



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:01 PM GMT

PDB ID : 4V84
Title : Crystal structure of a complex containing domain 3 of CrPV IGR IRES RNA bound to the 70S ribosome.
Authors : Zhu, J.; Korostelev, A.; Costantino, D.; Noller, H.F.; Kieft, J.S.
Deposited on : 2010-12-13
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

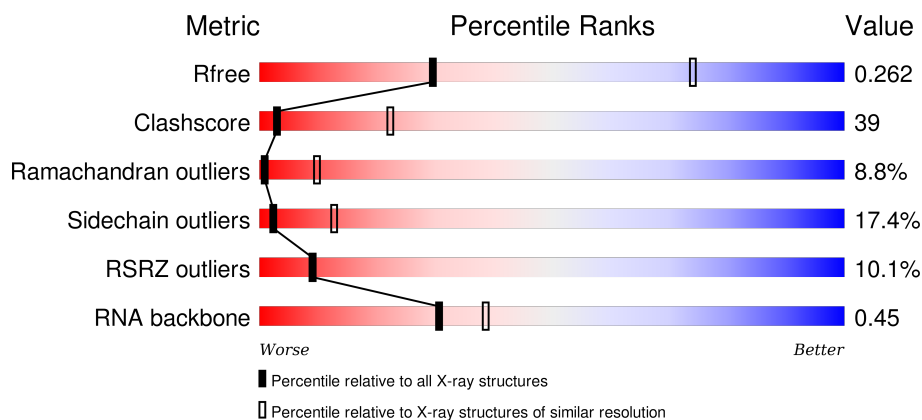
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| R_{free} | 91344 | 1476 (3.50-3.30) |
| Clashscore | 102246 | 1611 (3.50-3.30) |
| Ramachandran outliers | 100387 | 1571 (3.50-3.30) |
| Sidechain outliers | 100360 | 1571 (3.50-3.30) |
| RSRZ outliers | 91569 | 1485 (3.50-3.30) |
| RNA backbone | 2183 | 1041 (4.00-2.80) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1 | AA | 1506 | <div> <div>4%</div> <div>20%</div> <div>63%</div> <div>16%</div> <div>•</div> </div> |
| 1 | CA | 1506 | <div> <div>7%</div> <div>19%</div> <div>64%</div> <div>18%</div> </div> |
| 2 | AB | 234 | <div> <div>20%</div> <div>33%</div> <div>53%</div> <div>13%</div> </div> |
| 2 | CB | 234 | <div> <div>21%</div> <div>32%</div> <div>56%</div> <div>12%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3 | AC | 206 | |
| 3 | CC | 206 | |
| 4 | AD | 208 | |
| 4 | CD | 208 | |
| 5 | AE | 151 | |
| 5 | CE | 151 | |
| 6 | AF | 101 | |
| 6 | CF | 101 | |
| 7 | AG | 155 | |
| 7 | CG | 155 | |
| 8 | AH | 138 | |
| 8 | CH | 138 | |
| 9 | AI | 127 | |
| 9 | CI | 127 | |
| 10 | AJ | 98 | |
| 10 | CJ | 98 | |
| 11 | AK | 119 | |
| 11 | CK | 119 | |
| 12 | AL | 124 | |
| 12 | CL | 124 | |
| 13 | AM | 116 | |
| 13 | CM | 116 | |
| 14 | AN | 60 | |
| 14 | CN | 60 | |
| 15 | AO | 88 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 15 | CO | 88 | |
| 16 | AP | 83 | |
| 16 | CP | 83 | |
| 17 | AQ | 99 | |
| 17 | CQ | 99 | |
| 18 | AR | 70 | |
| 18 | CR | 70 | |
| 19 | AS | 78 | |
| 19 | CS | 78 | |
| 20 | AT | 99 | |
| 20 | CT | 99 | |
| 21 | AU | 24 | |
| 21 | CU | 24 | |
| 22 | AV | 43 | |
| 22 | CV | 43 | |
| 23 | BA | 2879 | |
| 23 | DA | 2879 | |
| 24 | BB | 119 | |
| 24 | DB | 119 | |
| 25 | BC | 271 | |
| 25 | DC | 271 | |
| 26 | BD | 204 | |
| 26 | DD | 204 | |
| 27 | BE | 202 | |
| 27 | DE | 202 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 28 | BF | 181 | |
| 28 | DF | 181 | |
| 29 | BG | 159 | |
| 29 | DG | 159 | |
| 30 | BH | 145 | |
| 30 | DH | 145 | |
| 31 | BI | 65 | |
| 31 | DI | 65 | |
| 32 | BJ | 137 | |
| 32 | DJ | 137 | |
| 33 | BK | 122 | |
| 33 | DK | 122 | |
| 34 | BL | 146 | |
| 34 | DL | 146 | |
| 35 | BM | 136 | |
| 35 | DM | 136 | |
| 36 | BN | 117 | |
| 36 | DN | 117 | |
| 37 | BO | 98 | |
| 37 | DO | 98 | |
| 38 | BP | 137 | |
| 38 | DP | 137 | |
| 39 | BQ | 116 | |
| 39 | DQ | 116 | |
| 40 | BR | 101 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 40 | DR | 101 | |
| 41 | BS | 112 | |
| 41 | DS | 112 | |
| 42 | BT | 92 | |
| 42 | DT | 92 | |
| 43 | BU | 100 | |
| 43 | DU | 100 | |
| 44 | BV | 188 | |
| 44 | DV | 188 | |
| 45 | BW | 76 | |
| 45 | DW | 76 | |
| 46 | BX | 88 | |
| 46 | DX | 88 | |
| 47 | BY | 62 | |
| 47 | DY | 62 | |
| 48 | BZ | 59 | |
| 48 | DZ | 59 | |
| 49 | B1 | 30 | |
| 49 | D1 | 30 | |
| 50 | B2 | 52 | |
| 50 | D2 | 52 | |
| 51 | B3 | 44 | |
| 51 | D3 | 44 | |
| 52 | B4 | 48 | |
| 52 | D4 | 48 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 53 | B5 | 63 | |
| 53 | D5 | 63 | |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 54 | MG | AA | 1601 | - | - | - | X |
| 54 | MG | AA | 1603 | - | - | - | X |
| 54 | MG | AA | 1621 | - | - | - | X |
| 54 | MG | AA | 1622 | - | - | - | X |
| 54 | MG | AA | 1624 | - | - | - | X |
| 54 | MG | AA | 1630 | - | - | - | X |
| 54 | MG | AA | 1636 | - | - | - | X |
| 54 | MG | AA | 1637 | - | - | - | X |
| 54 | MG | AA | 1647 | - | - | - | X |
| 54 | MG | AA | 1650 | - | - | - | X |
| 54 | MG | AA | 1679 | - | - | - | X |
| 54 | MG | AA | 1682 | - | - | - | X |
| 54 | MG | AA | 1695 | - | - | - | X |
| 54 | MG | AA | 1707 | - | - | - | X |
| 54 | MG | AA | 1713 | - | - | - | X |
| 54 | MG | AA | 1714 | - | - | - | X |
| 54 | MG | AA | 1721 | - | - | - | X |
| 54 | MG | AA | 1723 | - | - | - | X |
| 54 | MG | AA | 1728 | - | - | - | X |
| 54 | MG | AA | 1731 | - | - | - | X |
| 54 | MG | AA | 1742 | - | - | - | X |
| 54 | MG | AA | 1752 | - | - | - | X |
| 54 | MG | BA | 2901 | - | - | - | X |
| 54 | MG | BA | 2903 | - | - | - | X |
| 54 | MG | BA | 2904 | - | - | - | X |
| 54 | MG | BA | 2908 | - | - | - | X |
| 54 | MG | BA | 2909 | - | - | - | X |
| 54 | MG | BA | 2910 | - | - | - | X |
| 54 | MG | BA | 2911 | - | - | - | X |
| 54 | MG | BA | 2913 | - | - | - | X |
| 54 | MG | BA | 2914 | - | - | - | X |
| 54 | MG | BA | 2916 | - | - | - | X |
| 54 | MG | BA | 2917 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 54 | MG | BA | 2918 | - | - | - | X |
| 54 | MG | BA | 2920 | - | - | - | X |
| 54 | MG | BA | 2921 | - | - | - | X |
| 54 | MG | BA | 2922 | - | - | - | X |
| 54 | MG | BA | 2924 | - | - | - | X |
| 54 | MG | BA | 2925 | - | - | - | X |
| 54 | MG | BA | 2930 | - | - | - | X |
| 54 | MG | BA | 2931 | - | - | - | X |
| 54 | MG | BA | 2940 | - | - | - | X |
| 54 | MG | BA | 2941 | - | - | - | X |
| 54 | MG | BA | 2943 | - | - | - | X |
| 54 | MG | BA | 2952 | - | - | - | X |
| 54 | MG | BA | 2961 | - | - | - | X |
| 54 | MG | BA | 2967 | - | - | - | X |
| 54 | MG | BA | 2968 | - | - | - | X |
| 54 | MG | BA | 2970 | - | - | - | X |
| 54 | MG | BA | 2979 | - | - | - | X |
| 54 | MG | BA | 2980 | - | - | - | X |
| 54 | MG | BA | 2982 | - | - | - | X |
| 54 | MG | BA | 2998 | - | - | - | X |
| 54 | MG | BA | 2999 | - | - | - | X |
| 54 | MG | BA | 3004 | - | - | - | X |
| 54 | MG | BA | 3006 | - | - | - | X |
| 54 | MG | BA | 3019 | - | - | - | X |
| 54 | MG | BA | 3027 | - | - | - | X |
| 54 | MG | BA | 3046 | - | - | - | X |
| 54 | MG | BA | 3052 | - | - | - | X |
| 54 | MG | BA | 3088 | - | - | - | X |
| 54 | MG | BA | 3090 | - | - | - | X |
| 54 | MG | BA | 3091 | - | - | - | X |
| 54 | MG | BA | 3097 | - | - | - | X |
| 54 | MG | BA | 3118 | - | - | - | X |
| 54 | MG | BA | 3151 | - | - | - | X |
| 54 | MG | BA | 3152 | - | - | - | X |
| 54 | MG | BA | 3179 | - | - | - | X |
| 54 | MG | BA | 3180 | - | - | - | X |
| 54 | MG | BA | 3181 | - | - | - | X |
| 54 | MG | BA | 3182 | - | - | - | X |
| 54 | MG | BA | 3184 | - | - | - | X |
| 54 | MG | BA | 3185 | - | - | - | X |
| 54 | MG | BA | 3186 | - | - | - | X |
| 54 | MG | BA | 3188 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 54 | MG | BA | 3192 | - | - | - | X |
| 54 | MG | BA | 3204 | - | - | - | X |
| 54 | MG | BA | 3208 | - | - | - | X |
| 54 | MG | BA | 3220 | - | - | - | X |
| 54 | MG | BA | 3222 | - | - | - | X |
| 54 | MG | BA | 3226 | - | - | - | X |
| 54 | MG | BA | 3232 | - | - | - | X |
| 54 | MG | BA | 3242 | - | - | - | X |
| 54 | MG | BA | 3256 | - | - | - | X |
| 54 | MG | BA | 3257 | - | - | - | X |
| 54 | MG | BA | 3268 | - | - | - | X |
| 54 | MG | BA | 3270 | - | - | - | X |
| 54 | MG | BA | 3277 | - | - | - | X |
| 54 | MG | BA | 3284 | - | - | - | X |
| 54 | MG | CA | 1607 | - | - | - | X |
| 54 | MG | CA | 1609 | - | - | - | X |
| 54 | MG | CA | 1612 | - | - | - | X |
| 54 | MG | CA | 1617 | - | - | - | X |
| 54 | MG | CA | 1672 | - | - | - | X |
| 54 | MG | CA | 1691 | - | - | - | X |
| 54 | MG | CA | 1692 | - | - | - | X |
| 54 | MG | CA | 1698 | - | - | - | X |
| 54 | MG | CA | 1703 | - | - | - | X |
| 54 | MG | CA | 1715 | - | - | - | X |
| 54 | MG | CA | 1717 | - | - | - | X |
| 54 | MG | DA | 2901 | - | - | - | X |
| 54 | MG | DA | 2902 | - | - | - | X |
| 54 | MG | DA | 2904 | - | - | - | X |
| 54 | MG | DA | 2905 | - | - | - | X |
| 54 | MG | DA | 2906 | - | - | - | X |
| 54 | MG | DA | 2907 | - | - | - | X |
| 54 | MG | DA | 2908 | - | - | - | X |
| 54 | MG | DA | 2909 | - | - | - | X |
| 54 | MG | DA | 2911 | - | - | - | X |
| 54 | MG | DA | 2914 | - | - | - | X |
| 54 | MG | DA | 2915 | - | - | - | X |
| 54 | MG | DA | 2916 | - | - | - | X |
| 54 | MG | DA | 2917 | - | - | - | X |
| 54 | MG | DA | 2918 | - | - | - | X |
| 54 | MG | DA | 2921 | - | - | - | X |
| 54 | MG | DA | 2927 | - | - | - | X |
| 54 | MG | DA | 2932 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 54 | MG | DA | 2933 | - | - | - | X |
| 54 | MG | DA | 2934 | - | - | - | X |
| 54 | MG | DA | 2943 | - | - | - | X |
| 54 | MG | DA | 2944 | - | - | - | X |
| 54 | MG | DA | 2950 | - | - | - | X |
| 54 | MG | DA | 2955 | - | - | - | X |
| 54 | MG | DA | 2959 | - | - | - | X |
| 54 | MG | DA | 2965 | - | - | - | X |
| 54 | MG | DA | 2966 | - | - | - | X |
| 54 | MG | DA | 2968 | - | - | - | X |
| 54 | MG | DA | 2971 | - | - | - | X |
| 54 | MG | DA | 2976 | - | - | - | X |
| 54 | MG | DA | 2978 | - | - | - | X |
| 54 | MG | DA | 2989 | - | - | - | X |
| 54 | MG | DA | 2999 | - | - | - | X |
| 54 | MG | DA | 3000 | - | - | - | X |
| 54 | MG | DA | 3003 | - | - | - | X |
| 54 | MG | DA | 3012 | - | - | - | X |
| 54 | MG | DA | 3022 | - | - | - | X |
| 54 | MG | DA | 3023 | - | - | - | X |
| 54 | MG | DA | 3024 | - | - | - | X |
| 54 | MG | DA | 3033 | - | - | - | X |
| 54 | MG | DA | 3034 | - | - | - | X |
| 54 | MG | DA | 3036 | - | - | - | X |
| 54 | MG | DA | 3039 | - | - | - | X |
| 54 | MG | DA | 3047 | - | - | - | X |
| 54 | MG | DA | 3066 | - | - | - | X |
| 54 | MG | DA | 3070 | - | - | - | X |
| 54 | MG | DA | 3072 | - | - | - | X |
| 54 | MG | DA | 3079 | - | - | - | X |
| 54 | MG | DA | 3082 | - | - | - | X |
| 54 | MG | DA | 3083 | - | - | - | X |
| 54 | MG | DA | 3101 | - | - | - | X |
| 54 | MG | DA | 3105 | - | - | - | X |
| 54 | MG | DA | 3149 | - | - | - | X |
| 54 | MG | DA | 3154 | - | - | - | X |
| 54 | MG | DA | 3165 | - | - | - | X |
| 54 | MG | DA | 3174 | - | - | - | X |
| 54 | MG | DA | 3188 | - | - | - | X |
| 54 | MG | DA | 3190 | - | - | - | X |
| 54 | MG | DA | 3191 | - | - | - | X |
| 54 | MG | DA | 3192 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 54 | MG | DA | 3198 | - | - | - | X |
| 54 | MG | DA | 3201 | - | - | - | X |
| 54 | MG | DA | 3202 | - | - | - | X |
| 54 | MG | DA | 3208 | - | - | - | X |
| 54 | MG | DA | 3214 | - | - | - | X |
| 54 | MG | DA | 3215 | - | - | - | X |
| 54 | MG | DA | 3216 | - | - | - | X |
| 54 | MG | DA | 3223 | - | - | - | X |
| 54 | MG | DA | 3228 | - | - | - | X |
| 54 | MG | DA | 3232 | - | - | - | X |
| 54 | MG | DA | 3241 | - | - | - | X |
| 54 | MG | DA | 3251 | - | - | - | X |
| 54 | MG | DA | 3259 | - | - | - | X |
| 54 | MG | DA | 3272 | - | - | - | X |
| 54 | MG | DA | 3274 | - | - | - | X |
| 54 | MG | DA | 3298 | - | - | - | X |
| 54 | MG | DA | 3304 | - | - | - | X |
| 54 | MG | DA | 3306 | - | - | - | X |
| 54 | MG | DA | 3310 | - | - | - | X |
| 54 | MG | DA | 3313 | - | - | - | X |
| 54 | MG | DA | 3324 | - | - | - | X |
| 54 | MG | DG | 201 | - | - | - | X |

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 282142 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called ribosomal RNA 16S.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1 | AA | 1506 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32372 | 14409 | 5999 | 10459 | 1505 | | | |
| 1 | CA | 1506 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32372 | 14409 | 5999 | 10459 | 1505 | | | |

- Molecule 2 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2 | AB | 234 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1901 | 1213 | 341 | 342 | 5 | | | |
| 2 | CB | 234 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1901 | 1213 | 341 | 342 | 5 | | | |

- Molecule 3 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | AC | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1613 | 1016 | 314 | 282 | 1 | | | |
| 3 | CC | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1613 | 1016 | 314 | 282 | 1 | | | |

- Molecule 4 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4 | AD | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1703 | 1066 | 339 | 291 | 7 | | | |
| 4 | CD | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1703 | 1066 | 339 | 291 | 7 | | | |

- Molecule 5 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | AE | 151 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1156 | 729 | 218 | 205 | 4 | | | |
| 5 | CE | 151 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1156 | 729 | 218 | 205 | 4 | | | |

- Molecule 6 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | AF | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 843 | 531 | 155 | 154 | 3 | | | |
| 6 | CF | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 843 | 531 | 155 | 154 | 3 | | | |

- Molecule 7 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | AG | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1257 | 781 | 252 | 218 | 6 | | | |
| 7 | CG | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1257 | 781 | 252 | 218 | 6 | | | |

- Molecule 8 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | AH | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1116 | 705 | 215 | 193 | 3 | | | |
| 8 | CH | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1116 | 705 | 215 | 193 | 3 | | | |

- Molecule 9 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 9 | AI | 127 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 1011 | 639 | 198 | 174 | | | | |
| 9 | CI | 127 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 1011 | 639 | 198 | 174 | | | | |

- Molecule 10 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | AJ | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 795 | 499 | 156 | 139 | 1 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | CJ | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 795 | 499 | 156 | 139 | 1 | | | |

- Molecule 11 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | AK | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 885 | 549 | 168 | 165 | 3 | | | |
| 11 | CK | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 885 | 549 | 168 | 165 | 3 | | | |

- Molecule 12 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | AL | 124 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 971 | 611 | 195 | 164 | 1 | | | |
| 12 | CL | 124 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 971 | 611 | 195 | 164 | 1 | | | |

- Molecule 13 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | AM | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 929 | 574 | 191 | 162 | 2 | | | |
| 13 | CM | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 929 | 574 | 191 | 162 | 2 | | | |

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 14 | AN | 60 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 492 | 312 | 104 | 72 | 4 | | | |
| 14 | CN | 60 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 492 | 312 | 104 | 72 | 4 | | | |

- Molecule 15 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15 | AO | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 734 | 459 | 147 | 126 | 2 | | | |
| 15 | CO | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 734 | 459 | 147 | 126 | 2 | | | |

- Molecule 16 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | AP | 83 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 701 | 443 | 139 | 118 | 1 | | | |
| 16 | CP | 83 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 701 | 443 | 139 | 118 | 1 | | | |

- Molecule 17 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17 | AQ | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 824 | 528 | 152 | 142 | 2 | | | |
| 17 | CQ | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 824 | 528 | 152 | 142 | 2 | | | |

- Molecule 18 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 18 | AR | 70 | Total | C | N | O | 0 | 0 | 0 |
| | | | 574 | 367 | 112 | 95 | | | |
| 18 | CR | 70 | Total | C | N | O | 0 | 0 | 0 |
| | | | 574 | 367 | 112 | 95 | | | |

- Molecule 19 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | AS | 78 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 630 | 403 | 114 | 111 | 2 | | | |
| 19 | CS | 78 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 630 | 403 | 114 | 111 | 2 | | | |

- Molecule 20 is a protein called 30S ribosomal protein Thx.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | AT | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 762 | 469 | 162 | 129 | 2 | | | |
| 20 | CT | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 762 | 469 | 162 | 129 | 2 | | | |

- Molecule 21 is a protein called domain 3 of CrPV IGR IRES RNA.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 21 | AU | 24 | Total | C | N | O | 0 | 0 | 0 |
| | | | 209 | 128 | 50 | 31 | | | |
| 21 | CU | 24 | Total | C | N | O | 0 | 0 | 0 |
| | | | 209 | 128 | 50 | 31 | | | |

- Molecule 22 is a RNA chain called RNA (34-MER).

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 22 | AV | 34 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 719 | 323 | 125 | 238 | 33 | | | |
| 22 | CV | 34 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 719 | 323 | 125 | 238 | 33 | | | |

- Molecule 23 is a RNA chain called 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 23 | BA | 2760 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 59440 | 26455 | 11114 | 19112 | 2759 | | | |
| 23 | DA | 2760 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 59442 | 26456 | 11114 | 19113 | 2759 | | | |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|---------------|
| BA | 1142 | U | C | SEE REMARK 999 | GB AE017221.1 |
| BA | 2825 | U | G | SEE REMARK 999 | GB AE017221.1 |
| DA | 1142 | U | C | SEE REMARK 999 | GB AE017221.1 |
| DA | 2825 | U | G | SEE REMARK 999 | GB AE017221.1 |

- Molecule 24 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 24 | BB | 119 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2551 | 1136 | 471 | 826 | 118 | | | |
| 24 | DB | 119 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2551 | 1136 | 471 | 826 | 118 | | | |

- Molecule 25 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 25 | BC | 271 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2105 | 1329 | 416 | 357 | 3 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 25 | DC | 271 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2105 | 1329 | 416 | 357 | 3 | | | |

- Molecule 26 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26 | BD | 204 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1564 | 988 | 299 | 271 | 6 | | | |
| 26 | DD | 204 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1564 | 988 | 299 | 271 | 6 | | | |

- Molecule 27 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 27 | BE | 202 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1587 | 1011 | 297 | 276 | 3 | | | |
| 27 | DE | 202 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1587 | 1011 | 297 | 276 | 3 | | | |

- Molecule 28 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28 | BF | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1475 | 943 | 268 | 260 | 4 | | | |
| 28 | DF | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1475 | 943 | 268 | 260 | 4 | | | |

- Molecule 29 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 29 | BG | 159 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1223 | 773 | 228 | 221 | 1 | | | |
| 29 | DG | 159 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1223 | 773 | 228 | 221 | 1 | | | |

- Molecule 30 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30 | BH | 145 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1133 | 724 | 200 | 208 | 1 | | | |
| 30 | DH | 145 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1133 | 724 | 200 | 208 | 1 | | | |

- Molecule 31 is a protein called 50S ribosomal protein L10.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 31 | BI | 32 | Total | C | N | O | 0 | 0 | 0 |
| | | | 254 | 157 | 49 | 48 | | | |
| 31 | DI | 32 | Total | C | N | O | 0 | 0 | 0 |
| | | | 254 | 157 | 49 | 48 | | | |

- Molecule 32 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32 | BJ | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1097 | 707 | 205 | 182 | 3 | | | |
| 32 | DJ | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1097 | 707 | 205 | 182 | 3 | | | |

- Molecule 33 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33 | BK | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 932 | 587 | 171 | 170 | 4 | | | |
| 33 | DK | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 932 | 587 | 171 | 170 | 4 | | | |

- Molecule 34 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34 | BL | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1114 | 692 | 227 | 193 | 2 | | | |
| 34 | DL | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1114 | 692 | 227 | 193 | 2 | | | |

- Molecule 35 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35 | BM | 136 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1079 | 688 | 204 | 182 | 5 | | | |
| 35 | DM | 136 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1079 | 688 | 204 | 182 | 5 | | | |

- Molecule 36 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 36 | BN | 117 | Total | C | N | O | 0 | 0 | 0 |
| | | | 960 | 599 | 202 | 159 | | | |
| 36 | DN | 117 | Total | C | N | O | 0 | 0 | 0 |
| | | | 960 | 599 | 202 | 159 | | | |

- Molecule 37 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 37 | BO | 98 | Total | C | N | O | 0 | 0 | 0 |
| | | | 771 | 486 | 154 | 131 | | | |
| 37 | DO | 98 | Total | C | N | O | 0 | 0 | 0 |
| | | | 771 | 486 | 154 | 131 | | | |

- Molecule 38 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38 | BP | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1144 | 713 | 234 | 196 | 1 | | | |
| 38 | DP | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1144 | 713 | 234 | 196 | 1 | | | |

- Molecule 39 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39 | BQ | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 953 | 601 | 201 | 150 | 1 | | | |
| 39 | DQ | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 953 | 601 | 201 | 150 | 1 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| BQ | ? | - | PHE | DELETION | UNP Q72L76 |
| DQ | ? | - | PHE | DELETION | UNP Q72L76 |

- Molecule 40 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40 | BR | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 779 | 501 | 142 | 135 | 1 | | | |
| 40 | DR | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 779 | 501 | 142 | 135 | 1 | | | |

- Molecule 41 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41 | BS | 112 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 891 | 560 | 175 | 154 | 2 | | | |
| 41 | DS | 112 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 891 | 560 | 175 | 154 | 2 | | | |

- Molecule 42 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 42 | BT | 92 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 726 | 471 | 131 | 124 | | | | |
| 42 | DT | 92 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 726 | 471 | 131 | 124 | | | | |

- Molecule 43 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43 | BU | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 776 | 500 | 148 | 124 | 4 | | | |
| 43 | DU | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 776 | 500 | 148 | 124 | 4 | | | |

- Molecule 44 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44 | BV | 188 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1492 | 950 | 265 | 275 | 2 | | | |
| 44 | DV | 188 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1492 | 950 | 265 | 275 | 2 | | | |

- Molecule 45 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45 | BW | 76 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 605 | 376 | 126 | 102 | 1 | | | |
| 45 | DW | 76 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 605 | 376 | 126 | 102 | 1 | | | |

- Molecule 46 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 46 | BX | 88 | Total | C | N | O | 0 | 0 | 0 |
| | | | 695 | 435 | 141 | 119 | | | |
| 46 | DX | 88 | Total | C | N | O | 0 | 0 | 0 |
| | | | 695 | 435 | 141 | 119 | | | |

- Molecule 47 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 47 | BY | 62 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 521 | 325 | 102 | 92 | 2 | | | |
| 47 | DY | 62 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 521 | 325 | 102 | 92 | 2 | | | |

- Molecule 48 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 48 | BZ | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 468 | 298 | 90 | 79 | 1 | | | |
| 48 | DZ | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 468 | 298 | 90 | 79 | 1 | | | |

- Molecule 49 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 49 | B1 | 30 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 226 | 142 | 36 | 44 | 4 | | | |
| 49 | D1 | 30 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 226 | 142 | 36 | 44 | 4 | | | |

- Molecule 50 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 50 | B2 | 52 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 405 | 255 | 79 | 66 | 5 | | | |
| 50 | D2 | 52 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 405 | 255 | 79 | 66 | 5 | | | |

- Molecule 51 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 51 | B3 | 44 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 381 | 235 | 77 | 65 | 4 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 51 | D3 | 44 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 381 | 235 | 77 | 65 | 4 | | | |

- Molecule 52 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 52 | B4 | 48 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 419 | 257 | 104 | 56 | 2 | | | |
| 52 | D4 | 48 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 419 | 257 | 104 | 56 | 2 | | | |

- Molecule 53 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 53 | B5 | 63 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 508 | 326 | 101 | 79 | 2 | | | |
| 53 | D5 | 63 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 508 | 326 | 101 | 79 | 2 | | | |

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 54 | BB | 17 | Total | Mg | 0 | 0 |
| | | | 17 | 17 | | |
| 54 | DE | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 54 | BA | 408 | Total | Mg | 0 | 0 |
| | | | 408 | 408 | | |
| 54 | CA | 140 | Total | Mg | 0 | 0 |
| | | | 140 | 140 | | |
| 54 | DG | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 54 | CV | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 54 | AV | 4 | Total | Mg | 0 | 0 |
| | | | 4 | 4 | | |
| 54 | D2 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 54 | DA | 436 | Total | Mg | 0 | 0 |
| | | | 436 | 436 | | |
| 54 | B2 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 54 | CP | 1 | Total 1 | Mg 1 | 0 | 0 |
| 54 | AA | 163 | Total 163 | Mg 163 | 0 | 0 |
| 54 | D4 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 54 | BK | 1 | Total 1 | Mg 1 | 0 | 0 |
| 54 | AD | 1 | Total 1 | Mg 1 | 0 | 0 |
| 54 | DB | 17 | Total 17 | Mg 17 | 0 | 0 |

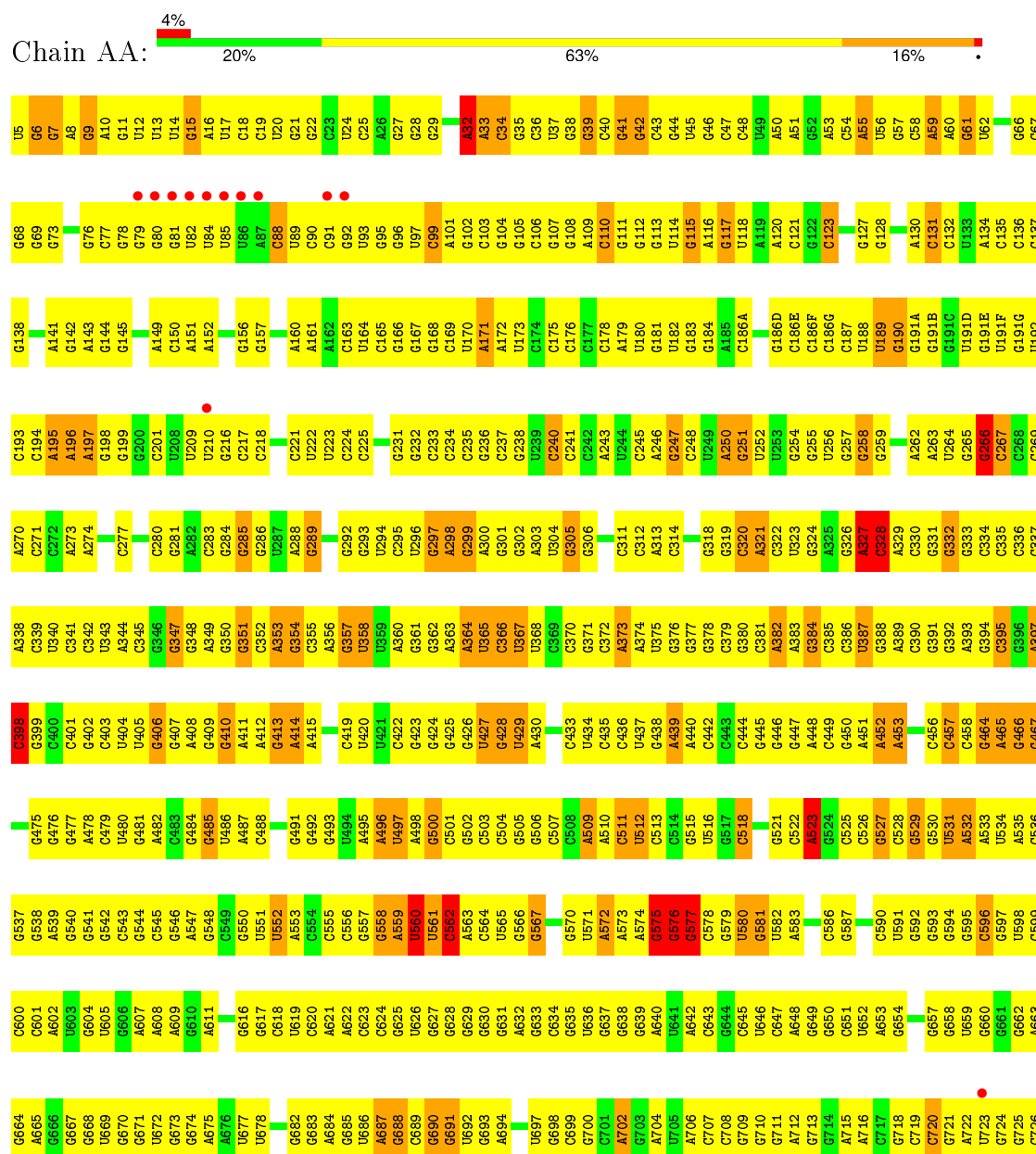
- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

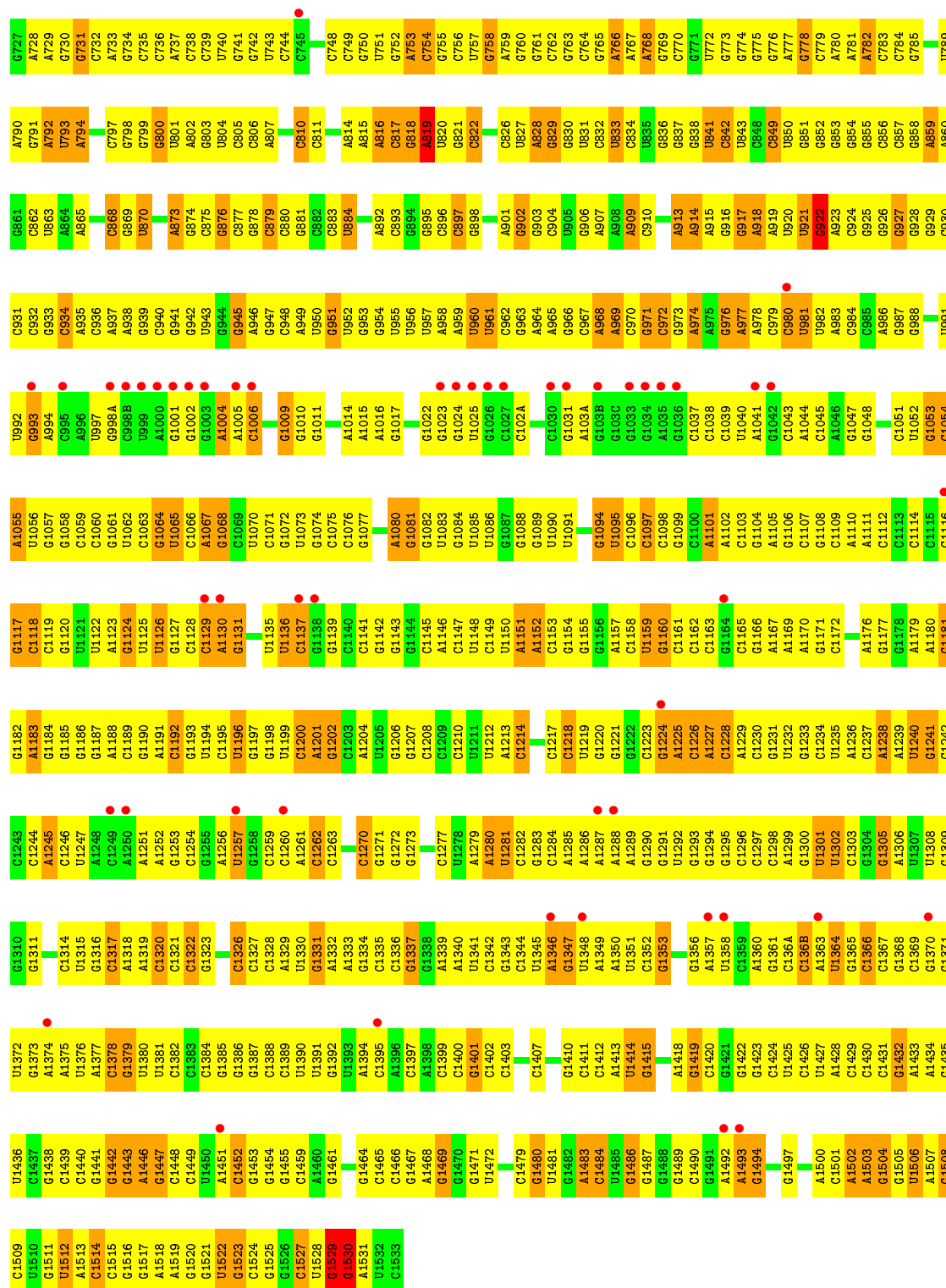
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 55 | CN | 1 | Total 1 | Zn 1 | 0 | 0 |
| 55 | AD | 1 | Total 1 | Zn 1 | 0 | 0 |
| 55 | CD | 1 | Total 1 | Zn 1 | 0 | 0 |
| 55 | AN | 1 | Total 1 | Zn 1 | 0 | 0 |

3 Residue-property plots

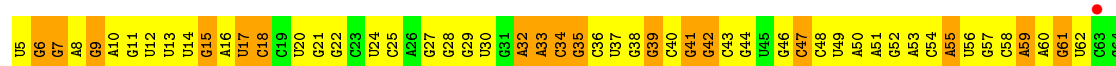
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: ribosomal RNA 16S

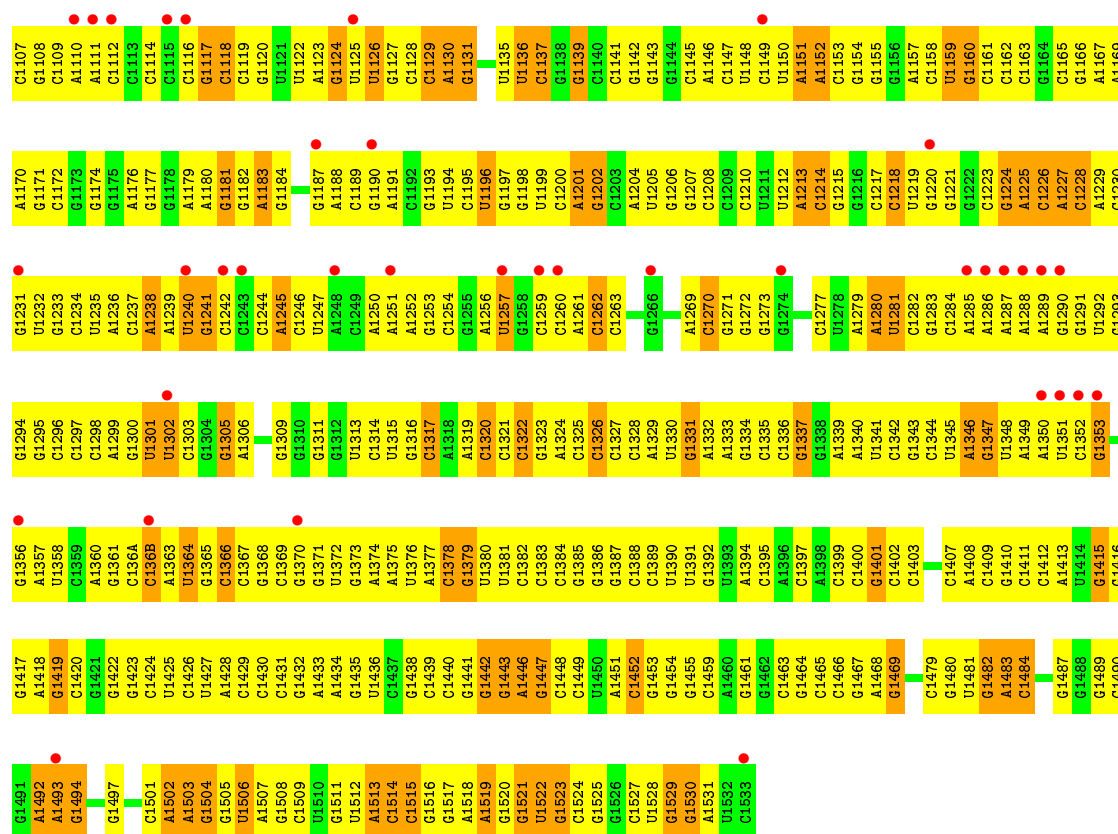




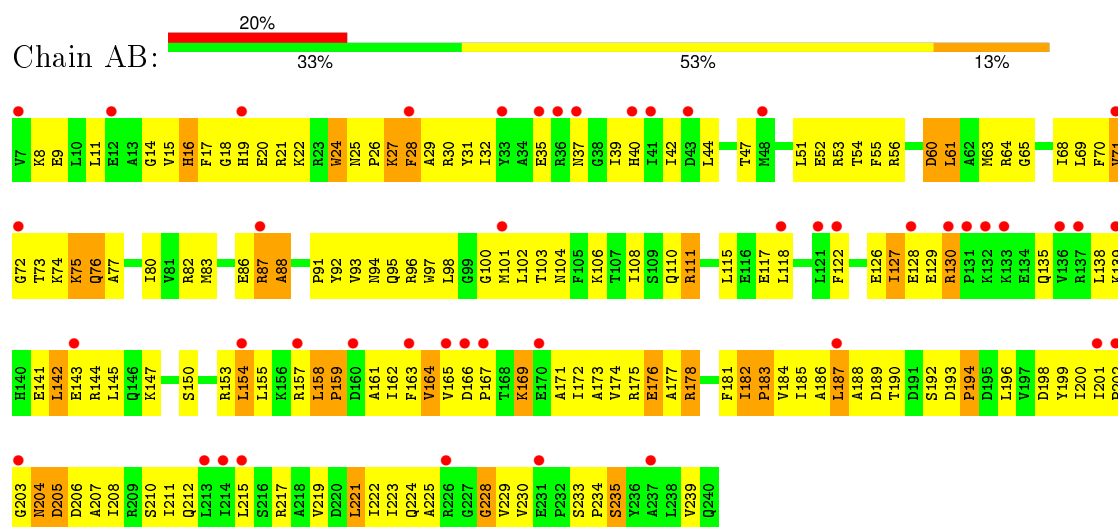
• Molecule 1: ribosomal RNA 16S



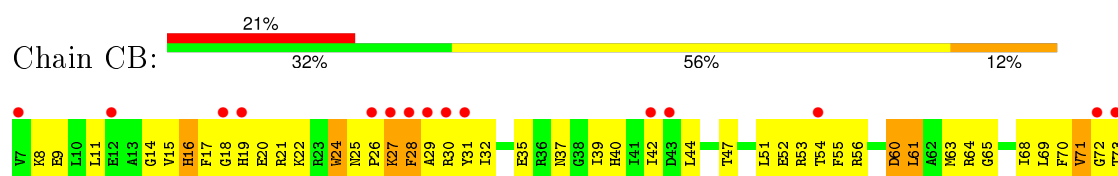
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| G1048 | C985 | A923 | G853 | A780 | A715 | U651 | U531 | U531 | G465 | C335 | C335 | C270 | C194 | C137 | C67 |
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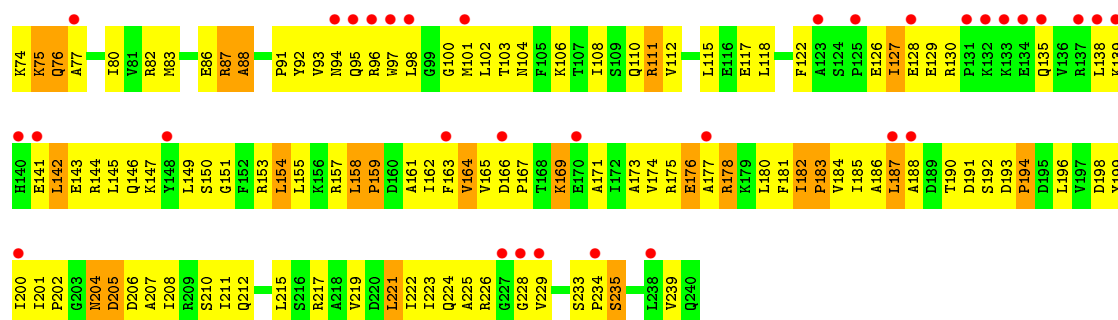


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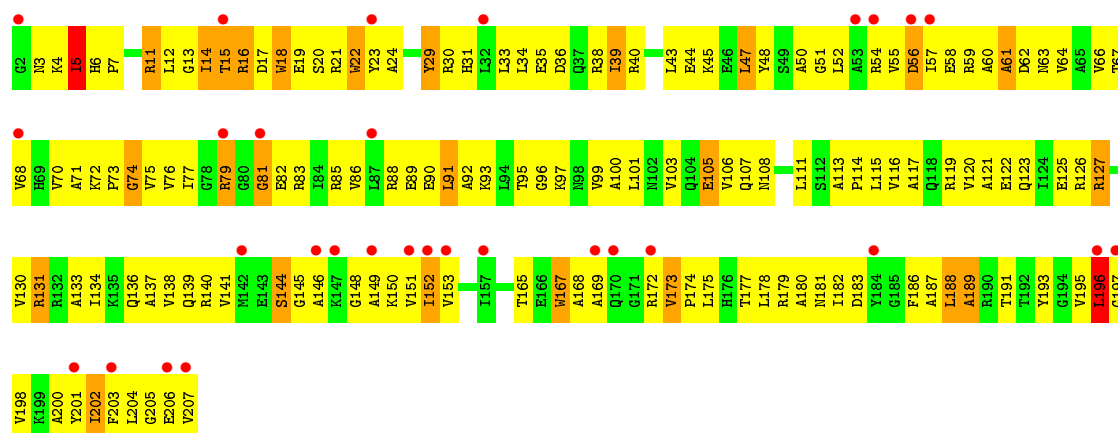


• Molecule 2: 30S ribosomal protein S2

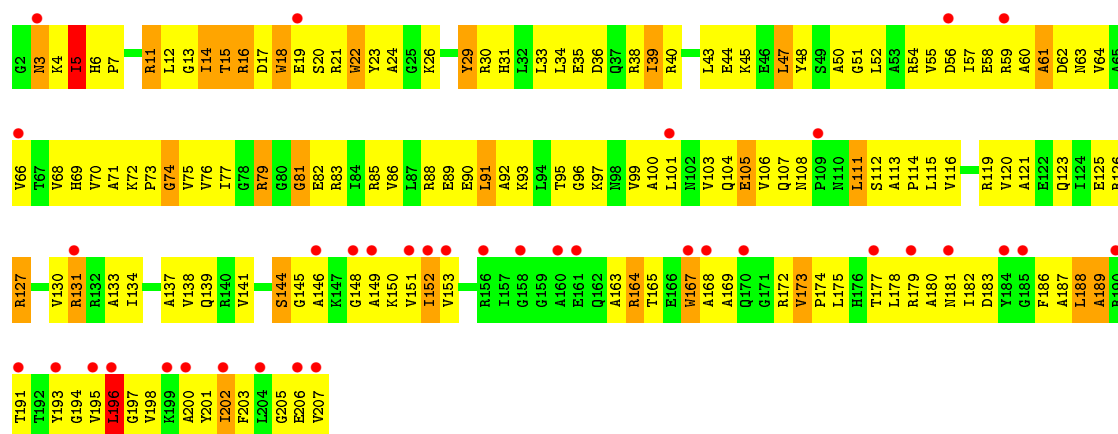




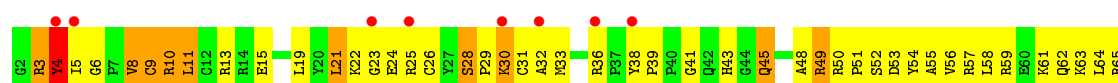
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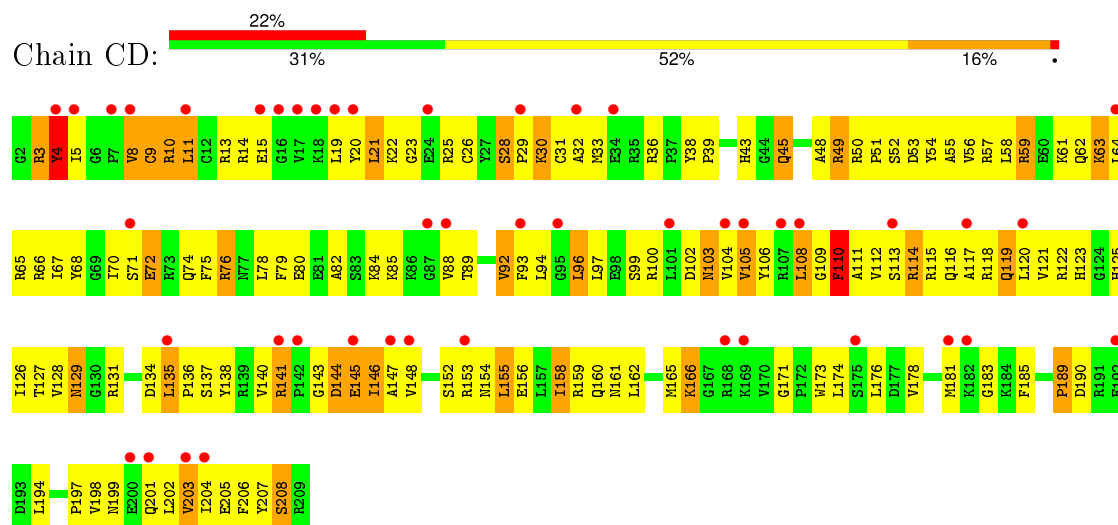
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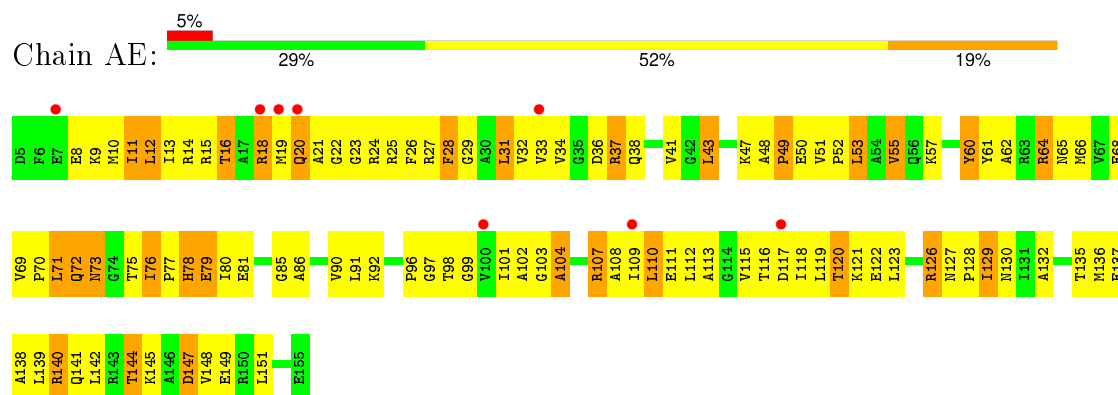
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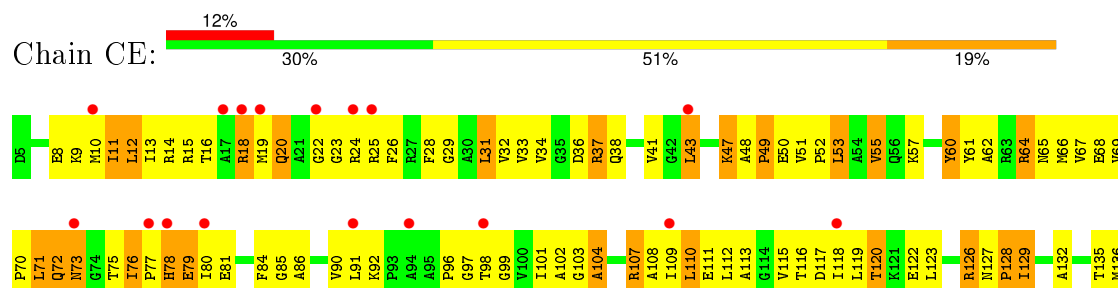
- Molecule 4: 30S ribosomal protein S4

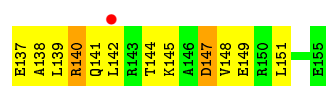


- Molecule 5: 30S ribosomal protein S5

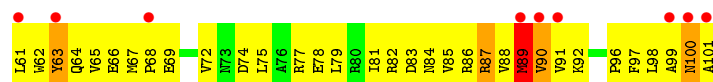


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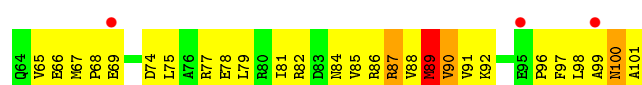




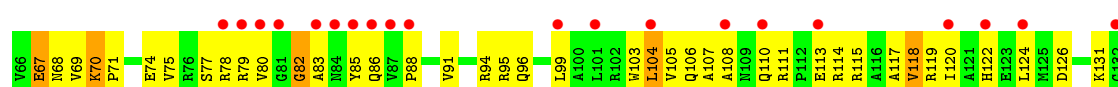
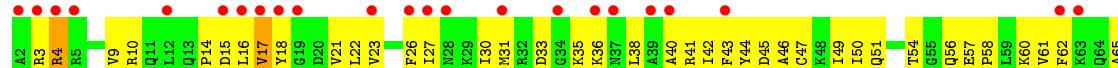
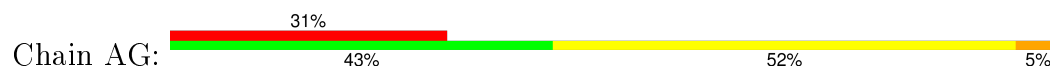
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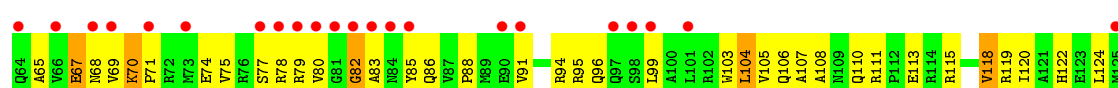
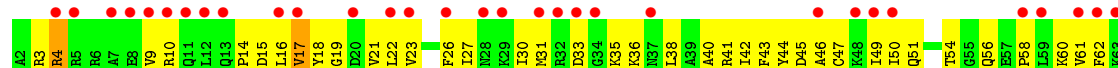
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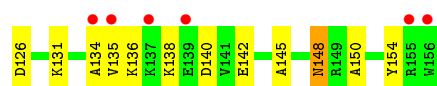


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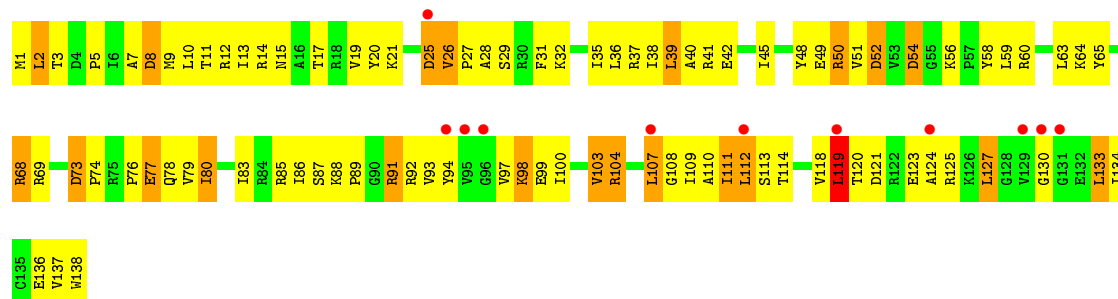


• Molecule 7: 30S ribosomal protein S7

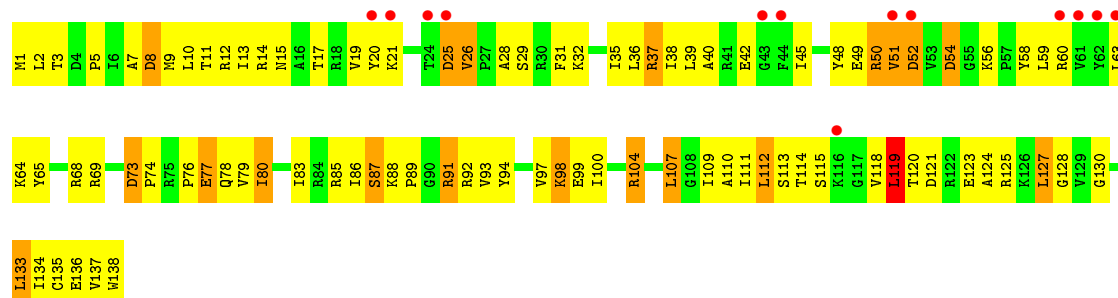




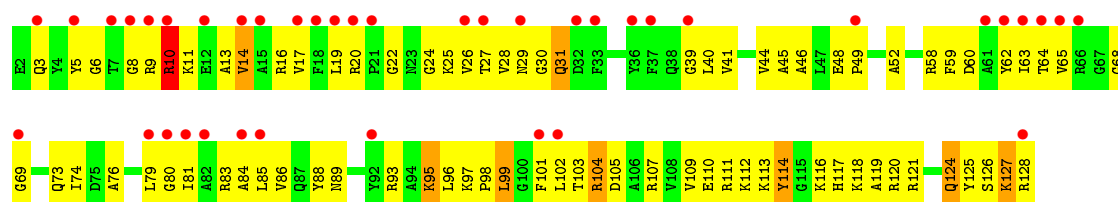
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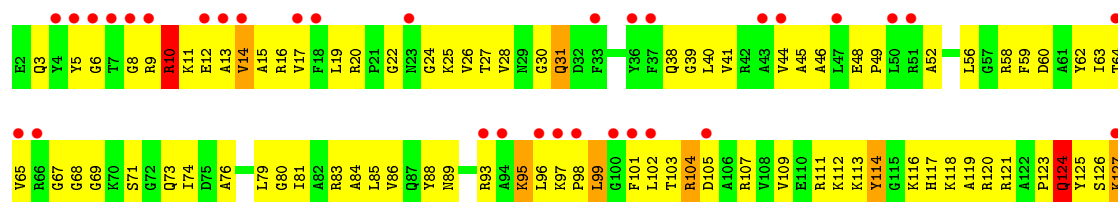
- Molecule 8: 30S ribosomal protein S8



- Molecule 9: 30S ribosomal protein S9

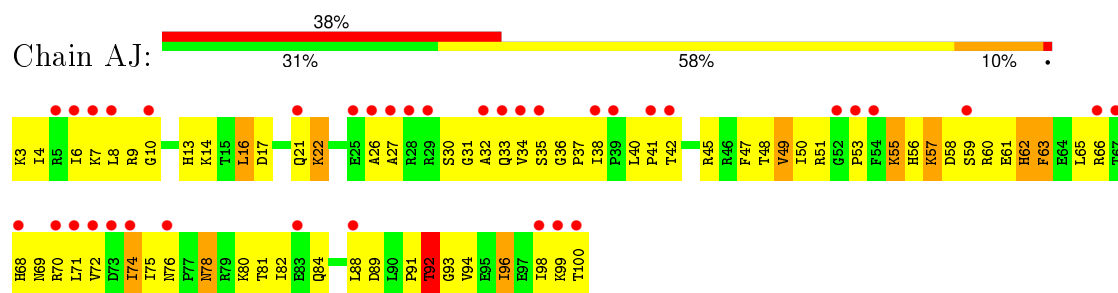


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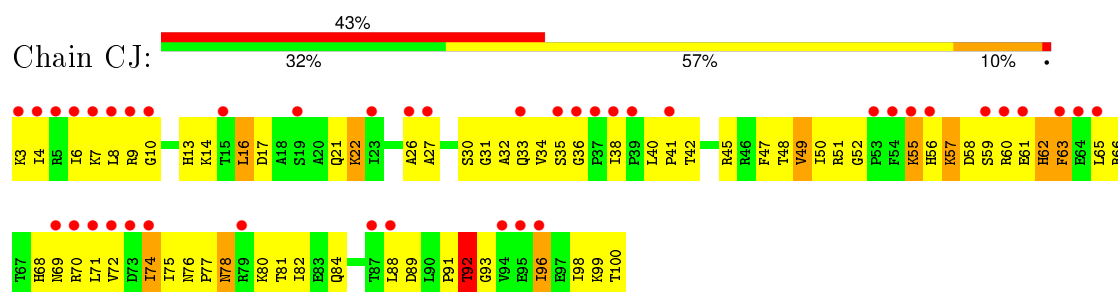


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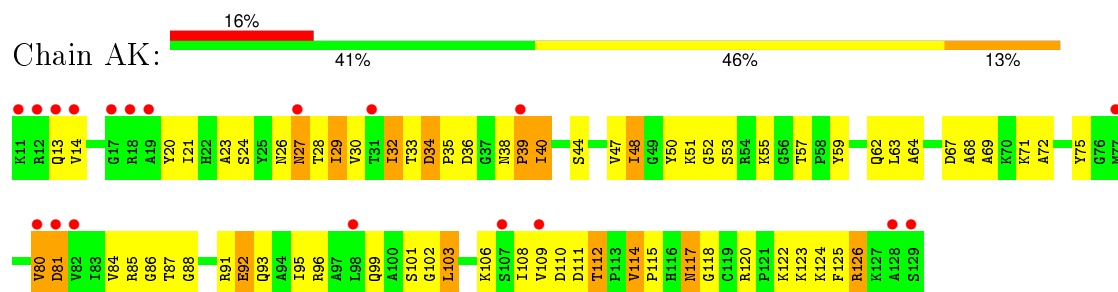
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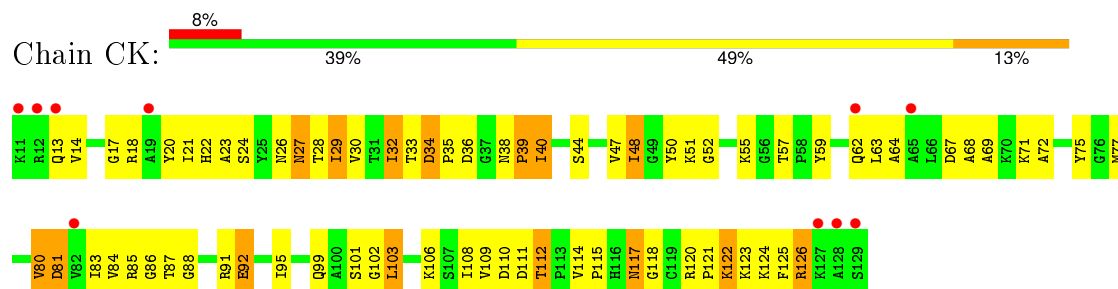
- Molecule 10: 30S ribosomal protein S10



- Molecule 11: 30S ribosomal protein S11



- Molecule 11: 30S ribosomal protein S11

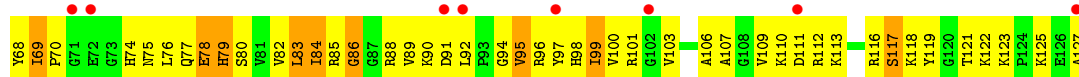
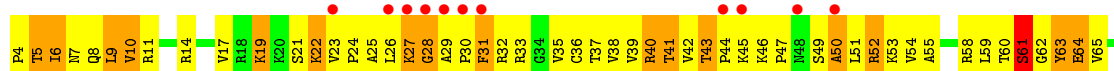


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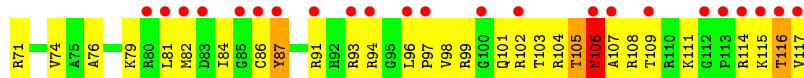
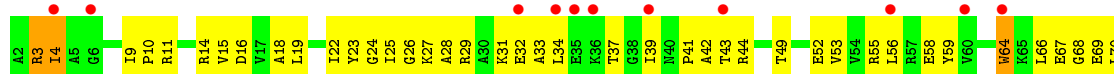




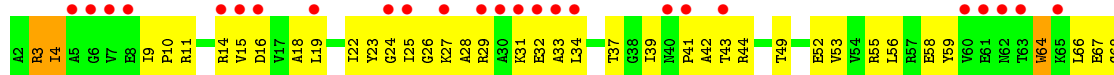
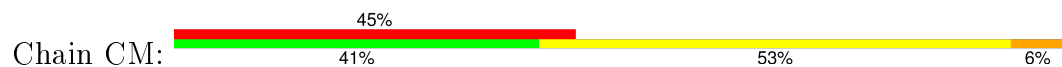
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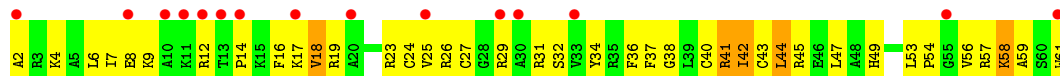
• Molecule 13: 30S ribosomal protein S13



• Molecule 13: 30S ribosomal protein S13

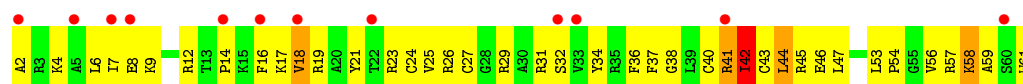


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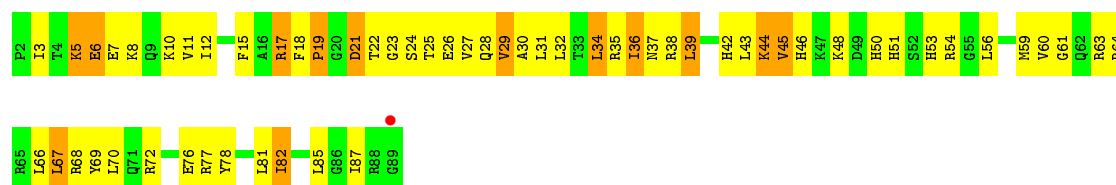


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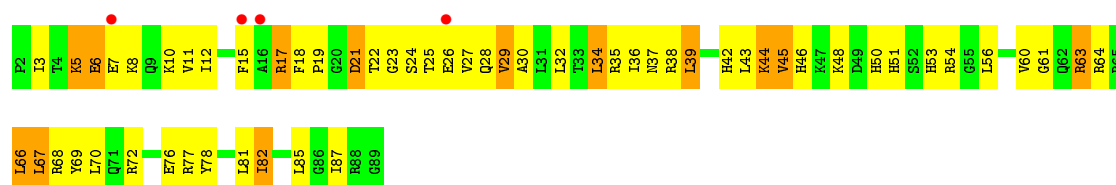




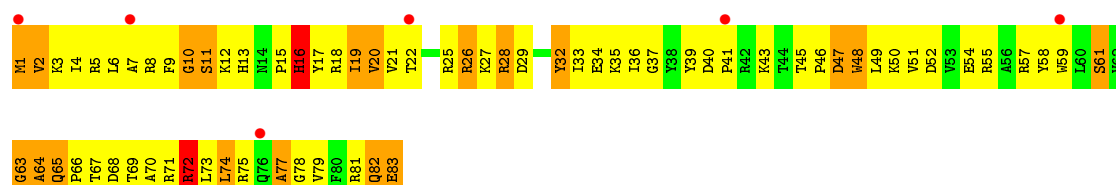
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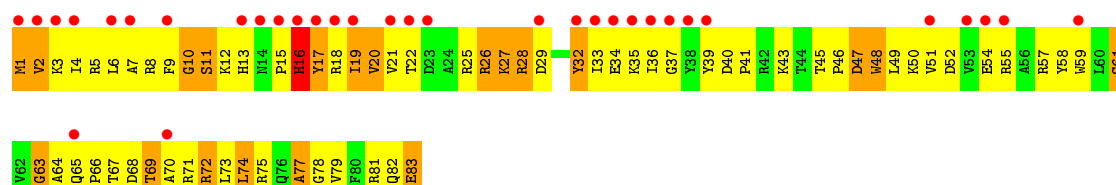
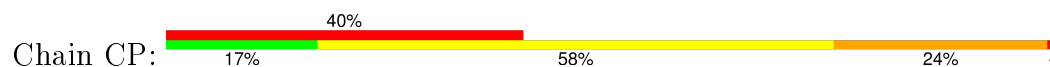
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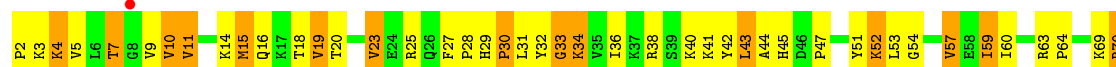
• Molecule 16: 30S ribosomal protein S16



• Molecule 16: 30S ribosomal protein S16

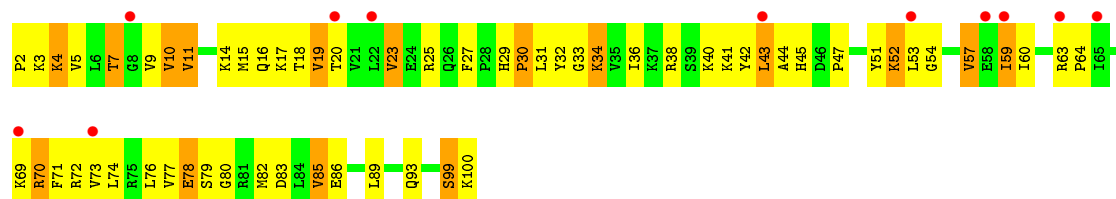
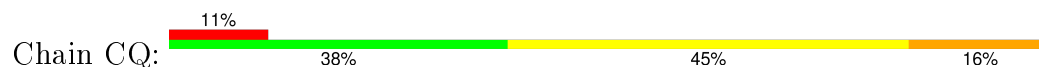


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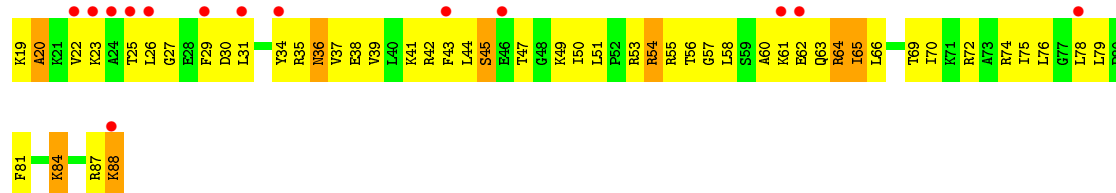




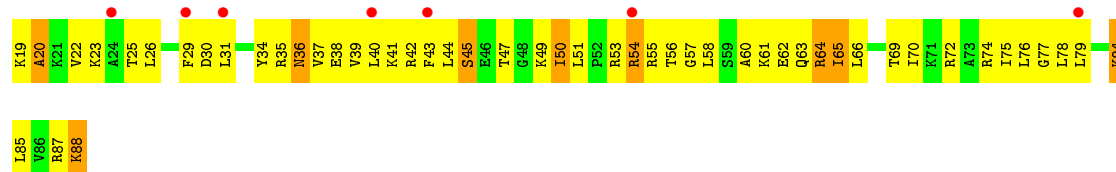
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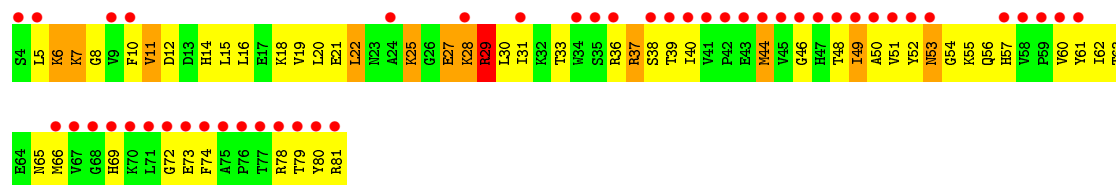
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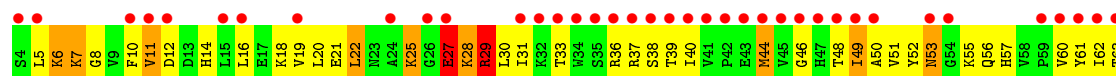
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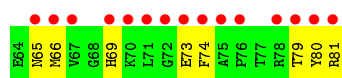


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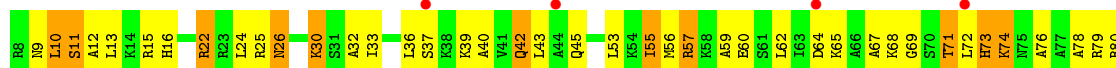


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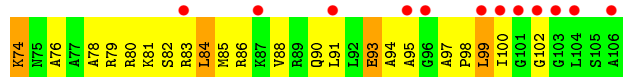
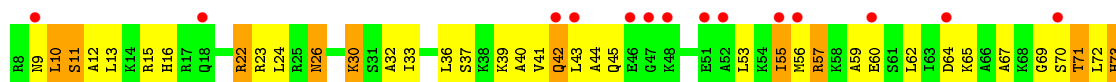




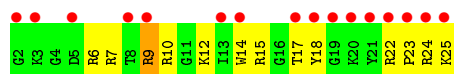
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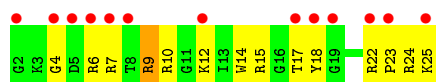
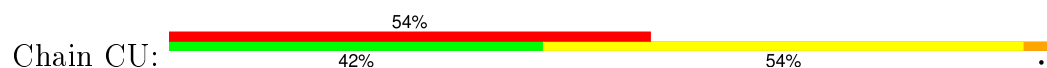
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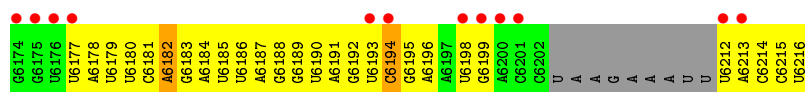
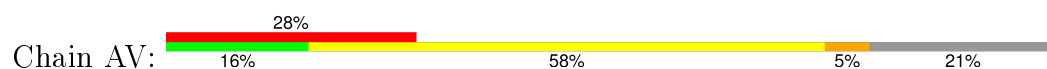
- Molecule 21: domain 3 of CrPV IGR IRES RNA



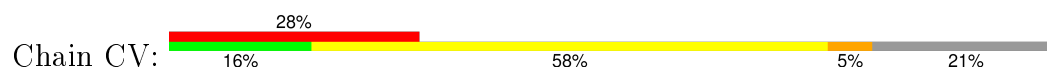
- Molecule 21: domain 3 of CrPV IGR IRES RNA

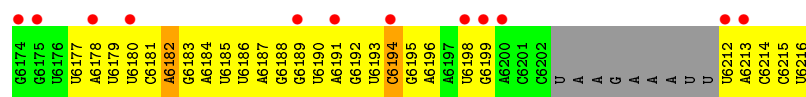


- Molecule 22: RNA (34-MER)

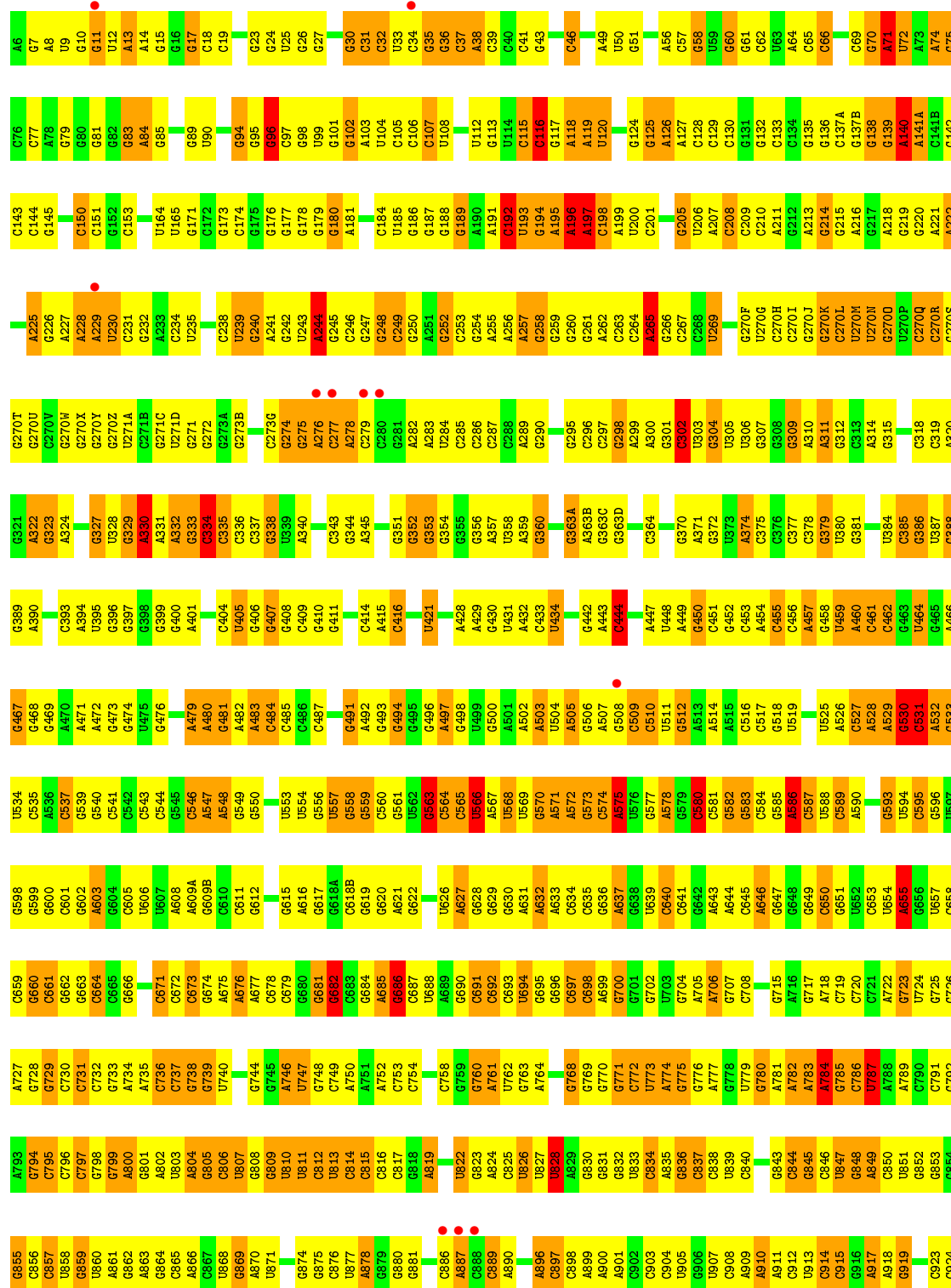
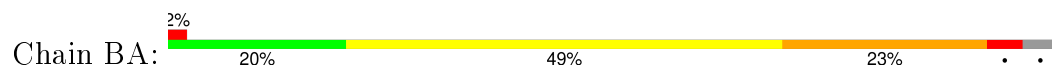


- Molecule 22: RNA (34-MER)



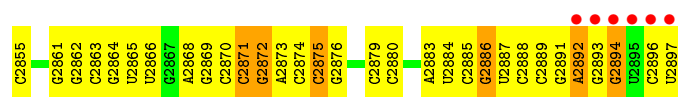


• Molecule 23: 23S ribosomal RNA

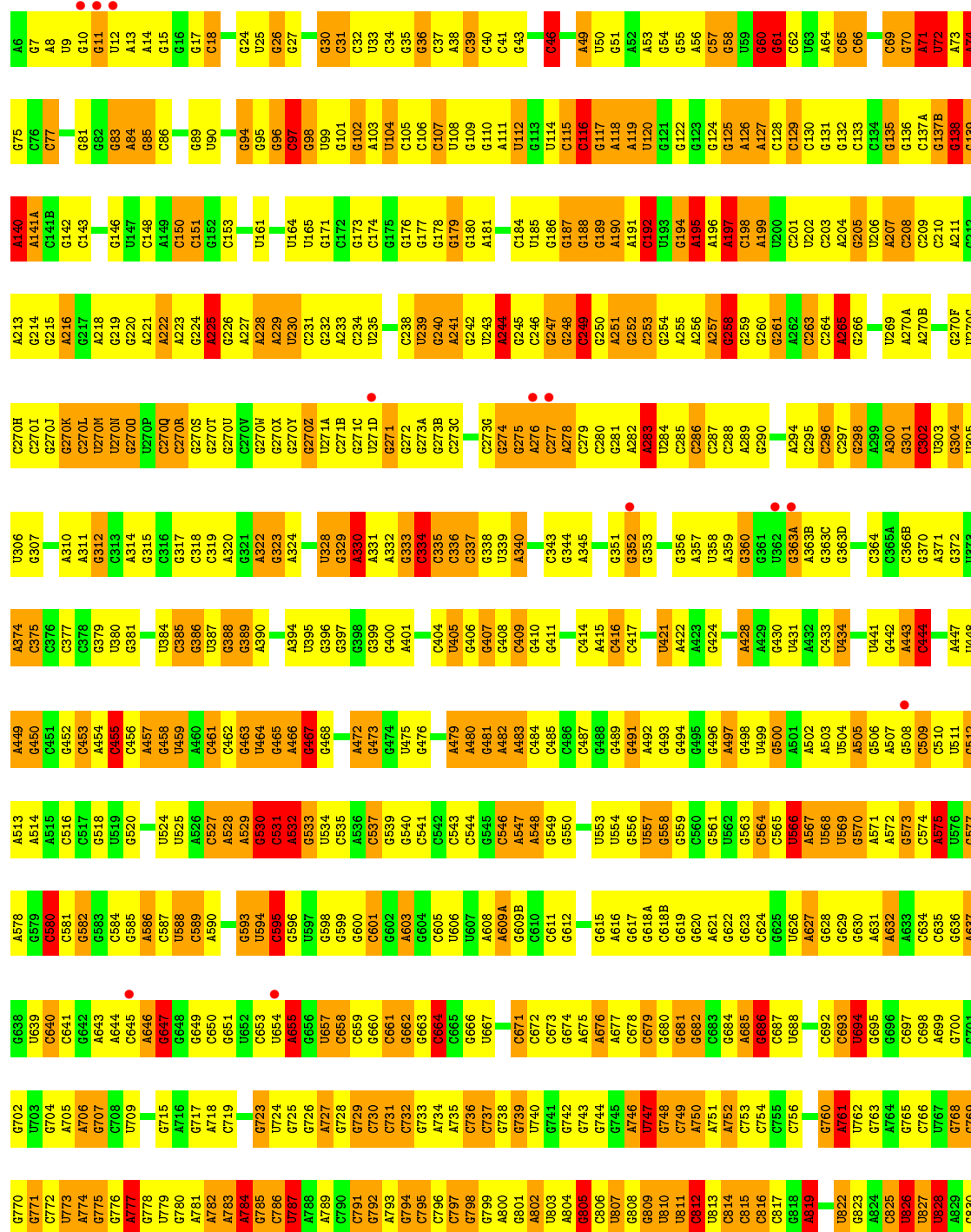
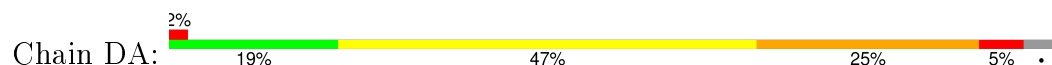


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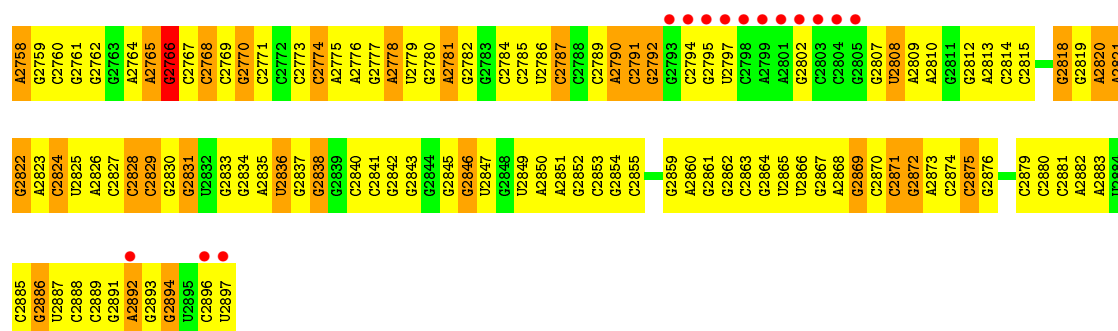


• Molecule 23: 23S ribosomal RNA

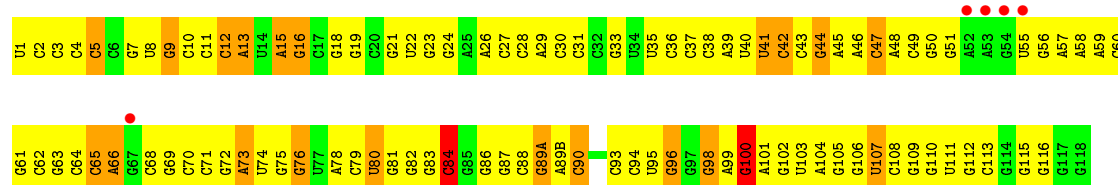


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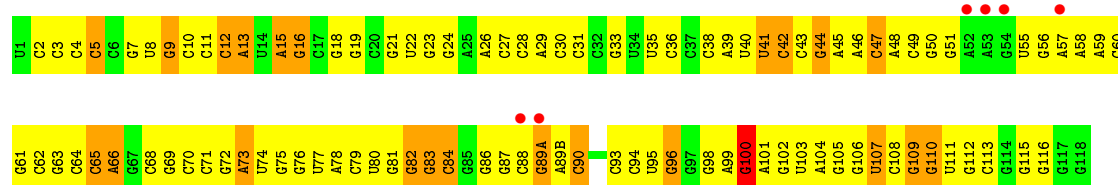
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| G2631 | G2632 | G2569 | G2505 | G2444 | G2384 | A2320 | G2259 | G2186 | A | C2063 | U1939 | G1870 | G1799 |
| A2632 | G2701 | G2570 | U2506 | G2445 | C2385 | G2321 | C2260 | G2187 | G | C2064 | G1945 | C1870 | C1800 |
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| C2664 | A2602 | C2602 | C2540 | A2478 | G2417 | C2356 | C2293 | G2232 | C | G2100 | A1977 | U1915 | C1838 |
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| G2675 | A2613 | A2613 | U2552 | G2489 | G2428 | G2367 | A2304 | U2243 | A | C | G1989 | C1924 | A1847 |
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| G2682 | C2620 | C2620 | C2559 | C2496 | A2435 | C2374 | A2311 | G2251 | C | U | G1996 | A1932 | G1856 |
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| C2684 | G2622 | G2622 | U2562 | G2498 | U2437 | A2376 | C2314 | G2253 | C | G | G1998 | C1934 | G1858 |
| U2685 | U2623 | U2623 | U2563 | C2499 | U2438 | A2377 | G2315 | C2254 | U | U | G1999 | A1935 | G1859 |
| G2686 | C2624 | C2624 | A2564 | U2500 | A2439 | A2378 | G2316 | G2255 | C | G | G2000 | A1936 | G1862 |
| U2687 | U2625 | U2625 | G2565 | C2501 | A2440 | G2379 | C2317 | G2256 | U | U | A2001 | A1937 | |
| C2688 | G2626 | G2626 | G2566 | G2502 | C2441 | C2380 | G2318 | U2257 | C | | | | |
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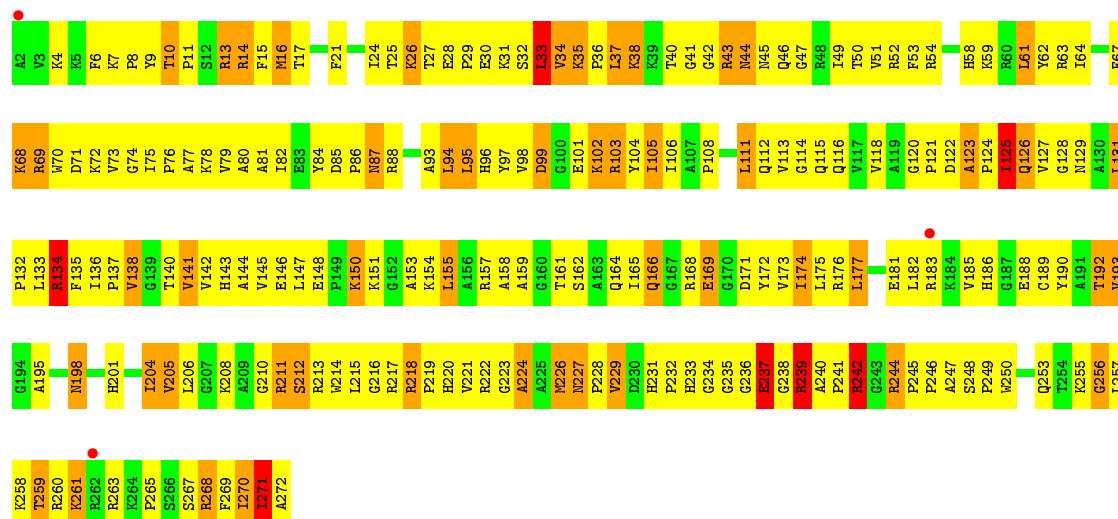
• Molecule 24: 5S ribosomal RNA



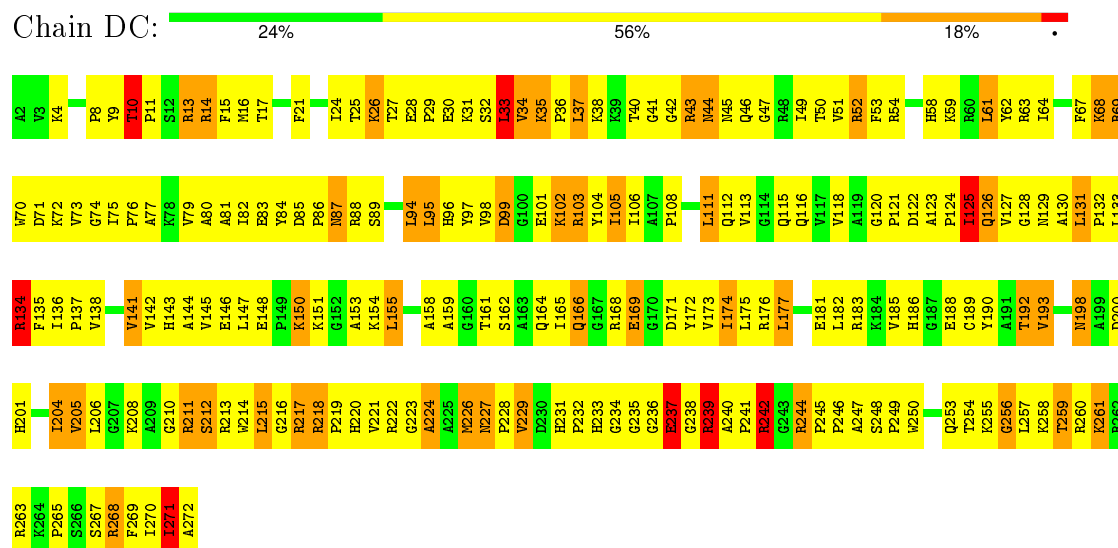
• Molecule 24: 5S ribosomal RNA



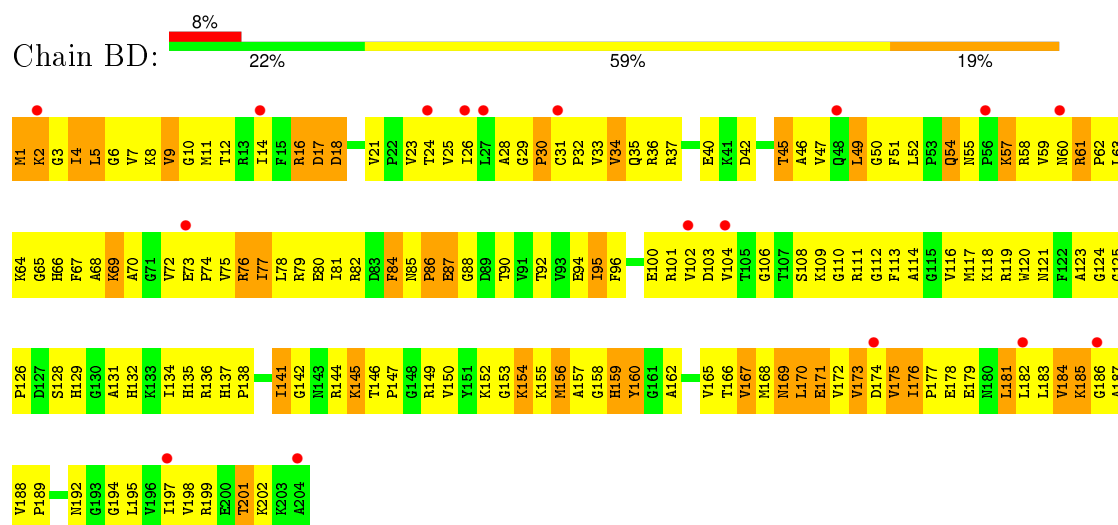
• Molecule 25: 50S ribosomal protein L2



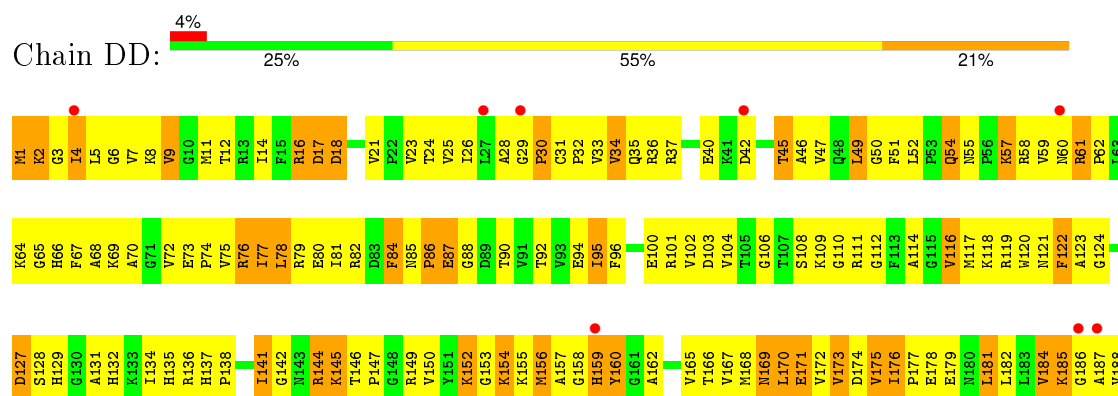
- Molecule 25: 50S ribosomal protein L2

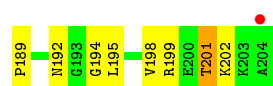


- Molecule 26: 50S ribosomal protein L3



- Molecule 26: 50S ribosomal protein L3





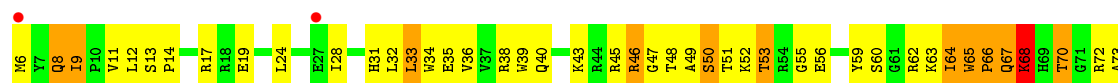
- Molecule 27: 50S ribosomal protein L4

Chain BE: 35% 47% 18%



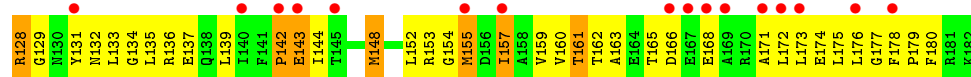
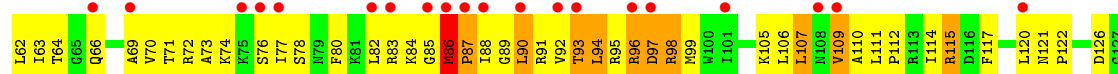
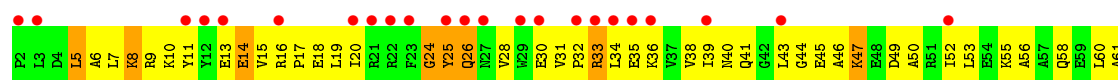
- Molecule 27: 50S ribosomal protein L4

Chain DE: 2% 34% 48% 16%



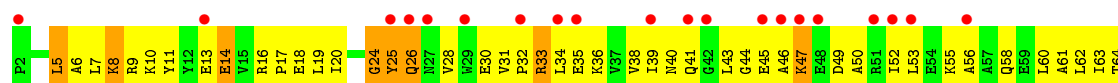
- Molecule 28: 50S ribosomal protein L5

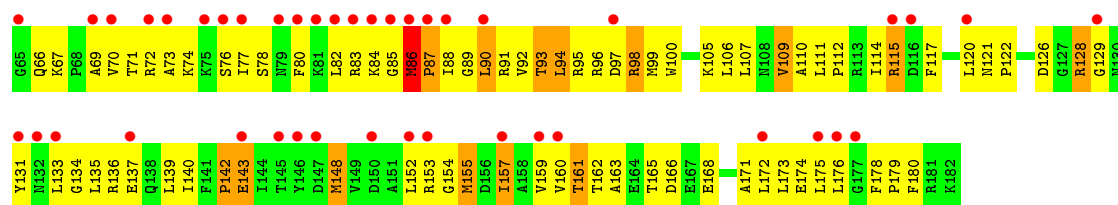
Chain BF: 33% 30% 56% 14%



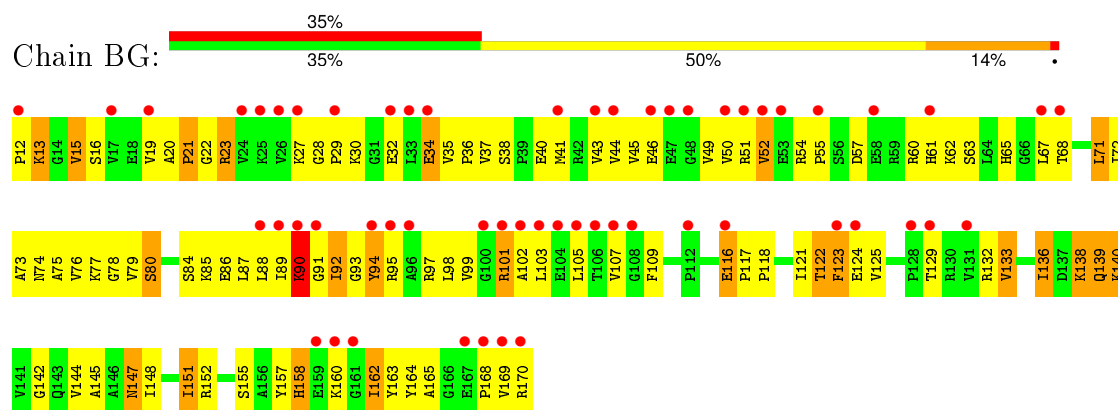
- Molecule 28: 50S ribosomal protein L5

Chain DF: 34% 30% 57% 12%

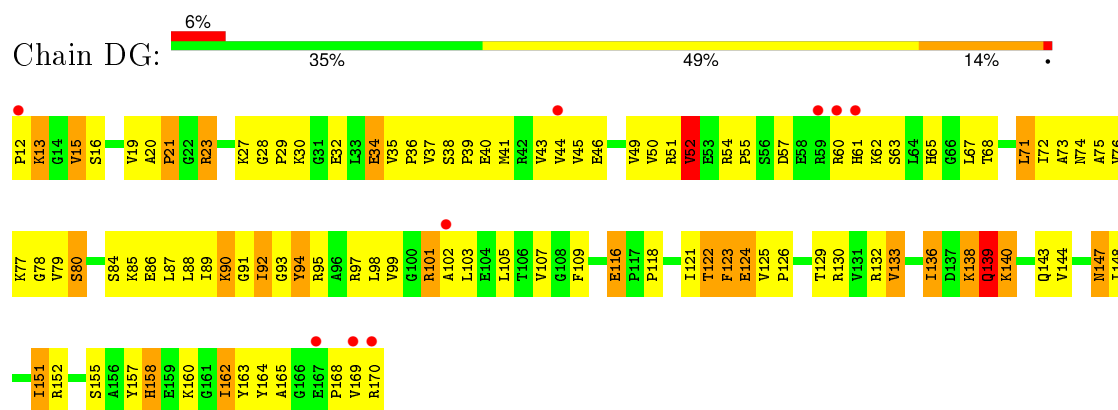




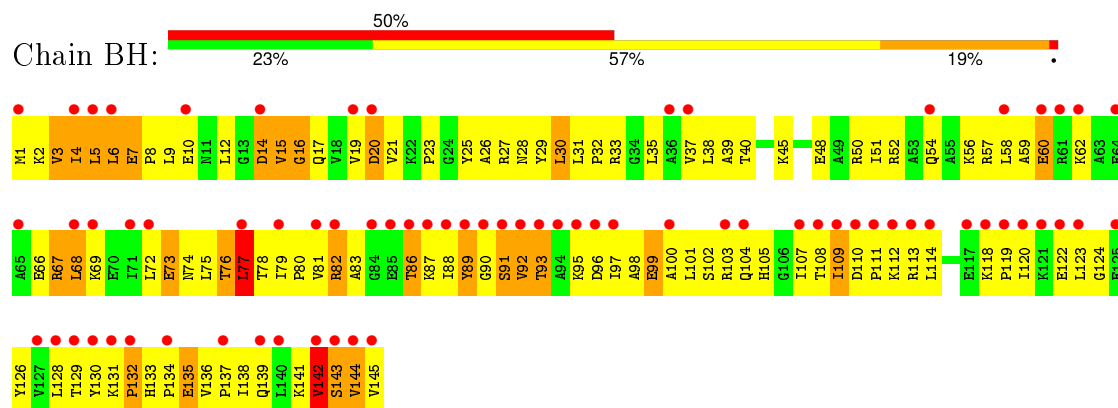
• Molecule 29: 50S ribosomal protein L6



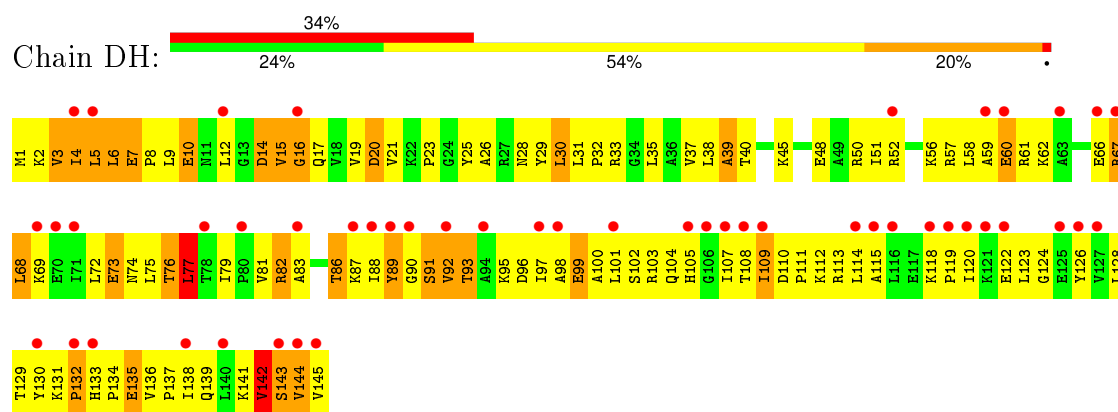
• Molecule 29: 50S ribosomal protein L6



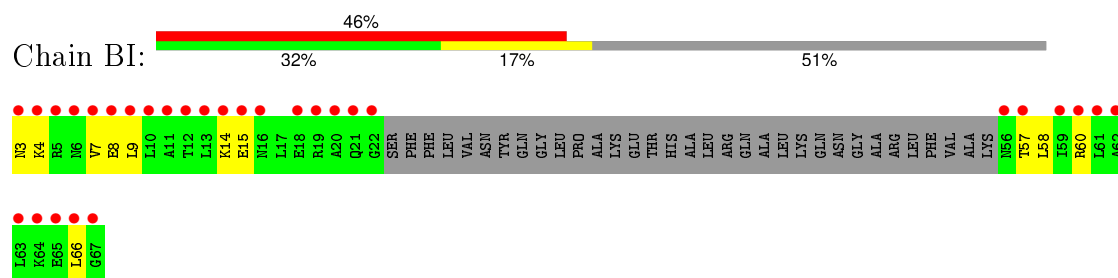
• Molecule 30: 50S ribosomal protein L9



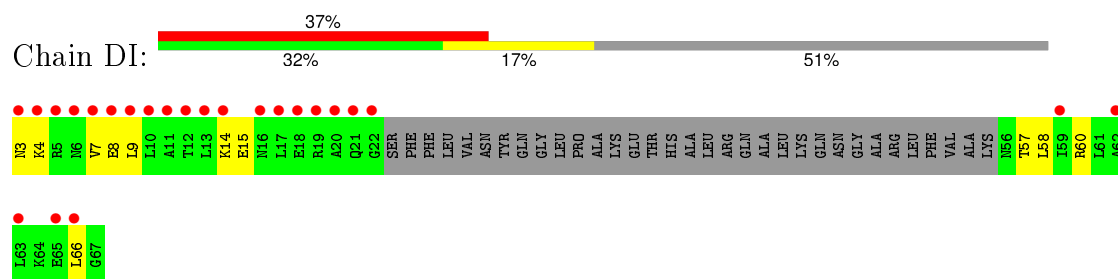
• Molecule 30: 50S ribosomal protein L9



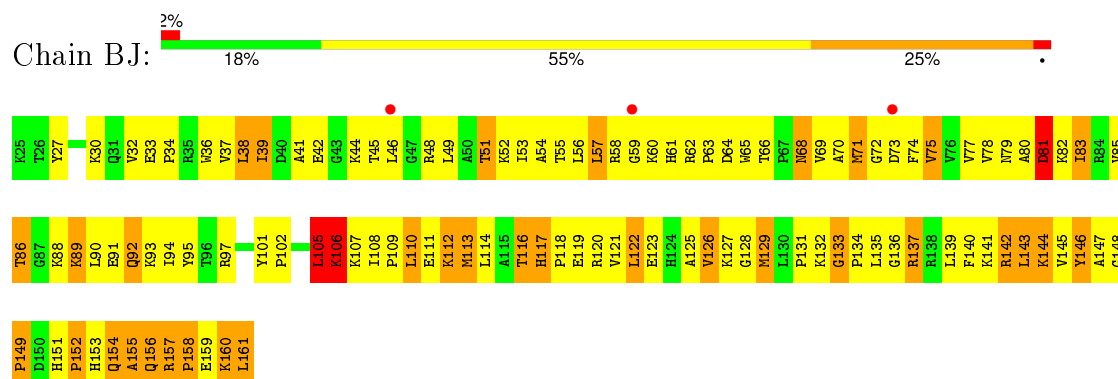
• Molecule 31: 50S ribosomal protein L10



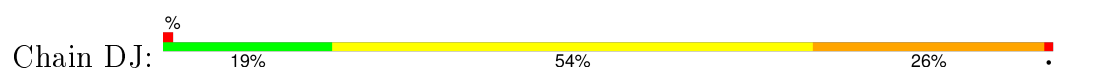
• Molecule 31: 50S ribosomal protein L10

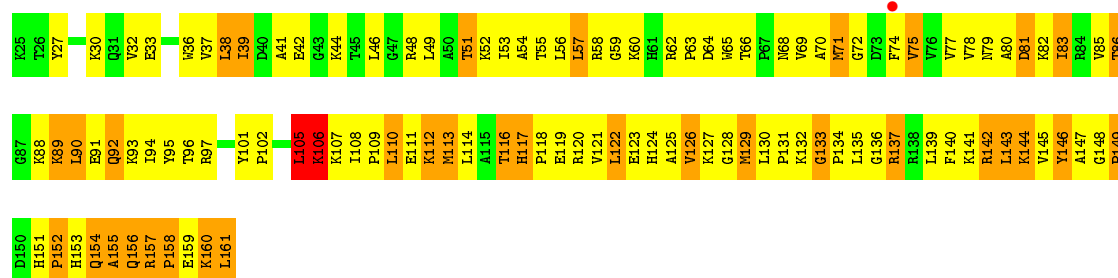


• Molecule 32: 50S ribosomal protein L13



• Molecule 32: 50S ribosomal protein L13





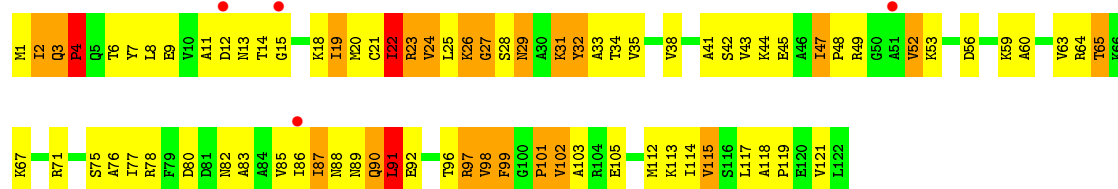
- Molecule 33: 50S ribosomal protein L14

Chain BK: 30% 49% 18%



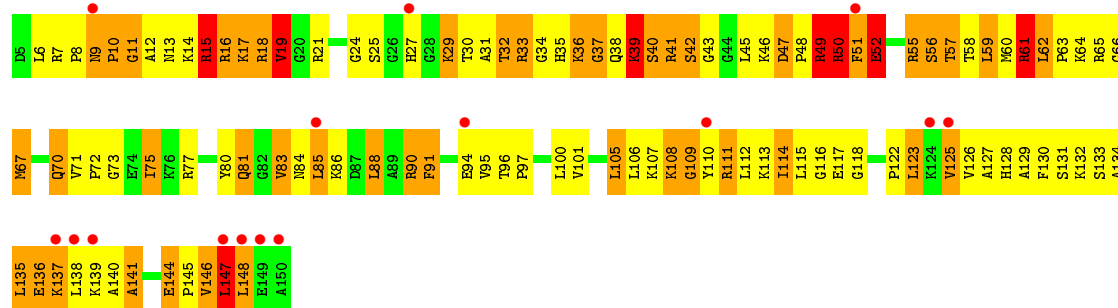
- Molecule 33: 50S ribosomal protein L14

Chain DK: 3% 34% 46% 17%



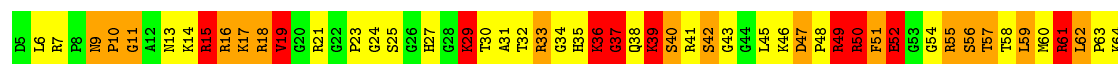
- Molecule 34: 50S ribosomal protein L15

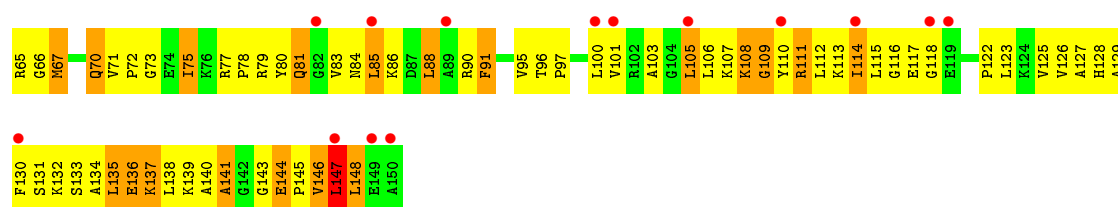
Chain BL: 10% 23% 42% 30% 5%



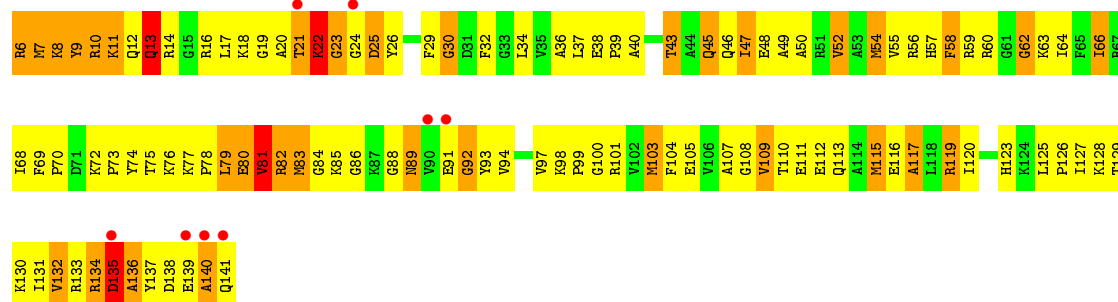
- Molecule 34: 50S ribosomal protein L15

Chain DL: 10% 21% 48% 24% 8%

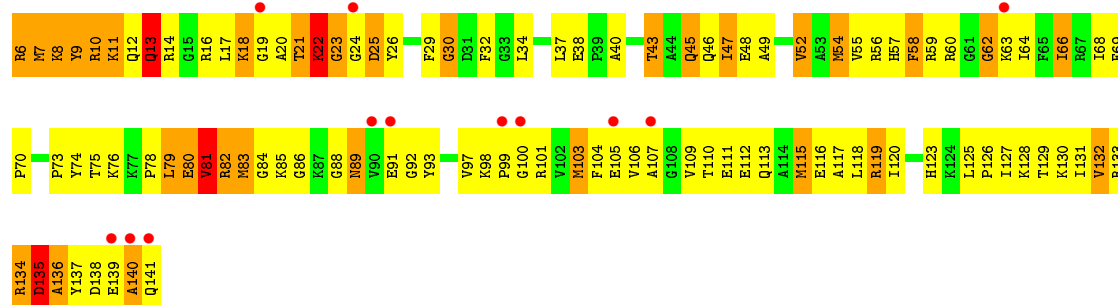




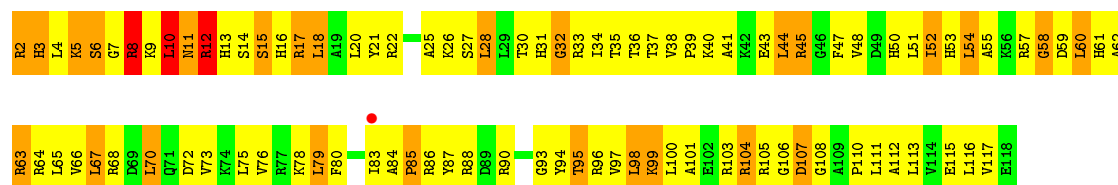
• Molecule 35: 50S ribosomal protein L16



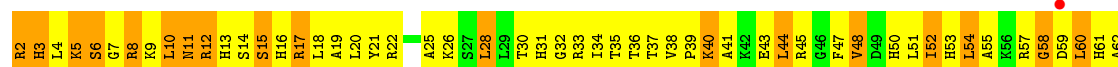
• Molecule 35: 50S ribosomal protein L16

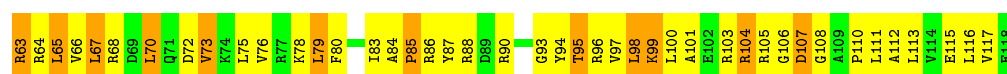


• Molecule 36: 50S ribosomal protein L17

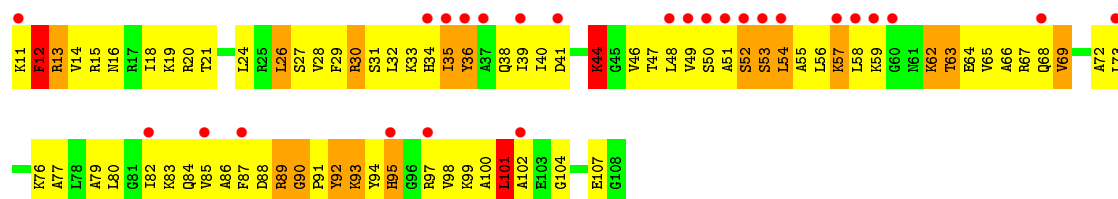


• Molecule 36: 50S ribosomal protein L17

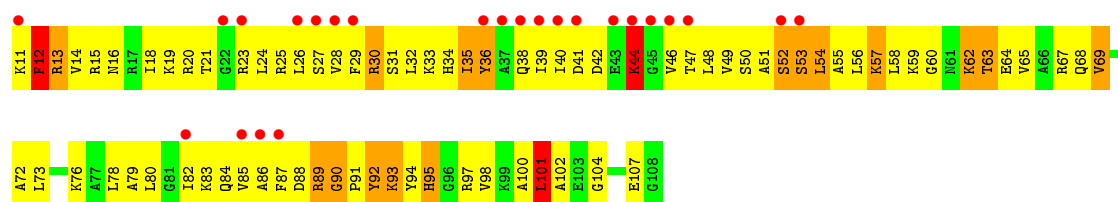




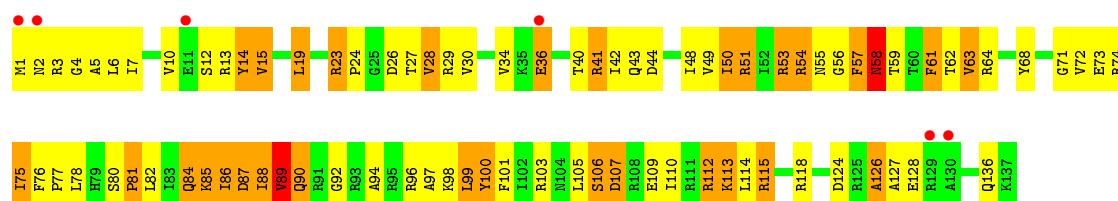
• Molecule 37: 50S ribosomal protein L18



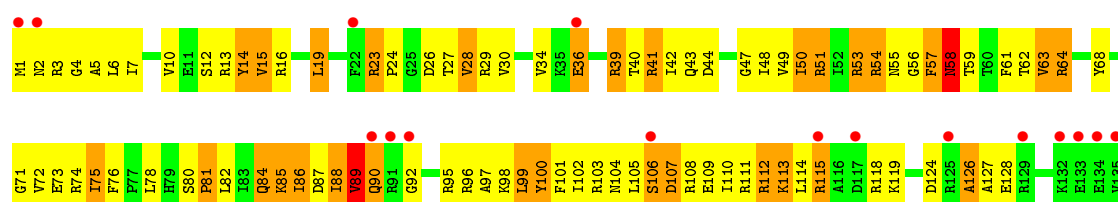
• Molecule 37: 50S ribosomal protein L18



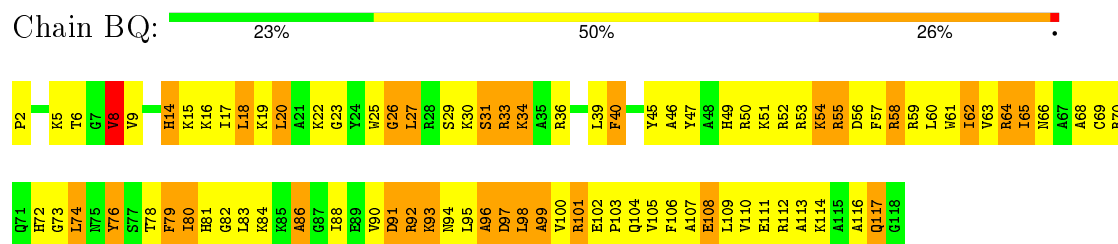
• Molecule 38: 50S ribosomal protein L19



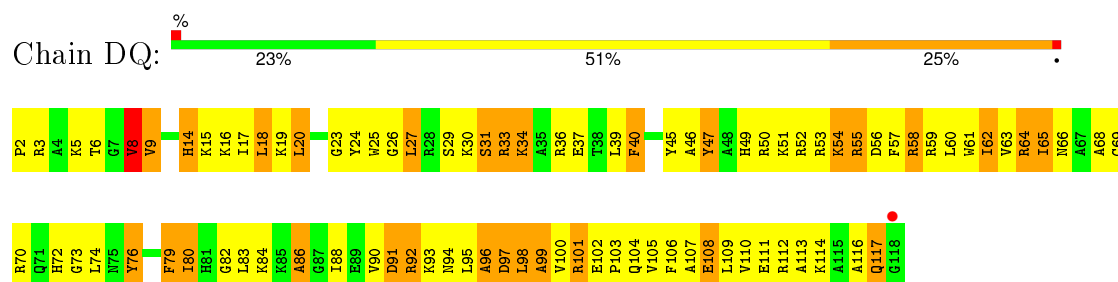
• Molecule 38: 50S ribosomal protein L19



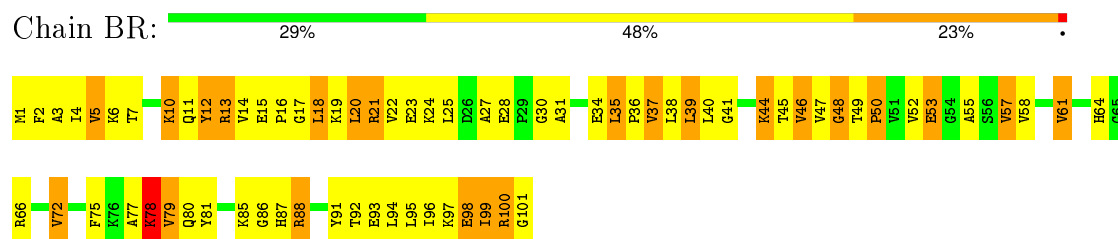
• Molecule 39: 50S ribosomal protein L20



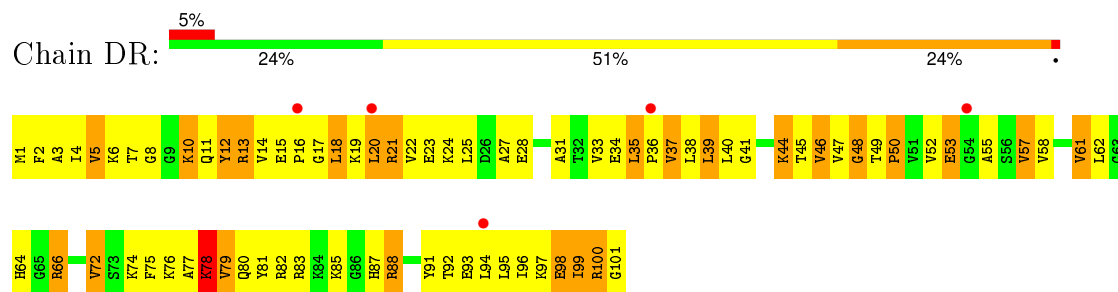
- Molecule 39: 50S ribosomal protein L20



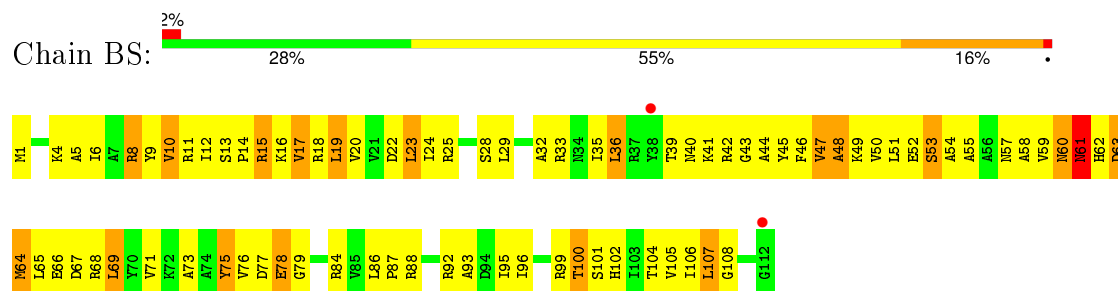
- Molecule 40: 50S ribosomal protein L21



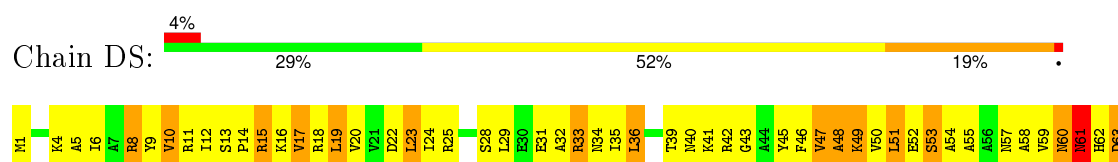
- Molecule 40: 50S ribosomal protein L21



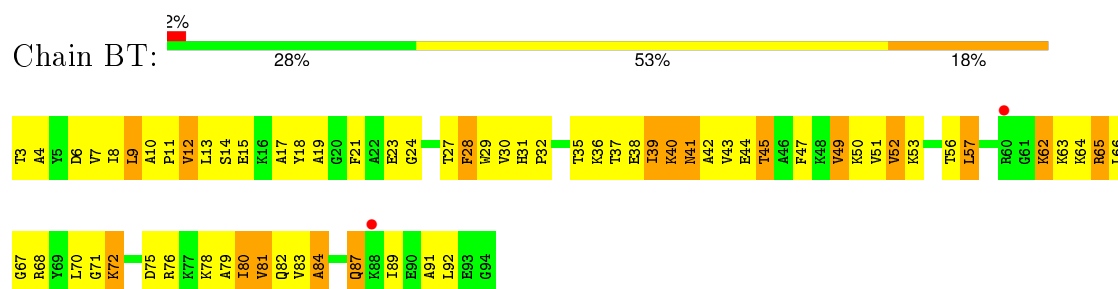
- Molecule 41: 50S ribosomal protein L22



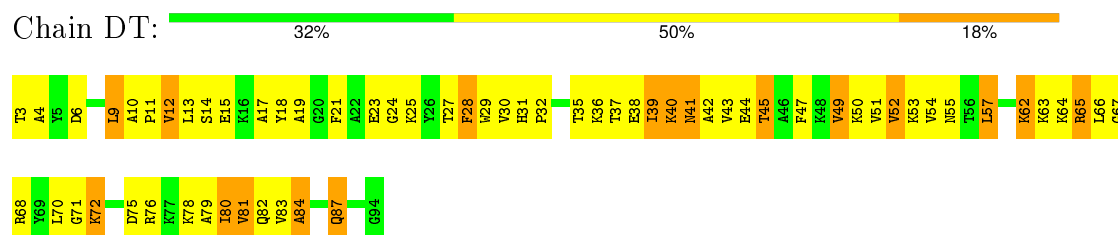
- Molecule 41: 50S ribosomal protein L22



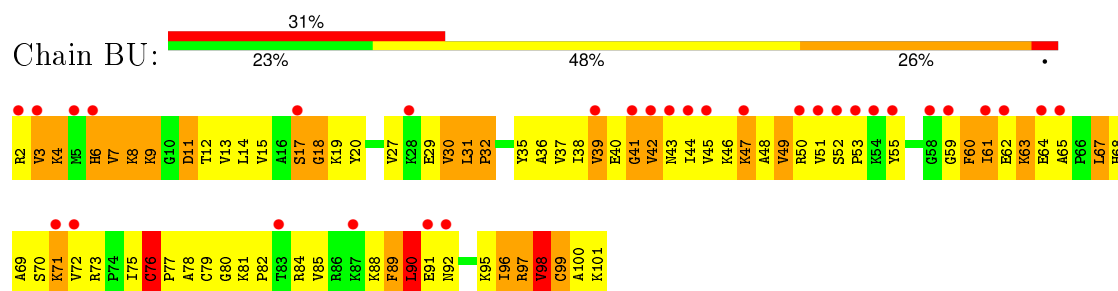
- Molecule 42: 50S ribosomal protein L23



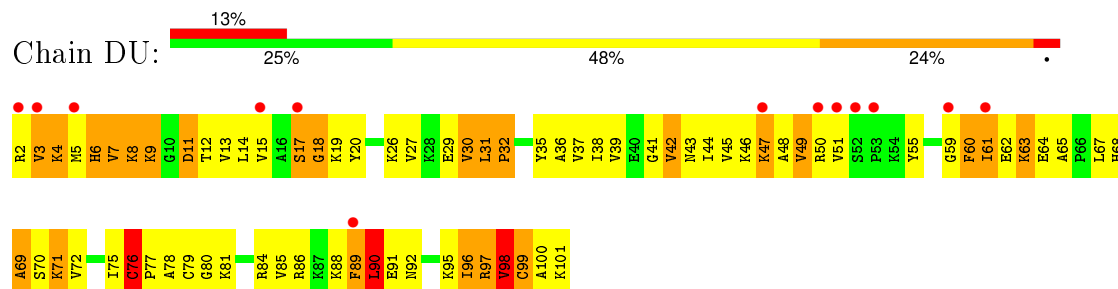
- Molecule 42: 50S ribosomal protein L23



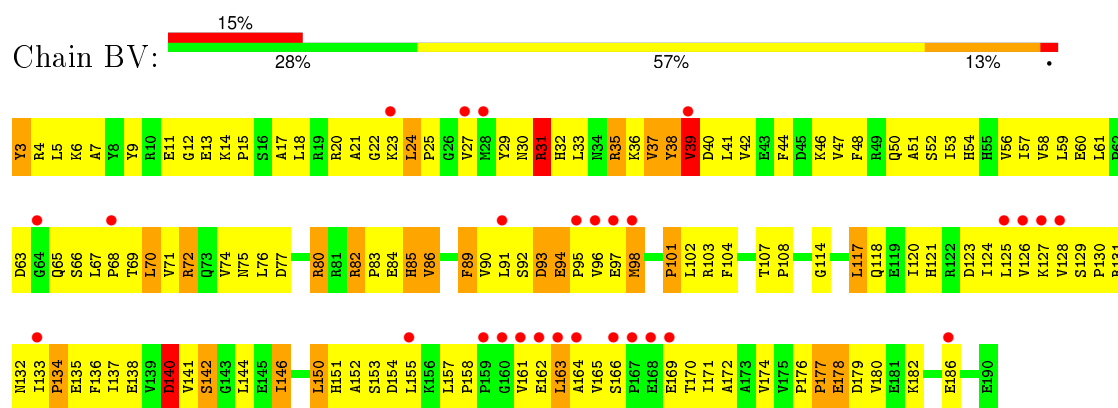
- Molecule 43: 50S ribosomal protein L24



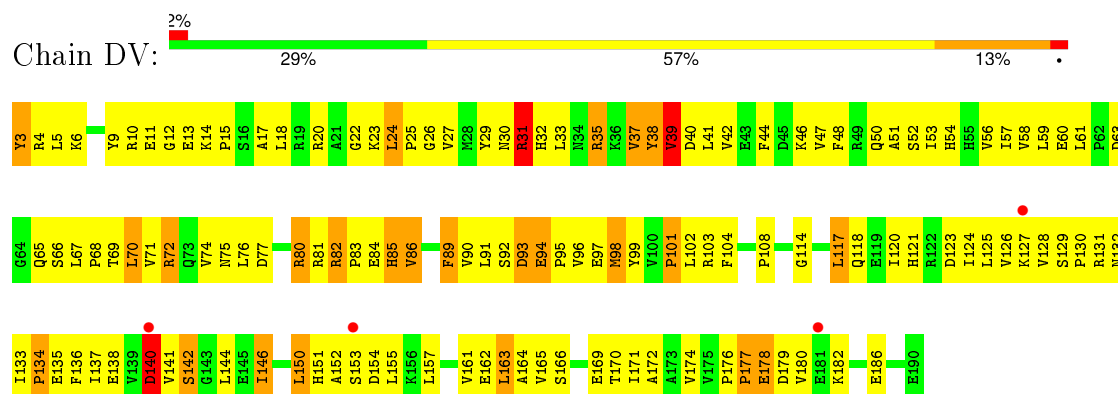
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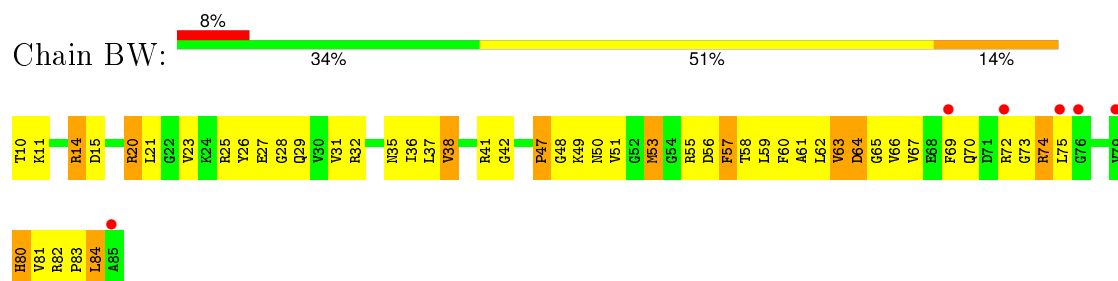
- Molecule 44: 50S ribosomal protein L25



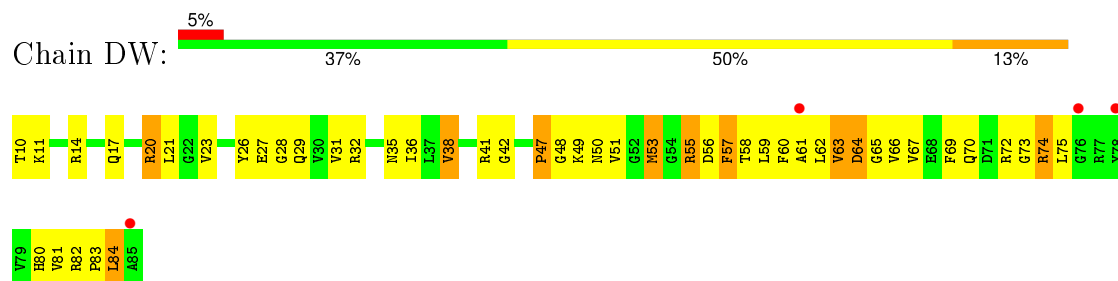
- Molecule 44: 50S ribosomal protein L25



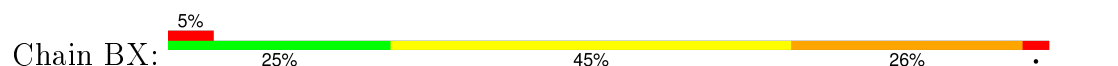
- Molecule 45: 50S ribosomal protein L27



- Molecule 45: 50S ribosomal protein L27

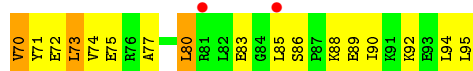


- Molecule 46: 50S ribosomal protein L28

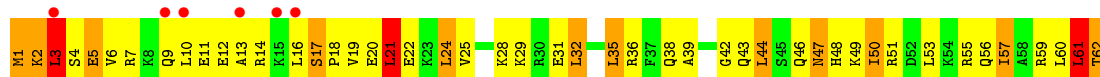




• Molecule 46: 50S ribosomal protein L28



• Molecule 47: 50S ribosomal protein L29



• Molecule 47: 50S ribosomal protein L29



• Molecule 48: 50S ribosomal protein L30

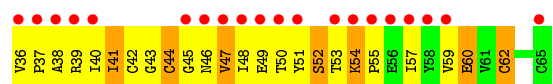


• Molecule 48: 50S ribosomal protein L30

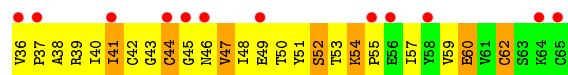
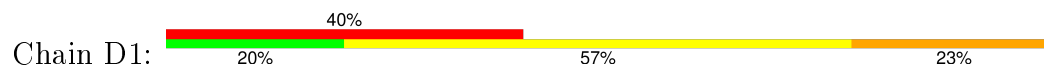


• Molecule 49: 50S ribosomal protein L31

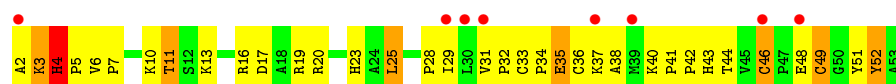




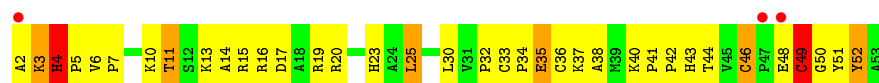
- Molecule 49: 50S ribosomal protein L31



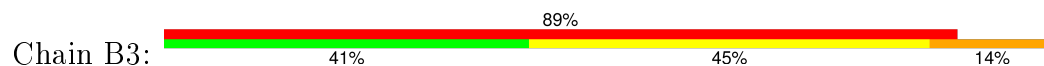
- Molecule 50: 50S ribosomal protein L32



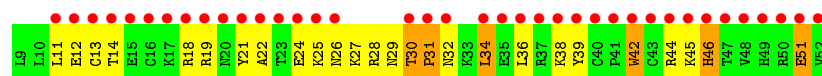
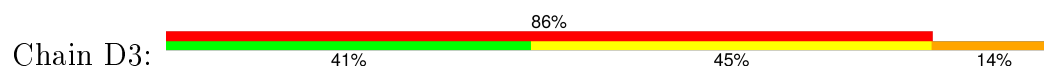
- Molecule 50: 50S ribosomal protein L32



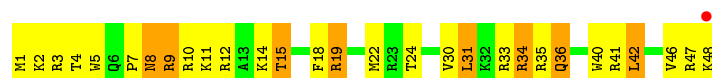
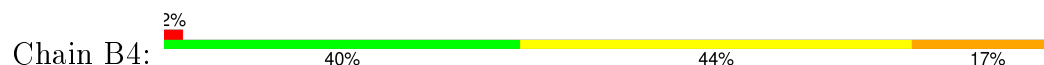
- Molecule 51: 50S ribosomal protein L33



- Molecule 51: 50S ribosomal protein L33



- Molecule 52: 50S ribosomal protein L34



- Molecule 52: 50S ribosomal protein L34

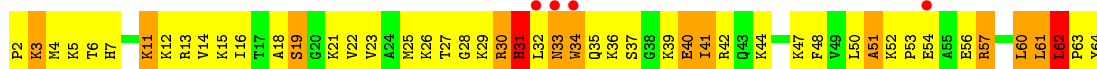




- Molecule 53: 50S ribosomal protein L35



- Molecule 53: 50S ribosomal protein L35



4 Data and refinement statistics

| Property | Value | Source |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 210.69Å 451.66Å 614.25Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 49.52 – 3.40 49.52 – 3.40 | Depositor EDS |
| % Data completeness (in resolution range) | 97.5 (49.52-3.40) 97.6 (49.52-3.40) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.28 (at 3.40Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: 1.6.1_357) | Depositor |
| R, R_{free} | 0.228 , 0.266 0.223 , 0.262 | Depositor DCC |
| R_{free} test set | 7680 reflections (0.99%) | DCC |
| Wilson B-factor (Å ²) | 86.0 | Xtriage |
| Anisotropy | 0.391 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.27 , 106.4 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$ | Xtriage |
| Outliers | 0 of 775950 reflections | Xtriage |
| F_o, F_c correlation | 0.91 | EDS |
| Total number of atoms | 282142 | wwPDB-VP |
| Average B, all atoms (Å ²) | 110.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|-----------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | AA | 0.63 | 4/36238 (0.0%) | 1.02 | 99/56561 (0.2%) |
| 1 | CA | 0.57 | 0/36238 | 0.96 | 75/56561 (0.1%) |
| 2 | AB | 0.31 | 0/1936 | 0.51 | 0/2609 |
| 2 | CB | 0.28 | 0/1936 | 0.50 | 0/2609 |
| 3 | AC | 0.31 | 0/1637 | 0.47 | 0/2205 |
| 3 | CC | 0.29 | 0/1637 | 0.47 | 0/2205 |
| 4 | AD | 0.41 | 0/1733 | 0.59 | 0/2318 |
| 4 | CD | 0.34 | 0/1733 | 0.56 | 0/2318 |
| 5 | AE | 0.41 | 0/1172 | 0.61 | 0/1576 |
| 5 | CE | 0.36 | 0/1172 | 0.57 | 0/1576 |
| 6 | AF | 0.33 | 0/856 | 0.57 | 0/1154 |
| 6 | CF | 0.37 | 0/856 | 0.59 | 0/1154 |
| 7 | AG | 0.27 | 0/1276 | 0.46 | 0/1709 |
| 7 | CG | 0.27 | 0/1276 | 0.46 | 0/1709 |
| 8 | AH | 0.39 | 0/1136 | 0.61 | 0/1527 |
| 8 | CH | 0.33 | 0/1136 | 0.58 | 0/1527 |
| 9 | AI | 0.29 | 0/1029 | 0.45 | 0/1378 |
| 9 | CI | 0.27 | 0/1029 | 0.45 | 0/1378 |
| 10 | AJ | 0.28 | 0/808 | 0.48 | 0/1085 |
| 10 | CJ | 0.27 | 0/808 | 0.46 | 0/1085 |
| 11 | AK | 0.39 | 0/900 | 0.59 | 0/1213 |
| 11 | CK | 0.41 | 0/900 | 0.61 | 0/1213 |
| 12 | AL | 0.47 | 0/987 | 0.70 | 1/1320 (0.1%) |
| 12 | CL | 0.44 | 0/987 | 0.68 | 0/1320 |
| 13 | AM | 0.25 | 0/939 | 0.44 | 0/1258 |
| 13 | CM | 0.24 | 0/939 | 0.44 | 0/1258 |
| 14 | AN | 0.31 | 0/501 | 0.50 | 0/664 |
| 14 | CN | 0.31 | 0/501 | 0.52 | 0/664 |
| 15 | AO | 0.39 | 0/745 | 0.57 | 0/992 |
| 15 | CO | 0.37 | 0/745 | 0.56 | 0/992 |
| 16 | AP | 0.42 | 0/717 | 0.62 | 0/963 |
| 16 | CP | 0.34 | 0/717 | 0.59 | 0/963 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|--------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | AQ | 0.43 | 0/837 | 0.60 | 0/1117 |
| 17 | CQ | 0.37 | 0/837 | 0.56 | 0/1117 |
| 18 | AR | 0.38 | 0/579 | 0.61 | 0/768 |
| 18 | CR | 0.37 | 0/579 | 0.60 | 0/768 |
| 19 | AS | 0.25 | 0/643 | 0.43 | 0/865 |
| 19 | CS | 0.25 | 0/643 | 0.42 | 0/865 |
| 20 | AT | 0.38 | 0/764 | 0.57 | 0/1006 |
| 20 | CT | 0.33 | 0/764 | 0.54 | 0/1006 |
| 21 | AU | 0.23 | 0/213 | 0.43 | 0/277 |
| 21 | CU | 0.24 | 0/213 | 0.42 | 0/277 |
| 22 | AV | 0.43 | 0/802 | 0.68 | 0/1245 |
| 22 | CV | 0.43 | 0/802 | 0.69 | 0/1245 |
| 23 | BA | 1.07 | 153/66570 (0.2%) | 1.48 | 1344/103918 (1.3%) |
| 23 | DA | 1.19 | 253/66575 (0.4%) | 1.59 | 1756/103930 (1.7%) |
| 24 | BB | 0.58 | 0/2853 | 1.00 | 9/4451 (0.2%) |
| 24 | DB | 0.59 | 0/2853 | 1.04 | 3/4451 (0.1%) |
| 25 | BC | 0.71 | 1/2155 (0.0%) | 0.90 | 3/2905 (0.1%) |
| 25 | DC | 0.74 | 1/2155 (0.0%) | 0.91 | 5/2905 (0.2%) |
| 26 | BD | 0.58 | 0/1597 | 0.77 | 0/2153 |
| 26 | DD | 0.62 | 1/1597 (0.1%) | 0.81 | 0/2153 |
| 27 | BE | 0.63 | 0/1622 | 0.77 | 0/2194 |
| 27 | DE | 0.67 | 0/1622 | 0.78 | 0/2194 |
| 28 | BF | 0.28 | 0/1500 | 0.49 | 0/2017 |
| 28 | DF | 0.28 | 0/1500 | 0.49 | 0/2017 |
| 29 | BG | 0.32 | 0/1246 | 0.58 | 0/1682 |
| 29 | DG | 0.44 | 0/1246 | 0.64 | 0/1682 |
| 30 | BH | 0.33 | 0/1148 | 0.56 | 0/1552 |
| 30 | DH | 0.38 | 0/1148 | 0.56 | 0/1552 |
| 31 | BI | 0.25 | 0/252 | 0.44 | 0/333 |
| 31 | DI | 0.27 | 0/252 | 0.46 | 0/333 |
| 32 | BJ | 0.56 | 0/1124 | 0.75 | 0/1515 |
| 32 | DJ | 0.59 | 0/1124 | 0.76 | 0/1515 |
| 33 | BK | 0.57 | 0/942 | 0.76 | 0/1268 |
| 33 | DK | 0.61 | 0/942 | 0.77 | 0/1268 |
| 34 | BL | 0.74 | 1/1131 (0.1%) | 1.01 | 1/1504 (0.1%) |
| 34 | DL | 0.75 | 2/1131 (0.2%) | 1.03 | 5/1504 (0.3%) |
| 35 | BM | 0.61 | 0/1099 | 0.83 | 2/1468 (0.1%) |
| 35 | DM | 0.60 | 0/1099 | 0.83 | 1/1468 (0.1%) |
| 36 | BN | 0.59 | 0/974 | 0.85 | 0/1302 |
| 36 | DN | 0.59 | 0/974 | 0.83 | 1/1302 (0.1%) |
| 37 | BO | 0.36 | 0/779 | 0.58 | 0/1036 |
| 37 | DO | 0.39 | 0/779 | 0.61 | 0/1036 |
| 38 | BP | 0.50 | 0/1158 | 0.68 | 0/1544 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------------|-------------|--------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 38 | DP | 0.51 | 0/1158 | 0.69 | 0/1544 |
| 39 | BQ | 0.63 | 0/970 | 0.81 | 0/1290 |
| 39 | DQ | 0.67 | 0/970 | 0.81 | 0/1290 |
| 40 | BR | 0.58 | 0/790 | 0.73 | 1/1057 (0.1%) |
| 40 | DR | 0.61 | 0/790 | 0.74 | 1/1057 (0.1%) |
| 41 | BS | 0.63 | 0/902 | 0.78 | 0/1209 |
| 41 | DS | 0.66 | 0/902 | 0.76 | 0/1209 |
| 42 | BT | 0.64 | 0/740 | 0.79 | 0/993 |
| 42 | DT | 0.74 | 0/740 | 0.84 | 0/993 |
| 43 | BU | 0.53 | 0/789 | 0.76 | 0/1051 |
| 43 | DU | 0.56 | 0/789 | 0.76 | 0/1051 |
| 44 | BV | 0.36 | 0/1524 | 0.57 | 0/2068 |
| 44 | DV | 0.38 | 0/1524 | 0.57 | 0/2068 |
| 45 | BW | 0.50 | 0/613 | 0.71 | 0/816 |
| 45 | DW | 0.52 | 0/613 | 0.72 | 0/816 |
| 46 | BX | 0.73 | 0/702 | 0.98 | 2/932 (0.2%) |
| 46 | DX | 0.82 | 0/702 | 1.04 | 2/932 (0.2%) |
| 47 | BY | 0.55 | 0/523 | 0.87 | 1/690 (0.1%) |
| 47 | DY | 0.72 | 0/523 | 0.98 | 3/690 (0.4%) |
| 48 | BZ | 0.52 | 0/473 | 0.68 | 0/634 |
| 48 | DZ | 0.50 | 0/473 | 0.65 | 0/634 |
| 49 | B1 | 0.23 | 0/229 | 0.40 | 0/309 |
| 49 | D1 | 0.22 | 0/229 | 0.41 | 0/309 |
| 50 | B2 | 0.61 | 0/419 | 0.80 | 0/567 |
| 50 | D2 | 0.58 | 0/419 | 0.79 | 0/567 |
| 51 | B3 | 0.28 | 0/388 | 0.46 | 0/518 |
| 51 | D3 | 0.27 | 0/388 | 0.46 | 0/518 |
| 52 | B4 | 0.72 | 0/427 | 0.89 | 0/561 |
| 52 | D4 | 0.84 | 0/427 | 1.05 | 1/561 (0.2%) |
| 53 | B5 | 0.68 | 0/516 | 0.88 | 0/679 |
| 53 | D5 | 0.69 | 0/516 | 0.88 | 1/679 (0.1%) |
| All | All | 0.85 | 416/305211 (0.1%) | 1.21 | 3317/456064 (0.7%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 25 | DC | 0 | 1 |
| 27 | BE | 0 | 1 |
| 27 | DE | 0 | 1 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 34 | BL | 0 | 5 |
| 34 | DL | 0 | 5 |
| 35 | BM | 0 | 1 |
| 35 | DM | 0 | 1 |
| 36 | BN | 0 | 1 |
| 36 | DN | 0 | 1 |
| 39 | BQ | 0 | 2 |
| 39 | DQ | 0 | 2 |
| All | All | 0 | 21 |

All (416) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 23 | DA | 774 | A | N9-C4 | -13.87 | 1.29 | 1.37 |
| 23 | DA | 1332 | G | N9-C4 | -11.99 | 1.28 | 1.38 |
| 23 | DA | 1602 | U | C4-O4 | 11.31 | 1.32 | 1.23 |
| 23 | BA | 1332 | G | N9-C4 | -11.02 | 1.29 | 1.38 |
| 23 | DA | 2249 | U | C4-O4 | 10.67 | 1.32 | 1.23 |
| 23 | DA | 1614 | A | N9-C4 | -10.65 | 1.31 | 1.37 |
| 23 | DA | 761 | A | C5-C4 | 10.24 | 1.46 | 1.38 |
| 23 | DA | 71 | A | N9-C4 | -10.23 | 1.31 | 1.37 |
| 23 | DA | 676 | A | N9-C4 | -9.99 | 1.31 | 1.37 |
| 23 | DA | 2593 | U | C4-O4 | 9.50 | 1.31 | 1.23 |
| 23 | BA | 570 | G | C6-O6 | 9.46 | 1.32 | 1.24 |
| 23 | DA | 761 | A | C6-N1 | 9.44 | 1.42 | 1.35 |
| 23 | BA | 676 | A | N9-C4 | -9.32 | 1.32 | 1.37 |
| 23 | BA | 1678 | G | N9-C4 | -9.10 | 1.30 | 1.38 |
| 23 | DA | 677 | A | N9-C4 | -9.09 | 1.32 | 1.37 |
| 23 | BA | 1783 | A | N3-C4 | -8.94 | 1.29 | 1.34 |
| 23 | DA | 1671 | U | C4-O4 | 8.93 | 1.30 | 1.23 |
| 23 | BA | 1786 | A | N3-C4 | -8.91 | 1.29 | 1.34 |
| 23 | DA | 774 | A | N3-C4 | -8.90 | 1.29 | 1.34 |
| 23 | BA | 774 | A | N9-C4 | -8.86 | 1.32 | 1.37 |
| 23 | DA | 677 | A | N3-C4 | -8.81 | 1.29 | 1.34 |
| 23 | BA | 1332 | G | C2-N3 | -8.54 | 1.25 | 1.32 |
| 23 | DA | 797 | C | N1-C6 | -8.37 | 1.32 | 1.37 |
| 23 | DA | 783 | A | N9-C4 | -8.32 | 1.32 | 1.37 |
| 23 | BA | 503 | A | N3-C4 | -8.11 | 1.29 | 1.34 |
| 23 | BA | 1971 | A | N3-C4 | -8.09 | 1.29 | 1.34 |
| 23 | DA | 575 | A | N9-C4 | -8.06 | 1.33 | 1.37 |
| 23 | BA | 761 | A | C6-N1 | 7.89 | 1.41 | 1.35 |
| 23 | BA | 2028 | U | C4-O4 | 7.87 | 1.29 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 23 | BA | 192 | C | N1-C6 | -7.77 | 1.32 | 1.37 |
| 34 | DL | 39 | LYS | CB-CG | 7.73 | 1.73 | 1.52 |
| 23 | DA | 1322 | A | N3-C4 | -7.73 | 1.30 | 1.34 |
| 23 | DA | 1678 | G | N9-C4 | -7.70 | 1.31 | 1.38 |
| 34 | BL | 39 | LYS | CB-CG | 7.70 | 1.73 | 1.52 |
| 23 | BA | 675 | A | N9-C4 | -7.63 | 1.33 | 1.37 |
| 23 | BA | 1783 | A | N9-C4 | -7.62 | 1.33 | 1.37 |
| 23 | BA | 800 | A | N9-C4 | -7.53 | 1.33 | 1.37 |
| 23 | BA | 2448 | A | N9-C4 | -7.52 | 1.33 | 1.37 |
| 23 | DA | 2028 | U | C4-O4 | 7.49 | 1.29 | 1.23 |
| 23 | BA | 1786 | A | N9-C4 | -7.48 | 1.33 | 1.37 |
| 23 | DA | 1829 | A | N9-C4 | -7.45 | 1.33 | 1.37 |
| 23 | DA | 945 | A | N7-C5 | -7.41 | 1.34 | 1.39 |
| 23 | DA | 265 | A | N9-C4 | -7.38 | 1.33 | 1.37 |
| 23 | DA | 2032 | G | N7-C5 | 7.32 | 1.43 | 1.39 |
| 23 | DA | 761 | A | C6-N6 | 7.30 | 1.39 | 1.33 |
| 23 | BA | 1308 | A | N9-C4 | -7.30 | 1.33 | 1.37 |
| 23 | DA | 1614 | A | N7-C5 | -7.27 | 1.34 | 1.39 |
| 23 | BA | 330 | A | N9-C4 | -7.22 | 1.33 | 1.37 |
| 23 | DA | 748 | G | C5-C4 | -7.22 | 1.33 | 1.38 |
| 23 | BA | 2057 | A | N3-C4 | -7.15 | 1.30 | 1.34 |
| 23 | BA | 2057 | A | N9-C4 | -7.15 | 1.33 | 1.37 |
| 23 | DA | 1367 | A | C6-N1 | -7.12 | 1.30 | 1.35 |
| 23 | BA | 2433 | A | N3-C4 | -7.11 | 1.30 | 1.34 |
| 23 | DA | 450 | G | C6-O6 | 7.10 | 1.30 | 1.24 |
| 23 | BA | 1021 | A | N9-C4 | -7.07 | 1.33 | 1.37 |
| 23 | DA | 678 | C | N3-C4 | -7.07 | 1.28 | 1.33 |
| 23 | BA | 1786 | A | N7-C5 | -7.01 | 1.35 | 1.39 |
| 23 | BA | 655 | A | N9-C4 | 6.99 | 1.42 | 1.37 |
| 23 | DA | 211 | A | N3-C4 | -6.96 | 1.30 | 1.34 |
| 23 | BA | 2518 | A | N9-C4 | -6.94 | 1.33 | 1.37 |
| 23 | BA | 1902 | C | N3-C4 | -6.94 | 1.29 | 1.33 |
| 23 | BA | 761 | A | C5-C4 | 6.92 | 1.43 | 1.38 |
| 23 | BA | 2028 | U | C2-N3 | 6.90 | 1.42 | 1.37 |
| 23 | DA | 1802 | A | N3-C4 | -6.88 | 1.30 | 1.34 |
| 23 | DA | 676 | A | N3-C4 | -6.87 | 1.30 | 1.34 |
| 23 | DA | 2497 | A | N9-C4 | -6.85 | 1.33 | 1.37 |
| 23 | BA | 1332 | G | N3-C4 | -6.83 | 1.30 | 1.35 |
| 23 | DA | 945 | A | C5-C6 | -6.81 | 1.34 | 1.41 |
| 23 | DA | 2518 | A | N9-C4 | -6.81 | 1.33 | 1.37 |
| 23 | DA | 761 | A | N1-C2 | 6.79 | 1.40 | 1.34 |
| 23 | DA | 2506 | U | N1-C2 | 6.78 | 1.44 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|-------|-------|-------------|----------|
| 23 | DA | 2028 | U | C2-N3 | 6.76 | 1.42 | 1.37 |
| 23 | BA | 584 | C | N1-C6 | -6.74 | 1.33 | 1.37 |
| 23 | DA | 1783 | A | N3-C4 | -6.73 | 1.30 | 1.34 |
| 23 | DA | 450 | G | N9-C8 | -6.72 | 1.33 | 1.37 |
| 23 | DA | 742 | G | C5-C4 | -6.72 | 1.33 | 1.38 |
| 23 | DA | 752 | A | N3-C4 | -6.72 | 1.30 | 1.34 |
| 23 | BA | 783 | A | N9-C4 | -6.72 | 1.33 | 1.37 |
| 23 | BA | 2010 | G | N7-C5 | -6.71 | 1.35 | 1.39 |
| 23 | DA | 2713 | A | N9-C4 | -6.70 | 1.33 | 1.37 |
| 23 | DA | 1378 | A | N3-C4 | -6.68 | 1.30 | 1.34 |
| 23 | DA | 114(B) | A | N9-C4 | -6.68 | 1.33 | 1.37 |
| 23 | DA | 1308 | A | N9-C4 | -6.67 | 1.33 | 1.37 |
| 23 | BA | 2506 | U | N1-C2 | 6.67 | 1.44 | 1.38 |
| 23 | DA | 774 | A | C5-C6 | -6.67 | 1.35 | 1.41 |
| 23 | BA | 528 | A | N9-C4 | -6.67 | 1.33 | 1.37 |
| 23 | BA | 764 | A | N9-C4 | -6.64 | 1.33 | 1.37 |
| 23 | DA | 2427 | C | N1-C6 | -6.64 | 1.33 | 1.37 |
| 23 | DA | 340 | A | N3-C4 | -6.64 | 1.30 | 1.34 |
| 23 | BA | 2713 | A | N9-C4 | -6.62 | 1.33 | 1.37 |
| 23 | BA | 1671 | U | C4-O4 | 6.62 | 1.28 | 1.23 |
| 23 | BA | 453 | C | N1-C6 | -6.61 | 1.33 | 1.37 |
| 23 | DA | 126 | A | C5-C4 | -6.61 | 1.34 | 1.38 |
| 23 | BA | 761 | A | C6-N6 | 6.61 | 1.39 | 1.33 |
| 23 | BA | 2058 | A | N3-C4 | -6.56 | 1.30 | 1.34 |
| 23 | DA | 2054 | A | N7-C5 | -6.56 | 1.35 | 1.39 |
| 23 | DA | 472 | A | N9-C4 | -6.55 | 1.33 | 1.37 |
| 23 | DA | 2061 | G | C6-O6 | 6.55 | 1.30 | 1.24 |
| 23 | DA | 778 | G | N1-C2 | -6.55 | 1.32 | 1.37 |
| 23 | DA | 575 | A | N7-C5 | -6.54 | 1.35 | 1.39 |
| 23 | BA | 945 | A | N7-C5 | -6.53 | 1.35 | 1.39 |
| 23 | DA | 2242 | G | N9-C8 | -6.51 | 1.33 | 1.37 |
| 23 | BA | 1827 | C | N1-C6 | -6.49 | 1.33 | 1.37 |
| 23 | BA | 457 | A | N9-C4 | -6.48 | 1.33 | 1.37 |
| 23 | DA | 570 | G | C6-O6 | 6.46 | 1.29 | 1.24 |
| 23 | DA | 752 | A | C6-N1 | -6.45 | 1.31 | 1.35 |
| 23 | BA | 677 | A | N9-C4 | -6.44 | 1.33 | 1.37 |
| 23 | DA | 71 | A | N3-C4 | -6.43 | 1.30 | 1.34 |
| 23 | BA | 1977 | A | N9-C4 | -6.43 | 1.33 | 1.37 |
| 23 | DA | 1609 | A | N9-C4 | -6.42 | 1.33 | 1.37 |
| 23 | DA | 1619 | G | N3-C4 | -6.42 | 1.30 | 1.35 |
| 23 | BA | 734 | A | N9-C4 | -6.41 | 1.34 | 1.37 |
| 23 | DA | 676 | A | C5-C4 | 6.41 | 1.43 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 23 | DA | 676 | A | N9-C8 | 6.40 | 1.42 | 1.37 |
| 23 | DA | 2430 | A | N7-C5 | -6.37 | 1.35 | 1.39 |
| 23 | DA | 1777 | U | C2-N3 | -6.36 | 1.33 | 1.37 |
| 23 | DA | 774 | A | N7-C5 | -6.33 | 1.35 | 1.39 |
| 23 | DA | 1780 | A | N7-C5 | -6.32 | 1.35 | 1.39 |
| 23 | BA | 568 | U | C4-O4 | 6.32 | 1.28 | 1.23 |
| 23 | DA | 1978 | A | N9-C4 | -6.32 | 1.34 | 1.37 |
| 23 | DA | 2588 | G | P-OP2 | 6.32 | 1.59 | 1.49 |
| 23 | BA | 570 | G | C5-C6 | 6.31 | 1.48 | 1.42 |
| 23 | DA | 116 | C | N1-C6 | -6.31 | 1.33 | 1.37 |
| 25 | DC | 239 | ARG | CG-CD | 6.30 | 1.67 | 1.51 |
| 23 | DA | 585 | G | C6-N1 | -6.30 | 1.35 | 1.39 |
| 23 | BA | 460 | A | N9-C4 | -6.29 | 1.34 | 1.37 |
| 23 | BA | 2009 | G | C5-C4 | -6.29 | 1.33 | 1.38 |
| 23 | DA | 457 | A | N9-C4 | -6.29 | 1.34 | 1.37 |
| 23 | BA | 764 | A | C5-C6 | -6.29 | 1.35 | 1.41 |
| 23 | DA | 2448 | A | N9-C4 | -6.28 | 1.34 | 1.37 |
| 23 | BA | 31 | C | N1-C6 | -6.26 | 1.33 | 1.37 |
| 23 | BA | 800 | A | N3-C4 | -6.25 | 1.31 | 1.34 |
| 25 | BC | 239 | ARG | CG-CD | 6.25 | 1.67 | 1.51 |
| 23 | DA | 1899 | G | N9-C4 | -6.25 | 1.32 | 1.38 |
| 23 | DA | 678 | C | N1-C6 | -6.22 | 1.33 | 1.37 |
| 23 | DA | 2057 | A | N3-C4 | -6.22 | 1.31 | 1.34 |
| 23 | BA | 1829 | A | N9-C4 | -6.22 | 1.34 | 1.37 |
| 23 | BA | 2069 | G | N9-C4 | -6.22 | 1.32 | 1.38 |
| 23 | DA | 2059 | A | N9-C4 | -6.21 | 1.34 | 1.37 |
| 23 | DA | 2432 | A | N9-C4 | -6.21 | 1.34 | 1.37 |
| 23 | DA | 1776 | G | C6-N1 | -6.20 | 1.35 | 1.39 |
| 23 | DA | 1614 | A | N3-C4 | -6.19 | 1.31 | 1.34 |
| 23 | BA | 2510 | C | N1-C6 | -6.19 | 1.33 | 1.37 |
| 23 | DA | 1783 | A | N9-C4 | -6.19 | 1.34 | 1.37 |
| 23 | BA | 575 | A | N9-C4 | -6.18 | 1.34 | 1.37 |
| 23 | DA | 1332 | G | C2-N3 | -6.18 | 1.27 | 1.32 |
| 23 | DA | 1271 | G | N9-C8 | -6.17 | 1.33 | 1.37 |
| 23 | BA | 808 | G | N9-C8 | -6.15 | 1.33 | 1.37 |
| 23 | BA | 2032 | G | N9-C8 | 6.15 | 1.42 | 1.37 |
| 23 | DA | 1770 | G | N3-C4 | -6.14 | 1.31 | 1.35 |
| 23 | BA | 1786 | A | C5-C6 | -6.13 | 1.35 | 1.41 |
| 23 | DA | 2689 | U | C2-N3 | -6.13 | 1.33 | 1.37 |
| 23 | DA | 1902 | C | N3-C4 | -6.12 | 1.29 | 1.33 |
| 1 | AA | 901 | A | N9-C4 | -6.12 | 1.34 | 1.37 |
| 23 | BA | 460 | A | N3-C4 | -6.11 | 1.31 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|-------|-------|-------------|----------|
| 23 | DA | 2058 | A | N3-C4 | -6.11 | 1.31 | 1.34 |
| 23 | BA | 2587 | A | N9-C4 | -6.11 | 1.34 | 1.37 |
| 23 | DA | 1569 | A | N3-C4 | -6.11 | 1.31 | 1.34 |
| 23 | DA | 1603 | A | N3-C4 | -6.10 | 1.31 | 1.34 |
| 23 | BA | 1313 | U | N1-C2 | -6.10 | 1.33 | 1.38 |
| 23 | BA | 265 | A | N9-C4 | -6.09 | 1.34 | 1.37 |
| 23 | BA | 1971 | A | N9-C4 | -6.06 | 1.34 | 1.37 |
| 23 | DA | 2717 | G | N9-C8 | -6.06 | 1.33 | 1.37 |
| 23 | DA | 2452 | C | N1-C6 | -6.05 | 1.33 | 1.37 |
| 23 | DA | 1332 | G | N9-C8 | 6.03 | 1.42 | 1.37 |
| 23 | DA | 1619 | G | C6-N1 | -6.03 | 1.35 | 1.39 |
| 23 | BA | 1978 | A | N9-C4 | -6.02 | 1.34 | 1.37 |
| 23 | DA | 655 | A | N9-C4 | 6.02 | 1.41 | 1.37 |
| 23 | DA | 2512 | C | N1-C6 | -6.02 | 1.33 | 1.37 |
| 23 | BA | 2453 | A | C6-N1 | -6.01 | 1.31 | 1.35 |
| 23 | DA | 783 | A | N3-C4 | -6.01 | 1.31 | 1.34 |
| 23 | BA | 2062 | A | P-O5' | -6.01 | 1.53 | 1.59 |
| 23 | BA | 2430 | A | N7-C5 | -6.01 | 1.35 | 1.39 |
| 23 | DA | 2591 | C | N1-C6 | -6.01 | 1.33 | 1.37 |
| 23 | DA | 1606 | G | C6-N1 | -6.00 | 1.35 | 1.39 |
| 23 | BA | 2497 | A | N9-C4 | -5.99 | 1.34 | 1.37 |
| 23 | BA | 676 | A | C5-C6 | -5.98 | 1.35 | 1.41 |
| 23 | BA | 1000 | A | C6-N1 | -5.98 | 1.31 | 1.35 |
| 23 | DA | 1378 | A | N9-C4 | -5.98 | 1.34 | 1.37 |
| 23 | DA | 567 | A | P-OP1 | 5.97 | 1.59 | 1.49 |
| 23 | DA | 2063 | C | N3-C4 | -5.96 | 1.29 | 1.33 |
| 23 | BA | 1352 | U | C2-N3 | -5.95 | 1.33 | 1.37 |
| 23 | DA | 2242 | G | C5-C4 | -5.95 | 1.34 | 1.38 |
| 23 | BA | 737 | C | N1-C6 | -5.94 | 1.33 | 1.37 |
| 23 | DA | 2256 | G | N3-C4 | -5.93 | 1.31 | 1.35 |
| 23 | BA | 2496 | C | N1-C6 | -5.92 | 1.33 | 1.37 |
| 23 | DA | 814 | C | N1-C6 | -5.92 | 1.33 | 1.37 |
| 23 | BA | 2060 | A | N9-C4 | -5.89 | 1.34 | 1.37 |
| 23 | DA | 706 | A | N9-C4 | -5.89 | 1.34 | 1.37 |
| 23 | DA | 2055 | C | N1-C6 | -5.89 | 1.33 | 1.37 |
| 23 | DA | 983 | A | N9-C4 | -5.88 | 1.34 | 1.37 |
| 23 | DA | 449 | A | C6-N1 | -5.87 | 1.31 | 1.35 |
| 23 | BA | 1774 | C | P-OP1 | 5.86 | 1.58 | 1.49 |
| 23 | DA | 2032 | G | N9-C8 | 5.85 | 1.42 | 1.37 |
| 23 | DA | 114(B) | A | N7-C5 | -5.85 | 1.35 | 1.39 |
| 23 | BA | 2601 | C | N1-C6 | -5.84 | 1.33 | 1.37 |
| 23 | DA | 216 | A | N7-C5 | -5.84 | 1.35 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|-------|-------|-------------|----------|
| 23 | BA | 1991 | U | C2-N3 | -5.84 | 1.33 | 1.37 |
| 23 | BA | 2430 | A | N3-C4 | -5.82 | 1.31 | 1.34 |
| 23 | DA | 2080 | G | C6-N1 | -5.81 | 1.35 | 1.39 |
| 23 | DA | 453 | C | N1-C6 | -5.79 | 1.33 | 1.37 |
| 23 | BA | 71 | A | N9-C4 | -5.78 | 1.34 | 1.37 |
| 23 | DA | 211 | A | N9-C4 | -5.76 | 1.34 | 1.37 |
| 23 | BA | 787 | U | P-OP1 | 5.75 | 1.58 | 1.49 |
| 23 | DA | 204 | A | N9-C4 | -5.75 | 1.34 | 1.37 |
| 23 | BA | 1780 | A | N9-C4 | -5.74 | 1.34 | 1.37 |
| 23 | BA | 2595 | G | C5-C4 | -5.74 | 1.34 | 1.38 |
| 23 | DA | 2577 | A | C6-N1 | -5.73 | 1.31 | 1.35 |
| 23 | BA | 114(B) | A | N7-C5 | -5.72 | 1.35 | 1.39 |
| 23 | DA | 2057 | A | N9-C4 | -5.72 | 1.34 | 1.37 |
| 23 | BA | 432 | A | N9-C4 | -5.72 | 1.34 | 1.37 |
| 23 | BA | 945 | A | C5-C6 | -5.72 | 1.35 | 1.41 |
| 23 | DA | 787 | U | P-OP1 | 5.72 | 1.58 | 1.49 |
| 23 | BA | 929 | G | N7-C5 | -5.71 | 1.35 | 1.39 |
| 23 | DA | 698 | C | C2-O2 | 5.71 | 1.29 | 1.24 |
| 23 | DA | 195 | A | N3-C4 | -5.71 | 1.31 | 1.34 |
| 23 | BA | 2005 | A | N9-C4 | -5.69 | 1.34 | 1.37 |
| 23 | DA | 1619 | G | C5-C4 | -5.67 | 1.34 | 1.38 |
| 23 | DA | 782 | A | N9-C4 | -5.66 | 1.34 | 1.37 |
| 23 | DA | 782 | A | C5-C4 | -5.65 | 1.34 | 1.38 |
| 23 | BA | 676 | A | N7-C5 | -5.62 | 1.35 | 1.39 |
| 23 | DA | 2033 | A | C6-N1 | -5.62 | 1.31 | 1.35 |
| 23 | BA | 1899 | G | N9-C8 | 5.62 | 1.41 | 1.37 |
| 23 | DA | 2054 | A | C5-C6 | -5.62 | 1.35 | 1.41 |
| 23 | DA | 1802 | A | N9-C4 | -5.62 | 1.34 | 1.37 |
| 23 | DA | 241 | A | N9-C4 | -5.61 | 1.34 | 1.37 |
| 23 | DA | 766 | C | N1-C6 | -5.61 | 1.33 | 1.37 |
| 23 | DA | 1616 | A | C5-C6 | -5.61 | 1.36 | 1.41 |
| 23 | DA | 2227 | A | N9-C4 | -5.58 | 1.34 | 1.37 |
| 23 | BA | 1664 | A | N9-C4 | -5.58 | 1.34 | 1.37 |
| 23 | BA | 1617 | C | N1-C6 | -5.58 | 1.33 | 1.37 |
| 23 | BA | 1678 | G | C2-N3 | -5.57 | 1.28 | 1.32 |
| 23 | DA | 1777 | U | N3-C4 | -5.57 | 1.33 | 1.38 |
| 23 | BA | 1676 | A | N3-C4 | -5.55 | 1.31 | 1.34 |
| 23 | DA | 2446 | G | C5-C4 | -5.55 | 1.34 | 1.38 |
| 23 | BA | 1841 | U | C4-O4 | 5.55 | 1.28 | 1.23 |
| 23 | DA | 199 | A | C5-C4 | -5.55 | 1.34 | 1.38 |
| 23 | DA | 2741 | A | N9-C4 | -5.54 | 1.34 | 1.37 |
| 23 | DA | 693 | C | N1-C6 | -5.53 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 23 | DA | 211 | A | C6-N1 | -5.53 | 1.31 | 1.35 |
| 23 | DA | 569 | U | N1-C6 | -5.53 | 1.32 | 1.38 |
| 23 | DA | 1201 | C | N1-C6 | -5.53 | 1.33 | 1.37 |
| 1 | AA | 1523 | G | N3-C4 | -5.52 | 1.31 | 1.35 |
| 23 | DA | 2346 | A | N3-C4 | -5.52 | 1.31 | 1.34 |
| 23 | DA | 387 | U | C4-O4 | 5.51 | 1.28 | 1.23 |
| 23 | BA | 1602 | U | C4-O4 | 5.51 | 1.28 | 1.23 |
| 23 | DA | 2242 | G | N7-C5 | -5.51 | 1.35 | 1.39 |
| 23 | BA | 2346 | A | N3-C4 | -5.51 | 1.31 | 1.34 |
| 23 | BA | 1571 | A | N9-C4 | -5.50 | 1.34 | 1.37 |
| 23 | DA | 1824 | G | N9-C8 | -5.50 | 1.34 | 1.37 |
| 23 | DA | 2070 | G | N9-C8 | -5.50 | 1.34 | 1.37 |
| 23 | DA | 2060 | A | N3-C4 | -5.49 | 1.31 | 1.34 |
| 23 | BA | 1827 | C | N3-C4 | -5.49 | 1.30 | 1.33 |
| 23 | BA | 764 | A | N7-C5 | -5.48 | 1.35 | 1.39 |
| 23 | DA | 2062 | A | C5'-C4' | -5.48 | 1.44 | 1.51 |
| 23 | BA | 244 | A | N3-C4 | -5.47 | 1.31 | 1.34 |
| 23 | DA | 1782 | C | N1-C6 | -5.47 | 1.33 | 1.37 |
| 23 | DA | 204 | A | C6-N1 | -5.46 | 1.31 | 1.35 |
| 23 | DA | 2054 | A | N9-C4 | -5.46 | 1.34 | 1.37 |
| 23 | BA | 575 | A | N3-C4 | -5.46 | 1.31 | 1.34 |
| 23 | DA | 1606 | G | C5-C4 | -5.46 | 1.34 | 1.38 |
| 23 | DA | 1662 | C | N3-C4 | -5.46 | 1.30 | 1.33 |
| 23 | BA | 1309 | G | N3-C4 | -5.46 | 1.31 | 1.35 |
| 23 | DA | 2085 | C | N1-C6 | -5.45 | 1.33 | 1.37 |
| 23 | DA | 1776 | G | C6-O6 | -5.44 | 1.19 | 1.24 |
| 23 | DA | 1633 | G | N7-C5 | -5.44 | 1.35 | 1.39 |
| 23 | DA | 1376 | C | C4-C5 | -5.43 | 1.38 | 1.43 |
| 23 | BA | 837 | C | C4-C5 | -5.42 | 1.38 | 1.43 |
| 23 | DA | 1775 | U | C2-N3 | -5.42 | 1.33 | 1.37 |
| 23 | DA | 1341 | U | C2-N3 | 5.42 | 1.41 | 1.37 |
| 23 | DA | 2447 | G | N3-C4 | -5.42 | 1.31 | 1.35 |
| 23 | DA | 57 | C | N1-C6 | -5.42 | 1.33 | 1.37 |
| 23 | BA | 2430 | A | N9-C4 | -5.41 | 1.34 | 1.37 |
| 23 | DA | 2231 | C | N1-C6 | -5.41 | 1.33 | 1.37 |
| 23 | BA | 114(B) | A | C5-C6 | -5.41 | 1.36 | 1.41 |
| 23 | DA | 2587 | A | N3-C4 | -5.40 | 1.31 | 1.34 |
| 23 | BA | 677 | A | N3-C4 | -5.40 | 1.31 | 1.34 |
| 23 | DA | 2447 | G | N9-C4 | -5.40 | 1.33 | 1.38 |
| 23 | DA | 1802 | A | N7-C5 | -5.40 | 1.36 | 1.39 |
| 23 | BA | 824 | A | N9-C4 | -5.40 | 1.34 | 1.37 |
| 23 | BA | 2681 | C | N3-C4 | -5.39 | 1.30 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|-------|-------|-------------|----------|
| 23 | DA | 2432 | A | N7-C5 | -5.39 | 1.36 | 1.39 |
| 23 | DA | 195 | A | N9-C4 | -5.39 | 1.34 | 1.37 |
| 23 | DA | 1609 | A | N3-C4 | -5.39 | 1.31 | 1.34 |
| 23 | DA | 794 | G | C6-N1 | -5.38 | 1.35 | 1.39 |
| 1 | AA | 909 | A | N9-C4 | -5.38 | 1.34 | 1.37 |
| 23 | DA | 2502 | G | N9-C8 | -5.38 | 1.34 | 1.37 |
| 23 | DA | 122 | G | N3-C4 | -5.37 | 1.31 | 1.35 |
| 23 | DA | 1616 | A | P-O5' | -5.37 | 1.54 | 1.59 |
| 23 | DA | 454 | A | N9-C4 | -5.36 | 1.34 | 1.37 |
| 23 | DA | 330 | A | N9-C4 | -5.36 | 1.34 | 1.37 |
| 23 | BA | 2054 | A | N7-C5 | -5.35 | 1.36 | 1.39 |
| 23 | DA | 2601 | C | N1-C6 | -5.35 | 1.33 | 1.37 |
| 23 | DA | 114(B) | A | N3-C4 | -5.35 | 1.31 | 1.34 |
| 23 | BA | 2595 | G | N9-C4 | -5.34 | 1.33 | 1.38 |
| 23 | BA | 2741 | A | N9-C4 | -5.34 | 1.34 | 1.37 |
| 23 | BA | 114(B) | A | N9-C4 | -5.34 | 1.34 | 1.37 |
| 23 | DA | 2445 | G | C6-N1 | -5.34 | 1.35 | 1.39 |
| 23 | DA | 330 | A | C5-C6 | -5.33 | 1.36 | 1.41 |
| 23 | DA | 1786 | A | N7-C5 | -5.33 | 1.36 | 1.39 |
| 23 | DA | 786 | C | N1-C6 | -5.32 | 1.33 | 1.37 |
| 23 | BA | 2440 | C | N1-C2 | -5.32 | 1.34 | 1.40 |
| 23 | BA | 2018 | G | C6-N1 | -5.32 | 1.35 | 1.39 |
| 23 | BA | 2060 | A | N3-C4 | -5.32 | 1.31 | 1.34 |
| 23 | BA | 585 | G | C6-N1 | -5.32 | 1.35 | 1.39 |
| 23 | DA | 2584 | U | C4-O4 | 5.31 | 1.27 | 1.23 |
| 23 | DA | 2448 | A | C5-C6 | -5.31 | 1.36 | 1.41 |
| 23 | DA | 2577 | A | N7-C5 | -5.31 | 1.36 | 1.39 |
| 23 | DA | 1331 | A | N9-C4 | -5.31 | 1.34 | 1.37 |
| 23 | BA | 1678 | G | N3-C4 | -5.30 | 1.31 | 1.35 |
| 23 | BA | 2440 | C | N1-C6 | -5.30 | 1.33 | 1.37 |
| 23 | DA | 1614 | A | N1-C2 | 5.30 | 1.39 | 1.34 |
| 23 | DA | 798 | G | N7-C5 | -5.29 | 1.36 | 1.39 |
| 23 | DA | 2256 | G | C5-C4 | -5.29 | 1.34 | 1.38 |
| 23 | DA | 1248 | G | C5-C4 | -5.29 | 1.34 | 1.38 |
| 23 | BA | 1776 | G | C8-N7 | -5.29 | 1.27 | 1.30 |
| 23 | DA | 2577 | A | C5-C4 | -5.28 | 1.35 | 1.38 |
| 23 | DA | 777 | A | N3-C4 | -5.28 | 1.31 | 1.34 |
| 23 | DA | 1029 | A | N9-C4 | -5.28 | 1.34 | 1.37 |
| 26 | DD | 127 | ASP | CB-CG | 5.27 | 1.62 | 1.51 |
| 23 | BA | 2059 | A | C5-C4 | -5.26 | 1.35 | 1.38 |
| 23 | DA | 1674 | G | N9-C8 | -5.26 | 1.34 | 1.37 |
| 23 | DA | 2058 | A | C5-C4 | -5.26 | 1.35 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|-------|-------|-------------|----------|
| 23 | DA | 2709 | G | N9-C8 | -5.26 | 1.34 | 1.37 |
| 23 | DA | 1332 | G | N3-C4 | -5.26 | 1.31 | 1.35 |
| 23 | DA | 2232 | U | C4-O4 | 5.26 | 1.27 | 1.23 |
| 23 | DA | 457 | A | C5-C4 | -5.25 | 1.35 | 1.38 |
| 23 | DA | 473 | G | C6-N1 | -5.25 | 1.35 | 1.39 |
| 23 | DA | 1257 | C | N1-C6 | -5.25 | 1.33 | 1.37 |
| 23 | DA | 36 | G | N3-C4 | -5.25 | 1.31 | 1.35 |
| 23 | DA | 1624 | G | C5-C4 | -5.25 | 1.34 | 1.38 |
| 23 | BA | 2433 | A | C6-N1 | -5.25 | 1.31 | 1.35 |
| 23 | DA | 46 | C | N3-C4 | -5.24 | 1.30 | 1.33 |
| 23 | BA | 2392 | A | N7-C5 | -5.24 | 1.36 | 1.39 |
| 23 | DA | 761 | A | C5-C6 | -5.24 | 1.36 | 1.41 |
| 23 | BA | 2010 | G | C5-C6 | -5.24 | 1.37 | 1.42 |
| 23 | DA | 2257 | U | N1-C2 | -5.24 | 1.33 | 1.38 |
| 23 | DA | 1698 | A | N9-C4 | -5.23 | 1.34 | 1.37 |
| 23 | BA | 764 | A | N3-C4 | -5.23 | 1.31 | 1.34 |
| 23 | BA | 1675 | C | N1-C6 | -5.22 | 1.34 | 1.37 |
| 23 | BA | 2448 | A | N3-C4 | -5.22 | 1.31 | 1.34 |
| 23 | DA | 36 | G | C6-N1 | -5.22 | 1.35 | 1.39 |
| 23 | DA | 531 | C | N1-C6 | -5.22 | 1.34 | 1.37 |
| 1 | AA | 32 | A | N3-C4 | -5.21 | 1.31 | 1.34 |
| 23 | BA | 676 | A | N3-C4 | -5.21 | 1.31 | 1.34 |
| 23 | DA | 116 | C | N3-C4 | -5.20 | 1.30 | 1.33 |
| 23 | DA | 223 | A | N9-C8 | -5.20 | 1.33 | 1.37 |
| 23 | DA | 2060 | A | C5-C4 | -5.20 | 1.35 | 1.38 |
| 23 | DA | 2084 | C | N1-C6 | -5.20 | 1.34 | 1.37 |
| 23 | DA | 2014 | A | N9-C4 | -5.19 | 1.34 | 1.37 |
| 23 | BA | 114(B) | A | N3-C4 | -5.19 | 1.31 | 1.34 |
| 23 | DA | 943 | U | N1-C2 | -5.19 | 1.33 | 1.38 |
| 23 | DA | 751 | A | C6-N1 | -5.18 | 1.31 | 1.35 |
| 23 | BA | 2517 | C | N1-C6 | -5.18 | 1.34 | 1.37 |
| 23 | DA | 1792 | G | N7-C5 | -5.18 | 1.36 | 1.39 |
| 23 | DA | 1815 | A | C6-N1 | -5.17 | 1.31 | 1.35 |
| 23 | DA | 2248 | C | N1-C6 | -5.17 | 1.34 | 1.37 |
| 23 | DA | 2227 | A | N3-C4 | -5.17 | 1.31 | 1.34 |
| 23 | DA | 678 | C | N1-C2 | -5.16 | 1.34 | 1.40 |
| 23 | DA | 251 | A | N7-C5 | -5.16 | 1.36 | 1.39 |
| 23 | DA | 1616 | A | N9-C4 | -5.15 | 1.34 | 1.37 |
| 23 | DA | 2588 | G | P-OP1 | 5.15 | 1.57 | 1.49 |
| 23 | DA | 2488 | A | C5-C4 | -5.14 | 1.35 | 1.38 |
| 23 | BA | 1671 | U | C2-N3 | 5.14 | 1.41 | 1.37 |
| 23 | DA | 812 | C | N1-C6 | -5.14 | 1.34 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 23 | DA | 2434 | A | N3-C4 | -5.13 | 1.31 | 1.34 |
| 34 | DL | 36 | LYS | CD-CE | 5.13 | 1.64 | 1.51 |
| 23 | DA | 2587 | A | N9-C4 | -5.12 | 1.34 | 1.37 |
| 23 | DA | 2588 | G | C6-N1 | -5.12 | 1.35 | 1.39 |
| 23 | BA | 575 | A | C5-C4 | -5.11 | 1.35 | 1.38 |
| 23 | DA | 2505 | G | N3-C4 | -5.11 | 1.31 | 1.35 |
| 23 | DA | 2765 | A | N7-C5 | -5.11 | 1.36 | 1.39 |
| 23 | BA | 1571 | A | N3-C4 | -5.11 | 1.31 | 1.34 |
| 23 | DA | 995 | C | N1-C6 | -5.10 | 1.34 | 1.37 |
| 23 | BA | 196 | A | C6-N1 | -5.10 | 1.31 | 1.35 |
| 23 | DA | 1606 | G | N1-C2 | -5.10 | 1.33 | 1.37 |
| 23 | BA | 836 | G | N9-C4 | -5.09 | 1.33 | 1.38 |
| 23 | BA | 1278 | A | N3-C4 | -5.09 | 1.31 | 1.34 |
| 23 | BA | 2249 | U | C4-O4 | 5.09 | 1.27 | 1.23 |
| 23 | BA | 1997 | G | C6-N1 | -5.09 | 1.35 | 1.39 |
| 23 | DA | 2588 | G | N3-C4 | -5.09 | 1.31 | 1.35 |
| 23 | BA | 2009 | G | N3-C4 | -5.08 | 1.31 | 1.35 |
| 23 | DA | 1776 | G | P-OP2 | 5.08 | 1.57 | 1.49 |
| 23 | DA | 799 | G | N1-C2 | -5.08 | 1.33 | 1.37 |
| 23 | DA | 805 | G | N7-C5 | -5.07 | 1.36 | 1.39 |
| 23 | DA | 2448 | A | N3-C4 | -5.07 | 1.31 | 1.34 |
| 23 | DA | 732 | C | N1-C6 | -5.07 | 1.34 | 1.37 |
| 23 | BA | 2198 | A | N9-C4 | -5.07 | 1.34 | 1.37 |
| 23 | DA | 769 | G | N1-C2 | -5.07 | 1.33 | 1.37 |
| 23 | DA | 784 | A | N9-C4 | -5.07 | 1.34 | 1.37 |
| 23 | BA | 2069 | G | N3-C4 | -5.06 | 1.31 | 1.35 |
| 23 | DA | 2510 | C | N1-C6 | -5.06 | 1.34 | 1.37 |
| 23 | DA | 473 | G | N3-C4 | -5.06 | 1.31 | 1.35 |
| 23 | DA | 751 | A | P-OP1 | 5.06 | 1.57 | 1.49 |
| 23 | BA | 684 | G | N3-C4 | -5.06 | 1.31 | 1.35 |
| 23 | BA | 1264 | G | N3-C4 | -5.05 | 1.31 | 1.35 |
| 23 | BA | 2199 | A | N3-C4 | -5.05 | 1.31 | 1.34 |
| 23 | BA | 2463 | C | N1-C6 | -5.05 | 1.34 | 1.37 |
| 23 | DA | 1780 | A | C5-C6 | -5.05 | 1.36 | 1.41 |
| 23 | DA | 1760 | A | C6-N1 | -5.05 | 1.32 | 1.35 |
| 23 | BA | 1941 | C | N1-C6 | -5.05 | 1.34 | 1.37 |
| 23 | DA | 1780 | A | N9-C4 | -5.04 | 1.34 | 1.37 |
| 23 | BA | 802 | A | N3-C4 | -5.03 | 1.31 | 1.34 |
| 23 | DA | 2451 | A | N3-C4 | -5.03 | 1.31 | 1.34 |
| 23 | DA | 564 | C | N3-C4 | -5.03 | 1.30 | 1.33 |
| 23 | DA | 582 | G | N9-C8 | -5.03 | 1.34 | 1.37 |
| 23 | DA | 467 | G | N9-C4 | -5.02 | 1.33 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 23 | DA | 566 | U | C2-N3 | -5.02 | 1.34 | 1.37 |
| 23 | BA | 1902 | C | C2-N3 | -5.02 | 1.31 | 1.35 |
| 23 | DA | 736 | C | N1-C6 | -5.02 | 1.34 | 1.37 |
| 23 | BA | 244 | A | N9-C4 | -5.02 | 1.34 | 1.37 |
| 23 | BA | 462 | C | N3-C4 | -5.02 | 1.30 | 1.33 |
| 23 | DA | 192 | C | N1-C6 | -5.02 | 1.34 | 1.37 |
| 23 | DA | 2062 | A | P-O5' | -5.01 | 1.54 | 1.59 |
| 23 | DA | 452 | G | N3-C4 | -5.00 | 1.31 | 1.35 |
| 23 | DA | 795 | C | N1-C6 | -5.00 | 1.34 | 1.37 |

All (3317) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 23 | DA | 761 | A | N1-C6-N6 | 30.82 | 137.09 | 118.60 |
| 23 | BA | 761 | A | N1-C6-N6 | 25.08 | 133.65 | 118.60 |
| 23 | DA | 1332 | G | N3-C4-N9 | -24.42 | 111.35 | 126.00 |
| 23 | DA | 1332 | G | N3-C4-C5 | 23.85 | 140.52 | 128.60 |
| 23 | BA | 1332 | G | N3-C4-N9 | -22.46 | 112.52 | 126.00 |
| 23 | DA | 761 | A | C6-C5-N7 | -21.62 | 117.17 | 132.30 |
| 23 | BA | 1332 | G | N3-C4-C5 | 21.41 | 139.31 | 128.60 |
| 23 | DA | 1602 | U | N3-C4-C5 | -19.94 | 102.64 | 114.60 |
| 23 | BA | 676 | A | C2-N3-C4 | -19.31 | 100.94 | 110.60 |
| 23 | DA | 761 | A | C5-C6-N1 | -19.15 | 108.12 | 117.70 |
| 23 | DA | 676 | A | C2-N3-C4 | -19.01 | 101.09 | 110.60 |
| 23 | DA | 761 | A | C5-N7-C8 | -18.20 | 94.80 | 103.90 |
| 23 | BA | 761 | A | C6-C5-N7 | -17.81 | 119.83 | 132.30 |
| 23 | DA | 761 | A | C4-C5-N7 | 17.34 | 119.37 | 110.70 |
| 23 | DA | 761 | A | N9-C4-C5 | -17.20 | 98.92 | 105.80 |
| 23 | DA | 2028 | U | N3-C4-C5 | -17.14 | 104.32 | 114.60 |
| 23 | DA | 1332 | G | C2-N3-C4 | -16.96 | 103.42 | 111.90 |
| 23 | DA | 774 | A | C2-N3-C4 | -16.91 | 102.14 | 110.60 |
| 23 | BA | 2028 | U | N3-C4-C5 | -16.41 | 104.75 | 114.60 |
| 23 | DA | 676 | A | C5-N7-C8 | -15.45 | 96.17 | 103.90 |
| 23 | BA | 761 | A | C5-N7-C8 | -14.95 | 96.42 | 103.90 |
| 23 | DA | 2028 | U | C6-N1-C2 | -14.94 | 112.03 | 121.00 |
| 23 | BA | 1678 | G | N3-C4-C5 | 14.81 | 136.01 | 128.60 |
| 23 | DA | 1999 | C | C6-N1-C2 | 14.72 | 126.19 | 120.30 |
| 23 | BA | 761 | A | C4-C5-N7 | 14.67 | 118.03 | 110.70 |
| 23 | BA | 1678 | G | N3-C4-N9 | -14.62 | 117.23 | 126.00 |
| 23 | DA | 2028 | U | N3-C4-O4 | 14.44 | 129.51 | 119.40 |
| 23 | DA | 1678 | G | N3-C4-C5 | 14.37 | 135.78 | 128.60 |
| 23 | DA | 1962 | C | N1-C2-O2 | 14.20 | 127.42 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 23 | DA | 761 | A | C2-N3-C4 | -14.19 | 103.50 | 110.60 |
| 23 | BA | 761 | A | N9-C4-C5 | -14.12 | 100.15 | 105.80 |
| 23 | DA | 1678 | G | N3-C4-N9 | -14.08 | 117.55 | 126.00 |
| 23 | BA | 2501 | C | C6-N1-C2 | 14.00 | 125.90 | 120.30 |
| 23 | DA | 783 | A | C5-N7-C8 | -13.85 | 96.98 | 103.90 |
| 23 | DA | 2505 | G | C5-C6-O6 | 13.63 | 136.78 | 128.60 |
| 23 | BA | 1962 | C | N1-C2-O2 | 13.58 | 127.05 | 118.90 |
| 23 | DA | 1671 | U | N3-C4-C5 | -13.42 | 106.55 | 114.60 |
| 23 | DA | 2249 | U | N3-C4-C5 | -13.40 | 106.56 | 114.60 |
| 23 | BA | 774 | A | C2-N3-C4 | -13.36 | 103.92 | 110.60 |
| 23 | BA | 1899 | G | N3-C4-N9 | -13.30 | 118.02 | 126.00 |
| 23 | BA | 2571 | C | C6-N1-C2 | 13.17 | 125.57 | 120.30 |
| 23 | BA | 1999 | C | C6-N1-C2 | 13.05 | 125.52 | 120.30 |
| 23 | DA | 2593 | U | N3-C4-C5 | -12.93 | 106.84 | 114.60 |
| 23 | DA | 761 | A | C4-C5-C6 | 12.90 | 123.45 | 117.00 |
| 23 | BA | 2028 | U | N3-C4-O4 | 12.80 | 128.36 | 119.40 |
| 23 | BA | 676 | A | C5-C6-N1 | -12.74 | 111.33 | 117.70 |
| 23 | DA | 450 | G | C5-C6-N1 | -12.71 | 105.15 | 111.50 |
| 23 | DA | 1602 | U | N3-C4-O4 | 12.71 | 128.29 | 119.40 |
| 23 | BA | 1332 | G | C2-N3-C4 | -12.68 | 105.56 | 111.90 |
| 23 | BA | 2028 | U | C6-N1-C2 | -12.61 | 113.43 | 121.00 |
| 23 | BA | 1786 | A | C5-N7-C8 | -12.59 | 97.60 | 103.90 |
| 23 | BA | 676 | A | C5-N7-C8 | -12.56 | 97.62 | 103.90 |
| 23 | BA | 761 | A | C5-C6-N1 | -12.54 | 111.43 | 117.70 |
| 23 | DA | 761 | A | N7-C8-N9 | 12.41 | 120.01 | 113.80 |
| 23 | DA | 1602 | U | C6-N1-C2 | -12.37 | 113.58 | 121.00 |
| 23 | BA | 1602 | U | C6-N1-C2 | -12.33 | 113.61 | 121.00 |
| 23 | BA | 570 | G | C5-C6-N1 | -12.25 | 105.37 | 111.50 |
| 23 | BA | 1602 | U | N3-C4-C5 | -12.24 | 107.26 | 114.60 |
| 23 | BA | 1671 | U | N3-C4-O4 | 12.21 | 127.94 | 119.40 |
| 23 | BA | 1671 | U | N3-C4-C5 | -12.16 | 107.30 | 114.60 |
| 23 | DA | 124 | G | C8-N9-C4 | 12.13 | 111.25 | 106.40 |
| 23 | DA | 945 | A | C6-C5-N7 | -12.12 | 123.81 | 132.30 |
| 23 | DA | 676 | A | N7-C8-N9 | 12.10 | 119.85 | 113.80 |
| 23 | DA | 1332 | G | N3-C2-N2 | -12.06 | 111.46 | 119.90 |
| 23 | DA | 2626 | C | C6-N1-C2 | 12.01 | 125.10 | 120.30 |
| 23 | BA | 945 | A | C6-C5-N7 | -11.99 | 123.91 | 132.30 |
| 23 | DA | 1602 | U | C4-C5-C6 | 11.96 | 126.88 | 119.70 |
| 23 | DA | 2579 | C | C6-N1-C2 | 11.96 | 125.08 | 120.30 |
| 23 | BA | 1332 | G | N3-C2-N2 | -11.92 | 111.56 | 119.90 |
| 23 | DA | 774 | A | C5-N7-C8 | -11.91 | 97.95 | 103.90 |
| 23 | BA | 1786 | A | N7-C8-N9 | 11.87 | 119.74 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 23 | DA | 1616 | A | C5-N7-C8 | -11.87 | 97.97 | 103.90 |
| 23 | DA | 783 | A | N7-C8-N9 | 11.85 | 119.73 | 113.80 |
| 23 | DA | 2619 | C | C6-N1-C2 | 11.84 | 125.03 | 120.30 |
| 23 | DA | 2830 | G | N1-C6-O6 | 11.77 | 126.96 | 119.90 |
| 23 | DA | 57 | C | C6-N1-C2 | 11.74 | 125.00 | 120.30 |
| 23 | BA | 1790 | C | N3-C4-C5 | 11.74 | 126.59 | 121.90 |
| 23 | BA | 1786 | A | C8-N9-C4 | -11.73 | 101.11 | 105.80 |
| 23 | DA | 1332 | G | C8-N9-C1' | 11.69 | 142.20 | 127.00 |
| 23 | DA | 1021 | A | C2-N3-C4 | -11.66 | 104.77 | 110.60 |
| 23 | DA | 1698 | A | C2-N3-C4 | -11.64 | 104.78 | 110.60 |
| 23 | BA | 2571 | C | C5-C6-N1 | -11.64 | 115.18 | 121.00 |
| 23 | BA | 1899 | G | C2-N3-C4 | -11.59 | 106.10 | 111.90 |
| 23 | DA | 1614 | A | C2-N3-C4 | -11.57 | 104.82 | 110.60 |
| 23 | BA | 2502 | G | N1-C6-O6 | 11.55 | 126.83 | 119.90 |
| 23 | DA | 676 | A | C4-C5-N7 | 11.44 | 116.42 | 110.70 |
| 23 | DA | 265 | A | C2-N3-C4 | -11.39 | 104.91 | 110.60 |
| 23 | BA | 761 | A | N7-C8-N9 | 11.35 | 119.48 | 113.80 |
| 23 | DA | 71 | A | C5-N7-C8 | -11.30 | 98.25 | 103.90 |
| 23 | BA | 570 | G | C4-C5-N7 | -11.29 | 106.28 | 110.80 |
| 23 | DA | 1899 | G | N3-C4-N9 | -11.29 | 119.23 | 126.00 |
| 23 | DA | 570 | G | C5-C6-O6 | 11.21 | 135.33 | 128.60 |
| 23 | BA | 570 | G | C5-C6-O6 | 11.20 | 135.32 | 128.60 |
| 23 | DA | 761 | A | C5-C6-N6 | -11.15 | 114.78 | 123.70 |
| 23 | DA | 1671 | U | N3-C4-O4 | 11.13 | 127.19 | 119.40 |
| 23 | DA | 2648 | C | C6-N1-C2 | 11.12 | 124.75 | 120.30 |
| 23 | BA | 1899 | G | N3-C4-C5 | 11.10 | 134.15 | 128.60 |
| 23 | BA | 2829 | C | C6-N1-C2 | 11.08 | 124.73 | 120.30 |
| 23 | DA | 2571 | C | C6-N1-C2 | 11.04 | 124.72 | 120.30 |
| 23 | DA | 201 | C | C6-N1-C2 | 11.03 | 124.71 | 120.30 |
| 23 | DA | 1332 | G | C4-N9-C1' | -10.98 | 112.22 | 126.50 |
| 23 | BA | 761 | A | C5-C6-N6 | -10.97 | 114.92 | 123.70 |
| 23 | DA | 2581 | G | C5-C6-O6 | 10.91 | 135.15 | 128.60 |
| 23 | BA | 1332 | G | C8-N9-C1' | 10.91 | 141.18 | 127.00 |
| 23 | BA | 2498 | C | C6-N1-C2 | 10.91 | 124.66 | 120.30 |
| 23 | DA | 570 | G | C4-C5-N7 | -10.89 | 106.44 | 110.80 |
| 23 | DA | 450 | G | C4-C5-C6 | 10.88 | 125.33 | 118.80 |
| 23 | DA | 1614 | A | C5-C6-N1 | -10.84 | 112.28 | 117.70 |
| 23 | DA | 676 | A | N3-C4-C5 | 10.82 | 134.38 | 126.80 |
| 23 | DA | 2501 | C | C6-N1-C2 | 10.80 | 124.62 | 120.30 |
| 23 | DA | 210 | C | C6-N1-C2 | 10.79 | 124.62 | 120.30 |
| 23 | BA | 210 | C | C6-N1-C2 | 10.74 | 124.60 | 120.30 |
| 23 | DA | 2689 | U | C5-C4-O4 | 10.71 | 132.33 | 125.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 23 | BA | 330 | A | C2-N3-C4 | -10.69 | 105.25 | 110.60 |
| 23 | DA | 1616 | A | N1-C6-N6 | 10.69 | 125.02 | 118.60 |
| 23 | DA | 1899 | G | N3-C4-C5 | 10.65 | 133.92 | 128.60 |
| 23 | BA | 2579 | C | C6-N1-C2 | 10.60 | 124.54 | 120.30 |
| 1 | CA | 123 | C | C6-N1-C2 | 10.59 | 124.53 | 120.30 |
| 23 | BA | 2502 | G | C5-C6-O6 | -10.58 | 122.25 | 128.60 |
| 23 | BA | 676 | A | N7-C8-N9 | 10.57 | 119.09 | 113.80 |
| 23 | BA | 2456 | C | N3-C4-C5 | 10.57 | 126.13 | 121.90 |
| 23 | DA | 2544 | G | N1-C6-O6 | 10.57 | 126.24 | 119.90 |
| 23 | BA | 1786 | A | C6-C5-N7 | -10.56 | 124.91 | 132.30 |
| 23 | DA | 208 | C | C6-N1-C2 | 10.56 | 124.53 | 120.30 |
| 23 | DA | 1786 | A | C5-N7-C8 | -10.55 | 98.63 | 103.90 |
| 23 | DA | 2050 | C | N1-C2-O2 | -10.54 | 112.58 | 118.90 |
| 23 | DA | 1007 | C | C6-N1-C2 | 10.53 | 124.51 | 120.30 |
| 23 | BA | 847 | U | C5-C6-N1 | -10.52 | 117.44 | 122.70 |
| 23 | DA | 2593 | U | N3-C4-O4 | 10.52 | 126.76 | 119.40 |
| 23 | BA | 678 | C | N3-C4-C5 | 10.50 | 126.10 | 121.90 |
| 23 | DA | 1786 | A | N7-C8-N9 | 10.43 | 119.01 | 113.80 |
| 23 | BA | 945 | A | N1-C6-N6 | 10.39 | 124.83 | 118.60 |
| 23 | DA | 676 | A | N1-C2-N3 | 10.39 | 134.50 | 129.30 |
| 23 | DA | 2689 | U | C2-N1-C1' | -10.37 | 105.26 | 117.70 |
| 23 | BA | 2648 | C | C6-N1-C2 | 10.32 | 124.43 | 120.30 |
| 23 | BA | 676 | A | N3-C4-C5 | 10.32 | 134.02 | 126.80 |
| 23 | BA | 1261 | C | C6-N1-C2 | 10.31 | 124.43 | 120.30 |
| 23 | DA | 1999 | C | C5-C6-N1 | -10.25 | 115.88 | 121.00 |
| 23 | BA | 761 | A | C4-C5-C6 | 10.24 | 122.12 | 117.00 |
| 23 | BA | 691 | C | C6-N1-C2 | 10.23 | 124.39 | 120.30 |
| 23 | BA | 2430 | A | C4-C5-C6 | 10.23 | 122.12 | 117.00 |
| 23 | BA | 1786 | A | C2-N3-C4 | -10.22 | 105.49 | 110.60 |
| 23 | DA | 1616 | A | C4-C5-N7 | 10.22 | 115.81 | 110.70 |
| 23 | BA | 2010 | G | C6-C5-N7 | -10.20 | 124.28 | 130.40 |
| 23 | DA | 1614 | A | C4-C5-C6 | 10.14 | 122.07 | 117.00 |
| 23 | BA | 676 | A | N1-C6-N6 | 10.05 | 124.63 | 118.60 |
| 23 | DA | 2028 | U | C4-C5-C6 | 10.05 | 125.73 | 119.70 |
| 23 | BA | 1790 | C | C2-N3-C4 | -10.03 | 114.89 | 119.90 |
| 23 | BA | 1332 | G | C4-N9-C1' | -10.01 | 113.49 | 126.50 |
| 23 | DA | 945 | A | N7-C8-N9 | 9.98 | 118.79 | 113.80 |
| 23 | DA | 408 | G | C8-N9-C4 | 9.97 | 110.39 | 106.40 |
| 23 | DA | 1698 | A | N1-C6-N6 | 9.97 | 124.58 | 118.60 |
| 23 | BA | 2330 | G | C8-N9-C4 | 9.97 | 110.39 | 106.40 |
| 23 | BA | 1021 | A | C2-N3-C4 | -9.95 | 105.63 | 110.60 |
| 23 | BA | 444 | C | C6-N1-C2 | 9.94 | 124.28 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | DA | 114(B) | A | C2-N3-C4 | -9.93 | 105.64 | 110.60 |
| 23 | DA | 2464 | C | C6-N1-C2 | 9.91 | 124.27 | 120.30 |
| 23 | DA | 209 | C | C6-N1-C2 | 9.90 | 124.26 | 120.30 |
| 23 | DA | 210 | C | C5-C6-N1 | -9.89 | 116.05 | 121.00 |
| 23 | DA | 2330 | G | C8-N9-C4 | 9.88 | 110.35 | 106.40 |
| 23 | BA | 2689 | U | C2-N1-C1' | -9.87 | 105.86 | 117.70 |
| 23 | DA | 461 | C | N1-C2-O2 | -9.86 | 112.99 | 118.90 |
| 23 | DA | 330 | A | N1-C6-N6 | 9.86 | 124.51 | 118.60 |
| 23 | DA | 1790 | C | C6-N1-C2 | 9.85 | 124.24 | 120.30 |
| 23 | DA | 1614 | A | C6-C5-N7 | -9.84 | 125.41 | 132.30 |
| 23 | DA | 265 | A | C5-N7-C8 | -9.83 | 98.99 | 103.90 |
| 23 | DA | 2518 | A | C5-N7-C8 | -9.82 | 98.99 | 103.90 |
| 23 | DA | 2430 | A | C6-C5-N7 | -9.79 | 125.45 | 132.30 |
| 23 | DA | 1791 | A | C8-N9-C4 | 9.78 | 109.71 | 105.80 |
| 23 | DA | 945 | A | C4-N9-C1' | 9.75 | 143.84 | 126.30 |
| 23 | BA | 2463 | C | C6-N1-C2 | 9.74 | 124.20 | 120.30 |
| 23 | BA | 1962 | C | C2-N1-C1' | 9.71 | 129.47 | 118.80 |
| 23 | DA | 2502 | G | C5-C6-O6 | -9.70 | 122.78 | 128.60 |
| 23 | DA | 2498 | C | C6-N1-C2 | 9.69 | 124.18 | 120.30 |
| 23 | DA | 71 | A | N1-C6-N6 | 9.69 | 124.41 | 118.60 |
| 23 | DA | 1572 | A | C8-N9-C4 | 9.68 | 109.67 | 105.80 |
| 23 | DA | 570 | G | C5-C6-N1 | -9.65 | 106.68 | 111.50 |
| 23 | DA | 2430 | A | N1-C6-N6 | 9.64 | 124.39 | 118.60 |
| 23 | BA | 1898 | U | C5-C4-O4 | 9.64 | 131.68 | 125.90 |
| 23 | BA | 2871 | C | C6-N1-C2 | 9.63 | 124.15 | 120.30 |
| 23 | DA | 774 | A | N1-C6-N6 | 9.63 | 124.38 | 118.60 |
| 23 | BA | 945 | A | C4-N9-C1' | 9.62 | 143.61 | 126.30 |
| 23 | DA | 809 | G | N1-C6-O6 | 9.61 | 125.66 | 119.90 |
| 23 | DA | 783 | A | C2-N3-C4 | -9.59 | 105.80 | 110.60 |
| 23 | DA | 1618 | A | N1-C6-N6 | 9.59 | 124.35 | 118.60 |
| 23 | DA | 1648 | C | N1-C2-O2 | -9.58 | 113.15 | 118.90 |
| 23 | DA | 141(A) | A | C5-N7-C8 | -9.58 | 99.11 | 103.90 |
| 23 | DA | 2689 | U | N3-C4-O4 | -9.58 | 112.69 | 119.40 |
| 23 | BA | 2044 | C | C6-N1-C2 | 9.57 | 124.13 | 120.30 |
| 23 | BA | 783 | A | N1-C6-N6 | 9.56 | 124.34 | 118.60 |
| 23 | BA | 1241 | A | C2-N3-C4 | -9.56 | 105.82 | 110.60 |
| 23 | DA | 2050 | C | C2-N3-C4 | -9.55 | 115.12 | 119.90 |
| 23 | DA | 397 | G | C8-N9-C4 | 9.55 | 110.22 | 106.40 |
| 23 | BA | 2713 | A | N1-C6-N6 | 9.54 | 124.32 | 118.60 |
| 23 | DA | 783 | A | C4-C5-N7 | 9.54 | 115.47 | 110.70 |
| 23 | DA | 2032 | G | C5-N7-C8 | -9.54 | 99.53 | 104.30 |
| 23 | BA | 2689 | U | C5-C4-O4 | 9.53 | 131.62 | 125.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 23 | BA | 664 | C | C6-N1-C2 | 9.51 | 124.11 | 120.30 |
| 23 | DA | 1331 | A | C2-N3-C4 | -9.51 | 105.84 | 110.60 |
| 23 | BA | 2032 | G | C5-N7-C8 | -9.50 | 99.55 | 104.30 |
| 23 | DA | 130 | C | N3-C4-C5 | 9.48 | 125.69 | 121.90 |
| 23 | BA | 2043 | C | C6-N1-C2 | 9.47 | 124.09 | 120.30 |
| 23 | DA | 2713 | A | N1-C6-N6 | 9.46 | 124.28 | 118.60 |
| 23 | DA | 1257 | C | C5-C6-N1 | -9.46 | 116.27 | 121.00 |
| 23 | DA | 1899 | G | C2-N3-C4 | -9.45 | 107.17 | 111.90 |
| 23 | DA | 330 | A | C2-N3-C4 | -9.44 | 105.88 | 110.60 |
| 23 | DA | 2829 | C | C6-N1-C2 | 9.40 | 124.06 | 120.30 |
| 23 | BA | 828 | U | N3-C4-O4 | -9.40 | 112.82 | 119.40 |
| 23 | BA | 2028 | U | C4-C5-C6 | 9.39 | 125.33 | 119.70 |
| 23 | BA | 2240 | C | C6-N1-C2 | 9.38 | 124.05 | 120.30 |
| 23 | DA | 1994 | C | C6-N1-C2 | 9.37 | 124.05 | 120.30 |
| 23 | BA | 2713 | A | C5-N7-C8 | -9.36 | 99.22 | 103.90 |
| 23 | BA | 2430 | A | N1-C6-N6 | 9.32 | 124.19 | 118.60 |
| 23 | BA | 2084 | C | C6-N1-C2 | 9.31 | 124.03 | 120.30 |
| 23 | DA | 586 | A | C8-N9-C4 | 9.29 | 109.52 | 105.80 |
| 23 | BA | 640 | C | C6-N1-C2 | 9.28 | 124.01 | 120.30 |
| 23 | DA | 979 | G | C4-C5-N7 | 9.28 | 114.51 | 110.80 |
| 23 | DA | 2580 | U | C5-C4-O4 | 9.27 | 131.46 | 125.90 |
| 23 | DA | 1671 | U | C4-C5-C6 | 9.27 | 125.26 | 119.70 |
| 23 | BA | 679 | C | N1-C2-O2 | -9.25 | 113.35 | 118.90 |
| 23 | DA | 2681 | C | C5-C6-N1 | -9.23 | 116.38 | 121.00 |
| 23 | BA | 2571 | C | C2-N3-C4 | -9.23 | 115.28 | 119.90 |
| 23 | DA | 1257 | C | C2-N3-C4 | -9.23 | 115.29 | 119.90 |
| 23 | BA | 2010 | G | C4-C5-N7 | 9.22 | 114.49 | 110.80 |
| 23 | DA | 2028 | U | C5-C6-N1 | 9.22 | 127.31 | 122.70 |
| 23 | DA | 784 | A | N1-C6-N6 | -9.22 | 113.07 | 118.60 |
| 23 | BA | 2502 | G | C6-C5-N7 | -9.21 | 124.88 | 130.40 |
| 23 | BA | 2619 | C | C6-N1-C2 | 9.19 | 123.98 | 120.30 |
| 23 | DA | 678 | C | N3-C4-C5 | 9.20 | 125.58 | 121.90 |
| 23 | BA | 1614 | A | C2-N3-C4 | -9.19 | 106.01 | 110.60 |
| 23 | DA | 2648 | C | N1-C2-O2 | -9.19 | 113.39 | 118.90 |
| 23 | DA | 397 | G | N1-C6-O6 | 9.18 | 125.41 | 119.90 |
| 23 | DA | 945 | A | C5-N7-C8 | -9.18 | 99.31 | 103.90 |
| 23 | BA | 330 | A | N1-C6-N6 | 9.18 | 124.11 | 118.60 |
| 23 | DA | 1264 | G | C8-N9-C4 | -9.17 | 102.73 | 106.40 |
| 23 | BA | 2084 | C | C5-C6-N1 | -9.17 | 116.42 | 121.00 |
| 23 | DA | 2066 | C | C6-N1-C2 | 9.16 | 123.97 | 120.30 |
| 23 | DA | 133 | C | C6-N1-C2 | 9.16 | 123.96 | 120.30 |
| 23 | DA | 527 | C | N3-C4-N4 | -9.15 | 111.59 | 118.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | BA | 2742 | C | C6-N1-C2 | 9.15 | 123.96 | 120.30 |
| 23 | DA | 2448 | A | N1-C6-N6 | 9.14 | 124.09 | 118.60 |
| 23 | BA | 580 | C | C5-C6-N1 | -9.14 | 116.43 | 121.00 |
| 23 | DA | 1616 | A | C6-C5-N7 | -9.13 | 125.91 | 132.30 |
| 23 | DA | 1614 | A | N1-C6-N6 | 9.11 | 124.07 | 118.60 |
| 23 | BA | 676 | A | C4-C5-N7 | 9.11 | 115.25 | 110.70 |
| 23 | BA | 2430 | A | C6-C5-N7 | -9.10 | 125.93 | 132.30 |
| 23 | DA | 1616 | A | N7-C8-N9 | 9.10 | 118.35 | 113.80 |
| 23 | DA | 130 | C | C6-N1-C2 | 9.09 | 123.94 | 120.30 |
| 23 | DA | 676 | A | C5-C6-N1 | -9.09 | 113.16 | 117.70 |
| 23 | DA | 2043 | C | C6-N1-C2 | 9.08 | 123.93 | 120.30 |
| 23 | BA | 2066 | C | N3-C4-C5 | 9.07 | 125.53 | 121.90 |
| 23 | DA | 189 | G | C8-N9-C4 | 9.04 | 110.02 | 106.40 |
| 23 | BA | 560 | C | C6-N1-C2 | 9.04 | 123.92 | 120.30 |
| 23 | DA | 2231 | C | N1-C2-O2 | -9.03 | 113.48 | 118.90 |
| 23 | DA | 774 | A | N1-C2-N3 | 9.01 | 133.81 | 129.30 |
| 23 | DA | 1678 | G | C4-N9-C1' | -9.01 | 114.79 | 126.50 |
| 23 | DA | 387 | U | N3-C4-C5 | -8.99 | 109.21 | 114.60 |
| 23 | BA | 708 | C | C6-N1-C2 | 8.98 | 123.89 | 120.30 |
| 23 | DA | 1698 | A | C5-N7-C8 | -8.98 | 99.41 | 103.90 |
| 23 | BA | 1934 | C | C6-N1-C2 | 8.98 | 123.89 | 120.30 |
| 23 | BA | 761 | A | C2-N3-C4 | -8.96 | 106.12 | 110.60 |
| 23 | BA | 1783 | A | N9-C4-C5 | 8.96 | 109.39 | 105.80 |
| 23 | BA | 1902 | C | N3-C4-N4 | -8.95 | 111.73 | 118.00 |
| 23 | BA | 945 | A | C4-C5-C6 | 8.95 | 121.48 | 117.00 |
| 23 | BA | 1779 | U | C6-N1-C2 | 8.95 | 126.37 | 121.00 |
| 23 | DA | 1962 | C | C2-N1-C1' | 8.94 | 128.63 | 118.80 |
| 23 | DA | 679 | C | C2-N3-C4 | -8.93 | 115.44 | 119.90 |
| 23 | DA | 1349 | A | N1-C6-N6 | 8.92 | 123.95 | 118.60 |
| 23 | BA | 1244 | G | C8-N9-C4 | 8.92 | 109.97 | 106.40 |
| 23 | BA | 1830 | C | N1-C2-O2 | -8.91 | 113.55 | 118.90 |
| 23 | DA | 659 | C | C6-N1-C2 | 8.91 | 123.86 | 120.30 |
| 23 | DA | 2571 | C | N3-C4-C5 | 8.90 | 125.46 | 121.90 |
| 23 | BA | 2391 | G | N1-C6-O6 | -8.87 | 114.58 | 119.90 |
| 23 | DA | 774 | A | N3-C4-C5 | 8.87 | 133.01 | 126.80 |
| 23 | DA | 2578 | G | C5-C6-O6 | -8.87 | 123.28 | 128.60 |
| 23 | BA | 528 | A | C2-N3-C4 | -8.85 | 106.17 | 110.60 |
| 23 | DA | 568 | U | N3-C4-C5 | -8.84 | 109.30 | 114.60 |
| 23 | DA | 783 | A | C6-C5-N7 | -8.82 | 126.12 | 132.30 |
| 23 | DA | 1786 | A | C6-C5-N7 | -8.82 | 126.12 | 132.30 |
| 23 | DA | 774 | A | C4-C5-N7 | 8.82 | 115.11 | 110.70 |
| 23 | DA | 2010 | G | N1-C6-O6 | 8.82 | 125.19 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | DA | 1678 | G | C8-N9-C1' | 8.82 | 138.47 | 127.00 |
| 1 | AA | 299 | G | C5-C6-N1 | -8.82 | 107.09 | 111.50 |
| 23 | BA | 676 | A | C6-C5-N7 | -8.81 | 126.13 | 132.30 |
| 23 | DA | 1786 | A | C2-N3-C4 | -8.81 | 106.19 | 110.60 |
| 23 | DA | 1979 | C | N1-C2-O2 | -8.81 | 113.61 | 118.90 |
| 23 | DA | 1790 | C | N3-C4-C5 | 8.79 | 125.42 | 121.90 |
| 23 | DA | 678 | C | C6-N1-C2 | 8.78 | 123.81 | 120.30 |
| 23 | BA | 2010 | G | N1-C6-O6 | 8.77 | 125.16 | 119.90 |
| 23 | BA | 945 | A | C8-N9-C1' | -8.76 | 111.94 | 127.70 |
| 23 | DA | 1605 | C | C6-N1-C2 | -8.75 | 116.80 | 120.30 |
| 23 | DA | 2830 | G | C5-C6-O6 | -8.73 | 123.36 | 128.60 |
| 23 | BA | 265 | A | C5-N7-C8 | -8.73 | 99.54 | 103.90 |
| 23 | DA | 1698 | A | C6-C5-N7 | -8.73 | 126.19 | 132.30 |
| 23 | DA | 2502 | G | N1-C6-O6 | 8.73 | 125.14 | 119.90 |
| 23 | BA | 2050 | C | N1-C2-O2 | -8.72 | 113.67 | 118.90 |
| 23 | BA | 847 | U | C2-N1-C1' | -8.72 | 107.24 | 117.70 |
| 23 | BA | 783 | A | C5-N7-C8 | -8.71 | 99.55 | 103.90 |
| 23 | BA | 1839 | G | N3-C4-N9 | -8.71 | 120.78 | 126.00 |
| 23 | DA | 945 | A | N1-C6-N6 | 8.70 | 123.82 | 118.60 |
| 23 | BA | 461 | C | N1-C2-O2 | -8.69 | 113.69 | 118.90 |
| 23 | DA | 774 | A | C6-C5-N7 | -8.69 | 126.22 | 132.30 |
| 23 | DA | 2505 | G | N1-C6-O6 | -8.69 | 114.69 | 119.90 |
| 23 | BA | 1614 | A | C5-C6-N1 | -8.69 | 113.36 | 117.70 |
| 23 | DA | 2581 | G | N1-C6-O6 | -8.69 | 114.69 | 119.90 |
| 23 | BA | 1572 | A | C8-N9-C4 | 8.68 | 109.27 | 105.80 |
| 23 | DA | 1616 | A | C2-N3-C4 | -8.68 | 106.26 | 110.60 |
| 23 | BA | 929 | G | N1-C6-O6 | 8.68 | 125.11 | 119.90 |
| 23 | DA | 2648 | C | C5-C6-N1 | -8.67 | 116.67 | 121.00 |
| 23 | BA | 2713 | A | C2-N3-C4 | -8.67 | 106.27 | 110.60 |
| 23 | DA | 671 | C | N1-C2-O2 | -8.66 | 113.70 | 118.90 |
| 23 | DA | 114(B) | A | C6-C5-N7 | -8.66 | 126.24 | 132.30 |
| 23 | DA | 57 | C | N3-C4-C5 | 8.65 | 125.36 | 121.90 |
| 23 | BA | 2693 | A | N1-C6-N6 | -8.65 | 113.41 | 118.60 |
| 23 | DA | 2496 | C | C6-N1-C2 | 8.65 | 123.76 | 120.30 |
| 23 | DA | 1698 | A | C4-C5-N7 | 8.64 | 115.02 | 110.70 |
| 23 | DA | 2248 | C | C2-N3-C4 | -8.64 | 115.58 | 119.90 |
| 23 | DA | 1678 | G | C2-N3-C4 | -8.64 | 107.58 | 111.90 |
| 23 | DA | 265 | A | C5-C6-N1 | -8.64 | 113.38 | 117.70 |
| 23 | BA | 1325 | G | N9-C4-C5 | 8.63 | 108.85 | 105.40 |
| 23 | BA | 1332 | G | N1-C2-N2 | 8.63 | 123.96 | 116.20 |
| 23 | DA | 945 | A | C4-C5-C6 | 8.63 | 121.31 | 117.00 |
| 23 | BA | 535 | C | C6-N1-C2 | 8.62 | 123.75 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | DA | 1602 | U | C2-N3-C4 | 8.62 | 132.17 | 127.00 |
| 23 | DA | 684 | G | C8-N9-C4 | -8.60 | 102.96 | 106.40 |
| 23 | DA | 211 | A | C2-N3-C4 | -8.59 | 106.31 | 110.60 |
| 23 | DA | 945 | A | C8-N9-C4 | -8.59 | 102.36 | 105.80 |
| 23 | DA | 2689 | U | C6-N1-C1' | 8.57 | 133.19 | 121.20 |
| 23 | DA | 2713 | A | C5-N7-C8 | -8.57 | 99.62 | 103.90 |
| 23 | DA | 211 | A | N1-C2-N3 | 8.56 | 133.58 | 129.30 |
| 23 | DA | 377 | C | C6-N1-C2 | 8.56 | 123.72 | 120.30 |
| 23 | DA | 676 | A | C6-C5-N7 | -8.55 | 126.31 | 132.30 |
| 23 | DA | 2647 | U | C5-C6-N1 | -8.55 | 118.42 | 122.70 |
| 23 | DA | 2451 | A | N9-C4-C5 | 8.54 | 109.22 | 105.80 |
| 23 | BA | 1698 | A | N1-C6-N6 | 8.54 | 123.72 | 118.60 |
| 23 | BA | 1614 | A | C6-C5-N7 | -8.54 | 126.33 | 132.30 |
| 23 | BA | 1788 | C | C5-C6-N1 | -8.51 | 116.75 | 121.00 |
| 23 | DA | 140 | A | C5-N7-C8 | -8.50 | 99.65 | 103.90 |
| 23 | DA | 570 | G | N9-C4-C5 | 8.49 | 108.80 | 105.40 |
| 23 | BA | 330 | A | N9-C4-C5 | -8.49 | 102.40 | 105.80 |
| 23 | BA | 2581 | G | C8-N9-C4 | -8.49 | 103.00 | 106.40 |
| 23 | DA | 2688 | U | C5-C4-O4 | 8.49 | 131.00 | 125.90 |
| 23 | DA | 677 | A | C2-N3-C4 | -8.48 | 106.36 | 110.60 |
| 23 | DA | 2010 | G | C6-C5-N7 | -8.48 | 125.31 | 130.40 |
| 23 | DA | 194 | G | C8-N9-C4 | 8.48 | 109.79 | 106.40 |
| 23 | BA | 2828 | C | C5-C6-N1 | -8.47 | 116.77 | 121.00 |
| 23 | BA | 2433 | A | N1-C2-N3 | 8.47 | 133.53 | 129.30 |
| 23 | BA | 1683 | C | N1-C2-O2 | -8.47 | 113.82 | 118.90 |
| 23 | BA | 2066 | C | C2-N3-C4 | -8.47 | 115.67 | 119.90 |
| 23 | BA | 2057 | A | N1-C2-N3 | 8.46 | 133.53 | 129.30 |
| 23 | BA | 970 | C | C6-N1-C2 | 8.44 | 123.67 | 120.30 |
| 23 | BA | 1772 | G | C8-N9-C4 | 8.43 | 109.77 | 106.40 |
| 23 | BA | 2057 | A | C2-N3-C4 | -8.42 | 106.39 | 110.60 |
| 23 | BA | 1979 | C | N1-C2-O2 | -8.42 | 113.85 | 118.90 |
| 23 | BA | 1261 | C | N3-C4-C5 | 8.42 | 125.27 | 121.90 |
| 23 | BA | 2430 | A | C2-N3-C4 | -8.41 | 106.39 | 110.60 |
| 23 | DA | 71 | A | C4-C5-N7 | 8.41 | 114.91 | 110.70 |
| 23 | BA | 783 | A | C2-N3-C4 | -8.41 | 106.40 | 110.60 |
| 23 | DA | 450 | G | C4-C5-N7 | -8.40 | 107.44 | 110.80 |
| 23 | DA | 2053 | G | N1-C6-O6 | 8.40 | 124.94 | 119.90 |
| 23 | BA | 397 | G | N1-C6-O6 | 8.40 | 124.94 | 119.90 |
| 23 | DA | 458 | G | C2-N3-C4 | 8.40 | 116.10 | 111.90 |
| 23 | DA | 2500 | U | C5-C6-N1 | -8.39 | 118.50 | 122.70 |
| 23 | BA | 2699 | C | C5-C6-N1 | -8.39 | 116.81 | 121.00 |
| 23 | DA | 1417 | C | C6-N1-C2 | 8.38 | 123.65 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | DA | 787 | U | C5-C6-N1 | -8.37 | 118.52 | 122.70 |
| 23 | BA | 671 | C | N1-C2-O2 | -8.37 | 113.88 | 118.90 |
| 23 | BA | 2010 | G | C8-N9-C4 | -8.37 | 103.05 | 106.40 |
| 23 | BA | 1602 | U | N3-C4-O4 | 8.37 | 125.26 | 119.40 |
| 23 | BA | 2689 | U | N3-C4-O4 | -8.37 | 113.54 | 119.40 |
| 23 | BA | 2505 | G | C5-C6-O6 | 8.36 | 133.61 | 128.60 |
| 23 | BA | 677 | A | C2-N3-C4 | -8.35 | 106.42 | 110.60 |
| 23 | BA | 2544 | G | N1-C6-O6 | 8.35 | 124.91 | 119.90 |
| 23 | BA | 1253 | A | C5-N7-C8 | -8.35 | 99.73 | 103.90 |
| 23 | DA | 945 | A | C4-C5-N7 | 8.35 | 114.87 | 110.70 |
| 23 | BA | 655 | A | C8-N9-C4 | -8.34 | 102.46 | 105.80 |
| 23 | BA | 1971 | A | N1-C6-N6 | 8.34 | 123.60 | 118.60 |
| 23 | BA | 2681 | C | N3-C4-N4 | -8.34 | 112.16 | 118.00 |
| 23 | DA | 2503 | A | N1-C2-N3 | -8.34 | 125.13 | 129.30 |
| 23 | DA | 568 | U | C4-C5-C6 | 8.34 | 124.70 | 119.70 |
| 23 | DA | 937 | U | C5-C6-N1 | -8.33 | 118.53 | 122.70 |
| 23 | BA | 2441 | C | C6-N1-C2 | 8.32 | 123.63 | 120.30 |
| 23 | DA | 1934 | C | C6-N1-C2 | 8.32 | 123.63 | 120.30 |
| 23 | BA | 2392 | A | C2-N3-C4 | -8.31 | 106.44 | 110.60 |
| 23 | DA | 761 | A | C8-N9-C1' | -8.31 | 112.74 | 127.70 |
| 23 | DA | 1962 | C | C6-N1-C1' | -8.31 | 110.83 | 120.80 |
| 23 | DA | 2057 | A | C2-N3-C4 | -8.30 | 106.45 | 110.60 |
| 23 | BA | 731 | C | C6-N1-C2 | 8.30 | 123.62 | 120.30 |
| 23 | DA | 1021 | A | C5-N7-C8 | -8.30 | 99.75 | 103.90 |
| 23 | DA | 1010 | A | C8-N9-C4 | 8.29 | 109.11 | 105.80 |
| 1 | AA | 123 | C | C6-N1-C2 | 8.28 | 123.61 | 120.30 |
| 23 | DA | 472 | A | C8-N9-C4 | 8.28 | 109.11 | 105.80 |
| 23 | DA | 2699 | C | C6-N1-C2 | 8.28 | 123.61 | 120.30 |
| 23 | DA | 2463 | C | C6-N1-C2 | 8.28 | 123.61 | 120.30 |
| 23 | BA | 189 | G | C8-N9-C4 | 8.28 | 109.71 | 106.40 |
| 23 | DA | 1935 | G | C8-N9-C4 | 8.27 | 109.71 | 106.40 |
| 23 | BA | 1771 | C | N1-C2-O2 | -8.27 | 113.94 | 118.90 |
| 23 | BA | 265 | A | C2-N3-C4 | -8.27 | 106.47 | 110.60 |
| 23 | DA | 2056 | G | C4-C5-N7 | 8.25 | 114.10 | 110.80 |
| 23 | BA | 1999 | C | C5-C6-N1 | -8.25 | 116.88 | 121.00 |
| 23 | BA | 2226 | C | C6-N1-C2 | 8.24 | 123.60 | 120.30 |
| 23 | BA | 2463 | C | C5-C6-N1 | -8.24 | 116.88 | 121.00 |
| 23 | DA | 2061 | G | C5-C6-N1 | -8.23 | 107.39 | 111.50 |
| 23 | DA | 2417 | C | C6-N1-C2 | 8.22 | 123.59 | 120.30 |
| 23 | BA | 828 | U | C5-C4-O4 | 8.21 | 130.83 | 125.90 |
| 23 | DA | 1264 | G | N9-C4-C5 | 8.20 | 108.68 | 105.40 |
| 23 | BA | 807 | U | C2-N1-C1' | -8.19 | 107.87 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | DA | 2432 | A | C2-N3-C4 | -8.19 | 106.51 | 110.60 |
| 23 | BA | 444 | C | C5-C6-N1 | -8.18 | 116.91 | 121.00 |
| 23 | BA | 676 | A | N3-C4-N9 | -8.18 | 120.85 | 127.40 |
| 23 | DA | 2706 | G | C5-C6-O6 | -8.18 | 123.69 | 128.60 |
| 23 | DA | 676 | A | N3-C4-N9 | -8.18 | 120.86 | 127.40 |
| 23 | DA | 1161 | C | C6-N1-C2 | -8.18 | 117.03 | 120.30 |
| 23 | DA | 2739 | U | C5-C6-N1 | -8.17 | 118.61 | 122.70 |
| 23 | DA | 270(B) | A | C8-N9-C4 | 8.16 | 109.06 | 105.80 |
| 23 | BA | 1962 | C | C6-N1-C1' | -8.16 | 111.01 | 120.80 |
| 23 | BA | 1653 | G | C8-N9-C4 | 8.15 | 109.66 | 106.40 |
| 23 | BA | 2713 | A | C4-C5-N7 | 8.15 | 114.78 | 110.70 |
| 23 | BA | 574 | C | C6-N1-C2 | 8.15 | 123.56 | 120.30 |
| 23 | DA | 2593 | U | C4-C5-C6 | 8.14 | 124.59 | 119.70 |
| 23 | DA | 2430 | A | C4-C5-C6 | 8.14 | 121.07 | 117.00 |
| 23 | BA | 2506 | U | N3-C2-O2 | -8.14 | 116.50 | 122.20 |
| 23 | BA | 2424 | C | C6-N1-C2 | 8.13 | 123.55 | 120.30 |
| 23 | DA | 2712 | U | N1-C2-N3 | 8.13 | 119.78 | 114.90 |
| 23 | BA | 1253 | A | C4-C5-C6 | -8.12 | 112.94 | 117.00 |
| 23 | BA | 1786 | A | N1-C2-N3 | 8.12 | 133.36 | 129.30 |
| 23 | BA | 1325 | G | C8-N9-C1' | 8.11 | 137.54 | 127.00 |
| 23 | BA | 1800 | C | C6-N1-C2 | 8.11 | 123.54 | 120.30 |
| 23 | DA | 1309 | G | C8-N9-C4 | 8.11 | 109.64 | 106.40 |
| 23 | BA | 1614 | A | C5-N7-C8 | -8.11 | 99.85 | 103.90 |
| 23 | BA | 764 | A | C5-N7-C8 | -8.09 | 99.85 | 103.90 |
| 23 | DA | 2515 | C | C6-N1-C2 | 8.09 | 123.54 | 120.30 |
| 23 | BA | 814 | C | C6-N1-C2 | 8.09 | 123.54 | 120.30 |
| 23 | DA | 786 | C | C5-C6-N1 | -8.08 | 116.96 | 121.00 |
| 23 | DA | 2681 | C | N3-C4-N4 | -8.08 | 112.34 | 118.00 |
| 23 | BA | 1204 | A | C5-N7-C8 | -8.08 | 99.86 | 103.90 |
| 23 | DA | 528 | A | C2-N3-C4 | -8.07 | 106.56 | 110.60 |
| 23 | DA | 71 | A | C2-N3-C4 | -8.07 | 106.57 | 110.60 |
| 23 | DA | 2510 | C | C6-N1-C2 | 8.07 | 123.53 | 120.30 |
| 23 | BA | 141(A) | A | C5-N7-C8 | -8.06 | 99.87 | 103.90 |
| 23 | BA | 840 | C | C6-N1-C2 | 8.05 | 123.52 | 120.30 |
| 23 | BA | 2081 | C | N1-C2-O2 | -8.06 | 114.07 | 118.90 |
| 23 | DA | 1783 | A | N9-C4-C5 | 8.06 | 109.02 | 105.80 |
| 23 | DA | 2626 | C | C5-C6-N1 | -8.06 | 116.97 | 121.00 |
| 23 | DA | 114(B) | A | N1-C6-N6 | 8.05 | 123.43 | 118.60 |
| 23 | DA | 408 | G | N7-C8-N9 | -8.05 | 109.08 | 113.10 |
| 23 | DA | 664 | C | C6-N1-C2 | 8.05 | 123.52 | 120.30 |
| 23 | BA | 2777 | G | C8-N9-C4 | 8.05 | 109.62 | 106.40 |
| 23 | BA | 1790 | C | C5-C6-N1 | -8.03 | 116.99 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | DA | 698 | C | C6-N1-C2 | 8.03 | 123.51 | 120.30 |
| 1 | AA | 1512 | U | C5-C6-N1 | -8.02 | 118.69 | 122.70 |
| 23 | DA | 2518 | A | C4-C5-N7 | 8.02 | 114.71 | 110.70 |
| 47 | DY | 21 | LEU | CA-CB-CG | 8.02 | 133.74 | 115.30 |
| 23 | BA | 945 | A | C5-N7-C8 | -8.01 | 99.89 | 103.90 |
| 23 | DA | 1022 | G | N1-C6-O6 | -8.00 | 115.10 | 119.90 |
| 23 | BA | 1678 | G | C8-N9-C1' | 8.00 | 137.40 | 127.00 |
| 23 | BA | 2596 | U | C2-N1-C1' | -8.00 | 108.11 | 117.70 |
| 23 | DA | 1627 | G | N1-C6-O6 | 8.00 | 124.70 | 119.90 |
| 23 | BA | 2028 | U | C5-C6-N1 | 7.99 | 126.70 | 122.70 |
| 23 | BA | 2017 | U | N1-C2-N3 | 7.99 | 119.69 | 114.90 |
| 23 | BA | 529 | A | N1-C6-N6 | 7.98 | 123.39 | 118.60 |
| 23 | DA | 840 | C | C6-N1-C2 | 7.98 | 123.49 | 120.30 |
| 23 | BA | 1898 | U | N3-C4-C5 | -7.98 | 109.81 | 114.60 |
| 23 | DA | 2505 | G | C4-C5-N7 | -7.98 | 107.61 | 110.80 |
| 23 | BA | 1820 | U | C5-C6-N1 | -7.98 | 118.71 | 122.70 |
| 23 | DA | 465 | G | C8-N9-C4 | -7.97 | 103.21 | 106.40 |
| 23 | DA | 1341 | U | N3-C4-O4 | 7.97 | 124.98 | 119.40 |
| 23 | BA | 32 | C | N1-C2-O2 | -7.96 | 114.12 | 118.90 |
| 23 | DA | 1644 | C | N1-C2-O2 | 7.96 | 123.68 | 118.90 |
| 23 | BA | 114(B) | A | C6-C5-N7 | -7.95 | 126.74 | 132.30 |
| 23 | DA | 1332 | G | C5-N7-C8 | -7.94 | 100.33 | 104.30 |
| 1 | CA | 285 | G | C8-N9-C4 | 7.94 | 109.58 | 106.40 |
| 23 | DA | 2014 | A | C8-N9-C4 | 7.94 | 108.97 | 105.80 |
| 23 | DA | 2581 | G | N9-C4-C5 | 7.94 | 108.58 | 105.40 |
| 23 | BA | 1614 | A | N7-C8-N9 | 7.93 | 117.77 | 113.80 |
| 23 | DA | 2591 | C | C5-C6-N1 | -7.93 | 117.03 | 121.00 |
| 23 | DA | 809 | G | C5-C6-O6 | -7.93 | 123.84 | 128.60 |
| 23 | BA | 1678 | G | C2-N3-C4 | -7.92 | 107.94 | 111.90 |
| 23 | BA | 535 | C | C5-C6-N1 | -7.92 | 117.04 | 121.00 |
| 23 | BA | 2346 | A | C2-N3-C4 | -7.91 | 106.64 | 110.60 |
| 23 | BA | 2699 | C | C6-N1-C2 | 7.91 | 123.46 | 120.30 |
| 23 | DA | 783 | A | C8-N9-C4 | -7.90 | 102.64 | 105.80 |
| 23 | BA | 189 | G | N9-C4-C5 | -7.90 | 102.24 | 105.40 |
| 23 | BA | 2028 | U | C2-N3-C4 | 7.90 | 131.74 | 127.00 |
| 23 | DA | 273(A) | G | C8-N9-C4 | 7.90 | 109.56 | 106.40 |
| 46 | BX | 35 | THR | N-CA-C | 7.90 | 132.33 | 111.00 |
| 23 | BA | 2499 | C | C2-N3-C4 | -7.90 | 115.95 | 119.90 |
| 23 | DA | 2567 | G | N1-C6-O6 | 7.90 | 124.64 | 119.90 |
| 23 | DA | 783 | A | N1-C6-N6 | 7.90 | 123.34 | 118.60 |
| 23 | BA | 2524 | G | C8-N9-C4 | 7.89 | 109.56 | 106.40 |
| 23 | BA | 1786 | A | C4-C5-N7 | 7.89 | 114.64 | 110.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | DA | 107 | C | C6-N1-C2 | 7.88 | 123.45 | 120.30 |
| 23 | BA | 2010 | G | C5-N7-C8 | -7.88 | 100.36 | 104.30 |
| 23 | DA | 971 | C | N1-C2-O2 | -7.88 | 114.17 | 118.90 |
| 23 | DA | 1989 | G | N1-C6-O6 | 7.88 | 124.63 | 119.90 |
| 23 | BA | 298 | G | C5-N7-C8 | -7.88 | 100.36 | 104.30 |
| 23 | DA | 2451 | A | C8-N9-C4 | -7.88 | 102.65 | 105.80 |
| 23 | BA | 2593 | U | N3-C4-C5 | -7.88 | 109.87 | 114.60 |
| 23 | DA | 736 | C | C6-N1-C2 | 7.87 | 123.45 | 120.30 |
| 23 | DA | 1007 | C | C5-C6-N1 | -7.87 | 117.06 | 121.00 |
| 23 | BA | 2518 | A | C5-N7-C8 | -7.87 | 99.97 | 103.90 |
| 47 | BY | 21 | LEU | CA-CB-CG | 7.87 | 133.39 | 115.30 |
| 23 | DA | 2424 | C | C6-N1-C2 | 7.86 | 123.44 | 120.30 |
| 23 | DA | 2324 | C | C5-C6-N1 | -7.85 | 117.07 | 121.00 |
| 23 | BA | 1671 | U | C5-C6-N1 | 7.85 | 126.62 | 122.70 |
| 23 | DA | 1820 | U | C5-C6-N1 | -7.85 | 118.78 | 122.70 |
| 1 | CA | 1053 | G | C4-N9-C1' | -7.85 | 116.30 | 126.50 |
| 23 | BA | 530 | G | C8-N9-C4 | -7.84 | 103.26 | 106.40 |
| 23 | DA | 2713 | A | C2-N3-C4 | -7.84 | 106.68 | 110.60 |
| 23 | DA | 2430 | A | C2-N3-C4 | -7.84 | 106.68 | 110.60 |
| 23 | DA | 814 | C | C6-N1-C2 | 7.84 | 123.43 | 120.30 |
| 23 | BA | 1704 | G | C8-N9-C4 | 7.83 | 109.53 | 106.40 |
| 23 | BA | 945 | A | C4-C5-N7 | 7.83 | 114.62 | 110.70 |
| 23 | BA | 1332 | G | C5-N7-C8 | -7.83 | 100.39 | 104.30 |
| 23 | DA | 1261 | C | C6-N1-C2 | 7.83 | 123.43 | 120.30 |
| 23 | BA | 1323 | U | N1-C2-O2 | -7.83 | 117.32 | 122.80 |
| 23 | DA | 2685 | G | C5-C6-N1 | -7.83 | 107.59 | 111.50 |
| 23 | DA | 141(A) | A | C4-C5-N7 | 7.82 | 114.61 | 110.70 |
| 23 | DA | 761 | A | C4-N9-C1' | 7.82 | 140.37 | 126.30 |
| 23 | DA | 1201 | C | C6-N1-C2 | 7.82 | 123.43 | 120.30 |
| 23 | BA | 1899 | G | C8-N9-C4 | -7.81 | 103.27 | 106.40 |
| 23 | DA | 945 | A | C8-N9-C1' | -7.81 | 113.64 | 127.70 |
| 23 | DA | 2232 | U | C5-C6-N1 | -7.81 | 118.80 | 122.70 |
| 23 | DA | 1600 | C | N1-C2-O2 | -7.80 | 114.22 | 118.90 |
| 23 | DA | 2053 | G | C5-C6-O6 | -7.79 | 123.92 | 128.60 |
| 23 | DA | 2544 | G | C5-C6-O6 | -7.79 | 123.93 | 128.60 |
| 23 | DA | 2244 | U | N3-C2-O2 | -7.78 | 116.75 | 122.20 |
| 23 | DA | 2054 | A | N1-C6-N6 | 7.77 | 123.27 | 118.60 |
| 23 | DA | 1592 | C | C6-N1-C2 | 7.77 | 123.41 | 120.30 |
| 23 | DA | 2066 | C | N3-C4-C5 | 7.76 | 125.01 | 121.90 |
| 23 | BA | 566 | U | C5-C6-N1 | -7.76 | 118.82 | 122.70 |
| 23 | BA | 783 | A | C6-C5-N7 | -7.76 | 126.87 | 132.30 |
| 23 | BA | 1827 | C | C2-N3-C4 | -7.75 | 116.02 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | BA | 676 | A | N1-C2-N3 | 7.75 | 133.17 | 129.30 |
| 23 | DA | 530 | G | C8-N9-C4 | -7.74 | 103.30 | 106.40 |
| 23 | DA | 601 | C | C6-N1-C2 | 7.74 | 123.39 | 120.30 |
| 23 | DA | 828 | U | C5-C4-O4 | 7.74 | 130.54 | 125.90 |
| 23 | BA | 1204 | A | N7-C8-N9 | 7.73 | 117.66 | 113.80 |
| 23 | BA | 2391 | G | C5-C6-O6 | 7.72 | 133.23 | 128.60 |
| 23 | DA | 2713 | A | C6-C5-N7 | -7.72 | 126.90 | 132.30 |
| 1 | AA | 896 | C | C6-N1-C2 | 7.72 | 123.39 | 120.30 |
| 23 | DA | 784 | A | N9-C4-C5 | 7.71 | 108.89 | 105.80 |
| 23 | BA | 2010 | G | N7-C8-N9 | 7.71 | 116.95 | 113.10 |
| 23 | BA | 929 | G | C6-C5-N7 | -7.70 | 125.78 | 130.40 |
| 23 | BA | 1648 | C | N1-C2-O2 | -7.70 | 114.28 | 118.90 |
| 23 | DA | 979 | G | C5-N7-C8 | -7.70 | 100.45 | 104.30 |
| 23 | DA | 1325 | G | C8-N9-C1' | 7.70 | 137.00 | 127.00 |
| 23 | BA | 2588 | G | N1-C2-N3 | 7.69 | 128.52 | 123.90 |
| 23 | BA | 835 | A | C8-N9-C4 | 7.69 | 108.88 | 105.80 |
| 23 | DA | 2061 | G | N1-C6-O6 | 7.69 | 124.52 | 119.90 |
| 23 | BA | 570 | G | N9-C4-C5 | 7.68 | 108.47 | 105.40 |
| 23 | DA | 450 | G | N1-C6-O6 | 7.68 | 124.51 | 119.90 |
| 23 | BA | 1994 | C | C6-N1-C2 | 7.68 | 123.37 | 120.30 |
| 23 | DA | 1618 | A | C5-C6-N6 | -7.68 | 117.56 | 123.70 |
| 23 | DA | 57 | C | C5-C6-N1 | -7.68 | 117.16 | 121.00 |
| 23 | DA | 2571 | C | C5-C6-N1 | -7.68 | 117.16 | 121.00 |
| 23 | DA | 2503 | A | C5-C6-N1 | 7.67 | 121.54 | 117.70 |
| 23 | DA | 1665 | A | N1-C6-N6 | 7.67 | 123.20 | 118.60 |
| 23 | BA | 945 | A | N7-C8-N9 | 7.67 | 117.64 | 113.80 |
| 23 | BA | 1154 | G | N1-C6-O6 | -7.67 | 115.30 | 119.90 |
| 23 | BA | 774 | A | N3-C4-C5 | 7.66 | 132.16 | 126.80 |
| 23 | BA | 1678 | G | C4-N9-C1' | -7.65 | 116.55 | 126.50 |
| 23 | DA | 2596 | U | C2-N1-C1' | -7.65 | 108.52 | 117.70 |
| 23 | BA | 83 | G | N3-C4-C5 | 7.65 | 132.43 | 128.60 |
| 23 | BA | 568 | U | N3-C4-C5 | -7.65 | 110.01 | 114.60 |
| 23 | DA | 2010 | G | C2-N3-C4 | -7.65 | 108.07 | 111.90 |
| 23 | BA | 774 | A | C5-C6-N1 | -7.65 | 113.88 | 117.70 |
| 23 | BA | 2689 | U | C6-N1-C1' | 7.64 | 131.90 | 121.20 |
| 1 | CA | 1415 | G | N1-C6-O6 | 7.64 | 124.48 | 119.90 |
| 23 | DA | 2827 | C | C5-C6-N1 | -7.64 | 117.18 | 121.00 |
| 23 | DA | 847 | U | C2-N1-C1' | -7.64 | 108.53 | 117.70 |
| 23 | BA | 779 | U | C6-N1-C2 | 7.64 | 125.58 | 121.00 |
| 23 | BA | 1627 | G | N1-C6-O6 | 7.63 | 124.48 | 119.90 |
| 23 | BA | 2091 | U | C5-C6-N1 | -7.63 | 118.88 | 122.70 |
| 23 | DA | 929 | G | N1-C6-O6 | 7.63 | 124.48 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | BA | 2454 | G | N7-C8-N9 | -7.62 | 109.29 | 113.10 |
| 23 | DA | 2502 | G | N9-C4-C5 | -7.62 | 102.35 | 105.40 |
| 23 | DA | 1786 | A | C8-N9-C4 | -7.62 | 102.75 | 105.80 |
| 23 | BA | 580 | C | C2-N3-C4 | -7.61 | 116.09 | 119.90 |
| 1 | CA | 117 | G | N1-C6-O6 | 7.61 | 124.47 | 119.90 |
| 23 | DA | 2346 | A | C2-N3-C4 | -7.61 | 106.79 | 110.60 |
| 23 | BA | 2841 | C | C6-N1-C2 | 7.61 | 123.34 | 120.30 |
| 23 | BA | 2505 | G | C4-C5-N7 | -7.60 | 107.76 | 110.80 |
| 23 | DA | 328 | U | C5-C6-N1 | -7.60 | 118.90 | 122.70 |
| 23 | BA | 210 | C | C5-C6-N1 | -7.60 | 117.20 | 121.00 |
| 23 | BA | 580 | C | C6-N1-C2 | 7.59 | 123.33 | 120.30 |
| 23 | BA | 31 | C | C6-N1-C2 | 7.58 | 123.33 | 120.30 |
| 23 | DA | 57 | C | C2-N3-C4 | -7.58 | 116.11 | 119.90 |
| 23 | BA | 2540 | C | C5-C6-N1 | -7.58 | 117.21 | 121.00 |
| 46 | DX | 35 | THR | N-CA-C | 7.58 | 131.45 | 111.00 |
| 23 | DA | 684 | G | N7-C8-N9 | 7.57 | 116.89 | 113.10 |
| 1 | AA | 903 | G | C8-N9-C4 | 7.57 | 109.43 | 106.40 |
| 23 | DA | 466 | A | C2-N3-C4 | -7.57 | 106.81 | 110.60 |
| 23 | DA | 956 | G | C8-N9-C4 | 7.57 | 109.43 | 106.40 |
| 23 | DA | 979 | G | N1-C6-O6 | 7.57 | 124.44 | 119.90 |
| 23 | DA | 580 | C | C6-N1-C2 | 7.57 | 123.33 | 120.30 |
| 23 | DA | 2601 | C | C2-N3-C4 | -7.57 | 116.12 | 119.90 |
| 23 | BA | 1614 | A | N1-C6-N6 | 7.56 | 123.14 | 118.60 |
| 24 | BB | 100 | G | C8-N9-C4 | 7.56 | 109.42 | 106.40 |
| 23 | DA | 2591 | C | C4-C5-C6 | 7.56 | 121.18 | 117.40 |
| 23 | DA | 265 | A | N7-C8-N9 | 7.55 | 117.58 | 113.80 |
| 23 | DA | 915 | C | C6-N1-C2 | -7.55 | 117.28 | 120.30 |
| 1 | AA | 34 | C | C6-N1-C2 | 7.54 | 123.32 | 120.30 |
| 23 | BA | 1349 | A | N1-C6-N6 | 7.54 | 123.12 | 118.60 |
| 23 | DA | 1839 | G | N3-C4-N9 | -7.54 | 121.48 | 126.00 |
| 23 | DA | 2614 | A | C5-C6-N1 | 7.54 | 121.47 | 117.70 |
| 1 | CA | 299 | G | C4-C5-N7 | -7.54 | 107.78 | 110.80 |
| 1 | AA | 901 | A | C2-N3-C4 | -7.54 | 106.83 | 110.60 |
| 23 | BA | 2699 | C | C2-N1-C1' | -7.54 | 110.51 | 118.80 |
| 23 | DA | 2510 | C | N3-C4-C5 | 7.54 | 124.91 | 121.90 |
| 23 | DA | 2248 | C | C5-C6-N1 | -7.53 | 117.23 | 121.00 |
| 23 | DA | 114(B) | A | N1-C2-N3 | 7.53 | 133.07 | 129.30 |
| 23 | DA | 1031 | G | N1-C6-O6 | 7.53 | 124.42 | 119.90 |
| 23 | DA | 148 | C | C5-C6-N1 | -7.52 | 117.24 | 121.00 |
| 23 | BA | 2626 | C | C6-N1-C2 | 7.52 | 123.31 | 120.30 |
| 23 | DA | 676 | A | C8-N9-C4 | -7.52 | 102.79 | 105.80 |
| 23 | BA | 2081 | C | C2-N3-C4 | -7.52 | 116.14 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | DA | 424 | G | C5-C6-O6 | -7.52 | 124.09 | 128.60 |
| 23 | DA | 530 | G | N1-C6-O6 | -7.51 | 115.39 | 119.90 |
| 23 | DA | 2065 | C | N3-C4-C5 | 7.51 | 124.91 | 121.90 |
| 23 | BA | 771 | G | N1-C6-O6 | 7.50 | 124.40 | 119.90 |
| 1 | CA | 1053 | G | C8-N9-C1' | 7.50 | 136.75 | 127.00 |
| 23 | BA | 2250 | G | C8-N9-C4 | -7.50 | 103.40 | 106.40 |
| 23 | BA | 1161 | C | C6-N1-C2 | -7.49 | 117.30 | 120.30 |
| 23 | DA | 1352 | U | C5-C6-N1 | -7.49 | 118.95 | 122.70 |
| 23 | BA | 1770 | G | N1-C2-N3 | 7.49 | 128.39 | 123.90 |
| 23 | DA | 141(A) | A | N7-C8-N9 | 7.48 | 117.54 | 113.80 |
| 23 | DA | 815 | C | N3-C4-C5 | 7.48 | 124.89 | 121.90 |
| 23 | BA | 784 | A | N1-C6-N6 | -7.47 | 114.12 | 118.60 |
| 23 | BA | 1671 | U | C6-N1-C2 | -7.47 | 116.52 | 121.00 |
| 23 | BA | 1686 | C | N1-C2-O2 | -7.47 | 114.42 | 118.90 |
| 23 | DA | 140 | A | C4-C5-N7 | 7.46 | 114.43 | 110.70 |
| 52 | D4 | 19 | ARG | NE-CZ-NH2 | -7.46 | 116.57 | 120.30 |
| 23 | DA | 786 | C | C6-N1-C2 | 7.46 | 123.28 | 120.30 |
| 23 | BA | 764 | A | C4-C5-N7 | 7.45 | 114.42 | 110.70 |
| 23 | BA | 2588 | G | C2-N3-C4 | -7.45 | 108.18 | 111.90 |
| 23 | DA | 2503 | A | C2-N3-C4 | 7.45 | 114.32 | 110.60 |
| 23 | DA | 1261 | C | N1-C2-O2 | -7.45 | 114.43 | 118.90 |
| 23 | DA | 1304 | C | C2-N3-C4 | -7.45 | 116.18 | 119.90 |
| 23 | BA | 557 | U | C5-C6-N1 | -7.43 | 118.98 | 122.70 |
| 23 | DA | 1349 | A | C2-N3-C4 | -7.43 | 106.89 | 110.60 |
| 23 | BA | 1793 | C | C6-N1-C2 | 7.43 | 123.27 | 120.30 |
| 23 | DA | 1348 | G | N1-C6-O6 | 7.43 | 124.36 | 119.90 |
| 23 | DA | 2363 | C | C6-N1-C2 | 7.42 | 123.27 | 120.30 |
| 23 | BA | 530 | G | N1-C6-O6 | -7.42 | 115.45 | 119.90 |
| 23 | BA | 2713 | A | C6-C5-N7 | -7.42 | 127.11 | 132.30 |
| 23 | DA | 595 | C | C5-C6-N1 | -7.42 | 117.29 | 121.00 |
| 23 | DA | 736 | C | N1-C2-O2 | -7.42 | 114.45 | 118.90 |
| 1 | AA | 868 | C | C6-N1-C2 | -7.42 | 117.33 | 120.30 |
| 23 | DA | 1215 | G | C8-N9-C4 | 7.41 | 109.36 | 106.40 |
| 23 | BA | 130 | C | C6-N1-C2 | 7.41 | 123.26 | 120.30 |
| 23 | BA | 512 | G | N3-C4-N9 | -7.41 | 121.55 | 126.00 |
| 23 | DA | 1786 | A | C4-C5-N7 | 7.41 | 114.41 | 110.70 |
| 23 | BA | 2828 | C | C2-N3-C4 | -7.40 | 116.20 | 119.90 |
| 23 | DA | 676 | A | N1-C6-N6 | 7.40 | 123.04 | 118.60 |
| 23 | DA | 1252 | G | C8-N9-C4 | 7.40 | 109.36 | 106.40 |
| 1 | AA | 1053 | G | C8-N9-C1' | 7.40 | 136.62 | 127.00 |
| 23 | DA | 2028 | U | C2-N3-C4 | 7.39 | 131.44 | 127.00 |
| 23 | DA | 2505 | G | N9-C4-C5 | 7.39 | 108.36 | 105.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | BA | 1224 | C | N1-C2-O2 | -7.39 | 114.47 | 118.90 |
| 23 | DA | 1998 | G | C8-N9-C4 | 7.39 | 109.36 | 106.40 |
| 23 | DA | 137(B) | G | N1-C6-O6 | 7.38 | 124.33 | 119.90 |
| 23 | BA | 2634 | G | C8-N9-C4 | 7.38 | 109.35 | 106.40 |
| 23 | BA | 826 | U | C5-C6-N1 | -7.38 | 119.01 | 122.70 |
| 23 | DA | 2547 | U | C5-C6-N1 | -7.38 | 119.01 | 122.70 |
| 23 | DA | 527 | C | N3-C4-C5 | 7.38 | 124.85 | 121.90 |
| 23 | BA | 2346 | A | N1-C2-N3 | 7.37 | 132.99 | 129.30 |
| 23 | BA | 2430 | A | C5-C6-N1 | -7.37 | 114.01 | 117.70 |
| 23 | BA | 1309 | G | C8-N9-C1' | -7.37 | 117.42 | 127.00 |
| 1 | CA | 552 | U | C5-C6-N1 | -7.37 | 119.02 | 122.70 |
| 23 | DA | 298 | G | C5-N7-C8 | -7.37 | 100.62 | 104.30 |
| 23 | DA | 513 | A | C8-N9-C4 | -7.36 | 102.86 | 105.80 |
| 23 | BA | 1254 | A | N1-C2-N3 | 7.36 | 132.98 | 129.30 |
| 23 | BA | 1769 | G | C8-N9-C4 | -7.36 | 103.45 | 106.40 |
| 23 | DA | 1653 | G | N1-C6-O6 | 7.36 | 124.32 | 119.90 |
| 23 | BA | 298 | G | C4-C5-N7 | 7.36 | 113.74 | 110.80 |
| 23 | BA | 2032 | G | N7-C8-N9 | 7.36 | 116.78 | 113.10 |
| 23 | BA | 2719 | G | N3-C4-N9 | 7.35 | 130.41 | 126.00 |
| 23 | BA | 2595 | G | C5-C6-O6 | -7.34 | 124.19 | 128.60 |
| 23 | DA | 141(A) | A | N1-C6-N6 | 7.34 | 123.01 | 118.60 |
| 23 | DA | 1325 | G | N9-C4-C5 | 7.34 | 108.34 | 105.40 |
| 23 | DA | 124 | G | N7-C8-N9 | -7.34 | 109.43 | 113.10 |
| 23 | BA | 1602 | U | C4-C5-C6 | 7.34 | 124.10 | 119.70 |
| 23 | BA | 1210 | A | C2-N3-C4 | -7.33 | 106.93 | 110.60 |
| 23 | BA | 1252 | G | C8-N9-C4 | 7.33 | 109.33 | 106.40 |
| 23 | BA | 2056 | G | C4-C5-N7 | 7.33 | 113.73 | 110.80 |
| 23 | DA | 265 | A | N1-C6-N6 | 7.33 | 123.00 | 118.60 |
| 23 | DA | 1652 | A | N1-C6-N6 | 7.32 | 122.99 | 118.60 |
| 23 | BA | 968 | G | C5-C6-O6 | -7.32 | 124.21 | 128.60 |
| 23 | DA | 330 | A | C6-C5-N7 | -7.32 | 127.18 | 132.30 |
| 23 | BA | 2648 | C | C5-C6-N1 | -7.32 | 117.34 | 121.00 |
| 23 | BA | 640 | C | C5-C6-N1 | -7.32 | 117.34 | 121.00 |
| 23 | BA | 1254 | A | C6-N1-C2 | -7.32 | 114.21 | 118.60 |
| 23 | DA | 2588 | G | N1-C2-N3 | 7.32 | 128.29 | 123.90 |
| 23 | DA | 2589 | A | C8-N9-C4 | 7.32 | 108.73 | 105.80 |
| 23 | BA | 114(B) | A | N1-C6-N6 | 7.31 | 122.99 | 118.60 |
| 23 | DA | 2037 | G | N1-C6-O6 | -7.31 | 115.52 | 119.90 |
| 23 | DA | 428 | A | C2-N3-C4 | -7.30 | 106.95 | 110.60 |
| 23 | BA | 2017 | U | C4-C5-C6 | 7.30 | 124.08 | 119.70 |
| 23 | DA | 679 | C | N3-C4-C5 | 7.30 | 124.82 | 121.90 |
| 23 | DA | 857 | C | N1-C2-O2 | -7.30 | 114.52 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | DA | 1996 | C | N1-C2-O2 | -7.30 | 114.52 | 118.90 |
| 23 | DA | 800 | A | N1-C6-N6 | -7.30 | 114.22 | 118.60 |
| 23 | DA | 2055 | C | N3-C4-C5 | -7.30 | 118.98 | 121.90 |
| 23 | BA | 2502 | G | C4-C5-N7 | 7.29 | 113.72 | 110.80 |
| 23 | DA | 2464 | C | C5-C6-N1 | -7.29 | 117.35 | 121.00 |
| 1 | AA | 1053 | G | C4-N9-C1' | -7.29 | 117.03 | 126.50 |
| 23 | DA | 761 | A | C6-N1-C2 | 7.28 | 122.97 | 118.60 |
| 23 | DA | 1024 | G | C8-N9-C4 | 7.28 | 109.31 | 106.40 |
| 23 | BA | 1201 | C | C6-N1-C2 | 7.28 | 123.21 | 120.30 |
| 23 | BA | 2595 | G | C8-N9-C4 | 7.27 | 109.31 | 106.40 |
| 23 | DA | 1209 | G | N1-C6-O6 | -7.27 | 115.54 | 119.90 |
| 23 | DA | 2593 | U | C6-N1-C2 | -7.27 | 116.64 | 121.00 |
| 23 | BA | 1261 | C | C5-C6-N1 | -7.27 | 117.36 | 121.00 |
| 23 | DA | 1663 | C | C5-C6-N1 | -7.27 | 117.36 | 121.00 |
| 23 | BA | 1999 | C | C2-N1-C1' | -7.27 | 110.81 | 118.80 |
| 23 | BA | 2081 | C | C5-C6-N1 | -7.26 | 117.37 | 121.00 |
| 23 | DA | 1898 | U | N3-C4-C5 | -7.26 | 110.24 | 114.60 |
| 23 | DA | 56 | A | C2-N3-C4 | -7.26 | 106.97 | 110.60 |
| 23 | DA | 2580 | U | N3-C4-C5 | -7.25 | 110.25 | 114.60 |
| 23 | BA | 772 | C | C6-N1-C2 | 7.25 | 123.20 | 120.30 |
| 23 | DA | 945 | A | C5-C6-N6 | -7.25 | 117.90 | 123.70 |
| 23 | DA | 197 | A | N1-C6-N6 | 7.25 | 122.95 | 118.60 |
| 23 | DA | 2532 | G | C5-C6-O6 | -7.24 | 124.25 | 128.60 |
| 23 | DA | 2712 | U | N3-C2-O2 | -7.24 | 117.13 | 122.20 |
| 23 | BA | 570 | G | C5-N7-C8 | 7.24 | 107.92 | 104.30 |
| 23 | DA | 961 | C | N3-C4-C5 | -7.24 | 119.00 | 121.90 |
| 23 | BA | 676 | A | C8-N9-C4 | -7.24 | 102.91 | 105.80 |
| 23 | BA | 1698 | A | C6-C5-N7 | -7.23 | 127.24 | 132.30 |
| 23 | DA | 756 | C | C6-N1-C2 | 7.23 | 123.19 | 120.30 |
| 23 | DA | 1332 | G | N1-C2-N2 | 7.23 | 122.70 | 116.20 |
| 23 | BA | 1328 | G | C6-C5-N7 | -7.22 | 126.06 | 130.40 |
| 23 | DA | 2249 | U | C4-C5-C6 | 7.22 | 124.03 | 119.70 |
| 23 | BA | 2581 | G | N9-C4-C5 | 7.22 | 108.29 | 105.40 |
| 23 | DA | 570 | G | C8-N9-C4 | -7.22 | 103.51 | 106.40 |
| 23 | DA | 2648 | C | N3-C2-O2 | 7.22 | 126.96 | 121.90 |
| 23 | DA | 1645 | G | C5-C6-N1 | 7.22 | 115.11 | 111.50 |
| 23 | DA | 2689 | U | N1-C2-N3 | 7.22 | 119.23 | 114.90 |
| 23 | BA | 471 | A | C8-N9-C4 | 7.22 | 108.69 | 105.80 |
| 23 | BA | 2825 | U | N3-C4-C5 | 7.22 | 118.93 | 114.60 |
| 23 | DA | 1367 | A | C2-N3-C4 | -7.21 | 106.99 | 110.60 |
| 23 | DA | 2448 | A | C5-C6-N6 | -7.21 | 117.93 | 123.70 |
| 23 | BA | 783 | A | C5-C6-N1 | -7.20 | 114.10 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | BA | 2447 | G | C4-N9-C1' | -7.20 | 117.14 | 126.50 |
| 23 | BA | 2007 | C | C6-N1-C2 | 7.20 | 123.18 | 120.30 |
| 23 | DA | 2532 | G | N1-C6-O6 | 7.20 | 124.22 | 119.90 |
| 23 | DA | 737 | C | C6-N1-C2 | 7.20 | 123.18 | 120.30 |
| 23 | DA | 774 | A | N3-C4-N9 | -7.20 | 121.64 | 127.40 |
| 23 | BA | 2700 | C | C5-C6-N1 | -7.20 | 117.40 | 121.00 |
| 23 | DA | 2081 | C | C5-C6-N1 | -7.20 | 117.40 | 121.00 |
| 23 | DA | 2700 | C | C6-N1-C2 | 7.19 | 123.18 | 120.30 |
| 23 | BA | 2451 | A | N9-C4-C5 | 7.19 | 108.68 | 105.80 |
| 23 | BA | 529 | A | C5-C6-N6 | -7.19 | 117.95 | 123.70 |
| 23 | BA | 808 | G | C8-N9-C4 | 7.19 | 109.28 | 106.40 |
| 23 | DA | 979 | G | C5-C6-O6 | -7.19 | 124.29 | 128.60 |
| 23 | DA | 189 | G | N9-C4-C5 | -7.19 | 102.53 | 105.40 |
| 23 | BA | 561 | G | C8-N9-C4 | 7.18 | 109.27 | 106.40 |
| 23 | DA | 747 | U | C5-C6-N1 | -7.18 | 119.11 | 122.70 |
| 23 | DA | 2448 | A | C5-N7-C8 | -7.18 | 100.31 | 103.90 |
| 23 | DA | 1614 | A | C5-N7-C8 | -7.18 | 100.31 | 103.90 |
| 23 | DA | 83 | G | N3-C4-N9 | -7.18 | 121.69 | 126.00 |
| 23 | DA | 1332 | G | C4-C5-C6 | -7.18 | 114.50 | 118.80 |
| 23 | BA | 2515 | C | N3-C4-C5 | 7.17 | 124.77 | 121.90 |
| 23 | DA | 1363 | C | C2-N3-C4 | -7.17 | 116.31 | 119.90 |
| 23 | DA | 458 | G | N3-C4-C5 | -7.17 | 125.01 | 128.60 |
| 23 | BA | 2498 | C | C5-C6-N1 | -7.17 | 117.41 | 121.00 |
| 23 | DA | 918 | A | N1-C6-N6 | 7.17 | 122.90 | 118.60 |
| 23 | DA | 2232 | U | C5-C4-O4 | 7.17 | 130.20 | 125.90 |
| 23 | DA | 298 | G | C4-C5-N7 | 7.16 | 113.67 | 110.80 |
| 23 | DA | 1021 | A | C4-C5-N7 | 7.16 | 114.28 | 110.70 |
| 23 | DA | 2871 | C | C6-N1-C2 | 7.16 | 123.16 | 120.30 |
| 23 | DA | 397 | G | N9-C4-C5 | -7.16 | 102.54 | 105.40 |
| 23 | DA | 2681 | C | C5-C4-N4 | 7.16 | 125.21 | 120.20 |
| 23 | BA | 760 | G | C4-C5-N7 | 7.15 | 113.66 | 110.80 |
| 23 | BA | 2392 | A | C8-N9-C4 | -7.15 | 102.94 | 105.80 |
| 23 | DA | 2257 | U | N3-C2-O2 | 7.15 | 127.20 | 122.20 |
| 23 | DA | 265 | A | C4-C5-N7 | 7.15 | 114.27 | 110.70 |
| 23 | DA | 2553 | G | C5-C6-O6 | -7.15 | 124.31 | 128.60 |
| 23 | BA | 836 | G | N3-C4-C5 | 7.14 | 132.17 | 128.60 |
| 23 | DA | 444 | C | C6-N1-C2 | 7.14 | 123.16 | 120.30 |
| 1 | AA | 297 | G | C8-N9-C4 | 7.13 | 109.25 | 106.40 |
| 23 | DA | 1902 | C | N3-C4-N4 | -7.13 | 113.01 | 118.00 |
| 23 | BA | 535 | C | N3-C4-C5 | 7.13 | 124.75 | 121.90 |
| 23 | BA | 698 | C | C6-N1-C2 | 7.12 | 123.15 | 120.30 |
| 23 | BA | 1698 | A | C5-N7-C8 | -7.12 | 100.34 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|----------|-------|-------------|----------|
| 23 | BA | 746 | A | C6-N1-C2 | -7.12 | 114.33 | 118.60 |
| 23 | DA | 1795 | C | N1-C2-O2 | -7.12 | 114.63 | 118.90 |
| 23 | DA | 2231 | C | C2-N3-C4 | -7.12 | 116.34 | 119.90 |
| 23 | BA | 2614 | A | C6-N1-C2 | -7.12 | 114.33 | 118.60 |
| 23 | DA | 2553 | G | C5-C6-N1 | 7.11 | 115.06 | 111.50 |
| 1 | CA | 43 | C | C6-N1-C2 | 7.11 | 123.14 | 120.30 |
| 23 | BA | 2441 | C | N3-C2-O2 | 7.11 | 126.87 | 121.90 |
| 23 | BA | 17 | G | C5-C6-O6 | -7.10 | 124.34 | 128.60 |
| 23 | DA | 737 | C | N3-C4-C5 | 7.10 | 124.74 | 121.90 |
| 23 | BA | 1655 | A | C8-N9-C4 | 7.10 | 108.64 | 105.80 |
| 23 | DA | 557 | U | C5-C6-N1 | -7.10 | 119.15 | 122.70 |
| 23 | DA | 1570 | A | C8-N9-C4 | 7.09 | 108.64 | 105.80 |
| 23 | BA | 1325 | G | C8-N9-C4 | -7.09 | 103.56 | 106.40 |
| 23 | DA | 2619 | C | N3-C4-C5 | 7.09 | 124.74 | 121.90 |
| 1 | AA | 43 | C | C6-N1-C2 | 7.09 | 123.14 | 120.30 |
| 1 | CA | 299 | G | C5-C6-O6 | 7.09 | 132.85 | 128.60 |
| 23 | DA | 124 | G | N9-C4-C5 | -7.09 | 102.56 | 105.40 |
| 23 | BA | 563 | G | N1-C6-O6 | -7.09 | 115.65 | 119.90 |
| 23 | BA | 1982 | C | N1-C2-O2 | -7.09 | 114.65 | 118.90 |
| 23 | DA | 2050 | C | C5-C6-N1 | -7.09 | 117.46 | 121.00 |
| 35 | BM | 81 | VAL | N-CA-C | 7.08 | 130.12 | 111.00 |
| 23 | BA | 708 | C | C5-C6-N1 | -7.08 | 117.46 | 121.00 |
| 23 | BA | 1602 | U | N1-C2-N3 | 7.07 | 119.14 | 114.90 |
| 1 | AA | 756 | C | C6-N1-C2 | 7.07 | 123.13 | 120.30 |
| 23 | DA | 2032 | G | N7-C8-N9 | 7.07 | 116.64 | 113.10 |
| 23 | BA | 974(A) | G | C8-N9-C4 | -7.07 | 103.57 | 106.40 |
| 23 | DA | 577 | G | C8-N9-C4 | 7.07 | 109.23 | 106.40 |
| 23 | DA | 1791 | A | N7-C8-N9 | -7.07 | 110.27 | 113.80 |
| 23 | BA | 2571 | C | N3-C4-C5 | 7.06 | 124.73 | 121.90 |
| 23 | BA | 2249 | U | N3-C4-C5 | -7.06 | 110.36 | 114.60 |
| 23 | DA | 377 | C | C5-C6-N1 | -7.06 | 117.47 | 121.00 |
| 23 | BA | 2430 | A | N1-C2-N3 | 7.05 | 132.83 | 129.30 |
| 23 | DA | 265 | A | C6-C5-N7 | -7.05 | 127.36 | 132.30 |
| 23 | BA | 1790 | C | N3-C4-N4 | -7.05 | 113.07 | 118.00 |
| 23 | DA | 210 | C | C2-N3-C4 | -7.05 | 116.38 | 119.90 |
| 23 | DA | 2515 | C | C5-C6-N1 | -7.05 | 117.48 | 121.00 |
| 1 | AA | 576 | G | N1-C6-O6 | 7.04 | 124.13 | 119.90 |
| 23 | DA | 2518 | A | N7-C8-N9 | 7.04 | 117.32 | 113.80 |
| 23 | DA | 1620 | G | C8-N9-C4 | 7.04 | 109.22 | 106.40 |
| 23 | BA | 1902 | C | C5-C4-N4 | 7.04 | 125.12 | 120.20 |
| 23 | DA | 1602 | U | N1-C2-N3 | 7.03 | 119.12 | 114.90 |
| 23 | BA | 2587 | A | C8-N9-C4 | 7.03 | 108.61 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | BA | 1786 | A | N1-C6-N6 | 7.03 | 122.82 | 118.60 |
| 1 | CA | 892 | A | N1-C6-N6 | 7.02 | 122.81 | 118.60 |
| 23 | BA | 30 | G | C8-N9-C4 | 7.02 | 109.21 | 106.40 |
| 23 | DA | 1900 | A | N1-C6-N6 | -7.02 | 114.39 | 118.60 |
| 23 | DA | 1138 | G | N3-C4-N9 | 7.02 | 130.21 | 126.00 |
| 23 | DA | 1698 | A | N1-C2-N3 | 7.02 | 132.81 | 129.30 |
| 23 | BA | 979 | G | C5-N7-C8 | -7.01 | 100.79 | 104.30 |
| 35 | DM | 81 | VAL | N-CA-C | 7.01 | 129.94 | 111.00 |
| 23 | DA | 678 | C | C5-C6-N1 | -7.01 | 117.50 | 121.00 |
| 23 | DA | 847 | U | C5-C6-N1 | -7.01 | 119.19 | 122.70 |
| 23 | DA | 2699 | C | C5-C6-N1 | -7.01 | 117.50 | 121.00 |
| 23 | DA | 2713 | A | C4-C5-N7 | 7.01 | 114.21 | 110.70 |
| 23 | DA | 330 | A | C5-C6-N1 | -7.01 | 114.20 | 117.70 |
| 23 | DA | 1304 | C | N3-C4-C5 | 7.00 | 124.70 | 121.90 |
| 23 | DA | 2394 | C | C5-C6-N1 | -7.00 | 117.50 | 121.00 |
| 23 | DA | 2500 | U | N1-C2-O2 | -7.00 | 117.90 | 122.80 |
| 23 | BA | 2499 | C | C5-C6-N1 | -7.00 | 117.50 | 121.00 |
| 23 | DA | 270(Y) | G | C5-C6-N1 | -7.00 | 108.00 | 111.50 |
| 23 | DA | 1380 | G | C8-N9-C4 | 7.00 | 109.20 | 106.40 |
| 23 | BA | 835 | A | N7-C8-N9 | -6.99 | 110.30 | 113.80 |
| 23 | DA | 77 | C | C6-N1-C2 | 6.99 | 123.10 | 120.30 |
| 23 | BA | 976 | C | C5-C6-N1 | -6.99 | 117.51 | 121.00 |
| 23 | DA | 734 | A | C8-N9-C4 | 6.99 | 108.60 | 105.80 |
| 23 | BA | 761 | A | C4-N9-C1' | 6.99 | 138.87 | 126.30 |
| 23 | DA | 993 | G | N1-C6-O6 | -6.98 | 115.71 | 119.90 |
| 23 | BA | 2050 | C | C2-N3-C4 | -6.97 | 116.42 | 119.90 |
| 23 | DA | 2260 | C | C6-N1-C2 | 6.97 | 123.09 | 120.30 |
| 23 | BA | 2386 | C | C5-C6-N1 | -6.97 | 117.52 | 121.00 |
| 23 | DA | 933 | A | C5-N7-C8 | -6.97 | 100.42 | 103.90 |
| 23 | BA | 1493 | C | C2-N1-C1' | 6.97 | 126.46 | 118.80 |
| 23 | BA | 2232 | U | N3-C4-C5 | -6.96 | 110.42 | 114.60 |
| 23 | BA | 736 | C | C6-N1-C2 | 6.96 | 123.08 | 120.30 |
| 23 | BA | 1698 | A | C4-C5-N7 | 6.96 | 114.18 | 110.70 |
| 23 | BA | 1830 | C | N3-C2-O2 | 6.96 | 126.77 | 121.90 |
| 23 | DA | 1615 | C | C6-N1-C2 | 6.96 | 123.08 | 120.30 |
| 23 | DA | 2579 | C | C5-C6-N1 | -6.96 | 117.52 | 121.00 |
| 23 | BA | 1332 | G | C4-C5-C6 | -6.95 | 114.63 | 118.80 |
| 23 | DA | 1204 | A | C2-N3-C4 | -6.95 | 107.12 | 110.60 |
| 23 | DA | 1776 | G | C5-C6-N1 | 6.95 | 114.98 | 111.50 |
| 23 | BA | 783 | A | N7-C8-N9 | 6.95 | 117.28 | 113.80 |
| 23 | BA | 671 | C | C4-C5-C6 | 6.95 | 120.87 | 117.40 |
| 23 | BA | 1332 | G | C5-C6-N1 | -6.95 | 108.03 | 111.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | DA | 2593 | U | N1-C2-O2 | -6.95 | 117.94 | 122.80 |
| 23 | BA | 561 | G | N7-C8-N9 | -6.95 | 109.63 | 113.10 |
| 23 | BA | 1323 | U | N3-C4-O4 | 6.94 | 124.26 | 119.40 |
| 23 | BA | 2236 | C | C6-N1-C2 | 6.94 | 123.08 | 120.30 |
| 23 | BA | 2454 | G | C5-N7-C8 | 6.93 | 107.77 | 104.30 |
| 23 | DA | 1341 | U | N3-C4-C5 | -6.93 | 110.44 | 114.60 |
| 23 | DA | 2399 | G | C8-N9-C4 | 6.93 | 109.17 | 106.40 |
| 23 | BA | 2386 | C | C6-N1-C2 | 6.93 | 123.07 | 120.30 |
| 23 | BA | 761 | A | C8-N9-C1' | -6.93 | 115.22 | 127.70 |
| 23 | BA | 1332 | G | N9-C4-C5 | 6.93 | 108.17 | 105.40 |
| 23 | DA | 1764 | G | N1-C6-O6 | -6.93 | 115.74 | 119.90 |
| 23 | BA | 640 | C | N3-C4-C5 | 6.93 | 124.67 | 121.90 |
| 23 | BA | 1788 | C | C2-N3-C4 | -6.93 | 116.44 | 119.90 |
| 23 | DA | 1493 | C | C2-N1-C1' | 6.92 | 126.42 | 118.80 |
| 23 | BA | 140 | A | N1-C6-N6 | 6.92 | 122.75 | 118.60 |
| 23 | DA | 2028 | U | N1-C2-N3 | 6.91 | 119.05 | 114.90 |
| 23 | BA | 771 | G | C5-C6-O6 | -6.91 | 124.45 | 128.60 |
| 23 | DA | 1309 | G | N1-C6-O6 | 6.91 | 124.05 | 119.90 |
| 23 | DA | 2787 | C | C6-N1-C2 | -6.91 | 117.54 | 120.30 |
| 23 | DA | 2430 | A | N1-C2-N3 | 6.91 | 132.75 | 129.30 |
| 23 | BA | 309 | G | C5-C6-N1 | -6.91 | 108.05 | 111.50 |
| 23 | BA | 2035 | G | N1-C6-O6 | -6.90 | 115.76 | 119.90 |
| 23 | BA | 1786 | A | C4-C5-C6 | 6.90 | 120.45 | 117.00 |
| 34 | DL | 37 | GLY | N-CA-C | 6.90 | 130.35 | 113.10 |
| 23 | DA | 2699 | C | C2-N1-C1' | -6.90 | 111.21 | 118.80 |
| 23 | BA | 837 | C | C6-N1-C2 | -6.89 | 117.54 | 120.30 |
| 23 | BA | 976 | C | C6-N1-C2 | 6.89 | 123.06 | 120.30 |
| 23 | DA | 746 | A | C6-N1-C2 | -6.89 | 114.46 | 118.60 |
| 23 | DA | 2515 | C | C2-N3-C4 | -6.89 | 116.45 | 119.90 |
| 23 | BA | 2441 | C | N1-C2-O2 | -6.89 | 114.77 | 118.90 |
| 23 | DA | 444 | C | C5-C6-N1 | -6.89 | 117.56 | 121.00 |
| 23 | DA | 450 | G | C4-N9-C1' | 6.88 | 135.45 | 126.50 |
| 23 | BA | 2044 | C | N3-C4-C5 | 6.88 | 124.65 | 121.90 |
| 23 | BA | 650 | C | C6-N1-C2 | 6.88 | 123.05 | 120.30 |
| 23 | BA | 2287 | A | C2-N3-C4 | -6.88 | 107.16 | 110.60 |
| 23 | DA | 140 | A | N7-C8-N9 | 6.88 | 117.24 | 113.80 |
| 23 | BA | 568 | U | C5-C4-O4 | 6.87 | 130.02 | 125.90 |
| 23 | BA | 1323 | U | C4-C5-C6 | 6.87 | 123.83 | 119.70 |
| 23 | DA | 2614 | A | C6-N1-C2 | -6.87 | 114.48 | 118.60 |
| 23 | BA | 1653 | G | N1-C6-O6 | 6.87 | 124.02 | 119.90 |
| 23 | DA | 2719 | G | C4-C5-N7 | 6.87 | 113.55 | 110.80 |
| 23 | BA | 83 | G | N3-C4-N9 | -6.86 | 121.88 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | DA | 397 | G | C2-N3-C4 | -6.86 | 108.47 | 111.90 |
| 23 | DA | 582 | G | C8-N9-C4 | 6.86 | 109.14 | 106.40 |
| 23 | DA | 1790 | C | C2-N1-C1' | -6.86 | 111.25 | 118.80 |
| 23 | DA | 2049 | G | C8-N9-C4 | 6.86 | 109.14 | 106.40 |
| 23 | BA | 1225 | G | C5-C6-O6 | 6.86 | 132.72 | 128.60 |
| 23 | DA | 2447 | G | C4-N9-C1' | -6.86 | 117.59 | 126.50 |
| 23 | DA | 678 | C | C2-N3-C4 | -6.85 | 116.47 | 119.90 |
| 23 | BA | 2828 | C | C6-N1-C2 | 6.85 | 123.04 | 120.30 |
| 23 | DA | 2503 | A | C5-C6-N6 | -6.85 | 118.22 | 123.70 |
| 23 | BA | 966 | G | C8-N9-C4 | 6.85 | 109.14 | 106.40 |
| 23 | BA | 2532 | G | N1-C6-O6 | 6.85 | 124.01 | 119.90 |
| 23 | BA | 2708 | G | C8-N9-C4 | 6.85 | 109.14 | 106.40 |
| 23 | BA | 1616 | A | C6-C5-N7 | -6.85 | 127.51 | 132.30 |
| 23 | DA | 1614 | A | N1-C2-N3 | 6.85 | 132.72 | 129.30 |
| 23 | DA | 223 | A | C4-C5-C6 | 6.84 | 120.42 | 117.00 |
| 23 | BA | 265 | A | N7-C8-N9 | 6.84 | 117.22 | 113.80 |
| 23 | BA | 1021 | A | C5-N7-C8 | -6.84 | 100.48 | 103.90 |
| 23 | DA | 1030 | G | C8-N9-C4 | 6.84 | 109.13 | 106.40 |
| 23 | DA | 1332 | G | C5-C6-N1 | -6.84 | 108.08 | 111.50 |
| 23 | BA | 1123 | C | C6-N1-C2 | 6.83 | 123.03 | 120.30 |
| 23 | BA | 929 | G | C5-C6-N1 | -6.83 | 108.08 | 111.50 |
| 23 | DA | 1962 | C | C5-C6-N1 | 6.83 | 124.41 | 121.00 |
| 23 | DA | 2451 | A | N1-C6-N6 | -6.83 | 114.50 | 118.60 |
| 23 | BA | 673 | C | N3-C4-C5 | 6.83 | 124.63 | 121.90 |
| 23 | DA | 2647 | U | C6-N1-C2 | 6.83 | 125.09 | 121.00 |
| 23 | DA | 1021 | A | N3-C4-C5 | 6.82 | 131.57 | 126.80 |
| 23 | BA | 1962 | C | N3-C2-O2 | -6.82 | 117.13 | 121.90 |
| 23 | DA | 1332 | G | N9-C4-C5 | 6.82 | 108.13 | 105.40 |
| 23 | BA | 494 | G | N1-C6-O6 | 6.82 | 123.99 | 119.90 |
| 23 | DA | 2826 | A | C2-N3-C4 | -6.82 | 107.19 | 110.60 |
| 23 | BA | 1898 | U | C6-N1-C1' | 6.81 | 130.73 | 121.20 |
| 23 | DA | 2517 | C | C6-N1-C2 | 6.81 | 123.02 | 120.30 |
| 23 | BA | 840 | C | N3-C4-C5 | 6.80 | 124.62 | 121.90 |
| 23 | DA | 1022 | G | C8-N9-C4 | -6.80 | 103.68 | 106.40 |
| 23 | DA | 192 | C | C6-N1-C2 | 6.80 | 123.02 | 120.30 |
| 23 | BA | 678 | C | C6-N1-C2 | 6.80 | 123.02 | 120.30 |
| 23 | BA | 1962 | C | C5-C6-N1 | 6.80 | 124.40 | 121.00 |
| 23 | DA | 375 | C | C6-N1-C2 | 6.80 | 123.02 | 120.30 |
| 23 | DA | 1261 | C | C5-C6-N1 | -6.80 | 117.60 | 121.00 |
| 23 | DA | 2504 | U | C5-C6-N1 | -6.80 | 119.30 | 122.70 |
| 23 | BA | 535 | C | C2-N3-C4 | -6.80 | 116.50 | 119.90 |
| 23 | BA | 1675 | C | N3-C4-C5 | -6.80 | 119.18 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | DA | 2520 | C | C6-N1-C2 | 6.80 | 123.02 | 120.30 |
| 23 | BA | 1323 | U | N1-C2-N3 | 6.80 | 118.98 | 114.90 |
| 23 | DA | 65 | C | N1-C2-O2 | -6.80 | 114.82 | 118.90 |
| 23 | DA | 1349 | A | C4-C5-N7 | 6.80 | 114.10 | 110.70 |
| 23 | DA | 1201 | C | C5-C6-N1 | -6.79 | 117.60 | 121.00 |
| 23 | BA | 141(A) | A | C4-C5-N7 | 6.79 | 114.10 | 110.70 |
| 23 | BA | 527 | C | N3-C4-N4 | -6.79 | 113.25 | 118.00 |
| 23 | BA | 1982 | C | C5-C4-N4 | -6.79 | 115.44 | 120.20 |
| 23 | DA | 697 | C | C6-N1-C2 | 6.79 | 123.02 | 120.30 |
| 23 | BA | 330 | A | C4-C5-N7 | 6.78 | 114.09 | 110.70 |
| 23 | DA | 543 | C | C6-N1-C2 | 6.78 | 123.01 | 120.30 |
| 23 | DA | 807 | U | C2-N1-C1' | -6.78 | 109.56 | 117.70 |
| 23 | DA | 450 | G | C8-N9-C1' | -6.78 | 118.19 | 127.00 |
| 23 | BA | 2447 | G | C8-N9-C1' | 6.78 | 135.81 | 127.00 |
| 23 | BA | 1775 | U | C5-C6-N1 | -6.78 | 119.31 | 122.70 |
| 23 | BA | 2010 | G | C5-C6-O6 | -6.78 | 124.53 | 128.60 |
| 23 | DA | 704 | G | C8-N9-C4 | 6.78 | 109.11 | 106.40 |
| 23 | DA | 2588 | G | C2-N3-C4 | -6.77 | 108.52 | 111.90 |
| 23 | BA | 729 | G | C4-C5-N7 | 6.76 | 113.50 | 110.80 |
| 23 | DA | 530 | G | N1-C2-N2 | -6.76 | 110.11 | 116.20 |
| 23 | BA | 141(A) | A | C2-N3-C4 | -6.76 | 107.22 | 110.60 |
| 23 | BA | 327 | G | N1-C6-O6 | 6.76 | 123.96 | 119.90 |
| 23 | DA | 71 | A | C6-C5-N7 | -6.76 | 127.57 | 132.30 |
| 23 | DA | 1333 | C | C6-N1-C2 | 6.76 | 123.00 | 120.30 |
| 23 | BA | 1814 | G | C8-N9-C4 | 6.75 | 109.10 | 106.40 |
| 23 | BA | 2500 | U | C5-C6-N1 | -6.75 | 119.32 | 122.70 |
| 23 | DA | 58 | G | C8-N9-C1' | -6.75 | 118.22 | 127.00 |
| 1 | AA | 357 | G | N1-C6-O6 | 6.75 | 123.95 | 119.90 |
| 23 | DA | 655 | A | C8-N9-C4 | -6.75 | 103.10 | 105.80 |
| 23 | BA | 330 | A | C6-C5-N7 | -6.74 | 127.58 | 132.30 |
| 23 | BA | 2392 | A | N7-C8-N9 | 6.74 | 117.17 | 113.80 |
| 23 | BA | 503 | A | N1-C2-N3 | 6.74 | 132.67 | 129.30 |
| 23 | DA | 2711 | A | C2-N3-C4 | -6.74 | 107.23 | 110.60 |
| 23 | BA | 2825 | U | C4-C5-C6 | -6.73 | 115.66 | 119.70 |
| 23 | BA | 2505 | G | N9-C4-C5 | 6.73 | 108.09 | 105.40 |
| 23 | DA | 774 | A | C5-C6-N1 | -6.73 | 114.34 | 117.70 |
| 23 | BA | 2709 | G | N1-C6-O6 | 6.72 | 123.94 | 119.90 |
| 23 | DA | 240 | G | C5-C6-O6 | 6.72 | 132.63 | 128.60 |
| 23 | DA | 2699 | C | C2-N3-C4 | -6.72 | 116.54 | 119.90 |
| 23 | DA | 828 | U | N3-C4-O4 | -6.72 | 114.70 | 119.40 |
| 23 | DA | 2434 | A | N9-C4-C5 | 6.72 | 108.49 | 105.80 |
| 23 | DA | 1651 | G | C5-C6-O6 | -6.71 | 124.57 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 23 | DA | 2597 | G | C8-N9-C4 | 6.71 | 109.08 | 106.40 |
| 23 | BA | 2053 | G | N1-C6-O6 | 6.71 | 123.93 | 119.90 |
| 23 | BA | 2544 | G | C5-C6-O6 | -6.71 | 124.57 | 128.60 |
| 23 | BA | 474 | G | N1-C6-O6 | -6.71 | 115.87 | 119.90 |
| 23 | DA | 2430 | A | C5-N7-C8 | -6.71 | 100.55 | 103.90 |
| 23 | BA | 267 | C | C6-N1-C2 | 6.71 | 122.98 | 120.30 |
| 23 | BA | 2489 | G | N1-C6-O6 | 6.71 | 123.92 | 119.90 |
| 23 | BA | 444 | C | N1-C2-O2 | -6.70 | 114.88 | 118.90 |
| 23 | DA | 1304 | C | C5-C6-N1 | -6.70 | 117.65 | 121.00 |
| 23 | DA | 2699 | C | N1-C2-O2 | -6.70 | 114.88 | 118.90 |
| 1 | AA | 822 | C | C6-N1-C2 | 6.70 | 122.98 | 120.30 |
| 23 | BA | 1200 | C | N1-C2-O2 | -6.70 | 114.88 | 118.90 |
| 23 | DA | 2248 | C | N3-C4-C5 | 6.70 | 124.58 | 121.90 |
| 23 | DA | 1815 | A | N1-C2-N3 | 6.70 | 132.65 | 129.30 |
| 23 | DA | 2438 | U | C5-C6-N1 | -6.70 | 119.35 | 122.70 |
| 23 | BA | 2053 | G | C5-C6-O6 | -6.69 | 124.58 | 128.60 |
| 23 | DA | 1653 | G | C8-N9-C4 | 6.69 | 109.08 | 106.40 |
| 23 | BA | 187 | G | N3-C4-N9 | 6.69 | 130.01 | 126.00 |
| 23 | BA | 2555 | U | C5-C4-O4 | 6.69 | 129.91 | 125.90 |
| 23 | DA | 1771 | C | N1-C2-O2 | -6.69 | 114.89 | 118.90 |
| 23 | DA | 2065 | C | C5-C4-N4 | -6.69 | 115.52 | 120.20 |
| 23 | BA | 265 | A | C5-C6-N1 | -6.69 | 114.36 | 117.70 |
| 1 | AA | 285 | G | C8-N9-C4 | 6.68 | 109.07 | 106.40 |
| 23 | DA | 1624 | G | C8-N9-C4 | 6.68 | 109.07 | 106.40 |
| 23 | BA | 808 | G | N7-C8-N9 | -6.68 | 109.76 | 113.10 |
| 23 | BA | 1652 | A | N1-C6-N6 | 6.68 | 122.61 | 118.60 |
| 23 | DA | 18 | C | C6-N1-C2 | 6.68 | 122.97 | 120.30 |
| 23 | DA | 1788 | C | N3-C4-C5 | 6.68 | 124.57 | 121.90 |
| 23 | DA | 2227 | A | C2-N3-C4 | -6.68 | 107.26 | 110.60 |
| 23 | BA | 971 | C | N1-C2-O2 | -6.68 | 114.89 | 118.90 |
| 1 | CA | 299 | G | N9-C4-C5 | 6.67 | 108.07 | 105.40 |
| 23 | BA | 248 | G | C4-C5-N7 | 6.67 | 113.47 | 110.80 |
| 23 | BA | 265 | A | N1-C6-N6 | 6.67 | 122.60 | 118.60 |
| 23 | DA | 1651 | G | N1-C6-O6 | 6.67 | 123.90 | 119.90 |
| 23 | DA | 2488 | A | C5-C6-N1 | 6.67 | 121.03 | 117.70 |
| 23 | DA | 2638 | G | N1-C6-O6 | -6.67 | 115.90 | 119.90 |
| 23 | BA | 659 | C | C6-N1-C2 | 6.67 | 122.97 | 120.30 |
| 23 | DA | 2699 | C | N3-C4-C5 | 6.66 | 124.57 | 121.90 |
| 23 | BA | 1648 | C | C2-N3-C4 | -6.66 | 116.57 | 119.90 |
| 23 | DA | 1253 | A | C4-C5-C6 | -6.66 | 113.67 | 117.00 |
| 23 | DA | 594 | U | C5-C4-O4 | 6.66 | 129.90 | 125.90 |
| 23 | DA | 657 | U | C5-C6-N1 | -6.66 | 119.37 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | BA | 129 | C | C5-C6-N1 | -6.66 | 117.67 | 121.00 |
| 23 | BA | 697 | C | C6-N1-C2 | 6.65 | 122.96 | 120.30 |
| 23 | BA | 949 | C | N3-C4-C5 | 6.65 | 124.56 | 121.90 |
| 23 | BA | 2681 | C | C5-C4-N4 | 6.65 | 124.86 | 120.20 |
| 23 | DA | 1210 | A | C2-N3-C4 | -6.65 | 107.28 | 110.60 |
| 23 | DA | 2383 | G | C6-C5-N7 | -6.65 | 126.41 | 130.40 |
| 23 | DA | 129 | C | C5-C6-N1 | -6.65 | 117.68 | 121.00 |
| 23 | DA | 1778 | U | C5-C6-N1 | -6.65 | 119.38 | 122.70 |
| 23 | DA | 2249 | U | C2-N3-C4 | 6.65 | 130.99 | 127.00 |
| 23 | DA | 36 | G | C4-C5-N7 | -6.64 | 108.14 | 110.80 |
| 23 | DA | 667 | U | C4-C5-C6 | 6.64 | 123.69 | 119.70 |
| 23 | DA | 1962 | C | C2-N3-C4 | 6.64 | 123.22 | 119.90 |
| 23 | BA | 587 | C | N3-C4-C5 | -6.64 | 119.24 | 121.90 |
| 23 | BA | 2271 | G | N3-C4-N9 | 6.64 | 129.98 | 126.00 |
| 23 | DA | 141(A) | A | C2-N3-C4 | -6.64 | 107.28 | 110.60 |
| 23 | BA | 602 | G | N7-C8-N9 | -6.64 | 109.78 | 113.10 |
| 23 | DA | 1572 | A | N7-C8-N9 | -6.64 | 110.48 | 113.80 |
| 23 | DA | 2397 | G | C8-N9-C4 | -6.64 | 103.75 | 106.40 |
| 23 | DA | 2706 | G | N1-C6-O6 | 6.63 | 123.88 | 119.90 |
| 1 | CA | 896 | C | C6-N1-C2 | 6.63 | 122.95 | 120.30 |
| 1 | AA | 576 | G | C6-C5-N7 | -6.63 | 126.42 | 130.40 |
| 23 | BA | 2036 | C | C6-N1-C2 | -6.63 | 117.65 | 120.30 |
| 23 | DA | 807 | U | C6-N1-C1' | 6.63 | 130.48 | 121.20 |
| 23 | BA | 1615 | C | C6-N1-C2 | 6.62 | 122.95 | 120.30 |
| 23 | BA | 1634 | A | N1-C6-N6 | -6.62 | 114.63 | 118.60 |
| 23 | DA | 1962 | C | N1-C2-N3 | -6.62 | 114.56 | 119.20 |
| 23 | DA | 530 | G | N7-C8-N9 | 6.62 | 116.41 | 113.10 |
| 23 | DA | 1309 | G | C8-N9-C1' | -6.62 | 118.40 | 127.00 |
| 23 | DA | 1999 | C | C2-N1-C1' | -6.62 | 111.52 | 118.80 |
| 23 | DA | 2514 | U | C5-C6-N1 | -6.62 | 119.39 | 122.70 |
| 23 | BA | 807 | U | C6-N1-C1' | 6.61 | 130.46 | 121.20 |
| 23 | BA | 1190 | G | C4-C5-N7 | 6.61 | 113.44 | 110.80 |
| 23 | BA | 2593 | U | C6-N1-C2 | -6.61 | 117.03 | 121.00 |
| 23 | BA | 782 | A | C8-N9-C4 | 6.61 | 108.44 | 105.80 |
| 23 | DA | 1775 | U | C5-C6-N1 | -6.61 | 119.40 | 122.70 |
| 23 | BA | 194 | G | C8-N9-C4 | 6.61 | 109.04 | 106.40 |
| 23 | BA | 650 | C | C5-C6-N1 | -6.61 | 117.70 | 121.00 |
| 23 | DA | 239 | U | C5-C6-N1 | -6.61 | 119.40 | 122.70 |
| 23 | DA | 114(B) | A | C4-C5-C6 | 6.61 | 120.30 | 117.00 |
| 23 | DA | 2689 | U | C5-C6-N1 | -6.60 | 119.40 | 122.70 |
| 23 | DA | 2709 | G | C8-N9-C4 | 6.60 | 109.04 | 106.40 |
| 23 | BA | 2544 | G | C4-C5-N7 | 6.60 | 113.44 | 110.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 23 | BA | 497 | A | C8-N9-C4 | 6.59 | 108.44 | 105.80 |
| 23 | DA | 1417 | C | C5-C6-N1 | -6.59 | 117.70 | 121.00 |
| 23 | BA | 2688 | U | C5-C4-O4 | 6.59 | 129.86 | 125.90 |
| 1 | AA | 328 | C | C6-N1-C2 | 6.59 | 122.94 | 120.30 |
| 1 | AA | 691 | G | N3-C4-N9 | 6.59 | 129.96 | 126.00 |
| 23 | DA | 580 | C | N3-C4-C5 | 6.59 | 124.54 | 121.90 |
| 23 | DA | 1443 | G | N1-C6-O6 | 6.59 | 123.85 | 119.90 |
| 23 | BA | 2464 | C | C6-N1-C2 | 6.59 | 122.94 | 120.30 |
| 23 | DA | 2830 | G | C6-C5-N7 | -6.59 | 126.45 | 130.40 |
| 23 | BA | 2032 | G | C4-C5-N7 | 6.59 | 113.44 | 110.80 |
| 23 | DA | 2346 | A | N1-C2-N3 | 6.58 | 132.59 | 129.30 |
| 23 | BA | 1680 | U | C5-C4-O4 | 6.58 | 129.85 | 125.90 |
| 23 | BA | 774 | A | N1-C6-N6 | 6.57 | 122.54 | 118.60 |
| 23 | BA | 814 | C | C5-C6-N1 | -6.57 | 117.71 | 121.00 |
| 23 | BA | 933 | A | C2-N3-C4 | -6.57 | 107.31 | 110.60 |
| 23 | BA | 2037 | G | N1-C2-N3 | 6.57 | 127.84 | 123.90 |
| 23 | DA | 2271 | G | N3-C4-N9 | 6.57 | 129.94 | 126.00 |
| 23 | BA | 2830 | G | N1-C6-O6 | 6.57 | 123.84 | 119.90 |
| 23 | DA | 2591 | C | C6-N1-C2 | 6.57 | 122.93 | 120.30 |
| 23 | DA | 2233 | U | C2-N3-C4 | -6.57 | 123.06 | 127.00 |
| 23 | DA | 2715 | C | N3-C4-C5 | 6.57 | 124.53 | 121.90 |
| 1 | AA | 264 | U | N3-C2-O2 | -6.57 | 117.60 | 122.20 |
| 23 | DA | 66 | C | C6-N1-C2 | 6.56 | 122.92 | 120.30 |
| 23 | BA | 2828 | C | N3-C4-C5 | 6.56 | 124.53 | 121.90 |
| 23 | DA | 458 | G | C5-C6-N1 | 6.56 | 114.78 | 111.50 |
| 23 | DA | 71 | A | N7-C8-N9 | 6.56 | 117.08 | 113.80 |
| 23 | DA | 1644 | C | N3-C2-O2 | -6.56 | 117.31 | 121.90 |
| 23 | DA | 937 | U | C6-N1-C2 | 6.55 | 124.93 | 121.00 |
| 23 | BA | 2438 | U | C5-C6-N1 | -6.55 | 119.42 | 122.70 |
| 23 | BA | 2084 | C | C2-N3-C4 | -6.55 | 116.63 | 119.90 |
| 23 | BA | 671 | C | N3-C4-C5 | -6.54 | 119.28 | 121.90 |
| 23 | BA | 1616 | A | N1-C6-N6 | 6.54 | 122.53 | 118.60 |
| 23 | DA | 397 | G | C5-C6-O6 | -6.54 | 124.68 | 128.60 |
| 23 | DA | 2330 | G | N9-C4-C5 | -6.54 | 102.78 | 105.40 |
| 23 | DA | 2072 | G | N3-C4-C5 | 6.54 | 131.87 | 128.60 |
| 23 | DA | 112 | U | C5-C6-N1 | -6.53 | 119.43 | 122.70 |
| 23 | BA | 1976 | U | N1-C2-N3 | 6.53 | 118.82 | 114.90 |
| 23 | DA | 667 | U | C5-C6-N1 | -6.53 | 119.44 | 122.70 |
| 23 | DA | 2007 | C | C5-C6-N1 | -6.53 | 117.74 | 121.00 |
| 23 | BA | 1815 | A | N1-C2-N3 | 6.52 | 132.56 | 129.30 |
| 1 | CA | 1519 | A | N1-C2-N3 | 6.52 | 132.56 | 129.30 |
| 23 | BA | 1969 | A | C8-N9-C4 | -6.52 | 103.19 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | DA | 2394 | C | C6-N1-C2 | 6.52 | 122.91 | 120.30 |
| 23 | DA | 1996 | C | C6-N1-C2 | 6.51 | 122.91 | 120.30 |
| 23 | DA | 933 | A | C6-C5-N7 | -6.51 | 127.74 | 132.30 |
| 23 | DA | 1783 | A | C8-N9-C4 | -6.51 | 103.20 | 105.80 |
| 23 | BA | 1698 | A | C2-N3-C4 | -6.51 | 107.35 | 110.60 |
| 23 | BA | 2378 | A | C8-N9-C4 | 6.51 | 108.40 | 105.80 |
| 23 | DA | 1027 | A | C8-N9-C4 | 6.51 | 108.40 | 105.80 |
| 23 | BA | 933 | A | N7-C8-N9 | 6.50 | 117.05 | 113.80 |
| 1 | CA | 1521 | G | C8-N9-C4 | -6.50 | 103.80 | 106.40 |
| 23 | DA | 114(B) | A | C5-N7-C8 | -6.50 | 100.65 | 103.90 |
| 23 | BA | 789 | A | C5-C6-N6 | -6.50 | 118.50 | 123.70 |
| 23 | BA | 1204 | A | C8-N9-C4 | -6.50 | 103.20 | 105.80 |
| 23 | DA | 1798 | U | N3-C4-C5 | 6.50 | 118.50 | 114.60 |
| 1 | CA | 768 | A | C8-N9-C4 | 6.50 | 108.40 | 105.80 |
| 23 | DA | 768 | G | N3-C4-N9 | 6.49 | 129.89 | 126.00 |
| 1 | AA | 529 | G | N1-C6-O6 | 6.49 | 123.79 | 119.90 |
| 1 | AA | 815 | A | N1-C6-N6 | -6.49 | 114.71 | 118.60 |
| 23 | DA | 2249 | U | N3-C4-O4 | 6.49 | 123.94 | 119.40 |
| 23 | DA | 2553 | G | N9-C4-C5 | -6.49 | 102.80 | 105.40 |
| 23 | BA | 561 | G | C5-N7-C8 | 6.49 | 107.54 | 104.30 |
| 23 | BA | 736 | C | N3-C4-C5 | 6.48 | 124.49 | 121.90 |
| 1 | AA | 1523 | G | N1-C6-O6 | 6.48 | 123.79 | 119.90 |
| 23 | DA | 935 | C | C6-N1-C2 | 6.48 | 122.89 | 120.30 |
| 23 | BA | 104 | U | C5-C6-N1 | -6.48 | 119.46 | 122.70 |
| 23 | BA | 1304 | C | C6-N1-C2 | 6.48 | 122.89 | 120.30 |
| 23 | BA | 2063 | C | N3-C4-C5 | -6.48 | 119.31 | 121.90 |
| 23 | BA | 2626 | C | N3-C4-C5 | 6.48 | 124.49 | 121.90 |
| 23 | DA | 795 | C | N1-C2-O2 | -6.48 | 115.01 | 118.90 |
| 23 | DA | 1322 | A | N9-C4-C5 | 6.48 | 108.39 | 105.80 |
| 23 | BA | 1329 | U | C5-C6-N1 | -6.47 | 119.46 | 122.70 |
| 23 | BA | 2647 | U | C5-C6-N1 | -6.47 | 119.46 | 122.70 |
| 24 | BB | 98 | G | C8-N9-C1' | -6.47 | 118.58 | 127.00 |
| 23 | DA | 1935 | G | N3-C4-C5 | 6.47 | 131.84 | 128.60 |
| 23 | BA | 2045 | C | C6-N1-C2 | 6.47 | 122.89 | 120.30 |
| 23 | BA | 2540 | C | C2-N3-C4 | -6.47 | 116.67 | 119.90 |
| 23 | DA | 2231 | C | C5-C6-N1 | -6.47 | 117.77 | 121.00 |
| 23 | DA | 204 | A | C2-N3-C4 | -6.46 | 107.37 | 110.60 |
| 23 | DA | 765 | G | C8-N9-C4 | 6.46 | 108.99 | 106.40 |
| 23 | BA | 265 | A | C4-C5-N7 | 6.46 | 113.93 | 110.70 |
| 23 | BA | 1190 | G | C5-C6-O6 | -6.46 | 124.72 | 128.60 |
| 23 | DA | 736 | C | N3-C2-O2 | 6.46 | 126.42 | 121.90 |
| 23 | DA | 1323 | U | N3-C4-C5 | -6.46 | 110.72 | 114.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | DA | 2432 | A | C5-N7-C8 | -6.46 | 100.67 | 103.90 |
| 23 | DA | 330 | A | C4-C5-N7 | 6.46 | 113.93 | 110.70 |
| 23 | DA | 1674 | G | C8-N9-C4 | 6.46 | 108.98 | 106.40 |
| 23 | DA | 2688 | U | N3-C2-O2 | -6.45 | 117.68 | 122.20 |
| 23 | BA | 512 | G | C8-N9-C1' | 6.45 | 135.38 | 127.00 |
| 23 | BA | 729 | G | C6-C5-N7 | -6.45 | 126.53 | 130.40 |
| 23 | BA | 1241 | A | C5-C6-N1 | -6.45 | 114.47 | 117.70 |
| 23 | BA | 1499 | C | C6-N1-C2 | 6.45 | 122.88 | 120.30 |
| 23 | BA | 2707 | G | C8-N9-C4 | 6.45 | 108.98 | 106.40 |
| 23 | DA | 2581 | G | N3-C4-N9 | -6.45 | 122.13 | 126.00 |
| 23 | DA | 815 | C | C6-N1-C2 | 6.45 | 122.88 | 120.30 |
| 23 | DA | 1786 | A | N1-C6-N6 | 6.44 | 122.47 | 118.60 |
| 1 | AA | 398 | C | C6-N1-C2 | 6.44 | 122.88 | 120.30 |
| 23 | BA | 1352 | U | C5-C6-N1 | -6.44 | 119.48 | 122.70 |
| 23 | BA | 2596 | U | N3-C4-O4 | -6.43 | 114.90 | 119.40 |
| 23 | DA | 802 | A | C8-N9-C1' | -6.43 | 116.12 | 127.70 |
| 23 | DA | 1444 | G | C8-N9-C4 | 6.43 | 108.97 | 106.40 |
| 23 | DA | 1310 | G | N1-C6-O6 | 6.43 | 123.76 | 119.90 |
| 23 | DA | 811 | U | C5-C6-N1 | -6.42 | 119.49 | 122.70 |
| 23 | BA | 2359 | C | C6-N1-C2 | 6.42 | 122.87 | 120.30 |
| 23 | DA | 2685 | G | N1-C6-O6 | 6.42 | 123.75 | 119.90 |
| 23 | DA | 1348 | G | C5-C6-O6 | -6.42 | 124.75 | 128.60 |
| 23 | DA | 434 | U | N3-C2-O2 | 6.42 | 126.69 | 122.20 |
| 23 | DA | 1355 | G | C5-C6-N1 | 6.42 | 114.71 | 111.50 |
| 23 | DA | 2206 | C | N3-C4-N4 | -6.42 | 113.51 | 118.00 |
| 23 | DA | 1257 | C | C4-C5-C6 | 6.42 | 120.61 | 117.40 |
| 23 | DA | 1493 | C | C5-C6-N1 | 6.42 | 124.21 | 121.00 |
| 23 | BA | 66 | C | C6-N1-C2 | 6.41 | 122.87 | 120.30 |
| 23 | BA | 1602 | U | C5-C6-N1 | 6.41 | 125.91 | 122.70 |
| 1 | CA | 1524 | C | N3-C4-C5 | 6.41 | 124.47 | 121.90 |
| 23 | DA | 2386 | C | C5-C6-N1 | -6.41 | 117.79 | 121.00 |
| 23 | DA | 1309 | G | N9-C4-C5 | -6.41 | 102.83 | 105.40 |
| 23 | DA | 2197 | U | C6-N1-C2 | 6.41 | 124.85 | 121.00 |
| 23 | DA | 1190 | G | C5-C6-O6 | -6.41 | 124.75 | 128.60 |
| 23 | DA | 1315 | C | C6-N1-C2 | -6.41 | 117.74 | 120.30 |
| 23 | DA | 1258 | C | C5-C6-N1 | -6.41 | 117.80 | 121.00 |
| 1 | AA | 903 | G | N7-C8-N9 | -6.40 | 109.90 | 113.10 |
| 1 | AA | 896 | C | C5-C6-N1 | -6.40 | 117.80 | 121.00 |
| 23 | DA | 1342 | A | N1-C6-N6 | 6.40 | 122.44 | 118.60 |
| 23 | BA | 2053 | G | C4-C5-N7 | 6.40 | 113.36 | 110.80 |
| 23 | DA | 1021 | A | N7-C8-N9 | 6.40 | 117.00 | 113.80 |
| 23 | BA | 809 | G | N1-C6-O6 | 6.39 | 123.73 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 23 | DA | 1824 | G | C6-N1-C2 | -6.39 | 121.27 | 125.10 |
| 23 | BA | 956 | G | C5-C6-N1 | -6.39 | 108.31 | 111.50 |
| 23 | DA | 1022 | G | N9-C4-C5 | 6.39 | 107.95 | 105.40 |
| 23 | BA | 728 | G | C8-N9-C4 | 6.39 | 108.95 | 106.40 |
| 23 | BA | 1443 | G | N1-C6-O6 | 6.39 | 123.73 | 119.90 |
| 23 | BA | 1804 | C | C5-C6-N1 | -6.39 | 117.81 | 121.00 |
| 23 | BA | 951 | C | C6-N1-C2 | 6.38 | 122.85 | 120.30 |
| 23 | BA | 1983 | C | N3-C4-C5 | 6.38 | 124.45 | 121.90 |
| 23 | DA | 2618 | G | N1-C2-N3 | 6.38 | 127.73 | 123.90 |
| 23 | DA | 1322 | A | N1-C2-N3 | 6.38 | 132.49 | 129.30 |
| 23 | DA | 1655 | A | C8-N9-C4 | 6.38 | 108.35 | 105.80 |
| 23 | BA | 789 | A | N1-C6-N6 | 6.38 | 122.43 | 118.60 |
| 23 | DA | 265 | A | N3-C4-C5 | 6.38 | 131.26 | 126.80 |
| 23 | DA | 1342 | A | C5-C6-N6 | -6.38 | 118.60 | 123.70 |
| 23 | DA | 2502 | G | N3-C4-N9 | 6.38 | 129.83 | 126.00 |
| 23 | BA | 2532 | G | C6-C5-N7 | -6.38 | 126.57 | 130.40 |
| 23 | BA | 36 | G | N7-C8-N9 | -6.38 | 109.91 | 113.10 |
| 23 | DA | 1779 | U | C6-N1-C2 | 6.38 | 124.83 | 121.00 |
| 23 | BA | 1355 | G | N1-C6-O6 | -6.37 | 116.08 | 119.90 |
| 23 | DA | 294 | A | C8-N9-C4 | 6.37 | 108.35 | 105.80 |
| 23 | DA | 2397 | G | N7-C8-N9 | 6.37 | 116.29 | 113.10 |
| 23 | BA | 840 | C | C5-C6-N1 | -6.37 | 117.81 | 121.00 |
| 23 | DA | 586 | A | N7-C8-N9 | -6.37 | 110.61 | 113.80 |
| 23 | BA | 2502 | G | C5-N7-C8 | -6.37 | 101.11 | 104.30 |
| 23 | DA | 330 | A | C5-N7-C8 | -6.37 | 100.72 | 103.90 |
| 23 | BA | 1605 | C | N1-C2-O2 | -6.37 | 115.08 | 118.90 |
| 23 | DA | 2010 | G | N1-C2-N3 | 6.37 | 127.72 | 123.90 |
| 1 | AA | 299 | G | C5-C6-O6 | 6.36 | 132.42 | 128.60 |
| 23 | DA | 1786 | A | C5-C6-N1 | -6.36 | 114.52 | 117.70 |
| 23 | DA | 1998 | G | N7-C8-N9 | -6.36 | 109.92 | 113.10 |
| 23 | DA | 1996 | C | N3-C2-O2 | 6.36 | 126.35 | 121.90 |
| 23 | DA | 2706 | G | C4-C5-N7 | 6.36 | 113.34 | 110.80 |
| 23 | BA | 602 | G | C8-N9-C4 | 6.36 | 108.94 | 106.40 |
| 23 | BA | 692 | C | N3-C4-C5 | 6.36 | 124.44 | 121.90 |
| 23 | BA | 949 | C | C6-N1-C2 | 6.36 | 122.84 | 120.30 |
| 23 | DA | 2502 | G | C6-C5-N7 | -6.36 | 126.59 | 130.40 |
| 25 | DC | 177 | LEU | CA-CB-CG | -6.36 | 100.68 | 115.30 |
| 23 | DA | 2454 | G | C8-N9-C4 | 6.35 | 108.94 | 106.40 |
| 23 | BA | 2043 | C | C5-C6-N1 | -6.35 | 117.82 | 121.00 |
| 23 | BA | 1128 | A | N7-C8-N9 | -6.34 | 110.63 | 113.80 |
| 23 | DA | 584 | C | N3-C4-C5 | 6.34 | 124.44 | 121.90 |
| 23 | DA | 1351 | C | C5-C6-N1 | -6.34 | 117.83 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | DA | 1633 | G | C6-C5-N7 | -6.34 | 126.60 | 130.40 |
| 1 | AA | 357 | G | C5-C6-N1 | -6.34 | 108.33 | 111.50 |
| 23 | DA | 746 | A | N1-C2-N3 | 6.34 | 132.47 | 129.30 |
| 23 | BA | 2387 | U | C5-C6-N1 | -6.33 | 119.53 | 122.70 |
| 23 | DA | 1144 | G | C4-C5-N7 | 6.33 | 113.33 | 110.80 |
| 23 | DA | 2518 | A | C2-N3-C4 | -6.33 | 107.43 | 110.60 |
| 23 | DA | 657 | U | N3-C2-O2 | -6.33 | 117.77 | 122.20 |
| 23 | DA | 2087 | G | C8-N9-C4 | 6.33 | 108.93 | 106.40 |
| 23 | DA | 2465 | C | N3-C4-C5 | 6.33 | 124.43 | 121.90 |
| 23 | DA | 2688 | U | N3-C4-O4 | -6.33 | 114.97 | 119.40 |
| 23 | DA | 2719 | G | N3-C4-N9 | 6.33 | 129.80 | 126.00 |
| 23 | DA | 1200 | C | N1-C2-O2 | -6.33 | 115.10 | 118.90 |
| 23 | DA | 2507 | C | C5-C6-N1 | -6.33 | 117.84 | 121.00 |
| 23 | BA | 783 | A | C4-C5-N7 | 6.33 | 113.86 | 110.70 |
| 23 | DA | 2448 | A | C4-C5-N7 | 6.33 | 113.86 | 110.70 |
| 23 | BA | 1798 | U | C5-C6-N1 | -6.32 | 119.54 | 122.70 |
| 23 | DA | 2250 | G | C8-N9-C4 | -6.32 | 103.87 | 106.40 |
| 23 | BA | 240 | G | C5-C6-N1 | -6.32 | 108.34 | 111.50 |
| 23 | BA | 691 | C | C5-C6-N1 | -6.32 | 117.84 | 121.00 |
| 23 | BA | 1138 | G | N3-C4-N9 | 6.32 | 129.79 | 126.00 |
| 23 | BA | 2555 | U | N1-C2-N3 | 6.32 | 118.69 | 114.90 |
| 23 | DA | 2043 | C | C5-C6-N1 | -6.32 | 117.84 | 121.00 |
| 23 | DA | 2332 | U | C5-C6-N1 | -6.32 | 119.54 | 122.70 |
| 23 | DA | 784 | A | C5-C6-N6 | 6.31 | 128.75 | 123.70 |
| 23 | DA | 1021 | A | C5-C6-N1 | -6.31 | 114.54 | 117.70 |
| 23 | BA | 2521 | C | C6-N1-C2 | 6.31 | 122.82 | 120.30 |
| 23 | DA | 2374 | C | C6-N1-C2 | 6.31 | 122.83 | 120.30 |
| 23 | BA | 124 | G | C8-N9-C4 | 6.31 | 108.92 | 106.40 |
| 23 | BA | 2742 | C | C5-C6-N1 | -6.31 | 117.85 | 121.00 |
| 23 | DA | 768 | G | C8-N9-C4 | 6.31 | 108.92 | 106.40 |
| 23 | BA | 2625 | G | C8-N9-C4 | 6.30 | 108.92 | 106.40 |
| 23 | DA | 1302 | A | N9-C4-C5 | 6.30 | 108.32 | 105.80 |
| 23 | BA | 2066 | C | C6-N1-C2 | 6.30 | 122.82 | 120.30 |
| 23 | DA | 2638 | G | N9-C4-C5 | 6.29 | 107.92 | 105.40 |
| 23 | BA | 298 | G | N7-C8-N9 | 6.29 | 116.25 | 113.10 |
| 23 | BA | 686 | G | C5-C6-O6 | -6.29 | 124.83 | 128.60 |
| 23 | DA | 2538 | C | C5-C6-N1 | -6.29 | 117.86 | 121.00 |
| 23 | BA | 298 | G | C5-C6-O6 | -6.29 | 124.83 | 128.60 |
| 23 | BA | 704 | G | C4-C5-N7 | 6.29 | 113.31 | 110.80 |
| 23 | BA | 1663 | C | C6-N1-C2 | 6.28 | 122.81 | 120.30 |
| 23 | DA | 1834 | U | C2-N1-C1' | 6.28 | 125.24 | 117.70 |
| 23 | DA | 2010 | G | C4-C5-N7 | 6.28 | 113.31 | 110.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | DA | 2056 | G | N9-C4-C5 | -6.28 | 102.89 | 105.40 |
| 23 | DA | 2206 | C | N3-C4-C5 | 6.28 | 124.41 | 121.90 |
| 23 | BA | 2501 | C | N3-C4-C5 | 6.28 | 124.41 | 121.90 |
| 23 | DA | 2227 | A | C5-C6-N1 | -6.28 | 114.56 | 117.70 |
| 23 | BA | 2206 | C | N3-C4-C5 | 6.28 | 124.41 | 121.90 |
| 23 | DA | 2080 | G | N1-C2-N3 | 6.28 | 127.67 | 123.90 |
| 23 | BA | 560 | C | C5-C6-N1 | -6.27 | 117.86 | 121.00 |
| 23 | DA | 798 | G | N1-C2-N3 | 6.27 | 127.66 | 123.90 |
| 24 | BB | 84 | C | C6-N1-C2 | -6.27 | 117.79 | 120.30 |
| 23 | DA | 774 | A | N7-C8-N9 | 6.27 | 116.94 | 113.80 |
| 23 | DA | 1832 | C | C2-N3-C4 | -6.27 | 116.77 | 119.90 |
| 1 | AA | 297 | G | N7-C8-N9 | -6.27 | 109.97 | 113.10 |
| 23 | BA | 1188 | U | N3-C2-O2 | -6.27 | 117.81 | 122.20 |
| 23 | DA | 748 | G | C5-C6-N1 | 6.27 | 114.63 | 111.50 |
| 23 | DA | 2091 | U | C5-C6-N1 | -6.27 | 119.57 | 122.70 |
| 23 | BA | 1899 | G | C5-C6-O6 | 6.27 | 132.36 | 128.60 |
| 23 | DA | 1802 | A | N1-C2-N3 | 6.27 | 132.43 | 129.30 |
| 23 | DA | 2427 | C | N3-C4-C5 | -6.26 | 119.39 | 121.90 |
| 23 | BA | 1964 | G | N3-C4-N9 | 6.26 | 129.76 | 126.00 |
| 23 | BA | 933 | A | C5-N7-C8 | -6.26 | 100.77 | 103.90 |
| 23 | BA | 2839 | G | N1-C6-O6 | 6.26 | 123.66 | 119.90 |
| 23 | DA | 750 | A | C5-N7-C8 | -6.26 | 100.77 | 103.90 |
| 23 | DA | 2462 | U | C6-N1-C2 | 6.26 | 124.76 | 121.00 |
| 23 | BA | 596 | G | N1-C6-O6 | 6.26 | 123.66 | 119.90 |
| 23 | DA | 2066 | C | C2-N3-C4 | -6.26 | 116.77 | 119.90 |
| 23 | DA | 2447 | G | C8-N9-C1' | 6.26 | 135.14 | 127.00 |
| 1 | AA | 691 | G | N9-C4-C5 | -6.26 | 102.90 | 105.40 |
| 23 | BA | 1323 | U | N3-C4-C5 | -6.26 | 110.85 | 114.60 |
| 23 | DA | 2501 | C | N3-C4-C5 | 6.26 | 124.40 | 121.90 |
| 23 | DA | 2638 | G | C5-C6-O6 | 6.26 | 132.35 | 128.60 |
| 23 | BA | 1780 | A | C2-N3-C4 | -6.25 | 107.47 | 110.60 |
| 23 | DA | 2061 | G | C4-C5-C6 | 6.25 | 122.55 | 118.80 |
| 23 | BA | 1935 | G | N3-C4-C5 | 6.25 | 131.73 | 128.60 |
| 23 | DA | 283 | A | N1-C6-N6 | -6.25 | 114.85 | 118.60 |
| 23 | DA | 1983 | C | C6-N1-C2 | 6.25 | 122.80 | 120.30 |
| 23 | BA | 2515 | C | C6-N1-C2 | 6.25 | 122.80 | 120.30 |
| 23 | BA | 802 | A | C8-N9-C1' | -6.25 | 116.45 | 127.70 |
| 23 | BA | 265 | A | C6-C5-N7 | -6.24 | 127.93 | 132.30 |
| 23 | BA | 444 | C | C2-N1-C1' | -6.24 | 111.93 | 118.80 |
| 23 | DA | 798 | G | C6-N1-C2 | -6.24 | 121.35 | 125.10 |
| 23 | DA | 98 | G | N1-C6-O6 | 6.24 | 123.64 | 119.90 |
| 23 | DA | 1824 | G | C5-C6-N1 | 6.24 | 114.62 | 111.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 23 | BA | 2713 | A | N9-C4-C5 | -6.24 | 103.31 | 105.80 |
| 23 | DA | 1773 | A | N1-C6-N6 | 6.24 | 122.34 | 118.60 |
| 24 | BB | 76 | G | C5-C6-O6 | -6.24 | 124.86 | 128.60 |
| 53 | D5 | 62 | LEU | CA-CB-CG | -6.24 | 100.96 | 115.30 |
| 23 | DA | 250 | G | C8-N9-C4 | -6.23 | 103.91 | 106.40 |
| 23 | BA | 2506 | U | N1-C2-O2 | 6.23 | 127.16 | 122.80 |
| 23 | BA | 13 | A | N1-C6-N6 | -6.23 | 114.86 | 118.60 |
| 23 | DA | 976 | C | C6-N1-C2 | 6.23 | 122.79 | 120.30 |
| 1 | AA | 815 | A | N9-C4-C5 | 6.23 | 108.29 | 105.80 |
| 23 | DA | 826 | U | C5-C6-N1 | -6.23 | 119.59 | 122.70 |
| 23 | BA | 1779 | U | C5-C6-N1 | -6.22 | 119.59 | 122.70 |
| 23 | BA | 2578 | G | C5-C6-O6 | -6.22 | 124.87 | 128.60 |
| 23 | BA | 2279 | G | N1-C6-O6 | -6.22 | 116.17 | 119.90 |
| 23 | BA | 2622 | C | N3-C4-C5 | 6.22 | 124.39 | 121.90 |
| 23 | DA | 1201 | C | N1-C2-O2 | -6.22 | 115.17 | 118.90 |
| 23 | DA | 1367 | A | N7-C8-N9 | -6.22 | 110.69 | 113.80 |
| 23 | BA | 1653 | G | N9-C4-C5 | -6.21 | 102.91 | 105.40 |
| 23 | DA | 1299 | G | N9-C4-C5 | -6.21 | 102.91 | 105.40 |
| 23 | DA | 1366 | A | C2-N3-C4 | -6.21 | 107.49 | 110.60 |
| 23 | DA | 2489 | G | N1-C6-O6 | 6.21 | 123.63 | 119.90 |
| 23 | DA | 2822 | G | C8-N9-C4 | 6.21 | 108.89 | 106.40 |
| 1 | AA | 1415 | G | N1-C6-O6 | 6.21 | 123.63 | 119.90 |
| 23 | BA | 594 | U | N1-C2-N3 | 6.21 | 118.63 | 114.90 |
| 23 | BA | 1776 | G | C5-C6-N1 | 6.21 | 114.60 | 111.50 |
| 23 | DA | 640 | C | C6-N1-C2 | 6.21 | 122.78 | 120.30 |
| 23 | BA | 1899 | G | N1-C2-N3 | 6.20 | 127.62 | 123.90 |
| 23 | DA | 1304 | C | C6-N1-C2 | 6.20 | 122.78 | 120.30 |
| 23 | BA | 512 | G | C5-N7-C8 | -6.20 | 101.20 | 104.30 |
| 23 | BA | 798 | G | N1-C2-N3 | 6.20 | 127.62 | 123.90 |
| 23 | BA | 2069 | G | C8-N9-C4 | 6.20 | 108.88 | 106.40 |
| 23 | DA | 328 | U | C4-C5-C6 | 6.20 | 123.42 | 119.70 |
| 23 | DA | 2559 | C | C2-N3-C4 | -6.20 | 116.80 | 119.90 |
| 23 | DA | 1480 | G | N1-C6-O6 | 6.20 | 123.62 | 119.90 |
| 23 | BA | 1264 | G | N1-C2-N3 | 6.20 | 127.62 | 123.90 |
| 23 | DA | 1698 | A | N9-C4-C5 | -6.20 | 103.32 | 105.80 |
| 23 | DA | 704 | G | N1-C6-O6 | 6.19 | 123.61 | 119.90 |
| 23 | BA | 1704 | G | N7-C8-N9 | -6.19 | 110.00 | 113.10 |
| 23 | BA | 2689 | U | C5-C6-N1 | -6.19 | 119.60 | 122.70 |
| 23 | DA | 965 | C | C6-N1-C2 | -6.19 | 117.82 | 120.30 |
| 23 | DA | 1253 | A | C5-N7-C8 | -6.19 | 100.81 | 103.90 |
| 23 | DA | 662 | G | C8-N9-C4 | 6.19 | 108.88 | 106.40 |
| 23 | BA | 1674 | G | C8-N9-C4 | 6.18 | 108.87 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | BA | 2005 | A | C2-N3-C4 | -6.18 | 107.51 | 110.60 |
| 23 | DA | 450 | G | C5-N7-C8 | 6.18 | 107.39 | 104.30 |
| 23 | DA | 686 | G | C5-C6-O6 | -6.18 | 124.89 | 128.60 |
| 23 | BA | 956 | G | N1-C6-O6 | 6.18 | 123.61 | 119.90 |
| 23 | BA | 2700 | C | C2-N3-C4 | -6.18 | 116.81 | 119.90 |
| 23 | BA | 2506 | U | C2-N1-C1' | 6.18 | 125.11 | 117.70 |
| 23 | DA | 466 | A | N1-C2-N3 | 6.18 | 132.39 | 129.30 |
| 23 | DA | 794 | G | N1-C2-N3 | 6.18 | 127.61 | 123.90 |
| 23 | BA | 528 | A | N1-C2-N3 | 6.18 | 132.39 | 129.30 |
| 23 | DA | 1341 | U | N3-C2-O2 | 6.18 | 126.52 | 122.20 |
| 23 | DA | 768 | G | N1-C2-N3 | 6.17 | 127.61 | 123.90 |
| 23 | DA | 1770 | G | N1-C2-N3 | 6.17 | 127.61 | 123.90 |
| 23 | DA | 2542 | A | N7-C8-N9 | -6.17 | 110.71 | 113.80 |
| 23 | BA | 1675 | C | C4-C5-C6 | 6.17 | 120.49 | 117.40 |
| 23 | BA | 1821 | A | C8-N9-C4 | 6.17 | 108.27 | 105.80 |
| 23 | BA | 1937 | A | N1-C2-N3 | 6.17 | 132.39 | 129.30 |
| 23 | DA | 2571 | C | C2-N3-C4 | -6.17 | 116.81 | 119.90 |
| 23 | BA | 847 | U | C2-N3-C4 | -6.17 | 123.30 | 127.00 |
| 23 | DA | 1403 | C | C5-C6-N1 | -6.17 | 117.92 | 121.00 |
| 23 | BA | 1792 | G | N9-C4-C5 | 6.17 | 107.87 | 105.40 |
| 23 | DA | 141(A) | A | C6-C5-N7 | -6.17 | 127.98 | 132.30 |
| 23 | DA | 58 | G | C4-N9-C1' | 6.16 | 134.51 | 126.50 |
| 23 | DA | 180 | G | C8-N9-C4 | 6.16 | 108.86 | 106.40 |
| 23 | DA | 1802 | A | N9-C4-C5 | 6.16 | 108.27 | 105.80 |
| 23 | DA | 2043 | C | C2-N3-C4 | -6.16 | 116.82 | 119.90 |
| 23 | BA | 197 | A | N1-C6-N6 | 6.16 | 122.30 | 118.60 |
| 23 | BA | 586 | A | C8-N9-C4 | 6.16 | 108.26 | 105.80 |
| 23 | BA | 945 | A | C5-C6-N6 | -6.16 | 118.77 | 123.70 |
| 1 | CA | 299 | G | C5-C6-N1 | -6.16 | 108.42 | 111.50 |
| 23 | DA | 2712 | U | C2-N3-C4 | -6.16 | 123.30 | 127.00 |
| 23 | BA | 2059 | A | C8-N9-C4 | 6.16 | 108.26 | 105.80 |
| 23 | DA | 94 | G | N3-C4-N9 | 6.16 | 129.69 | 126.00 |
| 23 | DA | 273(C) | C | C5-C6-N1 | -6.16 | 117.92 | 121.00 |
| 23 | DA | 933 | A | N7-C8-N9 | 6.16 | 116.88 | 113.80 |
| 23 | DA | 72 | U | N3-C2-O2 | -6.16 | 117.89 | 122.20 |
| 23 | BA | 564 | C | C6-N1-C2 | -6.15 | 117.84 | 120.30 |
| 23 | DA | 777 | A | N1-C2-N3 | 6.15 | 132.38 | 129.30 |
| 23 | BA | 458 | G | C5-C6-O6 | -6.15 | 124.91 | 128.60 |
| 23 | BA | 114(B) | A | C2-N3-C4 | -6.15 | 107.52 | 110.60 |
| 23 | BA | 1677 | A | C8-N9-C4 | -6.15 | 103.34 | 105.80 |
| 23 | BA | 2053 | G | N9-C4-C5 | -6.15 | 102.94 | 105.40 |
| 23 | BA | 2440 | C | N1-C2-O2 | -6.15 | 115.21 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | DA | 2724 | C | N1-C2-O2 | -6.15 | 115.21 | 118.90 |
| 23 | BA | 678 | C | C2-N3-C4 | -6.15 | 116.83 | 119.90 |
| 23 | DA | 971 | C | N3-C2-O2 | 6.15 | 126.20 | 121.90 |
| 23 | DA | 2517 | C | C5-C6-N1 | -6.15 | 117.93 | 121.00 |
| 23 | BA | 786 | C | C2-N3-C4 | -6.15 | 116.83 | 119.90 |
| 23 | BA | 1225 | G | N1-C6-O6 | -6.15 | 116.21 | 119.90 |
| 23 | BA | 2829 | C | C5-C6-N1 | -6.15 | 117.93 | 121.00 |
| 23 | DA | 273(A) | G | N7-C8-N9 | -6.15 | 110.03 | 113.10 |
| 1 | AA | 918 | A | N1-C6-N6 | -6.14 | 114.91 | 118.60 |
| 23 | DA | 1183 | G | N1-C6-O6 | 6.14 | 123.59 | 119.90 |
| 34 | BL | 61 | ARG | NE-CZ-NH1 | 6.14 | 123.37 | 120.30 |
| 23 | DA | 83 | G | N3-C4-C5 | 6.14 | 131.67 | 128.60 |
| 23 | DA | 132 | G | C8-N9-C4 | 6.14 | 108.86 | 106.40 |
| 23 | DA | 1138 | G | N3-C4-C5 | -6.14 | 125.53 | 128.60 |
| 23 | DA | 2550 | G | C8-N9-C4 | 6.14 | 108.86 | 106.40 |
| 23 | BA | 1010 | A | C8-N9-C4 | 6.14 | 108.25 | 105.80 |
| 23 | BA | 1678 | G | C4-C5-C6 | -6.14 | 115.12 | 118.80 |
| 23 | DA | 512 | G | C8-N9-C1' | 6.14 | 134.98 | 127.00 |
| 23 | DA | 1331 | A | N1-C2-N3 | 6.14 | 132.37 | 129.30 |
| 23 | DA | 2345 | G | C4-C5-N7 | -6.14 | 108.35 | 110.80 |
| 23 | BA | 509 | C | C6-N1-C2 | 6.13 | 122.75 | 120.30 |
| 23 | DA | 2510 | C | C2-N3-C4 | -6.13 | 116.84 | 119.90 |
| 23 | BA | 570 | G | C4-C5-C6 | 6.12 | 122.47 | 118.80 |
| 23 | BA | 760 | G | N3-C4-C5 | 6.12 | 131.66 | 128.60 |
| 23 | DA | 444 | C | C2-N3-C4 | -6.12 | 116.84 | 119.90 |
| 23 | DA | 933 | A | C4-C5-N7 | 6.12 | 113.76 | 110.70 |
| 23 | DA | 1898 | U | C5-C4-O4 | 6.12 | 129.57 | 125.90 |
| 23 | DA | 2044 | C | N3-C4-C5 | 6.12 | 124.35 | 121.90 |
| 23 | DA | 458 | G | N3-C4-N9 | 6.12 | 129.67 | 126.00 |
| 23 | DA | 752 | A | N1-C2-N3 | 6.12 | 132.36 | 129.30 |
| 23 | DA | 947 | G | C8-N9-C4 | 6.12 | 108.85 | 106.40 |
| 23 | DA | 1031 | G | C2-N3-C4 | -6.12 | 108.84 | 111.90 |
| 23 | DA | 582 | G | N7-C8-N9 | -6.11 | 110.04 | 113.10 |
| 23 | DA | 994 | C | C4-C5-C6 | 6.11 | 120.45 | 117.40 |
| 23 | DA | 2070 | G | N1-C2-N3 | 6.11 | 127.56 | 123.90 |
| 23 | DA | 2719 | G | C4-N9-C1' | 6.11 | 134.44 | 126.50 |
| 23 | DA | 1663 | C | C6-N1-C2 | 6.11 | 122.74 | 120.30 |
| 23 | BA | 787 | U | C5-C6-N1 | -6.11 | 119.65 | 122.70 |
| 23 | BA | 1614 | A | C4-C5-C6 | 6.11 | 120.05 | 117.00 |
| 23 | BA | 2681 | C | C5-C6-N1 | -6.10 | 117.95 | 121.00 |
| 23 | DA | 1790 | C | C5-C6-N1 | -6.10 | 117.95 | 121.00 |
| 23 | DA | 2838 | G | C5-C6-O6 | -6.10 | 124.94 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | BA | 494 | G | C5-C6-O6 | -6.10 | 124.94 | 128.60 |
| 23 | BA | 1208 | C | C6-N1-C2 | 6.10 | 122.74 | 120.30 |
| 23 | DA | 2463 | C | N1-C2-O2 | -6.10 | 115.24 | 118.90 |
| 23 | DA | 2675 | A | C8-N9-C4 | 6.10 | 108.24 | 105.80 |
| 23 | BA | 543 | C | C6-N1-C2 | 6.10 | 122.74 | 120.30 |
| 23 | BA | 1783 | A | N3-C4-N9 | -6.10 | 122.52 | 127.40 |
| 23 | DA | 86 | C | C6-N1-C2 | 6.10 | 122.74 | 120.30 |
| 23 | DA | 1392 | A | N1-C6-N6 | -6.10 | 114.94 | 118.60 |
| 23 | DA | 1790 | C | C2-N3-C4 | -6.10 | 116.85 | 119.90 |
| 23 | BA | 807 | U | C5-C6-N1 | -6.10 | 119.65 | 122.70 |
| 23 | DA | 564 | C | C6-N1-C2 | -6.10 | 117.86 | 120.30 |
| 23 | BA | 993 | G | N9-C4-C5 | 6.10 | 107.84 | 105.40 |
| 23 | DA | 801 | G | N9-C4-C5 | 6.10 | 107.84 | 105.40 |
| 23 | DA | 1022 | G | N3-C4-C5 | -6.10 | 125.55 | 128.60 |
| 23 | BA | 1827 | C | C5-C6-N1 | -6.09 | 117.95 | 121.00 |
| 23 | DA | 1830 | C | C6-N1-C2 | 6.09 | 122.74 | 120.30 |
| 23 | BA | 1648 | C | C5-C6-N1 | -6.09 | 117.95 | 121.00 |
| 23 | DA | 2249 | U | C6-N1-C2 | -6.09 | 117.35 | 121.00 |
| 1 | CA | 856 | C | C6-N1-C2 | -6.08 | 117.87 | 120.30 |
| 23 | BA | 450 | G | C8-N9-C1' | -6.08 | 119.09 | 127.00 |
| 23 | DA | 1400 | G | N3-C4-N9 | 6.08 | 129.65 | 126.00 |
| 24 | DB | 83 | G | N1-C6-O6 | 6.08 | 123.55 | 119.90 |
| 23 | DA | 1331 | A | C5-C6-N1 | -6.08 | 114.66 | 117.70 |
| 23 | BA | 2831 | G | N3-C4-N9 | -6.08 | 122.36 | 126.00 |
| 23 | DA | 126 | A | N1-C6-N6 | 6.08 | 122.25 | 118.60 |
| 23 | DA | 1655 | A | C2-N3-C4 | -6.08 | 107.56 | 110.60 |
| 23 | DA | 1902 | C | C5-C4-N4 | 6.08 | 124.45 | 120.20 |
| 23 | BA | 333 | G | C8-N9-C1' | -6.07 | 119.11 | 127.00 |
| 23 | DA | 1258 | C | C6-N1-C2 | 6.07 | 122.73 | 120.30 |
| 23 | DA | 2503 | A | C4-C5-C6 | -6.07 | 113.96 | 117.00 |
| 23 | BA | 83 | G | C4-N9-C1' | -6.07 | 118.61 | 126.50 |
| 23 | BA | 333 | G | C4-N9-C1' | 6.07 | 134.39 | 126.50 |
| 23 | BA | 1613 | G | N1-C6-O6 | -6.07 | 116.26 | 119.90 |
| 23 | BA | 1899 | G | N3-C2-N2 | -6.07 | 115.65 | 119.90 |
| 23 | DA | 2426 | A | C5-N7-C8 | -6.07 | 100.86 | 103.90 |
| 23 | BA | 2066 | C | C5-C6-N1 | -6.07 | 117.97 | 121.00 |
| 23 | DA | 2080 | G | C6-N1-C2 | -6.07 | 121.46 | 125.10 |
| 23 | DA | 141(A) | A | C8-N9-C4 | -6.07 | 103.37 | 105.80 |
| 23 | DA | 1937 | A | C2-N3-C4 | -6.07 | 107.57 | 110.60 |
| 23 | BA | 2250 | G | N1-C6-O6 | -6.06 | 116.26 | 119.90 |
| 23 | BA | 2510 | C | C5-C6-N1 | -6.06 | 117.97 | 121.00 |
| 23 | DA | 216 | A | C5-N7-C8 | -6.06 | 100.87 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | DA | 270(A) | A | C2-N3-C4 | -6.06 | 107.57 | 110.60 |
| 23 | BA | 2453 | A | N1-C2-N3 | 6.06 | 132.33 | 129.30 |
| 23 | DA | 60 | G | P-O3'-C3' | 6.06 | 126.98 | 119.70 |
| 23 | DA | 296 | C | C6-N1-C2 | 6.06 | 122.72 | 120.30 |
| 23 | DA | 1286 | A | N1-C2-N3 | 6.06 | 132.33 | 129.30 |
| 23 | BA | 1983 | C | C2-N3-C4 | -6.06 | 116.87 | 119.90 |
| 23 | BA | 528 | A | C5-N7-C8 | -6.06 | 100.87 | 103.90 |
| 23 | BA | 1248 | G | C5-C6-O6 | -6.06 | 124.96 | 128.60 |
| 23 | BA | 2330 | G | N7-C8-N9 | -6.06 | 110.07 | 113.10 |
| 23 | DA | 2436 | G | N1-C6-O6 | 6.06 | 123.53 | 119.90 |
| 23 | DA | 296 | C | C5-C6-N1 | -6.06 | 117.97 | 121.00 |
| 23 | DA | 2440 | C | C5-C4-N4 | 6.06 | 124.44 | 120.20 |
| 23 | DA | 133 | C | C5-C6-N1 | -6.05 | 117.97 | 121.00 |
| 23 | DA | 794 | G | N1-C6-O6 | -6.05 | 116.27 | 119.90 |
| 23 | BA | 2033 | A | N1-C2-N3 | 6.05 | 132.33 | 129.30 |
| 23 | DA | 104 | U | C5-C6-N1 | -6.05 | 119.67 | 122.70 |
| 23 | DA | 224 | G | C8-N9-C4 | 6.05 | 108.82 | 106.40 |
| 23 | BA | 1899 | G | N9-C4-C5 | 6.05 | 107.82 | 105.40 |
| 23 | DA | 198 | C | N3-C4-C5 | 6.05 | 124.32 | 121.90 |
| 23 | DA | 783 | A | C5-C6-N1 | -6.05 | 114.67 | 117.70 |
| 1 | AA | 876 | G | C8-N9-C4 | 6.05 | 108.82 | 106.40 |
| 23 | DA | 2681 | C | C2-N1-C1' | -6.05 | 112.15 | 118.80 |
| 23 | BA | 780 | G | C8-N9-C4 | 6.04 | 108.82 | 106.40 |
| 23 | BA | 974(B) | C | N3-C4-C5 | 6.04 | 124.32 | 121.90 |
| 23 | DA | 2456 | C | N3-C4-C5 | 6.04 | 124.32 | 121.90 |
| 23 | DA | 482 | A | N1-C6-N6 | 6.04 | 122.22 | 118.60 |
| 23 | DA | 528 | A | N1-C2-N3 | 6.04 | 132.32 | 129.30 |
| 23 | DA | 2584 | U | N3-C4-O4 | 6.04 | 123.63 | 119.40 |
| 23 | BA | 201 | C | C6-N1-C2 | 6.04 | 122.72 | 120.30 |
| 23 | BA | 209 | C | C6-N1-C2 | 6.04 | 122.72 | 120.30 |
| 23 | DA | 2058 | A | C8-N9-C4 | 6.04 | 108.21 | 105.80 |
| 23 | BA | 141(A) | A | N7-C8-N9 | 6.03 | 116.82 | 113.80 |
| 23 | BA | 2825 | U | N3-C4-O4 | -6.03 | 115.18 | 119.40 |
| 23 | BA | 1261 | C | C2-N3-C4 | -6.03 | 116.88 | 119.90 |
| 23 | DA | 1360 | A | C8-N9-C4 | -6.03 | 103.39 | 105.80 |
| 23 | DA | 1782 | C | C6-N1-C2 | 6.03 | 122.71 | 120.30 |
| 23 | BA | 2454 | G | C8-N9-C4 | 6.03 | 108.81 | 106.40 |
| 23 | DA | 1161 | C | C5-C6-N1 | 6.03 | 124.01 | 121.00 |
| 23 | DA | 1707 | G | C2-N3-C4 | -6.03 | 108.89 | 111.90 |
| 23 | DA | 1843 | C | N3-C4-C5 | 6.03 | 124.31 | 121.90 |
| 23 | DA | 2033 | A | N1-C2-N3 | 6.02 | 132.31 | 129.30 |
| 23 | BA | 595 | C | C6-N1-C2 | 6.02 | 122.71 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | BA | 2059 | A | C6-N1-C2 | -6.02 | 114.99 | 118.60 |
| 23 | DA | 204 | A | N7-C8-N9 | -6.02 | 110.79 | 113.80 |
| 23 | DA | 2681 | C | C2-N3-C4 | -6.02 | 116.89 | 119.90 |
| 23 | DA | 2719 | G | C8-N9-C1' | -6.02 | 119.17 | 127.00 |
| 23 | BA | 1677 | A | N7-C8-N9 | 6.02 | 116.81 | 113.80 |
| 23 | DA | 247 | G | C8-N9-C4 | 6.02 | 108.81 | 106.40 |
| 23 | DA | 1528 | A | C8-N9-C4 | -6.02 | 103.39 | 105.80 |
| 23 | BA | 808 | G | C5-N7-C8 | 6.02 | 107.31 | 104.30 |
| 23 | BA | 1837 | C | C6-N1-C2 | -6.02 | 117.89 | 120.30 |
| 23 | BA | 2032 | G | N3-C4-N9 | -6.02 | 122.39 | 126.00 |
| 23 | BA | 2390 | U | N3-C2-O2 | -6.02 | 117.99 | 122.20 |
| 23 | DA | 2056 | G | C5-N7-C8 | -6.02 | 101.29 | 104.30 |
| 23 | DA | 2595 | G | C5-C6-N1 | 6.02 | 114.51 | 111.50 |
| 23 | BA | 1000 | A | C5-C6-N6 | 6.01 | 128.51 | 123.70 |
| 23 | DA | 667 | U | N1-C2-N3 | 6.01 | 118.51 | 114.90 |
| 23 | DA | 1778 | U | C2-N3-C4 | -6.01 | 123.39 | 127.00 |
| 23 | BA | 1252 | G | N7-C8-N9 | -6.01 | 110.09 | 113.10 |
| 23 | BA | 2626 | C | C2-N1-C1' | -6.01 | 112.19 | 118.80 |
| 23 | BA | 1123 | C | C5-C6-N1 | -6.01 | 118.00 | 121.00 |
| 23 | DA | 747 | U | C2-N3-C4 | -6.01 | 123.39 | 127.00 |
| 23 | DA | 1614 | A | N7-C8-N9 | 6.01 | 116.81 | 113.80 |
| 23 | DA | 86 | C | C5-C6-N1 | -6.01 | 118.00 | 121.00 |
| 23 | DA | 1903 | G | N1-C6-O6 | -6.00 | 116.30 | 119.90 |
| 23 | DA | 2713 | A | C5-C6-N6 | -6.00 | 118.90 | 123.70 |
| 23 | DA | 1032 | A | C8-N9-C4 | 6.00 | 108.20 | 105.80 |
| 23 | DA | 2601 | C | C5-C6-N1 | -6.00 | 118.00 | 121.00 |
| 23 | BA | 843 | G | N1-C6-O6 | 6.00 | 123.50 | 119.90 |
| 23 | DA | 2283 | C | N1-C2-O2 | -6.00 | 115.30 | 118.90 |
| 23 | BA | 2508 | G | C8-N9-C4 | 6.00 | 108.80 | 106.40 |
| 23 | DA | 138 | G | C8-N9-C4 | -6.00 | 104.00 | 106.40 |
| 23 | DA | 2240 | C | C6-N1-C2 | 6.00 | 122.70 | 120.30 |
| 23 | BA | 509 | C | N3-C4-C5 | 6.00 | 124.30 | 121.90 |
| 23 | BA | 1977 | A | C2-N3-C4 | -6.00 | 107.60 | 110.60 |
| 23 | DA | 1367 | A | C8-N9-C4 | 6.00 | 108.20 | 105.80 |
| 23 | DA | 2249 | U | C5-C4-O4 | 6.00 | 129.50 | 125.90 |
| 23 | BA | 2345 | G | C4-C5-N7 | -6.00 | 108.40 | 110.80 |
| 23 | DA | 472 | A | N7-C8-N9 | -6.00 | 110.80 | 113.80 |
| 23 | DA | 2711 | A | C8-N9-C4 | 6.00 | 108.20 | 105.80 |
| 23 | DA | 31 | C | C5-C4-N4 | -5.99 | 116.00 | 120.20 |
| 23 | BA | 575 | A | C8-N9-C4 | 5.99 | 108.20 | 105.80 |
| 23 | DA | 434 | U | N1-C2-O2 | -5.99 | 118.61 | 122.80 |
| 23 | DA | 2283 | C | N3-C2-O2 | 5.99 | 126.09 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 23 | DA | 1204 | A | C5-N7-C8 | -5.99 | 100.91 | 103.90 |
| 23 | DA | 1963 | U | N1-C2-O2 | 5.99 | 126.99 | 122.80 |
| 23 | DA | 1815 | A | N9-C4-C5 | 5.99 | 108.20 | 105.80 |
| 23 | DA | 225 | A | C2-N3-C4 | -5.99 | 107.61 | 110.60 |
| 23 | DA | 1325 | G | C5-C6-N1 | 5.99 | 114.49 | 111.50 |
| 23 | BA | 571 | A | C4-C5-C6 | -5.99 | 114.01 | 117.00 |
| 23 | BA | 1309 | G | C8-N9-C4 | 5.99 | 108.79 | 106.40 |
| 23 | DA | 109 | G | C8-N9-C4 | 5.99 | 108.79 | 106.40 |
| 23 | DA | 197 | A | C5-N7-C8 | -5.99 | 100.91 | 103.90 |
| 23 | DA | 2770 | G | C4-C5-N7 | -5.99 | 108.41 | 110.80 |
| 23 | DA | 189 | G | C8-N9-C1' | -5.98 | 119.22 | 127.00 |
| 23 | DA | 945 | A | O4'-C1'-N9 | 5.98 | 112.99 | 108.20 |
| 23 | BA | 1839 | G | N3-C4-C5 | 5.98 | 131.59 | 128.60 |
| 23 | BA | 1839 | G | C5-C6-O6 | 5.98 | 132.19 | 128.60 |
| 23 | BA | 2498 | C | C2-N3-C4 | -5.98 | 116.91 | 119.90 |
| 23 | DA | 1825 | A | C6-N1-C2 | -5.98 | 115.01 | 118.60 |
| 23 | DA | 1977 | A | C2-N3-C4 | -5.98 | 107.61 | 110.60 |
| 23 | BA | 600 | G | N1-C6-O6 | 5.98 | 123.49 | 119.90 |
| 23 | BA | 1797 | C | C6-N1-C2 | 5.98 | 122.69 | 120.30 |
| 23 | DA | 537 | C | C6-N1-C2 | 5.98 | 122.69 | 120.30 |
| 23 | DA | 746 | A | C4-C5-C6 | 5.98 | 119.99 | 117.00 |
| 23 | BA | 114(B) | A | C4-C5-C6 | 5.98 | 119.99 | 117.00 |
| 23 | DA | 2596 | U | C5-C6-N1 | -5.98 | 119.71 | 122.70 |
| 23 | BA | 1804 | C | C2-N3-C4 | -5.97 | 116.91 | 119.90 |
| 23 | DA | 1617 | C | N1-C2-O2 | -5.97 | 115.31 | 118.90 |
| 23 | BA | 1796 | U | C5-C6-N1 | -5.97 | 119.71 | 122.70 |
| 23 | BA | 1961 | C | C5-C6-N1 | -5.97 | 118.01 | 121.00 |
| 23 | BA | 704 | G | N9-C4-C5 | -5.97 | 103.01 | 105.40 |
| 23 | DA | 26 | G | C8-N9-C4 | 5.97 | 108.79 | 106.40 |
| 23 | BA | 594 | U | N3-C2-O2 | -5.97 | 118.02 | 122.20 |
| 23 | DA | 2430 | A | N7-C8-N9 | 5.97 | 116.78 | 113.80 |
| 23 | DA | 2590 | A | N1-C2-N3 | 5.97 | 132.28 | 129.30 |
| 23 | BA | 129 | C | C6-N1-C2 | 5.96 | 122.69 | 120.30 |
| 23 | DA | 72 | U | C2-N3-C4 | -5.96 | 123.42 | 127.00 |
| 23 | DA | 584 | C | C2-N3-C4 | -5.96 | 116.92 | 119.90 |
| 23 | DA | 1841 | U | N3-C4-O4 | 5.96 | 123.58 | 119.40 |
| 23 | DA | 529 | A | C5-C6-N6 | -5.96 | 118.93 | 123.70 |
| 23 | DA | 2605 | U | C5-C4-O4 | 5.96 | 129.48 | 125.90 |
| 23 | DA | 2875 | C | C6-N1-C2 | 5.96 | 122.69 | 120.30 |
| 23 | DA | 840 | C | C5-C6-N1 | -5.96 | 118.02 | 121.00 |
| 23 | BA | 1956 | U | C5-C6-N1 | -5.96 | 119.72 | 122.70 |
| 23 | BA | 1980 | G | N3-C4-C5 | -5.96 | 125.62 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | DA | 322 | A | N1-C6-N6 | -5.96 | 115.03 | 118.60 |
| 23 | DA | 532 | A | N1-C6-N6 | -5.96 | 115.03 | 118.60 |
| 23 | DA | 1699 | G | C4-C5-N7 | -5.96 | 108.42 | 110.80 |
| 23 | DA | 2014 | A | N1-C6-N6 | 5.96 | 122.17 | 118.60 |
| 23 | DA | 270(Z) | G | C5-C6-O6 | 5.96 | 132.17 | 128.60 |
| 23 | BA | 2086 | U | C5-C4-O4 | 5.95 | 129.47 | 125.90 |
| 23 | BA | 2433 | A | C4-C5-C6 | 5.95 | 119.98 | 117.00 |
| 23 | DA | 1210 | A | N7-C8-N9 | 5.95 | 116.78 | 113.80 |
| 23 | DA | 1616 | A | C8-N9-C4 | -5.95 | 103.42 | 105.80 |
| 23 | DA | 2567 | G | C5-C6-O6 | -5.95 | 125.03 | 128.60 |
| 23 | DA | 2762 | G | C6-C5-N7 | -5.95 | 126.83 | 130.40 |
| 1 | CA | 926 | G | N9-C4-C5 | 5.95 | 107.78 | 105.40 |
| 23 | DA | 1261 | C | N3-C2-O2 | 5.95 | 126.06 | 121.90 |
| 23 | DA | 2061 | G | C8-N9-C1' | -5.95 | 119.27 | 127.00 |
| 23 | BA | 929 | G | C4-C5-C6 | 5.95 | 122.37 | 118.80 |
| 23 | BA | 933 | A | C6-C5-N7 | -5.95 | 128.14 | 132.30 |
| 23 | DA | 2521 | C | C6-N1-C2 | 5.95 | 122.68 | 120.30 |
| 47 | DY | 21 | LEU | CB-CG-CD1 | 5.95 | 121.11 | 111.00 |
| 1 | AA | 918 | A | N9-C4-C5 | 5.95 | 108.18 | 105.80 |
| 23 | BA | 138 | G | C8-N9-C4 | -5.95 | 104.02 | 106.40 |
| 23 | BA | 1164 | G | C4-N9-C1' | 5.95 | 134.23 | 126.50 |
| 23 | BA | 2719 | G | C6-C5-N7 | -5.95 | 126.83 | 130.40 |
| 23 | DA | 2532 | G | C6-C5-N7 | -5.95 | 126.83 | 130.40 |
| 23 | DA | 933 | A | C2-N3-C4 | -5.94 | 107.63 | 110.60 |
| 23 | DA | 2442 | C | C5-C6-N1 | -5.94 | 118.03 | 121.00 |
| 23 | BA | 2092 | U | C5-C4-O4 | 5.94 | 129.47 | 125.90 |
| 23 | BA | 2232 | U | C5-C4-O4 | 5.94 | 129.47 | 125.90 |
| 23 | DA | 2505 | G | C5-C6-N1 | -5.94 | 108.53 | 111.50 |
| 23 | DA | 273(C) | C | C6-N1-C2 | 5.94 | 122.68 | 120.30 |
| 23 | DA | 1820 | U | C6-N1-C2 | 5.94 | 124.56 | 121.00 |
| 23 | DA | 677 | A | C8-N9-C4 | 5.94 | 108.17 | 105.80 |
| 23 | DA | 1385 | G | C4-N9-C1' | -5.94 | 118.78 | 126.50 |
| 23 | DA | 1827 | C | C2-N3-C4 | -5.94 | 116.93 | 119.90 |
| 23 | DA | 2454 | G | N7-C8-N9 | -5.94 | 110.13 | 113.10 |
| 23 | DA | 2550 | G | N1-C6-O6 | 5.94 | 123.46 | 119.90 |
| 23 | DA | 2597 | G | N7-C8-N9 | -5.94 | 110.13 | 113.10 |
| 23 | BA | 1770 | G | C2-N3-C4 | -5.93 | 108.93 | 111.90 |
| 23 | DA | 1989 | G | C5-C6-O6 | -5.93 | 125.04 | 128.60 |
| 1 | AA | 299 | G | C4-C5-N7 | -5.93 | 108.43 | 110.80 |
| 23 | BA | 452 | G | C5-C6-O6 | -5.93 | 125.04 | 128.60 |
| 23 | BA | 1790 | C | C6-N1-C2 | 5.93 | 122.67 | 120.30 |
| 23 | BA | 1000 | A | N1-C6-N6 | -5.93 | 115.04 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | DA | 2006 | C | C5-C6-N1 | -5.93 | 118.04 | 121.00 |
| 23 | DA | 2233 | U | N3-C4-C5 | 5.93 | 118.16 | 114.60 |
| 23 | DA | 734 | A | N1-C6-N6 | 5.92 | 122.16 | 118.60 |
| 23 | DA | 2327 | A | C8-N9-C4 | 5.92 | 108.17 | 105.80 |
| 23 | BA | 570 | G | C8-N9-C4 | -5.92 | 104.03 | 106.40 |
| 23 | DA | 1126 | A | C8-N9-C4 | 5.92 | 108.17 | 105.80 |
| 23 | DA | 1679 | U | N1-C2-O2 | -5.92 | 118.65 | 122.80 |
| 23 | BA | 529 | A | C4-C5-N7 | 5.92 | 113.66 | 110.70 |
| 23 | BA | 140 | A | C5-N7-C8 | -5.92 | 100.94 | 103.90 |
| 1 | CA | 810 | C | C5-C6-N1 | -5.92 | 118.04 | 121.00 |
| 23 | DA | 2578 | G | N1-C6-O6 | 5.92 | 123.45 | 119.90 |
| 23 | BA | 2070 | G | C8-N9-C4 | 5.92 | 108.77 | 106.40 |
| 23 | BA | 2544 | G | C2-N3-C4 | -5.92 | 108.94 | 111.90 |
| 23 | BA | 1655 | A | N1-C6-N6 | 5.92 | 122.15 | 118.60 |
| 23 | BA | 1798 | U | N1-C2-O2 | -5.92 | 118.66 | 122.80 |
| 23 | DA | 187 | G | N3-C4-N9 | 5.91 | 129.55 | 126.00 |
| 23 | DA | 2518 | A | N3-C4-C5 | 5.91 | 130.94 | 126.80 |
| 23 | BA | 141(A) | A | N1-C6-N6 | 5.91 | 122.15 | 118.60 |
| 23 | BA | 1957 | C | C6-N1-C2 | 5.91 | 122.67 | 120.30 |
| 23 | BA | 2524 | G | N7-C8-N9 | -5.91 | 110.14 | 113.10 |
| 23 | DA | 187 | G | C8-N9-C1' | -5.91 | 119.32 | 127.00 |
| 23 | BA | 2007 | C | C5-C6-N1 | -5.91 | 118.05 | 121.00 |
| 23 | BA | 2719 | G | N9-C4-C5 | -5.91 | 103.04 | 105.40 |
| 23 | DA | 2057 | A | N1-C2-N3 | 5.91 | 132.25 | 129.30 |
| 23 | BA | 1121 | C | C6-N1-C2 | 5.91 | 122.66 | 120.30 |
| 23 | DA | 723 | G | C5-C6-N1 | -5.91 | 108.55 | 111.50 |
| 23 | DA | 1395 | A | N1-C2-N3 | -5.91 | 126.35 | 129.30 |
| 23 | BA | 1333 | C | C5-C4-N4 | -5.90 | 116.07 | 120.20 |
| 23 | BA | 2831 | G | N3-C4-C5 | 5.90 | 131.55 | 128.60 |
| 23 | DA | 543 | C | C5-C6-N1 | -5.90 | 118.05 | 121.00 |
| 23 | DA | 570 | G | C5-N7-C8 | 5.90 | 107.25 | 104.30 |
| 23 | DA | 2050 | C | N1-C2-N3 | 5.90 | 123.33 | 119.20 |
| 23 | BA | 806 | C | C6-N1-C2 | -5.90 | 117.94 | 120.30 |
| 23 | BA | 1264 | G | N9-C4-C5 | 5.90 | 107.76 | 105.40 |
| 23 | BA | 2593 | U | C4-C5-C6 | 5.90 | 123.24 | 119.70 |
| 23 | DA | 298 | G | N1-C6-O6 | 5.90 | 123.44 | 119.90 |
| 23 | BA | 1769 | G | N7-C8-N9 | 5.89 | 116.05 | 113.10 |
| 1 | AA | 810 | C | C5-C6-N1 | -5.89 | 118.05 | 121.00 |
| 23 | BA | 1901 | A | N1-C6-N6 | -5.89 | 115.07 | 118.60 |
| 23 | BA | 2719 | G | C8-N9-C1' | -5.89 | 119.34 | 127.00 |
| 23 | BA | 509 | C | C2-N1-C1' | -5.89 | 112.32 | 118.80 |
| 23 | DA | 693 | C | C4-C5-C6 | 5.89 | 120.34 | 117.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | DA | 1325 | G | C4-N9-C1' | -5.89 | 118.84 | 126.50 |
| 23 | BA | 530 | G | N7-C8-N9 | 5.89 | 116.04 | 113.10 |
| 23 | DA | 2232 | U | C4-C5-C6 | 5.88 | 123.23 | 119.70 |
| 23 | DA | 2510 | C | C5-C6-N1 | -5.88 | 118.06 | 121.00 |
| 23 | BA | 1313 | U | C5-C6-N1 | 5.88 | 125.64 | 122.70 |
| 23 | BA | 2593 | U | N1-C2-N3 | 5.88 | 118.43 | 114.90 |
| 23 | BA | 2719 | G | C4-N9-C1' | 5.88 | 134.15 | 126.50 |
| 23 | DA | 1783 | A | C6-N1-C2 | -5.88 | 115.07 | 118.60 |
| 23 | BA | 1291 | C | C6-N1-C2 | 5.88 | 122.65 | 120.30 |
| 1 | CA | 1513 | A | N7-C8-N9 | -5.88 | 110.86 | 113.80 |
| 23 | DA | 1266 | G | C8-N9-C4 | 5.88 | 108.75 | 106.40 |
| 23 | DA | 1335 | U | C5-C6-N1 | -5.88 | 119.76 | 122.70 |
| 23 | BA | 840 | C | C2-N3-C4 | -5.88 | 116.96 | 119.90 |
| 23 | BA | 2544 | G | C6-C5-N7 | -5.88 | 126.87 | 130.40 |
| 23 | BA | 847 | U | C6-N1-C1' | 5.88 | 129.43 | 121.20 |
| 1 | AA | 904 | C | C5-C6-N1 | -5.87 | 118.06 | 121.00 |
| 23 | BA | 1982 | C | N3-C4-N4 | 5.87 | 122.11 | 118.00 |
| 25 | BC | 177 | LEU | CA-CB-CG | -5.87 | 101.79 | 115.30 |
| 23 | DA | 808 | G | C6-N1-C2 | -5.87 | 121.58 | 125.10 |
| 23 | DA | 841 | A | C6-N1-C2 | -5.87 | 115.08 | 118.60 |
| 23 | DA | 2549 | G | N1-C2-N3 | 5.87 | 127.42 | 123.90 |
| 23 | BA | 1769 | G | C6-C5-N7 | -5.87 | 126.88 | 130.40 |
| 23 | BA | 2822 | G | C8-N9-C4 | 5.87 | 108.75 | 106.40 |
| 23 | DA | 263 | C | C6-N1-C2 | 5.87 | 122.65 | 120.30 |
| 23 | DA | 2587 | A | C8-N9-C4 | 5.87 | 108.15 | 105.80 |
| 23 | DA | 2506 | U | N3-C2-O2 | -5.87 | 118.09 | 122.20 |
| 23 | BA | 640 | C | N3-C4-N4 | -5.87 | 113.89 | 118.00 |
| 23 | DA | 940 | G | N3-C4-C5 | -5.87 | 125.67 | 128.60 |
| 23 | BA | 239 | U | C2-N1-C1' | -5.86 | 110.67 | 117.70 |
| 23 | BA | 1617 | C | C5-C6-N1 | -5.86 | 118.07 | 121.00 |
| 23 | DA | 298 | G | C5-C6-O6 | -5.86 | 125.08 | 128.60 |
| 23 | DA | 760 | G | C8-N9-C4 | 5.86 | 108.75 | 106.40 |
| 23 | DA | 1264 | G | C5-C6-O6 | 5.86 | 132.12 | 128.60 |
| 23 | DA | 1589 | C | C6-N1-C2 | -5.86 | 117.95 | 120.30 |
| 23 | DA | 2033 | A | C2-N3-C4 | -5.86 | 107.67 | 110.60 |
| 23 | DA | 2324 | C | C2-N3-C4 | -5.86 | 116.97 | 119.90 |
| 23 | BA | 968 | G | N1-C6-O6 | 5.86 | 123.42 | 119.90 |
| 23 | BA | 1250 | G | C8-N9-C4 | 5.86 | 108.75 | 106.40 |
| 23 | BA | 1666 | G | N3-C4-C5 | 5.86 | 131.53 | 128.60 |
| 23 | DA | 2497 | A | C2-N3-C4 | -5.86 | 107.67 | 110.60 |
| 23 | BA | 799 | G | C5-C6-N1 | 5.86 | 114.43 | 111.50 |
| 23 | DA | 40 | C | C5-C6-N1 | -5.86 | 118.07 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | DA | 224 | G | N3-C4-C5 | 5.86 | 131.53 | 128.60 |
| 23 | DA | 2550 | G | C5-C6-O6 | -5.86 | 125.08 | 128.60 |
| 23 | DA | 2278 | A | C8-N9-C4 | -5.86 | 103.46 | 105.80 |
| 1 | AA | 1522 | U | N1-C2-N3 | 5.86 | 118.41 | 114.90 |
| 23 | BA | 1325 | G | C4-N9-C1' | -5.86 | 118.89 | 126.50 |
| 23 | BA | 2003 | G | C8-N9-C4 | 5.86 | 108.74 | 106.40 |
| 23 | BA | 2496 | C | C2-N3-C4 | -5.86 | 116.97 | 119.90 |
| 23 | DA | 2392 | A | C8-N9-C4 | -5.85 | 103.46 | 105.80 |
| 23 | DA | 2581 | G | C4-C5-N7 | -5.85 | 108.46 | 110.80 |
| 23 | BA | 811 | U | C5-C6-N1 | -5.85 | 119.77 | 122.70 |
| 23 | BA | 2227 | A | C2-N3-C4 | -5.85 | 107.67 | 110.60 |
| 1 | CA | 1522 | U | N1-C2-N3 | 5.85 | 118.41 | 114.90 |
| 23 | DA | 1031 | G | C4-C5-N7 | 5.85 | 113.14 | 110.80 |
| 23 | DA | 1125 | G | N3-C4-C5 | 5.85 | 131.52 | 128.60 |
| 23 | BA | 734 | A | C2-N3-C4 | -5.85 | 107.68 | 110.60 |
| 23 | BA | 834 | C | C2-N3-C4 | -5.85 | 116.98 | 119.90 |
| 1 | CA | 1415 | G | C6-C5-N7 | -5.85 | 126.89 | 130.40 |
| 23 | BA | 1614 | A | C4-C5-N7 | 5.84 | 113.62 | 110.70 |
| 23 | DA | 1252 | G | N7-C8-N9 | -5.84 | 110.18 | 113.10 |
| 23 | DA | 1780 | A | C2-N3-C4 | -5.84 | 107.68 | 110.60 |
| 23 | DA | 2427 | C | C4-C5-C6 | 5.84 | 120.32 | 117.40 |
| 23 | BA | 94 | G | C6-C5-N7 | -5.84 | 126.89 | 130.40 |
| 23 | DA | 71 | A | N3-C4-C5 | 5.84 | 130.89 | 126.80 |
| 23 | DA | 213 | A | C8-N9-C4 | 5.84 | 108.14 | 105.80 |
| 23 | DA | 1215 | G | N7-C8-N9 | -5.84 | 110.18 | 113.10 |
| 23 | BA | 2032 | G | N3-C4-C5 | 5.84 | 131.52 | 128.60 |
| 23 | DA | 949 | C | C6-N1-C2 | 5.84 | 122.64 | 120.30 |
| 23 | DA | 1349 | A | C5-N7-C8 | -5.84 | 100.98 | 103.90 |
| 23 | DA | 377 | C | C2-N1-C1' | -5.84 | 112.38 | 118.80 |
| 23 | DA | 1302 | A | N1-C6-N6 | -5.84 | 115.10 | 118.60 |
| 23 | BA | 330 | A | N3-C4-C5 | 5.83 | 130.88 | 126.80 |
| 23 | DA | 204 | A | N1-C6-N6 | -5.83 | 115.10 | 118.60 |
| 23 | DA | 2447 | G | N3-C4-N9 | -5.83 | 122.50 | 126.00 |
| 23 | DA | 2553 | G | C4-C5-N7 | 5.83 | 113.13 | 110.80 |
| 1 | AA | 811 | C | C6-N1-C2 | 5.83 | 122.63 | 120.30 |
| 23 | BA | 1798 | U | C2-N3-C4 | -5.83 | 123.50 | 127.00 |
| 23 | DA | 752 | A | N1-C6-N6 | -5.83 | 115.10 | 118.60 |
| 23 | DA | 1286 | A | N9-C4-C5 | 5.83 | 108.13 | 105.80 |
| 23 | DA | 1402 | C | C6-N1-C2 | -5.83 | 117.97 | 120.30 |
| 23 | DA | 1898 | U | C6-N1-C1' | 5.83 | 129.37 | 121.20 |
| 23 | BA | 1253 | A | C4-C5-N7 | 5.83 | 113.62 | 110.70 |
| 23 | BA | 1965 | C | N1-C2-O2 | 5.83 | 122.40 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 23 | DA | 333 | G | C4-N9-C1' | 5.83 | 134.08 | 126.50 |
| 23 | DA | 1258 | C | C2-N3-C4 | -5.83 | 116.98 | 119.90 |
| 1 | CA | 811 | C | C2-N3-C4 | -5.83 | 116.99 | 119.90 |
| 23 | DA | 1297 | C | N1-C2-O2 | -5.83 | 115.40 | 118.90 |
| 23 | BA | 2281 | C | C6-N1-C2 | 5.83 | 122.63 | 120.30 |
| 23 | BA | 450 | G | C4-C5-C6 | 5.82 | 122.29 | 118.80 |
| 23 | BA | 1396 | U | C5-C6-N1 | -5.82 | 119.79 | 122.70 |
| 23 | BA | 2392 | A | C5-C6-N1 | -5.82 | 114.79 | 117.70 |
| 23 | DA | 1602 | U | C5-C6-N1 | 5.82 | 125.61 | 122.70 |
| 23 | DA | 2063 | C | C5-C4-N4 | 5.82 | 124.28 | 120.20 |
| 23 | DA | 658 | C | C5-C6-N1 | -5.82 | 118.09 | 121.00 |
| 23 | BA | 1609 | A | C2-N3-C4 | -5.82 | 107.69 | 110.60 |
| 23 | DA | 2004 | G | C6-C5-N7 | -5.82 | 126.91 | 130.40 |
| 23 | DA | 731 | C | C6-N1-C2 | 5.82 | 122.63 | 120.30 |
| 23 | BA | 138 | G | N3-C4-C5 | -5.82 | 125.69 | 128.60 |
| 23 | BA | 1369 | G | C5-C6-O6 | -5.82 | 125.11 | 128.60 |
| 23 | DA | 2086 | U | C5-C4-O4 | 5.82 | 129.39 | 125.90 |
| 1 | AA | 1486 | G | N1-C6-O6 | 5.82 | 123.39 | 119.90 |
| 23 | BA | 1161 | C | C2-N1-C1' | 5.82 | 125.20 | 118.80 |
| 23 | DA | 681 | G | C8-N9-C1' | -5.82 | 119.44 | 127.00 |
| 23 | DA | 847 | U | C6-N1-C1' | 5.82 | 129.34 | 121.20 |
| 23 | DA | 676 | A | O4'-C1'-N9 | 5.81 | 112.85 | 108.20 |
| 23 | BA | 2053 | G | C6-C5-N7 | -5.81 | 126.91 | 130.40 |
| 23 | DA | 1349 | A | C6-C5-N7 | -5.81 | 128.23 | 132.30 |
| 23 | DA | 2593 | U | N1-C2-N3 | 5.81 | 118.39 | 114.90 |
| 23 | BA | 2253 | G | C8-N9-C1' | -5.81 | 119.45 | 127.00 |
| 23 | DA | 1031 | G | C6-C5-N7 | -5.81 | 126.92 | 130.40 |
| 23 | DA | 1258 | C | N3-C4-C5 | 5.81 | 124.22 | 121.90 |
| 23 | DA | 1306 | C | N3-C4-C5 | 5.81 | 124.22 | 121.90 |
| 23 | DA | 2244 | U | N1-C2-O2 | 5.81 | 126.87 | 122.80 |
| 23 | BA | 1655 | A | C2-N3-C4 | -5.81 | 107.70 | 110.60 |
| 23 | BA | 248 | G | C5-C6-O6 | -5.80 | 125.12 | 128.60 |
| 23 | BA | 1841 | U | N3-C4-O4 | 5.80 | 123.46 | 119.40 |
| 23 | DA | 244 | A | C5-C6-N1 | 5.80 | 120.60 | 117.70 |
| 23 | BA | 2697 | G | N1-C6-O6 | 5.80 | 123.38 | 119.90 |
| 23 | DA | 784 | A | C8-N9-C1' | 5.80 | 138.14 | 127.70 |
| 23 | DA | 1190 | G | C4-C5-N7 | 5.80 | 113.12 | 110.80 |
| 1 | AA | 1512 | U | N1-C2-N3 | 5.80 | 118.38 | 114.90 |
| 23 | BA | 1392 | A | N1-C6-N6 | -5.80 | 115.12 | 118.60 |
| 23 | BA | 2876 | G | C8-N9-C4 | 5.80 | 108.72 | 106.40 |
| 23 | DA | 570 | G | C4-C5-C6 | 5.79 | 122.28 | 118.80 |
| 23 | DA | 2532 | G | C8-N9-C1' | -5.79 | 119.47 | 127.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | BA | 107 | C | C6-N1-C2 | 5.79 | 122.62 | 120.30 |
| 23 | BA | 655 | A | N7-C8-N9 | 5.79 | 116.70 | 113.80 |
| 23 | BA | 2280 | G | C5-C6-N1 | 5.79 | 114.40 | 111.50 |
| 23 | DA | 61 | G | C8-N9-C4 | 5.79 | 108.72 | 106.40 |
| 23 | DA | 407 | G | C8-N9-C1' | -5.79 | 119.47 | 127.00 |
| 23 | DA | 768 | G | C8-N9-C1' | -5.79 | 119.47 | 127.00 |
| 23 | DA | 1698 | A | C5-C6-N1 | -5.79 | 114.80 | 117.70 |
| 23 | BA | 764 | A | N1-C6-N6 | 5.79 | 122.08 | 118.60 |
| 23 | BA | 834 | C | C5-C6-N1 | -5.79 | 118.10 | 121.00 |
| 24 | BB | 76 | G | N1-C6-O6 | 5.79 | 123.38 | 119.90 |
| 23 | DA | 2056 | G | C5-C6-O6 | -5.79 | 125.12 | 128.60 |
| 1 | AA | 1200 | C | C6-N1-C2 | 5.79 | 122.62 | 120.30 |
| 23 | BA | 379 | G | C8-N9-C4 | 5.79 | 108.72 | 106.40 |
| 23 | BA | 1248 | G | C5-C6-N1 | 5.79 | 114.39 | 111.50 |
| 23 | BA | 1674 | G | C8-N9-C1' | -5.79 | 119.47 | 127.00 |
| 23 | BA | 1933 | G | N1-C6-O6 | -5.79 | 116.43 | 119.90 |
| 23 | DA | 1804 | C | C2-N3-C4 | -5.79 | 117.01 | 119.90 |
| 23 | DA | 787 | U | C2-N3-C4 | -5.78 | 123.53 | 127.00 |
| 23 | BA | 1324 | G | C4-C5-N7 | 5.78 | 113.11 | 110.80 |
| 23 | BA | 302 | C | C2-N1-C1' | -5.78 | 112.44 | 118.80 |
| 23 | BA | 377 | C | C2-N1-C1' | -5.78 | 112.44 | 118.80 |
| 23 | DA | 1396 | U | C5-C6-N1 | -5.78 | 119.81 | 122.70 |
| 23 | BA | 2456 | C | C6-N1-C2 | 5.78 | 122.61 | 120.30 |
| 23 | DA | 2436 | G | C5-C6-N1 | -5.78 | 108.61 | 111.50 |
| 23 | BA | 450 | G | C4-N9-C1' | 5.78 | 134.01 | 126.50 |
| 23 | DA | 2248 | C | C6-N1-C2 | 5.77 | 122.61 | 120.30 |
| 23 | BA | 847 | U | N1-C2-N3 | 5.77 | 118.36 | 114.90 |
| 23 | BA | 979 | G | N1-C6-O6 | 5.77 | 123.36 | 119.90 |
| 23 | DA | 39 | C | N1-C2-O2 | -5.77 | 115.44 | 118.90 |
| 23 | DA | 126 | A | C5-C6-N6 | -5.77 | 119.08 | 123.70 |
| 23 | BA | 2250 | G | N9-C4-C5 | 5.77 | 107.71 | 105.40 |
| 23 | BA | 2875 | C | N1-C2-O2 | -5.77 | 115.44 | 118.90 |
| 1 | AA | 1472 | U | N3-C4-O4 | -5.77 | 115.36 | 119.40 |
| 1 | CA | 297 | G | C8-N9-C4 | 5.77 | 108.71 | 106.40 |
| 23 | DA | 129 | C | C6-N1-C2 | 5.77 | 122.61 | 120.30 |
| 23 | DA | 240 | G | C5-C6-N1 | -5.77 | 108.62 | 111.50 |
| 23 | DA | 803 | U | C4-C5-C6 | 5.77 | 123.16 | 119.70 |
| 23 | DA | 1209 | G | C5-C6-O6 | 5.77 | 132.06 | 128.60 |
| 23 | DA | 2638 | G | C8-N9-C4 | -5.77 | 104.09 | 106.40 |
| 23 | BA | 2648 | C | N1-C2-O2 | -5.77 | 115.44 | 118.90 |
| 23 | DA | 1315 | C | N1-C2-N3 | 5.77 | 123.24 | 119.20 |
| 34 | DL | 61 | ARG | NE-CZ-NH1 | 5.77 | 123.18 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | BA | 1329 | U | C6-N1-C2 | 5.77 | 124.46 | 121.00 |
| 23 | DA | 661 | C | C5-C6-N1 | -5.77 | 118.12 | 121.00 |
| 23 | DA | 782 | A | C8-N9-C4 | 5.77 | 108.11 | 105.80 |
| 23 | DA | 2272 | U | C5-C6-N1 | 5.77 | 125.58 | 122.70 |
| 23 | DA | 2714 | G | C4-N9-C1' | 5.76 | 133.99 | 126.50 |
| 23 | DA | 1156 | A | C5-N7-C8 | -5.76 | 101.02 | 103.90 |
| 23 | BA | 1332 | G | N1-C6-O6 | 5.76 | 123.36 | 119.90 |
| 23 | DA | 333 | G | C8-N9-C1' | -5.76 | 119.51 | 127.00 |
| 23 | BA | 1262 | A | C5-C6-N1 | 5.76 | 120.58 | 117.70 |
| 1 | AA | 754 | C | N3-C2-O2 | -5.76 | 117.87 | 121.90 |
| 23 | BA | 1007 | C | C6-N1-C2 | 5.76 | 122.60 | 120.30 |
| 1 | CA | 896 | C | C5-C6-N1 | -5.76 | 118.12 | 121.00 |
| 23 | BA | 2042 | A | N1-C6-N6 | 5.75 | 122.05 | 118.60 |
| 23 | BA | 2253 | G | C4-N9-C1' | 5.75 | 133.98 | 126.50 |
| 23 | BA | 2700 | C | C6-N1-C2 | 5.75 | 122.60 | 120.30 |
| 23 | DA | 1764 | G | C5-C6-N1 | 5.75 | 114.38 | 111.50 |
| 23 | BA | 2050 | C | C5-C6-N1 | -5.75 | 118.12 | 121.00 |
| 23 | DA | 2043 | C | N3-C4-C5 | 5.75 | 124.20 | 121.90 |
| 23 | BA | 587 | C | C4-C5-C6 | 5.75 | 120.28 | 117.40 |
| 23 | DA | 1627 | G | C5-C6-N1 | -5.75 | 108.63 | 111.50 |
| 23 | BA | 2486 | G | N1-C6-O6 | 5.75 | 123.35 | 119.90 |
| 23 | DA | 530 | G | N3-C2-N2 | 5.75 | 123.92 | 119.90 |
| 23 | DA | 2614 | A | C5-C6-N6 | -5.75 | 119.10 | 123.70 |
| 23 | BA | 675 | A | N3-C4-C5 | 5.75 | 130.82 | 126.80 |
| 23 | DA | 1379 | A | N1-C6-N6 | 5.75 | 122.05 | 118.60 |
| 23 | BA | 675 | A | C2-N3-C4 | -5.74 | 107.73 | 110.60 |
| 23 | BA | 2501 | C | N1-C2-N3 | -5.74 | 115.18 | 119.20 |
| 23 | DA | 263 | C | C5-C6-N1 | -5.74 | 118.13 | 121.00 |
| 23 | DA | 2719 | G | N9-C4-C5 | -5.74 | 103.10 | 105.40 |
| 23 | BA | 575 | A | C2-N3-C4 | -5.74 | 107.73 | 110.60 |
| 23 | DA | 1021 | A | N1-C6-N6 | 5.74 | 122.05 | 118.60 |
| 23 | DA | 2501 | C | C5-C6-N1 | -5.74 | 118.13 | 121.00 |
| 23 | DA | 2625 | G | N1-C2-N3 | 5.74 | 127.34 | 123.90 |
| 23 | BA | 1308 | A | C2-N3-C4 | -5.74 | 107.73 | 110.60 |
| 23 | BA | 1333 | C | C6-N1-C1' | -5.74 | 113.91 | 120.80 |
| 23 | DA | 2500 | U | C4-C5-C6 | 5.74 | 123.14 | 119.70 |
| 23 | BA | 1821 | A | N1-C2-N3 | 5.74 | 132.17 | 129.30 |
| 23 | DA | 1403 | C | N1-C2-N3 | 5.74 | 123.22 | 119.20 |
| 23 | BA | 2596 | U | C5-C6-N1 | -5.74 | 119.83 | 122.70 |
| 23 | DA | 1680 | U | C6-N1-C2 | -5.74 | 117.56 | 121.00 |
| 23 | DA | 1901 | A | C5-C6-N1 | 5.74 | 120.57 | 117.70 |
| 23 | DA | 2072 | G | C2-N3-C4 | -5.74 | 109.03 | 111.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|----------|-------|-------------|----------|
| 23 | BA | 1376 | C | N1-C2-O2 | -5.74 | 115.46 | 118.90 |
| 23 | BA | 2386 | C | C2-N3-C4 | -5.74 | 117.03 | 119.90 |
| 23 | DA | 244 | A | C4-C5-C6 | -5.74 | 114.13 | 117.00 |
| 23 | BA | 1304 | C | N3-C4-C5 | 5.73 | 124.19 | 121.90 |
| 23 | DA | 769 | G | C5-C6-N1 | 5.73 | 114.37 | 111.50 |
| 23 | DA | 756 | C | C5-C6-N1 | -5.73 | 118.13 | 121.00 |
| 23 | DA | 802 | A | C6-N1-C2 | -5.73 | 115.16 | 118.60 |
| 23 | BA | 1809 | A | C4-C5-C6 | 5.73 | 119.87 | 117.00 |
| 23 | DA | 980 | A | C2-N3-C4 | -5.73 | 107.73 | 110.60 |
| 23 | DA | 1253 | A | N1-C2-N3 | -5.73 | 126.44 | 129.30 |
| 23 | DA | 1368 | G | C6-N1-C2 | -5.73 | 121.66 | 125.10 |
| 23 | BA | 114(B) | A | C5-N7-C8 | -5.73 | 101.04 | 103.90 |
| 23 | BA | 31 | C | C5-C6-N1 | -5.72 | 118.14 | 121.00 |
| 23 | BA | 1031 | G | C2-N3-C4 | -5.72 | 109.04 | 111.90 |
| 23 | BA | 1617 | C | C2-N3-C4 | -5.72 | 117.04 | 119.90 |
| 1 | CA | 758 | G | N1-C6-O6 | 5.72 | 123.33 | 119.90 |
| 23 | DA | 1325 | G | C8-N9-C4 | -5.72 | 104.11 | 106.40 |
| 23 | BA | 2518 | A | N7-C8-N9 | 5.72 | 116.66 | 113.80 |
| 23 | DA | 2084 | C | C5-C6-N1 | -5.72 | 118.14 | 121.00 |
| 23 | DA | 2502 | G | C8-N9-C4 | 5.72 | 108.69 | 106.40 |
| 23 | DA | 1210 | A | C6-C5-N7 | -5.72 | 128.29 | 132.30 |
| 23 | BA | 1671 | U | C4-C5-C6 | 5.72 | 123.13 | 119.70 |
| 23 | BA | 807 | U | C2-N3-C4 | -5.72 | 123.57 | 127.00 |
| 23 | BA | 2601 | C | C5-C6-N1 | -5.72 | 118.14 | 121.00 |
| 23 | BA | 594 | U | N3-C4-C5 | -5.72 | 111.17 | 114.60 |
| 23 | BA | 804 | A | N1-C2-N3 | 5.72 | 132.16 | 129.30 |
| 23 | BA | 2433 | A | C2-N3-C4 | -5.72 | 107.74 | 110.60 |
| 23 | DA | 816 | C | C5-C4-N4 | -5.72 | 116.20 | 120.20 |
| 23 | DA | 979 | G | N3-C4-C5 | 5.72 | 131.46 | 128.60 |
| 23 | DA | 1210 | A | C5-N7-C8 | -5.72 | 101.04 | 103.90 |
| 23 | DA | 1765 | C | N1-C2-O2 | -5.72 | 115.47 | 118.90 |
| 23 | DA | 1798 | U | C2-N3-C4 | -5.72 | 123.57 | 127.00 |
| 23 | DA | 2442 | C | C6-N1-C2 | 5.72 | 122.59 | 120.30 |
| 23 | BA | 37 | C | N3-C4-C5 | 5.71 | 124.19 | 121.90 |
| 23 | BA | 2451 | A | N1-C6-N6 | -5.71 | 115.17 | 118.60 |
| 23 | BA | 322 | A | N9-C4-C5 | 5.71 | 108.08 | 105.80 |
| 1 | AA | 904 | C | C2-N3-C4 | -5.71 | 117.04 | 119.90 |
| 23 | DA | 2503 | A | C4-C5-N7 | 5.71 | 113.56 | 110.70 |
| 23 | BA | 71 | A | C4-C5-N7 | 5.71 | 113.55 | 110.70 |
| 23 | DA | 1123 | C | C6-N1-C2 | 5.71 | 122.58 | 120.30 |
| 23 | DA | 424 | G | N1-C6-O6 | 5.71 | 123.32 | 119.90 |
| 23 | DA | 1901 | A | N1-C6-N6 | -5.71 | 115.18 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | DA | 580 | C | C5-C6-N1 | -5.70 | 118.15 | 121.00 |
| 23 | DA | 2640 | G | C8-N9-C4 | 5.70 | 108.68 | 106.40 |
| 1 | AA | 529 | G | C5-C6-O6 | -5.70 | 125.18 | 128.60 |
| 23 | BA | 566 | U | C2-N1-C1' | -5.70 | 110.86 | 117.70 |
| 1 | CA | 880 | C | C5-C6-N1 | -5.70 | 118.15 | 121.00 |
| 23 | DA | 2066 | C | C5-C6-N1 | -5.70 | 118.15 | 121.00 |
| 23 | BA | 1841 | U | N1-C2-O2 | -5.70 | 118.81 | 122.80 |
| 23 | BA | 2713 | A | N7-C8-N9 | 5.70 | 116.65 | 113.80 |
| 23 | DA | 2463 | C | N3-C2-O2 | 5.70 | 125.89 | 121.90 |
| 23 | DA | 2553 | G | C8-N9-C4 | 5.70 | 108.68 | 106.40 |
| 23 | BA | 36 | G | C5-N7-C8 | 5.70 | 107.15 | 104.30 |
| 23 | DA | 2059 | A | C8-N9-C4 | 5.70 | 108.08 | 105.80 |
| 23 | BA | 71 | A | C5-N7-C8 | -5.70 | 101.05 | 103.90 |
| 25 | DC | 242 | ARG | N-CA-C | -5.70 | 95.62 | 111.00 |
| 23 | BA | 330 | A | C5-C6-N1 | -5.69 | 114.85 | 117.70 |
| 23 | DA | 2443 | C | N3-C4-C5 | 5.69 | 124.18 | 121.90 |
| 23 | BA | 1804 | C | N1-C2-O2 | -5.69 | 115.48 | 118.90 |
| 23 | BA | 1827 | C | N3-C4-C5 | 5.69 | 124.18 | 121.90 |
| 23 | BA | 2510 | C | C2-N3-C4 | -5.69 | 117.05 | 119.90 |
| 23 | DA | 2515 | C | N3-C4-C5 | 5.69 | 124.18 | 121.90 |
| 23 | BA | 847 | U | C5-C4-O4 | 5.69 | 129.31 | 125.90 |
| 23 | DA | 197 | A | C6-C5-N7 | -5.69 | 128.32 | 132.30 |
| 23 | DA | 374 | A | C2-N3-C4 | -5.69 | 107.75 | 110.60 |
| 23 | DA | 407 | G | C4-N9-C1' | 5.69 | 133.90 | 126.50 |
| 1 | AA | 1523 | G | N3-C2-N2 | -5.69 | 115.92 | 119.90 |
| 23 | DA | 2518 | A | N1-C6-N6 | 5.69 | 122.01 | 118.60 |
| 23 | DA | 1819 | A | N1-C2-N3 | 5.69 | 132.14 | 129.30 |
| 23 | DA | 1839 | G | N3-C4-C5 | 5.69 | 131.44 | 128.60 |
| 23 | DA | 2048 | G | N1-C6-O6 | -5.69 | 116.49 | 119.90 |
| 23 | DA | 2292 | C | C6-N1-C2 | 5.68 | 122.57 | 120.30 |
| 23 | DA | 568 | U | C5-C4-O4 | 5.68 | 129.31 | 125.90 |
| 23 | DA | 1310 | G | C5-C6-O6 | -5.68 | 125.19 | 128.60 |
| 23 | DA | 1555 | G | C8-N9-C1' | -5.68 | 119.61 | 127.00 |
| 23 | DA | 2742 | C | C5-C6-N1 | -5.68 | 118.16 | 121.00 |
| 23 | DA | 1499 | C | C6-N1-C2 | 5.68 | 122.57 | 120.30 |
| 23 | BA | 330 | A | C8-N9-C4 | 5.68 | 108.07 | 105.80 |
| 23 | BA | 1935 | G | C8-N9-C4 | 5.68 | 108.67 | 106.40 |
| 23 | BA | 1948 | G | N1-C6-O6 | -5.68 | 116.49 | 119.90 |
| 23 | DA | 2084 | C | C6-N1-C2 | 5.68 | 122.57 | 120.30 |
| 23 | BA | 38 | A | C5-C6-N1 | 5.67 | 120.54 | 117.70 |
| 23 | BA | 836 | G | C8-N9-C4 | 5.67 | 108.67 | 106.40 |
| 23 | DA | 61 | G | N7-C8-N9 | -5.67 | 110.26 | 113.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 23 | DA | 794 | G | C2-N3-C4 | -5.67 | 109.06 | 111.90 |
| 23 | DA | 2544 | G | C6-C5-N7 | -5.67 | 127.00 | 130.40 |
| 23 | BA | 2232 | U | C4-C5-C6 | 5.67 | 123.10 | 119.70 |
| 23 | DA | 2506 | U | C2-N1-C1' | 5.67 | 124.51 | 117.70 |
| 23 | DA | 146 | G | C5-C6-O6 | -5.67 | 125.20 | 128.60 |
| 23 | DA | 1241 | A | C5-C6-N1 | -5.67 | 114.86 | 117.70 |
| 23 | BA | 810 | U | N3-C2-O2 | -5.67 | 118.23 | 122.20 |
| 23 | BA | 1330 | C | N3-C4-C5 | 5.67 | 124.17 | 121.90 |
| 23 | DA | 1333 | C | C6-N1-C1' | -5.67 | 114.00 | 120.80 |
| 1 | AA | 879 | C | C6-N1-C2 | 5.67 | 122.57 | 120.30 |
| 23 | BA | 512 | G | N3-C4-C5 | 5.67 | 131.43 | 128.60 |
| 23 | BA | 2648 | C | C2-N1-C1' | -5.67 | 112.57 | 118.80 |
| 23 | DA | 794 | G | N1-C2-N2 | -5.67 | 111.10 | 116.20 |
| 23 | DA | 837 | C | C6-N1-C2 | -5.67 | 118.03 | 120.30 |
| 23 | DA | 1815 | A | N1-C6-N6 | -5.67 | 115.20 | 118.60 |
| 23 | DA | 1970 | A | C6-N1-C2 | -5.67 | 115.20 | 118.60 |
| 23 | DA | 2592 | G | N3-C4-C5 | -5.67 | 125.77 | 128.60 |
| 23 | BA | 2392 | A | N1-C2-N3 | 5.66 | 132.13 | 129.30 |
| 23 | BA | 798 | G | N3-C4-N9 | 5.66 | 129.40 | 126.00 |
| 23 | DA | 848 | G | C8-N9-C4 | 5.66 | 108.67 | 106.40 |
| 23 | DA | 2744 | G | N3-C4-C5 | 5.66 | 131.43 | 128.60 |
| 23 | DA | 2054 | A | C2-N3-C4 | -5.66 | 107.77 | 110.60 |
| 23 | BA | 1496 | A | C8-N9-C4 | -5.66 | 103.54 | 105.80 |
| 1 | CA | 501 | C | C6-N1-C2 | -5.66 | 118.04 | 120.30 |
| 23 | DA | 497 | A | N1-C6-N6 | 5.66 | 122.00 | 118.60 |
| 23 | DA | 1633 | G | C8-N9-C4 | -5.66 | 104.14 | 106.40 |
| 23 | DA | 2440 | C | C2-N1-C1' | -5.66 | 112.58 | 118.80 |
| 23 | DA | 1123 | C | C5-C6-N1 | -5.66 | 118.17 | 121.00 |
| 23 | DA | 1323 | U | N1-C2-O2 | -5.66 | 118.84 | 122.80 |
| 1 | AA | 117 | G | N1-C6-O6 | 5.66 | 123.29 | 119.90 |
| 23 | BA | 779 | U | C5-C6-N1 | -5.66 | 119.87 | 122.70 |
| 23 | DA | 529 | A | N1-C6-N6 | 5.66 | 121.99 | 118.60 |
| 23 | DA | 2057 | A | C8-N9-C4 | 5.66 | 108.06 | 105.80 |
| 23 | DA | 2253 | G | C4-N9-C1' | 5.66 | 133.85 | 126.50 |
| 23 | BA | 945 | A | O4'-C1'-N9 | 5.65 | 112.72 | 108.20 |
| 23 | DA | 194 | G | N9-C4-C5 | -5.65 | 103.14 | 105.40 |
| 23 | DA | 589 | C | C5-C6-N1 | -5.65 | 118.17 | 121.00 |
| 23 | BA | 1820 | U | C6-N1-C2 | 5.65 | 124.39 | 121.00 |
| 23 | DA | 1131 | G | C8-N9-C4 | 5.65 | 108.66 | 106.40 |
| 23 | BA | 1313 | U | N3-C4-O4 | 5.65 | 123.35 | 119.40 |
| 23 | DA | 272 | G | C4-N9-C1' | -5.65 | 119.16 | 126.50 |
| 23 | DA | 994 | C | N1-C2-N3 | 5.65 | 123.15 | 119.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | DA | 1994 | C | C5-C6-N1 | -5.65 | 118.17 | 121.00 |
| 23 | BA | 2453 | A | C2-N3-C4 | -5.65 | 107.78 | 110.60 |
| 35 | BM | 81 | VAL | CB-CA-C | -5.65 | 100.67 | 111.40 |
| 23 | DA | 1128 | A | N1-C6-N6 | -5.65 | 115.21 | 118.60 |
| 23 | DA | 1271 | G | C8-N9-C4 | 5.65 | 108.66 | 106.40 |
| 23 | DA | 2520 | C | C5-C6-N1 | -5.65 | 118.18 | 121.00 |
| 23 | BA | 1982 | C | N3-C2-O2 | 5.65 | 125.85 | 121.90 |
| 23 | DA | 684 | G | C5-N7-C8 | -5.65 | 101.48 | 104.30 |
| 23 | BA | 968 | G | C4-C5-N7 | 5.64 | 113.06 | 110.80 |
| 23 | BA | 1605 | C | C6-N1-C2 | -5.64 | 118.04 | 120.30 |
| 23 | DA | 2510 | C | C5-C4-N4 | -5.64 | 116.25 | 120.20 |
| 23 | BA | 2032 | G | C8-N9-C4 | -5.64 | 104.14 | 106.40 |
| 23 | DA | 1617 | C | C6-N1-C2 | 5.64 | 122.56 | 120.30 |
| 23 | BA | 964 | C | C4-C5-C6 | -5.64 | 114.58 | 117.40 |
| 23 | BA | 974(B) | C | C2-N3-C4 | -5.64 | 117.08 | 119.90 |
| 23 | DA | 729 | G | C4-C5-N7 | 5.64 | 113.06 | 110.80 |
| 23 | DA | 1620 | G | N7-C8-N9 | -5.64 | 110.28 | 113.10 |
| 23 | DA | 1999 | C | N3-C4-C5 | 5.64 | 124.16 | 121.90 |
| 23 | BA | 1271 | G | N3-C4-N9 | 5.64 | 129.38 | 126.00 |
| 23 | DA | 801 | G | N1-C6-O6 | -5.64 | 116.52 | 119.90 |
| 23 | DA | 1264 | G | C4-C5-N7 | -5.64 | 108.55 | 110.80 |
| 23 | BA | 484 | C | N3-C4-C5 | 5.63 | 124.15 | 121.90 |
| 23 | BA | 1899 | G | C5-N7-C8 | -5.63 | 101.48 | 104.30 |
| 23 | BA | 1976 | U | N3-C2-O2 | -5.63 | 118.26 | 122.20 |
| 23 | DA | 253 | C | N3-C4-C5 | -5.63 | 119.65 | 121.90 |
| 23 | DA | 2346 | A | C5-C6-N1 | -5.63 | 114.88 | 117.70 |
| 23 | DA | 2540 | C | C5-C6-N1 | -5.63 | 118.18 | 121.00 |
| 23 | BA | 537 | C | C6-N1-C2 | 5.63 | 122.55 | 120.30 |
| 23 | BA | 1776 | G | C8-N9-C4 | 5.63 | 108.65 | 106.40 |
| 23 | BA | 2009 | G | N9-C4-C5 | 5.63 | 107.65 | 105.40 |
| 23 | DA | 1980 | G | N1-C2-N3 | 5.63 | 127.28 | 123.90 |
| 23 | DA | 2324 | C | C2-N1-C1' | -5.63 | 112.61 | 118.80 |
| 1 | CA | 576 | G | C4-N9-C1' | 5.63 | 133.82 | 126.50 |
| 23 | BA | 330 | A | C5-N7-C8 | -5.63 | 101.09 | 103.90 |
| 23 | BA | 580 | C | N3-C4-C5 | 5.63 | 124.15 | 121.90 |
| 23 | BA | 1655 | A | N9-C4-C5 | -5.63 | 103.55 | 105.80 |
| 23 | BA | 1898 | U | C2-N1-C1' | -5.63 | 110.95 | 117.70 |
| 23 | BA | 1979 | C | N3-C2-O2 | 5.63 | 125.84 | 121.90 |
| 23 | DA | 77 | C | N3-C4-C5 | 5.63 | 124.15 | 121.90 |
| 23 | BA | 671 | C | N1-C2-N3 | 5.63 | 123.14 | 119.20 |
| 23 | BA | 1314 | C | C2-N1-C1' | 5.63 | 124.99 | 118.80 |
| 23 | BA | 2035 | G | C5-C6-N1 | 5.63 | 114.31 | 111.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 23 | DA | 1678 | G | C4-C5-C6 | -5.63 | 115.42 | 118.80 |
| 23 | DA | 2869 | G | C8-N9-C4 | -5.63 | 104.15 | 106.40 |
| 23 | DA | 2589 | A | N7-C8-N9 | -5.62 | 110.99 | 113.80 |
| 23 | BA | 1031 | G | N1-C6-O6 | 5.62 | 123.27 | 119.90 |
| 23 | DA | 30 | G | C8-N9-C4 | 5.62 | 108.65 | 106.40 |
| 23 | DA | 1304 | C | N1-C2-O2 | -5.62 | 115.53 | 118.90 |
| 23 | BA | 1021 | A | N3-C4-C5 | 5.62 | 130.73 | 126.80 |
| 23 | BA | 2640 | G | C8-N9-C4 | 5.62 | 108.65 | 106.40 |
| 23 | BA | 529 | A | C6-C5-N7 | -5.62 | 128.37 | 132.30 |
| 23 | BA | 809 | G | C5-C6-N1 | -5.62 | 108.69 | 111.50 |
| 23 | BA | 1671 | U | C2-N3-C4 | 5.62 | 130.37 | 127.00 |
| 23 | DA | 116 | C | C5-C6-N1 | -5.62 | 118.19 | 121.00 |
| 23 | BA | 58 | G | C4-N9-C1' | 5.62 | 133.80 | 126.50 |
| 23 | DA | 1302 | A | C5-C6-N6 | 5.62 | 128.19 | 123.70 |
| 23 | BA | 1979 | C | C2-N1-C1' | -5.62 | 112.62 | 118.80 |
| 1 | AA | 576 | G | C4-N9-C1' | 5.61 | 133.80 | 126.50 |
| 23 | BA | 530 | G | C5-C6-O6 | 5.61 | 131.97 | 128.60 |
| 23 | BA | 1286 | A | C4-C5-C6 | 5.61 | 119.81 | 117.00 |
| 23 | DA | 197 | A | C4-C5-N7 | 5.61 | 113.51 | 110.70 |
| 23 | DA | 836 | G | N3-C4-C5 | 5.61 | 131.41 | 128.60 |
| 1 | AA | 756 | C | C5-C6-N1 | -5.61 | 118.19 | 121.00 |
| 23 | BA | 809 | G | C4-C5-C6 | 5.61 | 122.17 | 118.80 |
| 23 | BA | 1926 | U | C2-N1-C1' | -5.61 | 110.97 | 117.70 |
| 23 | BA | 2073 | C | C5-C6-N1 | -5.61 | 118.19 | 121.00 |
| 23 | DA | 961 | C | C4-C5-C6 | 5.61 | 120.20 | 117.40 |
| 23 | DA | 1674 | G | C8-N9-C1' | -5.61 | 119.71 | 127.00 |
| 23 | DA | 1801 | G | C5-C6-O6 | -5.61 | 125.23 | 128.60 |
| 23 | BA | 2624 | G | C8-N9-C4 | 5.61 | 108.64 | 106.40 |
| 23 | BA | 760 | G | C2-N3-C4 | -5.61 | 109.10 | 111.90 |
| 23 | BA | 1309 | G | C4-N9-C1' | 5.61 | 133.79 | 126.50 |
| 23 | BA | 2271 | G | C8-N9-C1' | -5.61 | 119.71 | 127.00 |
| 23 | DA | 1287 | A | C5-N7-C8 | -5.61 | 101.10 | 103.90 |
| 23 | BA | 2606 | C | N1-C2-O2 | -5.61 | 115.54 | 118.90 |
| 23 | DA | 188 | G | C6-C5-N7 | -5.61 | 127.04 | 130.40 |
| 23 | DA | 580 | C | C2-N3-C4 | -5.61 | 117.10 | 119.90 |
| 23 | DA | 1323 | U | N3-C4-O4 | 5.61 | 123.32 | 119.40 |
| 23 | BA | 60 | G | O4'-C1'-N9 | 5.60 | 112.68 | 108.20 |
| 23 | BA | 2324 | C | C2-N1-C1' | -5.60 | 112.64 | 118.80 |
| 23 | DA | 1444 | G | N7-C8-N9 | -5.60 | 110.30 | 113.10 |
| 23 | BA | 1678 | G | C5-N7-C8 | -5.60 | 101.50 | 104.30 |
| 1 | CA | 314 | C | C6-N1-C2 | -5.60 | 118.06 | 120.30 |
| 23 | DA | 2719 | G | C6-C5-N7 | -5.60 | 127.04 | 130.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | BA | 1007 | C | C5-C6-N1 | -5.60 | 118.20 | 121.00 |
| 23 | BA | 434 | U | N1-C2-O2 | -5.60 | 118.88 | 122.80 |
| 23 | DA | 210 | C | N3-C4-C5 | 5.60 | 124.14 | 121.90 |
| 23 | DA | 1271 | G | N3-C4-N9 | 5.60 | 129.36 | 126.00 |
| 23 | DA | 2634 | G | C8-N9-C4 | 5.60 | 108.64 | 106.40 |
| 23 | DA | 2675 | A | N7-C8-N9 | -5.60 | 111.00 | 113.80 |
| 23 | DA | 845 | G | C4-N9-C1' | 5.60 | 133.78 | 126.50 |
| 23 | BA | 1154 | G | C5-C6-O6 | 5.59 | 131.96 | 128.60 |
| 23 | DA | 248 | G | C8-N9-C4 | 5.59 | 108.64 | 106.40 |
| 23 | DA | 2056 | G | C6-C5-N7 | -5.59 | 127.04 | 130.40 |
| 23 | DA | 2456 | C | C6-N1-C2 | 5.59 | 122.54 | 120.30 |
| 23 | DA | 148 | C | C4-C5-C6 | 5.59 | 120.20 | 117.40 |
| 23 | BA | 1834 | U | C2-N1-C1' | 5.59 | 124.41 | 117.70 |
| 23 | BA | 2056 | G | C6-C5-N7 | -5.59 | 127.05 | 130.40 |
| 23 | DA | 322 | A | N9-C4-C5 | 5.59 | 108.04 | 105.80 |
| 23 | DA | 340 | A | N1-C2-N3 | 5.59 | 132.09 | 129.30 |
| 23 | DA | 1901 | A | C6-N1-C2 | -5.59 | 115.25 | 118.60 |
| 23 | BA | 469 | G | C8-N9-C4 | 5.59 | 108.63 | 106.40 |
| 23 | BA | 659 | C | C5-C6-N1 | -5.59 | 118.21 | 121.00 |
| 23 | DA | 71 | A | C5-C6-N1 | -5.59 | 114.91 | 117.70 |
| 23 | DA | 1570 | A | N7-C8-N9 | -5.59 | 111.01 | 113.80 |
| 23 | DA | 1821 | A | C8-N9-C4 | 5.59 | 108.03 | 105.80 |
| 23 | DA | 2009 | G | C4-C5-N7 | -5.59 | 108.57 | 110.80 |
| 23 | DA | 70 | G | C8-N9-C4 | -5.58 | 104.17 | 106.40 |
| 23 | DA | 657 | U | N1-C2-O2 | 5.58 | 126.71 | 122.80 |
| 23 | DA | 1325 | G | N1-C6-O6 | -5.58 | 116.55 | 119.90 |
| 23 | DA | 2233 | U | C5-C6-N1 | -5.58 | 119.91 | 122.70 |
| 23 | BA | 697 | C | N3-C4-C5 | 5.58 | 124.13 | 121.90 |
| 23 | BA | 773 | U | C5-C6-N1 | -5.58 | 119.91 | 122.70 |
| 23 | DA | 127 | A | C5-C6-N1 | 5.58 | 120.49 | 117.70 |
| 1 | CA | 815 | A | N9-C4-C5 | 5.58 | 108.03 | 105.80 |
| 23 | DA | 2496 | C | C5-C6-N1 | -5.58 | 118.21 | 121.00 |
| 23 | BA | 1841 | U | N3-C4-C5 | -5.58 | 111.25 | 114.60 |
| 23 | DA | 815 | C | C2-N3-C4 | -5.58 | 117.11 | 119.90 |
| 23 | DA | 1826 | G | N7-C8-N9 | -5.58 | 110.31 | 113.10 |
| 23 | BA | 2235 | G | C5-C6-O6 | -5.58 | 125.25 | 128.60 |
| 23 | DA | 2206 | C | C6-N1-C2 | 5.58 | 122.53 | 120.30 |
| 36 | DN | 65 | LEU | CA-CB-CG | -5.58 | 102.47 | 115.30 |
| 23 | BA | 1341 | U | C5-C6-N1 | 5.58 | 125.49 | 122.70 |
| 23 | BA | 1385 | G | C4-N9-C1' | -5.58 | 119.25 | 126.50 |
| 23 | DA | 1603 | A | C8-N9-C4 | -5.58 | 103.57 | 105.80 |
| 23 | DA | 1613 | G | N3-C2-N2 | 5.58 | 123.80 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | DA | 1804 | C | N1-C2-N3 | 5.58 | 123.10 | 119.20 |
| 23 | DA | 843 | G | N1-C6-O6 | 5.57 | 123.24 | 119.90 |
| 23 | DA | 1022 | G | C5-C6-O6 | 5.57 | 131.94 | 128.60 |
| 23 | BA | 1787 | A | C8-N9-C4 | 5.57 | 108.03 | 105.80 |
| 23 | DA | 1332 | G | N1-C6-O6 | 5.57 | 123.24 | 119.90 |
| 23 | DA | 2053 | G | C4-C5-N7 | 5.57 | 113.03 | 110.80 |
| 47 | DY | 60 | LEU | CA-CB-CG | -5.57 | 102.48 | 115.30 |
| 1 | AA | 523 | A | N1-C6-N6 | 5.57 | 121.94 | 118.60 |
| 23 | BA | 332 | A | N1-C2-N3 | 5.57 | 132.09 | 129.30 |
| 23 | BA | 1309 | G | N1-C2-N3 | 5.57 | 127.24 | 123.90 |
| 23 | BA | 2510 | C | C6-N1-C2 | 5.57 | 122.53 | 120.30 |
| 23 | DA | 1770 | G | N1-C6-O6 | 5.57 | 123.24 | 119.90 |
| 23 | DA | 2507 | C | C2-N3-C4 | -5.57 | 117.11 | 119.90 |
| 23 | BA | 2647 | U | C6-N1-C2 | 5.57 | 124.34 | 121.00 |
| 23 | DA | 535 | C | N1-C2-O2 | -5.57 | 115.56 | 118.90 |
| 23 | BA | 192 | C | C5-C6-N1 | -5.57 | 118.22 | 121.00 |
| 23 | DA | 1898 | U | C2-N1-C1' | -5.57 | 111.02 | 117.70 |
| 23 | DA | 2488 | A | C6-N1-C2 | -5.57 | 115.26 | 118.60 |
| 1 | AA | 552 | U | C5-C6-N1 | -5.57 | 119.92 | 122.70 |
| 23 | BA | 700 | G | N1-C6-O6 | 5.57 | 123.24 | 119.90 |
| 23 | BA | 1842 | G | N1-C6-O6 | 5.57 | 123.24 | 119.90 |
| 23 | BA | 2450 | A | C6-N1-C2 | -5.57 | 115.26 | 118.60 |
| 23 | DA | 2279 | G | N1-C6-O6 | -5.57 | 116.56 | 119.90 |
| 23 | DA | 2698 | U | C5-C6-N1 | -5.57 | 119.92 | 122.70 |
| 24 | DB | 84 | C | C6-N1-C2 | -5.57 | 118.07 | 120.30 |
| 23 | BA | 180 | G | C8-N9-C4 | 5.56 | 108.62 | 106.40 |
| 23 | BA | 1769 | G | C4-N9-C1' | 5.56 | 133.73 | 126.50 |
| 23 | BA | 2700 | C | N1-C2-O2 | -5.56 | 115.56 | 118.90 |
| 23 | BA | 1576 | U | N3-C2-O2 | -5.56 | 118.31 | 122.20 |
| 23 | BA | 1839 | G | N9-C4-C5 | 5.56 | 107.62 | 105.40 |
| 23 | BA | 2614 | A | C5-C6-N1 | 5.56 | 120.48 | 117.70 |
| 23 | DA | 1496 | A | N7-C8-N9 | 5.56 | 116.58 | 113.80 |
| 23 | DA | 1692 | U | N3-C4-O4 | -5.56 | 115.51 | 119.40 |
| 23 | BA | 1270 | C | C2-N1-C1' | -5.56 | 112.69 | 118.80 |
| 23 | DA | 826 | U | C6-N1-C2 | 5.56 | 124.33 | 121.00 |
| 23 | DA | 2506 | U | N1-C2-O2 | 5.56 | 126.69 | 122.80 |
| 23 | DA | 2239 | G | C2-N3-C4 | -5.56 | 109.12 | 111.90 |
| 23 | DA | 2430 | A | C4-C5-N7 | 5.56 | 113.48 | 110.70 |
| 1 | AA | 768 | A | N1-C2-N3 | 5.55 | 132.08 | 129.30 |
| 23 | BA | 115 | C | C4-C5-C6 | 5.55 | 120.18 | 117.40 |
| 23 | BA | 2056 | G | N9-C4-C5 | -5.55 | 103.18 | 105.40 |
| 23 | DA | 2010 | G | C5-C6-O6 | -5.55 | 125.27 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | BA | 1443 | G | N9-C4-C5 | -5.55 | 103.18 | 105.40 |
| 23 | BA | 847 | U | N1-C2-O2 | -5.55 | 118.91 | 122.80 |
| 23 | BA | 1899 | G | N7-C8-N9 | 5.55 | 115.88 | 113.10 |
| 23 | DA | 85 | G | C8-N9-C4 | 5.55 | 108.62 | 106.40 |
| 23 | DA | 1191 | G | C4-C5-N7 | -5.55 | 108.58 | 110.80 |
| 23 | DA | 1665 | A | C6-C5-N7 | -5.55 | 128.41 | 132.30 |
| 23 | DA | 2542 | A | C8-N9-C4 | 5.55 | 108.02 | 105.80 |
| 23 | BA | 512 | G | C4-N9-C1' | -5.55 | 119.29 | 126.50 |
| 23 | DA | 194 | G | N7-C8-N9 | -5.55 | 110.33 | 113.10 |
| 23 | DA | 2417 | C | C5-C6-N1 | -5.55 | 118.22 | 121.00 |
| 23 | DA | 2235 | G | C4-C5-N7 | 5.55 | 113.02 | 110.80 |
| 23 | DA | 2827 | C | C6-N1-C2 | 5.55 | 122.52 | 120.30 |
| 23 | BA | 1402 | C | C6-N1-C2 | -5.55 | 118.08 | 120.30 |
| 23 | DA | 340 | A | C2-N3-C4 | -5.55 | 107.83 | 110.60 |
| 23 | BA | 1260 | G | C5-C6-N1 | 5.54 | 114.27 | 111.50 |
| 23 | BA | 2072 | G | C5-C6-N1 | -5.54 | 108.73 | 111.50 |
| 23 | DA | 1962 | C | N3-C2-O2 | -5.54 | 118.02 | 121.90 |
| 23 | BA | 214 | G | C8-N9-C1' | 5.54 | 134.20 | 127.00 |
| 23 | BA | 587 | C | C5-C4-N4 | 5.54 | 124.08 | 120.20 |
| 23 | DA | 73 | A | N1-C6-N6 | -5.54 | 115.28 | 118.60 |
| 23 | DA | 1287 | A | N1-C6-N6 | 5.54 | 121.92 | 118.60 |
| 23 | DA | 111 | A | C2-N3-C4 | -5.54 | 107.83 | 110.60 |
| 1 | AA | 1522 | U | C5-C4-O4 | 5.54 | 129.22 | 125.90 |
| 23 | BA | 213 | A | C8-N9-C4 | 5.54 | 108.02 | 105.80 |
| 23 | DA | 933 | A | N1-C6-N6 | 5.54 | 121.92 | 118.60 |
| 23 | DA | 239 | U | C2-N1-C1' | -5.54 | 111.06 | 117.70 |
| 23 | DA | 1232 | G | N1-C6-O6 | 5.54 | 123.22 | 119.90 |
| 23 | BA | 1128 | A | C8-N9-C4 | 5.53 | 108.01 | 105.80 |
| 23 | BA | 1328 | G | C4-C5-N7 | 5.53 | 113.01 | 110.80 |
| 23 | DA | 2081 | C | C6-N1-C2 | 5.53 | 122.51 | 120.30 |
| 23 | DA | 2426 | A | N7-C8-N9 | 5.53 | 116.57 | 113.80 |
| 23 | DA | 2441 | C | N1-C2-O2 | -5.53 | 115.58 | 118.90 |
| 23 | BA | 1780 | A | N1-C2-N3 | 5.53 | 132.07 | 129.30 |
| 23 | BA | 453 | C | N3-C4-N4 | 5.53 | 121.87 | 118.00 |
| 23 | BA | 2361 | A | C8-N9-C4 | 5.53 | 108.01 | 105.80 |
| 23 | DA | 2075 | U | C6-N1-C2 | 5.53 | 124.32 | 121.00 |
| 23 | BA | 794 | G | C2-N3-C4 | -5.53 | 109.14 | 111.90 |
| 23 | BA | 1349 | A | C4-C5-N7 | 5.53 | 113.46 | 110.70 |
| 1 | CA | 892 | A | C5-C6-N6 | -5.53 | 119.28 | 123.70 |
| 23 | BA | 1977 | A | C8-N9-C4 | 5.53 | 108.01 | 105.80 |
| 23 | BA | 2241 | A | C2-N3-C4 | -5.52 | 107.84 | 110.60 |
| 23 | BA | 2614 | A | C5-C6-N6 | -5.52 | 119.28 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | DA | 114(B) | A | C4-C5-N7 | 5.52 | 113.46 | 110.70 |
| 23 | DA | 2257 | U | N1-C2-O2 | -5.52 | 118.93 | 122.80 |
| 1 | AA | 576 | G | C8-N9-C1' | -5.52 | 119.83 | 127.00 |
| 23 | DA | 2042 | A | N1-C6-N6 | 5.52 | 121.91 | 118.60 |
| 23 | BA | 94 | G | N3-C4-C5 | -5.52 | 125.84 | 128.60 |
| 23 | DA | 216 | A | C4-C5-N7 | 5.52 | 113.46 | 110.70 |
| 23 | BA | 527 | C | N3-C4-C5 | 5.51 | 124.11 | 121.90 |
| 23 | DA | 799 | G | C5-C6-N1 | 5.51 | 114.26 | 111.50 |
| 23 | DA | 1855 | G | C8-N9-C4 | 5.51 | 108.61 | 106.40 |
| 23 | DA | 2544 | G | N9-C4-C5 | -5.51 | 103.19 | 105.40 |
| 23 | BA | 461 | C | N3-C2-O2 | 5.51 | 125.76 | 121.90 |
| 23 | DA | 2431 | U | C5-C6-N1 | -5.51 | 119.94 | 122.70 |
| 23 | BA | 83 | G | C8-N9-C4 | 5.51 | 108.60 | 106.40 |
| 23 | BA | 1976 | U | C6-N1-C2 | -5.51 | 117.69 | 121.00 |
| 23 | DA | 1791 | A | N9-C4-C5 | -5.51 | 103.60 | 105.80 |
| 1 | AA | 691 | G | C5-C6-O6 | -5.51 | 125.29 | 128.60 |
| 23 | BA | 1571 | A | C8-N9-C4 | 5.51 | 108.00 | 105.80 |
| 1 | CA | 918 | A | N9-C4-C5 | 5.51 | 108.00 | 105.80 |
| 23 | DA | 513 | A | N7-C8-N9 | 5.51 | 116.56 | 113.80 |
| 23 | DA | 825 | C | C4-C5-C6 | 5.51 | 120.16 | 117.40 |
| 23 | DA | 1496 | A | C4-N9-C1' | 5.51 | 136.22 | 126.30 |
| 23 | DA | 1960 | A | C8-N9-C4 | 5.51 | 108.00 | 105.80 |
| 23 | DA | 2521 | C | C5-C6-N1 | -5.51 | 118.25 | 121.00 |
| 23 | BA | 664 | C | C5-C6-N1 | -5.51 | 118.25 | 121.00 |
| 23 | BA | 844 | C | C2-N3-C4 | -5.51 | 117.15 | 119.90 |
| 23 | BA | 789 | A | C4-C5-N7 | 5.50 | 113.45 | 110.70 |
| 23 | BA | 676 | A | C6-N1-C2 | 5.50 | 121.90 | 118.60 |
| 23 | BA | 1286 | A | N9-C4-C5 | 5.50 | 108.00 | 105.80 |
| 23 | BA | 2646 | C | N1-C2-O2 | -5.50 | 115.60 | 118.90 |
| 1 | CA | 695 | A | C2-N3-C4 | -5.50 | 107.85 | 110.60 |
| 1 | CA | 1524 | C | C6-N1-C2 | 5.50 | 122.50 | 120.30 |
| 23 | DA | 409 | C | C6-N1-C2 | 5.50 | 122.50 | 120.30 |
| 23 | DA | 1983 | C | C5-C6-N1 | -5.50 | 118.25 | 121.00 |
| 23 | DA | 2635 | C | C5-C6-N1 | -5.50 | 118.25 | 121.00 |
| 23 | BA | 1840 | G | N1-C6-O6 | 5.50 | 123.20 | 119.90 |
| 23 | DA | 1670 | C | N1-C2-O2 | -5.50 | 115.60 | 118.90 |
| 23 | BA | 23 | G | N3-C2-N2 | -5.50 | 116.05 | 119.90 |
| 23 | DA | 1622 | G | N1-C2-N3 | 5.50 | 127.20 | 123.90 |
| 23 | DA | 2022 | U | C5-C4-O4 | -5.50 | 122.60 | 125.90 |
| 23 | DA | 2702 | U | C5-C6-N1 | -5.50 | 119.95 | 122.70 |
| 23 | BA | 972 | G | N3-C4-N9 | 5.49 | 129.30 | 126.00 |
| 23 | DA | 2044 | C | C6-N1-C2 | 5.49 | 122.50 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | DA | 148 | C | C2-N3-C4 | -5.49 | 117.15 | 119.90 |
| 23 | DA | 737 | C | C5-C4-N4 | -5.49 | 116.36 | 120.20 |
| 23 | BA | 2053 | G | C2-N3-C4 | -5.49 | 109.16 | 111.90 |
| 23 | DA | 734 | A | N9-C4-C5 | -5.49 | 103.60 | 105.80 |
| 23 | BA | 564 | C | N3-C4-C5 | -5.49 | 119.70 | 121.90 |
| 23 | BA | 804 | A | C6-N1-C2 | -5.49 | 115.31 | 118.60 |
| 23 | DA | 1832 | C | C5-C6-N1 | -5.49 | 118.26 | 121.00 |
| 1 | AA | 720 | C | C2-N1-C1' | 5.48 | 124.83 | 118.80 |
| 23 | DA | 1295 | C | C5-C6-N1 | -5.48 | 118.26 | 121.00 |
| 23 | BA | 1616 | A | C5-N7-C8 | -5.48 | 101.16 | 103.90 |
| 23 | DA | 388 | G | C6-C5-N7 | 5.48 | 133.69 | 130.40 |
| 23 | DA | 1157 | G | N1-C6-O6 | 5.48 | 123.19 | 119.90 |
| 23 | BA | 2005 | A | N1-C6-N6 | 5.48 | 121.89 | 118.60 |
| 1 | CA | 799 | G | N1-C6-O6 | 5.48 | 123.19 | 119.90 |
| 23 | DA | 1704 | G | C8-N9-C4 | 5.48 | 108.59 | 106.40 |
| 23 | BA | 36 | G | C4-C5-N7 | -5.48 | 108.61 | 110.80 |
| 23 | BA | 126 | A | N1-C6-N6 | 5.48 | 121.89 | 118.60 |
| 23 | BA | 571 | A | C8-N9-C4 | -5.48 | 103.61 | 105.80 |
| 23 | BA | 408 | G | N3-C4-C5 | 5.48 | 131.34 | 128.60 |
| 23 | BA | 589 | C | N1-C2-O2 | -5.48 | 115.61 | 118.90 |
| 23 | DA | 1782 | C | N1-C2-O2 | 5.48 | 122.19 | 118.90 |
| 23 | BA | 334 | C | N1-C2-O2 | -5.47 | 115.62 | 118.90 |
| 23 | BA | 845 | G | C4-N9-C1' | 5.47 | 133.62 | 126.50 |
| 23 | BA | 1190 | G | N1-C6-O6 | 5.47 | 123.19 | 119.90 |
| 23 | BA | 2076 | U | C5-C4-O4 | 5.47 | 129.18 | 125.90 |
| 23 | DA | 513 | A | N1-C2-N3 | 5.47 | 132.04 | 129.30 |
| 23 | DA | 114(B) | A | C5-C6-N1 | -5.47 | 114.96 | 117.70 |
| 23 | DA | 1683 | C | N1-C2-O2 | -5.47 | 115.61 | 118.90 |
| 23 | DA | 2085 | C | C5-C6-N1 | -5.47 | 118.26 | 121.00 |
| 23 | BA | 768 | G | C4-C5-C6 | 5.47 | 122.08 | 118.80 |
| 23 | BA | 786 | C | C5-C6-N1 | -5.47 | 118.26 | 121.00 |
| 23 | DA | 2358 | G | C8-N9-C4 | -5.47 | 104.21 | 106.40 |
| 12 | AL | 9 | LEU | CA-CB-CG | -5.47 | 102.72 | 115.30 |
| 23 | DA | 1830 | C | C5-C4-N4 | -5.47 | 116.37 | 120.20 |
| 23 | BA | 675 | A | C5-C6-N1 | -5.47 | 114.97 | 117.70 |
| 23 | BA | 2719 | G | C4-C5-N7 | 5.47 | 112.99 | 110.80 |
| 23 | DA | 784 | A | N3-C4-N9 | -5.47 | 123.02 | 127.40 |
| 23 | DA | 1657 | C | N1-C2-O2 | -5.47 | 115.62 | 118.90 |
| 23 | BA | 2513 | G | N1-C6-O6 | -5.47 | 116.62 | 119.90 |
| 1 | AA | 55 | A | C8-N9-C4 | -5.47 | 103.61 | 105.80 |
| 23 | BA | 2634 | G | N7-C8-N9 | -5.47 | 110.37 | 113.10 |
| 1 | CA | 35 | G | N1-C6-O6 | 5.47 | 123.18 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 23 | DA | 2676 | C | N1-C2-O2 | -5.47 | 115.62 | 118.90 |
| 23 | BA | 512 | G | N1-C6-O6 | -5.46 | 116.62 | 119.90 |
| 23 | DA | 512 | G | N3-C4-N9 | -5.46 | 122.72 | 126.00 |
| 23 | DA | 2007 | C | C2-N3-C4 | -5.46 | 117.17 | 119.90 |
| 23 | BA | 94 | G | N3-C4-N9 | 5.46 | 129.28 | 126.00 |
| 23 | BA | 1309 | G | N1-C6-O6 | 5.46 | 123.18 | 119.90 |
| 23 | BA | 2556 | C | N3-C4-N4 | 5.46 | 121.82 | 118.00 |
| 23 | DA | 681 | G | C8-N9-C4 | 5.46 | 108.58 | 106.40 |
| 23 | DA | 2254 | C | N1-C2-O2 | -5.46 | 115.62 | 118.90 |
| 1 | AA | 1484 | C | C6-N1-C2 | 5.46 | 122.48 | 120.30 |
| 23 | DA | 1368 | G | C5-C6-N1 | 5.46 | 114.23 | 111.50 |
| 23 | BA | 2244 | U | N3-C2-O2 | -5.46 | 118.38 | 122.20 |
| 23 | BA | 2601 | C | C6-N1-C2 | 5.46 | 122.48 | 120.30 |
| 23 | BA | 2619 | C | C5-C6-N1 | -5.46 | 118.27 | 121.00 |
| 23 | DA | 1604 | C | N3-C4-N4 | 5.46 | 121.82 | 118.00 |
| 25 | BC | 46 | GLN | N-CA-C | -5.46 | 96.27 | 111.00 |
| 1 | CA | 117 | G | C5-C6-O6 | -5.46 | 125.33 | 128.60 |
| 23 | DA | 802 | A | N1-C2-N3 | 5.46 | 132.03 | 129.30 |
| 23 | BA | 494 | G | C8-N9-C4 | 5.45 | 108.58 | 106.40 |
| 23 | BA | 1235 | G | C5-C6-N1 | -5.45 | 108.77 | 111.50 |
| 23 | DA | 261 | G | N1-C6-O6 | 5.45 | 123.17 | 119.90 |
| 23 | DA | 1669 | A | C8-N9-C4 | -5.45 | 103.62 | 105.80 |
| 23 | DA | 1839 | G | N3-C2-N2 | -5.45 | 116.08 | 119.90 |
| 23 | BA | 71 | A | C2-N3-C4 | -5.45 | 107.88 | 110.60 |
| 23 | DA | 333 | G | N1-C6-O6 | 5.45 | 123.17 | 119.90 |
| 23 | DA | 1294 | U | N3-C2-O2 | -5.45 | 118.39 | 122.20 |
| 23 | DA | 1325 | G | C6-C5-N7 | 5.45 | 133.67 | 130.40 |
| 23 | BA | 722 | A | C2-N3-C4 | -5.45 | 107.88 | 110.60 |
| 23 | DA | 749 | C | N3-C4-C5 | 5.45 | 124.08 | 121.90 |
| 23 | DA | 1982 | C | N1-C2-O2 | -5.45 | 115.63 | 118.90 |
| 23 | DA | 249 | C | C6-N1-C2 | 5.45 | 122.48 | 120.30 |
| 23 | BA | 1677 | A | N1-C2-N3 | 5.45 | 132.02 | 129.30 |
| 23 | BA | 2708 | G | C5-C6-N1 | -5.45 | 108.78 | 111.50 |
| 23 | DA | 1902 | C | C5-C6-N1 | -5.45 | 118.28 | 121.00 |
| 1 | AA | 1432 | G | C5-C6-N1 | -5.44 | 108.78 | 111.50 |
| 23 | BA | 774 | A | N1-C2-N3 | 5.44 | 132.02 | 129.30 |
| 23 | DA | 2000 | G | N1-C6-O6 | -5.44 | 116.63 | 119.90 |
| 1 | AA | 45 | U | C6-N1-C2 | 5.44 | 124.27 | 121.00 |
| 1 | AA | 1414 | U | C6-N1-C2 | 5.44 | 124.27 | 121.00 |
| 23 | BA | 972 | G | N3-C4-C5 | -5.44 | 125.88 | 128.60 |
| 23 | BA | 2253 | G | C6-C5-N7 | -5.44 | 127.13 | 130.40 |
| 23 | DA | 2061 | G | C6-C5-N7 | -5.44 | 127.13 | 130.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | DA | 466 | A | C8-N9-C4 | 5.44 | 107.98 | 105.80 |
| 23 | DA | 1624 | G | C6-N1-C2 | -5.44 | 121.83 | 125.10 |
| 23 | DA | 1964 | G | N3-C4-N9 | 5.44 | 129.26 | 126.00 |
| 23 | BA | 104 | U | C2-N1-C1' | -5.44 | 111.17 | 117.70 |
| 23 | BA | 1271 | G | C8-N9-C1' | -5.44 | 119.93 | 127.00 |
| 23 | BA | 150 | C | C6-N1-C2 | 5.44 | 122.47 | 120.30 |
| 23 | DA | 915 | C | C5-C6-N1 | 5.44 | 123.72 | 121.00 |
| 23 | BA | 1616 | A | C2-N3-C4 | -5.43 | 107.88 | 110.60 |
| 23 | DA | 512 | G | C4-N9-C1' | -5.43 | 119.44 | 126.50 |
| 23 | DA | 2448 | A | C6-C5-N7 | -5.43 | 128.50 | 132.30 |
| 23 | DA | 2648 | C | C2-N1-C1' | -5.43 | 112.82 | 118.80 |
| 23 | DA | 2766 | G | C4-N9-C1' | 5.43 | 133.57 | 126.50 |
| 23 | BA | 807 | U | N1-C2-N3 | 5.43 | 118.16 | 114.90 |
| 23 | BA | 1991 | U | C5-C6-N1 | -5.43 | 119.98 | 122.70 |
| 23 | DA | 1332 | G | C6-C5-N7 | 5.43 | 133.66 | 130.40 |
| 23 | BA | 1763 | G | C2-N3-C4 | -5.43 | 109.19 | 111.90 |
| 23 | DA | 1689 | A | N1-C6-N6 | -5.43 | 115.34 | 118.60 |
| 23 | DA | 387 | U | N3-C4-O4 | 5.43 | 123.20 | 119.40 |
| 23 | BA | 1516 | U | N3-C2-O2 | -5.43 | 118.40 | 122.20 |
| 23 | DA | 979 | G | N7-C8-N9 | 5.43 | 115.81 | 113.10 |
| 23 | DA | 2253 | G | C6-C5-N7 | -5.43 | 127.14 | 130.40 |
| 23 | DA | 2544 | G | C4-C5-N7 | 5.43 | 112.97 | 110.80 |
| 1 | AA | 327 | A | C8-N9-C4 | -5.43 | 103.63 | 105.80 |
| 1 | CA | 1523 | G | C8-N9-C4 | 5.43 | 108.57 | 106.40 |
| 23 | DA | 116 | C | N1-C2-O2 | -5.43 | 115.64 | 118.90 |
| 23 | BA | 58 | G | C8-N9-C1' | -5.42 | 119.95 | 127.00 |
| 23 | BA | 2028 | U | N1-C2-O2 | -5.42 | 119.00 | 122.80 |
| 1 | CA | 791 | G | C8-N9-C4 | 5.42 | 108.57 | 106.40 |
| 23 | BA | 239 | U | N1-C2-O2 | -5.42 | 119.00 | 122.80 |
| 23 | BA | 510 | C | N1-C2-O2 | -5.42 | 115.65 | 118.90 |
| 23 | BA | 799 | G | C5-C6-O6 | -5.42 | 125.35 | 128.60 |
| 23 | BA | 1994 | C | C5-C6-N1 | -5.42 | 118.29 | 121.00 |
| 23 | DA | 2498 | C | N1-C2-O2 | -5.42 | 115.65 | 118.90 |
| 23 | DA | 694 | U | N1-C2-O2 | 5.42 | 126.59 | 122.80 |
| 23 | DA | 1213 | A | C8-N9-C4 | 5.42 | 107.97 | 105.80 |
| 23 | DA | 1323 | U | C4-C5-C6 | 5.42 | 122.95 | 119.70 |
| 23 | DA | 1302 | A | C4-C5-N7 | -5.42 | 107.99 | 110.70 |
| 23 | DA | 2544 | G | C8-N9-C4 | 5.42 | 108.57 | 106.40 |
| 1 | AA | 1527 | C | C6-N1-C2 | 5.41 | 122.47 | 120.30 |
| 23 | BA | 2675 | A | C8-N9-C4 | 5.41 | 107.97 | 105.80 |
| 23 | DA | 286 | C | C6-N1-C2 | 5.41 | 122.47 | 120.30 |
| 23 | DA | 1403 | C | C2-N3-C4 | -5.41 | 117.19 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | DA | 1572 | A | N9-C4-C5 | -5.41 | 103.64 | 105.80 |
| 23 | DA | 444 | C | C2-N1-C1' | -5.41 | 112.85 | 118.80 |
| 23 | DA | 1842 | G | C8-N9-C4 | 5.41 | 108.56 | 106.40 |
| 23 | BA | 2502 | G | N9-C4-C5 | -5.41 | 103.24 | 105.40 |
| 23 | DA | 258 | G | N1-C6-O6 | 5.41 | 123.14 | 119.90 |
| 23 | DA | 936 | C | C5-C6-N1 | -5.41 | 118.30 | 121.00 |
| 23 | DA | 130 | C | C2-N3-C4 | -5.41 | 117.20 | 119.90 |
| 23 | BA | 2249 | U | C6-N1-C2 | -5.41 | 117.76 | 121.00 |
| 23 | DA | 2590 | A | C2-N3-C4 | -5.41 | 107.90 | 110.60 |
| 23 | BA | 193 | U | C5-C6-N1 | -5.40 | 120.00 | 122.70 |
| 23 | BA | 723 | G | C8-N9-C4 | 5.40 | 108.56 | 106.40 |
| 23 | DA | 968 | G | C8-N9-C4 | 5.40 | 108.56 | 106.40 |
| 23 | BA | 208 | C | C6-N1-C2 | 5.40 | 122.46 | 120.30 |
| 23 | BA | 1789 | A | C5-C6-N1 | 5.40 | 120.40 | 117.70 |
| 23 | DA | 271(B) | C | C6-N1-C2 | 5.40 | 122.46 | 120.30 |
| 23 | DA | 461 | C | N3-C2-O2 | 5.40 | 125.68 | 121.90 |
| 23 | DA | 793 | A | C8-N9-C4 | -5.40 | 103.64 | 105.80 |
| 23 | DA | 2619 | C | C2-N1-C1' | -5.40 | 112.86 | 118.80 |
| 23 | BA | 397 | G | C6-C5-N7 | -5.40 | 127.16 | 130.40 |
| 23 | BA | 1496 | A | N7-C8-N9 | 5.40 | 116.50 | 113.80 |
| 1 | CA | 503 | C | C5-C6-N1 | 5.40 | 123.70 | 121.00 |
| 23 | DA | 204 | A | C8-N9-C4 | 5.40 | 107.96 | 105.80 |
| 1 | AA | 577 | G | C8-N9-C4 | 5.40 | 108.56 | 106.40 |
| 1 | AA | 766 | A | N1-C6-N6 | 5.40 | 121.84 | 118.60 |
| 23 | BA | 594 | U | C4-C5-C6 | 5.40 | 122.94 | 119.70 |
| 23 | BA | 845 | G | N3-C4-N9 | 5.40 | 129.24 | 126.00 |
| 23 | DA | 729 | G | C4-N9-C1' | 5.40 | 133.52 | 126.50 |
| 23 | DA | 2383 | G | C4-N9-C1' | 5.39 | 133.51 | 126.50 |
| 23 | BA | 124 | G | N1-C6-O6 | 5.39 | 123.14 | 119.90 |
| 25 | BC | 242 | ARG | N-CA-C | -5.39 | 96.44 | 111.00 |
| 23 | DA | 1204 | A | N7-C8-N9 | 5.39 | 116.50 | 113.80 |
| 23 | DA | 2392 | A | N7-C8-N9 | 5.39 | 116.50 | 113.80 |
| 23 | DA | 2519 | U | C5-C6-N1 | -5.39 | 120.00 | 122.70 |
| 23 | BA | 309 | G | N1-C6-O6 | 5.39 | 123.13 | 119.90 |
| 23 | BA | 459 | U | C5-C6-N1 | -5.39 | 120.01 | 122.70 |
| 1 | CA | 899 | C | C6-N1-C2 | 5.39 | 122.46 | 120.30 |
| 23 | DA | 2841 | C | C6-N1-C2 | 5.39 | 122.46 | 120.30 |
| 23 | DA | 976 | C | C5-C6-N1 | -5.39 | 118.31 | 121.00 |
| 23 | DA | 1646 | C | C6-N1-C2 | 5.39 | 122.45 | 120.30 |
| 23 | DA | 2846 | G | C4-C5-N7 | 5.39 | 112.95 | 110.80 |
| 23 | BA | 535 | C | N1-C2-O2 | -5.39 | 115.67 | 118.90 |
| 23 | BA | 1290 | C | C5-C6-N1 | -5.39 | 118.31 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | DA | 312 | G | C8-N9-C4 | 5.39 | 108.56 | 106.40 |
| 23 | DA | 1521 | G | C8-N9-C4 | -5.39 | 104.25 | 106.40 |
| 23 | DA | 1802 | A | C4-C5-C6 | 5.39 | 119.69 | 117.00 |
| 23 | DA | 2253 | G | C8-N9-C1' | -5.39 | 120.00 | 127.00 |
| 23 | BA | 1683 | C | N3-C2-O2 | 5.38 | 125.67 | 121.90 |
| 1 | CA | 918 | A | C8-N9-C4 | -5.38 | 103.65 | 105.80 |
| 23 | BA | 1628 | G | N1-C6-O6 | 5.38 | 123.13 | 119.90 |
| 23 | BA | 602 | G | C6-C5-N7 | 5.38 | 133.63 | 130.40 |
| 23 | BA | 1204 | A | C6-C5-N7 | -5.38 | 128.53 | 132.30 |
| 23 | DA | 211 | A | N7-C8-N9 | -5.38 | 111.11 | 113.80 |
| 23 | DA | 814 | C | C5-C6-N1 | -5.38 | 118.31 | 121.00 |
| 23 | DA | 993 | G | C6-C5-N7 | 5.38 | 133.63 | 130.40 |
| 23 | BA | 83 | G | C6-N1-C2 | 5.38 | 128.33 | 125.10 |
| 23 | DA | 1801 | G | C4-C5-N7 | 5.38 | 112.95 | 110.80 |
| 23 | BA | 1244 | G | N7-C8-N9 | -5.38 | 110.41 | 113.10 |
| 23 | DA | 375 | C | C5-C6-N1 | -5.38 | 118.31 | 121.00 |
| 23 | DA | 1309 | G | N7-C8-N9 | -5.38 | 110.41 | 113.10 |
| 23 | DA | 1423 | G | C8-N9-C4 | 5.38 | 108.55 | 106.40 |
| 23 | DA | 1662 | C | N1-C2-N3 | 5.38 | 122.97 | 119.20 |
| 23 | BA | 682 | G | N1-C6-O6 | -5.38 | 116.67 | 119.90 |
| 23 | BA | 2061 | G | N1-C6-O6 | 5.38 | 123.13 | 119.90 |
| 23 | BA | 2496 | C | N3-C2-O2 | -5.38 | 118.14 | 121.90 |
| 23 | DA | 1792 | G | N9-C4-C5 | 5.38 | 107.55 | 105.40 |
| 23 | BA | 1792 | G | C8-N9-C4 | -5.38 | 104.25 | 106.40 |
| 23 | DA | 1600 | C | N3-C2-O2 | 5.38 | 125.66 | 121.90 |
| 23 | BA | 956 | G | C8-N9-C4 | 5.37 | 108.55 | 106.40 |
| 23 | BA | 1934 | C | C2-N1-C1' | -5.37 | 112.89 | 118.80 |
| 23 | DA | 1698 | A | N7-C8-N9 | 5.37 | 116.49 | 113.80 |
| 23 | DA | 2592 | G | C6-N1-C2 | -5.37 | 121.88 | 125.10 |
| 23 | DA | 1164 | G | C8-N9-C1' | -5.37 | 120.02 | 127.00 |
| 23 | BA | 2044 | C | C5-C4-N4 | -5.37 | 116.44 | 120.20 |
| 23 | BA | 2688 | U | N3-C4-O4 | -5.37 | 115.64 | 119.40 |
| 23 | DA | 55 | G | C6-N1-C2 | -5.37 | 121.88 | 125.10 |
| 23 | BA | 2596 | U | C5-C4-O4 | 5.37 | 129.12 | 125.90 |
| 23 | DA | 681 | G | N7-C8-N9 | -5.37 | 110.42 | 113.10 |
| 23 | DA | 798 | G | C5-C6-O6 | -5.37 | 125.38 | 128.60 |
| 25 | DC | 46 | GLN | N-CA-C | -5.37 | 96.50 | 111.00 |
| 23 | BA | 1286 | A | C4-C5-N7 | -5.37 | 108.02 | 110.70 |
| 23 | DA | 1980 | G | N1-C2-N2 | -5.37 | 111.37 | 116.20 |
| 23 | BA | 1264 | G | C8-N9-C4 | -5.37 | 104.25 | 106.40 |
| 23 | DA | 138 | G | N7-C8-N9 | 5.37 | 115.78 | 113.10 |
| 1 | AA | 562 | C | N3-C4-C5 | 5.36 | 124.05 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | BA | 1616 | A | C4-C5-N7 | 5.36 | 113.38 | 110.70 |
| 23 | BA | 2005 | A | C8-N9-C4 | 5.36 | 107.94 | 105.80 |
| 23 | DA | 704 | G | C5-C6-O6 | -5.36 | 125.38 | 128.60 |
| 23 | BA | 1788 | C | N3-C4-C5 | 5.36 | 124.04 | 121.90 |
| 23 | DA | 298 | G | N7-C8-N9 | 5.36 | 115.78 | 113.10 |
| 23 | DA | 1555 | G | C4-N9-C1' | 5.36 | 133.47 | 126.50 |
| 23 | DA | 2824 | C | N1-C2-O2 | -5.36 | 115.68 | 118.90 |
| 23 | BA | 1161 | C | C5-C6-N1 | 5.36 | 123.68 | 121.00 |
| 23 | DA | 1268 | A | N1-C2-N3 | 5.36 | 131.98 | 129.30 |
| 23 | BA | 272 | G | C4-N9-C1' | -5.36 | 119.53 | 126.50 |
| 23 | BA | 1385 | G | C8-N9-C1' | 5.36 | 133.97 | 127.00 |
| 23 | DA | 2713 | A | N1-C2-N3 | 5.36 | 131.98 | 129.30 |
| 1 | AA | 266 | G | N3-C4-C5 | 5.36 | 131.28 | 128.60 |
| 23 | BA | 746 | A | C5-C6-N1 | 5.36 | 120.38 | 117.70 |
| 23 | BA | 1555 | G | C4-N9-C1' | 5.36 | 133.46 | 126.50 |
| 23 | BA | 2022 | U | N1-C2-N3 | -5.36 | 111.69 | 114.90 |
| 23 | DA | 489 | G | C8-N9-C4 | -5.36 | 104.26 | 106.40 |
| 23 | DA | 1429 | G | C5-C6-O6 | 5.36 | 131.81 | 128.60 |
| 23 | DA | 2219 | G | C8-N9-C4 | 5.36 | 108.54 | 106.40 |
| 23 | DA | 2743 | C | N1-C2-O2 | -5.36 | 115.69 | 118.90 |
| 23 | DA | 841 | A | C5-C6-N1 | 5.35 | 120.38 | 117.70 |
| 23 | DA | 2082 | A | C5-C6-N6 | -5.35 | 119.42 | 123.70 |
| 1 | AA | 1480 | G | C5-C6-O6 | -5.35 | 125.39 | 128.60 |
| 23 | BA | 1783 | A | N1-C2-N3 | 5.35 | 131.98 | 129.30 |
| 23 | BA | 2447 | G | C5-C6-O6 | -5.35 | 125.39 | 128.60 |
| 23 | BA | 2507 | C | N3-C4-N4 | -5.35 | 114.25 | 118.00 |
| 23 | DA | 83 | G | C6-N1-C2 | 5.35 | 128.31 | 125.10 |
| 23 | DA | 2010 | G | C5-N7-C8 | -5.35 | 101.62 | 104.30 |
| 23 | DA | 586 | A | N9-C4-C5 | -5.35 | 103.66 | 105.80 |
| 23 | DA | 1802 | A | C6-N1-C2 | -5.35 | 115.39 | 118.60 |
| 23 | BA | 1385 | G | N3-C4-N9 | -5.35 | 122.79 | 126.00 |
| 23 | DA | 661 | C | C2-N3-C4 | -5.35 | 117.22 | 119.90 |
| 23 | BA | 434 | U | N3-C2-O2 | 5.35 | 125.94 | 122.20 |
| 23 | DA | 133 | C | C2-N3-C4 | -5.35 | 117.23 | 119.90 |
| 23 | BA | 773 | U | N1-C2-O2 | -5.35 | 119.06 | 122.80 |
| 23 | BA | 797 | C | C5-C6-N1 | -5.35 | 118.33 | 121.00 |
| 23 | BA | 208 | C | N3-C4-C5 | 5.34 | 124.04 | 121.90 |
| 23 | DA | 729 | G | C6-C5-N7 | -5.34 | 127.19 | 130.40 |
| 23 | DA | 2748 | A | C8-N9-C4 | -5.34 | 103.66 | 105.80 |
| 23 | BA | 578 | A | N1-C6-N6 | -5.34 | 115.39 | 118.60 |
| 23 | BA | 1163 | G | N3-C2-N2 | -5.34 | 116.16 | 119.90 |
| 23 | DA | 967 | C | C5-C6-N1 | -5.34 | 118.33 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | DA | 2208 | U | N3-C2-O2 | 5.34 | 125.94 | 122.20 |
| 23 | DA | 2324 | C | N3-C4-N4 | -5.34 | 114.26 | 118.00 |
| 23 | BA | 1022 | G | C8-N9-C4 | -5.34 | 104.27 | 106.40 |
| 23 | DA | 322 | A | C8-N9-C4 | -5.34 | 103.67 | 105.80 |
| 23 | DA | 827 | U | C6-N1-C2 | 5.34 | 124.20 | 121.00 |
| 23 | DA | 2514 | U | C6-N1-C2 | 5.34 | 124.20 | 121.00 |
| 23 | DA | 2707 | G | C8-N9-C4 | 5.34 | 108.53 | 106.40 |
| 23 | BA | 1555 | G | N3-C4-N9 | 5.33 | 129.20 | 126.00 |
| 23 | BA | 1400 | G | N3-C4-C5 | -5.33 | 125.93 | 128.60 |
| 23 | BA | 1496 | A | C4-N9-C1' | 5.33 | 135.90 | 126.30 |
| 23 | BA | 2280 | G | C2-N3-C4 | 5.33 | 114.57 | 111.90 |
| 23 | DA | 179 | G | N1-C6-O6 | 5.33 | 123.10 | 119.90 |
| 23 | DA | 2081 | C | C2-N3-C4 | -5.33 | 117.23 | 119.90 |
| 23 | BA | 1937 | A | C2-N3-C4 | -5.33 | 107.93 | 110.60 |
| 23 | BA | 2840 | C | C6-N1-C2 | 5.33 | 122.43 | 120.30 |
| 1 | CA | 17 | U | N3-C2-O2 | -5.33 | 118.47 | 122.20 |
| 23 | DA | 2075 | U | C5-C6-N1 | -5.33 | 120.03 | 122.70 |
| 23 | DA | 2826 | A | N1-C2-N3 | 5.33 | 131.97 | 129.30 |
| 23 | BA | 1495 | A | N1-C2-N3 | -5.33 | 126.64 | 129.30 |
| 23 | BA | 2507 | C | C5-C6-N1 | -5.33 | 118.33 | 121.00 |
| 23 | DA | 2007 | C | C6-N1-C2 | 5.33 | 122.43 | 120.30 |
| 46 | DX | 29 | GLY | N-CA-C | -5.33 | 99.78 | 113.10 |
| 23 | DA | 459 | U | C5-C6-N1 | -5.33 | 120.04 | 122.70 |
| 23 | BA | 1617 | C | C6-N1-C2 | 5.33 | 122.43 | 120.30 |
| 23 | DA | 1317 | A | C8-N9-C4 | 5.33 | 107.93 | 105.80 |
| 23 | BA | 211 | A | C8-N9-C4 | 5.32 | 107.93 | 105.80 |
| 23 | BA | 1791 | A | C8-N9-C4 | 5.32 | 107.93 | 105.80 |
| 23 | DA | 727 | A | N1-C6-N6 | 5.32 | 121.79 | 118.60 |
| 23 | DA | 1700 | A | N1-C6-N6 | 5.32 | 121.80 | 118.60 |
| 23 | DA | 1348 | G | C4-C5-N7 | 5.32 | 112.93 | 110.80 |
| 23 | DA | 1606 | G | C5-C6-N1 | 5.32 | 114.16 | 111.50 |
| 23 | DA | 1790 | C | N3-C4-N4 | -5.32 | 114.28 | 118.00 |
| 23 | DA | 2232 | U | N3-C4-C5 | -5.32 | 111.41 | 114.60 |
| 23 | DA | 2519 | U | C6-N1-C2 | 5.32 | 124.19 | 121.00 |
| 23 | BA | 1191 | G | N1-C6-O6 | -5.32 | 116.71 | 119.90 |
| 23 | BA | 1664 | A | C2-N3-C4 | -5.32 | 107.94 | 110.60 |
| 23 | DA | 151 | C | C6-N1-C2 | 5.32 | 122.43 | 120.30 |
| 23 | DA | 707 | G | C8-N9-C4 | 5.32 | 108.53 | 106.40 |
| 23 | DA | 2419 | U | C5-C4-O4 | 5.32 | 129.09 | 125.90 |
| 23 | DA | 1286 | A | N1-C6-N6 | -5.32 | 115.41 | 118.60 |
| 23 | DA | 2005 | A | C5-C6-N1 | -5.32 | 115.04 | 117.70 |
| 23 | BA | 2056 | G | C8-N9-C1' | -5.32 | 120.09 | 127.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | CA | 34 | C | C6-N1-C2 | 5.32 | 122.43 | 120.30 |
| 1 | CA | 926 | G | C4-C5-N7 | -5.32 | 108.67 | 110.80 |
| 23 | DA | 2433 | A | C5-N7-C8 | -5.32 | 101.24 | 103.90 |
| 23 | BA | 583 | G | C5-C6-N1 | 5.32 | 114.16 | 111.50 |
| 23 | BA | 1200 | C | N3-C2-O2 | 5.32 | 125.62 | 121.90 |
| 23 | BA | 1671 | U | N1-C2-O2 | -5.32 | 119.08 | 122.80 |
| 23 | DA | 2227 | A | N3-C4-N9 | -5.32 | 123.15 | 127.40 |
| 23 | DA | 1843 | C | C2-N3-C4 | -5.31 | 117.24 | 119.90 |
| 23 | DA | 2397 | G | C6-C5-N7 | -5.31 | 127.21 | 130.40 |
| 23 | DA | 2762 | G | N1-C6-O6 | 5.31 | 123.09 | 119.90 |
| 34 | DL | 54 | GLY | N-CA-C | -5.31 | 99.82 | 113.10 |
| 23 | BA | 1342 | A | C4-C5-N7 | 5.31 | 113.36 | 110.70 |
| 23 | BA | 2004 | G | N1-C6-O6 | 5.31 | 123.09 | 119.90 |
| 23 | DA | 958 | U | C2-N1-C1' | 5.31 | 124.08 | 117.70 |
| 23 | DA | 1327 | C | N3-C4-C5 | -5.31 | 119.78 | 121.90 |
| 23 | BA | 661 | C | C5-C6-N1 | -5.31 | 118.34 | 121.00 |
| 23 | BA | 1765 | C | N1-C2-O2 | -5.31 | 115.71 | 118.90 |
| 23 | BA | 2519 | U | C5-C6-N1 | -5.31 | 120.05 | 122.70 |
| 23 | DA | 408 | G | N3-C4-C5 | 5.31 | 131.25 | 128.60 |
| 23 | BA | 211 | A | N7-C8-N9 | -5.31 | 111.15 | 113.80 |
| 23 | DA | 197 | A | C5-C6-N6 | -5.31 | 119.45 | 123.70 |
| 23 | DA | 300 | A | N1-C6-N6 | 5.31 | 121.78 | 118.60 |
| 23 | DA | 1164 | G | C4-N9-C1' | 5.31 | 133.40 | 126.50 |
| 1 | AA | 1192 | C | C5-C6-N1 | 5.31 | 123.65 | 121.00 |
| 23 | BA | 1775 | U | N3-C4-O4 | -5.31 | 115.69 | 119.40 |
| 1 | AA | 1053 | G | N3-C4-C5 | 5.30 | 131.25 | 128.60 |
| 23 | BA | 1971 | A | C5-C6-N6 | -5.30 | 119.46 | 123.70 |
| 23 | DA | 2828 | C | C6-N1-C2 | 5.30 | 122.42 | 120.30 |
| 23 | BA | 2345 | G | C5-C6-O6 | 5.30 | 131.78 | 128.60 |
| 23 | DA | 138 | G | C5-C6-N1 | 5.30 | 114.15 | 111.50 |
| 23 | BA | 116 | C | C4-C5-C6 | 5.30 | 120.05 | 117.40 |
| 23 | DA | 115 | C | C2-N3-C4 | -5.30 | 117.25 | 119.90 |
| 23 | DA | 2271 | G | C8-N9-C1' | -5.30 | 120.11 | 127.00 |
| 23 | BA | 1964 | G | C8-N9-C1' | -5.30 | 120.11 | 127.00 |
| 23 | BA | 1204 | A | C4-C5-N7 | 5.30 | 113.35 | 110.70 |
| 23 | DA | 1802 | A | C8-N9-C4 | -5.30 | 103.68 | 105.80 |
| 23 | BA | 126 | A | C8-N9-C4 | 5.30 | 107.92 | 105.80 |
| 23 | BA | 945 | A | N9-C4-C5 | -5.30 | 103.68 | 105.80 |
| 23 | BA | 2688 | U | C5-C6-N1 | -5.30 | 120.05 | 122.70 |
| 23 | DA | 1400 | G | N3-C4-C5 | -5.30 | 125.95 | 128.60 |
| 23 | DA | 1613 | G | N1-C2-N2 | -5.30 | 111.43 | 116.20 |
| 23 | DA | 2250 | G | N9-C4-C5 | 5.30 | 107.52 | 105.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | DA | 811 | U | C2-N1-C1' | -5.29 | 111.35 | 117.70 |
| 23 | DA | 180 | G | N9-C4-C5 | -5.29 | 103.28 | 105.40 |
| 23 | DA | 334 | C | N1-C2-O2 | -5.29 | 115.72 | 118.90 |
| 23 | DA | 1268 | A | C6-N1-C2 | -5.29 | 115.42 | 118.60 |
| 23 | DA | 2399 | G | N7-C8-N9 | -5.29 | 110.45 | 113.10 |
| 23 | BA | 772 | C | N3-C4-C5 | 5.29 | 124.02 | 121.90 |
| 23 | BA | 859 | G | C8-N9-C4 | 5.29 | 108.52 | 106.40 |
| 23 | BA | 1309 | G | C2-N3-C4 | -5.29 | 109.25 | 111.90 |
| 24 | BB | 80 | U | C5-C6-N1 | -5.29 | 120.05 | 122.70 |
| 23 | DA | 783 | A | N3-C4-C5 | 5.29 | 130.50 | 126.80 |
| 23 | DA | 1835 | G | C5-C6-N1 | 5.29 | 114.14 | 111.50 |
| 23 | DA | 210 | C | C2-N1-C1' | -5.29 | 112.98 | 118.80 |
| 23 | DA | 178 | G | C8-N9-C4 | 5.29 | 108.52 | 106.40 |
| 23 | BA | 141(A) | A | C6-C5-N7 | -5.29 | 128.60 | 132.30 |
| 23 | BA | 2075 | U | C5-C6-N1 | -5.29 | 120.06 | 122.70 |
| 1 | CA | 1415 | G | C8-N9-C1' | -5.29 | 120.13 | 127.00 |
| 23 | DA | 2280 | G | C5-C6-N1 | 5.29 | 114.14 | 111.50 |
| 23 | BA | 1138 | G | N3-C4-C5 | -5.28 | 125.96 | 128.60 |
| 23 | BA | 1615 | C | N1-C2-O2 | -5.28 | 115.73 | 118.90 |
| 23 | BA | 1942 | C | C5-C6-N1 | 5.28 | 123.64 | 121.00 |
| 23 | DA | 72 | U | N1-C2-N3 | 5.28 | 118.07 | 114.90 |
| 23 | DA | 1524 | G | N3-C4-C5 | -5.28 | 125.96 | 128.60 |
| 23 | DA | 2440 | C | N3-C4-C5 | -5.28 | 119.79 | 121.90 |
| 1 | CA | 55 | A | C8-N9-C4 | -5.28 | 103.69 | 105.80 |
| 23 | DA | 450 | G | C6-C5-N7 | -5.28 | 127.23 | 130.40 |
| 23 | DA | 687 | C | N3-C4-C5 | 5.28 | 124.01 | 121.90 |
| 23 | DA | 1602 | U | C5-C4-O4 | 5.28 | 129.07 | 125.90 |
| 23 | DA | 2524 | G | N7-C8-N9 | -5.28 | 110.46 | 113.10 |
| 23 | DA | 2626 | C | C2-N1-C1' | -5.28 | 112.99 | 118.80 |
| 23 | DA | 2762 | G | C4-C5-N7 | 5.28 | 112.91 | 110.80 |
| 23 | DA | 270(B) | A | N7-C8-N9 | -5.28 | 111.16 | 113.80 |
| 23 | DA | 2685 | G | C4-C5-C6 | 5.28 | 121.97 | 118.80 |
| 23 | BA | 244 | A | C2-N3-C4 | -5.28 | 107.96 | 110.60 |
| 23 | BA | 1614 | A | C4-N9-C1' | 5.28 | 135.80 | 126.30 |
| 23 | BA | 2081 | C | C6-N1-C2 | 5.28 | 122.41 | 120.30 |
| 23 | BA | 2252 | G | N1-C2-N3 | 5.28 | 127.07 | 123.90 |
| 23 | BA | 2271 | G | N3-C2-N2 | 5.28 | 123.59 | 119.90 |
| 23 | BA | 2499 | C | C4-C5-C6 | 5.28 | 120.04 | 117.40 |
| 1 | CA | 1515 | C | C5-C6-N1 | -5.28 | 118.36 | 121.00 |
| 23 | DA | 798 | G | C6-C5-N7 | -5.28 | 127.23 | 130.40 |
| 23 | DA | 802 | A | C8-N9-C4 | 5.28 | 107.91 | 105.80 |
| 23 | BA | 94 | G | C4-N9-C1' | 5.28 | 133.36 | 126.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23 | BA | 531 | C | C2-N3-C4 | -5.28 | 117.26 | 119.90 |
| 23 | BA | 2513 | G | C5-C6-N1 | 5.28 | 114.14 | 111.50 |
| 23 | DA | 2713 | A | N7-C8-N9 | 5.28 | 116.44 | 113.80 |
| 23 | DA | 1385 | G | C8-N9-C1' | 5.27 | 133.86 | 127.00 |
| 23 | DA | 2252 | G | C8-N9-C4 | 5.27 | 108.51 | 106.40 |
| 23 | DA | 2578 | G | C8-N9-C4 | 5.27 | 108.51 | 106.40 |
| 23 | BA | 32 | C | N3-C2-O2 | 5.27 | 125.59 | 121.90 |
| 23 | BA | 388 | G | N3-C4-N9 | -5.27 | 122.84 | 126.00 |
| 23 | BA | 937 | U | C5-C6-N1 | -5.27 | 120.06 | 122.70 |
| 23 | BA | 2783 | G | N3-C4-N9 | 5.27 | 129.16 | 126.00 |
| 23 | DA | 1349 | A | C5-C6-N6 | -5.27 | 119.48 | 123.70 |
| 23 | DA | 2383 | G | C8-N9-C1' | -5.27 | 120.15 | 127.00 |
| 23 | BA | 397 | G | C8-N9-C4 | 5.27 | 108.51 | 106.40 |
| 23 | BA | 2574 | G | N1-C2-N3 | 5.27 | 127.06 | 123.90 |
| 23 | DA | 2432 | A | C4-C5-N7 | 5.27 | 113.33 | 110.70 |
| 23 | BA | 197 | A | C5-C6-N6 | -5.27 | 119.49 | 123.70 |
| 23 | BA | 720 | C | C6-N1-C2 | 5.27 | 122.41 | 120.30 |
| 23 | BA | 738 | G | C5-C6-O6 | -5.27 | 125.44 | 128.60 |
| 23 | BA | 845 | G | C8-N9-C1' | -5.27 | 120.15 | 127.00 |
| 23 | DA | 214 | G | C4-N9-C1' | -5.27 | 119.65 | 126.50 |
| 23 | DA | 2276 | G | C5-C6-O6 | -5.27 | 125.44 | 128.60 |
| 23 | DA | 2564 | A | N1-C6-N6 | 5.27 | 121.76 | 118.60 |
| 25 | DC | 52 | ARG | NE-CZ-NH1 | -5.27 | 117.67 | 120.30 |
| 23 | DA | 861 | A | N7-C8-N9 | 5.27 | 116.43 | 113.80 |
| 23 | DA | 945 | A | C1'-O4'-C4' | -5.27 | 105.69 | 109.90 |
| 23 | DA | 2555 | U | C2-N1-C1' | -5.27 | 111.38 | 117.70 |
| 1 | CA | 819 | A | N1-C6-N6 | 5.26 | 121.76 | 118.60 |
| 23 | DA | 2092 | U | N1-C2-N3 | 5.26 | 118.06 | 114.90 |
| 23 | DA | 2271 | G | N3-C2-N2 | 5.26 | 123.58 | 119.90 |
| 23 | DA | 2524 | G | C8-N9-C4 | 5.26 | 108.51 | 106.40 |
| 23 | BA | 768 | G | C8-N9-C1' | -5.26 | 120.16 | 127.00 |
| 1 | CA | 552 | U | C2-N3-C4 | -5.26 | 123.84 | 127.00 |
| 23 | DA | 677 | A | N1-C2-N3 | 5.26 | 131.93 | 129.30 |
| 23 | DA | 2035 | G | C4-C5-N7 | -5.26 | 108.69 | 110.80 |
| 23 | BA | 806 | C | C2-N1-C1' | 5.26 | 124.59 | 118.80 |
| 23 | BA | 847 | U | N3-C4-O4 | -5.26 | 115.72 | 119.40 |
| 1 | CA | 918 | A | N1-C6-N6 | -5.26 | 115.44 | 118.60 |
| 23 | DA | 138 | G | N3-C4-C5 | -5.26 | 125.97 | 128.60 |
| 23 | DA | 1182 | A | C8-N9-C4 | -5.26 | 103.70 | 105.80 |
| 23 | BA | 1824 | G | C6-N1-C2 | -5.26 | 121.94 | 125.10 |
| 23 | DA | 340 | A | C5-C6-N1 | -5.26 | 115.07 | 117.70 |
| 23 | DA | 777 | A | N1-C6-N6 | -5.26 | 115.44 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23 | DA | 1261 | C | C2-N1-C1' | -5.26 | 113.02 | 118.80 |
| 23 | BA | 979 | G | N7-C8-N9 | 5.26 | 115.73 | 113.10 |
| 23 | BA | 568 | U | C2-N3-C4 | 5.25 | 130.15 | 127.00 |
| 23 | DA | 1282 | U | C6-N1-C2 | -5.25 | 117.85 | 121.00 |
| 23 | BA | 1493 | C | C6-N1-C1' | -5.25 | 114.50 | 120.80 |
| 23 | DA | 1008 | C | C6-N1-C2 | 5.25 | 122.40 | 120.30 |
| 23 | DA | 1322 | A | C6-N1-C2 | -5.25 | 115.45 | 118.60 |
| 23 | DA | 2570 | G | C2-N3-C4 | -5.25 | 109.27 | 111.90 |
| 23 | DA | 114 | U | C2-N1-C1' | 5.25 | 124.00 | 117.70 |
| 23 | DA | 2251 | G | C6-N1-C2 | -5.25 | 121.95 | 125.10 |
| 23 | DA | 2624 | G | C8-N9-C4 | 5.25 | 108.50 | 106.40 |
| 23 | DA | 2055 | C | C4-C5-C6 | 5.25 | 120.03 | 117.40 |
| 23 | DA | 1663 | C | C2-N3-C4 | -5.25 | 117.28 | 119.90 |
| 23 | BA | 801 | G | N9-C4-C5 | 5.25 | 107.50 | 105.40 |
| 24 | BB | 98 | G | C4-N9-C1' | 5.25 | 133.32 | 126.50 |
| 23 | DA | 704 | G | N9-C4-C5 | -5.25 | 103.30 | 105.40 |
| 23 | DA | 746 | A | C8-N9-C4 | -5.25 | 103.70 | 105.80 |
| 23 | DA | 1190 | G | N1-C6-O6 | 5.25 | 123.05 | 119.90 |
| 23 | DA | 1658 | C | N3-C4-C5 | 5.25 | 124.00 | 121.90 |
| 23 | BA | 945 | A | C1'-O4'-C4' | -5.25 | 105.70 | 109.90 |
| 23 | BA | 2501 | C | C2-N1-C1' | -5.25 | 113.03 | 118.80 |
| 23 | DA | 1306 | C | C6-N1-C2 | 5.25 | 122.40 | 120.30 |
| 23 | DA | 49 | A | N1-C2-N3 | -5.24 | 126.68 | 129.30 |
| 23 | DA | 1271 | G | C8-N9-C1' | -5.24 | 120.18 | 127.00 |
| 23 | DA | 2789 | C | C6-N1-C2 | 5.24 | 122.40 | 120.30 |
| 23 | BA | 444 | C | N3-C2-O2 | 5.24 | 125.57 | 121.90 |
| 23 | BA | 1138 | G | C4-N9-C1' | 5.24 | 133.31 | 126.50 |
| 23 | BA | 1190 | G | C5-N7-C8 | -5.24 | 101.68 | 104.30 |
| 23 | BA | 2392 | A | C4-C5-C6 | 5.24 | 119.62 | 117.00 |
| 23 | BA | 2464 | C | C5-C6-N1 | -5.24 | 118.38 | 121.00 |
| 23 | DA | 2391 | G | C4-C5-N7 | -5.24 | 108.70 | 110.80 |
| 23 | DA | 2574 | G | N3-C4-N9 | 5.24 | 129.14 | 126.00 |
| 23 | DA | 929 | G | C6-C5-N7 | -5.24 | 127.26 | 130.40 |
| 23 | DA | 1655 | A | N9-C4-C5 | -5.24 | 103.70 | 105.80 |
| 23 | BA | 1647 | G | C8-N9-C4 | 5.24 | 108.50 | 106.40 |
| 23 | DA | 2053 | G | C6-C5-N7 | -5.24 | 127.26 | 130.40 |
| 1 | CA | 1513 | A | C8-N9-C4 | 5.24 | 107.89 | 105.80 |
| 23 | DA | 1345 | C | C2-N3-C4 | -5.24 | 117.28 | 119.90 |
| 23 | DA | 2378 | A | C8-N9-C4 | 5.24 | 107.89 | 105.80 |
| 23 | DA | 2439 | A | P-O3'-C3' | 5.23 | 125.98 | 119.70 |
| 1 | AA | 1053 | G | N3-C4-N9 | -5.23 | 122.86 | 126.00 |
| 23 | BA | 1348 | G | N1-C6-O6 | 5.23 | 123.04 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | CA | 576 | G | C6-C5-N7 | -5.23 | 127.26 | 130.40 |
| 1 | CA | 781 | A | C4-C5-N7 | 5.23 | 113.32 | 110.70 |
| 23 | DA | 56 | A | N1-C2-N3 | 5.23 | 131.92 | 129.30 |
| 23 | DA | 1898 | U | C4-C5-C6 | 5.23 | 122.84 | 119.70 |
| 23 | DA | 1905 | C | C6-N1-C2 | 5.23 | 122.39 | 120.30 |
| 23 | DA | 1977 | A | C8-N9-C4 | 5.23 | 107.89 | 105.80 |
| 23 | DA | 2504 | U | C5-C4-O4 | 5.23 | 129.04 | 125.90 |
| 23 | BA | 2236 | C | C5-C6-N1 | -5.23 | 118.39 | 121.00 |
| 23 | DA | 845 | G | C8-N9-C1' | -5.23 | 120.20 | 127.00 |
| 23 | DA | 2250 | G | N1-C6-O6 | -5.23 | 116.76 | 119.90 |
| 23 | DA | 2581 | G | C6-C5-N7 | 5.23 | 133.54 | 130.40 |
| 23 | BA | 1842 | G | C8-N9-C1' | -5.23 | 120.20 | 127.00 |
| 1 | AA | 770 | C | N3-C4-C5 | 5.23 | 123.99 | 121.90 |
| 23 | BA | 996 | A | N1-C6-N6 | 5.23 | 121.74 | 118.60 |
| 23 | BA | 1558 | A | C2-N3-C4 | -5.23 | 107.99 | 110.60 |
| 23 | BA | 1980 | G | N3-C4-N9 | 5.23 | 129.14 | 126.00 |
| 23 | DA | 1318 | C | N3-C4-C5 | 5.23 | 123.99 | 121.90 |
| 23 | DA | 2049 | G | C5-C6-O6 | -5.23 | 125.47 | 128.60 |
| 23 | BA | 474 | G | N3-C4-C5 | -5.22 | 125.99 | 128.60 |
| 23 | BA | 723 | G | C2-N3-C4 | -5.22 | 109.29 | 111.90 |
| 23 | BA | 1612 | C | C4-C5-C6 | 5.22 | 120.01 | 117.40 |
| 23 | BA | 2059 | A | C5-C6-N1 | 5.22 | 120.31 | 117.70 |
| 23 | DA | 258 | G | C5-C6-N1 | -5.22 | 108.89 | 111.50 |
| 23 | DA | 1671 | U | C6-N1-C2 | -5.22 | 117.87 | 121.00 |
| 23 | DA | 993 | G | N9-C4-C5 | 5.22 | 107.49 | 105.40 |
| 23 | BA | 1760 | A | N1-C6-N6 | -5.22 | 115.47 | 118.60 |
| 23 | BA | 811 | U | C2-N1-C1' | -5.22 | 111.44 | 117.70 |
| 23 | DA | 698 | C | C2-N1-C1' | -5.22 | 113.06 | 118.80 |
| 23 | DA | 727 | A | C5-N7-C8 | -5.22 | 101.29 | 103.90 |
| 23 | DA | 2247 | A | N1-C2-N3 | 5.22 | 131.91 | 129.30 |
| 23 | BA | 1790 | C | C2-N1-C1' | -5.22 | 113.06 | 118.80 |
| 23 | DA | 1842 | G | C8-N9-C1' | -5.22 | 120.22 | 127.00 |
| 23 | DA | 2014 | A | N9-C4-C5 | -5.22 | 103.71 | 105.80 |
| 23 | BA | 1313 | U | N1-C2-O2 | -5.22 | 119.15 | 122.80 |
| 23 | DA | 131 | G | C5-C6-N1 | 5.22 | 114.11 | 111.50 |
| 23 | DA | 810 | U | N3-C2-O2 | -5.22 | 118.55 | 122.20 |
| 23 | DA | 1021 | A | C6-C5-N7 | -5.22 | 128.65 | 132.30 |
| 23 | DA | 1617 | C | N3-C2-O2 | 5.22 | 125.55 | 121.90 |
| 23 | BA | 705 | A | C2-N3-C4 | -5.21 | 107.99 | 110.60 |
| 23 | BA | 2091 | U | C4-C5-C6 | 5.21 | 122.83 | 119.70 |
| 1 | CA | 811 | C | C5-C6-N1 | -5.21 | 118.39 | 121.00 |
| 23 | DA | 1496 | A | C8-N9-C4 | -5.21 | 103.71 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 23 | DA | 1677 | A | C4-C5-C6 | 5.21 | 119.61 | 117.00 |
| 23 | DA | 1783 | A | N1-C6-N6 | -5.21 | 115.47 | 118.60 |
| 23 | BA | 1204 | A | C2-N3-C4 | -5.21 | 107.99 | 110.60 |
| 23 | DA | 729 | G | C5-N7-C8 | -5.21 | 101.69 | 104.30 |
| 23 | DA | 2427 | C | N1-C2-O2 | -5.21 | 115.77 | 118.90 |
| 23 | BA | 1821 | A | N7-C8-N9 | -5.21 | 111.19 | 113.80 |
| 23 | DA | 1589 | C | N3-C4-C5 | -5.21 | 119.81 | 121.90 |
| 23 | BA | 393 | C | N1-C2-O2 | -5.21 | 115.77 | 118.90 |
| 23 | DA | 945 | A | C6-N1-C2 | -5.21 | 115.47 | 118.60 |
| 23 | DA | 2088 | G | N1-C2-N3 | 5.21 | 127.03 | 123.90 |
| 23 | DA | 2438 | U | C2-N3-C4 | -5.21 | 123.87 | 127.00 |
| 23 | BA | 1779 | U | C5-C4-O4 | -5.21 | 122.78 | 125.90 |
| 23 | BA | 2595 | G | N9-C4-C5 | -5.21 | 103.32 | 105.40 |
| 1 | AA | 904 | C | N3-C2-O2 | -5.21 | 118.25 | 121.90 |
| 23 | BA | 2328 | A | C8-N9-C4 | 5.21 | 107.88 | 105.80 |
| 1 | CA | 1515 | C | C4-C5-C6 | 5.21 | 120.00 | 117.40 |
| 23 | DA | 40 | C | C2-N3-C4 | -5.21 | 117.30 | 119.90 |
| 23 | DA | 2239 | G | N1-C2-N3 | 5.21 | 127.02 | 123.90 |
| 24 | BB | 100 | G | N9-C4-C5 | -5.21 | 103.32 | 105.40 |
| 23 | BA | 1619 | G | C8-N9-C4 | 5.20 | 108.48 | 106.40 |
| 23 | BA | 1663 | C | C5-C6-N1 | -5.20 | 118.40 | 121.00 |
| 23 | DA | 1624 | G | N7-C8-N9 | -5.20 | 110.50 | 113.10 |
| 23 | DA | 1699 | G | N9-C4-C5 | 5.20 | 107.48 | 105.40 |
| 1 | AA | 1524 | C | C6-N1-C2 | 5.20 | 122.38 | 120.30 |
| 23 | DA | 140 | A | N1-C6-N6 | 5.20 | 121.72 | 118.60 |
| 23 | DA | 1398 | C | N3-C4-C5 | -5.20 | 119.82 | 121.90 |
| 23 | DA | 2377 | A | C8-N9-C4 | 5.20 | 107.88 | 105.80 |
| 23 | DA | 2434 | A | C8-N9-C4 | -5.20 | 103.72 | 105.80 |
| 24 | DB | 100 | G | C8-N9-C4 | 5.20 | 108.48 | 106.40 |
| 23 | DA | 74 | A | C8-N9-C4 | -5.20 | 103.72 | 105.80 |
| 23 | DA | 332 | A | N1-C2-N3 | 5.20 | 131.90 | 129.30 |
| 23 | DA | 1443 | G | C5-C6-O6 | -5.20 | 125.48 | 128.60 |
| 23 | DA | 1605 | C | C5-C6-N1 | 5.20 | 123.60 | 121.00 |
| 23 | BA | 679 | C | N3-C2-O2 | 5.20 | 125.54 | 121.90 |
| 23 | BA | 1355 | G | C5-C6-N1 | 5.20 | 114.10 | 111.50 |
| 23 | BA | 116 | C | C5-C6-N1 | -5.20 | 118.40 | 121.00 |
| 23 | BA | 959 | A | C2-N3-C4 | -5.20 | 108.00 | 110.60 |
| 23 | BA | 1645 | G | N1-C6-O6 | -5.20 | 116.78 | 119.90 |
| 23 | BA | 1776 | G | N9-C4-C5 | -5.20 | 103.32 | 105.40 |
| 23 | BA | 2241 | A | N1-C2-N3 | 5.20 | 131.90 | 129.30 |
| 23 | BA | 2249 | U | C5-C4-O4 | 5.20 | 129.02 | 125.90 |
| 23 | DA | 1030 | G | N7-C8-N9 | -5.20 | 110.50 | 113.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | DA | 2717 | G | N3-C4-C5 | -5.20 | 126.00 | 128.60 |
| 1 | CA | 720 | C | N1-C2-O2 | 5.19 | 122.02 | 118.90 |
| 23 | DA | 1330 | C | N3-C2-O2 | 5.19 | 125.54 | 121.90 |
| 23 | DA | 2498 | C | N3-C2-O2 | 5.19 | 125.54 | 121.90 |
| 23 | DA | 2774 | C | C6-N1-C2 | 5.19 | 122.38 | 120.30 |
| 23 | BA | 773 | U | N1-C2-N3 | 5.19 | 118.02 | 114.90 |
| 23 | BA | 1409 | C | C6-N1-C2 | 5.19 | 122.38 | 120.30 |
| 23 | DA | 83 | G | C5-C6-O6 | 5.19 | 131.72 | 128.60 |
| 23 | DA | 211 | A | C5-C6-N6 | 5.19 | 127.85 | 123.70 |
| 23 | DA | 678 | C | N3-C4-N4 | -5.19 | 114.36 | 118.00 |
| 23 | DA | 1241 | A | C2-N3-C4 | -5.19 | 108.00 | 110.60 |
| 23 | DA | 2197 | U | C5-C6-N1 | -5.19 | 120.10 | 122.70 |
| 23 | BA | 1690 | A | N1-C6-N6 | -5.19 | 115.49 | 118.60 |
| 23 | DA | 247 | G | N9-C4-C5 | -5.19 | 103.32 | 105.40 |
| 23 | DA | 270(Z) | G | N3-C4-N9 | -5.19 | 122.89 | 126.00 |
| 23 | DA | 1632 | A | N1-C6-N6 | 5.19 | 121.72 | 118.60 |
| 23 | DA | 422 | A | N1-C6-N6 | -5.19 | 115.49 | 118.60 |
| 23 | BA | 298 | G | C8-N9-C4 | -5.19 | 104.33 | 106.40 |
| 23 | BA | 407 | G | C4-N9-C1' | 5.19 | 133.25 | 126.50 |
| 23 | DA | 443 | A | N9-C4-C5 | 5.19 | 107.88 | 105.80 |
| 23 | DA | 647 | G | C8-N9-C4 | -5.19 | 104.33 | 106.40 |
| 23 | DA | 1558 | A | C2-N3-C4 | -5.19 | 108.01 | 110.60 |
| 23 | DA | 2522 | U | C5-C6-N1 | -5.19 | 120.11 | 122.70 |
| 23 | DA | 2670 | A | C8-N9-C4 | 5.19 | 107.88 | 105.80 |
| 23 | DA | 69 | C | C4-C5-C6 | 5.19 | 119.99 | 117.40 |
| 23 | DA | 70 | G | N3-C4-C5 | -5.18 | 126.01 | 128.60 |
| 23 | DA | 397 | G | N3-C4-C5 | 5.18 | 131.19 | 128.60 |
| 23 | DA | 2032 | G | N3-C4-N9 | -5.18 | 122.89 | 126.00 |
| 23 | DA | 2876 | G | C8-N9-C4 | 5.18 | 108.47 | 106.40 |
| 23 | BA | 1555 | G | C8-N9-C1' | -5.18 | 120.27 | 127.00 |
| 23 | DA | 2070 | G | C5-N7-C8 | 5.18 | 106.89 | 104.30 |
| 1 | AA | 576 | G | C5-C6-N1 | -5.18 | 108.91 | 111.50 |
| 23 | BA | 849 | A | C4-C5-N7 | 5.18 | 113.29 | 110.70 |
| 23 | DA | 74 | A | N1-C6-N6 | -5.18 | 115.49 | 118.60 |
| 23 | DA | 473 | G | N1-C2-N3 | 5.18 | 127.01 | 123.90 |
| 23 | DA | 2093 | G | N1-C6-O6 | 5.18 | 123.01 | 119.90 |
| 23 | DA | 2547 | U | C2-N3-C4 | -5.18 | 123.89 | 127.00 |
| 1 | AA | 778 | G | C4-N9-C1' | 5.18 | 133.23 | 126.50 |
| 23 | DA | 455 | C | N3-C4-C5 | 5.18 | 123.97 | 121.90 |
| 23 | BA | 458 | G | N3-C4-N9 | 5.18 | 129.11 | 126.00 |
| 23 | BA | 774 | A | N3-C4-N9 | -5.18 | 123.26 | 127.40 |
| 23 | DA | 1926 | U | C2-N1-C1' | -5.18 | 111.49 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | DA | 1671 | U | N1-C2-O2 | -5.17 | 119.18 | 122.80 |
| 23 | BA | 1244 | G | N9-C4-C5 | -5.17 | 103.33 | 105.40 |
| 23 | DA | 1963 | U | N3-C2-O2 | -5.17 | 118.58 | 122.20 |
| 23 | BA | 2017 | U | C5-C6-N1 | -5.17 | 120.11 | 122.70 |
| 23 | BA | 2450 | A | N1-C2-N3 | 5.17 | 131.89 | 129.30 |
| 1 | CA | 691 | G | N9-C4-C5 | -5.17 | 103.33 | 105.40 |
| 23 | DA | 1604 | C | C5-C4-N4 | -5.17 | 116.58 | 120.20 |
| 23 | DA | 1827 | C | C5-C6-N1 | -5.17 | 118.41 | 121.00 |
| 23 | BA | 849 | A | N1-C6-N6 | 5.17 | 121.70 | 118.60 |
| 23 | DA | 116 | C | C4-C5-C6 | 5.17 | 119.98 | 117.40 |
| 23 | DA | 1971 | A | N9-C4-C5 | -5.17 | 103.73 | 105.80 |
| 1 | AA | 395 | C | C6-N1-C2 | 5.17 | 122.37 | 120.30 |
| 23 | BA | 935 | C | C6-N1-C2 | 5.17 | 122.37 | 120.30 |
| 23 | BA | 1677 | A | C5-N7-C8 | -5.17 | 101.32 | 103.90 |
| 23 | BA | 2456 | C | C4-C5-C6 | -5.17 | 114.82 | 117.40 |
| 23 | DA | 1603 | A | N7-C8-N9 | 5.17 | 116.38 | 113.80 |
| 1 | AA | 1508 | G | C8-N9-C4 | 5.17 | 108.47 | 106.40 |
| 23 | BA | 1245 | G | C8-N9-C4 | 5.17 | 108.47 | 106.40 |
| 23 | BA | 1769 | G | N1-C2-N3 | 5.17 | 127.00 | 123.90 |
| 23 | DA | 271 | G | C2-N3-C4 | -5.17 | 109.32 | 111.90 |
| 1 | AA | 815 | A | C5-C6-N6 | 5.17 | 127.83 | 123.70 |
| 23 | BA | 575 | A | N7-C8-N9 | -5.16 | 111.22 | 113.80 |
| 23 | BA | 1681 | G | N1-C6-O6 | 5.16 | 123.00 | 119.90 |
| 23 | DA | 861 | A | C8-N9-C4 | -5.16 | 103.73 | 105.80 |
| 23 | DA | 1138 | G | C8-N9-C1' | -5.16 | 120.29 | 127.00 |
| 23 | DA | 2253 | G | N1-C6-O6 | 5.16 | 123.00 | 119.90 |
| 23 | DA | 2578 | G | C4-C5-N7 | 5.16 | 112.86 | 110.80 |
| 23 | BA | 1783 | A | C8-N9-C4 | -5.16 | 103.73 | 105.80 |
| 23 | BA | 2675 | A | N3-C4-C5 | 5.16 | 130.41 | 126.80 |
| 23 | DA | 1622 | G | C2-N3-C4 | -5.16 | 109.32 | 111.90 |
| 23 | BA | 96 | G | C8-N9-C1' | -5.16 | 120.29 | 127.00 |
| 23 | BA | 2773 | C | C6-N1-C2 | 5.16 | 122.36 | 120.30 |
| 23 | DA | 734 | A | C2-N3-C4 | -5.16 | 108.02 | 110.60 |
| 23 | DA | 1321 | A | C2-N3-C4 | -5.16 | 108.02 | 110.60 |
| 23 | DA | 1555 | G | N3-C4-N9 | 5.16 | 129.10 | 126.00 |
| 23 | DA | 2017 | U | N1-C2-N3 | 5.16 | 118.00 | 114.90 |
| 23 | DA | 520 | G | N3-C4-N9 | 5.16 | 129.09 | 126.00 |
| 23 | DA | 819 | A | C5-N7-C8 | -5.16 | 101.32 | 103.90 |
| 23 | BA | 813 | U | N1-C2-N3 | 5.16 | 117.99 | 114.90 |
| 23 | BA | 1666 | G | N3-C4-N9 | -5.16 | 122.91 | 126.00 |
| 23 | BA | 2824 | C | C6-N1-C2 | 5.16 | 122.36 | 120.30 |
| 23 | DA | 809 | G | C6-C5-N7 | -5.16 | 127.31 | 130.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | DA | 2846 | G | N1-C6-O6 | 5.16 | 122.99 | 119.90 |
| 23 | BA | 802 | A | C8-N9-C4 | 5.16 | 107.86 | 105.80 |
| 23 | BA | 1803 | A | N7-C8-N9 | -5.16 | 111.22 | 113.80 |
| 1 | CA | 1484 | C | C6-N1-C2 | 5.16 | 122.36 | 120.30 |
| 23 | DA | 908 | C | N1-C2-O2 | -5.16 | 115.81 | 118.90 |
| 23 | DA | 1770 | G | C6-C5-N7 | -5.16 | 127.31 | 130.40 |
| 23 | DA | 2532 | G | N9-C4-C5 | -5.16 | 103.34 | 105.40 |
| 23 | BA | 384 | U | C5-C6-N1 | -5.15 | 120.12 | 122.70 |
| 23 | DA | 1996 | C | C5-C6-N1 | -5.15 | 118.42 | 121.00 |
| 23 | BA | 803 | U | C4-C5-C6 | 5.15 | 122.79 | 119.70 |
| 23 | BA | 2688 | U | N3-C2-O2 | -5.15 | 118.59 | 122.20 |
| 23 | DA | 1395 | A | C5-C6-N1 | 5.15 | 120.28 | 117.70 |
| 1 | AA | 264 | U | N1-C2-N3 | 5.15 | 117.99 | 114.90 |
| 23 | BA | 114(B) | A | C4-C5-N7 | 5.15 | 113.28 | 110.70 |
| 23 | BA | 2253 | G | N1-C6-O6 | 5.15 | 122.99 | 119.90 |
| 46 | BX | 27 | GLU | N-CA-C | 5.15 | 124.91 | 111.00 |
| 23 | DA | 302 | C | C2-N1-C1' | -5.15 | 113.14 | 118.80 |
| 23 | BA | 706 | A | C2-N3-C4 | -5.15 | 108.03 | 110.60 |
| 23 | BA | 2395 | C | C6-N1-C2 | 5.15 | 122.36 | 120.30 |
| 23 | BA | 140 | A | N7-C8-N9 | 5.15 | 116.37 | 113.80 |
| 23 | BA | 397 | G | C2-N3-C4 | -5.15 | 109.33 | 111.90 |
| 23 | BA | 530 | G | N1-C2-N2 | -5.15 | 111.57 | 116.20 |
| 23 | BA | 660 | G | C8-N9-C4 | 5.15 | 108.46 | 106.40 |
| 23 | BA | 2681 | C | C2-N3-C4 | -5.15 | 117.33 | 119.90 |
| 34 | DL | 61 | ARG | NE-CZ-NH2 | -5.15 | 117.73 | 120.30 |
| 23 | BA | 1832 | C | N1-C2-O2 | -5.14 | 115.81 | 118.90 |
| 23 | DA | 1616 | A | C5-C6-N6 | -5.14 | 119.58 | 123.70 |
| 23 | DA | 2419 | U | C2-N1-C1' | -5.14 | 111.53 | 117.70 |
| 23 | DA | 2605 | U | N1-C2-N3 | 5.14 | 117.99 | 114.90 |
| 23 | DA | 2724 | C | N3-C4-C5 | 5.14 | 123.96 | 121.90 |
| 23 | DA | 1815 | A | C4-C5-N7 | -5.14 | 108.13 | 110.70 |
| 23 | DA | 2505 | G | N3-C4-N9 | -5.14 | 122.92 | 126.00 |
| 23 | BA | 460 | A | C2-N3-C4 | -5.14 | 108.03 | 110.60 |
| 23 | BA | 1122 | G | C4-N9-C1' | -5.14 | 119.82 | 126.50 |
| 23 | DA | 2766 | G | C8-N9-C4 | -5.14 | 104.34 | 106.40 |
| 1 | AA | 1415 | G | C5-C6-N1 | -5.14 | 108.93 | 111.50 |
| 1 | CA | 576 | G | N1-C6-O6 | 5.14 | 122.98 | 119.90 |
| 23 | DA | 114(B) | A | N7-C8-N9 | 5.14 | 116.37 | 113.80 |
| 23 | BA | 2584 | U | N3-C4-O4 | 5.14 | 123.00 | 119.40 |
| 1 | CA | 768 | A | N7-C8-N9 | -5.14 | 111.23 | 113.80 |
| 23 | DA | 2078 | C | N3-C4-C5 | 5.14 | 123.95 | 121.90 |
| 23 | BA | 1841 | U | N3-C2-O2 | 5.14 | 125.80 | 122.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | DA | 750 | A | C5-C6-N6 | -5.14 | 119.59 | 123.70 |
| 23 | DA | 1005 | C | N3-C4-C5 | 5.14 | 123.95 | 121.90 |
| 23 | DA | 1024 | G | N9-C4-C5 | -5.14 | 103.34 | 105.40 |
| 23 | DA | 1573 | G | C8-N9-C4 | 5.14 | 108.45 | 106.40 |
| 23 | DA | 2626 | C | N3-C4-C5 | 5.14 | 123.95 | 121.90 |
| 23 | BA | 429 | A | C6-N1-C2 | -5.13 | 115.52 | 118.60 |
| 23 | BA | 774 | A | C5-N7-C8 | -5.13 | 101.33 | 103.90 |
| 23 | BA | 1157 | G | N1-C6-O6 | 5.13 | 122.98 | 119.90 |
| 1 | CA | 674 | G | N1-C6-O6 | 5.13 | 122.98 | 119.90 |
| 1 | CA | 1053 | G | N3-C4-C5 | 5.13 | 131.17 | 128.60 |
| 23 | DA | 588 | U | N3-C4-C5 | -5.13 | 111.52 | 114.60 |
| 40 | DR | 18 | LEU | CA-CB-CG | 5.13 | 127.11 | 115.30 |
| 23 | BA | 1670 | C | N1-C2-O2 | -5.13 | 115.82 | 118.90 |
| 23 | DA | 681 | G | N1-C2-N3 | 5.13 | 126.98 | 123.90 |
| 23 | BA | 2454 | G | C4-C5-N7 | -5.13 | 108.75 | 110.80 |
| 23 | BA | 2590 | A | N1-C6-N6 | 5.13 | 121.68 | 118.60 |
| 23 | BA | 2597 | G | N3-C4-C5 | 5.13 | 131.17 | 128.60 |
| 24 | BB | 80 | U | C2-N1-C1' | -5.13 | 111.54 | 117.70 |
| 23 | DA | 62 | C | C5-C6-N1 | -5.13 | 118.43 | 121.00 |
| 23 | DA | 104 | U | C2-N1-C1' | -5.13 | 111.54 | 117.70 |
| 23 | DA | 2564 | A | C5-N7-C8 | -5.13 | 101.33 | 103.90 |
| 1 | CA | 43 | C | C5-C6-N1 | -5.13 | 118.44 | 121.00 |
| 23 | DA | 1363 | C | N1-C2-N3 | 5.13 | 122.79 | 119.20 |
| 23 | BA | 140 | A | C6-C5-N7 | -5.13 | 128.71 | 132.30 |
| 23 | BA | 795 | C | C2-N3-C4 | -5.13 | 117.33 | 119.90 |
| 23 | DA | 2345 | G | C5-C6-N1 | -5.13 | 108.94 | 111.50 |
| 1 | AA | 922 | G | N1-C6-O6 | 5.13 | 122.98 | 119.90 |
| 23 | BA | 2555 | U | C6-N1-C1' | 5.13 | 128.38 | 121.20 |
| 23 | DA | 1673 | U | C5-C4-O4 | -5.13 | 122.82 | 125.90 |
| 23 | DA | 561 | G | C8-N9-C4 | 5.12 | 108.45 | 106.40 |
| 23 | DA | 2762 | G | C5-C6-O6 | -5.12 | 125.53 | 128.60 |
| 1 | AA | 758 | G | N1-C6-O6 | 5.12 | 122.97 | 119.90 |
| 23 | BA | 1680 | U | N3-C2-O2 | -5.12 | 118.61 | 122.20 |
| 23 | DA | 1666 | G | N3-C4-N9 | -5.12 | 122.93 | 126.00 |
| 23 | DA | 2445 | G | C2-N3-C4 | -5.12 | 109.34 | 111.90 |
| 23 | DA | 2502 | G | C4-C5-N7 | 5.12 | 112.85 | 110.80 |
| 23 | DA | 2680 | C | C6-N1-C2 | 5.12 | 122.35 | 120.30 |
| 23 | BA | 2563 | U | C5-C6-N1 | -5.12 | 120.14 | 122.70 |
| 23 | DA | 2078 | C | C5-C4-N4 | -5.12 | 116.61 | 120.20 |
| 23 | DA | 2244 | U | C2-N1-C1' | 5.12 | 123.85 | 117.70 |
| 23 | DA | 2330 | G | N3-C4-C5 | 5.12 | 131.16 | 128.60 |
| 23 | DA | 934 | G | N1-C6-O6 | 5.12 | 122.97 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | BA | 2002 | G | C4-C5-C6 | -5.12 | 115.73 | 118.80 |
| 23 | DA | 802 | A | C4-N9-C1' | 5.12 | 135.51 | 126.30 |
| 23 | DA | 1788 | C | C2-N3-C4 | -5.12 | 117.34 | 119.90 |
| 23 | BA | 979 | G | N3-C2-N2 | -5.12 | 116.32 | 119.90 |
| 1 | CA | 1482 | G | N9-C4-C5 | -5.12 | 103.35 | 105.40 |
| 23 | DA | 1235 | G | C8-N9-C1' | -5.12 | 120.35 | 127.00 |
| 23 | DA | 2627 | G | C4-C5-N7 | 5.12 | 112.85 | 110.80 |
| 23 | BA | 378 | C | N1-C2-O2 | -5.11 | 115.83 | 118.90 |
| 23 | BA | 387 | U | N1-C2-N3 | 5.11 | 117.97 | 114.90 |
| 23 | BA | 687 | C | N1-C2-O2 | -5.11 | 115.83 | 118.90 |
| 23 | BA | 1902 | C | N3-C2-O2 | -5.11 | 118.32 | 121.90 |
| 23 | BA | 2433 | A | C6-N1-C2 | -5.11 | 115.53 | 118.60 |
| 23 | DA | 97 | C | C5-C6-N1 | -5.11 | 118.44 | 121.00 |
| 23 | DA | 150 | C | N3-C4-C5 | 5.11 | 123.94 | 121.90 |
| 23 | DA | 773 | U | N1-C2-N3 | 5.11 | 117.97 | 114.90 |
| 23 | DA | 2054 | A | C6-C5-N7 | -5.11 | 128.72 | 132.30 |
| 23 | DA | 2681 | C | C4-C5-C6 | 5.11 | 119.96 | 117.40 |
| 1 | AA | 1053 | G | N1-C2-N3 | -5.11 | 120.83 | 123.90 |
| 23 | BA | 338 | G | N3-C4-N9 | 5.11 | 129.07 | 126.00 |
| 23 | BA | 572 | A | C5-C6-N6 | -5.11 | 119.61 | 123.70 |
| 23 | BA | 1224 | C | N3-C2-O2 | 5.11 | 125.48 | 121.90 |
| 23 | BA | 2041 | U | C2-N3-C4 | -5.11 | 123.93 | 127.00 |
| 23 | BA | 2432 | A | C4-C5-C6 | 5.11 | 119.56 | 117.00 |
| 23 | BA | 2574 | G | C6-N1-C2 | -5.11 | 122.03 | 125.10 |
| 23 | DA | 336 | C | C4-C5-C6 | 5.11 | 119.96 | 117.40 |
| 23 | DA | 2392 | A | C2-N3-C4 | -5.11 | 108.05 | 110.60 |
| 23 | DA | 2600 | A | C8-N9-C4 | 5.11 | 107.84 | 105.80 |
| 23 | BA | 1309 | G | C6-C5-N7 | -5.11 | 127.33 | 130.40 |
| 23 | BA | 1612 | C | N1-C2-O2 | -5.11 | 115.83 | 118.90 |
| 23 | BA | 1980 | G | C5-C6-N1 | 5.11 | 114.06 | 111.50 |
| 1 | CA | 583 | A | N1-C6-N6 | 5.11 | 121.67 | 118.60 |
| 1 | CA | 898 | G | C8-N9-C4 | 5.11 | 108.44 | 106.40 |
| 23 | BA | 1138 | G | C8-N9-C1' | -5.11 | 120.36 | 127.00 |
| 23 | BA | 1627 | G | C6-C5-N7 | -5.11 | 127.33 | 130.40 |
| 23 | BA | 2056 | G | C5-N7-C8 | -5.11 | 101.75 | 104.30 |
| 23 | BA | 2581 | G | N3-C4-N9 | -5.11 | 122.94 | 126.00 |
| 23 | DA | 428 | A | N1-C2-N3 | 5.11 | 131.85 | 129.30 |
| 23 | DA | 768 | G | C5-N7-C8 | 5.11 | 106.85 | 104.30 |
| 23 | DA | 1603 | A | N1-C2-N3 | 5.11 | 131.85 | 129.30 |
| 23 | DA | 2681 | C | C6-N1-C2 | 5.11 | 122.34 | 120.30 |
| 23 | BA | 559 | G | C8-N9-C4 | 5.11 | 108.44 | 106.40 |
| 23 | BA | 760 | G | N9-C4-C5 | -5.11 | 103.36 | 105.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | BA | 1778 | U | C5-C6-N1 | -5.11 | 120.15 | 122.70 |
| 23 | BA | 1962 | C | C2-N3-C4 | 5.11 | 122.45 | 119.90 |
| 23 | DA | 1710 | C | C6-N1-C2 | 5.11 | 122.34 | 120.30 |
| 23 | DA | 1899 | G | C5-C6-N1 | -5.11 | 108.95 | 111.50 |
| 23 | DA | 1960 | A | N7-C8-N9 | -5.11 | 111.25 | 113.80 |
| 23 | DA | 2036 | C | N3-C4-N4 | 5.11 | 121.57 | 118.00 |
| 23 | BA | 1325 | G | C6-C5-N7 | 5.10 | 133.46 | 130.40 |
| 23 | BA | 1941 | C | C6-N1-C2 | 5.10 | 122.34 | 120.30 |
| 23 | DA | 845 | G | C6-C5-N7 | -5.10 | 127.34 | 130.40 |
| 23 | BA | 970 | C | C5-C4-N4 | -5.10 | 116.63 | 120.20 |
| 23 | BA | 987 | G | N3-C2-N2 | -5.10 | 116.33 | 119.90 |
| 23 | DA | 2048 | G | C5-C6-N1 | 5.10 | 114.05 | 111.50 |
| 23 | DA | 2539 | C | C5-C6-N1 | -5.10 | 118.45 | 121.00 |
| 23 | DA | 2673 | G | C6-C5-N7 | -5.10 | 127.34 | 130.40 |
| 1 | AA | 895 | G | C8-N9-C4 | 5.10 | 108.44 | 106.40 |
| 23 | DA | 207 | A | C6-N1-C2 | -5.10 | 115.54 | 118.60 |
| 23 | BA | 1253 | A | C5-C6-N1 | 5.10 | 120.25 | 117.70 |
| 23 | DA | 65 | C | N3-C2-O2 | 5.10 | 125.47 | 121.90 |
| 23 | DA | 120 | U | C6-N1-C2 | 5.10 | 124.06 | 121.00 |
| 23 | DA | 203 | C | C5-C6-N1 | -5.10 | 118.45 | 121.00 |
| 23 | DA | 1611 | C | C5-C4-N4 | -5.10 | 116.63 | 120.20 |
| 23 | DA | 2086 | U | N3-C2-O2 | -5.10 | 118.63 | 122.20 |
| 23 | DA | 2232 | U | C2-N1-C1' | -5.10 | 111.58 | 117.70 |
| 23 | BA | 1942 | C | C6-N1-C2 | -5.10 | 118.26 | 120.30 |
| 23 | DA | 190 | A | C6-N1-C2 | -5.10 | 115.54 | 118.60 |
| 23 | DA | 332 | A | N9-C4-C5 | 5.10 | 107.84 | 105.80 |
| 23 | DA | 452 | G | C5-C6-O6 | -5.10 | 125.54 | 128.60 |
| 23 | DA | 746 | A | N9-C4-C5 | 5.10 | 107.84 | 105.80 |
| 23 | DA | 2742 | C | C6-N1-C2 | 5.10 | 122.34 | 120.30 |
| 23 | BA | 1444 | G | C8-N9-C4 | 5.10 | 108.44 | 106.40 |
| 23 | DA | 655 | A | N7-C8-N9 | 5.10 | 116.35 | 113.80 |
| 23 | BA | 1776 | G | N1-C2-N2 | -5.09 | 111.61 | 116.20 |
| 23 | DA | 1341 | U | C2-N3-C4 | 5.09 | 130.06 | 127.00 |
| 23 | DA | 98 | G | C4-C5-N7 | 5.09 | 112.84 | 110.80 |
| 23 | DA | 2580 | U | C6-N1-C1' | 5.09 | 128.33 | 121.20 |
| 23 | BA | 2032 | G | C4-C5-C6 | -5.09 | 115.75 | 118.80 |
| 23 | BA | 2841 | C | N3-C4-C5 | 5.09 | 123.94 | 121.90 |
| 23 | DA | 140 | A | C6-C5-N7 | -5.09 | 128.74 | 132.30 |
| 23 | DA | 465 | G | C6-C5-N7 | -5.09 | 127.34 | 130.40 |
| 23 | DA | 640 | C | N3-C4-C5 | 5.09 | 123.94 | 121.90 |
| 23 | BA | 1342 | A | C5-N7-C8 | -5.09 | 101.36 | 103.90 |
| 23 | BA | 1551 | C | C6-N1-C2 | -5.09 | 118.26 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | BA | 1573 | G | N7-C8-N9 | -5.09 | 110.56 | 113.10 |
| 23 | BA | 2061 | G | C6-C5-N7 | -5.09 | 127.35 | 130.40 |
| 23 | DA | 211 | A | C8-N9-C4 | 5.09 | 107.83 | 105.80 |
| 23 | DA | 595 | C | C2-N3-C4 | -5.09 | 117.36 | 119.90 |
| 23 | DA | 1817 | G | C2-N3-C4 | -5.09 | 109.36 | 111.90 |
| 23 | BA | 387 | U | N1-C2-O2 | -5.09 | 119.24 | 122.80 |
| 23 | BA | 2714 | G | C4-N9-C1' | 5.09 | 133.11 | 126.50 |
| 23 | DA | 135 | G | N1-C6-O6 | 5.09 | 122.95 | 119.90 |
| 23 | DA | 677 | A | N7-C8-N9 | -5.09 | 111.26 | 113.80 |
| 23 | DA | 784 | A | C4-N9-C1' | -5.09 | 117.14 | 126.30 |
| 23 | DA | 2006 | C | C4-C5-C6 | 5.09 | 119.94 | 117.40 |
| 23 | DA | 2462 | U | C5-C4-O4 | -5.09 | 122.85 | 125.90 |
| 23 | DA | 294 | A | N9-C4-C5 | -5.08 | 103.77 | 105.80 |
| 23 | DA | 795 | C | C6-N1-C2 | 5.08 | 122.33 | 120.30 |
| 23 | BA | 566 | U | C2-N3-C4 | -5.08 | 123.95 | 127.00 |
| 23 | BA | 848 | G | N9-C4-C5 | -5.08 | 103.37 | 105.40 |
| 23 | BA | 114(B) | A | C4-N9-C1' | 5.08 | 135.45 | 126.30 |
| 23 | DA | 847 | U | N1-C2-N3 | 5.08 | 117.95 | 114.90 |
| 23 | DA | 2619 | C | N3-C2-O2 | 5.08 | 125.46 | 121.90 |
| 23 | BA | 565 | C | N3-C4-C5 | -5.08 | 119.87 | 121.90 |
| 23 | BA | 677 | A | N3-C4-C5 | 5.08 | 130.36 | 126.80 |
| 23 | DA | 458 | G | N3-C2-N2 | 5.08 | 123.46 | 119.90 |
| 23 | DA | 566 | U | C5-C6-N1 | -5.08 | 120.16 | 122.70 |
| 23 | BA | 2489 | G | C2-N3-C4 | -5.08 | 109.36 | 111.90 |
| 23 | DA | 98 | G | C6-C5-N7 | -5.08 | 127.35 | 130.40 |
| 23 | DA | 1904 | G | N1-C6-O6 | -5.08 | 116.85 | 119.90 |
| 23 | DA | 2497 | A | N3-C4-C5 | 5.08 | 130.35 | 126.80 |
| 25 | DC | 215 | LEU | CA-CB-CG | -5.08 | 103.62 | 115.30 |
| 23 | BA | 1137 | G | N1-C6-O6 | 5.08 | 122.95 | 119.90 |
| 23 | BA | 1662 | C | C5-C6-N1 | -5.08 | 118.46 | 121.00 |
| 23 | BA | 1803 | A | C8-N9-C4 | 5.08 | 107.83 | 105.80 |
| 23 | DA | 1672 | C | N3-C4-N4 | 5.08 | 121.55 | 118.00 |
| 23 | DA | 2724 | C | C2-N3-C4 | -5.08 | 117.36 | 119.90 |
| 23 | BA | 640 | C | C2-N3-C4 | -5.08 | 117.36 | 119.90 |
| 23 | DA | 532 | A | C5-N7-C8 | 5.08 | 106.44 | 103.90 |
| 23 | DA | 789 | A | N1-C6-N6 | 5.08 | 121.64 | 118.60 |
| 23 | DA | 1378 | A | N9-C4-C5 | 5.08 | 107.83 | 105.80 |
| 23 | DA | 1571 | A | C8-N9-C4 | 5.08 | 107.83 | 105.80 |
| 23 | DA | 2238 | G | C6-C5-N7 | -5.08 | 127.36 | 130.40 |
| 23 | BA | 2279 | G | N3-C4-C5 | -5.07 | 126.06 | 128.60 |
| 1 | CA | 907 | A | C8-N9-C4 | -5.07 | 103.77 | 105.80 |
| 23 | DA | 1825 | A | C5-C6-N1 | 5.07 | 120.24 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | DA | 867 | C | N3-C4-C5 | -5.07 | 119.87 | 121.90 |
| 23 | BA | 582 | G | C8-N9-C4 | 5.07 | 108.43 | 106.40 |
| 23 | BA | 738 | G | N1-C6-O6 | 5.07 | 122.94 | 119.90 |
| 23 | BA | 2544 | G | C5-N7-C8 | -5.07 | 101.77 | 104.30 |
| 23 | DA | 240 | G | C4-C5-N7 | -5.07 | 108.77 | 110.80 |
| 23 | DA | 509 | C | C5-C6-N1 | -5.07 | 118.47 | 121.00 |
| 23 | DA | 1592 | C | C5-C6-N1 | -5.07 | 118.46 | 121.00 |
| 23 | DA | 2698 | U | C4-C5-C6 | 5.07 | 122.74 | 119.70 |
| 34 | DL | 50 | ARG | NE-CZ-NH2 | -5.07 | 117.77 | 120.30 |
| 1 | AA | 560 | U | C2-N1-C1' | 5.07 | 123.78 | 117.70 |
| 23 | BA | 2004 | G | C2-N3-C4 | -5.07 | 109.37 | 111.90 |
| 23 | BA | 2697 | G | C2-N3-C4 | -5.07 | 109.37 | 111.90 |
| 23 | DA | 1128 | A | C5-C6-N1 | 5.07 | 120.23 | 117.70 |
| 23 | DA | 1128 | A | C2-N3-C4 | 5.07 | 113.13 | 110.60 |
| 23 | DA | 2715 | C | C6-N1-C2 | 5.07 | 122.33 | 120.30 |
| 23 | BA | 844 | C | C5-C6-N1 | -5.07 | 118.47 | 121.00 |
| 23 | BA | 1332 | G | C6-C5-N7 | 5.07 | 133.44 | 130.40 |
| 23 | BA | 2432 | A | C2-N3-C4 | -5.07 | 108.07 | 110.60 |
| 23 | DA | 366(B) | C | N1-C2-O2 | -5.07 | 115.86 | 118.90 |
| 23 | DA | 748 | G | N7-C8-N9 | -5.07 | 110.57 | 113.10 |
| 23 | DA | 1024 | G | C8-N9-C1' | -5.07 | 120.42 | 127.00 |
| 23 | DA | 797 | C | C4-C5-C6 | 5.06 | 119.93 | 117.40 |
| 23 | DA | 1286 | A | C5-C6-N6 | 5.06 | 127.75 | 123.70 |
| 23 | BA | 2028 | U | N1-C2-N3 | 5.06 | 117.94 | 114.90 |
| 23 | BA | 2346 | A | C8-N9-C4 | -5.06 | 103.78 | 105.80 |
| 23 | DA | 500 | G | C8-N9-C4 | 5.06 | 108.42 | 106.40 |
| 23 | DA | 582 | G | N1-C2-N3 | 5.06 | 126.94 | 123.90 |
| 23 | DA | 1225 | G | N3-C2-N2 | 5.06 | 123.44 | 119.90 |
| 23 | DA | 1825 | A | N1-C2-N3 | 5.06 | 131.83 | 129.30 |
| 23 | DA | 2435 | A | C5-N7-C8 | -5.06 | 101.37 | 103.90 |
| 23 | BA | 189 | G | C8-N9-C1' | -5.06 | 120.42 | 127.00 |
| 23 | BA | 2035 | G | C6-C5-N7 | 5.06 | 133.44 | 130.40 |
| 23 | BA | 2084 | C | N3-C4-C5 | 5.06 | 123.92 | 121.90 |
| 40 | BR | 18 | LEU | CA-CB-CG | 5.06 | 126.94 | 115.30 |
| 23 | DA | 771 | G | C5-C6-O6 | -5.06 | 125.56 | 128.60 |
| 23 | DA | 2087 | G | N1-C6-O6 | 5.06 | 122.94 | 119.90 |
| 1 | AA | 901 | A | C5-N7-C8 | -5.06 | 101.37 | 103.90 |
| 23 | BA | 1998 | G | C8-N9-C4 | 5.06 | 108.42 | 106.40 |
| 23 | DA | 201 | C | C5-C6-N1 | -5.06 | 118.47 | 121.00 |
| 23 | DA | 600 | G | C8-N9-C4 | 5.06 | 108.42 | 106.40 |
| 23 | DA | 956 | G | C2-N3-C4 | -5.06 | 109.37 | 111.90 |
| 23 | DA | 1631 | A | N1-C2-N3 | 5.06 | 131.83 | 129.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23 | DA | 2233 | U | N1-C2-O2 | -5.06 | 119.26 | 122.80 |
| 1 | AA | 1529 | G | C4-N9-C1' | 5.06 | 133.07 | 126.50 |
| 23 | DA | 2876 | G | N9-C4-C5 | -5.06 | 103.38 | 105.40 |
| 1 | AA | 819 | A | N1-C6-N6 | 5.05 | 121.63 | 118.60 |
| 23 | BA | 120 | U | C6-N1-C2 | 5.05 | 124.03 | 121.00 |
| 23 | BA | 1807 | G | N1-C6-O6 | -5.05 | 116.87 | 119.90 |
| 23 | BA | 2698 | U | C5-C4-O4 | 5.05 | 128.93 | 125.90 |
| 23 | DA | 263 | C | N3-C4-C5 | 5.05 | 123.92 | 121.90 |
| 23 | DA | 2026 | C | N1-C2-O2 | -5.05 | 115.87 | 118.90 |
| 23 | BA | 70 | G | N3-C4-C5 | -5.05 | 126.07 | 128.60 |
| 23 | BA | 1240 | U | N3-C4-C5 | -5.05 | 111.57 | 114.60 |
| 23 | BA | 2056 | G | C5-C6-O6 | -5.05 | 125.57 | 128.60 |
| 23 | BA | 2391 | G | N9-C4-C5 | 5.05 | 107.42 | 105.40 |
| 1 | AA | 1512 | U | C4-C5-C6 | 5.05 | 122.73 | 119.70 |
| 23 | BA | 761 | A | N3-C4-N9 | 5.05 | 131.44 | 127.40 |
| 23 | BA | 1634 | A | N9-C4-C5 | 5.05 | 107.82 | 105.80 |
| 23 | DA | 771 | G | C4-C5-N7 | 5.05 | 112.82 | 110.80 |
| 23 | BA | 374 | A | C8-N9-C4 | 5.05 | 107.82 | 105.80 |
| 23 | BA | 2059 | A | N7-C8-N9 | -5.05 | 111.28 | 113.80 |
| 23 | BA | 2346 | A | N7-C8-N9 | 5.05 | 116.33 | 113.80 |
| 23 | DA | 1686 | C | N1-C2-O2 | -5.05 | 115.87 | 118.90 |
| 23 | DA | 1496 | A | C6-C5-N7 | -5.05 | 128.77 | 132.30 |
| 23 | DA | 1677 | A | N9-C4-C5 | 5.05 | 107.82 | 105.80 |
| 23 | DA | 1951 | U | C5-C6-N1 | -5.05 | 120.18 | 122.70 |
| 23 | BA | 334 | C | C3'-C2'-C1' | 5.05 | 105.54 | 101.50 |
| 23 | BA | 675 | A | C5-N7-C8 | -5.05 | 101.38 | 103.90 |
| 23 | BA | 681 | G | C8-N9-C1' | -5.05 | 120.44 | 127.00 |
| 23 | BA | 807 | U | N3-C4-O4 | -5.05 | 115.87 | 119.40 |
| 23 | BA | 1649 | G | C2-N3-C4 | -5.05 | 109.38 | 111.90 |
| 23 | DA | 1634 | A | C8-N9-C4 | 5.05 | 107.82 | 105.80 |
| 23 | DA | 1687 | G | C5-C6-N1 | -5.05 | 108.98 | 111.50 |
| 23 | BA | 2426 | A | C5-N7-C8 | -5.04 | 101.38 | 103.90 |
| 23 | BA | 2518 | A | C2-N3-C4 | -5.04 | 108.08 | 110.60 |
| 23 | BA | 2777 | G | N7-C8-N9 | -5.04 | 110.58 | 113.10 |
| 23 | DA | 1658 | C | C6-N1-C1' | -5.04 | 114.75 | 120.80 |
| 23 | DA | 2497 | A | N3-C4-N9 | -5.04 | 123.36 | 127.40 |
| 1 | AA | 1530 | G | N1-C6-O6 | 5.04 | 122.93 | 119.90 |
| 1 | CA | 691 | G | C6-C5-N7 | -5.04 | 127.37 | 130.40 |
| 23 | DA | 334 | C | C3'-C2'-C1' | 5.04 | 105.53 | 101.50 |
| 23 | DA | 1368 | G | N1-C6-O6 | -5.04 | 116.87 | 119.90 |
| 23 | BA | 1210 | A | C5-C6-N1 | -5.04 | 115.18 | 117.70 |
| 23 | BA | 1903 | G | C8-N9-C4 | 5.04 | 108.42 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | BA | 2580 | U | N1-C2-N3 | 5.04 | 117.92 | 114.90 |
| 1 | CA | 720 | C | C2-N1-C1' | 5.04 | 124.35 | 118.80 |
| 23 | DA | 389 | G | C8-N9-C4 | 5.04 | 108.42 | 106.40 |
| 1 | AA | 810 | C | C4-C5-C6 | 5.04 | 119.92 | 117.40 |
| 23 | BA | 19 | C | C2-N3-C4 | -5.04 | 117.38 | 119.90 |
| 23 | BA | 1198 | U | N1-C2-N3 | 5.04 | 117.92 | 114.90 |
| 23 | DA | 337 | C | C2-N1-C1' | -5.04 | 113.26 | 118.80 |
| 23 | DA | 441 | U | C6-N1-C2 | 5.04 | 124.02 | 121.00 |
| 23 | DA | 2572 | A | N1-C6-N6 | 5.04 | 121.62 | 118.60 |
| 23 | DA | 2448 | A | C2-N3-C4 | -5.04 | 108.08 | 110.60 |
| 23 | BA | 543 | C | C5-C6-N1 | -5.04 | 118.48 | 121.00 |
| 23 | BA | 1155 | A | C8-N9-C4 | -5.04 | 103.79 | 105.80 |
| 23 | DA | 1203 | G | C4-C5-N7 | -5.04 | 108.79 | 110.80 |
| 23 | DA | 1351 | C | C6-N1-C2 | 5.04 | 122.31 | 120.30 |
| 23 | DA | 1633 | G | C5-C6-N1 | -5.04 | 108.98 | 111.50 |
| 23 | DA | 1644 | C | C2-N1-C1' | 5.04 | 124.34 | 118.80 |
| 23 | DA | 2323 | G | C8-N9-C4 | 5.04 | 108.41 | 106.40 |
| 23 | DA | 2327 | A | N1-C6-N6 | 5.04 | 121.62 | 118.60 |
| 1 | AA | 1097 | C | C6-N1-C2 | -5.03 | 118.29 | 120.30 |
| 23 | DA | 681 | G | N3-C4-N9 | 5.03 | 129.02 | 126.00 |
| 23 | DA | 1122 | G | C4-N9-C1' | -5.03 | 119.96 | 126.50 |
| 1 | AA | 575 | G | N1-C6-O6 | -5.03 | 116.88 | 119.90 |
| 23 | BA | 784 | A | C4-N9-C1' | -5.03 | 117.24 | 126.30 |
| 23 | BA | 2538 | C | C5-C6-N1 | -5.03 | 118.48 | 121.00 |
| 23 | DA | 686 | G | N1-C6-O6 | 5.03 | 122.92 | 119.90 |
| 23 | BA | 1899 | G | C8-N9-C1' | 5.03 | 133.54 | 127.00 |
| 23 | BA | 2327 | A | C8-N9-C4 | 5.03 | 107.81 | 105.80 |
| 23 | BA | 2839 | G | C5-C6-O6 | -5.03 | 125.58 | 128.60 |
| 23 | DA | 31 | C | N3-C4-C5 | 5.03 | 123.91 | 121.90 |
| 23 | DA | 202 | U | C5-C4-O4 | -5.03 | 122.88 | 125.90 |
| 23 | DA | 1022 | G | N1-C2-N3 | 5.03 | 126.92 | 123.90 |
| 23 | DA | 2490 | G | N9-C4-C5 | -5.03 | 103.39 | 105.40 |
| 23 | DA | 1653 | G | C8-N9-C1' | -5.03 | 120.46 | 127.00 |
| 23 | BA | 1558 | A | C5-C6-N1 | -5.03 | 115.19 | 117.70 |
| 23 | BA | 1971 | A | C4-C5-N7 | 5.03 | 113.21 | 110.70 |
| 23 | DA | 809 | G | N1-C2-N3 | 5.03 | 126.92 | 123.90 |
| 23 | DA | 1365 | A | C5-N7-C8 | -5.03 | 101.39 | 103.90 |
| 23 | DA | 1499 | C | C2-N1-C1' | -5.03 | 113.27 | 118.80 |
| 23 | DA | 2731 | G | C5-C6-N1 | 5.03 | 114.01 | 111.50 |
| 23 | BA | 2440 | C | C2-N1-C1' | -5.03 | 113.27 | 118.80 |
| 23 | BA | 2597 | G | C2-N3-C4 | -5.03 | 109.39 | 111.90 |
| 23 | DA | 1661 | G | C5-C6-N1 | 5.03 | 114.01 | 111.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | BA | 835 | A | C5-N7-C8 | 5.02 | 106.41 | 103.90 |
| 23 | DA | 855 | G | C8-N9-C4 | -5.02 | 104.39 | 106.40 |
| 23 | DA | 1299 | G | C8-N9-C4 | 5.02 | 108.41 | 106.40 |
| 23 | BA | 834 | C | N3-C4-N4 | -5.02 | 114.48 | 118.00 |
| 1 | CA | 552 | U | N3-C4-O4 | -5.02 | 115.89 | 119.40 |
| 23 | DA | 671 | C | N3-C4-N4 | 5.02 | 121.52 | 118.00 |
| 23 | DA | 1022 | G | C4-C5-N7 | -5.02 | 108.79 | 110.80 |
| 23 | BA | 802 | A | C4-N9-C1' | 5.02 | 135.34 | 126.30 |
| 23 | DA | 450 | G | N3-C4-C5 | -5.02 | 126.09 | 128.60 |
| 23 | DA | 727 | A | C8-N9-C4 | -5.02 | 103.79 | 105.80 |
| 23 | DA | 2333 | A | C8-N9-C4 | 5.02 | 107.81 | 105.80 |
| 23 | BA | 2766 | G | C4-N9-C1' | 5.02 | 133.03 | 126.50 |
| 23 | DA | 473 | G | C8-N9-C4 | 5.02 | 108.41 | 106.40 |
| 23 | DA | 1493 | C | C6-N1-C1' | -5.02 | 114.78 | 120.80 |
| 23 | DA | 1792 | G | C8-N9-C4 | -5.02 | 104.39 | 106.40 |
| 23 | BA | 1270 | C | C6-N1-C1' | 5.02 | 126.82 | 120.80 |
| 23 | DA | 1375 | C | C5-C4-N4 | -5.02 | 116.69 | 120.20 |
| 23 | BA | 789 | A | N9-C4-C5 | -5.01 | 103.79 | 105.80 |
| 23 | BA | 2064 | C | C6-N1-C2 | -5.01 | 118.29 | 120.30 |
| 23 | BA | 2555 | U | C2-N1-C1' | -5.01 | 111.68 | 117.70 |
| 23 | DA | 803 | U | N1-C2-N3 | 5.01 | 117.91 | 114.90 |
| 23 | DA | 968 | G | N9-C4-C5 | -5.01 | 103.39 | 105.40 |
| 23 | DA | 1185 | C | N3-C4-C5 | 5.01 | 123.91 | 121.90 |
| 23 | BA | 2448 | A | C2-N3-C4 | -5.01 | 108.09 | 110.60 |
| 23 | DA | 2330 | G | N7-C8-N9 | -5.01 | 110.59 | 113.10 |
| 1 | AA | 917 | G | C4-N9-C1' | 5.01 | 133.01 | 126.50 |
| 23 | BA | 964 | C | N3-C4-C5 | 5.01 | 123.91 | 121.90 |
| 23 | BA | 1325 | G | N3-C4-N9 | -5.01 | 122.99 | 126.00 |
| 23 | BA | 1948 | G | N3-C4-C5 | -5.01 | 126.09 | 128.60 |
| 23 | BA | 2443 | C | N1-C2-O2 | 5.01 | 121.91 | 118.90 |
| 23 | BA | 2596 | U | C6-N1-C2 | 5.01 | 124.01 | 121.00 |
| 23 | DA | 530 | G | C5-C6-O6 | 5.01 | 131.61 | 128.60 |
| 23 | BA | 815 | C | N3-C4-C5 | 5.01 | 123.90 | 121.90 |
| 23 | BA | 2056 | G | C6-N1-C2 | -5.01 | 122.09 | 125.10 |
| 23 | BA | 2498 | C | N1-C2-O2 | -5.01 | 115.89 | 118.90 |
| 23 | DA | 728 | G | N1-C2-N3 | 5.01 | 126.91 | 123.90 |
| 23 | DA | 1652 | A | C5-C6-N6 | -5.01 | 119.69 | 123.70 |
| 23 | DA | 2374 | C | C5-C6-N1 | -5.01 | 118.50 | 121.00 |
| 23 | BA | 1310 | G | C5-C6-O6 | -5.01 | 125.59 | 128.60 |
| 23 | BA | 1330 | C | C4-C5-C6 | -5.01 | 114.90 | 117.40 |
| 23 | BA | 1188 | U | C6-N1-C2 | -5.01 | 118.00 | 121.00 |
| 1 | CA | 18 | C | C6-N1-C2 | -5.01 | 118.30 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 23 | DA | 1397 | U | N1-C2-O2 | 5.01 | 126.30 | 122.80 |
| 23 | DA | 1429 | G | N1-C2-N3 | 5.01 | 126.90 | 123.90 |
| 23 | DA | 1677 | A | C8-N9-C4 | -5.01 | 103.80 | 105.80 |
| 23 | DA | 1928 | A | C8-N9-C4 | 5.01 | 107.80 | 105.80 |
| 23 | DA | 2447 | G | N1-C2-N3 | 5.01 | 126.90 | 123.90 |
| 23 | BA | 62 | C | C6-N1-C2 | 5.00 | 122.30 | 120.30 |
| 23 | BA | 2252 | G | C8-N9-C4 | 5.00 | 108.40 | 106.40 |
| 23 | DA | 961 | C | N3-C2-O2 | -5.00 | 118.40 | 121.90 |
| 23 | BA | 1632 | A | N1-C6-N6 | 5.00 | 121.60 | 118.60 |
| 23 | DA | 337 | C | C6-N1-C2 | 5.00 | 122.30 | 120.30 |
| 23 | DA | 2831 | G | N3-C4-N9 | -5.00 | 123.00 | 126.00 |
| 23 | BA | 1677 | A | C2-N3-C4 | -5.00 | 108.10 | 110.60 |

There are no chirality outliers.

All (21) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 27 | BE | 47 | GLY | Peptide |
| 34 | BL | 29 | LYS | Peptide |
| 34 | BL | 37 | GLY | Peptide |
| 34 | BL | 39 | LYS | Peptide |
| 34 | BL | 52 | GLU | Peptide |
| 34 | BL | 9 | ASN | Peptide |
| 35 | BM | 7 | MET | Peptide |
| 36 | BN | 11 | ASN | Peptide |
| 39 | BQ | 33 | ARG | Peptide |
| 39 | BQ | 91 | ASP | Peptide |
| 25 | DC | 237 | GLU | Peptide |
| 27 | DE | 47 | GLY | Peptide |
| 34 | DL | 29 | LYS | Peptide |
| 34 | DL | 37 | GLY | Peptide |
| 34 | DL | 39 | LYS | Peptide |
| 34 | DL | 52 | GLU | Peptide |
| 34 | DL | 9 | ASN | Peptide |
| 35 | DM | 7 | MET | Peptide |
| 36 | DN | 11 | ASN | Peptide |
| 39 | DQ | 33 | ARG | Peptide |
| 39 | DQ | 91 | ASP | Peptide |

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | AA | 32372 | 0 | 16339 | 1680 | 0 |
| 1 | CA | 32372 | 0 | 16339 | 1784 | 0 |
| 2 | AB | 1901 | 0 | 1951 | 173 | 0 |
| 2 | CB | 1901 | 0 | 1951 | 180 | 0 |
| 3 | AC | 1613 | 0 | 1677 | 180 | 0 |
| 3 | CC | 1613 | 0 | 1677 | 186 | 0 |
| 4 | AD | 1703 | 0 | 1764 | 192 | 0 |
| 4 | CD | 1703 | 0 | 1764 | 182 | 1 |
| 5 | AE | 1156 | 0 | 1213 | 141 | 0 |
| 5 | CE | 1156 | 0 | 1213 | 141 | 0 |
| 6 | AF | 843 | 0 | 857 | 96 | 1 |
| 6 | CF | 843 | 0 | 857 | 93 | 0 |
| 7 | AG | 1257 | 0 | 1296 | 95 | 0 |
| 7 | CG | 1257 | 0 | 1296 | 92 | 0 |
| 8 | AH | 1116 | 0 | 1177 | 133 | 0 |
| 8 | CH | 1116 | 0 | 1177 | 140 | 0 |
| 9 | AI | 1011 | 0 | 1043 | 100 | 0 |
| 9 | CI | 1011 | 0 | 1043 | 112 | 0 |
| 10 | AJ | 795 | 0 | 840 | 93 | 0 |
| 10 | CJ | 795 | 0 | 840 | 92 | 0 |
| 11 | AK | 885 | 0 | 904 | 76 | 0 |
| 11 | CK | 885 | 0 | 904 | 72 | 0 |
| 12 | AL | 971 | 0 | 1057 | 126 | 0 |
| 12 | CL | 971 | 0 | 1057 | 139 | 0 |
| 13 | AM | 929 | 0 | 987 | 83 | 0 |
| 13 | CM | 929 | 0 | 987 | 83 | 0 |
| 14 | AN | 492 | 0 | 530 | 49 | 0 |
| 14 | CN | 492 | 0 | 532 | 61 | 0 |
| 15 | AO | 734 | 0 | 771 | 66 | 0 |
| 15 | CO | 734 | 0 | 771 | 60 | 0 |
| 16 | AP | 701 | 0 | 720 | 96 | 0 |
| 16 | CP | 701 | 0 | 720 | 90 | 0 |
| 17 | AQ | 824 | 0 | 893 | 66 | 0 |
| 17 | CQ | 824 | 0 | 893 | 77 | 0 |
| 18 | AR | 574 | 0 | 644 | 70 | 0 |
| 18 | CR | 574 | 0 | 644 | 70 | 0 |
| 19 | AS | 630 | 0 | 652 | 70 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 19 | CS | 630 | 0 | 652 | 60 | 0 |
| 20 | AT | 762 | 0 | 859 | 64 | 0 |
| 20 | CT | 762 | 0 | 859 | 70 | 0 |
| 21 | AU | 209 | 0 | 221 | 16 | 0 |
| 21 | CU | 209 | 0 | 221 | 17 | 0 |
| 22 | AV | 719 | 0 | 366 | 58 | 0 |
| 22 | CV | 719 | 0 | 366 | 57 | 0 |
| 23 | BA | 59440 | 0 | 29964 | 2618 | 0 |
| 23 | DA | 59442 | 0 | 29965 | 2593 | 0 |
| 24 | BB | 2551 | 0 | 1295 | 147 | 0 |
| 24 | DB | 2551 | 0 | 1295 | 148 | 0 |
| 25 | BC | 2105 | 0 | 2182 | 353 | 0 |
| 25 | DC | 2105 | 0 | 2182 | 347 | 0 |
| 26 | BD | 1564 | 0 | 1629 | 224 | 0 |
| 26 | DD | 1564 | 0 | 1629 | 224 | 0 |
| 27 | BE | 1587 | 0 | 1632 | 147 | 0 |
| 27 | DE | 1587 | 0 | 1632 | 155 | 0 |
| 28 | BF | 1475 | 0 | 1537 | 155 | 0 |
| 28 | DF | 1475 | 0 | 1537 | 150 | 0 |
| 29 | BG | 1223 | 0 | 1282 | 114 | 0 |
| 29 | DG | 1223 | 0 | 1282 | 121 | 0 |
| 30 | BH | 1133 | 0 | 1220 | 131 | 0 |
| 30 | DH | 1133 | 0 | 1220 | 133 | 0 |
| 31 | BI | 254 | 0 | 275 | 8 | 0 |
| 31 | DI | 254 | 0 | 275 | 8 | 0 |
| 32 | BJ | 1097 | 0 | 1168 | 170 | 0 |
| 32 | DJ | 1097 | 0 | 1168 | 158 | 0 |
| 33 | BK | 932 | 0 | 994 | 97 | 0 |
| 33 | DK | 932 | 0 | 994 | 100 | 0 |
| 34 | BL | 1114 | 0 | 1187 | 270 | 0 |
| 34 | DL | 1114 | 0 | 1187 | 279 | 0 |
| 35 | BM | 1079 | 0 | 1127 | 170 | 0 |
| 35 | DM | 1079 | 0 | 1127 | 172 | 0 |
| 36 | BN | 960 | 0 | 1021 | 153 | 0 |
| 36 | DN | 960 | 0 | 1021 | 142 | 0 |
| 37 | BO | 771 | 0 | 832 | 95 | 0 |
| 37 | DO | 771 | 0 | 832 | 100 | 0 |
| 38 | BP | 1144 | 0 | 1211 | 129 | 0 |
| 38 | DP | 1144 | 0 | 1211 | 132 | 0 |
| 39 | BQ | 953 | 0 | 1013 | 150 | 0 |
| 39 | DQ | 953 | 0 | 1013 | 155 | 0 |
| 40 | BR | 779 | 0 | 852 | 131 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 40 | DR | 779 | 0 | 852 | 128 | 0 |
| 41 | BS | 891 | 0 | 951 | 106 | 0 |
| 41 | DS | 891 | 0 | 951 | 110 | 0 |
| 42 | BT | 726 | 0 | 778 | 88 | 0 |
| 42 | DT | 726 | 0 | 778 | 92 | 0 |
| 43 | BU | 776 | 0 | 870 | 138 | 0 |
| 43 | DU | 776 | 0 | 870 | 139 | 0 |
| 44 | BV | 1492 | 0 | 1513 | 174 | 0 |
| 44 | DV | 1492 | 0 | 1513 | 171 | 0 |
| 45 | BW | 605 | 0 | 628 | 71 | 0 |
| 45 | DW | 605 | 0 | 628 | 63 | 0 |
| 46 | BX | 695 | 0 | 764 | 112 | 0 |
| 46 | DX | 695 | 0 | 764 | 106 | 0 |
| 47 | BY | 521 | 0 | 575 | 81 | 0 |
| 47 | DY | 521 | 0 | 575 | 81 | 0 |
| 48 | BZ | 468 | 0 | 523 | 46 | 0 |
| 48 | DZ | 468 | 0 | 523 | 46 | 0 |
| 49 | B1 | 226 | 0 | 225 | 23 | 0 |
| 49 | D1 | 226 | 0 | 225 | 24 | 0 |
| 50 | B2 | 405 | 0 | 420 | 61 | 0 |
| 50 | D2 | 405 | 0 | 420 | 64 | 0 |
| 51 | B3 | 381 | 0 | 391 | 25 | 0 |
| 51 | D3 | 381 | 0 | 391 | 26 | 0 |
| 52 | B4 | 419 | 0 | 467 | 50 | 0 |
| 52 | D4 | 419 | 0 | 467 | 48 | 0 |
| 53 | B5 | 508 | 0 | 576 | 111 | 0 |
| 53 | D5 | 508 | 0 | 576 | 110 | 0 |
| 54 | AA | 163 | 0 | 0 | 0 | 0 |
| 54 | AD | 1 | 0 | 0 | 0 | 0 |
| 54 | AV | 4 | 0 | 0 | 0 | 0 |
| 54 | B2 | 1 | 0 | 0 | 0 | 0 |
| 54 | BA | 408 | 0 | 0 | 0 | 0 |
| 54 | BB | 17 | 0 | 0 | 0 | 0 |
| 54 | BK | 1 | 0 | 0 | 0 | 0 |
| 54 | CA | 140 | 0 | 0 | 0 | 0 |
| 54 | CP | 1 | 0 | 0 | 0 | 0 |
| 54 | CV | 1 | 0 | 0 | 0 | 0 |
| 54 | D2 | 1 | 0 | 0 | 0 | 0 |
| 54 | D4 | 1 | 0 | 0 | 0 | 0 |
| 54 | DA | 436 | 0 | 0 | 0 | 0 |
| 54 | DB | 17 | 0 | 0 | 0 | 0 |
| 54 | DE | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 54 | DG | 1 | 0 | 0 | 0 | 0 |
| 55 | AD | 1 | 0 | 0 | 0 | 0 |
| 55 | AN | 1 | 0 | 0 | 0 | 0 |
| 55 | CD | 1 | 0 | 0 | 0 | 0 |
| 55 | CN | 1 | 0 | 0 | 0 | 0 |
| All | All | 282142 | 0 | 191729 | 18333 | 1 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 39.

All (18333) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:DL:59:LEU:HA | 34:DL:61:ARG:NE | 1.55 | 1.20 |
| 34:DL:57:THR:HG23 | 34:DL:59:LEU:HD22 | 1.22 | 1.20 |
| 35:BM:81:VAL:O | 35:BM:82:ARG:HG2 | 1.39 | 1.19 |
| 34:BL:57:THR:HG23 | 34:BL:59:LEU:HD22 | 1.21 | 1.19 |
| 52:D4:8:ASN:C | 52:D4:8:ASN:HD22 | 1.42 | 1.18 |
| 47:BY:2:LYS:H | 47:BY:2:LYS:HE2 | 1.08 | 1.16 |
| 23:BA:2389:G:H5'' | 23:BA:2390:U:H5' | 1.19 | 1.16 |
| 43:BU:7:VAL:HG12 | 43:BU:8:LYS:HG3 | 1.25 | 1.16 |
| 47:DY:2:LYS:HE2 | 47:DY:2:LYS:H | 1.02 | 1.15 |
| 34:DL:114:ILE:HD12 | 34:DL:114:ILE:H | 1.11 | 1.15 |
| 1:AA:1123:A:H4' | 10:AJ:36:GLY:HA3 | 1.30 | 1.14 |
| 52:B4:8:ASN:C | 52:B4:8:ASN:HD22 | 1.46 | 1.14 |
| 23:DA:2015:A:H1' | 50:D2:2:ALA:HA | 1.30 | 1.14 |
| 23:DA:2439:A:H5' | 23:DA:2439:A:C8 | 1.83 | 1.13 |
| 34:BL:59:LEU:HA | 34:BL:61:ARG:NE | 1.63 | 1.13 |
| 26:BD:201:THR:HG22 | 26:BD:202:LYS:H | 1.08 | 1.12 |
| 23:BA:2015:A:H1' | 50:B2:2:ALA:HA | 1.28 | 1.12 |
| 47:DY:2:LYS:N | 47:DY:2:LYS:HE2 | 1.63 | 1.12 |
| 35:DM:81:VAL:O | 35:DM:82:ARG:HG2 | 1.49 | 1.11 |
| 26:DD:101:ARG:HD3 | 26:DD:169:ASN:HD21 | 1.13 | 1.11 |
| 36:DN:12:ARG:HG2 | 36:DN:16:HIS:CD2 | 1.84 | 1.11 |
| 47:BY:2:LYS:HE2 | 47:BY:2:LYS:N | 1.65 | 1.11 |
| 23:BA:1174:A:H3' | 23:BA:1175:U:H5'' | 1.24 | 1.11 |
| 23:BA:2781:A:H5'' | 23:BA:2782:G:H5' | 1.11 | 1.11 |
| 23:DA:1541:U:H3' | 23:DA:1542:G:H3' | 1.13 | 1.11 |
| 10:AJ:48:THR:HA | 10:AJ:62:HIS:HB3 | 1.32 | 1.11 |
| 45:BW:23:VAL:HA | 45:BW:38:VAL:HG22 | 1.26 | 1.11 |
| 45:DW:23:VAL:HA | 45:DW:38:VAL:HG22 | 1.28 | 1.11 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BA:1541:U:H3' | 23:BA:1542:G:H3' | 1.13 | 1.10 |
| 25:BC:155:LEU:HD23 | 25:BC:177:LEU:HD21 | 1.32 | 1.10 |
| 7:CG:113:GLU:HB2 | 7:CG:119:ARG:HG2 | 1.32 | 1.10 |
| 43:DU:7:VAL:HG12 | 43:DU:8:LYS:HG3 | 1.20 | 1.10 |
| 23:BA:2272:U:H6 | 23:BA:2272:U:H5'' | 1.16 | 1.10 |
| 23:DA:1174:A:H3' | 23:DA:1175:U:H5'' | 1.24 | 1.09 |
| 38:DP:51:ARG:HG3 | 38:DP:51:ARG:HH11 | 1.08 | 1.09 |
| 28:DF:60:LEU:HD11 | 28:DF:92:VAL:HG11 | 1.33 | 1.09 |
| 2:AB:185:ILE:HG22 | 2:AB:199:TYR:HB2 | 1.29 | 1.09 |
| 34:BL:128:HIS:HA | 34:BL:147:LEU:HB3 | 1.14 | 1.09 |
| 23:DA:2781:A:H5'' | 23:DA:2782:G:H5' | 1.15 | 1.09 |
| 23:BA:807:U:OP2 | 34:BL:39:LYS:HG3 | 1.52 | 1.09 |
| 1:AA:82:U:H2' | 1:AA:85:U:H5 | 1.18 | 1.09 |
| 34:DL:128:HIS:HA | 34:DL:147:LEU:HB3 | 1.15 | 1.09 |
| 1:CA:1347:G:C8 | 9:CI:107:ARG:HB3 | 1.87 | 1.09 |
| 1:AA:979:C:H3' | 1:AA:980:C:H5'' | 1.34 | 1.09 |
| 26:DD:201:THR:HG22 | 26:DD:202:LYS:H | 1.07 | 1.08 |
| 26:BD:101:ARG:HD3 | 26:BD:169:ASN:HD21 | 1.16 | 1.08 |
| 23:BA:2439:A:H5' | 23:BA:2439:A:C8 | 1.87 | 1.08 |
| 2:CB:111:ARG:HG2 | 2:CB:111:ARG:HH11 | 1.10 | 1.08 |
| 22:AV:6194:C:H2' | 22:AV:6195:G:H8 | 1.14 | 1.08 |
| 28:BF:60:LEU:HD11 | 28:BF:92:VAL:HG11 | 1.31 | 1.08 |
| 7:AG:113:GLU:HB2 | 7:AG:119:ARG:HG2 | 1.33 | 1.08 |
| 10:CJ:48:THR:HA | 10:CJ:62:HIS:HB3 | 1.32 | 1.08 |
| 1:CA:82:U:H2' | 1:CA:85:U:H5 | 1.18 | 1.07 |
| 34:BL:33:ARG:N | 34:BL:36:LYS:HE2 | 1.70 | 1.07 |
| 36:BN:12:ARG:HG2 | 36:BN:16:HIS:CD2 | 1.88 | 1.07 |
| 1:AA:365:U:H5'' | 1:AA:366:C:OP1 | 1.52 | 1.07 |
| 5:CE:101:ILE:HD11 | 5:CE:119:LEU:HD23 | 1.31 | 1.07 |
| 2:AB:111:ARG:HG2 | 2:AB:111:ARG:HH11 | 1.11 | 1.07 |
| 23:BA:2186:G:H2' | 23:BA:2187:G:H8 | 1.17 | 1.07 |
| 25:BC:10:THR:HG23 | 25:BC:13:ARG:HB3 | 1.31 | 1.07 |
| 22:CV:6194:C:H2' | 22:CV:6195:G:H8 | 1.16 | 1.07 |
| 38:DP:54:ARG:HG3 | 38:DP:54:ARG:HH11 | 1.14 | 1.07 |
| 23:DA:807:U:OP2 | 34:DL:39:LYS:HG3 | 1.55 | 1.06 |
| 23:DA:2389:G:H5'' | 23:DA:2390:U:H5' | 1.20 | 1.06 |
| 1:CA:979:C:H3' | 1:CA:980:C:H5'' | 1.32 | 1.06 |
| 5:AE:101:ILE:HD11 | 5:AE:119:LEU:HD23 | 1.31 | 1.06 |
| 38:BP:51:ARG:HG3 | 38:BP:51:ARG:HH11 | 1.15 | 1.06 |
| 1:AA:955:U:H1' | 1:AA:1227:A:H61 | 1.18 | 1.06 |
| 1:CA:365:U:H5'' | 1:CA:366:C:OP1 | 1.56 | 1.06 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:BE:67:GLN:O | 27:BE:67:GLN:HG3 | 1.56 | 1.06 |
| 27:DE:67:GLN:O | 27:DE:67:GLN:HG3 | 1.54 | 1.06 |
| 53:B5:30:ARG:O | 53:B5:31:HIS:HB3 | 1.52 | 1.06 |
| 34:BL:114:ILE:HD12 | 34:BL:114:ILE:H | 1.17 | 1.05 |
| 34:DL:62:LEU:HD22 | 34:DL:62:LEU:H | 1.19 | 1.05 |
| 23:BA:2502:G:H5' | 23:BA:2503:A:H5'' | 1.36 | 1.05 |
| 42:DT:63:LYS:HD2 | 42:DT:72:LYS:HA | 1.05 | 1.05 |
| 38:BP:54:ARG:HG3 | 38:BP:54:ARG:HH11 | 1.15 | 1.05 |
| 37:BO:11:LYS:HG2 | 37:BO:12:PHE:H | 1.18 | 1.05 |
| 34:DL:33:ARG:H | 34:DL:36:LYS:HE2 | 1.21 | 1.05 |
| 2:CB:185:ILE:HG22 | 2:CB:199:TYR:HB2 | 1.30 | 1.05 |
| 26:DD:201:THR:O | 26:DD:202:LYS:HD3 | 1.57 | 1.04 |
| 23:DA:2272:U:H6 | 23:DA:2272:U:H5'' | 1.20 | 1.04 |
| 32:BJ:157:ARG:H | 32:BJ:158:PRO:HD3 | 1.18 | 1.04 |
| 23:DA:1899:G:H22 | 23:DA:1902:C:N4 | 1.54 | 1.04 |
| 23:DA:2186:G:H2' | 23:DA:2187:G:H8 | 1.18 | 1.04 |
| 1:CA:1123:A:H4' | 10:CJ:36:GLY:HA3 | 1.37 | 1.04 |
| 23:BA:1899:G:H22 | 23:BA:1902:C:N4 | 1.56 | 1.04 |
| 23:DA:2502:G:H5' | 23:DA:2503:A:H5'' | 1.34 | 1.03 |
| 25:DC:10:THR:HG23 | 25:DC:13:ARG:HB3 | 1.36 | 1.03 |
| 34:DL:33:ARG:HE | 34:DL:36:LYS:HD3 | 1.23 | 1.02 |
| 26:BD:132:HIS:CD2 | 26:BD:135:HIS:NE2 | 2.27 | 1.02 |
| 34:BL:64:LYS:O | 34:BL:66:GLY:N | 1.92 | 1.02 |
| 1:CA:955:U:H1' | 1:CA:1227:A:H61 | 1.19 | 1.02 |
| 34:BL:57:THR:CG2 | 34:BL:59:LEU:HD22 | 1.88 | 1.02 |
| 34:BL:62:LEU:HD22 | 34:BL:62:LEU:H | 1.19 | 1.02 |
| 34:DL:33:ARG:N | 34:DL:36:LYS:HE2 | 1.73 | 1.02 |
| 26:BD:201:THR:O | 26:BD:202:LYS:HD3 | 1.59 | 1.01 |
| 23:BA:1021:A:H62 | 23:BA:1141:U:H3 | 1.04 | 1.01 |
| 27:BE:164:ARG:HH11 | 27:BE:164:ARG:HG2 | 1.23 | 1.01 |
| 23:BA:973:A:OP2 | 40:BR:78:LYS:NZ | 1.91 | 1.01 |
| 34:BL:33:ARG:H | 34:BL:36:LYS:HE2 | 1.22 | 1.01 |
| 29:DG:101:ARG:NE | 29:DG:101:ARG:H | 1.57 | 1.01 |
| 42:BT:63:LYS:HD2 | 42:BT:72:LYS:HA | 1.05 | 1.01 |
| 29:BG:101:ARG:H | 29:BG:101:ARG:NE | 1.58 | 1.01 |
| 42:DT:50:LYS:H | 42:DT:87:GLN:HE22 | 1.07 | 1.01 |
| 32:DJ:157:ARG:H | 32:DJ:158:PRO:HD3 | 1.20 | 1.01 |
| 23:DA:1658:C:OP1 | 26:DD:132:HIS:ND1 | 1.94 | 1.01 |
| 36:DN:38:VAL:HB | 36:DN:39:PRO:HD3 | 1.42 | 1.01 |
| 23:DA:1264:G:H5' | 50:D2:11:THR:HG21 | 1.42 | 1.01 |
| 41:BS:12:ILE:HD13 | 41:BS:17:VAL:HG13 | 1.40 | 1.01 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:B4:9:ARG:HE | 52:B4:48:LYS:HB2 | 1.24 | 1.00 |
| 23:BA:676:A:H8 | 23:BA:2069:G:H21 | 1.06 | 1.00 |
| 27:DE:164:ARG:HG2 | 27:DE:164:ARG:HH11 | 1.22 | 1.00 |
| 23:BA:603:A:H61 | 23:BA:655:A:C4' | 1.75 | 1.00 |
| 47:DY:14:ARG:HA | 47:DY:17:SER:HB2 | 1.41 | 1.00 |
| 23:BA:919:G:H5' | 24:BB:81:G:H1' | 1.44 | 1.00 |
| 28:BF:84:LYS:HG3 | 28:BF:85:GLY:H | 1.27 | 1.00 |
| 52:D4:9:ARG:HE | 52:D4:48:LYS:HB2 | 1.22 | 1.00 |
| 23:BA:2579:C:O3' | 26:BD:131:ALA:HB2 | 1.61 | 1.00 |
| 9:CI:13:ALA:HB2 | 9:CI:68:GLY:HA3 | 1.44 | 1.00 |
| 39:DQ:88:ILE:HB | 39:DQ:90:VAL:HG12 | 1.42 | 1.00 |
| 34:BL:33:ARG:HE | 34:BL:36:LYS:HD3 | 1.25 | 0.99 |
| 32:BJ:157:ARG:H | 32:BJ:158:PRO:CD | 1.70 | 0.99 |
| 25:DC:33:LEU:O | 25:DC:35:LYS:N | 1.93 | 0.99 |
| 35:DM:75:THR:HA | 35:DM:88:GLY:HA2 | 1.43 | 0.99 |
| 32:DJ:157:ARG:H | 32:DJ:158:PRO:CD | 1.72 | 0.99 |
| 23:BA:1899:G:H22 | 23:BA:1902:C:H41 | 1.01 | 0.99 |
| 23:DA:1614:A:H62 | 41:DS:93:ALA:HB2 | 1.25 | 0.99 |
| 25:BC:106:ILE:H | 25:BC:106:ILE:HD12 | 1.28 | 0.99 |
| 23:DA:860:U:H5 | 23:DA:917:A:N7 | 1.59 | 0.99 |
| 23:BA:1826:G:H4' | 25:BC:242:ARG:HE | 1.27 | 0.99 |
| 34:DL:40:SER:O | 34:DL:41:ARG:HD3 | 1.62 | 0.99 |
| 32:BJ:154:GLN:HE21 | 32:BJ:155:ALA:HB3 | 1.28 | 0.99 |
| 23:BA:810:U:H3 | 34:BL:36:LYS:HZ3 | 1.03 | 0.98 |
| 42:BT:50:LYS:H | 42:BT:87:GLN:HE22 | 1.07 | 0.98 |
| 9:AI:13:ALA:HB2 | 9:AI:68:GLY:HA3 | 1.44 | 0.98 |
| 32:DJ:154:GLN:HE21 | 32:DJ:155:ALA:HB3 | 1.27 | 0.98 |
| 1:AA:673:G:H2' | 1:AA:674:G:C8 | 1.98 | 0.98 |
| 38:DP:24:PRO:HA | 38:DP:49:VAL:HG13 | 1.45 | 0.98 |
| 50:B2:20:ARG:HA | 50:B2:23:HIS:HD2 | 1.25 | 0.98 |
| 28:DF:84:LYS:HG3 | 28:DF:85:GLY:H | 1.24 | 0.98 |
| 23:DA:1021:A:H62 | 23:DA:1141:U:H3 | 1.03 | 0.98 |
| 16:CP:4:ILE:HG12 | 16:CP:21:VAL:HG12 | 1.45 | 0.98 |
| 3:AC:20:SER:HB2 | 3:AC:40:ARG:HH12 | 1.27 | 0.98 |
| 50:D2:20:ARG:HA | 50:D2:23:HIS:HD2 | 1.28 | 0.98 |
| 30:BH:83:ALA:HB2 | 30:BH:123:LEU:HD12 | 1.45 | 0.98 |
| 41:DS:12:ILE:HD13 | 41:DS:17:VAL:HG13 | 1.44 | 0.98 |
| 23:BA:1544:C:OP1 | 23:BA:1544:C:H6 | 1.45 | 0.98 |
| 34:DL:64:LYS:O | 34:DL:66:GLY:N | 1.94 | 0.98 |
| 40:BR:2:PHE:CE2 | 40:BR:13:ARG:HD3 | 1.97 | 0.98 |
| 53:D5:30:ARG:O | 53:D5:31:HIS:HB3 | 1.61 | 0.98 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:BT:11:PRO:HA | 42:BT:28:PHE:HB3 | 1.43 | 0.98 |
| 39:BQ:88:ILE:HB | 39:BQ:90:VAL:HG12 | 1.45 | 0.97 |
| 4:AD:49:ARG:NH2 | 4:AD:50:ARG:HB2 | 1.79 | 0.97 |
| 23:BA:1614:A:H62 | 41:BS:93:ALA:HB2 | 1.29 | 0.97 |
| 1:CA:673:G:H2' | 1:CA:674:G:C8 | 1.99 | 0.97 |
| 23:BA:2729:G:H1' | 26:BD:187:ALA:HB2 | 1.47 | 0.97 |
| 26:DD:201:THR:HG22 | 26:DD:202:LYS:N | 1.80 | 0.97 |
| 23:DA:2729:G:H1' | 26:DD:187:ALA:HB2 | 1.44 | 0.97 |
| 34:BL:40:SER:O | 34:BL:41:ARG:HD3 | 1.65 | 0.97 |
| 28:DF:128:ARG:HE | 28:DF:129:GLY:H | 1.12 | 0.97 |
| 37:DO:11:LYS:HG2 | 37:DO:12:PHE:H | 1.25 | 0.97 |
| 23:BA:1541:U:C3' | 23:BA:1542:G:H3' | 1.95 | 0.97 |
| 47:BY:14:ARG:HA | 47:BY:17:SER:HB2 | 1.44 | 0.97 |
| 25:BC:87:ASN:HD22 | 25:BC:87:ASN:H | 1.06 | 0.97 |
| 16:AP:4:ILE:HG12 | 16:AP:21:VAL:HG12 | 1.43 | 0.97 |
| 25:DC:155:LEU:HD23 | 25:DC:177:LEU:HD21 | 1.46 | 0.97 |
| 4:CD:49:ARG:NH2 | 4:CD:50:ARG:HB2 | 1.79 | 0.97 |
| 3:CC:20:SER:HB2 | 3:CC:40:ARG:HH12 | 1.26 | 0.97 |
| 32:BJ:38:LEU:HD23 | 32:BJ:157:ARG:HG3 | 1.46 | 0.97 |
| 23:DA:2579:C:O3' | 26:DD:131:ALA:HB2 | 1.65 | 0.97 |
| 43:BU:29:GLU:HB3 | 43:BU:38:ILE:HB | 1.46 | 0.97 |
| 3:AC:182:ILE:HG12 | 3:AC:203:PHE:HA | 1.45 | 0.96 |
| 23:DA:676:A:H8 | 23:DA:2069:G:H21 | 1.11 | 0.96 |
| 23:BA:1658:C:OP1 | 26:BD:132:HIS:ND1 | 1.98 | 0.96 |
| 4:AD:104:VAL:HG11 | 4:AD:146:ILE:HD13 | 1.45 | 0.96 |
| 42:DT:84:ALA:HB3 | 42:DT:87:GLN:HE21 | 1.27 | 0.96 |
| 23:DA:603:A:H61 | 23:DA:655:A:C4' | 1.77 | 0.96 |
| 12:AL:26:LEU:HG | 12:AL:32:ARG:HH11 | 1.28 | 0.96 |
| 4:CD:65:ARG:HG3 | 4:CD:75:PHE:CD1 | 1.99 | 0.96 |
| 25:BC:33:LEU:O | 25:BC:35:LYS:N | 1.98 | 0.96 |
| 23:DA:1541:U:C3' | 23:DA:1542:G:H3' | 1.93 | 0.96 |
| 23:BA:860:U:H5 | 23:BA:917:A:N7 | 1.61 | 0.96 |
| 42:BT:63:LYS:HD2 | 42:BT:72:LYS:CA | 1.96 | 0.96 |
| 32:DJ:38:LEU:HD23 | 32:DJ:157:ARG:HG3 | 1.45 | 0.96 |
| 1:CA:392:G:H2' | 1:CA:393:A:H8 | 1.30 | 0.96 |
| 33:BK:119:PRO:HB2 | 38:BP:68:TYR:CE1 | 2.01 | 0.96 |
| 23:BA:252:G:OP2 | 34:BL:50:ARG:NH2 | 1.98 | 0.96 |
| 4:AD:9:CYS:HB3 | 4:AD:32:ALA:HB2 | 1.47 | 0.96 |
| 52:D4:19:ARG:HG3 | 52:D4:19:ARG:HH11 | 1.27 | 0.96 |
| 3:CC:182:ILE:HG12 | 3:CC:203:PHE:HA | 1.46 | 0.96 |
| 4:CD:104:VAL:HG11 | 4:CD:146:ILE:HD13 | 1.47 | 0.96 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:BL:62:LEU:HD22 | 34:BL:62:LEU:N | 1.80 | 0.96 |
| 1:AA:1320:C:H42 | 19:AS:36:ARG:HG3 | 1.28 | 0.96 |
| 40:DR:2:PHE:CE2 | 40:DR:13:ARG:HD3 | 2.01 | 0.96 |
| 35:BM:75:THR:HA | 35:BM:88:GLY:CA | 1.94 | 0.96 |
| 23:DA:1813:G:H1' | 25:DC:50:THR:HG21 | 1.47 | 0.96 |
| 34:DL:57:THR:CG2 | 34:DL:59:LEU:HD22 | 1.94 | 0.96 |
| 35:DM:75:THR:HA | 35:DM:88:GLY:CA | 1.96 | 0.95 |
| 4:CD:22:LYS:HB2 | 4:CD:26:CYS:SG | 2.05 | 0.95 |
| 23:DA:1541:U:H3' | 23:DA:1542:G:C3' | 1.95 | 0.95 |
| 47:DY:6:VAL:HG12 | 47:DY:10:LEU:HD11 | 1.48 | 0.95 |
| 25:DC:106:ILE:HD12 | 25:DC:106:ILE:H | 1.30 | 0.95 |
| 47:BY:35:LEU:HD12 | 47:BY:53:LEU:HD12 | 1.45 | 0.95 |
| 2:CB:174:VAL:O | 2:CB:178:ARG:HB2 | 1.66 | 0.95 |
| 1:AA:691:G:C6 | 11:AK:52:GLY:HA2 | 2.02 | 0.95 |
| 42:DT:11:PRO:HA | 42:DT:28:PHE:HB3 | 1.48 | 0.95 |
| 13:CM:52:GLU:HA | 13:CM:55:ARG:HB3 | 1.46 | 0.95 |
| 47:BY:6:VAL:HG12 | 47:BY:10:LEU:HD11 | 1.48 | 0.94 |
| 23:BA:1813:G:H1' | 25:BC:50:THR:HG21 | 1.46 | 0.94 |
| 30:DH:83:ALA:HB2 | 30:DH:123:LEU:HD12 | 1.47 | 0.94 |
| 20:AT:26:ASN:HB2 | 20:AT:71:THR:HG23 | 1.47 | 0.94 |
| 13:AM:52:GLU:HA | 13:AM:55:ARG:HB3 | 1.46 | 0.94 |
| 26:BD:36:ARG:HD3 | 26:BD:85:ASN:HD21 | 1.29 | 0.94 |
| 16:AP:28:ARG:HG2 | 16:AP:28:ARG:HH11 | 1.30 | 0.94 |
| 25:DC:158:ALA:HB3 | 25:DC:161:THR:HG21 | 1.47 | 0.94 |
| 23:BA:1541:U:H3' | 23:BA:1542:G:C3' | 1.97 | 0.94 |
| 34:BL:114:ILE:HD11 | 34:BL:127:ALA:HB3 | 1.48 | 0.94 |
| 1:AA:1097:C:H2' | 1:AA:1098:C:H6 | 1.32 | 0.94 |
| 1:AA:1253:G:H1 | 1:AA:1284:C:H42 | 1.14 | 0.94 |
| 23:DA:2712:U:H1' | 23:DA:712(B):A:C8 | 2.00 | 0.94 |
| 4:AD:22:LYS:HB2 | 4:AD:26:CYS:SG | 2.07 | 0.94 |
| 1:AA:1435:G:H2' | 1:AA:1436:U:C6 | 2.02 | 0.94 |
| 23:DA:1544:C:H6 | 23:DA:1544:C:OP1 | 1.49 | 0.94 |
| 25:BC:96:HIS:CD2 | 25:BC:102:LYS:HD3 | 2.02 | 0.94 |
| 25:BC:31:LYS:O | 25:BC:35:LYS:HB2 | 1.67 | 0.94 |
| 23:BA:197:A:H5' | 23:BA:197:A:H8 | 1.30 | 0.94 |
| 43:DU:14:LEU:HD23 | 43:DU:15:VAL:N | 1.83 | 0.94 |
| 34:DL:62:LEU:N | 34:DL:62:LEU:HD22 | 1.80 | 0.94 |
| 29:DG:101:ARG:HE | 29:DG:101:ARG:N | 1.66 | 0.94 |
| 40:BR:39:LEU:HD12 | 40:BR:47:VAL:HG11 | 1.49 | 0.94 |
| 39:BQ:55:ARG:HA | 39:BQ:58:ARG:HD2 | 1.47 | 0.94 |
| 35:BM:75:THR:HA | 35:BM:88:GLY:HA2 | 1.44 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:BA:94:G:H21 | 47:BY:47:ASN:ND2 | 1.64 | 0.94 |
| 8:CH:121:ASP:O | 8:CH:125:ARG:HB2 | 1.68 | 0.94 |
| 23:DA:973:A:OP2 | 40:DR:78:LYS:NZ | 2.00 | 0.94 |
| 52:D4:8:ASN:C | 52:D4:8:ASN:ND2 | 2.18 | 0.94 |
| 34:DL:38:GLN:HG3 | 34:DL:39:LYS:H | 1.33 | 0.94 |
| 3:CC:172:ARG:O | 3:CC:173:VAL:HG23 | 1.66 | 0.94 |
| 3:CC:173:VAL:O | 3:CC:173:VAL:HG12 | 1.69 | 0.93 |
| 34:DL:114:ILE:HD11 | 34:DL:127:ALA:HB3 | 1.49 | 0.93 |
| 23:BA:804:A:H5' | 23:BA:805:G:OP1 | 1.68 | 0.93 |
| 28:DF:38:VAL:HG22 | 28:DF:93:THR:HG23 | 1.49 | 0.93 |
| 1:CA:91:C:H2' | 1:CA:92:G:H8 | 1.33 | 0.93 |
| 23:BA:1210:A:H8 | 23:BA:1210:A:C5' | 1.81 | 0.93 |
| 35:BM:74:TYR:HD2 | 35:BM:91:GLU:HB2 | 1.29 | 0.93 |
| 35:BM:74:TYR:CD2 | 35:BM:91:GLU:HB2 | 2.04 | 0.93 |
| 52:D4:11:LYS:O | 52:D4:15:THR:HG23 | 1.69 | 0.93 |
| 16:CP:28:ARG:HH11 | 16:CP:28:ARG:HG2 | 1.34 | 0.93 |
| 20:CT:26:ASN:HB2 | 20:CT:71:THR:HG23 | 1.48 | 0.93 |
| 28:DF:5:LEU:HD21 | 49:D1:50:THR:HG23 | 1.51 | 0.93 |
| 28:BF:128:ARG:HE | 28:BF:129:GLY:H | 1.14 | 0.93 |
| 23:BA:1287:A:N7 | 36:BN:107:ASP:HB3 | 1.84 | 0.93 |
| 39:DQ:92:ARG:HG2 | 40:DR:11:GLN:NE2 | 1.84 | 0.93 |
| 23:BA:2210:G:N2 | 23:BA:2211:G:H5' | 1.84 | 0.93 |
| 39:BQ:92:ARG:HG2 | 40:BR:11:GLN:NE2 | 1.81 | 0.93 |
| 23:BA:547:A:H2' | 23:BA:548:A:C8 | 2.03 | 0.93 |
| 4:AD:65:ARG:HG3 | 4:AD:75:PHE:CD1 | 2.03 | 0.93 |
| 23:DA:252:G:OP2 | 34:DL:50:ARG:NH2 | 2.02 | 0.93 |
| 23:DA:547:A:H2' | 23:DA:548:A:C8 | 2.03 | 0.93 |
| 23:BA:1405:U:H2' | 23:BA:1406:U:C6 | 2.04 | 0.93 |
| 49:D1:59:VAL:HG12 | 49:D1:60:GLU:H | 1.34 | 0.93 |
| 22:AV:6213:A:H2' | 22:AV:6214:C:C6 | 2.04 | 0.93 |
| 2:AB:174:VAL:O | 2:AB:178:ARG:HB2 | 1.69 | 0.93 |
| 26:BD:201:THR:HG22 | 26:BD:202:LYS:N | 1.83 | 0.93 |
| 23:DA:919:G:H5' | 24:DB:81:G:H1' | 1.49 | 0.93 |
| 2:CB:187:LEU:HA | 2:CB:201:ILE:HB | 1.51 | 0.93 |
| 42:DT:63:LYS:HD2 | 42:DT:72:LYS:CA | 1.97 | 0.92 |
| 35:DM:74:TYR:HD2 | 35:DM:91:GLU:HB2 | 1.35 | 0.92 |
| 1:AA:38:G:N2 | 1:AA:397:A:H5' | 1.84 | 0.92 |
| 23:BA:140:A:H8 | 23:BA:1408:C:HO2' | 0.96 | 0.92 |
| 23:DA:1287:A:N7 | 36:DN:107:ASP:HB3 | 1.84 | 0.92 |
| 32:DJ:105:LEU:HD12 | 32:DJ:106:LYS:H | 1.34 | 0.92 |
| 3:CC:134:ILE:HG23 | 3:CC:151:VAL:HB | 1.51 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:DA:1826:G:H4' | 25:DC:242:ARG:HE | 1.32 | 0.92 |
| 23:DA:1899:G:H22 | 23:DA:1902:C:H41 | 1.05 | 0.92 |
| 29:BG:101:ARG:HE | 29:BG:101:ARG:N | 1.67 | 0.92 |
| 28:BF:38:VAL:HG22 | 28:BF:93:THR:HG23 | 1.51 | 0.92 |
| 23:BA:2439:A:H5' | 23:BA:2439:A:H8 | 1.31 | 0.92 |
| 23:BA:1209:G:H21 | 23:BA:1210:A:H62 | 1.15 | 0.92 |
| 23:DA:1170:G:H1 | 23:DA:1179:C:H42 | 1.17 | 0.92 |
| 4:AD:108:LEU:HD21 | 4:AD:183:GLY:HA3 | 1.52 | 0.92 |
| 8:AH:121:ASP:O | 8:AH:125:ARG:HB2 | 1.70 | 0.92 |
| 44:DV:48:PHE:HA | 44:DV:51:ALA:HB3 | 1.51 | 0.92 |
| 12:CL:26:LEU:HG | 12:CL:32:ARG:HH11 | 1.32 | 0.92 |
| 42:BT:84:ALA:HB3 | 42:BT:87:GLN:HE21 | 1.34 | 0.92 |
| 16:AP:19:ILE:HG22 | 16:AP:36:ILE:HG13 | 1.51 | 0.92 |
| 23:DA:94:G:H21 | 47:DY:47:ASN:ND2 | 1.67 | 0.92 |
| 1:AA:91:C:H2' | 1:AA:92:G:H8 | 1.34 | 0.92 |
| 35:BM:47:ILE:HG22 | 35:BM:48:GLU:N | 1.82 | 0.92 |
| 26:BD:5:LEU:HB2 | 26:BD:51:PHE:HD2 | 1.34 | 0.92 |
| 26:DD:132:HIS:CD2 | 26:DD:135:HIS:NE2 | 2.37 | 0.92 |
| 29:BG:68:THR:O | 29:BG:72:ILE:HG12 | 1.70 | 0.92 |
| 27:DE:9:ILE:HD11 | 27:DE:125:LEU:HG | 1.48 | 0.92 |
| 23:DA:1021:A:H3' | 23:DA:1021:A:H8 | 1.34 | 0.92 |
| 41:BS:75:TYR:CE2 | 41:BS:104:THR:HB | 2.04 | 0.92 |
| 1:CA:38:G:N2 | 1:CA:397:A:H5' | 1.84 | 0.92 |
| 23:DA:330:A:HO2' | 23:DA:331:A:H8 | 1.16 | 0.92 |
| 23:DA:860:U:O2' | 23:DA:861:A:H5' | 1.69 | 0.92 |
| 39:BQ:91:ASP:OD1 | 39:BQ:96:ALA:HB2 | 1.68 | 0.92 |
| 23:DA:2210:G:N2 | 23:DA:2211:G:H5' | 1.85 | 0.92 |
| 25:DC:31:LYS:O | 25:DC:35:LYS:HB2 | 1.70 | 0.91 |
| 23:BA:1405:U:H2' | 23:BA:1406:U:H6 | 1.30 | 0.91 |
| 23:BA:2219:G:C2' | 23:BA:2224:G:H5' | 2.01 | 0.91 |
| 23:DA:2068:U:H3 | 23:DA:2430:A:H2 | 0.93 | 0.91 |
| 23:BA:1021:A:H3' | 23:BA:1021:A:H8 | 1.32 | 0.91 |
| 39:BQ:83:LEU:HG | 39:BQ:88:ILE:HD11 | 1.50 | 0.91 |
| 23:BA:1170:G:H1 | 23:BA:1179:C:H42 | 1.16 | 0.91 |
| 39:BQ:92:ARG:NH2 | 40:BR:11:GLN:H | 1.67 | 0.91 |
| 3:AC:172:ARG:O | 3:AC:173:VAL:HG23 | 1.69 | 0.91 |
| 23:BA:2681:C:H5 | 23:BA:2725:A:H62 | 0.96 | 0.91 |
| 3:CC:14:ILE:HG23 | 3:CC:15:THR:H | 1.35 | 0.91 |
| 23:DA:2392:A:H2 | 23:DA:2424:C:H42 | 1.17 | 0.91 |
| 23:DA:2267:A:H5'' | 23:DA:2268:A:H5' | 1.51 | 0.91 |
| 23:BA:2219:G:H2' | 23:BA:2224:G:H5' | 1.49 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DA:363(A):G:H2' | 23:DA:363(B):A:H8 | 1.33 | 0.91 |
| 23:DA:1405:U:H2' | 23:DA:1406:U:H6 | 1.32 | 0.91 |
| 23:DA:1405:U:H2' | 23:DA:1406:U:C6 | 2.05 | 0.91 |
| 23:BA:363(A):G:H2' | 23:BA:363(B):A:H8 | 1.34 | 0.91 |
| 23:DA:662:G:OP1 | 34:DL:18:ARG:HD2 | 1.71 | 0.91 |
| 47:DY:2:LYS:CE | 47:DY:2:LYS:H | 1.84 | 0.91 |
| 23:BA:2887:U:H2' | 23:BA:2888:C:H6 | 1.34 | 0.91 |
| 3:CC:33:LEU:HD21 | 14:CN:53:LEU:HD22 | 1.52 | 0.91 |
| 23:BA:2068:U:N3 | 23:BA:2430:A:H2 | 1.67 | 0.91 |
| 1:AA:392:G:H2' | 1:AA:393:A:H8 | 1.34 | 0.91 |
| 26:DD:101:ARG:HD3 | 26:DD:169:ASN:ND2 | 1.85 | 0.91 |
| 45:BW:23:VAL:HA | 45:BW:38:VAL:CG2 | 2.01 | 0.91 |
| 23:DA:197:A:H8 | 23:DA:197:A:H5' | 1.34 | 0.91 |
| 25:BC:158:ALA:HB3 | 25:BC:161:THR:HG21 | 1.50 | 0.91 |
| 3:AC:33:LEU:HD21 | 14:AN:53:LEU:HD22 | 1.52 | 0.91 |
| 2:AB:71:VAL:HG23 | 2:AB:164:VAL:HG13 | 1.52 | 0.91 |
| 34:DL:35:HIS:O | 34:DL:36:LYS:HB2 | 1.69 | 0.91 |
| 40:DR:39:LEU:HD12 | 40:DR:47:VAL:HG11 | 1.51 | 0.91 |
| 28:DF:76:SER:HB3 | 28:DF:82:LEU:HB3 | 1.52 | 0.91 |
| 1:CA:265:G:H2' | 1:CA:266:G:H5'' | 1.52 | 0.91 |
| 27:BE:167:ALA:HB1 | 27:BE:173:VAL:HG11 | 1.52 | 0.91 |
| 27:DE:64:ILE:HD12 | 27:DE:64:ILE:O | 1.71 | 0.90 |
| 42:DT:63:LYS:CD | 42:DT:72:LYS:HA | 2.00 | 0.90 |
| 40:DR:38:LEU:O | 40:DR:39:LEU:HD13 | 1.71 | 0.90 |
| 6:CF:86:ARG:O | 6:CF:87:ARG:HB2 | 1.71 | 0.90 |
| 23:BA:2272:U:H5'' | 23:BA:2272:U:C6 | 2.06 | 0.90 |
| 23:BA:2712:U:H1' | 23:BA:712(B):A:C8 | 2.06 | 0.90 |
| 26:DD:36:ARG:HD3 | 26:DD:85:ASN:HD21 | 1.32 | 0.90 |
| 53:D5:33:ASN:HD22 | 53:D5:34:TRP:H | 1.15 | 0.90 |
| 23:BA:2267:A:H5'' | 23:BA:2268:A:H5' | 1.51 | 0.90 |
| 23:BA:141(A):A:H8 | 23:BA:1595:G:H21 | 1.18 | 0.90 |
| 1:CA:1201:A:H1' | 1:CA:1202:G:OP2 | 1.71 | 0.90 |
| 4:CD:9:CYS:HB3 | 4:CD:32:ALA:HB2 | 1.52 | 0.90 |
| 23:DA:1771:C:HO2' | 23:DA:1786:A:H8 | 0.98 | 0.90 |
| 22:AV:6194:C:H2' | 22:AV:6195:G:C8 | 2.05 | 0.90 |
| 1:CA:38:G:H22 | 1:CA:397:A:H5' | 1.35 | 0.90 |
| 26:DD:49:LEU:HD22 | 26:DD:49:LEU:H | 1.36 | 0.90 |
| 45:DW:23:VAL:HA | 45:DW:38:VAL:CG2 | 2.02 | 0.90 |
| 23:BA:2185:C:H2' | 23:BA:2186:G:C8 | 2.06 | 0.90 |
| 23:DA:1264:G:H5' | 50:D2:11:THR:CG2 | 2.01 | 0.90 |
| 47:DY:35:LEU:HD12 | 47:DY:53:LEU:HD12 | 1.51 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 39:DQ:55:ARG:HA | 39:DQ:58:ARG:HD2 | 1.52 | 0.90 |
| 49:B1:59:VAL:HG12 | 49:B1:60:GLU:H | 1.34 | 0.90 |
| 23:DA:2185:C:H2' | 23:DA:2186:G:C8 | 2.07 | 0.90 |
| 39:DQ:91:ASP:OD1 | 39:DQ:96:ALA:HB2 | 1.72 | 0.90 |
| 5:CE:43:LEU:HD22 | 5:CE:136:MET:HG3 | 1.51 | 0.90 |
| 41:BS:4:LYS:HA | 41:BS:106:ILE:HG22 | 1.53 | 0.90 |
| 34:DL:59:LEU:HA | 34:DL:61:ARG:CD | 2.01 | 0.90 |
| 6:AF:86:ARG:O | 6:AF:87:ARG:HB2 | 1.70 | 0.90 |
| 1:AA:38:G:H22 | 1:AA:397:A:H5' | 1.36 | 0.90 |
| 1:CA:1435:G:H2' | 1:CA:1436:U:C6 | 2.05 | 0.90 |
| 36:DN:10:LEU:HB3 | 36:DN:17:ARG:NE | 1.87 | 0.90 |
| 44:BV:48:PHE:HA | 44:BV:51:ALA:HB3 | 1.52 | 0.90 |
| 25:DC:96:HIS:CD2 | 25:DC:102:LYS:HD3 | 2.06 | 0.90 |
| 23:BA:810:U:H3 | 34:BL:36:LYS:NZ | 1.70 | 0.90 |
| 22:CV:6213:A:H2' | 22:CV:6214:C:C6 | 2.06 | 0.90 |
| 22:CV:6194:C:H2' | 22:CV:6195:G:C8 | 2.07 | 0.90 |
| 1:CA:1253:G:H1 | 1:CA:1284:C:H42 | 1.15 | 0.90 |
| 1:CA:737:A:H2' | 1:CA:738:C:C6 | 2.07 | 0.90 |
| 5:AE:43:LEU:HD22 | 5:AE:136:MET:HG3 | 1.53 | 0.90 |
| 30:DH:56:LYS:HA | 30:DH:59:ALA:HB3 | 1.53 | 0.90 |
| 43:DU:29:GLU:HB3 | 43:DU:38:ILE:HB | 1.53 | 0.90 |
| 23:DA:2887:U:H2' | 23:DA:2888:C:H6 | 1.35 | 0.90 |
| 16:CP:19:ILE:HG22 | 16:CP:36:ILE:HG13 | 1.54 | 0.89 |
| 3:AC:134:ILE:HG23 | 3:AC:151:VAL:HB | 1.53 | 0.89 |
| 4:AD:15:GLU:HG2 | 4:AD:63:LYS:HG3 | 1.52 | 0.89 |
| 25:BC:231:HIS:HD2 | 25:BC:249:PRO:HA | 1.35 | 0.89 |
| 20:AT:57:ARG:NH1 | 20:AT:102:GLY:HA2 | 1.87 | 0.89 |
| 30:BH:56:LYS:HA | 30:BH:59:ALA:HB3 | 1.54 | 0.89 |
| 37:DO:69:VAL:O | 37:DO:72:ALA:HB3 | 1.70 | 0.89 |
| 23:BA:2186:G:H2' | 23:BA:2187:G:C8 | 2.06 | 0.89 |
| 23:BA:1899:G:N2 | 23:BA:1902:C:H41 | 1.70 | 0.89 |
| 1:AA:199:G:H1 | 1:AA:218:C:H42 | 1.17 | 0.89 |
| 34:BL:57:THR:HG23 | 34:BL:59:LEU:CD2 | 2.02 | 0.89 |
| 23:BA:860:U:O2' | 23:BA:861:A:H5' | 1.72 | 0.89 |
| 2:CB:111:ARG:NH1 | 2:CB:111:ARG:HG2 | 1.83 | 0.89 |
| 37:DO:11:LYS:HG2 | 37:DO:12:PHE:N | 1.87 | 0.89 |
| 26:DD:5:LEU:HB2 | 26:DD:51:PHE:HD2 | 1.37 | 0.89 |
| 1:CA:1097:C:H2' | 1:CA:1098:C:H6 | 1.35 | 0.89 |
| 12:AL:69:ILE:HG23 | 12:AL:99:ILE:HG21 | 1.53 | 0.89 |
| 23:DA:810:U:H3 | 34:DL:36:LYS:HZ1 | 1.18 | 0.89 |
| 23:DA:1286:A:O2' | 23:DA:1288:U:OP2 | 1.89 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:AE:51:VAL:HB | 5:AE:52:PRO:HD3 | 1.53 | 0.89 |
| 24:DB:79:C:H2' | 24:DB:80:U:O4' | 1.72 | 0.89 |
| 23:DA:2542:A:N3 | 23:DA:2542:A:H5'' | 1.87 | 0.89 |
| 1:CA:1070:U:H2' | 1:CA:1071:C:H6 | 1.37 | 0.89 |
| 23:DA:2439:A:C5' | 23:DA:2439:A:H8 | 1.85 | 0.89 |
| 28:BF:76:SER:HB3 | 28:BF:82:LEU:HB3 | 1.52 | 0.89 |
| 35:BM:68:ILE:HD13 | 35:BM:103:MET:HG2 | 1.55 | 0.89 |
| 44:BV:132:ASN:O | 44:BV:134:PRO:HD3 | 1.71 | 0.89 |
| 11:AK:57:THR:HG22 | 11:AK:59:TYR:H | 1.36 | 0.89 |
| 41:BS:9:TYR:H | 41:BS:102:HIS:HD2 | 1.21 | 0.89 |
| 42:BT:35:THR:O | 42:BT:39:ILE:HG12 | 1.73 | 0.89 |
| 23:DA:94:G:H21 | 47:DY:47:ASN:HD22 | 1.19 | 0.89 |
| 23:BA:2542:A:H5'' | 23:BA:2542:A:N3 | 1.87 | 0.89 |
| 13:CM:10:PRO:HB2 | 13:CM:18:ALA:HB1 | 1.55 | 0.89 |
| 39:DQ:92:ARG:NH2 | 40:DR:11:GLN:H | 1.70 | 0.89 |
| 1:AA:386:C:H2' | 1:AA:387:U:H5'' | 1.54 | 0.89 |
| 6:CF:91:VAL:HG12 | 6:CF:92:LYS:O | 1.73 | 0.89 |
| 28:BF:5:LEU:HD21 | 49:B1:50:THR:HG23 | 1.52 | 0.89 |
| 8:AH:91:ARG:HH11 | 8:AH:91:ARG:CG | 1.85 | 0.89 |
| 34:DL:114:ILE:HD13 | 34:DL:130:PHE:CD1 | 2.08 | 0.88 |
| 1:AA:955:U:H1' | 1:AA:1227:A:N6 | 1.87 | 0.88 |
| 23:BA:94:G:H21 | 47:BY:47:ASN:HD22 | 1.17 | 0.88 |
| 2:CB:187:LEU:HD11 | 2:CB:205:ASP:HB3 | 1.54 | 0.88 |
| 25:DC:87:ASN:H | 25:DC:87:ASN:HD22 | 1.16 | 0.88 |
| 8:AH:92:ARG:HB3 | 8:AH:94:TYR:HE2 | 1.39 | 0.88 |
| 23:BA:1771:C:HO2' | 23:BA:1786:A:H8 | 0.94 | 0.88 |
| 29:DG:68:THR:O | 29:DG:72:ILE:HG12 | 1.71 | 0.88 |
| 23:DA:2439:A:C5' | 23:DA:2439:A:C8 | 2.56 | 0.88 |
| 23:BA:1021:A:C8 | 23:BA:1021:A:H3' | 2.08 | 0.88 |
| 11:CK:57:THR:HG22 | 11:CK:59:TYR:H | 1.35 | 0.88 |
| 23:DA:1437:C:H2' | 23:DA:1438:U:H6 | 1.37 | 0.88 |
| 52:B4:19:ARG:HG3 | 52:B4:19:ARG:HH11 | 1.37 | 0.88 |
| 1:AA:1070:U:H2' | 1:AA:1071:C:H6 | 1.38 | 0.88 |
| 41:DS:4:LYS:HA | 41:DS:106:ILE:HG22 | 1.55 | 0.88 |
| 23:DA:2439:A:H5' | 23:DA:2439:A:H8 | 1.34 | 0.88 |
| 25:DC:67:PHE:CE2 | 25:DC:106:ILE:HD11 | 2.07 | 0.88 |
| 19:CS:63:THR:HG22 | 19:CS:66:MET:HG2 | 1.55 | 0.88 |
| 2:AB:111:ARG:NH1 | 2:AB:111:ARG:HG2 | 1.85 | 0.88 |
| 34:DL:33:ARG:HB3 | 34:DL:36:LYS:HG3 | 1.54 | 0.88 |
| 23:DA:2186:G:H2' | 23:DA:2187:G:C8 | 2.07 | 0.88 |
| 1:CA:386:C:H2' | 1:CA:387:U:H5'' | 1.55 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:BZ:40:THR:HG23 | 48:BZ:43:ILE:HG12 | 1.52 | 0.88 |
| 7:AG:107:ALA:HB2 | 7:AG:134:ALA:HB2 | 1.54 | 0.88 |
| 1:CA:955:U:H1' | 1:CA:1227:A:N6 | 1.87 | 0.88 |
| 4:CD:119:GLN:HG3 | 4:CD:123:HIS:CD2 | 2.09 | 0.88 |
| 25:DC:231:HIS:HD2 | 25:DC:249:PRO:HA | 1.37 | 0.88 |
| 1:CA:199:G:H1 | 1:CA:218:C:H42 | 1.17 | 0.88 |
| 2:AB:187:LEU:HD11 | 2:AB:205:ASP:HB3 | 1.54 | 0.88 |
| 6:AF:7:ASN:HD21 | 18:AR:34:TYR:HE1 | 1.21 | 0.88 |
| 53:B5:33:ASN:HD22 | 53:B5:34:TRP:N | 1.71 | 0.88 |
| 35:DM:74:TYR:CD2 | 35:DM:91:GLU:HB2 | 2.08 | 0.88 |
| 48:DZ:40:THR:HG23 | 48:DZ:43:ILE:HG12 | 1.56 | 0.88 |
| 32:BJ:105:LEU:HD12 | 32:BJ:106:LYS:H | 1.36 | 0.88 |
| 9:CI:3:GLN:HG2 | 9:CI:20:ARG:HG2 | 1.55 | 0.88 |
| 1:AA:265:G:H2' | 1:AA:266:G:H5'' | 1.53 | 0.88 |
| 23:BA:2353:G:N1 | 23:BA:2353:G:C5 | 2.36 | 0.88 |
| 1:CA:1329:A:H5'' | 13:CM:26:GLY:H | 1.38 | 0.88 |
| 25:BC:70:TRP:HZ3 | 25:BC:146:GLU:OE1 | 1.57 | 0.88 |
| 37:DO:24:LEU:HD12 | 37:DO:84:GLN:HB3 | 1.56 | 0.88 |
| 3:CC:92:ALA:HB2 | 3:CC:99:VAL:HG13 | 1.56 | 0.88 |
| 3:AC:14:ILE:HG23 | 3:AC:15:THR:H | 1.37 | 0.88 |
| 50:B2:25:LEU:H | 50:B2:25:LEU:HD12 | 1.39 | 0.88 |
| 41:DS:13:SER:HB3 | 41:DS:16:LYS:HD3 | 1.54 | 0.88 |
| 27:BE:9:ILE:HD11 | 27:BE:125:LEU:HG | 1.55 | 0.88 |
| 46:DX:13:ILE:HG12 | 46:DX:63:ALA:HB2 | 1.55 | 0.88 |
| 53:D5:33:ASN:HD22 | 53:D5:34:TRP:N | 1.70 | 0.87 |
| 37:BO:11:LYS:HG2 | 37:BO:12:PHE:N | 1.84 | 0.87 |
| 1:AA:1201:A:H1' | 1:AA:1202:G:OP2 | 1.73 | 0.87 |
| 23:BA:96:G:H4' | 47:BY:48:HIS:CE1 | 2.09 | 0.87 |
| 11:CK:24:SER:HB3 | 11:CK:27:ASN:O | 1.73 | 0.87 |
| 26:BD:101:ARG:HD3 | 26:BD:169:ASN:ND2 | 1.89 | 0.87 |
| 40:DR:35:LEU:HB2 | 40:DR:57:VAL:HG13 | 1.55 | 0.87 |
| 10:CJ:32:ALA:HB3 | 10:CJ:76:ASN:HB2 | 1.54 | 0.87 |
| 9:AI:3:GLN:HG2 | 9:AI:20:ARG:HG2 | 1.55 | 0.87 |
| 35:BM:81:VAL:O | 35:BM:82:ARG:CG | 2.22 | 0.87 |
| 23:DA:1899:G:N2 | 23:DA:1902:C:H41 | 1.71 | 0.87 |
| 50:B2:20:ARG:HA | 50:B2:23:HIS:CD2 | 2.09 | 0.87 |
| 28:BF:34:LEU:HD23 | 28:BF:161:THR:HG23 | 1.55 | 0.87 |
| 1:AA:448:A:O2' | 1:AA:449:C:H5' | 1.74 | 0.87 |
| 53:D5:32:LEU:HD23 | 53:D5:33:ASN:H | 1.37 | 0.87 |
| 37:DO:24:LEU:O | 37:DO:86:ALA:HB3 | 1.73 | 0.87 |
| 36:DN:55:ALA:HA | 36:DN:80:PHE:CE1 | 2.09 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 37:BO:24:LEU:HD12 | 37:BO:84:GLN:HB3 | 1.55 | 0.87 |
| 34:DL:59:LEU:CA | 34:DL:61:ARG:NE | 2.37 | 0.87 |
| 23:DA:1021:A:C8 | 23:DA:1021:A:H3' | 2.08 | 0.87 |
| 12:CL:69:ILE:HG23 | 12:CL:99:ILE:HG21 | 1.54 | 0.87 |
| 1:CA:57:G:H2' | 1:CA:58:C:H6 | 1.40 | 0.87 |
| 34:BL:59:LEU:HA | 34:BL:61:ARG:CD | 2.05 | 0.87 |
| 23:BA:744:G:OP1 | 26:BD:132:HIS:HB3 | 1.75 | 0.87 |
| 2:AB:187:LEU:HA | 2:AB:201:ILE:HB | 1.55 | 0.87 |
| 23:DA:2681:C:H5 | 23:DA:2725:A:H62 | 0.91 | 0.87 |
| 52:B4:8:ASN:HD21 | 52:B4:11:LYS:H | 1.22 | 0.87 |
| 46:BX:73:LEU:HD11 | 46:BX:94:LEU:HB3 | 1.56 | 0.87 |
| 43:DU:81:LYS:HD3 | 43:DU:97:ARG:H | 1.39 | 0.87 |
| 23:BA:1437:C:H2' | 23:BA:1438:U:H6 | 1.39 | 0.87 |
| 37:DO:89:ARG:HG3 | 37:DO:94:TYR:HB2 | 1.57 | 0.87 |
| 30:DH:77:LEU:O | 30:DH:143:SER:HB3 | 1.75 | 0.87 |
| 4:AD:153:ARG:HH11 | 4:AD:181:MET:HE3 | 1.38 | 0.87 |
| 10:AJ:32:ALA:HB3 | 10:AJ:76:ASN:HB2 | 1.55 | 0.87 |
| 26:BD:49:LEU:HD22 | 26:BD:49:LEU:H | 1.38 | 0.87 |
| 24:BB:66:A:N6 | 24:BB:107:U:H2' | 1.90 | 0.87 |
| 23:DA:84:A:H5'' | 43:DU:9:LYS:HD2 | 1.55 | 0.87 |
| 2:CB:71:VAL:HG23 | 2:CB:164:VAL:HG13 | 1.54 | 0.87 |
| 36:BN:11:ASN:OD1 | 36:BN:12:ARG:N | 2.08 | 0.86 |
| 1:CA:1295:G:H21 | 1:CA:1302:U:H3 | 1.23 | 0.86 |
| 8:CH:91:ARG:CG | 8:CH:91:ARG:HH11 | 1.87 | 0.86 |
| 5:CE:126:ARG:CG | 5:CE:126:ARG:HH11 | 1.88 | 0.86 |
| 1:CA:688:G:H2' | 1:CA:689:C:H6 | 1.40 | 0.86 |
| 26:BD:120:TRP:CD2 | 26:BD:155:LYS:HD3 | 2.09 | 0.86 |
| 1:AA:1347:G:C8 | 9:AI:107:ARG:HB3 | 2.09 | 0.86 |
| 23:DA:2267:A:H5'' | 23:DA:2268:A:C5' | 2.05 | 0.86 |
| 23:DA:2068:U:N3 | 23:DA:2430:A:H2 | 1.72 | 0.86 |
| 25:BC:87:ASN:HD22 | 25:BC:87:ASN:N | 1.71 | 0.86 |
| 3:CC:88:ARG:HB3 | 3:CC:99:VAL:HG21 | 1.55 | 0.86 |
| 23:BA:323:G:H5' | 27:BE:169:ASN:HD21 | 1.40 | 0.86 |
| 8:AH:20:TYR:HA | 8:AH:65:TYR:CE2 | 2.10 | 0.86 |
| 42:BT:71:GLY:O | 42:BT:72:LYS:HG3 | 1.75 | 0.86 |
| 4:AD:108:LEU:HB3 | 4:AD:110:PHE:CE2 | 2.10 | 0.86 |
| 23:DA:1209:G:H21 | 23:DA:1210:A:H62 | 1.21 | 0.86 |
| 36:DN:51:LEU:HD23 | 36:DN:66:VAL:HG22 | 1.57 | 0.86 |
| 50:D2:25:LEU:HD12 | 50:D2:25:LEU:H | 1.40 | 0.86 |
| 11:AK:24:SER:HB3 | 11:AK:27:ASN:O | 1.72 | 0.86 |
| 11:AK:59:TYR:CE1 | 11:AK:63:LEU:HD21 | 2.10 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:BN:10:LEU:HB3 | 36:BN:17:ARG:NE | 1.91 | 0.86 |
| 25:BC:172:TYR:CD1 | 25:BC:186:HIS:HA | 2.09 | 0.86 |
| 4:AD:128:VAL:HG12 | 4:AD:129:ASN:OD1 | 1.75 | 0.86 |
| 43:BU:17:SER:HA | 43:BU:71:LYS:HD2 | 1.57 | 0.86 |
| 35:DM:58:PHE:HD1 | 35:DM:58:PHE:O | 1.59 | 0.86 |
| 25:DC:172:TYR:CD1 | 25:DC:186:HIS:HA | 2.10 | 0.86 |
| 40:BR:38:LEU:O | 40:BR:39:LEU:HD13 | 1.75 | 0.86 |
| 28:DF:34:LEU:HD23 | 28:DF:161:THR:HG23 | 1.55 | 0.86 |
| 26:DD:120:TRP:CD2 | 26:DD:155:LYS:HD3 | 2.11 | 0.86 |
| 23:DA:1587:A:H2' | 23:DA:1588:C:C6 | 2.11 | 0.86 |
| 52:D4:19:ARG:CG | 52:D4:19:ARG:HH11 | 1.87 | 0.86 |
| 46:DX:13:ILE:HB | 46:DX:62:VAL:HG23 | 1.57 | 0.86 |
| 20:CT:57:ARG:NH1 | 20:CT:102:GLY:HA2 | 1.90 | 0.86 |
| 5:AE:122:GLU:O | 5:AE:123:LEU:HD23 | 1.76 | 0.86 |
| 52:D4:8:ASN:HD22 | 52:D4:9:ARG:N | 1.73 | 0.86 |
| 23:BA:1529:A:H62 | 23:BA:1542:G:N2 | 1.74 | 0.86 |
| 23:BA:2439:A:C5' | 23:BA:2439:A:H8 | 1.88 | 0.86 |
| 23:DA:603:A:H61 | 23:DA:655:A:H4' | 1.41 | 0.86 |
| 3:AC:92:ALA:HB2 | 3:AC:99:VAL:HG13 | 1.56 | 0.86 |
| 44:DV:132:ASN:O | 44:DV:134:PRO:HD3 | 1.75 | 0.86 |
| 12:CL:52:ARG:CG | 12:CL:52:ARG:HH11 | 1.89 | 0.86 |
| 23:BA:674:G:H1' | 27:BE:74:ARG:HD3 | 1.54 | 0.86 |
| 1:CA:250:A:H4' | 1:CA:251:G:O5' | 1.75 | 0.86 |
| 40:DR:66:ARG:HD2 | 40:DR:88:ARG:CZ | 2.06 | 0.86 |
| 24:BB:79:C:H2' | 24:BB:80:U:O4' | 1.76 | 0.86 |
| 1:CA:965:A:C2 | 1:CA:969:A:C2 | 2.64 | 0.86 |
| 42:DT:71:GLY:O | 42:DT:72:LYS:HG3 | 1.74 | 0.86 |
| 2:CB:138:LEU:HD12 | 2:CB:141:GLU:HG3 | 1.58 | 0.86 |
| 38:BP:24:PRO:HA | 38:BP:49:VAL:HG13 | 1.55 | 0.86 |
| 34:DL:59:LEU:HA | 34:DL:61:ARG:HE | 1.35 | 0.85 |
| 20:AT:26:ASN:HD22 | 20:AT:26:ASN:H | 1.21 | 0.85 |
| 1:AA:1295:G:H21 | 1:AA:1302:U:H3 | 1.21 | 0.85 |
| 24:DB:66:A:N6 | 24:DB:107:U:H2' | 1.90 | 0.85 |
| 23:BA:2015:A:C1' | 50:B2:2:ALA:HA | 2.06 | 0.85 |
| 1:AA:971:G:C8 | 1:AA:1365:G:H4' | 2.11 | 0.85 |
| 19:AS:63:THR:HG22 | 19:AS:66:MET:HG2 | 1.55 | 0.85 |
| 1:CA:1124:G:H5' | 10:CJ:35:SER:HB2 | 1.57 | 0.85 |
| 41:DS:29:LEU:HD21 | 41:DS:33:ARG:HE | 1.41 | 0.85 |
| 3:AC:88:ARG:HB3 | 3:AC:99:VAL:HG21 | 1.56 | 0.85 |
| 23:DA:2219:G:H2' | 23:DA:2224:G:H5' | 1.57 | 0.85 |
| 37:DO:51:ALA:HB1 | 37:DO:72:ALA:HB1 | 1.58 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:DM:47:ILE:HG22 | 35:DM:48:GLU:N | 1.91 | 0.85 |
| 1:CA:59:A:H1' | 1:CA:354:G:N2 | 1.92 | 0.85 |
| 36:BN:55:ALA:HA | 36:BN:80:PHE:CE1 | 2.11 | 0.85 |
| 43:BU:14:LEU:HD23 | 43:BU:15:VAL:N | 1.90 | 0.85 |
| 43:DU:17:SER:HA | 43:DU:71:LYS:HD2 | 1.57 | 0.85 |
| 53:B5:32:LEU:HD23 | 53:B5:33:ASN:H | 1.42 | 0.85 |
| 24:DB:80:U:H2' | 24:DB:81:G:H21 | 1.39 | 0.85 |
| 23:DA:2219:G:C2' | 23:DA:2224:G:H5' | 2.06 | 0.85 |
| 23:DA:2272:U:C6 | 23:DA:2272:U:H5'' | 2.11 | 0.85 |
| 4:CD:15:GLU:HG2 | 4:CD:63:LYS:HG3 | 1.56 | 0.85 |
| 23:BA:197:A:C8 | 23:BA:197:A:H5' | 2.12 | 0.85 |
| 41:DS:75:TYR:CE2 | 41:DS:104:THR:HB | 2.11 | 0.85 |
| 23:BA:1264:G:H5' | 50:B2:11:THR:HG21 | 1.58 | 0.85 |
| 35:DM:81:VAL:O | 35:DM:82:ARG:CG | 2.25 | 0.85 |
| 38:DP:56:GLY:O | 38:DP:59:THR:HG22 | 1.76 | 0.85 |
| 33:BK:77:ILE:HD13 | 38:BP:74:ARG:HG3 | 1.56 | 0.85 |
| 53:B5:34:TRP:CG | 53:B5:35:GLN:N | 2.40 | 0.85 |
| 4:AD:119:GLN:HG3 | 4:AD:123:HIS:CD2 | 2.11 | 0.85 |
| 2:AB:26:PRO:HG2 | 2:AB:27:LYS:HD3 | 1.57 | 0.85 |
| 6:CF:35:ALA:HB1 | 6:CF:65:VAL:HG21 | 1.58 | 0.85 |
| 43:BU:15:VAL:HG22 | 43:BU:72:VAL:HG12 | 1.59 | 0.85 |
| 26:BD:201:THR:CG2 | 26:BD:202:LYS:H | 1.90 | 0.85 |
| 12:CL:26:LEU:HG | 12:CL:32:ARG:NH1 | 1.92 | 0.85 |
| 1:CA:737:A:H2' | 1:CA:738:C:H6 | 1.39 | 0.85 |
| 30:BH:113:ARG:HB2 | 30:BH:130:TYR:CZ | 2.11 | 0.85 |
| 36:BN:38:VAL:HB | 36:BN:39:PRO:HD3 | 1.56 | 0.85 |
| 23:DA:1343:G:H5' | 23:DA:1343:G:C8 | 2.11 | 0.85 |
| 30:BH:77:LEU:O | 30:BH:143:SER:HB3 | 1.76 | 0.85 |
| 1:CA:392:G:H2' | 1:CA:393:A:C8 | 2.11 | 0.85 |
| 41:BS:29:LEU:HD21 | 41:BS:33:ARG:HE | 1.41 | 0.85 |
| 23:BA:2875:C:H4' | 38:BP:5:ALA:HB2 | 1.59 | 0.85 |
| 13:AM:10:PRO:HB2 | 13:AM:18:ALA:HB1 | 1.57 | 0.85 |
| 6:CF:7:ASN:HD21 | 18:CR:34:TYR:HE1 | 1.21 | 0.85 |
| 29:DG:44:VAL:HG12 | 29:DG:45:VAL:H | 1.42 | 0.85 |
| 1:AA:1124:G:H5' | 10:AJ:35:SER:HB2 | 1.59 | 0.85 |
| 1:CA:320:C:H5'' | 1:CA:321:A:OP2 | 1.77 | 0.85 |
| 1:CA:82:U:H2' | 1:CA:85:U:C5 | 2.10 | 0.85 |
| 25:BC:67:PHE:CE2 | 25:BC:106:ILE:HD11 | 2.11 | 0.85 |
| 23:DA:141(A):A:H8 | 23:DA:1595:G:H21 | 1.20 | 0.85 |
| 23:BA:2377:A:H2' | 23:BA:2378:A:C8 | 2.11 | 0.85 |
| 29:DG:19:VAL:HG12 | 29:DG:20:ALA:H | 1.42 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 45:DW:42:GLY:HA2 | 45:DW:57:PHE:CD2 | 2.11 | 0.85 |
| 23:BA:529:A:H62 | 23:BA:2041:U:H3 | 1.22 | 0.85 |
| 7:CG:107:ALA:HB2 | 7:CG:134:ALA:HB2 | 1.56 | 0.85 |
| 23:DA:2502:G:H5' | 23:DA:2503:A:C5' | 2.07 | 0.84 |
| 50:D2:20:ARG:HA | 50:D2:23:HIS:CD2 | 2.11 | 0.84 |
| 34:DL:16:ARG:HE | 34:DL:16:ARG:C | 1.79 | 0.84 |
| 4:CD:128:VAL:HG12 | 4:CD:129:ASN:OD1 | 1.77 | 0.84 |
| 29:DG:148:ILE:O | 29:DG:151:ILE:HG12 | 1.77 | 0.84 |
| 27:BE:164:ARG:HG3 | 27:BE:175:THR:OG1 | 1.78 | 0.84 |
| 3:AC:66:VAL:HB | 3:AC:101:LEU:HD23 | 1.59 | 0.84 |
| 1:AA:57:G:H2' | 1:AA:58:C:H6 | 1.42 | 0.84 |
| 40:DR:27:ALA:HB3 | 40:DR:61:VAL:HG11 | 1.59 | 0.84 |
| 1:CA:971:G:C8 | 1:CA:1365:G:H4' | 2.12 | 0.84 |
| 12:AL:26:LEU:HG | 12:AL:32:ARG:NH1 | 1.91 | 0.84 |
| 26:DD:31:CYS:HB3 | 26:DD:49:LEU:HB3 | 1.56 | 0.84 |
| 23:DA:1156:A:C8 | 39:DQ:51:LYS:HD2 | 2.12 | 0.84 |
| 12:AL:52:ARG:HH11 | 12:AL:52:ARG:CG | 1.90 | 0.84 |
| 23:DA:322:A:H3' | 27:DE:169:ASN:ND2 | 1.91 | 0.84 |
| 5:AE:126:ARG:CG | 5:AE:126:ARG:HH11 | 1.89 | 0.84 |
| 23:BA:2781:A:C5' | 23:BA:2782:G:H5' | 2.02 | 0.84 |
| 34:DL:33:ARG:HB3 | 34:DL:36:LYS:CD | 2.07 | 0.84 |
| 5:AE:78:HIS:HD2 | 8:AH:104:ARG:HG2 | 1.42 | 0.84 |
| 3:AC:195:VAL:HG12 | 3:AC:196:LEU:H | 1.43 | 0.84 |
| 8:CH:92:ARG:HB3 | 8:CH:94:TYR:HE2 | 1.41 | 0.84 |
| 18:CR:58:LEU:HD23 | 18:CR:62:GLU:HB3 | 1.59 | 0.84 |
| 1:AA:250:A:H4' | 1:AA:251:G:O5' | 1.76 | 0.84 |
| 42:DT:9:LEU:HB2 | 42:DT:29:TRP:O | 1.77 | 0.84 |
| 32:DJ:142:ARG:HG3 | 32:DJ:142:ARG:HH11 | 1.42 | 0.84 |
| 46:DX:27:GLU:HB2 | 46:DX:33:LYS:HA | 1.59 | 0.84 |
| 23:BA:2391:G:OP1 | 53:B5:32:LEU:HB2 | 1.77 | 0.84 |
| 37:BO:89:ARG:HG3 | 37:BO:94:TYR:HB2 | 1.56 | 0.84 |
| 32:BJ:85:VAL:HG22 | 32:BJ:89:LYS:HG3 | 1.59 | 0.84 |
| 39:DQ:91:ASP:CG | 39:DQ:96:ALA:HB2 | 1.98 | 0.84 |
| 42:DT:35:THR:O | 42:DT:39:ILE:HG12 | 1.77 | 0.84 |
| 30:DH:113:ARG:HB2 | 30:DH:130:TYR:CZ | 2.12 | 0.84 |
| 12:CL:68:TYR:O | 12:CL:99:ILE:HG22 | 1.77 | 0.84 |
| 1:CA:57:G:H2' | 1:CA:58:C:C6 | 2.11 | 0.84 |
| 35:BM:6:ARG:O | 35:BM:7:MET:HG3 | 1.77 | 0.84 |
| 23:BA:2307:G:H2' | 23:BA:2308:G:H5' | 1.59 | 0.84 |
| 23:DA:2307:G:H2' | 23:DA:2308:G:H5' | 1.59 | 0.84 |
| 3:CC:195:VAL:HG12 | 3:CC:196:LEU:H | 1.42 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:BP:62:THR:HG22 | 38:BP:75:ILE:HG13 | 1.59 | 0.84 |
| 11:CK:108:ILE:HG21 | 18:CR:88:LYS:HG2 | 1.59 | 0.84 |
| 23:BA:1379:A:H4' | 23:BA:1380:G:OP2 | 1.78 | 0.84 |
| 29:BG:84:SER:HA | 29:BG:133:VAL:O | 1.77 | 0.84 |
| 6:AF:35:ALA:HB1 | 6:AF:65:VAL:HG21 | 1.59 | 0.84 |
| 53:D5:34:TRP:CG | 53:D5:35:GLN:N | 2.40 | 0.84 |
| 34:BL:38:GLN:HG3 | 34:BL:39:LYS:H | 1.42 | 0.84 |
| 5:CE:122:GLU:O | 5:CE:123:LEU:HD23 | 1.78 | 0.84 |
| 29:DG:46:GLU:HG3 | 29:DG:51:ARG:NE | 1.91 | 0.84 |
| 23:BA:84:A:H5'' | 43:BU:9:LYS:HD2 | 1.59 | 0.84 |
| 23:DA:1495:A:H5'' | 23:DA:1496:A:OP2 | 1.78 | 0.84 |
| 46:DX:73:LEU:HD11 | 46:DX:94:LEU:HB3 | 1.57 | 0.84 |
| 26:BD:111:ARG:HD2 | 26:BD:160:TYR:HE1 | 1.42 | 0.84 |
| 43:BU:81:LYS:CD | 43:BU:97:ARG:HB3 | 2.07 | 0.84 |
| 24:BB:80:U:H2' | 24:BB:81:G:H21 | 1.42 | 0.84 |
| 32:DJ:53:ILE:HG23 | 32:DJ:75:VAL:HG11 | 1.60 | 0.84 |
| 41:BS:13:SER:HB3 | 41:BS:16:LYS:HD3 | 1.59 | 0.84 |
| 12:AL:68:TYR:O | 12:AL:99:ILE:HG22 | 1.77 | 0.84 |
| 23:BA:2562:U:H1' | 33:BK:23:ARG:HH11 | 1.42 | 0.84 |
| 23:DA:2577:A:H5'' | 23:DA:2578:G:H5' | 1.60 | 0.84 |
| 46:BX:11:ARG:HB3 | 46:BX:12:PRO:CD | 2.08 | 0.84 |
| 23:BA:1343:G:H5' | 23:BA:1343:G:C8 | 2.12 | 0.84 |
| 47:BY:2:LYS:H | 47:BY:2:LYS:CE | 1.90 | 0.84 |
| 34:BL:33:ARG:HB3 | 34:BL:36:LYS:HG3 | 1.58 | 0.84 |
| 20:CT:26:ASN:H | 20:CT:26:ASN:HD22 | 1.25 | 0.84 |
| 1:CA:721:G:H4' | 1:CA:722:A:O4' | 1.77 | 0.84 |
| 33:BK:35:VAL:HG23 | 33:BK:65:THR:HG23 | 1.60 | 0.84 |
| 23:BA:1544:C:OP1 | 23:BA:1544:C:C6 | 2.30 | 0.84 |
| 1:AA:965:A:C2 | 1:AA:969:A:C2 | 2.66 | 0.84 |
| 35:DM:75:THR:CA | 35:DM:88:GLY:HA2 | 2.08 | 0.84 |
| 40:BR:39:LEU:HB3 | 40:BR:47:VAL:HG21 | 1.60 | 0.84 |
| 41:DS:9:TYR:H | 41:DS:102:HIS:HD2 | 1.23 | 0.84 |
| 26:BD:9:VAL:HG13 | 26:BD:25:VAL:O | 1.77 | 0.84 |
| 2:AB:87:ARG:HG3 | 2:AB:233:SER:HB3 | 1.60 | 0.84 |
| 1:CA:1320:C:H42 | 19:CS:36:ARG:HG3 | 1.43 | 0.84 |
| 24:BB:11:C:H3' | 24:BB:12:C:H6 | 1.42 | 0.83 |
| 23:DA:322:A:H3' | 27:DE:169:ASN:HD21 | 1.41 | 0.83 |
| 1:CA:448:A:O2' | 1:CA:449:C:H5' | 1.78 | 0.83 |
| 23:BA:2808:U:H2' | 23:BA:2809:A:H5' | 1.60 | 0.83 |
| 23:BA:2786:U:H4' | 26:BD:65:GLY:O | 1.77 | 0.83 |
| 1:AA:1329:A:H5'' | 13:AM:26:GLY:H | 1.41 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:AB:138:LEU:HD12 | 2:AB:141:GLU:HG3 | 1.58 | 0.83 |
| 1:AA:82:U:H2' | 1:AA:85:U:C5 | 2.10 | 0.83 |
| 39:DQ:83:LEU:HG | 39:DQ:88:ILE:HD11 | 1.59 | 0.83 |
| 39:BQ:83:LEU:HD12 | 39:BQ:113:ALA:HB2 | 1.61 | 0.83 |
| 47:BY:17:SER:HB3 | 47:BY:18:PRO:HD3 | 1.59 | 0.83 |
| 43:DU:81:LYS:CD | 43:DU:97:ARG:HB3 | 2.08 | 0.83 |
| 15:CO:18:PHE:CE1 | 15:CO:21:ASP:HB2 | 2.12 | 0.83 |
| 5:CE:51:VAL:HB | 5:CE:52:PRO:HD3 | 1.59 | 0.83 |
| 34:DL:114:ILE:N | 34:DL:114:ILE:HD12 | 1.92 | 0.83 |
| 1:CA:877:C:H5'' | 8:CH:88:LYS:HD3 | 1.60 | 0.83 |
| 23:DA:96:G:H4' | 47:DY:48:HIS:CE1 | 2.12 | 0.83 |
| 30:BH:133:HIS:CD2 | 30:BH:135:GLU:HG2 | 2.13 | 0.83 |
| 29:DG:84:SER:HA | 29:DG:133:VAL:O | 1.77 | 0.83 |
| 23:DA:1401:G:H2' | 23:DA:1402:C:H6 | 1.43 | 0.83 |
| 23:DA:2391:G:OP1 | 53:D5:32:LEU:HB2 | 1.79 | 0.83 |
| 26:DD:201:THR:CG2 | 26:DD:202:LYS:H | 1.91 | 0.83 |
| 43:DU:8:LYS:HZ2 | 43:DU:8:LYS:H | 1.24 | 0.83 |
| 32:DJ:85:VAL:HG22 | 32:DJ:89:LYS:HG3 | 1.59 | 0.83 |
| 1:AA:57:G:H2' | 1:AA:58:C:C6 | 2.14 | 0.83 |
| 23:BA:1495:A:H5'' | 23:BA:1496:A:OP2 | 1.78 | 0.83 |
| 23:BA:1858:G:H1' | 23:BA:1884:A:N6 | 1.94 | 0.83 |
| 23:DA:2015:A:C1' | 50:D2:2:ALA:HA | 2.07 | 0.83 |
| 41:BS:40:ASN:O | 41:BS:41:LYS:HG2 | 1.78 | 0.83 |
| 46:BX:27:GLU:HB2 | 46:BX:33:LYS:HA | 1.58 | 0.83 |
| 38:DP:53:ARG:HH11 | 38:DP:53:ARG:HG2 | 1.42 | 0.83 |
| 25:BC:79:VAL:HG21 | 25:BC:111:LEU:HD11 | 1.61 | 0.83 |
| 29:BG:46:GLU:HG3 | 29:BG:51:ARG:NE | 1.94 | 0.83 |
| 40:BR:27:ALA:HB3 | 40:BR:61:VAL:HG11 | 1.58 | 0.83 |
| 23:BA:2267:A:H5'' | 23:BA:2268:A:C5' | 2.07 | 0.83 |
| 23:DA:2781:A:C5' | 23:DA:2782:G:H5' | 2.04 | 0.83 |
| 53:B5:33:ASN:HD22 | 53:B5:34:TRP:H | 1.21 | 0.83 |
| 30:DH:100:ALA:HA | 30:DH:103:ARG:HB2 | 1.61 | 0.83 |
| 27:DE:167:ALA:HB1 | 27:DE:173:VAL:HG11 | 1.60 | 0.83 |
| 35:DM:6:ARG:O | 35:DM:7:MET:HG3 | 1.79 | 0.83 |
| 23:BA:2790:A:H2' | 23:BA:2791:C:H5'' | 1.60 | 0.83 |
| 4:CD:153:ARG:HH11 | 4:CD:181:MET:HE3 | 1.42 | 0.83 |
| 4:AD:92:VAL:HG12 | 4:AD:96:LEU:HD23 | 1.61 | 0.83 |
| 52:B4:8:ASN:ND2 | 52:B4:8:ASN:C | 2.23 | 0.83 |
| 23:BA:2577:A:H5'' | 23:BA:2578:G:H5' | 1.59 | 0.83 |
| 23:DA:1019:U:H3 | 23:DA:114(B):A:N6 | 1.77 | 0.83 |
| 23:DA:2787:C:H1' | 26:DD:62:PRO:HB3 | 1.60 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:CD:108:LEU:HD21 | 4:CD:183:GLY:HA3 | 1.58 | 0.83 |
| 52:B4:11:LYS:O | 52:B4:15:THR:HG23 | 1.78 | 0.83 |
| 2:CB:111:ARG:HH11 | 2:CB:111:ARG:CG | 1.92 | 0.83 |
| 39:BQ:91:ASP:CG | 39:BQ:96:ALA:HB2 | 1.98 | 0.83 |
| 23:BA:1210:A:H5'' | 23:BA:1210:A:H8 | 1.43 | 0.83 |
| 23:BA:1264:G:H5' | 50:B2:11:THR:CG2 | 2.09 | 0.83 |
| 8:CH:20:TYR:HA | 8:CH:65:TYR:CE2 | 2.12 | 0.83 |
| 2:CB:26:PRO:HG2 | 2:CB:27:LYS:HD3 | 1.60 | 0.83 |
| 19:AS:19:VAL:HG21 | 19:AS:44:MET:HG3 | 1.60 | 0.83 |
| 40:BR:35:LEU:HB2 | 40:BR:57:VAL:HG13 | 1.61 | 0.83 |
| 30:DH:92:VAL:HG23 | 30:DH:96:ASP:HB2 | 1.60 | 0.83 |
| 46:BX:13:ILE:HG12 | 46:BX:63:ALA:HB2 | 1.61 | 0.83 |
| 23:DA:1510:A:H2' | 23:DA:1511:A:C8 | 2.14 | 0.83 |
| 23:DA:848:G:H2' | 23:DA:849:A:C8 | 2.14 | 0.83 |
| 46:BX:19:GLN:HG3 | 46:BX:41:ARG:HE | 1.43 | 0.83 |
| 42:BT:9:LEU:HB2 | 42:BT:29:TRP:O | 1.79 | 0.83 |
| 4:CD:126:ILE:HG22 | 4:CD:127:THR:H | 1.43 | 0.83 |
| 23:DA:2598:A:OP1 | 25:DC:235:GLY:HA3 | 1.79 | 0.83 |
| 27:BE:101:LEU:HD12 | 27:BE:102:PRO:HD2 | 1.58 | 0.83 |
| 6:CF:26:ILE:O | 6:CF:30:LEU:HD12 | 1.78 | 0.83 |
| 25:BC:132:PRO:HD3 | 25:BC:190:TYR:CZ | 2.14 | 0.83 |
| 1:AA:320:C:H5'' | 1:AA:321:A:OP2 | 1.77 | 0.83 |
| 22:AV:6213:A:H2' | 22:AV:6214:C:H6 | 1.43 | 0.82 |
| 23:DA:674:G:H1' | 27:DE:74:ARG:HD3 | 1.59 | 0.82 |
| 23:BA:2502:G:H5' | 23:BA:2503:A:C5' | 2.08 | 0.82 |
| 47:BY:9:GLN:O | 47:BY:12:GLU:HB3 | 1.78 | 0.82 |
| 23:DA:1055:G:H2' | 23:DA:1056:G:C8 | 2.14 | 0.82 |
| 47:DY:9:GLN:O | 47:DY:12:GLU:HB3 | 1.78 | 0.82 |
| 1:AA:1238:A:N7 | 1:AA:1303:C:H1' | 1.94 | 0.82 |
| 39:DQ:82:GLY:HA3 | 39:DQ:113:ALA:HB1 | 1.62 | 0.82 |
| 35:DM:68:ILE:HD13 | 35:DM:103:MET:HG2 | 1.60 | 0.82 |
| 23:DA:2327:A:H2' | 23:DA:2328:A:C8 | 2.14 | 0.82 |
| 52:D4:12:ARG:HH11 | 52:D4:12:ARG:HG3 | 1.43 | 0.82 |
| 1:AA:818:G:O2' | 1:AA:819:A:H5' | 1.80 | 0.82 |
| 23:BA:1188:U:O2' | 23:BA:1189:A:H5' | 1.78 | 0.82 |
| 2:CB:87:ARG:HG3 | 2:CB:233:SER:HB3 | 1.61 | 0.82 |
| 32:BJ:53:ILE:HG23 | 32:BJ:75:VAL:HG11 | 1.61 | 0.82 |
| 26:BD:31:CYS:HB3 | 26:BD:49:LEU:HB3 | 1.59 | 0.82 |
| 1:CA:1294:G:H2' | 1:CA:1295:G:C8 | 2.15 | 0.82 |
| 1:AA:1152:A:H2' | 1:AA:1153:C:H6 | 1.44 | 0.82 |
| 1:AA:737:A:H2' | 1:AA:738:C:C6 | 2.14 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:987:G:H1 | 1:AA:1218:C:H42 | 1.28 | 0.82 |
| 8:CH:83:ILE:HG13 | 8:CH:137:VAL:HG22 | 1.60 | 0.82 |
| 23:BA:2009:G:H2' | 23:BA:2010:G:H5' | 1.60 | 0.82 |
| 25:DC:166:GLN:CA | 25:DC:166:GLN:HE21 | 1.93 | 0.82 |
| 1:AA:475:G:H2' | 1:AA:476:G:H8 | 1.45 | 0.82 |
| 52:D4:8:ASN:HD21 | 52:D4:11:LYS:H | 1.27 | 0.82 |
| 25:BC:106:ILE:N | 25:BC:106:ILE:HD12 | 1.95 | 0.82 |
| 32:DJ:93:LYS:HE3 | 32:DJ:95:TYR:HE1 | 1.45 | 0.82 |
| 23:DA:528:A:H3' | 23:DA:528:A:H8 | 1.44 | 0.82 |
| 40:BR:24:LYS:HA | 40:BR:92:THR:HG23 | 1.62 | 0.82 |
| 23:BA:1587:A:H2' | 23:BA:1588:C:C6 | 2.14 | 0.82 |
| 8:CH:12:ARG:HH12 | 8:CH:26:VAL:HA | 1.44 | 0.82 |
| 43:BU:8:LYS:H | 43:BU:8:LYS:HZ2 | 1.24 | 0.82 |
| 34:BL:33:ARG:HG2 | 34:BL:34:GLY:N | 1.93 | 0.82 |
| 1:CA:1154:G:H2' | 1:CA:1155:G:H8 | 1.44 | 0.82 |
| 33:DK:113:LYS:O | 33:DK:117:LEU:HD12 | 1.79 | 0.82 |
| 33:DK:77:ILE:HD13 | 38:DP:74:ARG:HG3 | 1.62 | 0.82 |
| 34:BL:35:HIS:O | 34:BL:36:LYS:HB2 | 1.79 | 0.82 |
| 23:BA:242:G:H5'' | 53:B5:63:PRO:HG2 | 1.62 | 0.82 |
| 1:AA:877:C:H5'' | 8:AH:88:LYS:HD3 | 1.61 | 0.82 |
| 23:BA:2306:C:H3' | 23:BA:2307:G:C8 | 2.15 | 0.82 |
| 39:BQ:92:ARG:CD | 39:BQ:94:ASN:HB3 | 2.10 | 0.82 |
| 33:DK:99:PHE:N | 33:DK:99:PHE:HD1 | 1.77 | 0.82 |
| 23:DA:2808:U:H2' | 23:DA:2809:A:H5' | 1.59 | 0.82 |
| 34:DL:33:ARG:HB3 | 34:DL:36:LYS:CG | 2.10 | 0.82 |
| 46:DX:11:ARG:HB3 | 46:DX:12:PRO:CD | 2.10 | 0.82 |
| 29:BG:148:ILE:O | 29:BG:151:ILE:HG12 | 1.78 | 0.82 |
| 27:DE:101:LEU:HD12 | 27:DE:102:PRO:HD2 | 1.60 | 0.82 |
| 25:DC:21:PHE:HB3 | 25:DC:24:ILE:HD12 | 1.59 | 0.82 |
| 25:BC:21:PHE:HB3 | 25:BC:24:ILE:HD12 | 1.60 | 0.82 |
| 27:DE:8:GLN:CD | 27:DE:8:GLN:H | 1.82 | 0.82 |
| 18:CR:54:ARG:HD2 | 18:CR:54:ARG:H | 1.44 | 0.82 |
| 23:BA:1614:A:N6 | 41:BS:87:PRO:HA | 1.95 | 0.81 |
| 23:DA:2377:A:H2' | 23:DA:2378:A:C8 | 2.15 | 0.81 |
| 1:AA:1294:G:H2' | 1:AA:1295:G:C8 | 2.15 | 0.81 |
| 23:DA:2306:C:H3' | 23:DA:2307:G:H8 | 1.45 | 0.81 |
| 4:CD:108:LEU:HB3 | 4:CD:110:PHE:CE2 | 2.15 | 0.81 |
| 8:AH:112:LEU:HA | 8:AH:134:ILE:HG12 | 1.62 | 0.81 |
| 40:DR:34:GLU:O | 40:DR:36:PRO:HD3 | 1.80 | 0.81 |
| 23:BA:1510:A:H2' | 23:BA:1511:A:C8 | 2.14 | 0.81 |
| 53:D5:28:GLY:O | 53:D5:32:LEU:HD21 | 1.80 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DA:2393:A:H5'' | 34:DL:62:LEU:HD12 | 1.60 | 0.81 |
| 35:BM:75:THR:CA | 35:BM:88:GLY:HA2 | 2.08 | 0.81 |
| 23:BA:2787:C:H1' | 26:BD:62:PRO:HB3 | 1.62 | 0.81 |
| 48:DZ:43:ILE:N | 48:DZ:43:ILE:HD13 | 1.94 | 0.81 |
| 15:AO:18:PHE:CE1 | 15:AO:21:ASP:HB2 | 2.15 | 0.81 |
| 19:CS:19:VAL:HG21 | 19:CS:44:MET:HG3 | 1.60 | 0.81 |
| 1:CA:624:C:H4' | 16:CP:11:SER:H | 1.43 | 0.81 |
| 40:DR:24:LYS:HA | 40:DR:92:THR:HG23 | 1.61 | 0.81 |
| 17:AQ:53:LEU:HD11 | 17:AQ:85:VAL:HG21 | 1.62 | 0.81 |
| 23:DA:1529:A:H62 | 23:DA:1542:G:N2 | 1.78 | 0.81 |
| 23:DA:1544:C:C6 | 23:DA:1544:C:OP1 | 2.33 | 0.81 |
| 23:DA:1174:A:C3' | 23:DA:1175:U:H5'' | 2.10 | 0.81 |
| 32:BJ:142:ARG:HG3 | 32:BJ:142:ARG:HH11 | 1.44 | 0.81 |
| 23:BA:603:A:H61 | 23:BA:655:A:H4' | 1.45 | 0.81 |
| 23:DA:996:A:H4' | 39:DQ:92:ARG:NH1 | 1.95 | 0.81 |
| 23:DA:860:U:C5 | 23:DA:917:A:N7 | 2.48 | 0.81 |
| 23:DA:242:G:H5'' | 53:D5:63:PRO:HG2 | 1.61 | 0.81 |
| 23:BA:2068:U:H3 | 23:BA:2430:A:H2 | 0.86 | 0.81 |
| 5:CE:76:ILE:HG12 | 5:CE:77:PRO:HD2 | 1.62 | 0.81 |
| 5:AE:76:ILE:HG12 | 5:AE:77:PRO:HD2 | 1.61 | 0.81 |
| 23:DA:2887:U:H2' | 23:DA:2888:C:C6 | 2.15 | 0.81 |
| 46:DX:27:GLU:CD | 46:DX:33:LYS:HE3 | 2.01 | 0.81 |
| 23:DA:1401:G:H2' | 23:DA:1402:C:C6 | 2.15 | 0.81 |
| 37:DO:104:GLY:HA2 | 37:DO:107:GLU:HG2 | 1.63 | 0.81 |
| 23:BA:2777:G:H5'' | 23:BA:2778:A:H5' | 1.61 | 0.81 |
| 29:BG:19:VAL:HG12 | 29:BG:20:ALA:H | 1.43 | 0.81 |
| 23:BA:1055:G:H2' | 23:BA:1056:G:C8 | 2.14 | 0.81 |
| 11:CK:34:ASP:N | 11:CK:40:ILE:HD11 | 1.95 | 0.81 |
| 23:DA:1858:G:H1' | 23:DA:1884:A:N6 | 1.96 | 0.81 |
| 23:BA:1110:G:HO2' | 23:BA:1111:A:H8 | 0.84 | 0.81 |
| 38:BP:53:ARG:HG2 | 38:BP:53:ARG:HH11 | 1.45 | 0.81 |
| 37:BO:104:GLY:HA2 | 37:BO:107:GLU:HG2 | 1.62 | 0.81 |
| 7:CG:115:ARG:O | 7:CG:118:VAL:HG22 | 1.80 | 0.81 |
| 37:BO:69:VAL:O | 37:BO:72:ALA:HB3 | 1.80 | 0.81 |
| 33:BK:113:LYS:O | 33:BK:117:LEU:HD12 | 1.79 | 0.81 |
| 27:BE:64:ILE:O | 27:BE:64:ILE:HD12 | 1.80 | 0.81 |
| 1:AA:721:G:H4' | 1:AA:722:A:O4' | 1.81 | 0.81 |
| 36:BN:63:ARG:HH11 | 36:BN:63:ARG:HB2 | 1.45 | 0.81 |
| 42:DT:53:LYS:HB3 | 42:DT:82:GLN:HB3 | 1.62 | 0.81 |
| 33:BK:19:ILE:H | 33:BK:19:ILE:HD13 | 1.43 | 0.81 |
| 33:DK:35:VAL:HG23 | 33:DK:65:THR:HG23 | 1.60 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:AB:111:ARG:HH11 | 2:AB:111:ARG:CG | 1.93 | 0.81 |
| 23:DA:330:A:O2' | 23:DA:331:A:H8 | 1.62 | 0.81 |
| 23:BA:2306:C:H3' | 23:BA:2307:G:H8 | 1.45 | 0.81 |
| 1:CA:818:G:O2' | 1:CA:819:A:H5' | 1.80 | 0.81 |
| 37:BO:31:SER:HB3 | 37:BO:34:HIS:HB2 | 1.63 | 0.81 |
| 23:BA:910:A:C5 | 35:BM:13:GLN:OE1 | 2.33 | 0.81 |
| 23:BA:1286:A:O2' | 23:BA:1288:U:OP2 | 1.98 | 0.81 |
| 11:AK:108:ILE:HG21 | 18:AR:88:LYS:HG2 | 1.62 | 0.81 |
| 1:CA:979:C:H42 | 14:CN:18:VAL:HG12 | 1.44 | 0.81 |
| 34:BL:114:ILE:HD13 | 34:BL:130:PHE:CD1 | 2.15 | 0.81 |
| 30:BH:92:VAL:HG23 | 30:BH:96:ASP:HB2 | 1.63 | 0.81 |
| 23:BA:848:G:H2' | 23:BA:849:A:C8 | 2.16 | 0.81 |
| 45:DW:42:GLY:HA2 | 45:DW:57:PHE:CE2 | 2.15 | 0.81 |
| 42:BT:53:LYS:HB3 | 42:BT:82:GLN:HB3 | 1.61 | 0.81 |
| 16:CP:39:TYR:CD1 | 16:CP:73:LEU:HD13 | 2.16 | 0.81 |
| 38:DP:51:ARG:HH11 | 38:DP:51:ARG:CG | 1.93 | 0.81 |
| 23:BA:996:A:H4' | 39:BQ:92:ARG:NH1 | 1.96 | 0.81 |
| 23:BA:2887:U:H2' | 23:BA:2888:C:C6 | 2.14 | 0.81 |
| 26:DD:111:ARG:HD2 | 26:DD:160:TYR:HE1 | 1.41 | 0.81 |
| 5:AE:31:LEU:HD21 | 5:AE:43:LEU:HD12 | 1.63 | 0.81 |
| 5:AE:57:LYS:O | 5:AE:61:TYR:HD2 | 1.63 | 0.81 |
| 4:CD:100:ARG:HH21 | 4:CD:118:ARG:HH12 | 1.29 | 0.81 |
| 23:BA:2009:G:C2' | 23:BA:2010:G:H5' | 2.11 | 0.81 |
| 1:CA:1152:A:H2' | 1:CA:1153:C:H6 | 1.45 | 0.81 |
| 16:AP:39:TYR:CD1 | 16:AP:73:LEU:HD13 | 2.16 | 0.81 |
| 42:DT:41:ASN:O | 42:DT:45:THR:HG23 | 1.81 | 0.81 |
| 23:DA:1418:G:H8 | 23:DA:1418:G:O5' | 1.63 | 0.81 |
| 24:BB:82:G:O2' | 24:BB:83:G:H5' | 1.80 | 0.81 |
| 5:CE:78:HIS:HD2 | 8:CH:104:ARG:HG2 | 1.43 | 0.81 |
| 8:AH:92:ARG:HB3 | 8:AH:94:TYR:CE2 | 2.15 | 0.81 |
| 41:DS:40:ASN:O | 41:DS:41:LYS:HG2 | 1.81 | 0.81 |
| 25:DC:27:THR:HG23 | 25:DC:27:THR:O | 1.79 | 0.81 |
| 23:DA:810:U:H3 | 34:DL:36:LYS:NZ | 1.79 | 0.81 |
| 39:DQ:83:LEU:HD12 | 39:DQ:113:ALA:HB2 | 1.61 | 0.81 |
| 28:DF:128:ARG:NE | 28:DF:129:GLY:H | 1.78 | 0.81 |
| 1:AA:1281:U:H4' | 1:AA:1282:C:OP2 | 1.81 | 0.81 |
| 20:CT:45:GLN:HB2 | 20:CT:91:LEU:HD13 | 1.63 | 0.81 |
| 23:BA:2327:A:H2' | 23:BA:2328:A:C8 | 2.16 | 0.80 |
| 53:D5:62:LEU:HB3 | 53:D5:63:PRO:HD3 | 1.61 | 0.80 |
| 2:CB:167:PRO:O | 2:CB:171:ALA:HB2 | 1.80 | 0.80 |
| 44:DV:125:LEU:HD22 | 44:DV:164:ALA:HB3 | 1.63 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:CK:59:TYR:CE1 | 11:CK:63:LEU:HD21 | 2.16 | 0.80 |
| 46:BX:13:ILE:HB | 46:BX:62:VAL:HG23 | 1.60 | 0.80 |
| 4:AD:166:LYS:HE2 | 25:DC:134:ARG:HH21 | 1.45 | 0.80 |
| 1:AA:957:U:H4' | 19:AS:79:THR:HB | 1.62 | 0.80 |
| 1:AA:781:A:C3' | 1:AA:782:A:H5' | 2.11 | 0.80 |
| 25:BC:87:ASN:ND2 | 25:BC:87:ASN:H | 1.79 | 0.80 |
| 23:DA:1210:A:C5' | 23:DA:1210:A:H8 | 1.94 | 0.80 |
| 1:AA:392:G:H2' | 1:AA:393:A:C8 | 2.16 | 0.80 |
| 36:DN:63:ARG:HB2 | 36:DN:63:ARG:HH11 | 1.46 | 0.80 |
| 23:DA:2306:C:H3' | 23:DA:2307:G:C8 | 2.16 | 0.80 |
| 23:BA:661:C:H4' | 34:BL:18:ARG:HG2 | 1.62 | 0.80 |
| 23:DA:875:G:H4' | 44:DV:170:THR:HG21 | 1.63 | 0.80 |
| 38:DP:62:THR:HG22 | 38:DP:75:ILE:HG13 | 1.64 | 0.80 |
| 7:AG:115:ARG:O | 7:AG:118:VAL:HG22 | 1.80 | 0.80 |
| 23:DA:804:A:H5'' | 23:DA:805:G:OP1 | 1.80 | 0.80 |
| 23:DA:744:G:OP1 | 26:DD:132:HIS:HB3 | 1.81 | 0.80 |
| 2:AB:187:LEU:CD1 | 2:AB:205:ASP:HB3 | 2.11 | 0.80 |
| 37:BO:24:LEU:O | 37:BO:86:ALA:HB3 | 1.81 | 0.80 |
| 23:DA:529:A:H62 | 23:DA:2041:U:H3 | 1.27 | 0.80 |
| 32:DJ:118:PRO:O | 32:DJ:121:VAL:HG22 | 1.81 | 0.80 |
| 4:AD:25:ARG:HG2 | 4:AD:30:LYS:HG3 | 1.63 | 0.80 |
| 34:DL:16:ARG:HH21 | 34:DL:17:LYS:HA | 1.46 | 0.80 |
| 1:CA:1070:U:H2' | 1:CA:1071:C:C6 | 2.16 | 0.80 |
| 1:AA:1064:G:H21 | 1:AA:1190:G:H2' | 1.45 | 0.80 |
| 6:AF:91:VAL:HG12 | 6:AF:92:LYS:O | 1.81 | 0.80 |
| 8:AH:12:ARG:HH12 | 8:AH:26:VAL:HA | 1.43 | 0.80 |
| 1:CA:1238:A:N7 | 1:CA:1303:C:H1' | 1.96 | 0.80 |
| 23:DA:329:G:OP2 | 43:DU:71:LYS:HE3 | 1.82 | 0.80 |
| 53:B5:28:GLY:O | 53:B5:32:LEU:HD21 | 1.82 | 0.80 |
| 39:DQ:92:ARG:HB2 | 39:DQ:92:ARG:HH11 | 1.44 | 0.80 |
| 25:BC:233:HIS:HE1 | 25:BC:247:ALA:H | 1.29 | 0.80 |
| 44:BV:69:THR:HG22 | 44:BV:90:VAL:HA | 1.62 | 0.80 |
| 1:AA:737:A:H2' | 1:AA:738:C:H6 | 1.46 | 0.80 |
| 1:CA:1281:U:H4' | 1:CA:1282:C:OP2 | 1.82 | 0.80 |
| 1:AA:175:C:H2' | 1:AA:176:C:H6 | 1.46 | 0.80 |
| 27:BE:157:VAL:HB | 27:BE:194:MET:HB3 | 1.62 | 0.80 |
| 1:AA:324:G:N2 | 1:AA:327:A:C8 | 2.50 | 0.80 |
| 3:AC:173:VAL:HG12 | 3:AC:173:VAL:O | 1.81 | 0.80 |
| 1:AA:1191:A:H5'' | 3:AC:4:LYS:NZ | 1.96 | 0.80 |
| 2:AB:167:PRO:O | 2:AB:171:ALA:HB2 | 1.81 | 0.80 |
| 41:BS:29:LEU:CD2 | 41:BS:33:ARG:HE | 1.94 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BA:1487:G:H2' | 23:BA:1488:G:H8 | 1.46 | 0.80 |
| 1:AA:59:A:H1' | 1:AA:354:G:N2 | 1.96 | 0.80 |
| 23:BA:7:G:H1 | 23:BA:2896:C:H42 | 1.28 | 0.80 |
| 27:BE:8:GLN:H | 27:BE:8:GLN:CD | 1.83 | 0.80 |
| 8:CH:112:LEU:HA | 8:CH:134:ILE:HG12 | 1.64 | 0.80 |
| 34:DL:147:LEU:HD13 | 34:DL:148:LEU:O | 1.81 | 0.80 |
| 23:BA:1174:A:C3' | 23:BA:1175:U:H5'' | 2.10 | 0.80 |
| 39:DQ:92:ARG:CD | 39:DQ:94:ASN:HB3 | 2.12 | 0.80 |
| 23:DA:363(A):G:H2' | 23:DA:363(B):A:C8 | 2.17 | 0.80 |
| 3:CC:66:VAL:HB | 3:CC:101:LEU:HD23 | 1.61 | 0.80 |
| 2:AB:77:ALA:HB2 | 2:AB:211:ILE:HD13 | 1.64 | 0.80 |
| 23:DA:528:A:H2 | 23:DA:2043:C:C5' | 1.95 | 0.80 |
| 30:DH:133:HIS:CD2 | 30:DH:135:GLU:HG2 | 2.16 | 0.80 |
| 18:AR:54:ARG:H | 18:AR:54:ARG:HD2 | 1.45 | 0.80 |
| 53:D5:57:ARG:HB2 | 53:D5:57:ARG:NH1 | 1.96 | 0.80 |
| 23:DA:1658:C:OP1 | 26:DD:132:HIS:O | 2.00 | 0.80 |
| 26:BD:54:GLN:HG2 | 26:BD:76:ARG:HG3 | 1.64 | 0.80 |
| 6:CF:26:ILE:HG22 | 6:CF:30:LEU:HD11 | 1.64 | 0.80 |
| 1:AA:625:G:C4 | 1:AA:626:U:C5 | 2.70 | 0.80 |
| 27:DE:89:VAL:HG12 | 27:DE:90:PHE:N | 1.97 | 0.80 |
| 1:CA:324:G:N2 | 1:CA:327:A:C8 | 2.49 | 0.80 |
| 22:CV:6213:A:H2' | 22:CV:6214:C:H6 | 1.46 | 0.80 |
| 32:BJ:27:TYR:CD2 | 39:BQ:100:VAL:HG11 | 2.17 | 0.80 |
| 47:DY:46:GLN:HB2 | 47:DY:49:LYS:NZ | 1.96 | 0.80 |
| 27:DE:103:LYS:HA | 27:DE:106:ARG:HG3 | 1.62 | 0.80 |
| 1:AA:1117:G:H21 | 1:AA:1180:A:H1' | 1.45 | 0.80 |
| 8:AH:83:ILE:HG13 | 8:AH:137:VAL:HG22 | 1.63 | 0.80 |
| 40:BR:100:ARG:HG3 | 40:BR:100:ARG:O | 1.80 | 0.80 |
| 40:BR:66:ARG:HD2 | 40:BR:88:ARG:CZ | 2.10 | 0.80 |
| 23:DA:2777:G:H5'' | 23:DA:2778:A:H5' | 1.64 | 0.80 |
| 33:DK:101:PRO:O | 33:DK:102:VAL:HG13 | 1.82 | 0.80 |
| 23:DA:910:A:C5 | 35:DM:13:GLN:OE1 | 2.34 | 0.80 |
| 23:DA:197:A:H5' | 23:DA:197:A:C8 | 2.17 | 0.80 |
| 5:AE:126:ARG:HG2 | 5:AE:126:ARG:HH11 | 1.47 | 0.80 |
| 42:BT:24:GLY:HA3 | 42:BT:82:GLN:HE22 | 1.47 | 0.80 |
| 23:DA:1110:G:HO2' | 23:DA:1111:A:H8 | 0.81 | 0.80 |
| 1:CA:710:G:OP1 | 6:CF:54:LYS:HE2 | 1.82 | 0.80 |
| 23:BA:605:C:H1' | 23:BA:657:U:O2' | 1.82 | 0.80 |
| 24:DB:11:C:H3' | 24:DB:12:C:H6 | 1.46 | 0.80 |
| 1:AA:1154:G:H2' | 1:AA:1155:G:H8 | 1.46 | 0.80 |
| 23:BA:733:G:N7 | 23:BA:761:A:C6 | 2.50 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BM:58:PHE:O | 35:BM:58:PHE:HD1 | 1.65 | 0.80 |
| 23:DA:557:U:H2' | 23:DA:558:G:H8 | 1.46 | 0.79 |
| 23:BA:1373:A:H2' | 23:BA:1374:G:O4' | 1.82 | 0.79 |
| 25:BC:8:PRO:HB3 | 25:BC:14:ARG:HB2 | 1.62 | 0.79 |
| 28:BF:39:ILE:HG12 | 28:BF:157:ILE:HG22 | 1.64 | 0.79 |
| 23:BA:875:G:H4' | 44:BV:170:THR:HG21 | 1.64 | 0.79 |
| 33:DK:119:PRO:HB2 | 38:DP:68:TYR:CE1 | 2.18 | 0.79 |
| 3:CC:43:LEU:HD22 | 3:CC:47:LEU:HD22 | 1.62 | 0.79 |
| 2:AB:101:MET:HA | 2:AB:108:ILE:HG13 | 1.63 | 0.79 |
| 34:BL:33:ARG:HB3 | 34:BL:36:LYS:CD | 2.12 | 0.79 |
| 47:DY:17:SER:HB3 | 47:DY:18:PRO:HD3 | 1.63 | 0.79 |
| 23:BA:330:A:HO2' | 23:BA:331:A:H8 | 1.30 | 0.79 |
| 2:CB:187:LEU:CD1 | 2:CB:205:ASP:HB3 | 2.13 | 0.79 |
| 5:CE:57:LYS:O | 5:CE:61:TYR:HD2 | 1.66 | 0.79 |
| 5:CE:126:ARG:HG2 | 5:CE:126:ARG:HH11 | 1.45 | 0.79 |
| 23:DA:1110:G:O2' | 23:DA:1111:A:H8 | 1.64 | 0.79 |
| 23:DA:752:A:H3' | 52:D4:1:MET:HE3 | 1.65 | 0.79 |
| 1:CA:475:G:H2' | 1:CA:476:G:C8 | 2.17 | 0.79 |
| 38:BP:54:ARG:HH11 | 38:BP:54:ARG:CG | 1.94 | 0.79 |
| 3:AC:152:ILE:HD11 | 3:AC:167:TRP:CD1 | 2.17 | 0.79 |
| 8:AH:20:TYR:HA | 8:AH:65:TYR:HE2 | 1.47 | 0.79 |
| 1:CA:475:G:H2' | 1:CA:476:G:H8 | 1.45 | 0.79 |
| 15:CO:30:ALA:HA | 15:CO:85:LEU:HD11 | 1.64 | 0.79 |
| 1:AA:828:A:H5'' | 1:AA:859:A:C2 | 2.17 | 0.79 |
| 1:CA:828:A:H5'' | 1:CA:859:A:C2 | 2.16 | 0.79 |
| 23:DA:1952:A:C5 | 33:DK:22:ILE:HD11 | 2.18 | 0.79 |
| 34:BL:59:LEU:HA | 34:BL:61:ARG:HE | 1.46 | 0.79 |
| 40:DR:39:LEU:HB3 | 40:DR:47:VAL:HG21 | 1.65 | 0.79 |
| 25:DC:70:TRP:HZ3 | 25:DC:146:GLU:OE1 | 1.65 | 0.79 |
| 23:DA:1487:G:H2' | 23:DA:1488:G:H8 | 1.45 | 0.79 |
| 45:DW:36:ILE:HD12 | 45:DW:58:THR:HG21 | 1.63 | 0.79 |
| 42:BT:41:ASN:O | 42:BT:45:THR:HG23 | 1.81 | 0.79 |
| 23:DA:605:C:H1' | 23:DA:657:U:O2' | 1.82 | 0.79 |
| 23:BA:1019:U:H3 | 23:BA:114(B):A:N6 | 1.79 | 0.79 |
| 3:CC:138:VAL:HG23 | 3:CC:151:VAL:HG23 | 1.64 | 0.79 |
| 3:CC:152:ILE:HD11 | 3:CC:167:TRP:CD1 | 2.17 | 0.79 |
| 44:DV:69:THR:HG22 | 44:DV:90:VAL:HA | 1.63 | 0.79 |
| 26:BD:51:PHE:CD1 | 26:BD:52:LEU:HD12 | 2.18 | 0.79 |
| 23:BA:363(A):G:H2' | 23:BA:363(B):A:C8 | 2.17 | 0.79 |
| 12:CL:52:ARG:HG3 | 12:CL:52:ARG:HH11 | 1.46 | 0.79 |
| 37:DO:31:SER:HB3 | 37:DO:34:HIS:HB2 | 1.64 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:556:C:O2 | 1:AA:556:C:H2' | 1.83 | 0.79 |
| 4:CD:92:VAL:HG12 | 4:CD:96:LEU:HD23 | 1.63 | 0.79 |
| 23:DA:2208:U:O2' | 23:DA:2209:C:H5' | 1.82 | 0.79 |
| 23:DA:2790:A:H2' | 23:DA:2791:C:H5'' | 1.61 | 0.79 |
| 29:BG:44:VAL:HG12 | 29:BG:45:VAL:H | 1.45 | 0.79 |
| 52:B4:8:ASN:ND2 | 52:B4:11:LYS:H | 1.81 | 0.79 |
| 23:BA:857:C:H4' | 45:BW:23:VAL:HG21 | 1.64 | 0.79 |
| 19:AS:6:LYS:HG2 | 19:AS:7:LYS:HD3 | 1.63 | 0.79 |
| 30:BH:83:ALA:CB | 30:BH:123:LEU:HD12 | 2.13 | 0.79 |
| 41:DS:29:LEU:CD2 | 41:DS:33:ARG:HE | 1.94 | 0.79 |
| 1:AA:1329:A:H5'' | 13:AM:26:GLY:N | 1.97 | 0.79 |
| 33:DK:90:GLN:O | 33:DK:91:LEU:HB2 | 1.83 | 0.79 |
| 30:BH:66:GLU:HG2 | 30:BH:67:ARG:NH2 | 1.96 | 0.79 |
| 3:AC:43:LEU:HD22 | 3:AC:47:LEU:HD22 | 1.63 | 0.79 |
| 34:DL:132:LYS:H | 34:DL:132:LYS:HD3 | 1.48 | 0.79 |
| 39:BQ:92:ARG:HB2 | 39:BQ:92:ARG:HH11 | 1.47 | 0.79 |
| 23:DA:1437:C:H2' | 23:DA:1438:U:C6 | 2.18 | 0.79 |
| 52:B4:19:ARG:HH11 | 52:B4:19:ARG:CG | 1.96 | 0.79 |
| 46:DX:13:ILE:HG12 | 46:DX:63:ALA:CB | 2.13 | 0.79 |
| 34:BL:16:ARG:NH1 | 34:BL:18:ARG:HG3 | 1.97 | 0.79 |
| 23:BA:760:G:C2' | 23:BA:761:A:H5' | 2.13 | 0.79 |
| 18:CR:26:LEU:HD11 | 18:CR:42:ARG:HD2 | 1.62 | 0.79 |
| 43:BU:17:SER:CA | 43:BU:71:LYS:HD2 | 2.12 | 0.79 |
| 1:AA:950:U:OP2 | 13:AM:102:ARG:HG3 | 1.81 | 0.79 |
| 42:DT:84:ALA:HB3 | 42:DT:87:GLN:NE2 | 1.97 | 0.79 |
| 1:AA:91:C:H2' | 1:AA:92:G:C8 | 2.18 | 0.79 |
| 1:AA:832:C:H42 | 1:AA:854:G:H1 | 1.31 | 0.79 |
| 1:CA:370:C:O2' | 1:CA:371:G:H5' | 1.82 | 0.79 |
| 28:DF:39:ILE:HG12 | 28:DF:157:ILE:HG22 | 1.64 | 0.79 |
| 13:CM:67:GLU:HG3 | 13:CM:68:GLY:H | 1.48 | 0.79 |
| 38:DP:51:ARG:NH1 | 38:DP:51:ARG:HG3 | 1.88 | 0.79 |
| 1:CA:1371:G:OP1 | 9:CI:11:LYS:HB3 | 1.82 | 0.79 |
| 1:AA:1070:U:H2' | 1:AA:1071:C:C6 | 2.18 | 0.79 |
| 4:AD:126:ILE:HG22 | 4:AD:127:THR:H | 1.48 | 0.79 |
| 34:BL:16:ARG:C | 34:BL:16:ARG:HE | 1.85 | 0.79 |
| 27:BE:132:VAL:HG23 | 27:BE:133:ASN:H | 1.49 | 0.79 |
| 53:B5:57:ARG:HB2 | 53:B5:57:ARG:NH1 | 1.97 | 0.79 |
| 23:DA:1373:A:H2' | 23:DA:1374:G:O4' | 1.82 | 0.79 |
| 6:AF:98:LEU:HD13 | 6:AF:101:ALA:HB2 | 1.64 | 0.79 |
| 15:AO:56:LEU:O | 15:AO:60:VAL:HG23 | 1.83 | 0.79 |
| 34:BL:59:LEU:CA | 34:BL:61:ARG:NE | 2.45 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:DQ:91:ASP:OD2 | 39:DQ:96:ALA:HB2 | 1.81 | 0.78 |
| 2:CB:101:MET:HA | 2:CB:108:ILE:HG13 | 1.64 | 0.78 |
| 1:CA:556:C:O2 | 1:CA:556:C:H2' | 1.83 | 0.78 |
| 23:BA:780:G:H21 | 23:BA:783:A:H62 | 1.27 | 0.78 |
| 38:DP:54:ARG:CG | 38:DP:54:ARG:HH11 | 1.94 | 0.78 |
| 38:BP:51:ARG:HG3 | 38:BP:51:ARG:NH1 | 1.94 | 0.78 |
| 5:AE:78:HIS:CD2 | 8:AH:104:ARG:HG2 | 2.19 | 0.78 |
| 1:AA:476:G:H2' | 1:AA:477:G:H8 | 1.48 | 0.78 |
| 23:BA:2531:A:H5' | 29:BG:157:TYR:CZ | 2.18 | 0.78 |
| 40:DR:100:ARG:HG3 | 40:DR:100:ARG:O | 1.81 | 0.78 |
| 46:DX:19:GLN:HG3 | 46:DX:41:ARG:HE | 1.47 | 0.78 |
| 27:BE:53:THR:HG23 | 27:BE:56:GLU:OE1 | 1.83 | 0.78 |
| 43:DU:17:SER:CA | 43:DU:71:LYS:HD2 | 2.13 | 0.78 |
| 4:AD:100:ARG:NH1 | 4:AD:137:SER:HA | 1.99 | 0.78 |
| 28:BF:41:GLN:HB3 | 28:BF:43:LEU:HD13 | 1.66 | 0.78 |
| 23:BA:2219:G:H2' | 23:BA:2224:G:C5' | 2.14 | 0.78 |
| 1:CA:266:G:H5' | 1:CA:267:C:C5 | 2.18 | 0.78 |
| 8:CH:92:ARG:HB3 | 8:CH:94:TYR:CE2 | 2.17 | 0.78 |
| 32:DJ:63:PRO:O | 39:DQ:64:ARG:HD2 | 1.81 | 0.78 |
| 3:AC:59:ARG:HG2 | 3:AC:64:VAL:HG22 | 1.65 | 0.78 |
| 3:CC:105:GLU:HG2 | 3:CC:106:VAL:H | 1.48 | 0.78 |
| 23:DA:528:A:H3' | 23:DA:528:A:C8 | 2.19 | 0.78 |
| 30:BH:100:ALA:HA | 30:BH:103:ARG:HB2 | 1.64 | 0.78 |
| 52:B4:12:ARG:HH11 | 52:B4:12:ARG:HG3 | 1.49 | 0.78 |
| 1:AA:99:C:O2' | 1:AA:101:A:H5'' | 1.84 | 0.78 |
| 42:BT:63:LYS:CD | 42:BT:72:LYS:HA | 2.01 | 0.78 |
| 53:B5:62:LEU:HB3 | 53:B5:63:PRO:HD3 | 1.65 | 0.78 |
| 1:CA:91:C:H2' | 1:CA:92:G:C8 | 2.18 | 0.78 |
| 1:CA:1154:G:H2' | 1:CA:1155:G:C8 | 2.17 | 0.78 |
| 23:DA:1046:A:H3' | 23:DA:1047:G:H5'' | 1.66 | 0.78 |
| 18:AR:58:LEU:HD23 | 18:AR:62:GLU:HB3 | 1.63 | 0.78 |
| 13:AM:67:GLU:HG3 | 13:AM:68:GLY:H | 1.48 | 0.78 |
| 27:DE:157:VAL:HB | 27:DE:194:MET:HB3 | 1.65 | 0.78 |
| 30:BH:5:LEU:H | 30:BH:5:LEU:HD23 | 1.47 | 0.78 |
| 23:DA:106:C:H1' | 43:DU:2:ARG:HE | 1.49 | 0.78 |
| 52:B4:8:ASN:HD22 | 52:B4:9:ARG:N | 1.82 | 0.78 |
| 34:BL:114:ILE:HD11 | 34:BL:127:ALA:CB | 2.12 | 0.78 |
| 23:DA:1658:C:OP1 | 26:DD:132:HIS:CE1 | 2.36 | 0.78 |
| 42:DT:57:LEU:CD1 | 42:DT:78:LYS:HB2 | 2.14 | 0.78 |
| 3:CC:195:VAL:HG12 | 3:CC:196:LEU:N | 1.99 | 0.78 |
| 29:BG:144:VAL:O | 29:BG:148:ILE:HG12 | 1.82 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:987:G:H1 | 1:CA:1218:C:H42 | 1.32 | 0.78 |
| 20:AT:45:GLN:HB2 | 20:AT:91:LEU:HD13 | 1.64 | 0.78 |
| 1:CA:1010:G:H2' | 1:CA:1011:G:C8 | 2.19 | 0.78 |
| 23:DA:971:C:H2' | 23:DA:972:G:H5' | 1.65 | 0.78 |
| 50:D2:41:PRO:HG2 | 50:D2:44:THR:HG21 | 1.65 | 0.78 |
| 13:AM:91:ARG:HH11 | 19:AS:81:ARG:HH22 | 1.31 | 0.78 |
| 1:AA:688:G:H2' | 1:AA:689:C:H6 | 1.48 | 0.78 |
| 23:BA:1209:G:H21 | 23:BA:1210:A:N6 | 1.81 | 0.78 |
| 23:DA:661:C:H4' | 34:DL:18:ARG:HG2 | 1.64 | 0.78 |
| 5:AE:50:GLU:OE2 | 5:AE:51:VAL:HG23 | 1.83 | 0.78 |
| 1:AA:475:G:H2' | 1:AA:476:G:C8 | 2.18 | 0.78 |
| 42:DT:24:GLY:HA3 | 42:DT:82:GLN:HE22 | 1.48 | 0.78 |
| 25:DC:8:PRO:HB3 | 25:DC:14:ARG:HB2 | 1.65 | 0.78 |
| 1:AA:601:C:H2' | 1:AA:602:A:C8 | 2.19 | 0.78 |
| 1:AA:495:A:H4' | 1:AA:496:A:OP1 | 1.83 | 0.78 |
| 24:BB:49:C:OP1 | 37:BO:97:ARG:HG3 | 1.84 | 0.78 |
| 29:BG:95:ARG:HH22 | 29:BG:97:ARG:NH2 | 1.82 | 0.78 |
| 28:BF:109:VAL:HG11 | 28:BF:142:PRO:HG3 | 1.66 | 0.78 |
| 10:AJ:51:ARG:HB2 | 10:AJ:60:ARG:HA | 1.66 | 0.78 |
| 34:DL:33:ARG:HB3 | 34:DL:36:LYS:HD3 | 1.66 | 0.78 |
| 44:BV:125:LEU:HD22 | 44:BV:164:ALA:HB3 | 1.66 | 0.78 |
| 26:DD:51:PHE:CD1 | 26:DD:52:LEU:HD12 | 2.18 | 0.78 |
| 25:DC:87:ASN:N | 25:DC:87:ASN:HD22 | 1.79 | 0.78 |
| 26:BD:111:ARG:HA | 36:BN:2:ARG:HH11 | 1.49 | 0.78 |
| 43:DU:2:ARG:HG2 | 43:DU:3:VAL:HG23 | 1.66 | 0.78 |
| 23:BA:1520:U:H2' | 23:BA:1521:G:O4' | 1.84 | 0.78 |
| 23:DA:2875:C:H4' | 38:DP:5:ALA:HB2 | 1.66 | 0.78 |
| 2:CB:8:LYS:HA | 2:CB:217:ARG:HH12 | 1.49 | 0.78 |
| 36:DN:38:VAL:HB | 36:DN:39:PRO:CD | 2.14 | 0.78 |
| 39:BQ:82:GLY:HA3 | 39:BQ:113:ALA:HB1 | 1.64 | 0.78 |
| 3:AC:195:VAL:HG12 | 3:AC:196:LEU:N | 1.99 | 0.78 |
| 25:BC:27:THR:HG23 | 25:BC:27:THR:O | 1.83 | 0.78 |
| 1:AA:1129:C:H1' | 1:AA:1130:A:OP2 | 1.84 | 0.78 |
| 1:CA:1117:G:H21 | 1:CA:1180:A:H1' | 1.47 | 0.78 |
| 4:AD:3:ARG:HD3 | 4:AD:5:ILE:HD11 | 1.64 | 0.77 |
| 23:DA:389:G:N1 | 34:DL:71:VAL:HG23 | 1.99 | 0.77 |
| 3:AC:105:GLU:HG2 | 3:AC:106:VAL:H | 1.49 | 0.77 |
| 1:AA:509:A:H5' | 4:AD:54:TYR:HD2 | 1.49 | 0.77 |
| 29:DG:30:LYS:HE2 | 29:DG:80:SER:O | 1.84 | 0.77 |
| 32:BJ:81:ASP:CG | 32:BJ:147:ALA:HB1 | 2.04 | 0.77 |
| 4:AD:204:ILE:HG21 | 5:AE:98:THR:O | 1.84 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:DL:114:ILE:HD13 | 34:DL:130:PHE:CE1 | 2.20 | 0.77 |
| 36:DN:11:ASN:OD1 | 36:DN:12:ARG:N | 2.17 | 0.77 |
| 32:BJ:93:LYS:HE3 | 32:BJ:95:TYR:HE1 | 1.49 | 0.77 |
| 42:DT:49:VAL:HG21 | 42:DT:83:VAL:HG12 | 1.65 | 0.77 |
| 23:DA:1021:A:N6 | 23:DA:1141:U:H3 | 1.82 | 0.77 |
| 23:BA:1437:C:H2' | 23:BA:1438:U:C6 | 2.19 | 0.77 |
| 23:BA:662:G:OP1 | 34:BL:18:ARG:HD2 | 1.83 | 0.77 |
| 25:DC:125:ILE:O | 25:DC:125:ILE:HG22 | 1.84 | 0.77 |
| 23:BA:1658:C:OP1 | 26:BD:132:HIS:CE1 | 2.37 | 0.77 |
| 25:DC:106:ILE:HD12 | 25:DC:106:ILE:N | 1.98 | 0.77 |
| 24:BB:15:A:H5' | 24:BB:16:G:C8 | 2.19 | 0.77 |
| 2:AB:97:TRP:HZ2 | 2:AB:102:LEU:HD13 | 1.48 | 0.77 |
| 1:AA:1154:G:H2' | 1:AA:1155:G:C8 | 2.19 | 0.77 |
| 2:AB:8:LYS:HA | 2:AB:217:ARG:HH12 | 1.49 | 0.77 |
| 25:DC:28:GLU:HB3 | 25:DC:29:PRO:HD3 | 1.67 | 0.77 |
| 34:DL:97:PRO:HD3 | 34:DL:126:VAL:HG12 | 1.66 | 0.77 |
| 25:DC:33:LEU:O | 25:DC:36:PRO:HD2 | 1.84 | 0.77 |
| 1:CA:377:G:OP1 | 16:CP:3:LYS:HD2 | 1.84 | 0.77 |
| 25:BC:33:LEU:O | 25:BC:36:PRO:HD2 | 1.84 | 0.77 |
| 34:DL:16:ARG:O | 34:DL:16:ARG:NE | 2.17 | 0.77 |
| 36:DN:2:ARG:C | 36:DN:4:LEU:H | 1.87 | 0.77 |
| 10:AJ:75:ILE:HG13 | 10:AJ:76:ASN:H | 1.49 | 0.77 |
| 40:BR:34:GLU:O | 40:BR:36:PRO:HD3 | 1.84 | 0.77 |
| 6:CF:78:GLU:O | 6:CF:81:ILE:HG13 | 1.84 | 0.77 |
| 32:DJ:81:ASP:CG | 32:DJ:147:ALA:HB1 | 2.04 | 0.77 |
| 10:AJ:48:THR:HG22 | 10:AJ:62:HIS:ND1 | 2.00 | 0.77 |
| 23:BA:860:U:C5 | 23:BA:917:A:N7 | 2.52 | 0.77 |
| 23:BA:1546:A:N7 | 23:BA:154(B):C:O2 | 2.18 | 0.77 |
| 34:BL:147:LEU:HD13 | 34:BL:148:LEU:O | 1.84 | 0.77 |
| 27:DE:164:ARG:HG3 | 27:DE:175:THR:OG1 | 1.84 | 0.77 |
| 42:BT:49:VAL:HG21 | 42:BT:83:VAL:HG12 | 1.67 | 0.77 |
| 4:AD:108:LEU:HB3 | 4:AD:110:PHE:HE2 | 1.47 | 0.77 |
| 23:DA:2687:U:C4 | 23:DA:2688:U:C5 | 2.73 | 0.77 |
| 33:DK:99:PHE:CD1 | 33:DK:99:PHE:N | 2.50 | 0.77 |
| 1:CA:625:G:C4 | 1:CA:626:U:C5 | 2.72 | 0.77 |
| 29:DG:88:LEU:HB3 | 29:DG:90:LYS:HD3 | 1.67 | 0.77 |
| 23:DA:2562:U:H1' | 33:DK:23:ARG:HH11 | 1.49 | 0.77 |
| 23:DA:2531:A:H5' | 29:DG:157:TYR:CZ | 2.19 | 0.77 |
| 23:DA:2286:A:H4' | 23:DA:2287:A:O4' | 1.85 | 0.77 |
| 43:BU:44:ILE:HG22 | 43:BU:45:VAL:H | 1.49 | 0.77 |
| 23:BA:1963:U:H2' | 23:BA:1963:U:O2 | 1.84 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1129:C:H1' | 1:CA:1130:A:OP2 | 1.84 | 0.77 |
| 52:D4:11:LYS:HD2 | 52:D4:15:THR:CG2 | 2.14 | 0.77 |
| 1:AA:790:A:H5' | 22:AV:6192:G:H4' | 1.67 | 0.77 |
| 23:DA:114(B):A:H4' | 32:DJ:48:ARG:HH22 | 1.48 | 0.77 |
| 23:BA:380:U:C2 | 46:BX:20:ARG:NH2 | 2.52 | 0.77 |
| 13:AM:23:TYR:CZ | 13:AM:71:ARG:HD3 | 2.20 | 0.77 |
| 32:DJ:38:LEU:CD2 | 32:DJ:157:ARG:HG3 | 2.15 | 0.77 |
| 47:BY:6:VAL:O | 47:BY:10:LEU:HG | 1.85 | 0.77 |
| 4:CD:25:ARG:HG2 | 4:CD:30:LYS:HG3 | 1.65 | 0.77 |
| 26:DD:77:ILE:HD13 | 26:DD:195:LEU:HD12 | 1.65 | 0.77 |
| 23:BA:528:A:H2 | 23:BA:2043:C:C5' | 1.98 | 0.77 |
| 23:BA:528:A:H8 | 23:BA:528:A:H3' | 1.49 | 0.77 |
| 36:BN:2:ARG:C | 36:BN:4:LEU:H | 1.87 | 0.77 |
| 33:DK:98:VAL:HG11 | 33:DK:114:ILE:HG23 | 1.66 | 0.77 |
| 1:AA:1010:G:H2' | 1:AA:1011:G:C8 | 2.20 | 0.77 |
| 1:CA:1064:G:H21 | 1:CA:1190:G:H2' | 1.48 | 0.77 |
| 25:BC:125:ILE:O | 25:BC:125:ILE:HG22 | 1.85 | 0.77 |
| 33:BK:99:PHE:N | 33:BK:99:PHE:HD1 | 1.81 | 0.77 |
| 47:BY:1:MET:SD | 47:BY:5:GLU:HG2 | 2.25 | 0.77 |
| 25:DC:10:THR:HG23 | 25:DC:13:ARG:CB | 2.13 | 0.77 |
| 29:DG:101:ARG:HE | 29:DG:101:ARG:H | 0.81 | 0.77 |
| 10:CJ:75:ILE:HG13 | 10:CJ:76:ASN:H | 1.49 | 0.77 |
| 23:DA:323:G:H5' | 27:DE:169:ASN:HD21 | 1.48 | 0.77 |
| 23:BA:1046:A:H3' | 23:BA:1047:G:H5'' | 1.66 | 0.77 |
| 1:AA:370:C:O2' | 1:AA:371:G:H5' | 1.85 | 0.77 |
| 23:DA:7:G:H1 | 23:DA:2896:C:H42 | 1.31 | 0.77 |
| 1:CA:781:A:C3' | 1:CA:782:A:H5' | 2.14 | 0.77 |
| 23:BA:2781:A:H5'' | 23:BA:2782:G:C5' | 2.05 | 0.77 |
| 43:DU:7:VAL:HG12 | 43:DU:8:LYS:CG | 2.07 | 0.77 |
| 25:BC:233:HIS:CE1 | 25:BC:247:ALA:H | 2.03 | 0.77 |
| 35:BM:76:LYS:N | 35:BM:88:GLY:HA2 | 1.99 | 0.77 |
| 42:DT:31:HIS:ND1 | 42:DT:32:PRO:HD2 | 2.00 | 0.77 |
| 28:BF:128:ARG:NE | 28:BF:129:GLY:H | 1.81 | 0.77 |
| 4:CD:28:SER:HB3 | 4:CD:29:PRO:HD2 | 1.67 | 0.77 |
| 1:AA:1073:U:H2' | 1:AA:1074:G:H8 | 1.50 | 0.77 |
| 25:DC:25:THR:CG2 | 25:DC:82:ILE:H | 1.98 | 0.77 |
| 1:CA:1191:A:H5'' | 3:CC:4:LYS:NZ | 2.00 | 0.77 |
| 43:BU:50:ARG:HD3 | 43:BU:51:VAL:H | 1.48 | 0.77 |
| 53:D5:52:LYS:H | 53:D5:53:PRO:HD2 | 1.50 | 0.77 |
| 53:D5:62:LEU:HB3 | 53:D5:63:PRO:CD | 2.15 | 0.77 |
| 39:BQ:98:LEU:O | 39:BQ:100:VAL:N | 2.17 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 32:DJ:105:LEU:CD1 | 32:DJ:106:LYS:H | 1.98 | 0.77 |
| 23:BA:2353:G:O6 | 23:BA:2353:G:C5 | 2.38 | 0.77 |
| 28:BF:77:ILE:HG22 | 28:BF:80:PHE:H | 1.50 | 0.77 |
| 23:BA:389:G:N1 | 34:BL:71:VAL:HG23 | 2.01 | 0.77 |
| 11:CK:21:ILE:HA | 11:CK:30:VAL:HG12 | 1.67 | 0.77 |
| 34:DL:7:ARG:O | 34:DL:10:PRO:HD3 | 1.85 | 0.77 |
| 24:DB:78:A:C2 | 24:DB:99:A:C4 | 2.73 | 0.77 |
| 34:BL:33:ARG:HB3 | 34:BL:36:LYS:CG | 2.15 | 0.76 |
| 23:BA:1210:A:C8 | 23:BA:1210:A:C5' | 2.67 | 0.76 |
| 8:AH:58:TYR:O | 8:AH:59:LEU:HD23 | 1.85 | 0.76 |
| 1:AA:625:G:H2' | 1:AA:626:U:H6 | 1.47 | 0.76 |
| 23:BA:2688:U:H3' | 23:BA:2688:U:O2 | 1.85 | 0.76 |
| 43:DU:44:ILE:HG22 | 43:DU:45:VAL:H | 1.48 | 0.76 |
| 23:BA:2598:A:OP1 | 25:BC:235:GLY:HA3 | 1.84 | 0.76 |
| 23:BA:2393:A:H5'' | 34:BL:62:LEU:HD12 | 1.66 | 0.76 |
| 23:BA:1019:U:H2' | 23:BA:1020:A:H8 | 1.50 | 0.76 |
| 53:B5:62:LEU:HB3 | 53:B5:63:PRO:CD | 2.15 | 0.76 |
| 23:DA:71:A:H2 | 42:DT:31:HIS:CE1 | 2.03 | 0.76 |
| 1:AA:735:C:H2' | 1:AA:736:C:H6 | 1.50 | 0.76 |
| 30:DH:5:LEU:H | 30:DH:5:LEU:HD23 | 1.50 | 0.76 |
| 23:DA:1520:U:H2' | 23:DA:1521:G:O4' | 1.84 | 0.76 |
| 1:AA:106:C:O2' | 1:AA:107:G:H5' | 1.85 | 0.76 |
| 27:DE:203:GLN:HA | 27:DE:206:ILE:O | 1.85 | 0.76 |
| 25:BC:28:GLU:HB3 | 25:BC:29:PRO:HD3 | 1.67 | 0.76 |
| 1:CA:106:C:O2' | 1:CA:107:G:H5' | 1.85 | 0.76 |
| 38:BP:42:ILE:O | 38:BP:42:ILE:HD12 | 1.86 | 0.76 |
| 23:DA:733:G:N7 | 23:DA:761:A:C6 | 2.53 | 0.76 |
| 23:BA:1683:C:H42 | 23:BA:1705:G:H1 | 1.31 | 0.76 |
| 25:BC:238:GLY:O | 25:BC:239:ARG:C | 2.22 | 0.76 |
| 4:AD:100:ARG:HH21 | 4:AD:118:ARG:HH12 | 1.32 | 0.76 |
| 48:BZ:43:ILE:HD13 | 48:BZ:43:ILE:N | 2.01 | 0.76 |
| 40:BR:27:ALA:CB | 40:BR:61:VAL:HG11 | 2.14 | 0.76 |
| 23:DA:270(H):C:H2' | 23:DA:270(I):C:H6 | 1.49 | 0.76 |
| 23:BA:256:A:C2' | 23:BA:257:A:H5' | 2.15 | 0.76 |
| 1:CA:738:C:H2' | 1:CA:739:C:C6 | 2.20 | 0.76 |
| 27:DE:34:TRP:HB2 | 34:DL:10:PRO:O | 1.86 | 0.76 |
| 25:BC:166:GLN:HE21 | 25:BC:166:GLN:CA | 1.97 | 0.76 |
| 1:AA:1422:G:H5'' | 33:BK:48:PRO:HB3 | 1.67 | 0.76 |
| 23:DA:226:G:N2 | 23:DA:228:A:H62 | 1.83 | 0.76 |
| 34:DL:33:ARG:HG2 | 34:DL:34:GLY:N | 2.00 | 0.76 |
| 23:BA:114(B):A:H4' | 32:BJ:48:ARG:HH22 | 1.51 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:DC:87:ASN:N | 25:DC:87:ASN:ND2 | 2.32 | 0.76 |
| 23:DA:911:A:H2' | 35:DM:9:TYR:OH | 1.83 | 0.76 |
| 23:BA:270(H):C:H2' | 23:BA:270(I):C:H6 | 1.49 | 0.76 |
| 1:AA:262:A:H2' | 1:AA:263:A:C8 | 2.20 | 0.76 |
| 45:BW:36:ILE:HD12 | 45:BW:58:THR:HG21 | 1.65 | 0.76 |
| 23:DA:960:A:H5'' | 23:DA:961:C:OP2 | 1.85 | 0.76 |
| 10:CJ:48:THR:HG22 | 10:CJ:62:HIS:ND1 | 1.99 | 0.76 |
| 25:BC:10:THR:HG23 | 25:BC:13:ARG:CB | 2.11 | 0.76 |
| 28:DF:128:ARG:HE | 28:DF:129:GLY:N | 1.84 | 0.76 |
| 34:DL:16:ARG:NH1 | 34:DL:18:ARG:HG3 | 2.01 | 0.76 |
| 5:CE:78:HIS:CD2 | 8:CH:104:ARG:HG2 | 2.20 | 0.76 |
| 1:AA:266:G:H5' | 1:AA:267:C:C5 | 2.21 | 0.76 |
| 1:CA:476:G:H2' | 1:CA:477:G:H8 | 1.49 | 0.76 |
| 53:B5:22:VAL:HB | 53:B5:54:GLU:HG3 | 1.68 | 0.76 |
| 23:BA:1475:G:N2 | 23:BA:1519:G:C4 | 2.54 | 0.76 |
| 1:CA:170:U:O2' | 1:CA:171:A:H5' | 1.84 | 0.76 |
| 13:AM:27:LYS:HE2 | 13:AM:31:LYS:HE3 | 1.66 | 0.76 |
| 3:CC:59:ARG:HG2 | 3:CC:64:VAL:HG22 | 1.67 | 0.76 |
| 1:CA:957:U:H4' | 19:CS:79:THR:HB | 1.67 | 0.76 |
| 2:AB:63:MET:HG2 | 2:AB:225:ALA:HB1 | 1.67 | 0.76 |
| 45:BW:56:ASP:O | 45:BW:57:PHE:HB2 | 1.85 | 0.76 |
| 36:DN:97:VAL:HA | 36:DN:113:LEU:O | 1.85 | 0.76 |
| 22:AV:6182:A:C2 | 22:AV:6183:G:C4 | 2.74 | 0.76 |
| 23:DA:1614:A:H62 | 41:DS:93:ALA:CB | 1.98 | 0.76 |
| 40:BR:40:LEU:HD23 | 40:BR:47:VAL:HG23 | 1.68 | 0.76 |
| 25:DC:233:HIS:CE1 | 25:DC:247:ALA:H | 2.03 | 0.76 |
| 26:DD:54:GLN:HG2 | 26:DD:76:ARG:HG3 | 1.66 | 0.76 |
| 6:AF:26:ILE:O | 6:AF:30:LEU:HD12 | 1.85 | 0.76 |
| 40:DR:25:LEU:H | 40:DR:92:THR:HG21 | 1.47 | 0.76 |
| 1:CA:625:G:H2' | 1:CA:626:U:H6 | 1.50 | 0.76 |
| 11:AK:34:ASP:N | 11:AK:40:ILE:HD11 | 2.00 | 0.76 |
| 23:BA:65:C:H2' | 23:BA:66:C:C6 | 2.20 | 0.76 |
| 43:BU:42:VAL:HG12 | 43:BU:65:ALA:HB3 | 1.66 | 0.76 |
| 19:CS:6:LYS:HG2 | 19:CS:7:LYS:HD3 | 1.67 | 0.76 |
| 27:BE:34:TRP:HB2 | 34:BL:10:PRO:O | 1.86 | 0.76 |
| 1:AA:624:C:H4' | 16:AP:11:SER:H | 1.51 | 0.76 |
| 23:BA:2250:G:C6 | 35:BM:82:ARG:HD2 | 2.21 | 0.76 |
| 22:CV:6182:A:C2 | 22:CV:6183:G:C4 | 2.74 | 0.76 |
| 38:BP:56:GLY:O | 38:BP:59:THR:HG22 | 1.84 | 0.76 |
| 39:BQ:91:ASP:OD2 | 39:BQ:96:ALA:HB2 | 1.85 | 0.76 |
| 26:BD:4:ILE:HG12 | 26:BD:28:ALA:HB1 | 1.68 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:CH:58:TYR:O | 8:CH:59:LEU:HD23 | 1.84 | 0.76 |
| 1:AA:555:C:H2' | 1:AA:556:C:H6 | 1.51 | 0.76 |
| 10:AJ:74:ILE:H | 10:AJ:74:ILE:HD13 | 1.49 | 0.76 |
| 29:BG:30:LYS:HE2 | 29:BG:80:SER:O | 1.86 | 0.76 |
| 23:DA:286:C:H2' | 23:DA:287:C:H6 | 1.48 | 0.76 |
| 36:BN:51:LEU:HD23 | 36:BN:66:VAL:HG22 | 1.66 | 0.76 |
| 43:DU:15:VAL:HG22 | 43:DU:72:VAL:HG12 | 1.66 | 0.76 |
| 32:BJ:38:LEU:CD2 | 32:BJ:157:ARG:HG3 | 2.16 | 0.76 |
| 34:DL:50:ARG:HD2 | 34:DL:51:PHE:N | 2.01 | 0.76 |
| 4:AD:110:PHE:H | 4:AD:110:PHE:HD2 | 1.34 | 0.76 |
| 1:CA:265:G:H5' | 17:CQ:64:PRO:O | 1.86 | 0.76 |
| 43:BU:81:LYS:HD3 | 43:BU:97:ARG:H | 1.51 | 0.76 |
| 1:CA:643:C:H5' | 8:CH:31:PHE:CE1 | 2.20 | 0.76 |
| 23:DA:780:G:H21 | 23:DA:783:A:H62 | 1.34 | 0.76 |
| 23:DA:256:A:C2' | 23:DA:257:A:H5' | 2.16 | 0.76 |
| 13:CM:27:LYS:HE2 | 13:CM:31:LYS:HE3 | 1.67 | 0.76 |
| 29:DG:85:LYS:HD3 | 29:DG:86:GLU:OE2 | 1.85 | 0.76 |
| 26:BD:5:LEU:HB2 | 26:BD:51:PHE:CD2 | 2.21 | 0.76 |
| 3:AC:138:VAL:HG23 | 3:AC:151:VAL:HG23 | 1.68 | 0.76 |
| 23:DA:760:G:C2' | 23:DA:761:A:H5' | 2.16 | 0.76 |
| 4:CD:117:ALA:O | 4:CD:121:VAL:HG23 | 1.86 | 0.76 |
| 28:DF:77:ILE:HG22 | 28:DF:80:PHE:H | 1.50 | 0.76 |
| 33:BK:90:GLN:O | 33:BK:91:LEU:HB2 | 1.85 | 0.76 |
| 23:DA:1379:A:H4' | 23:DA:1380:G:OP2 | 1.86 | 0.76 |
| 18:AR:26:LEU:HD11 | 18:AR:42:ARG:HD2 | 1.67 | 0.76 |
| 23:DA:2786:U:H4' | 26:DD:65:GLY:O | 1.85 | 0.76 |
| 32:DJ:27:TYR:CD2 | 39:DQ:100:VAL:HG11 | 2.21 | 0.76 |
| 43:DU:50:ARG:HD3 | 43:DU:51:VAL:H | 1.50 | 0.76 |
| 34:DL:57:THR:HG23 | 34:DL:59:LEU:CD2 | 2.12 | 0.75 |
| 38:DP:100:TYR:HB3 | 38:DP:103:ARG:NH1 | 2.01 | 0.75 |
| 1:CA:971:G:H1' | 1:CA:1365:G:O2' | 1.86 | 0.75 |
| 20:AT:26:ASN:ND2 | 20:AT:26:ASN:H | 1.83 | 0.75 |
| 20:CT:26:ASN:ND2 | 20:CT:26:ASN:H | 1.84 | 0.75 |
| 27:BE:103:LYS:HA | 27:BE:106:ARG:HG3 | 1.68 | 0.75 |
| 23:DA:1045:A:H5'' | 23:DA:1047:G:O4' | 1.86 | 0.75 |
| 18:CR:26:LEU:HD21 | 18:CR:42:ARG:HH11 | 1.49 | 0.75 |
| 45:BW:53:MET:HB2 | 45:BW:59:LEU:HD23 | 1.68 | 0.75 |
| 23:DA:966:G:H2' | 23:DA:967:C:H6 | 1.49 | 0.75 |
| 25:BC:182:LEU:H | 25:BC:272:ALA:HB3 | 1.51 | 0.75 |
| 28:DF:114:ILE:HB | 28:DF:117:PHE:HB2 | 1.67 | 0.75 |
| 2:AB:72:GLY:O | 2:AB:94:ASN:HA | 1.86 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:BU:2:ARG:HG2 | 43:BU:3:VAL:HG23 | 1.67 | 0.75 |
| 23:DA:1778:U:H2' | 23:DA:1784:A:N6 | 2.01 | 0.75 |
| 17:CQ:15:MET:HB3 | 17:CQ:18:THR:HB | 1.68 | 0.75 |
| 32:BJ:118:PRO:O | 32:BJ:121:VAL:HG22 | 1.86 | 0.75 |
| 23:BA:2439:A:C5' | 23:BA:2439:A:C8 | 2.63 | 0.75 |
| 3:CC:18:TRP:CD1 | 14:CN:54:PRO:HA | 2.21 | 0.75 |
| 2:AB:178:ARG:HH22 | 2:AB:196:LEU:HA | 1.51 | 0.75 |
| 44:DV:136:PHE:C | 44:DV:137:ILE:HD12 | 2.05 | 0.75 |
| 23:BA:1434:A:H61 | 23:BA:1558:A:N6 | 1.84 | 0.75 |
| 38:BP:26:ASP:HB2 | 38:BP:90:GLN:O | 1.86 | 0.75 |
| 15:AO:30:ALA:HA | 15:AO:85:LEU:HD11 | 1.67 | 0.75 |
| 43:BU:47:LYS:HA | 43:BU:60:PHE:CE2 | 2.21 | 0.75 |
| 23:DA:2593:U:H2' | 23:DA:2594:C:C6 | 2.21 | 0.75 |
| 17:CQ:40:LYS:HD2 | 17:CQ:42:TYR:CE1 | 2.22 | 0.75 |
| 47:BY:46:GLN:HB2 | 47:BY:49:LYS:NZ | 2.01 | 0.75 |
| 23:DA:857:C:H4' | 45:DW:23:VAL:HG21 | 1.68 | 0.75 |
| 25:BC:77:ALA:HB2 | 25:BC:97:TYR:HA | 1.68 | 0.75 |
| 23:BA:1110:G:O2' | 23:BA:1111:A:H8 | 1.65 | 0.75 |
| 23:BA:733:G:N7 | 23:BA:761:A:N6 | 2.34 | 0.75 |
| 43:DU:76:CYS:HB3 | 43:DU:77:PRO:HD2 | 1.68 | 0.75 |
| 26:DD:117:MET:CE | 26:DD:124:GLY:HA3 | 2.17 | 0.75 |
| 27:DE:132:VAL:HG23 | 27:DE:133:ASN:H | 1.51 | 0.75 |
| 23:BA:773:U:C4' | 25:BC:47:GLY:HA3 | 2.17 | 0.75 |
| 24:BB:78:A:C2 | 24:BB:99:A:C4 | 2.73 | 0.75 |
| 52:D4:8:ASN:ND2 | 52:D4:11:LYS:H | 1.85 | 0.75 |
| 24:DB:8:U:H5'' | 37:DO:15:ARG:HH22 | 1.51 | 0.75 |
| 28:DF:41:GLN:HB3 | 28:DF:43:LEU:HD13 | 1.67 | 0.75 |
| 23:BA:330:A:O2' | 23:BA:331:A:H8 | 1.69 | 0.75 |
| 23:DA:547:A:H2' | 23:DA:548:A:H8 | 1.48 | 0.75 |
| 4:CD:9:CYS:CB | 4:CD:32:ALA:HB2 | 2.15 | 0.75 |
| 24:DB:66:A:H61 | 24:DB:107:U:H2' | 1.50 | 0.75 |
| 23:DA:1475:G:N2 | 23:DA:1519:G:C4 | 2.54 | 0.75 |
| 15:CO:56:LEU:O | 15:CO:60:VAL:HG23 | 1.87 | 0.75 |
| 23:BA:1679:U:C2' | 23:BA:1680:U:H5' | 2.17 | 0.75 |
| 23:BA:580:C:H2' | 23:BA:581:C:H6 | 1.52 | 0.75 |
| 1:AA:712:A:O2' | 1:AA:713:G:H5' | 1.87 | 0.75 |
| 13:CM:9:ILE:HG22 | 13:CM:11:ARG:HG3 | 1.69 | 0.75 |
| 47:BY:1:MET:HE1 | 47:BY:5:GLU:HG2 | 1.69 | 0.75 |
| 25:DC:242:ARG:HH11 | 25:DC:242:ARG:HG2 | 1.51 | 0.75 |
| 24:DB:15:A:H5' | 24:DB:16:G:C8 | 2.22 | 0.75 |
| 1:CA:1073:U:H2' | 1:CA:1074:G:H8 | 1.49 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:DX:46:LEU:HD21 | 46:DX:61:ARG:HE | 1.52 | 0.75 |
| 43:DU:81:LYS:HD3 | 43:DU:97:ARG:N | 2.01 | 0.75 |
| 23:BA:557:U:H2' | 23:BA:558:G:H8 | 1.49 | 0.75 |
| 26:BD:111:ARG:HA | 36:BN:2:ARG:HD3 | 1.69 | 0.75 |
| 23:BA:388:G:OP1 | 46:BX:33:LYS:HB3 | 1.86 | 0.75 |
| 46:BX:27:GLU:CD | 46:BX:33:LYS:HE3 | 2.07 | 0.75 |
| 25:DC:133:LEU:C | 25:DC:135:PHE:H | 1.89 | 0.75 |
| 28:BF:114:ILE:HB | 28:BF:117:PHE:HB2 | 1.68 | 0.75 |
| 22:CV:6177:U:H2' | 22:CV:6178:A:C8 | 2.20 | 0.75 |
| 23:BA:2593:U:H2' | 23:BA:2594:C:C6 | 2.22 | 0.75 |
| 22:AV:6177:U:H2' | 22:AV:6178:A:C8 | 2.20 | 0.75 |
| 23:DA:773:U:H4' | 25:DC:47:GLY:HA3 | 1.69 | 0.75 |
| 12:CL:32:ARG:O | 12:CL:84:ILE:HD12 | 1.85 | 0.75 |
| 37:BO:15:ARG:O | 37:BO:19:LYS:HG3 | 1.87 | 0.75 |
| 29:BG:101:ARG:HE | 29:BG:101:ARG:H | 0.82 | 0.75 |
| 23:DA:861:A:H2' | 23:DA:862:G:H5' | 1.68 | 0.75 |
| 23:DA:2210:G:H3' | 23:DA:2210:G:N3 | 2.02 | 0.75 |
| 25:DC:87:ASN:H | 25:DC:87:ASN:ND2 | 1.84 | 0.75 |
| 8:AH:12:ARG:NH1 | 8:AH:26:VAL:HA | 2.01 | 0.75 |
| 28:DF:109:VAL:HG11 | 28:DF:142:PRO:HG3 | 1.66 | 0.75 |
| 40:DR:20:LEU:HD23 | 40:DR:94:LEU:HB2 | 1.69 | 0.75 |
| 29:DG:95:ARG:HH22 | 29:DG:97:ARG:NH2 | 1.83 | 0.75 |
| 29:BG:92:ILE:HG22 | 29:BG:93:GLY:N | 2.02 | 0.75 |
| 23:DA:1132:A:O2' | 23:DA:1133:U:H5' | 1.86 | 0.75 |
| 1:CA:1226:C:N4 | 13:CM:104:ARG:HD2 | 2.01 | 0.75 |
| 34:BL:114:ILE:HD13 | 34:BL:130:PHE:CE1 | 2.21 | 0.75 |
| 23:BA:1021:A:N6 | 23:BA:1141:U:H3 | 1.83 | 0.75 |
| 25:BC:72:LYS:HD2 | 25:BC:75:ILE:HD12 | 1.68 | 0.75 |
| 2:CB:54:THR:HG21 | 2:CB:201:ILE:HD11 | 1.67 | 0.75 |
| 42:BT:31:HIS:ND1 | 42:BT:32:PRO:HD2 | 2.00 | 0.75 |
| 6:CF:98:LEU:HD13 | 6:CF:101:ALA:HB2 | 1.68 | 0.75 |
| 24:BB:21:G:H1 | 24:BB:62:C:H42 | 1.34 | 0.75 |
| 27:BE:183:VAL:O | 27:BE:187:VAL:HG23 | 1.86 | 0.75 |
| 24:BB:75:G:H21 | 44:BV:85:HIS:HE1 | 1.33 | 0.75 |
| 11:AK:21:ILE:HA | 11:AK:30:VAL:HG12 | 1.69 | 0.75 |
| 25:DC:131:LEU:HA | 25:DC:190:TYR:CE2 | 2.22 | 0.75 |
| 36:BN:97:VAL:HA | 36:BN:113:LEU:O | 1.87 | 0.75 |
| 23:DA:2015:A:H1' | 50:D2:2:ALA:CA | 2.14 | 0.75 |
| 25:BC:155:LEU:CD2 | 25:BC:177:LEU:HD21 | 2.14 | 0.75 |
| 43:DU:27:VAL:HG23 | 43:DU:27:VAL:O | 1.85 | 0.75 |
| 13:CM:91:ARG:HH11 | 19:CS:81:ARG:HH22 | 1.31 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:DR:40:LEU:HD23 | 40:DR:47:VAL:HG23 | 1.67 | 0.75 |
| 30:DH:83:ALA:CB | 30:DH:123:LEU:HD12 | 2.16 | 0.75 |
| 23:BA:2210:G:H3' | 23:BA:2210:G:N3 | 2.01 | 0.75 |
| 26:BD:5:LEU:HD23 | 26:BD:5:LEU:N | 2.00 | 0.75 |
| 23:DA:2688:U:O2 | 23:DA:2688:U:H3' | 1.86 | 0.75 |
| 24:BB:15:A:H5' | 24:BB:16:G:H8 | 1.52 | 0.75 |
| 5:AE:77:PRO:HD2 | 5:AE:142:LEU:HD22 | 1.69 | 0.75 |
| 36:BN:54:LEU:HD22 | 36:BN:66:VAL:HG23 | 1.69 | 0.75 |
| 23:BA:1401:G:H2' | 23:BA:1402:C:C6 | 2.21 | 0.75 |
| 23:BA:1418:G:H8 | 23:BA:1418:G:O5' | 1.70 | 0.75 |
| 23:BA:2637:U:H5'' | 26:BD:82:ARG:NH2 | 2.00 | 0.75 |
| 30:BH:2:LYS:HG3 | 30:BH:39:ALA:HB3 | 1.69 | 0.75 |
| 23:DA:1541:U:H5'' | 23:DA:1543:A:P | 2.27 | 0.75 |
| 25:BC:106:ILE:H | 25:BC:106:ILE:CD1 | 2.00 | 0.75 |
| 42:BT:28:PHE:CD1 | 42:BT:28:PHE:N | 2.55 | 0.75 |
| 26:DD:111:ARG:HA | 36:DN:2:ARG:HD3 | 1.68 | 0.75 |
| 1:AA:1152:A:H2' | 1:AA:1153:C:C6 | 2.21 | 0.75 |
| 46:BX:11:ARG:HG3 | 46:BX:11:ARG:HH11 | 1.52 | 0.75 |
| 5:CE:50:GLU:OE2 | 5:CE:51:VAL:HG23 | 1.87 | 0.75 |
| 23:BA:380:U:O2' | 46:BX:20:ARG:HB3 | 1.86 | 0.75 |
| 23:BA:1679:U:H2' | 23:BA:1680:U:H5' | 1.69 | 0.75 |
| 25:DC:132:PRO:HG3 | 25:DC:190:TYR:CE1 | 2.22 | 0.75 |
| 1:AA:913:A:H1' | 1:AA:914:A:OP2 | 1.87 | 0.75 |
| 43:BU:7:VAL:HG12 | 43:BU:8:LYS:CG | 2.12 | 0.74 |
| 23:DA:1543:A:H3' | 23:DA:1543:A:H8 | 1.51 | 0.74 |
| 23:BA:1543:A:H8 | 23:BA:1543:A:H3' | 1.51 | 0.74 |
| 23:DA:917:A:H5' | 23:DA:918:A:OP2 | 1.87 | 0.74 |
| 3:AC:18:TRP:CD1 | 14:AN:54:PRO:HA | 2.21 | 0.74 |
| 47:DY:6:VAL:O | 47:DY:10:LEU:HG | 1.86 | 0.74 |
| 28:BF:128:ARG:HE | 28:BF:129:GLY:N | 1.84 | 0.74 |
| 43:BU:27:VAL:O | 43:BU:27:VAL:HG23 | 1.86 | 0.74 |
| 1:CA:1152:A:H2' | 1:CA:1153:C:C6 | 2.22 | 0.74 |
| 23:BA:773:U:H4' | 25:BC:47:GLY:HA3 | 1.67 | 0.74 |
| 35:DM:66:ILE:HG22 | 35:DM:104:PHE:CD2 | 2.22 | 0.74 |
| 24:DB:18:G:H1 | 24:DB:65:C:H42 | 1.35 | 0.74 |
| 9:CI:19:LEU:HD21 | 9:CI:59:PHE:HB3 | 1.68 | 0.74 |
| 12:AL:110:LYS:O | 12:AL:111:ASP:HB2 | 1.86 | 0.74 |
| 43:DU:47:LYS:HA | 43:DU:60:PHE:CE2 | 2.21 | 0.74 |
| 43:DU:8:LYS:HD2 | 43:DU:13:VAL:HG21 | 1.69 | 0.74 |
| 1:CA:1226:C:H2' | 13:CM:103:THR:HB | 1.69 | 0.74 |
| 1:AA:691:G:O6 | 11:AK:52:GLY:HA2 | 1.87 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BA:547:A:H2' | 23:BA:548:A:H8 | 1.48 | 0.74 |
| 23:DA:1596:A:C2' | 23:DA:1597:A:H5' | 2.17 | 0.74 |
| 26:DD:5:LEU:N | 26:DD:5:LEU:HD23 | 2.02 | 0.74 |
| 23:BA:2747:G:O6 | 23:BA:2755:C:H5'' | 1.87 | 0.74 |
| 3:AC:43:LEU:O | 3:AC:47:LEU:HB3 | 1.88 | 0.74 |
| 23:DA:257:A:H2' | 23:DA:258:G:O5' | 1.87 | 0.74 |
| 1:CA:1259:C:H1' | 1:CA:1283:G:H21 | 1.53 | 0.74 |
| 33:BK:31:LYS:HB3 | 33:BK:32:TYR:CE1 | 2.23 | 0.74 |
| 1:CA:832:C:H42 | 1:CA:854:G:H1 | 1.35 | 0.74 |
| 21:CU:18:TYR:HD2 | 21:CU:22:ARG:HG2 | 1.52 | 0.74 |
| 38:DP:26:ASP:HB2 | 38:DP:90:GLN:O | 1.87 | 0.74 |
| 1:AA:337:C:H2' | 1:AA:338:A:H8 | 1.52 | 0.74 |
| 40:DR:40:LEU:H | 40:DR:47:VAL:HG22 | 1.51 | 0.74 |
| 37:DO:15:ARG:O | 37:DO:19:LYS:HG3 | 1.87 | 0.74 |
| 20:AT:72:LEU:HD23 | 20:AT:73:HIS:N | 2.02 | 0.74 |
| 23:DA:662:G:P | 34:DL:18:ARG:HD2 | 2.27 | 0.74 |
| 44:BV:58:VAL:HA | 44:BV:67:LEU:O | 1.87 | 0.74 |
| 32:DJ:38:LEU:HD12 | 32:DJ:39:ILE:N | 2.02 | 0.74 |
| 42:DT:28:PHE:CD1 | 42:DT:28:PHE:N | 2.55 | 0.74 |
| 23:DA:1209:G:H21 | 23:DA:1210:A:N6 | 1.85 | 0.74 |
| 23:DA:1331:A:HO2' | 23:DA:1332:G:H8 | 1.36 | 0.74 |
| 42:BT:30:VAL:HG12 | 42:BT:31:HIS:N | 2.02 | 0.74 |
| 23:DA:388:G:OP1 | 46:DX:33:LYS:HB3 | 1.86 | 0.74 |
| 1:AA:39:G:C2 | 1:AA:40:C:C6 | 2.75 | 0.74 |
| 7:AG:131:LYS:HE3 | 7:AG:136:LYS:NZ | 2.03 | 0.74 |
| 23:DA:333:G:C6 | 23:DA:334:C:N4 | 2.55 | 0.74 |
| 2:AB:127:ILE:N | 2:AB:127:ILE:HD13 | 2.02 | 0.74 |
| 23:DA:737:C:C2' | 23:DA:738:G:H5' | 2.18 | 0.74 |
| 1:CA:376:G:OP2 | 16:CP:67:THR:HG21 | 1.86 | 0.74 |
| 16:CP:22:THR:HG22 | 16:CP:32:TYR:HB3 | 1.68 | 0.74 |
| 33:BK:119:PRO:HB2 | 38:BP:68:TYR:HE1 | 1.53 | 0.74 |
| 23:DA:1188:U:O2' | 23:DA:1189:A:H5' | 1.87 | 0.74 |
| 25:DC:238:GLY:O | 25:DC:239:ARG:C | 2.26 | 0.74 |
| 46:DX:31:GLY:O | 46:DX:32:LYS:HB2 | 1.87 | 0.74 |
| 46:BX:11:ARG:HH12 | 46:BX:61:ARG:H | 1.35 | 0.74 |
| 23:BA:911:A:H2' | 35:BM:9:TYR:OH | 1.87 | 0.74 |
| 3:CC:43:LEU:O | 3:CC:47:LEU:HB3 | 1.87 | 0.74 |
| 35:BM:120:ILE:O | 35:BM:123:HIS:HB2 | 1.87 | 0.74 |
| 1:CA:175:C:H2' | 1:CA:176:C:H6 | 1.53 | 0.74 |
| 44:DV:179:ASP:OD1 | 44:DV:180:VAL:HG13 | 1.87 | 0.74 |
| 33:BK:98:VAL:HG11 | 33:BK:114:ILE:HG23 | 1.69 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:979:C:H3' | 1:AA:980:C:C5' | 2.16 | 0.74 |
| 40:DR:13:ARG:C | 40:DR:13:ARG:HD2 | 2.08 | 0.74 |
| 12:AL:32:ARG:O | 12:AL:84:ILE:HD12 | 1.87 | 0.74 |
| 2:CB:77:ALA:HB2 | 2:CB:211:ILE:HD13 | 1.69 | 0.74 |
| 47:DY:28:LYS:HE3 | 47:DY:56:GLN:HE22 | 1.50 | 0.74 |
| 4:CD:3:ARG:HD3 | 4:CD:5:ILE:HD11 | 1.69 | 0.74 |
| 32:BJ:105:LEU:CD1 | 32:BJ:106:LYS:H | 1.99 | 0.74 |
| 1:AA:1347:G:N2 | 1:AA:1373:G:H2' | 2.03 | 0.74 |
| 23:BA:528:A:H2 | 23:BA:2043:C:H5' | 1.51 | 0.74 |
| 25:BC:132:PRO:HG3 | 25:BC:190:TYR:CE1 | 2.23 | 0.74 |
| 23:BA:1401:G:H2' | 23:BA:1402:C:H6 | 1.51 | 0.74 |
| 23:DA:17:G:H4' | 39:DQ:25:TRP:CH2 | 2.22 | 0.74 |
| 1:AA:841:U:O2' | 1:AA:842:C:H5'' | 1.86 | 0.74 |
| 1:CA:495:A:H4' | 1:CA:496:A:OP1 | 1.87 | 0.74 |
| 50:D2:40:LYS:NZ | 50:D2:49:CYS:HB3 | 2.03 | 0.74 |
| 43:BU:63:LYS:HG3 | 43:BU:64:GLU:H | 1.53 | 0.74 |
| 4:AD:117:ALA:O | 4:AD:121:VAL:HG23 | 1.86 | 0.74 |
| 16:CP:17:TYR:H | 16:CP:17:TYR:HD1 | 1.33 | 0.74 |
| 40:BR:13:ARG:HD2 | 40:BR:13:ARG:C | 2.08 | 0.74 |
| 1:CA:262:A:H2' | 1:CA:263:A:C8 | 2.23 | 0.74 |
| 1:CA:1329:A:N7 | 21:CU:7:ARG:NH2 | 2.36 | 0.74 |
| 24:BB:66:A:H61 | 24:BB:107:U:H2' | 1.50 | 0.74 |
| 40:BR:64:HIS:CD2 | 40:BR:92:THR:HG22 | 2.22 | 0.74 |
| 1:AA:170:U:O2' | 1:AA:171:A:H5' | 1.88 | 0.74 |
| 29:BG:95:ARG:HH22 | 29:BG:97:ARG:HH21 | 1.34 | 0.74 |
| 40:DR:91:TYR:CG | 40:DR:91:TYR:O | 2.39 | 0.74 |
| 23:DA:1434:A:H61 | 23:DA:1558:A:N6 | 1.83 | 0.74 |
| 1:CA:1057:G:H4' | 3:CC:197:GLY:H | 1.52 | 0.74 |
| 22:CV:6192:G:H2' | 22:CV:6193:U:C6 | 2.23 | 0.74 |
| 23:DA:2846:G:H2' | 23:DA:2847:U:H6 | 1.53 | 0.74 |
| 23:DA:1566:A:OP1 | 25:DC:211:ARG:NH1 | 2.21 | 0.74 |
| 23:DA:1614:A:N6 | 41:DS:87:PRO:HA | 2.02 | 0.74 |
| 23:DA:1019:U:H3 | 23:DA:114(B):A:H62 | 1.35 | 0.74 |
| 23:DA:1639:U:C2' | 23:DA:1640:C:H5'' | 2.18 | 0.74 |
| 41:BS:9:TYR:H | 41:BS:102:HIS:CD2 | 2.04 | 0.74 |
| 23:BA:966:G:H2' | 23:BA:967:C:H6 | 1.52 | 0.74 |
| 1:CA:1513:A:H2' | 1:CA:1514:C:C6 | 2.23 | 0.74 |
| 25:DC:79:VAL:HG21 | 25:DC:111:LEU:HD11 | 1.70 | 0.74 |
| 23:DA:1799:G:H8 | 25:DC:181:GLU:OE1 | 1.69 | 0.74 |
| 23:DA:2681:C:H5 | 23:DA:2725:A:N6 | 1.76 | 0.74 |
| 23:DA:2219:G:H2' | 23:DA:2224:G:C5' | 2.18 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:828:A:H2' | 1:AA:829:G:O4' | 1.88 | 0.74 |
| 13:CM:23:TYR:CZ | 13:CM:71:ARG:HD3 | 2.22 | 0.74 |
| 23:BA:2815:C:O2' | 50:B2:43:HIS:HD2 | 1.69 | 0.74 |
| 30:DH:66:GLU:HG2 | 30:DH:67:ARG:NH2 | 2.02 | 0.74 |
| 18:CR:66:LEU:O | 18:CR:70:ILE:HG13 | 1.87 | 0.74 |
| 26:BD:170:LEU:HD23 | 26:BD:170:LEU:N | 2.03 | 0.74 |
| 27:DE:164:ARG:HG2 | 27:DE:164:ARG:NH1 | 1.98 | 0.74 |
| 34:DL:47:ASP:OD1 | 34:DL:49:ARG:HG2 | 1.88 | 0.74 |
| 32:DJ:154:GLN:NE2 | 32:DJ:155:ALA:HB3 | 2.03 | 0.74 |
| 3:CC:20:SER:HB2 | 3:CC:40:ARG:NH1 | 2.03 | 0.74 |
| 20:CT:72:LEU:HD23 | 20:CT:73:HIS:N | 2.03 | 0.74 |
| 23:DA:1826:G:OP1 | 25:DC:233:HIS:HD2 | 1.71 | 0.74 |
| 23:DA:1404:C:O2 | 23:DA:1404:C:H2' | 1.87 | 0.74 |
| 25:BC:231:HIS:CD2 | 25:BC:249:PRO:HA | 2.21 | 0.74 |
| 2:AB:54:THR:HG21 | 2:AB:201:ILE:HD11 | 1.67 | 0.74 |
| 1:CA:828:A:H2' | 1:CA:829:G:O4' | 1.88 | 0.74 |
| 24:DB:49:C:OP1 | 37:DO:97:ARG:HG3 | 1.87 | 0.74 |
| 23:BA:1952:A:C5 | 33:BK:22:ILE:HD11 | 2.22 | 0.74 |
| 20:CT:13:LEU:H | 20:CT:13:LEU:HD12 | 1.53 | 0.74 |
| 23:BA:2208:U:O2' | 23:BA:2209:C:H5' | 1.87 | 0.74 |
| 13:AM:9:ILE:HG22 | 13:AM:11:ARG:HG3 | 1.69 | 0.74 |
| 25:DC:176:ARG:HG2 | 25:DC:176:ARG:HH11 | 1.52 | 0.74 |
| 23:BA:1541:U:H5" | 23:BA:1543:A:P | 2.27 | 0.73 |
| 25:BC:76:PRO:HB3 | 25:BC:116:GLN:HE21 | 1.53 | 0.73 |
| 1:CA:735:C:H2' | 1:CA:736:C:H6 | 1.52 | 0.73 |
| 8:CH:91:ARG:HH11 | 8:CH:91:ARG:HG3 | 1.52 | 0.73 |
| 36:DN:54:LEU:HD22 | 36:DN:66:VAL:HG23 | 1.70 | 0.73 |
| 27:BE:101:LEU:O | 27:BE:106:ARG:NH1 | 2.20 | 0.73 |
| 53:B5:51:ALA:H | 53:B5:54:GLU:HB2 | 1.52 | 0.73 |
| 10:AJ:4:ILE:HD12 | 10:AJ:100:THR:HG22 | 1.70 | 0.73 |
| 28:DF:36:LYS:HB3 | 28:DF:160:VAL:HB | 1.70 | 0.73 |
| 10:CJ:51:ARG:HB2 | 10:CJ:60:ARG:HA | 1.70 | 0.73 |
| 6:CF:87:ARG:HG3 | 6:CF:87:ARG:HH11 | 1.51 | 0.73 |
| 4:AD:9:CYS:CB | 4:AD:32:ALA:HB2 | 2.17 | 0.73 |
| 1:CA:93:U:H2' | 1:CA:95:G:C8 | 2.23 | 0.73 |
| 1:CA:99:C:O2' | 1:CA:101:A:H5" | 1.87 | 0.73 |
| 18:AR:26:LEU:HD21 | 18:AR:42:ARG:HH11 | 1.52 | 0.73 |
| 43:BU:30:VAL:HG23 | 43:BU:37:VAL:HG12 | 1.71 | 0.73 |
| 24:DB:21:G:H1 | 24:DB:62:C:H42 | 1.36 | 0.73 |
| 4:CD:36:ARG:HG2 | 4:CD:38:TYR:OH | 1.89 | 0.73 |
| 17:AQ:31:LEU:HD23 | 17:AQ:32:TYR:CZ | 2.22 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:AI:19:LEU:HG | 9:AI:60:ASP:O | 1.87 | 0.73 |
| 23:BA:2015:A:H1' | 50:B2:2:ALA:CA | 2.13 | 0.73 |
| 22:AV:6192:G:H2' | 22:AV:6193:U:C6 | 2.23 | 0.73 |
| 6:AF:87:ARG:HH11 | 6:AF:87:ARG:HG3 | 1.53 | 0.73 |
| 23:DA:140:A:H8 | 23:DA:1408:C:HO2' | 1.36 | 0.73 |
| 12:AL:45:LYS:HG3 | 12:AL:91:ASP:O | 1.87 | 0.73 |
| 34:BL:7:ARG:O | 34:BL:10:PRO:HD3 | 1.87 | 0.73 |
| 23:DA:2784:C:H1' | 26:DD:37:ARG:HH12 | 1.53 | 0.73 |
| 38:BP:89:VAL:O | 38:BP:90:GLN:HB2 | 1.87 | 0.73 |
| 25:BC:201:HIS:O | 25:BC:204:ILE:HG13 | 1.89 | 0.73 |
| 23:BA:2101:G:H2' | 23:BA:2102:U:H5' | 1.70 | 0.73 |
| 10:CJ:74:ILE:H | 10:CJ:74:ILE:HD13 | 1.53 | 0.73 |
| 1:CA:1432:G:OP1 | 38:DP:107:ASP:HB2 | 1.87 | 0.73 |
| 1:CA:659:U:O2' | 1:CA:660:G:H5' | 1.87 | 0.73 |
| 34:DL:38:GLN:CG | 34:DL:39:LYS:H | 2.00 | 0.73 |
| 23:DA:2389:G:H5" | 23:DA:2390:U:C5' | 2.12 | 0.73 |
| 1:CA:136(A):C:C2' | 1:CA:136(B):C:H5" | 2.18 | 0.73 |
| 23:BA:322:A:H3' | 27:BE:169:ASN:ND2 | 2.03 | 0.73 |
| 20:AT:57:ARG:HH11 | 20:AT:102:GLY:HA2 | 1.53 | 0.73 |
| 1:AA:17:U:H1' | 1:AA:1080:A:N3 | 2.04 | 0.73 |
| 37:BO:51:ALA:HB1 | 37:BO:72:ALA:HB1 | 1.68 | 0.73 |
| 4:AD:166:LYS:HE2 | 25:DC:134:ARG:NH2 | 2.03 | 0.73 |
| 34:BL:16:ARG:O | 34:BL:16:ARG:NE | 2.19 | 0.73 |
| 35:DM:54:MET:HG2 | 35:DM:64:ILE:HD13 | 1.70 | 0.73 |
| 46:BX:37:ILE:HG23 | 46:BX:38:SER:N | 2.02 | 0.73 |
| 23:BA:971:C:H2' | 23:BA:972:G:H5' | 1.69 | 0.73 |
| 1:AA:136(A):C:C2' | 1:AA:136(B):C:H5" | 2.17 | 0.73 |
| 23:BA:2286:A:H4' | 23:BA:2287:A:O4' | 1.88 | 0.73 |
| 35:BM:141:GLN:H | 44:BV:53:ILE:HB | 1.53 | 0.73 |
| 5:AE:50:GLU:HG3 | 5:AE:52:PRO:HD2 | 1.69 | 0.73 |
| 23:BA:71:A:H2 | 42:BT:31:HIS:CE1 | 2.07 | 0.73 |
| 25:DC:223:GLY:HA3 | 25:DC:231:HIS:CE1 | 2.23 | 0.73 |
| 35:DM:58:PHE:CD1 | 35:DM:58:PHE:O | 2.41 | 0.73 |
| 23:DA:1495:A:N3 | 23:DA:1496:A:C2 | 2.56 | 0.73 |
| 1:CA:601:C:H2' | 1:CA:602:A:C8 | 2.22 | 0.73 |
| 26:DD:167:VAL:HG22 | 26:DD:170:LEU:HD21 | 1.71 | 0.73 |
| 1:CA:1347:G:N2 | 1:CA:1373:G:H2' | 2.04 | 0.73 |
| 1:AA:971:G:H1' | 1:AA:1365:G:O2' | 1.87 | 0.73 |
| 1:AA:973:G:H3' | 1:AA:974:A:H5" | 1.69 | 0.73 |
| 40:BR:40:LEU:H | 40:BR:47:VAL:HG22 | 1.53 | 0.73 |
| 23:BA:330:A:H2 | 23:BA:1210:A:H2' | 1.53 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DM:141:GLN:H | 44:DV:53:ILE:HB | 1.52 | 0.73 |
| 23:DA:1210:A:H5'' | 23:DA:1210:A:H8 | 1.51 | 0.73 |
| 44:BV:30:ASN:OD1 | 44:BV:33:LEU:HB3 | 1.88 | 0.73 |
| 1:AA:457:C:O2 | 1:AA:457:C:H2' | 1.87 | 0.73 |
| 1:CA:457:C:H2' | 1:CA:457:C:O2 | 1.89 | 0.73 |
| 23:BA:1270:C:H5'' | 23:BA:1271:G:O5' | 1.88 | 0.73 |
| 29:DG:92:ILE:HG22 | 29:DG:93:GLY:N | 2.01 | 0.73 |
| 23:BA:1388:G:H2' | 23:BA:1389:G:H8 | 1.54 | 0.73 |
| 35:DM:20:ALA:HB1 | 35:DM:99:PRO:O | 1.89 | 0.73 |
| 23:DA:2101:G:H2' | 23:DA:2102:U:H5' | 1.70 | 0.73 |
| 27:DE:183:VAL:O | 27:DE:187:VAL:HG23 | 1.87 | 0.73 |
| 47:BY:35:LEU:CD1 | 47:BY:53:LEU:HD12 | 2.19 | 0.73 |
| 23:BA:2210:G:H21 | 23:BA:2211:G:C5' | 2.01 | 0.73 |
| 2:AB:173:ALA:O | 2:AB:176:GLU:HB2 | 1.89 | 0.73 |
| 6:AF:26:ILE:HG22 | 6:AF:30:LEU:HD11 | 1.71 | 0.73 |
| 1:AA:659:U:O2' | 1:AA:660:G:H5' | 1.88 | 0.73 |
| 23:DA:1358:G:O2' | 23:DA:1359:A:H5'' | 1.89 | 0.73 |
| 44:DV:58:VAL:HA | 44:DV:67:LEU:O | 1.88 | 0.73 |
| 28:BF:36:LYS:HB3 | 28:BF:160:VAL:HB | 1.69 | 0.73 |
| 27:DE:101:LEU:HD12 | 27:DE:102:PRO:CD | 2.18 | 0.73 |
| 34:BL:16:ARG:NH2 | 34:BL:18:ARG:H | 1.87 | 0.73 |
| 23:BA:105:C:H2' | 23:BA:106:C:H6 | 1.53 | 0.73 |
| 8:CH:5:PRO:O | 8:CH:8:ASP:HB3 | 1.89 | 0.73 |
| 23:DA:1963:U:O2 | 23:DA:1963:U:H2' | 1.87 | 0.73 |
| 43:DU:42:VAL:HG12 | 43:DU:65:ALA:HB3 | 1.71 | 0.73 |
| 24:BB:8:U:H5'' | 37:BO:15:ARG:HH22 | 1.51 | 0.73 |
| 23:BA:1019:U:H3 | 23:BA:114(B):A:H62 | 1.36 | 0.73 |
| 23:BA:1022:G:H8 | 32:BJ:92:GLN:HE22 | 1.37 | 0.73 |
| 34:DL:49:ARG:CG | 34:DL:50:ARG:H | 2.02 | 0.73 |
| 23:DA:2210:G:H21 | 23:DA:2211:G:C5' | 2.02 | 0.73 |
| 2:CB:97:TRP:HZ2 | 2:CB:102:LEU:HD13 | 1.52 | 0.73 |
| 46:DX:11:ARG:HG3 | 46:DX:11:ARG:HH11 | 1.54 | 0.73 |
| 1:CA:820:U:H4' | 1:CA:821:G:OP2 | 1.88 | 0.73 |
| 11:CK:44:SER:OG | 11:CK:47:VAL:HG23 | 1.89 | 0.73 |
| 1:CA:555:C:H2' | 1:CA:556:C:H6 | 1.54 | 0.73 |
| 23:BA:65:C:H2' | 23:BA:66:C:H6 | 1.54 | 0.73 |
| 10:CJ:4:ILE:HD12 | 10:CJ:100:THR:HG22 | 1.70 | 0.73 |
| 23:BA:286:C:H2' | 23:BA:287:C:H6 | 1.54 | 0.73 |
| 1:AA:1259:C:H1' | 1:AA:1283:G:H21 | 1.52 | 0.73 |
| 39:BQ:5:LYS:HG2 | 39:BQ:6:THR:N | 2.03 | 0.73 |
| 25:DC:31:LYS:HG3 | 25:DC:33:LEU:HG | 1.71 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:DM:76:LYS:N | 35:DM:88:GLY:HA2 | 2.04 | 0.73 |
| 25:DC:233:HIS:HE1 | 25:DC:247:ALA:H | 1.37 | 0.73 |
| 5:CE:31:LEU:HD21 | 5:CE:43:LEU:HD12 | 1.70 | 0.73 |
| 26:DD:111:ARG:HA | 36:DN:2:ARG:HH11 | 1.53 | 0.73 |
| 5:CE:50:GLU:HG3 | 5:CE:52:PRO:HD2 | 1.71 | 0.73 |
| 1:AA:1014:A:H5' | 19:AS:14:HIS:CD2 | 2.24 | 0.73 |
| 30:BH:5:LEU:HD23 | 30:BH:5:LEU:N | 2.03 | 0.73 |
| 23:DA:2658:C:H4' | 29:DG:158:HIS:CE1 | 2.24 | 0.73 |
| 1:CA:1064:G:H1' | 1:CA:1065:U:OP2 | 1.89 | 0.73 |
| 4:CD:134:ASP:O | 4:CD:136:PRO:HD3 | 1.89 | 0.73 |
| 4:AD:134:ASP:O | 4:AD:136:PRO:HD3 | 1.87 | 0.73 |
| 21:AU:18:TYR:HD2 | 21:AU:22:ARG:HG2 | 1.53 | 0.73 |
| 8:CH:51:VAL:HG21 | 8:CH:60:ARG:HG3 | 1.71 | 0.73 |
| 17:CQ:53:LEU:HD11 | 17:CQ:85:VAL:HG21 | 1.69 | 0.73 |
| 35:BM:20:ALA:HB1 | 35:BM:99:PRO:O | 1.89 | 0.73 |
| 25:BC:176:ARG:HH11 | 25:BC:176:ARG:HG2 | 1.54 | 0.73 |
| 23:BA:941:A:H4' | 34:BL:35:HIS:CE1 | 2.24 | 0.72 |
| 23:BA:2392:A:H2 | 23:BA:2424:C:H42 | 1.35 | 0.72 |
| 34:DL:33:ARG:HE | 34:DL:36:LYS:CD | 2.00 | 0.72 |
| 24:DB:70:C:H2' | 24:DB:71:C:H6 | 1.54 | 0.72 |
| 3:CC:91:LEU:HD22 | 3:CC:99:VAL:HG12 | 1.71 | 0.72 |
| 46:DX:11:ARG:HB2 | 46:DX:13:ILE:HG22 | 1.71 | 0.72 |
| 46:DX:27:GLU:CB | 46:DX:33:LYS:HG3 | 2.19 | 0.72 |
| 41:DS:9:TYR:H | 41:DS:102:HIS:CD2 | 2.07 | 0.72 |
| 8:CH:20:TYR:HA | 8:CH:65:TYR:HE2 | 1.52 | 0.72 |
| 1:CA:1281:U:H5' | 1:CA:1282:C:H5 | 1.54 | 0.72 |
| 1:AA:556:C:C2' | 1:AA:557:G:H5' | 2.19 | 0.72 |
| 8:AH:51:VAL:HG21 | 8:AH:60:ARG:HG3 | 1.70 | 0.72 |
| 12:CL:45:LYS:HG3 | 12:CL:91:ASP:O | 1.89 | 0.72 |
| 23:BA:1156:A:C8 | 39:BQ:51:LYS:HD2 | 2.24 | 0.72 |
| 1:AA:216:G:H2' | 1:AA:217:C:C6 | 2.24 | 0.72 |
| 23:DA:540:G:H2' | 23:DA:541:C:H6 | 1.54 | 0.72 |
| 7:CG:131:LYS:HE3 | 7:CG:136:LYS:NZ | 2.02 | 0.72 |
| 1:CA:841:U:O2' | 1:CA:842:C:H5'' | 1.88 | 0.72 |
| 25:DC:30:GLU:HG3 | 25:DC:63:ARG:CZ | 2.18 | 0.72 |
| 1:AA:1234:C:H1' | 1:AA:1364:U:O2 | 1.88 | 0.72 |
| 34:BL:33:ARG:HB3 | 34:BL:36:LYS:HD3 | 1.69 | 0.72 |
| 1:AA:1097:C:H2' | 1:AA:1098:C:C6 | 2.21 | 0.72 |
| 2:CB:27:LYS:HG3 | 2:CB:194:PRO:HD2 | 1.71 | 0.72 |
| 40:DR:64:HIS:CD2 | 40:DR:92:THR:HG22 | 2.23 | 0.72 |
| 23:BA:954:G:C5 | 23:BA:955:C:C5 | 2.77 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:DX:40:ARG:HG2 | 46:DX:41:ARG:N | 2.04 | 0.72 |
| 45:BW:42:GLY:HA2 | 45:BW:57:PHE:CD2 | 2.24 | 0.72 |
| 44:BV:179:ASP:OD1 | 44:BV:180:VAL:HG13 | 1.89 | 0.72 |
| 1:AA:706:A:O4' | 11:AK:29:ILE:HD11 | 1.87 | 0.72 |
| 32:BJ:63:PRO:O | 39:BQ:64:ARG:HD2 | 1.89 | 0.72 |
| 34:DL:114:ILE:HD11 | 34:DL:127:ALA:CB | 2.18 | 0.72 |
| 47:DY:1:MET:SD | 47:DY:5:GLU:HG2 | 2.29 | 0.72 |
| 23:BA:2846:G:H2' | 23:BA:2847:U:H6 | 1.54 | 0.72 |
| 24:DB:82:G:O2' | 24:DB:83:G:H5' | 1.89 | 0.72 |
| 23:BA:2353:G:H5'' | 45:BW:32:ARG:NH2 | 2.05 | 0.72 |
| 46:DX:46:LEU:CD2 | 46:DX:61:ARG:HE | 2.03 | 0.72 |
| 23:DA:966:G:C4 | 23:DA:967:C:C5 | 2.76 | 0.72 |
| 6:AF:78:GLU:O | 6:AF:81:ILE:HG13 | 1.89 | 0.72 |
| 2:CB:72:GLY:O | 2:CB:94:ASN:HA | 1.88 | 0.72 |
| 23:BA:1871:A:H2' | 23:BA:1872:A:C8 | 2.23 | 0.72 |
| 1:CA:1468:A:H2' | 1:CA:1469:G:O4' | 1.89 | 0.72 |
| 23:DA:277:C:H3' | 23:DA:278:A:H5'' | 1.71 | 0.72 |
| 44:DV:13:GLU:HB3 | 44:DV:18:LEU:HD11 | 1.71 | 0.72 |
| 12:CL:110:LYS:O | 12:CL:111:ASP:HB2 | 1.89 | 0.72 |
| 2:CB:70:PHE:O | 2:CB:92:TYR:HA | 1.89 | 0.72 |
| 40:DR:38:LEU:O | 40:DR:52:VAL:HG12 | 1.89 | 0.72 |
| 1:AA:376:G:OP2 | 16:AP:67:THR:HG21 | 1.90 | 0.72 |
| 23:BA:2210:G:H21 | 23:BA:2211:G:H5' | 1.52 | 0.72 |
| 23:BA:1639:U:C2' | 23:BA:1640:C:H5'' | 2.19 | 0.72 |
| 47:DY:31:GLU:O | 47:DY:35:LEU:HB2 | 1.89 | 0.72 |
| 2:CB:173:ALA:O | 2:CB:176:GLU:HB2 | 1.89 | 0.72 |
| 26:DD:120:TRP:CE3 | 26:DD:155:LYS:HD3 | 2.23 | 0.72 |
| 23:BA:2658:C:H4' | 29:BG:158:HIS:CE1 | 2.24 | 0.72 |
| 27:DE:50:SER:HA | 27:DE:92:PRO:O | 1.90 | 0.72 |
| 25:DC:228:PRO:HD3 | 25:DC:234:GLY:O | 1.89 | 0.72 |
| 23:DA:2415:G:H1' | 34:DL:67:MET:HE1 | 1.71 | 0.72 |
| 43:DU:13:VAL:HG11 | 43:DU:72:VAL:HB | 1.72 | 0.72 |
| 53:B5:30:ARG:O | 53:B5:31:HIS:CB | 2.30 | 0.72 |
| 40:DR:13:ARG:HD2 | 40:DR:14:VAL:N | 2.03 | 0.72 |
| 40:BR:2:PHE:HE2 | 40:BR:13:ARG:HD3 | 1.50 | 0.72 |
| 35:BM:76:LYS:H | 35:BM:88:GLY:HA2 | 1.54 | 0.72 |
| 1:CA:38:G:C2 | 1:CA:397:A:C2 | 2.77 | 0.72 |
| 26:DD:5:LEU:HB2 | 26:DD:51:PHE:CD2 | 2.23 | 0.72 |
| 23:BA:1045:A:H5'' | 23:BA:1047:G:O4' | 1.89 | 0.72 |
| 23:BA:1331:A:HO2' | 23:BA:1332:G:H8 | 1.34 | 0.72 |
| 27:DE:117:ARG:HD2 | 27:DE:190:GLU:O | 1.89 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:BB:18:G:H1 | 24:BB:65:C:H42 | 1.37 | 0.72 |
| 25:DC:76:PRO:HB3 | 25:DC:116:GLN:HE21 | 1.54 | 0.72 |
| 29:BG:88:LEU:HB3 | 29:BG:90:LYS:HD3 | 1.69 | 0.72 |
| 38:DP:1:MET:C | 38:DP:3:ARG:H | 1.91 | 0.72 |
| 39:DQ:5:LYS:HG2 | 39:DQ:6:THR:N | 2.03 | 0.72 |
| 1:AA:950:U:O4 | 13:AM:105:THR:HG21 | 1.89 | 0.72 |
| 32:BJ:38:LEU:HD12 | 32:BJ:39:ILE:N | 2.04 | 0.72 |
| 32:DJ:38:LEU:HD23 | 32:DJ:157:ARG:CG | 2.19 | 0.72 |
| 3:AC:18:TRP:HB3 | 3:AC:20:SER:O | 1.89 | 0.72 |
| 25:DC:106:ILE:CD1 | 25:DC:106:ILE:H | 2.03 | 0.72 |
| 1:CA:39:G:C2 | 1:CA:40:C:C6 | 2.77 | 0.72 |
| 4:CD:100:ARG:NH1 | 4:CD:137:SER:HA | 2.04 | 0.72 |
| 4:CD:108:LEU:HB3 | 4:CD:110:PHE:HE2 | 1.54 | 0.72 |
| 25:BC:131:LEU:HA | 25:BC:190:TYR:CE2 | 2.23 | 0.72 |
| 23:BA:534:U:O2' | 39:BQ:49:HIS:CD2 | 2.43 | 0.72 |
| 23:DA:2009:G:C2' | 23:DA:2010:G:H5' | 2.19 | 0.72 |
| 23:BA:300:A:OP1 | 43:BU:84:ARG:NH2 | 2.21 | 0.72 |
| 39:DQ:114:LYS:O | 39:DQ:117:GLN:HB2 | 1.90 | 0.72 |
| 1:CA:1053:G:H3' | 1:CA:1054:C:H5' | 1.72 | 0.72 |
| 46:DX:10:LYS:O | 46:DX:11:ARG:HG2 | 1.88 | 0.72 |
| 29:DG:144:VAL:O | 29:DG:148:ILE:HG12 | 1.89 | 0.72 |
| 42:BT:57:LEU:CD1 | 42:BT:78:LYS:HB2 | 2.20 | 0.72 |
| 1:CA:556:C:C2' | 1:CA:557:G:H5' | 2.20 | 0.72 |
| 23:BA:2687:U:C4 | 23:BA:2688:U:C5 | 2.78 | 0.72 |
| 23:DA:774:A:H2 | 23:DA:787:U:HO2' | 1.37 | 0.72 |
| 23:DA:534:U:O2' | 39:DQ:49:HIS:CD2 | 2.42 | 0.72 |
| 8:CH:86:ILE:HB | 8:CH:133:LEU:HD22 | 1.71 | 0.72 |
| 27:BE:89:VAL:HG12 | 27:BE:90:PHE:N | 2.04 | 0.72 |
| 23:DA:301:G:C4 | 23:DA:302:C:C5 | 2.77 | 0.72 |
| 21:AU:6:ARG:HG3 | 21:AU:15:ARG:NH1 | 2.05 | 0.72 |
| 1:CA:1234:C:H1' | 1:CA:1364:U:O2 | 1.89 | 0.72 |
| 25:BC:31:LYS:HG3 | 25:BC:33:LEU:HG | 1.72 | 0.72 |
| 12:AL:52:ARG:HH11 | 12:AL:52:ARG:HG3 | 1.51 | 0.72 |
| 1:CA:556:C:H2' | 1:CA:557:G:H5' | 1.72 | 0.72 |
| 23:DA:2285:C:H2' | 23:DA:2286:A:H5'' | 1.71 | 0.72 |
| 1:CA:216:G:H2' | 1:CA:217:C:C6 | 2.25 | 0.72 |
| 23:BA:1966:A:H4' | 23:BA:1967:C:OP1 | 1.89 | 0.72 |
| 23:BA:1348:G:H2' | 23:BA:1349:A:H5'' | 1.71 | 0.72 |
| 1:AA:1220:G:H2' | 1:AA:1221:G:H8 | 1.53 | 0.72 |
| 23:DA:1019:U:H2' | 23:DA:1020:A:H8 | 1.55 | 0.72 |
| 40:BR:38:LEU:O | 40:BR:52:VAL:HG12 | 1.89 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:93:U:H2' | 1:AA:95:G:C8 | 2.24 | 0.72 |
| 23:DA:2787:C:C1' | 26:DD:62:PRO:HB3 | 2.18 | 0.72 |
| 52:D4:12:ARG:NH1 | 52:D4:12:ARG:HG3 | 2.04 | 0.72 |
| 1:CA:1129:C:H4' | 1:CA:1130:A:O5' | 1.89 | 0.72 |
| 9:AI:19:LEU:HD21 | 9:AI:59:PHE:HB3 | 1.69 | 0.72 |
| 23:BA:2850:A:OP2 | 23:BA:2866:U:H5 | 1.72 | 0.72 |
| 23:DA:1396:U:H2' | 23:DA:1396:U:O2 | 1.88 | 0.72 |
| 50:B2:33:CYS:HG | 50:B2:49:CYS:HG | 1.31 | 0.72 |
| 33:DK:2:ILE:HG12 | 33:DK:8:LEU:HD11 | 1.72 | 0.72 |
| 32:BJ:160:LYS:HE3 | 32:BJ:161:LEU:H | 1.54 | 0.72 |
| 2:AB:70:PHE:O | 2:AB:92:TYR:HA | 1.90 | 0.72 |
| 38:BP:51:ARG:HH11 | 38:BP:51:ARG:CG | 1.99 | 0.72 |
| 27:BE:67:GLN:CG | 27:BE:67:GLN:O | 2.35 | 0.72 |
| 2:CB:162:ILE:O | 2:CB:185:ILE:HG12 | 1.90 | 0.72 |
| 42:BT:84:ALA:HB3 | 42:BT:87:GLN:NE2 | 2.04 | 0.72 |
| 39:BQ:79:PHE:C | 39:BQ:79:PHE:CD1 | 2.62 | 0.72 |
| 34:BL:45:LEU:HD23 | 34:BL:46:LYS:N | 2.05 | 0.72 |
| 23:BA:330:A:C2 | 23:BA:1210:A:H2' | 2.25 | 0.72 |
| 1:AA:91:C:O2' | 1:AA:92:G:H5' | 1.90 | 0.72 |
| 1:CA:266:G:H5' | 1:CA:267:C:H5 | 1.53 | 0.72 |
| 43:DU:81:LYS:NZ | 43:DU:98:VAL:HG12 | 2.05 | 0.72 |
| 34:BL:16:ARG:HH21 | 34:BL:17:LYS:HA | 1.54 | 0.72 |
| 1:CA:1191:A:H5'' | 3:CC:4:LYS:HZ2 | 1.51 | 0.72 |
| 23:BA:256:A:O2' | 23:BA:257:A:H5' | 1.90 | 0.72 |
| 23:DA:1388:G:H2' | 23:DA:1389:G:H8 | 1.55 | 0.72 |
| 16:AP:74:LEU:O | 16:AP:79:VAL:HG23 | 1.89 | 0.72 |
| 23:BA:1007:C:O2' | 32:BJ:131:PRO:HA | 1.90 | 0.72 |
| 1:CA:913:A:H1' | 1:CA:914:A:OP2 | 1.89 | 0.72 |
| 25:BC:30:GLU:HG3 | 25:BC:63:ARG:CZ | 2.19 | 0.72 |
| 34:BL:61:ARG:C | 34:BL:62:LEU:HD13 | 2.11 | 0.71 |
| 23:BA:917:A:H5' | 23:BA:918:A:OP2 | 1.91 | 0.71 |
| 2:CB:178:ARG:HH22 | 2:CB:196:LEU:HA | 1.53 | 0.71 |
| 1:CA:1329:A:H5'' | 13:CM:26:GLY:N | 2.04 | 0.71 |
| 23:BA:528:A:C8 | 23:BA:528:A:H3' | 2.25 | 0.71 |
| 40:DR:27:ALA:CB | 40:DR:61:VAL:HG11 | 2.20 | 0.71 |
| 23:BA:1495:A:N3 | 23:BA:1496:A:C2 | 2.58 | 0.71 |
| 23:BA:1332:G:N2 | 23:BA:1610:A:C8 | 2.57 | 0.71 |
| 3:CC:58:GLU:O | 3:CC:59:ARG:HG3 | 1.90 | 0.71 |
| 4:CD:204:ILE:HG21 | 5:CE:98:THR:O | 1.89 | 0.71 |
| 1:CA:1443:G:N2 | 38:DP:119:LYS:HA | 2.05 | 0.71 |
| 35:DM:120:ILE:O | 35:DM:123:HIS:HB2 | 1.90 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1136:U:H5'' | 1:AA:1137:C:OP2 | 1.90 | 0.71 |
| 40:BR:20:LEU:HD23 | 40:BR:94:LEU:HB2 | 1.72 | 0.71 |
| 34:BL:132:LYS:H | 34:BL:132:LYS:HD3 | 1.55 | 0.71 |
| 53:D5:30:ARG:O | 53:D5:31:HIS:CB | 2.37 | 0.71 |
| 43:BU:8:LYS:HD2 | 43:BU:13:VAL:HG21 | 1.71 | 0.71 |
| 26:DD:11:MET:HB2 | 26:DD:23:VAL:O | 1.89 | 0.71 |
| 23:DA:2781:A:H5'' | 23:DA:2782:G:C5' | 2.09 | 0.71 |
| 37:DO:87:PHE:CE1 | 37:DO:102:ALA:HB2 | 2.25 | 0.71 |
| 25:BC:87:ASN:ND2 | 25:BC:87:ASN:N | 2.29 | 0.71 |
| 47:BY:28:LYS:HE3 | 47:BY:56:GLN:HE22 | 1.55 | 0.71 |
| 30:DH:79:ILE:HG22 | 30:DH:81:VAL:HG23 | 1.72 | 0.71 |
| 24:BB:70:C:H2' | 24:BB:71:C:H6 | 1.55 | 0.71 |
| 1:CA:1097:C:H2' | 1:CA:1098:C:C6 | 2.24 | 0.71 |
| 28:BF:5:LEU:CD2 | 28:BF:6:ALA:H | 2.04 | 0.71 |
| 1:CA:1053:G:C3' | 1:CA:1054:C:H5' | 2.20 | 0.71 |
| 23:DA:2443:C:O2' | 23:DA:2444:G:H5' | 1.89 | 0.71 |
| 29:BG:85:LYS:HD3 | 29:BG:86:GLU:OE2 | 1.90 | 0.71 |
| 17:AQ:15:MET:HB3 | 17:AQ:18:THR:HB | 1.72 | 0.71 |
| 27:BE:205:ARG:O | 27:BE:206:ILE:HG23 | 1.90 | 0.71 |
| 20:AT:13:LEU:HD12 | 20:AT:13:LEU:H | 1.54 | 0.71 |
| 23:DA:1541:U:O3' | 23:DA:1543:A:OP1 | 2.07 | 0.71 |
| 40:BR:5:VAL:CG1 | 40:BR:14:VAL:HG21 | 2.20 | 0.71 |
| 1:AA:430:A:OP1 | 4:AD:9:CYS:HB2 | 1.90 | 0.71 |
| 1:CA:91:C:O2' | 1:CA:92:G:H5' | 1.90 | 0.71 |
| 24:DB:15:A:H5' | 24:DB:16:G:H8 | 1.54 | 0.71 |
| 25:BC:231:HIS:CD2 | 25:BC:232:PRO:HD2 | 2.25 | 0.71 |
| 1:AA:1191:A:H5'' | 3:AC:4:LYS:HZ2 | 1.52 | 0.71 |
| 46:BX:11:ARG:HB2 | 46:BX:13:ILE:HG22 | 1.71 | 0.71 |
| 23:BA:1329:U:H5'' | 23:BA:1330:C:H5 | 1.54 | 0.71 |
| 23:BA:1799:G:H8 | 25:BC:181:GLU:OE1 | 1.73 | 0.71 |
| 23:DA:773:U:C4' | 25:DC:47:GLY:HA3 | 2.20 | 0.71 |
| 9:CI:19:LEU:HG | 9:CI:60:ASP:O | 1.90 | 0.71 |
| 23:DA:2639:A:H2' | 23:DA:2640:G:H5' | 1.72 | 0.71 |
| 23:BA:2092:U:C5 | 23:BA:2226:C:OP2 | 2.42 | 0.71 |
| 43:BU:76:CYS:HB3 | 43:BU:77:PRO:HD2 | 1.70 | 0.71 |
| 44:DV:23:LYS:HB3 | 44:DV:38:TYR:HD1 | 1.54 | 0.71 |
| 26:BD:11:MET:HE3 | 26:BD:186:GLY:HA2 | 1.72 | 0.71 |
| 22:CV:6182:A:N1 | 22:CV:6195:G:C2 | 2.59 | 0.71 |
| 28:DF:84:LYS:HG3 | 28:DF:85:GLY:N | 2.04 | 0.71 |
| 40:BR:13:ARG:HD2 | 40:BR:14:VAL:N | 2.06 | 0.71 |
| 1:CA:393:A:C2 | 1:CA:394:G:C8 | 2.78 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:690:G:H2' | 1:AA:691:G:C8 | 2.24 | 0.71 |
| 1:CA:1530:G:OP1 | 1:CA:1530:G:H4' | 1.90 | 0.71 |
| 1:AA:1289:A:OP1 | 21:AU:10:ARG:HD3 | 1.90 | 0.71 |
| 23:BA:813:U:H2' | 23:BA:814:C:C6 | 2.24 | 0.71 |
| 33:DK:19:ILE:H | 33:DK:19:ILE:HD13 | 1.54 | 0.71 |
| 34:BL:114:ILE:N | 34:BL:114:ILE:HD12 | 1.99 | 0.71 |
| 23:BA:2294:C:H2' | 23:BA:2295:C:C6 | 2.24 | 0.71 |
| 32:BJ:38:LEU:HD23 | 32:BJ:157:ARG:CG | 2.20 | 0.71 |
| 34:BL:50:ARG:HD2 | 34:BL:51:PHE:N | 2.04 | 0.71 |
| 4:AD:28:SER:HB3 | 4:AD:29:PRO:HD2 | 1.72 | 0.71 |
| 20:AT:26:ASN:HD22 | 20:AT:26:ASN:N | 1.88 | 0.71 |
| 26:BD:36:ARG:HD3 | 26:BD:85:ASN:ND2 | 2.06 | 0.71 |
| 34:DL:16:ARG:NH2 | 34:DL:18:ARG:H | 1.89 | 0.71 |
| 1:CA:735:C:O2' | 1:CA:736:C:H5' | 1.89 | 0.71 |
| 23:BA:2353:G:O6 | 23:BA:2353:G:N1 | 2.23 | 0.71 |
| 1:CA:691:G:C6 | 11:CK:52:GLY:HA2 | 2.25 | 0.71 |
| 9:AI:113:LYS:HG2 | 9:AI:119:ALA:HA | 1.73 | 0.71 |
| 23:DA:2305:A:H5'' | 28:DF:134:GLY:HA3 | 1.73 | 0.71 |
| 25:BC:133:LEU:C | 25:BC:135:PHE:H | 1.93 | 0.71 |
| 44:BV:39:VAL:HG21 | 44:BV:44:PHE:HB2 | 1.72 | 0.71 |
| 12:CL:86:GLY:HA2 | 12:CL:97:TYR:HA | 1.71 | 0.71 |
| 35:BM:66:ILE:HG22 | 35:BM:104:PHE:CD2 | 2.25 | 0.71 |
| 21:CU:6:ARG:HG3 | 21:CU:15:ARG:NH1 | 2.04 | 0.71 |
| 2:CB:63:MET:HG2 | 2:CB:225:ALA:HB1 | 1.70 | 0.71 |
| 34:DL:101:VAL:HB | 34:DL:106:LEU:HB3 | 1.71 | 0.71 |
| 23:DA:1543:A:H3' | 23:DA:1543:A:C8 | 2.26 | 0.71 |
| 2:AB:162:ILE:O | 2:AB:185:ILE:HG12 | 1.91 | 0.71 |
| 28:DF:5:LEU:CD2 | 28:DF:6:ALA:H | 2.03 | 0.71 |
| 28:BF:25:TYR:CD1 | 28:BF:30:GLU:HB3 | 2.25 | 0.71 |
| 27:DE:9:ILE:HD11 | 27:DE:125:LEU:CG | 2.21 | 0.71 |
| 45:BW:72:ARG:CZ | 45:BW:75:LEU:HD13 | 2.21 | 0.71 |
| 25:DC:121:PRO:HB3 | 25:DC:135:PHE:CE2 | 2.25 | 0.71 |
| 1:AA:1117:G:O3' | 9:AI:104:ARG:HG3 | 1.89 | 0.71 |
| 1:CA:712:A:O2' | 1:CA:713:G:H5' | 1.91 | 0.71 |
| 1:AA:556:C:H2' | 1:AA:557:G:H5' | 1.71 | 0.71 |
| 23:DA:256:A:O2' | 23:DA:257:A:H5' | 1.90 | 0.71 |
| 23:DA:2469:A:H2 | 23:DA:2481:G:H21 | 1.39 | 0.71 |
| 44:DV:39:VAL:HG21 | 44:DV:44:PHE:HB2 | 1.71 | 0.71 |
| 23:DA:1817:G:OP1 | 25:DC:88:ARG:NH2 | 2.21 | 0.71 |
| 1:CA:650:G:O2' | 1:CA:651:C:H5' | 1.90 | 0.71 |
| 1:AA:1053:G:C3' | 1:AA:1054:C:H5' | 2.20 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:BF:174:GLU:HG2 | 28:BF:180:PHE:CE1 | 2.26 | 0.71 |
| 23:BA:2346:A:H5'' | 23:BA:2383:G:H1' | 1.73 | 0.71 |
| 23:BA:404:C:H4' | 23:BA:405:U:H5' | 1.72 | 0.71 |
| 23:BA:1778:U:H2' | 23:BA:1784:A:N6 | 2.05 | 0.71 |
| 23:DA:1966:A:H4' | 23:DA:1967:C:OP1 | 1.91 | 0.71 |
| 2:CB:167:PRO:HG2 | 2:CB:192:SER:OG | 1.91 | 0.71 |
| 23:BA:2768:C:C4 | 23:BA:2769:C:C5 | 2.79 | 0.71 |
| 1:AA:1281:U:H5' | 1:AA:1282:C:H5 | 1.54 | 0.71 |
| 38:DP:53:ARG:NH1 | 38:DP:53:ARG:HG2 | 2.01 | 0.71 |
| 1:AA:1530:G:H4' | 1:AA:1530:G:OP1 | 1.91 | 0.71 |
| 1:AA:820:U:H4' | 1:AA:821:G:OP2 | 1.89 | 0.71 |
| 1:CA:819:A:H4' | 1:CA:820:U:OP2 | 1.90 | 0.71 |
| 1:AA:1129:C:H4' | 1:AA:1130:A:O5' | 1.91 | 0.71 |
| 23:BA:105:C:H2' | 23:BA:106:C:C6 | 2.25 | 0.71 |
| 3:CC:23:TYR:CD2 | 3:CC:24:ALA:N | 2.59 | 0.71 |
| 44:BV:13:GLU:HB3 | 44:BV:18:LEU:HD11 | 1.72 | 0.71 |
| 46:DX:37:ILE:HG23 | 46:DX:38:SER:N | 2.06 | 0.71 |
| 33:BK:101:PRO:O | 33:BK:102:VAL:HG13 | 1.90 | 0.71 |
| 23:BA:960:A:H5'' | 23:BA:961:C:OP2 | 1.90 | 0.71 |
| 23:BA:2415:G:H1' | 34:BL:67:MET:HE1 | 1.73 | 0.71 |
| 26:BD:101:ARG:HH21 | 26:BD:171:GLU:HB3 | 1.54 | 0.71 |
| 34:BL:33:ARG:HG2 | 34:BL:34:GLY:H | 1.56 | 0.71 |
| 34:DL:49:ARG:HG3 | 34:DL:50:ARG:H | 1.54 | 0.71 |
| 1:AA:376:G:O2' | 1:AA:377:G:H5' | 1.90 | 0.71 |
| 1:AA:386:C:C2' | 1:AA:387:U:H5'' | 2.20 | 0.71 |
| 23:DA:1329:U:H5'' | 23:DA:1330:C:H5 | 1.56 | 0.71 |
| 8:AH:91:ARG:HG3 | 8:AH:91:ARG:HH11 | 1.55 | 0.71 |
| 1:AA:266:G:H5' | 1:AA:267:C:H5 | 1.54 | 0.71 |
| 43:DU:81:LYS:HZ3 | 43:DU:98:VAL:N | 1.88 | 0.71 |
| 23:BA:2784:C:H1' | 26:BD:37:ARG:HH12 | 1.55 | 0.71 |
| 23:DA:580:C:H2' | 23:DA:581:C:H6 | 1.55 | 0.71 |
| 12:AL:86:GLY:HA2 | 12:AL:97:TYR:HA | 1.72 | 0.71 |
| 28:DF:50:ALA:O | 28:DF:53:LEU:HB3 | 1.91 | 0.71 |
| 23:DA:357:A:H2' | 23:DA:358:U:H6 | 1.54 | 0.71 |
| 17:AQ:40:LYS:HD2 | 17:AQ:42:TYR:CE1 | 2.26 | 0.71 |
| 1:CA:1136:U:H5'' | 1:CA:1137:C:OP2 | 1.90 | 0.71 |
| 34:DL:146:VAL:HG13 | 34:DL:147:LEU:HD12 | 1.73 | 0.71 |
| 23:BA:1528:A:C2 | 23:BA:1529:A:C2 | 2.79 | 0.71 |
| 22:CV:6188:G:N2 | 22:CV:6216:U:C2 | 2.58 | 0.71 |
| 28:DF:25:TYR:CD1 | 28:DF:30:GLU:HB3 | 2.25 | 0.71 |
| 5:CE:77:PRO:HD2 | 5:CE:142:LEU:HD22 | 1.72 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:BN:7:GLY:O | 36:BN:8:ARG:HB3 | 1.91 | 0.71 |
| 43:BU:81:LYS:HD3 | 43:BU:97:ARG:HB3 | 1.72 | 0.71 |
| 1:AA:735:C:O2' | 1:AA:736:C:H5' | 1.91 | 0.71 |
| 16:AP:8:ARG:O | 16:AP:9:PHE:CD2 | 2.44 | 0.71 |
| 25:BC:25:THR:HG21 | 25:BC:81:ALA:HA | 1.72 | 0.71 |
| 1:AA:914:A:H2' | 1:AA:915:A:H5' | 1.73 | 0.71 |
| 26:DD:108:SER:O | 26:DD:162:ALA:HA | 1.90 | 0.71 |
| 23:DA:1270:C:H5'' | 23:DA:1271:G:O5' | 1.91 | 0.71 |
| 52:B4:9:ARG:NE | 52:B4:48:LYS:HB2 | 2.04 | 0.71 |
| 25:BC:70:TRP:C | 25:BC:70:TRP:CD1 | 2.64 | 0.71 |
| 3:AC:20:SER:HB2 | 3:AC:40:ARG:NH1 | 2.04 | 0.71 |
| 39:BQ:92:ARG:CG | 40:BR:11:GLN:NE2 | 2.53 | 0.71 |
| 47:DY:6:VAL:HG12 | 47:DY:10:LEU:CD1 | 2.20 | 0.71 |
| 2:AB:27:LYS:HG3 | 2:AB:194:PRO:HD2 | 1.72 | 0.71 |
| 30:DH:62:LYS:HB2 | 30:DH:133:HIS:CE1 | 2.25 | 0.71 |
| 29:DG:95:ARG:HH22 | 29:DG:97:ARG:HH21 | 1.36 | 0.71 |
| 17:AQ:19:VAL:HG23 | 17:AQ:44:ALA:HB3 | 1.72 | 0.71 |
| 23:DA:1679:U:C2' | 23:DA:1680:U:H5' | 2.20 | 0.71 |
| 1:CA:538:G:O3' | 12:CL:113:LYS:HG3 | 1.90 | 0.71 |
| 23:DA:404:C:H4' | 23:DA:405:U:H5' | 1.73 | 0.71 |
| 43:DU:8:LYS:HZ3 | 43:DU:8:LYS:C | 1.93 | 0.70 |
| 2:CB:162:ILE:HD11 | 2:CB:184:VAL:HG13 | 1.73 | 0.70 |
| 40:DR:5:VAL:CG1 | 40:DR:14:VAL:HG21 | 2.20 | 0.70 |
| 39:BQ:79:PHE:C | 39:BQ:79:PHE:HD1 | 1.93 | 0.70 |
| 23:DA:2768:C:C4 | 23:DA:2769:C:C5 | 2.79 | 0.70 |
| 36:DN:57:ARG:HG2 | 36:DN:58:GLY:H | 1.56 | 0.70 |
| 23:BA:784:A:H5' | 23:BA:785:G:OP1 | 1.90 | 0.70 |
| 3:AC:58:GLU:O | 3:AC:59:ARG:HG3 | 1.91 | 0.70 |
| 25:DC:125:ILE:CG2 | 25:DC:125:ILE:O | 2.39 | 0.70 |
| 35:DM:23:GLY:HA3 | 35:DM:98:LYS:HB2 | 1.73 | 0.70 |
| 1:CA:337:C:H2' | 1:CA:338:A:H8 | 1.54 | 0.70 |
| 26:DD:46:ALA:HB2 | 26:DD:82:ARG:HA | 1.73 | 0.70 |
| 16:CP:74:LEU:O | 16:CP:79:VAL:HG23 | 1.91 | 0.70 |
| 23:DA:1290:C:H2' | 23:DA:1291:C:H6 | 1.56 | 0.70 |
| 43:BU:8:LYS:N | 43:BU:8:LYS:HZ2 | 1.88 | 0.70 |
| 23:DA:1546:A:N7 | 23:DA:154(B):C:O2 | 2.24 | 0.70 |
| 1:CA:1347:G:H8 | 9:CI:107:ARG:HB3 | 1.55 | 0.70 |
| 23:DA:861:A:C2' | 23:DA:862:G:H5' | 2.20 | 0.70 |
| 30:DH:68:LEU:O | 30:DH:138:ILE:HD13 | 1.91 | 0.70 |
| 1:CA:323:U:O3' | 20:CT:22:ARG:HG2 | 1.91 | 0.70 |
| 1:AA:16:A:O2' | 1:AA:17:U:H5' | 1.91 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:AB:167:PRO:HG2 | 2:AB:192:SER:OG | 1.91 | 0.70 |
| 26:BD:120:TRP:CE3 | 26:BD:155:LYS:HD3 | 2.26 | 0.70 |
| 25:BC:121:PRO:HB3 | 25:BC:135:PHE:CE2 | 2.25 | 0.70 |
| 23:DA:588:U:H2' | 23:DA:589:C:C6 | 2.26 | 0.70 |
| 23:DA:733:G:N7 | 23:DA:761:A:N6 | 2.39 | 0.70 |
| 23:DA:784:A:H5' | 23:DA:785:G:OP1 | 1.90 | 0.70 |
| 23:BA:863:A:OP1 | 35:BM:21:THR:HB | 1.90 | 0.70 |
| 1:AA:1053:G:H3' | 1:AA:1054:C:H5' | 1.72 | 0.70 |
| 23:DA:249:C:O2 | 53:D5:12:LYS:HE3 | 1.91 | 0.70 |
| 17:CQ:19:VAL:HG23 | 17:CQ:44:ALA:HB3 | 1.73 | 0.70 |
| 41:DS:22:ASP:HA | 41:DS:25:ARG:HH12 | 1.56 | 0.70 |
| 23:BA:1794:U:H2' | 23:BA:1795:C:H6 | 1.56 | 0.70 |
| 23:BA:333:G:C6 | 23:BA:334:C:N4 | 2.59 | 0.70 |
| 23:BA:861:A:H2' | 23:BA:862:G:H5' | 1.73 | 0.70 |
| 22:AV:6182:A:N1 | 22:AV:6195:G:C2 | 2.59 | 0.70 |
| 47:BY:6:VAL:HG12 | 47:BY:10:LEU:CD1 | 2.22 | 0.70 |
| 16:AP:22:THR:HG22 | 16:AP:32:TYR:HB3 | 1.73 | 0.70 |
| 4:AD:3:ARG:N | 4:AD:3:ARG:HD2 | 2.06 | 0.70 |
| 6:AF:79:LEU:HB2 | 6:AF:88:VAL:HG21 | 1.72 | 0.70 |
| 8:CH:12:ARG:NH1 | 8:CH:26:VAL:HA | 2.06 | 0.70 |
| 8:AH:86:ILE:HB | 8:AH:133:LEU:HD22 | 1.73 | 0.70 |
| 23:DA:910:A:H62 | 35:DM:12:GLN:HA | 1.56 | 0.70 |
| 30:DH:5:LEU:N | 30:DH:5:LEU:HD23 | 2.05 | 0.70 |
| 23:BA:1386:C:H2' | 23:BA:1387:C:H6 | 1.54 | 0.70 |
| 23:BA:2631:G:N3 | 23:BA:2810:A:H2 | 1.88 | 0.70 |
| 23:DA:2402:C:H5' | 23:DA:2403:C:OP2 | 1.90 | 0.70 |
| 1:CA:979:C:H3' | 1:CA:980:C:C5' | 2.15 | 0.70 |
| 32:BJ:154:GLN:NE2 | 32:BJ:155:ALA:HB3 | 2.03 | 0.70 |
| 37:DO:38:GLN:HB3 | 37:DO:47:THR:HG21 | 1.73 | 0.70 |
| 1:AA:1066:C:H2' | 1:AA:1066:C:O2 | 1.89 | 0.70 |
| 1:AA:255:G:H2' | 1:AA:256:U:H6 | 1.57 | 0.70 |
| 12:CL:44:PRO:HG3 | 12:CL:52:ARG:HE | 1.55 | 0.70 |
| 36:BN:2:ARG:C | 36:BN:4:LEU:N | 2.43 | 0.70 |
| 6:CF:79:LEU:HB2 | 6:CF:88:VAL:HG21 | 1.72 | 0.70 |
| 38:BP:53:ARG:HG2 | 38:BP:53:ARG:NH1 | 2.03 | 0.70 |
| 23:BA:1358:G:O2' | 23:BA:1359:A:H5'' | 1.90 | 0.70 |
| 43:DU:2:ARG:O | 43:DU:4:LYS:N | 2.23 | 0.70 |
| 1:CA:105:G:H2' | 1:CA:106:C:H6 | 1.55 | 0.70 |
| 25:DC:132:PRO:HD3 | 25:DC:190:TYR:CZ | 2.27 | 0.70 |
| 26:BD:108:SER:O | 26:BD:162:ALA:HA | 1.91 | 0.70 |
| 23:DA:18:C:O3' | 39:DQ:23:GLY:HA2 | 1.90 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:AF:3:ARG:HG3 | 6:AF:66:GLU:HG2 | 1.72 | 0.70 |
| 23:DA:1728:G:O5' | 23:DA:1728:G:H8 | 1.74 | 0.70 |
| 23:BA:1309:G:H3' | 52:B4:9:ARG:NH1 | 2.05 | 0.70 |
| 34:BL:97:PRO:HD3 | 34:BL:126:VAL:HG12 | 1.72 | 0.70 |
| 27:BE:63:LYS:NZ | 27:BE:67:GLN:HE21 | 1.88 | 0.70 |
| 12:AL:26:LEU:HB3 | 12:AL:29:ALA:HB3 | 1.74 | 0.70 |
| 1:AA:1064:G:H1' | 1:AA:1065:U:OP2 | 1.90 | 0.70 |
| 12:CL:44:PRO:HG3 | 12:CL:52:ARG:NE | 2.07 | 0.70 |
| 23:DA:2747:G:O6 | 23:DA:2755:C:H5'' | 1.91 | 0.70 |
| 8:CH:97:VAL:O | 8:CH:100:ILE:HG13 | 1.91 | 0.70 |
| 33:BK:99:PHE:N | 33:BK:99:PHE:CD1 | 2.52 | 0.70 |
| 27:DE:205:ARG:O | 27:DE:206:ILE:HG23 | 1.92 | 0.70 |
| 32:BJ:69:VAL:HG13 | 32:BJ:71:MET:HG3 | 1.73 | 0.70 |
| 34:BL:85:LEU:HA | 34:BL:88:LEU:HB2 | 1.73 | 0.70 |
| 29:DG:55:PRO:HG2 | 29:DG:61:HIS:CE1 | 2.27 | 0.70 |
| 23:BA:828:U:O2 | 23:BA:828:U:H3' | 1.91 | 0.70 |
| 28:BF:50:ALA:O | 28:BF:53:LEU:HB3 | 1.92 | 0.70 |
| 23:BA:2639:A:H2' | 23:BA:2640:G:H5' | 1.74 | 0.70 |
| 23:BA:1541:U:O3' | 23:BA:1543:A:OP1 | 2.10 | 0.70 |
| 1:CA:1346:A:N1 | 1:CA:1374:A:H5'' | 2.07 | 0.70 |
| 23:DA:125:G:H4' | 23:DA:126:A:OP2 | 1.90 | 0.70 |
| 23:BA:140:A:H8 | 23:BA:1408:C:O2' | 1.70 | 0.70 |
| 26:BD:77:ILE:HD13 | 26:BD:195:LEU:HD12 | 1.74 | 0.70 |
| 3:CC:206:GLU:HG2 | 3:CC:207:VAL:HG23 | 1.73 | 0.70 |
| 11:AK:57:THR:HG22 | 11:AK:59:TYR:N | 2.07 | 0.70 |
| 23:BA:126:A:O5' | 52:B4:19:ARG:HG2 | 1.92 | 0.70 |
| 40:DR:98:GLU:HG2 | 40:DR:100:ARG:HD3 | 1.74 | 0.70 |
| 50:B2:40:LYS:NZ | 50:B2:49:CYS:HB3 | 2.06 | 0.70 |
| 1:CA:1423:G:H5'' | 33:DK:49:ARG:HH22 | 1.56 | 0.70 |
| 23:DA:2661:G:O2' | 23:DA:2662:A:H5' | 1.91 | 0.70 |
| 9:CI:97:LYS:HD3 | 9:CI:102:LEU:HD12 | 1.72 | 0.70 |
| 1:CA:922:G:C6 | 1:CA:923:A:C6 | 2.80 | 0.70 |
| 1:CA:579:G:H2' | 1:CA:580:U:H6 | 1.57 | 0.70 |
| 23:BA:774:A:H2 | 23:BA:787:U:HO2' | 1.37 | 0.70 |
| 23:DA:1170:G:H1 | 23:DA:1179:C:N4 | 1.90 | 0.70 |
| 40:DR:2:PHE:HE2 | 40:DR:13:ARG:HD3 | 1.56 | 0.70 |
| 34:DL:45:LEU:HD23 | 34:DL:46:LYS:N | 2.07 | 0.70 |
| 1:CA:386:C:C2' | 1:CA:387:U:H5'' | 2.21 | 0.70 |
| 16:CP:20:VAL:HG23 | 16:CP:34:GLU:O | 1.92 | 0.70 |
| 1:AA:38:G:C2 | 1:AA:397:A:C2 | 2.80 | 0.70 |
| 23:BA:547:A:C6 | 23:BA:548:A:C6 | 2.80 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BA:1596:A:C2' | 23:BA:1597:A:H5' | 2.20 | 0.70 |
| 34:DL:18:ARG:HB3 | 34:DL:18:ARG:NH1 | 2.07 | 0.70 |
| 1:AA:393:A:C2 | 1:AA:394:G:C8 | 2.80 | 0.70 |
| 5:CE:43:LEU:HD22 | 5:CE:136:MET:CG | 2.21 | 0.70 |
| 11:CK:57:THR:HG22 | 11:CK:59:TYR:N | 2.06 | 0.70 |
| 48:BZ:28:LEU:N | 48:BZ:28:LEU:HD12 | 2.06 | 0.70 |
| 45:BW:49:LYS:HB2 | 45:BW:80:HIS:HB3 | 1.74 | 0.70 |
| 29:DG:19:VAL:HG12 | 29:DG:20:ALA:N | 2.05 | 0.70 |
| 46:BX:31:GLY:O | 46:BX:32:LYS:HB2 | 1.91 | 0.70 |
| 8:AH:58:TYR:C | 8:AH:59:LEU:HD23 | 2.12 | 0.70 |
| 38:DP:89:VAL:O | 38:DP:90:GLN:HB2 | 1.90 | 0.70 |
| 23:BA:1396:U:H2' | 23:BA:1396:U:O2 | 1.90 | 0.70 |
| 1:AA:1157:A:H4' | 1:AA:1158:C:O5' | 1.92 | 0.70 |
| 29:DG:27:LYS:HG2 | 29:DG:32:GLU:HG3 | 1.74 | 0.70 |
| 17:CQ:31:LEU:HD23 | 17:CQ:32:TYR:CZ | 2.27 | 0.70 |
| 16:CP:8:ARG:O | 16:CP:9:PHE:CD2 | 2.45 | 0.70 |
| 1:AA:579:G:H2' | 1:AA:580:U:H6 | 1.55 | 0.70 |
| 9:AI:97:LYS:HD3 | 9:AI:102:LEU:HD12 | 1.72 | 0.70 |
| 1:AA:940:C:C2 | 1:AA:941:G:C8 | 2.79 | 0.70 |
| 8:AH:5:PRO:O | 8:AH:8:ASP:HB3 | 1.91 | 0.70 |
| 23:BA:1543:A:C8 | 23:BA:1543:A:H3' | 2.26 | 0.70 |
| 4:AD:51:PRO:HB3 | 4:AD:55:ALA:HB3 | 1.73 | 0.70 |
| 23:BA:1411:C:H2' | 23:BA:1412:A:H8 | 1.57 | 0.70 |
| 44:DV:30:ASN:O | 44:DV:32:HIS:N | 2.25 | 0.70 |
| 1:CA:1292:U:H2' | 1:CA:1293:G:H8 | 1.56 | 0.70 |
| 53:B5:52:LYS:H | 53:B5:53:PRO:HD2 | 1.57 | 0.70 |
| 23:DA:1411:C:H2' | 23:DA:1412:A:H8 | 1.55 | 0.70 |
| 30:DH:2:LYS:HG3 | 30:DH:39:ALA:HB3 | 1.72 | 0.70 |
| 45:DW:49:LYS:HB2 | 45:DW:80:HIS:HB3 | 1.74 | 0.70 |
| 44:BV:37:VAL:HG23 | 44:BV:38:TYR:N | 2.06 | 0.70 |
| 23:DA:2353:G:H5" | 45:DW:32:ARG:NH2 | 2.07 | 0.70 |
| 1:CA:505:G:C6 | 1:CA:535:A:C2 | 2.80 | 0.70 |
| 30:BH:62:LYS:HB2 | 30:BH:133:HIS:CE1 | 2.27 | 0.70 |
| 29:DG:77:LYS:HA | 29:DG:80:SER:HB2 | 1.72 | 0.70 |
| 34:BL:14:LYS:O | 34:BL:15:ARG:HB2 | 1.90 | 0.70 |
| 29:BG:30:LYS:HB2 | 29:BG:79:VAL:HA | 1.74 | 0.70 |
| 2:AB:126:GLU:C | 2:AB:127:ILE:HD13 | 2.12 | 0.70 |
| 11:AK:23:ALA:HA | 11:AK:28:THR:OG1 | 1.92 | 0.70 |
| 41:BS:59:VAL:HG12 | 41:BS:60:ASN:OD1 | 1.92 | 0.70 |
| 23:BA:116:C:H2' | 23:BA:117:G:C8 | 2.27 | 0.70 |
| 23:BA:1728:G:H8 | 23:BA:1728:G:O5' | 1.75 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:AP:43:LYS:HG2 | 16:AP:48:TRP:CD2 | 2.27 | 0.70 |
| 53:D5:22:VAL:HB | 53:D5:54:GLU:HG3 | 1.74 | 0.70 |
| 23:BA:729:G:OP2 | 25:BC:13:ARG:NH1 | 2.25 | 0.70 |
| 25:DC:70:TRP:CD1 | 25:DC:70:TRP:C | 2.64 | 0.70 |
| 4:CD:67:ILE:HG22 | 4:CD:68:TYR:CD1 | 2.26 | 0.70 |
| 28:DF:41:GLN:HG2 | 28:DF:155:MET:HB3 | 1.74 | 0.70 |
| 1:CA:668:G:H1' | 15:CO:46:HIS:HD2 | 1.56 | 0.70 |
| 5:AE:57:LYS:O | 5:AE:61:TYR:CD2 | 2.45 | 0.70 |
| 6:CF:90:VAL:HG12 | 6:CF:91:VAL:N | 2.06 | 0.70 |
| 3:AC:206:GLU:HG2 | 3:AC:207:VAL:HG23 | 1.73 | 0.70 |
| 12:CL:44:PRO:HG3 | 12:CL:52:ARG:CD | 2.22 | 0.70 |
| 1:AA:1295:G:N2 | 1:AA:1302:U:H3 | 1.90 | 0.70 |
| 23:DA:1046:A:N3 | 31:DI:4:LYS:HD3 | 2.07 | 0.70 |
| 1:AA:66:G:H4' | 1:AA:173:U:C5 | 2.26 | 0.70 |
| 23:DA:2346:A:H5'' | 23:DA:2383:G:H1' | 1.72 | 0.70 |
| 39:DQ:98:LEU:O | 39:DQ:100:VAL:N | 2.25 | 0.70 |
| 1:AA:914:A:C2' | 1:AA:915:A:H5' | 2.22 | 0.70 |
| 1:CA:862:C:C2' | 1:CA:863:U:H5' | 2.22 | 0.70 |
| 44:BV:23:LYS:HB3 | 44:BV:38:TYR:HD1 | 1.55 | 0.70 |
| 1:AA:1022:G:H2' | 1:AA:1023:G:H8 | 1.57 | 0.70 |
| 8:AH:97:VAL:HG13 | 8:AH:98:LYS:H | 1.57 | 0.70 |
| 23:BA:301:G:C4 | 23:BA:302:C:C5 | 2.80 | 0.70 |
| 23:BA:1170:G:H1 | 23:BA:1179:C:N4 | 1.89 | 0.69 |
| 3:AC:91:LEU:HD22 | 3:AC:99:VAL:HG12 | 1.74 | 0.69 |
| 23:BA:1639:U:H2' | 23:BA:1640:C:H5'' | 1.74 | 0.69 |
| 1:AA:15:G:H4' | 5:AE:24:ARG:HH12 | 1.56 | 0.69 |
| 4:CD:3:ARG:N | 4:CD:3:ARG:HD2 | 2.07 | 0.69 |
| 1:AA:1346:A:N1 | 1:AA:1374:A:H5'' | 2.06 | 0.69 |
| 20:CT:57:ARG:HH11 | 20:CT:102:GLY:HA2 | 1.55 | 0.69 |
| 40:BR:25:LEU:H | 40:BR:92:THR:HG21 | 1.57 | 0.69 |
| 1:CA:729:A:H2' | 1:CA:730:G:H8 | 1.56 | 0.69 |
| 23:BA:1857:G:N2 | 23:BA:1886:C:N4 | 2.40 | 0.69 |
| 23:DA:1309:G:H3' | 52:D4:9:ARG:NH1 | 2.07 | 0.69 |
| 9:CI:113:LYS:HG2 | 9:CI:119:ALA:HA | 1.73 | 0.69 |
| 23:BA:2731:G:C6 | 23:BA:2732:G:O6 | 2.45 | 0.69 |
| 4:CD:119:GLN:HG3 | 4:CD:123:HIS:HD2 | 1.55 | 0.69 |
| 36:BN:2:ARG:O | 36:BN:4:LEU:N | 2.25 | 0.69 |
| 43:BU:81:LYS:NZ | 43:BU:98:VAL:HG12 | 2.07 | 0.69 |
| 45:DW:53:MET:HB2 | 45:DW:59:LEU:HD23 | 1.73 | 0.69 |
| 9:AI:22:GLY:HA3 | 9:AI:60:ASP:OD2 | 1.92 | 0.69 |
| 27:BE:203:GLN:HA | 27:BE:206:ILE:O | 1.92 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 44:DV:22:GLY:O | 44:DV:41:LEU:HB2 | 1.91 | 0.69 |
| 23:BA:826:U:H4' | 34:BL:55:ARG:HB2 | 1.72 | 0.69 |
| 23:DA:987:G:H2' | 23:DA:988:A:H5' | 1.74 | 0.69 |
| 33:BK:25:LEU:HB2 | 33:BK:38:VAL:O | 1.91 | 0.69 |
| 32:DJ:160:LYS:HE3 | 32:DJ:161:LEU:H | 1.55 | 0.69 |
| 23:BA:990:A:H5'' | 23:BA:991:C:P | 2.32 | 0.69 |
| 23:DA:1871:A:H2' | 23:DA:1872:A:C8 | 2.27 | 0.69 |
| 26:DD:101:ARG:HH21 | 26:DD:171:GLU:HB3 | 1.57 | 0.69 |
| 34:BL:49:ARG:CG | 34:BL:50:ARG:H | 2.04 | 0.69 |
| 45:BW:72:ARG:HB3 | 45:BW:75:LEU:HD12 | 1.73 | 0.69 |
| 13:CM:10:PRO:HG3 | 13:CM:22:ILE:HD11 | 1.74 | 0.69 |
| 1:AA:1292:U:H2' | 1:AA:1293:G:H8 | 1.57 | 0.69 |
| 46:DX:86:SER:O | 46:DX:90:ILE:HG12 | 1.93 | 0.69 |
| 1:CA:625:G:H4' | 16:CP:16:HIS:CD2 | 2.26 | 0.69 |
| 27:DE:199:TRP:O | 27:DE:203:GLN:HG2 | 1.92 | 0.69 |
| 29:BG:77:LYS:HA | 29:BG:80:SER:HB2 | 1.75 | 0.69 |
| 26:DD:37:ARG:O | 26:DD:45:THR:HA | 1.92 | 0.69 |
| 35:BM:23:GLY:HA3 | 35:BM:98:LYS:HB2 | 1.74 | 0.69 |
| 25:DC:77:ALA:HB2 | 25:DC:97:TYR:HA | 1.74 | 0.69 |
| 23:DA:1679:U:H2' | 23:DA:1680:U:H5' | 1.72 | 0.69 |
| 1:CA:1426:C:H2' | 1:CA:1427:U:H6 | 1.58 | 0.69 |
| 23:BA:314:A:O2' | 23:BA:315:G:H5' | 1.92 | 0.69 |
| 6:CF:3:ARG:HG3 | 6:CF:66:GLU:HG2 | 1.74 | 0.69 |
| 40:BR:91:TYR:O | 40:BR:91:TYR:CD2 | 2.44 | 0.69 |
| 1:CA:940:C:C2 | 1:CA:941:G:C8 | 2.79 | 0.69 |
| 51:D3:42:TRP:HA | 51:D3:42:TRP:CE3 | 2.27 | 0.69 |
| 23:BA:1607:C:H4' | 23:BA:1608:A:O5' | 1.92 | 0.69 |
| 32:DJ:57:LEU:O | 32:DJ:72:GLY:HA3 | 1.92 | 0.69 |
| 1:AA:963:G:H2' | 1:AA:964:A:H8 | 1.58 | 0.69 |
| 32:BJ:142:ARG:HG3 | 32:BJ:142:ARG:NH1 | 2.07 | 0.69 |
| 16:CP:17:TYR:N | 16:CP:17:TYR:CD1 | 2.59 | 0.69 |
| 25:BC:35:LYS:HE2 | 25:BC:103:ARG:HA | 1.74 | 0.69 |
| 1:CA:690:G:H2' | 1:CA:691:G:C8 | 2.26 | 0.69 |
| 23:DA:863:A:OP1 | 35:DM:21:THR:HB | 1.93 | 0.69 |
| 8:AH:51:VAL:HG21 | 8:AH:60:ARG:CG | 2.22 | 0.69 |
| 1:AA:650:G:O2' | 1:AA:651:C:H5' | 1.91 | 0.69 |
| 36:BN:52:ILE:HG21 | 36:BN:94:TYR:CG | 2.27 | 0.69 |
| 34:BL:101:VAL:HB | 34:BL:106:LEU:HB3 | 1.74 | 0.69 |
| 27:DE:67:GLN:O | 27:DE:67:GLN:CG | 2.32 | 0.69 |
| 23:BA:603:A:N6 | 23:BA:655:A:H4' | 2.07 | 0.69 |
| 23:BA:1826:G:OP1 | 25:BC:233:HIS:HD2 | 1.74 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 47:BY:31:GLU:O | 47:BY:35:LEU:HB2 | 1.92 | 0.69 |
| 44:DV:94:GLU:H | 44:DV:94:GLU:CD | 1.94 | 0.69 |
| 47:DY:9:GLN:C | 47:DY:12:GLU:HB3 | 2.12 | 0.69 |
| 27:DE:89:VAL:HG12 | 27:DE:90:PHE:H | 1.57 | 0.69 |
| 53:B5:22:VAL:HG12 | 53:B5:50:LEU:HD12 | 1.73 | 0.69 |
| 23:DA:737:C:H2' | 23:DA:738:G:H5' | 1.73 | 0.69 |
| 26:DD:4:ILE:HG12 | 26:DD:28:ALA:HB1 | 1.73 | 0.69 |
| 23:DA:2092:U:C5 | 23:DA:2226:C:OP2 | 2.45 | 0.69 |
| 28:DF:7:LEU:HD23 | 28:DF:10:LYS:HD2 | 1.75 | 0.69 |
| 29:BG:98:LEU:HD12 | 29:BG:99:VAL:N | 2.06 | 0.69 |
| 23:DA:1746:G:C2 | 23:DA:1747:G:C8 | 2.80 | 0.69 |
| 50:B2:41:PRO:HG2 | 50:B2:44:THR:HG21 | 1.73 | 0.69 |
| 23:BA:861:A:C2' | 23:BA:862:G:H5' | 2.22 | 0.69 |
| 34:BL:112:LEU:HD23 | 34:BL:113:LYS:N | 2.07 | 0.69 |
| 37:BO:87:PHE:CE1 | 37:BO:102:ALA:HB2 | 2.28 | 0.69 |
| 26:DD:2:LYS:HE2 | 26:DD:95:ILE:O | 1.93 | 0.69 |
| 36:DN:7:GLY:O | 36:DN:8:ARG:HB3 | 1.93 | 0.69 |
| 44:BV:53:ILE:HG22 | 44:BV:71:VAL:O | 1.92 | 0.69 |
| 29:BG:19:VAL:HG12 | 29:BG:20:ALA:N | 2.07 | 0.69 |
| 1:CA:833:U:H2' | 1:CA:834:C:C6 | 2.28 | 0.69 |
| 40:BR:91:TYR:O | 40:BR:91:TYR:CG | 2.45 | 0.69 |
| 27:BE:46:ARG:HG2 | 27:BE:46:ARG:HH11 | 1.57 | 0.69 |
| 1:CA:255:G:H2' | 1:CA:256:U:H6 | 1.57 | 0.69 |
| 23:DA:1248:G:OP1 | 39:DQ:2:PRO:HD2 | 1.92 | 0.69 |
| 1:CA:909:A:H2' | 1:CA:910:C:O4' | 1.92 | 0.69 |
| 23:DA:924:C:H2' | 23:DA:925:C:H6 | 1.57 | 0.69 |
| 1:AA:1446:A:H61 | 38:BP:118:ARG:NH2 | 1.89 | 0.69 |
| 23:DA:1348:G:H2' | 23:DA:1349:A:H5'' | 1.75 | 0.69 |
| 3:CC:76:VAL:HG21 | 3:CC:103:VAL:HG11 | 1.75 | 0.69 |
| 34:DL:59:LEU:CA | 34:DL:61:ARG:HE | 2.01 | 0.69 |
| 34:DL:62:LEU:HD23 | 34:DL:62:LEU:O | 1.92 | 0.69 |
| 26:BD:11:MET:HB2 | 26:BD:23:VAL:O | 1.93 | 0.69 |
| 23:DA:603:A:N6 | 23:DA:655:A:H4' | 2.07 | 0.69 |
| 25:BC:96:HIS:HD2 | 25:BC:102:LYS:HD3 | 1.57 | 0.69 |
| 25:BC:77:ALA:CB | 25:BC:97:TYR:HA | 2.22 | 0.69 |
| 23:BA:2787:C:C1' | 26:BD:62:PRO:HB3 | 2.22 | 0.69 |
| 43:DU:78:ALA:HB3 | 43:DU:81:LYS:HE3 | 1.74 | 0.69 |
| 1:CA:1220:G:H2' | 1:CA:1221:G:H8 | 1.54 | 0.69 |
| 1:AA:819:A:H4' | 1:AA:820:U:OP2 | 1.92 | 0.69 |
| 23:DA:105:C:H2' | 23:DA:106:C:H6 | 1.58 | 0.69 |
| 23:DA:2815:C:O2' | 50:D2:43:HIS:HD2 | 1.75 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 26:BD:46:ALA:HB2 | 26:BD:82:ARG:HA | 1.72 | 0.69 |
| 23:BA:2285:C:H2' | 23:BA:2286:A:H5'' | 1.73 | 0.69 |
| 25:DC:72:LYS:HD2 | 25:DC:75:ILE:HD12 | 1.74 | 0.69 |
| 1:CA:1194:U:H2' | 1:CA:1195:C:C6 | 2.28 | 0.69 |
| 20:CT:90:GLN:O | 20:CT:93:GLU:HB3 | 1.93 | 0.69 |
| 1:CA:1157:A:H4' | 1:CA:1158:C:O5' | 1.92 | 0.69 |
| 13:CM:76:ALA:HA | 13:CM:79:LYS:HE2 | 1.73 | 0.69 |
| 1:AA:862:C:C2' | 1:AA:863:U:H5' | 2.23 | 0.69 |
| 23:BA:277:C:H3' | 23:BA:278:A:H5'' | 1.72 | 0.69 |
| 23:DA:1754:C:OP1 | 38:DP:96:ARG:NH1 | 2.23 | 0.69 |
| 1:CA:16:A:O2' | 1:CA:17:U:H5' | 1.93 | 0.69 |
| 23:BA:1909:C:C2 | 23:BA:1922:G:N2 | 2.61 | 0.69 |
| 33:DK:31:LYS:HB3 | 33:DK:32:TYR:CE1 | 2.27 | 0.69 |
| 23:DA:2850:A:OP2 | 23:DA:2866:U:H5 | 1.76 | 0.69 |
| 23:DA:65:C:H2' | 23:DA:66:C:C6 | 2.27 | 0.69 |
| 34:DL:138:LEU:HD11 | 34:DL:144:GLU:HB3 | 1.75 | 0.69 |
| 23:BA:2415:G:H4' | 34:BL:66:GLY:CA | 2.23 | 0.69 |
| 52:D4:9:ARG:NE | 52:D4:48:LYS:HB2 | 2.03 | 0.69 |
| 1:CA:1368:G:O2' | 1:CA:1369:C:H5' | 1.93 | 0.69 |
| 1:AA:979:C:H5'' | 1:AA:980:C:OP2 | 1.93 | 0.69 |
| 10:AJ:55:LYS:HD2 | 10:AJ:55:LYS:O | 1.93 | 0.69 |
| 13:AM:107:ALA:O | 13:AM:111:LYS:HG3 | 1.92 | 0.69 |
| 34:BL:33:ARG:HE | 34:BL:36:LYS:CD | 2.04 | 0.69 |
| 23:BA:1021:A:H2' | 23:BA:1023:U:H5' | 1.73 | 0.69 |
| 23:BA:1021:A:C3' | 23:BA:1021:A:C8 | 2.75 | 0.69 |
| 40:BR:79:VAL:O | 40:BR:79:VAL:HG13 | 1.91 | 0.69 |
| 39:BQ:108:GLU:HG3 | 40:BR:44:LYS:HG2 | 1.72 | 0.69 |
| 44:DV:30:ASN:OD1 | 44:DV:33:LEU:HB3 | 1.92 | 0.69 |
| 12:AL:44:PRO:HG3 | 12:AL:52:ARG:CD | 2.23 | 0.69 |
| 42:DT:57:LEU:HD11 | 42:DT:78:LYS:HB2 | 1.74 | 0.69 |
| 19:AS:19:VAL:O | 19:AS:22:LEU:HB2 | 1.93 | 0.69 |
| 27:BE:39:TRP:O | 27:BE:43:LYS:HG2 | 1.93 | 0.69 |
| 23:BA:1046:A:N3 | 31:BI:4:LYS:HD3 | 2.08 | 0.69 |
| 53:B5:50:LEU:O | 53:B5:51:ALA:HB2 | 1.93 | 0.69 |
| 1:AA:600:C:H2' | 1:AA:601:C:C6 | 2.28 | 0.69 |
| 25:BC:25:THR:CG2 | 25:BC:82:ILE:H | 2.04 | 0.69 |
| 23:DA:9:U:C4 | 23:DA:2629:A:C6 | 2.80 | 0.69 |
| 45:BW:42:GLY:HA2 | 45:BW:57:PHE:CE2 | 2.27 | 0.69 |
| 1:AA:1356:G:H2' | 1:AA:1357:A:C8 | 2.28 | 0.69 |
| 8:AH:97:VAL:HG13 | 8:AH:98:LYS:N | 2.08 | 0.69 |
| 1:CA:1426:C:H2' | 1:CA:1427:U:C6 | 2.26 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BA:1606:G:H5'' | 23:BA:1607:C:OP1 | 1.92 | 0.69 |
| 38:BP:1:MET:C | 38:BP:3:ARG:H | 1.96 | 0.69 |
| 8:AH:77:GLU:HG3 | 8:AH:78:GLN:N | 2.08 | 0.69 |
| 13:AM:76:ALA:HA | 13:AM:79:LYS:HE2 | 1.73 | 0.69 |
| 23:DA:273(G):C:H2' | 23:DA:274:G:H5'' | 1.74 | 0.69 |
| 23:BA:2433:A:H5'' | 23:BA:2434:A:P | 2.32 | 0.69 |
| 25:BC:228:PRO:HD3 | 25:BC:234:GLY:O | 1.93 | 0.69 |
| 23:BA:1537:C:H2' | 23:BA:1538:G:O4' | 1.93 | 0.69 |
| 23:BA:1290:C:H2' | 23:BA:1291:C:H6 | 1.57 | 0.69 |
| 23:BA:2402:C:H5' | 23:BA:2403:C:OP2 | 1.92 | 0.69 |
| 1:CA:1022:G:H2' | 1:CA:1023:G:H8 | 1.57 | 0.69 |
| 53:D5:32:LEU:HD23 | 53:D5:33:ASN:N | 2.08 | 0.69 |
| 47:DY:1:MET:CE | 47:DY:5:GLU:HG2 | 2.22 | 0.69 |
| 39:DQ:79:PHE:CD1 | 39:DQ:79:PHE:C | 2.66 | 0.69 |
| 23:BA:993:G:C5 | 23:BA:994:C:H5 | 2.10 | 0.69 |
| 40:BR:47:VAL:O | 40:BR:49:THR:O | 2.11 | 0.69 |
| 23:DA:1812:A:C2' | 23:DA:1813:G:H5' | 2.23 | 0.69 |
| 23:BA:1404:C:O2 | 23:BA:1404:C:H2' | 1.92 | 0.69 |
| 43:BU:78:ALA:HB3 | 43:BU:81:LYS:HE3 | 1.75 | 0.69 |
| 43:BU:81:LYS:HD3 | 43:BU:97:ARG:N | 2.08 | 0.69 |
| 30:BH:66:GLU:HG2 | 30:BH:67:ARG:CZ | 2.23 | 0.69 |
| 38:BP:88:ILE:HD12 | 38:BP:89:VAL:H | 1.58 | 0.69 |
| 32:DJ:77:VAL:HB | 32:DJ:145:VAL:HG22 | 1.74 | 0.69 |
| 25:BC:226:MET:C | 25:BC:227:ASN:HD22 | 1.95 | 0.69 |
| 43:DU:8:LYS:HZ2 | 43:DU:8:LYS:N | 1.91 | 0.69 |
| 23:DA:1264:G:C5' | 50:D2:11:THR:HG21 | 2.22 | 0.69 |
| 1:AA:482:A:N3 | 1:AA:482:A:H2' | 2.08 | 0.69 |
| 16:AP:28:ARG:HH11 | 16:AP:28:ARG:CG | 2.05 | 0.69 |
| 23:DA:2712:U:H1' | 23:DA:712(B):A:H8 | 1.57 | 0.69 |
| 23:BA:94:G:N2 | 47:BY:47:ASN:ND2 | 2.39 | 0.69 |
| 40:DR:79:VAL:O | 40:DR:79:VAL:HG13 | 1.91 | 0.69 |
| 23:DA:1332:G:N2 | 23:DA:1610:A:C8 | 2.61 | 0.69 |
| 44:BV:136:PHE:C | 44:BV:137:ILE:HD12 | 2.13 | 0.69 |
| 1:AA:1081:G:OP1 | 5:AE:18:ARG:HG2 | 1.93 | 0.69 |
| 25:DC:231:HIS:CD2 | 25:DC:249:PRO:HA | 2.26 | 0.69 |
| 43:DU:81:LYS:HD3 | 43:DU:97:ARG:HB3 | 1.74 | 0.69 |
| 1:CA:688:G:H2' | 1:CA:689:C:C6 | 2.25 | 0.69 |
| 23:DA:1343:G:H5' | 23:DA:1343:G:H8 | 1.56 | 0.69 |
| 45:DW:56:ASP:O | 45:DW:57:PHE:HB2 | 1.92 | 0.69 |
| 29:DG:140:LYS:O | 29:DG:144:VAL:HG23 | 1.93 | 0.69 |
| 25:DC:25:THR:HG21 | 25:DC:81:ALA:CA | 2.23 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BA:760:G:H2' | 23:BA:761:A:H5' | 1.72 | 0.69 |
| 1:AA:833:U:H2' | 1:AA:834:C:H6 | 1.58 | 0.69 |
| 25:BC:25:THR:HG21 | 25:BC:81:ALA:CA | 2.22 | 0.69 |
| 1:CA:833:U:H2' | 1:CA:834:C:H6 | 1.57 | 0.69 |
| 50:D2:33:CYS:HG | 50:D2:49:CYS:HG | 1.34 | 0.69 |
| 23:BA:1386:C:OP2 | 23:BA:1396:U:H5 | 1.75 | 0.69 |
| 11:AK:44:SER:OG | 11:AK:47:VAL:HG23 | 1.92 | 0.69 |
| 27:BE:199:TRP:O | 27:BE:203:GLN:HG2 | 1.92 | 0.69 |
| 23:DA:987:G:C2' | 23:DA:988:A:H5' | 2.22 | 0.69 |
| 11:CK:23:ALA:HA | 11:CK:28:THR:OG1 | 1.93 | 0.69 |
| 23:DA:1024:G:O5' | 23:DA:1024:G:H8 | 1.76 | 0.69 |
| 1:CA:1483:A:H5'' | 1:CA:1484:C:OP2 | 1.93 | 0.69 |
| 1:CA:1410:G:O2' | 1:CA:1411:C:H5' | 1.93 | 0.69 |
| 23:DA:1276:A:H1' | 36:DN:16:HIS:HE1 | 1.58 | 0.68 |
| 26:BD:167:VAL:HG22 | 26:BD:170:LEU:HD21 | 1.74 | 0.68 |
| 3:CC:13:GLY:CA | 14:CN:57:ARG:HE | 2.07 | 0.68 |
| 53:B5:31:HIS:C | 53:B5:33:ASN:N | 2.45 | 0.68 |
| 13:CM:39:ILE:HD11 | 13:CM:52:GLU:HG2 | 1.74 | 0.68 |
| 1:CA:397:A:H3' | 1:CA:397:A:N3 | 2.08 | 0.68 |
| 24:BB:11:C:H3' | 24:BB:12:C:C6 | 2.26 | 0.68 |
| 1:CA:105:G:H2' | 1:CA:106:C:C6 | 2.27 | 0.68 |
| 27:BE:31:HIS:ND1 | 34:BL:13:ASN:HB2 | 2.07 | 0.68 |
| 29:BG:102:ALA:HB2 | 29:BG:116:GLU:HA | 1.75 | 0.68 |
| 43:DU:6:HIS:HD2 | 43:DU:35:TYR:CE1 | 2.11 | 0.68 |
| 23:DA:609(B):G:N2 | 23:DA:619:G:H1' | 2.07 | 0.68 |
| 6:AF:33:TYR:CE1 | 6:AF:75:LEU:HA | 2.28 | 0.68 |
| 2:AB:22:LYS:HA | 2:AB:22:LYS:HZ2 | 1.57 | 0.68 |
| 23:BA:2364:C:C2' | 23:BA:2365:G:H5' | 2.22 | 0.68 |
| 28:DF:174:GLU:HG2 | 28:DF:180:PHE:CE1 | 2.28 | 0.68 |
| 23:DA:630:G:N2 | 23:DA:632:A:H3' | 2.09 | 0.68 |
| 13:AM:96:LEU:HB3 | 13:AM:97:PRO:HD2 | 1.75 | 0.68 |
| 32:DJ:157:ARG:N | 32:DJ:158:PRO:CD | 2.52 | 0.68 |
| 43:BU:29:GLU:CB | 43:BU:38:ILE:HB | 2.21 | 0.68 |
| 23:DA:330:A:H2 | 23:DA:1210:A:H2' | 1.58 | 0.68 |
| 36:BN:57:ARG:HG2 | 36:BN:58:GLY:H | 1.56 | 0.68 |
| 23:BA:2724:C:OP1 | 26:BD:118:LYS:HE3 | 1.92 | 0.68 |
| 1:AA:332:G:OP2 | 20:AT:10:LEU:HD23 | 1.93 | 0.68 |
| 1:CA:600:C:H2' | 1:CA:601:C:C6 | 2.29 | 0.68 |
| 40:BR:98:GLU:HG2 | 40:BR:100:ARG:HD3 | 1.73 | 0.68 |
| 1:CA:1066:C:O2 | 1:CA:1066:C:H2' | 1.92 | 0.68 |
| 27:DE:31:HIS:ND1 | 34:DL:13:ASN:HB2 | 2.08 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 23:BA:2636:U:H4' | 26:BD:80:GLU:CD | 2.13 | 0.68 |
| 23:DA:580:C:H2' | 23:DA:581:C:C6 | 2.29 | 0.68 |
| 1:AA:729:A:H2' | 1:AA:730:G:H8 | 1.58 | 0.68 |
| 23:BA:270(J):G:HO2' | 23:BA:270(K):G:H8 | 1.41 | 0.68 |
| 13:AM:25:ILE:HD11 | 13:AM:66:LEU:HD13 | 1.75 | 0.68 |
| 28:BF:84:LYS:O | 28:BF:86:MET:HG3 | 1.93 | 0.68 |
| 23:DA:993:G:C5 | 23:DA:994:C:H5 | 2.11 | 0.68 |
| 28:DF:5:LEU:HD23 | 28:DF:6:ALA:H | 1.59 | 0.68 |
| 23:DA:330:A:C2 | 23:DA:1210:A:H2' | 2.29 | 0.68 |
| 1:CA:1073:U:H2' | 1:CA:1074:G:C8 | 2.29 | 0.68 |
| 23:BA:2305:A:H5'' | 28:BF:134:GLY:HA3 | 1.76 | 0.68 |
| 6:CF:33:TYR:CE1 | 6:CF:75:LEU:HA | 2.28 | 0.68 |
| 23:DA:481:G:C4 | 23:DA:507:A:C2 | 2.81 | 0.68 |
| 23:DA:2009:G:H2' | 23:DA:2010:G:H5' | 1.74 | 0.68 |
| 10:AJ:40:LEU:HB2 | 10:AJ:69:ASN:HB3 | 1.75 | 0.68 |
| 1:CA:1356:G:H2' | 1:CA:1357:A:C8 | 2.28 | 0.68 |
| 23:BA:651:G:OP1 | 53:B5:19:SER:HB3 | 1.93 | 0.68 |
| 23:BA:999:U:H5'' | 23:BA:1154:G:O6 | 1.93 | 0.68 |
| 41:BS:65:LEU:HB2 | 41:BS:68:ARG:HE | 1.57 | 0.68 |
| 25:DC:257:LEU:C | 25:DC:257:LEU:HD23 | 2.13 | 0.68 |
| 1:AA:498:A:H4' | 1:AA:500:G:OP1 | 1.93 | 0.68 |
| 34:BL:62:LEU:O | 34:BL:62:LEU:HD23 | 1.93 | 0.68 |
| 47:BY:1:MET:CE | 47:BY:5:GLU:HG2 | 2.24 | 0.68 |
| 38:DP:74:ARG:HD3 | 38:DP:76:PHE:CE2 | 2.28 | 0.68 |
| 5:AE:101:ILE:O | 5:AE:120:THR:HG23 | 1.92 | 0.68 |
| 23:BA:603:A:C2 | 23:BA:655:A:N3 | 2.61 | 0.68 |
| 39:DQ:88:ILE:HD12 | 39:DQ:90:VAL:CG1 | 2.23 | 0.68 |
| 35:DM:76:LYS:H | 35:DM:88:GLY:HA2 | 1.56 | 0.68 |
| 3:AC:153:VAL:HG12 | 3:AC:198:VAL:HG22 | 1.75 | 0.68 |
| 23:BA:1786:A:H4' | 23:BA:1787:A:OP2 | 1.92 | 0.68 |
| 47:BY:9:GLN:C | 47:BY:12:GLU:HB3 | 2.12 | 0.68 |
| 8:CH:58:TYR:C | 8:CH:59:LEU:HD23 | 2.14 | 0.68 |
| 45:BW:36:ILE:HG23 | 45:BW:58:THR:HG23 | 1.76 | 0.68 |
| 23:DA:1386:C:OP2 | 23:DA:1396:U:H5 | 1.77 | 0.68 |
| 1:CA:914:A:C2' | 1:CA:915:A:H5' | 2.24 | 0.68 |
| 3:AC:89:GLU:O | 3:AC:93:LYS:HB2 | 1.92 | 0.68 |
| 29:BG:27:LYS:HG2 | 29:BG:32:GLU:HG3 | 1.76 | 0.68 |
| 23:DA:813:U:H2' | 23:DA:814:C:C6 | 2.28 | 0.68 |
| 27:BE:36:VAL:O | 27:BE:40:GLN:HG3 | 1.93 | 0.68 |
| 47:DY:1:MET:HE1 | 47:DY:5:GLU:HG2 | 1.74 | 0.68 |
| 23:DA:2438:U:O3' | 23:DA:2439:A:H3' | 1.94 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 38:DP:51:ARG:HD3 | 38:DP:62:THR:HG23 | 1.75 | 0.68 |
| 2:AB:185:ILE:CG2 | 2:AB:199:TYR:HB2 | 2.17 | 0.68 |
| 23:BA:1899:G:O2' | 23:BA:1900:A:OP2 | 2.10 | 0.68 |
| 40:DR:6:LYS:HG3 | 40:DR:11:GLN:HG2 | 1.76 | 0.68 |
| 1:AA:674:G:H2' | 1:AA:675:A:H8 | 1.58 | 0.68 |
| 41:BS:73:ALA:O | 41:BS:106:ILE:HG12 | 1.94 | 0.68 |
| 25:DC:166:GLN:HA | 25:DC:166:GLN:HE21 | 1.59 | 0.68 |
| 36:DN:99:LYS:CD | 36:DN:99:LYS:H | 2.04 | 0.68 |
| 44:BV:22:GLY:O | 44:BV:41:LEU:HB2 | 1.93 | 0.68 |
| 26:DD:9:VAL:HG13 | 26:DD:25:VAL:O | 1.92 | 0.68 |
| 10:AJ:45:ARG:HB3 | 10:AJ:47:PHE:CZ | 2.29 | 0.68 |
| 1:CA:482:A:N3 | 1:CA:482:A:H2' | 2.08 | 0.68 |
| 23:DA:300:A:OP1 | 43:DU:84:ARG:NH2 | 2.26 | 0.68 |
| 23:BA:329:G:OP2 | 43:BU:71:LYS:HE3 | 1.94 | 0.68 |
| 47:DY:2:LYS:HA | 47:DY:5:GLU:OE2 | 1.94 | 0.68 |
| 23:DA:84:A:C5' | 43:DU:9:LYS:HD2 | 2.24 | 0.68 |
| 34:BL:109:GLY:O | 34:BL:111:ARG:N | 2.27 | 0.68 |
| 10:CJ:48:THR:HA | 10:CJ:62:HIS:CB | 2.18 | 0.68 |
| 34:DL:38:GLN:HG3 | 34:DL:39:LYS:N | 2.07 | 0.68 |
| 38:BP:100:TYR:HB3 | 38:BP:103:ARG:NH1 | 2.08 | 0.68 |
| 16:CP:19:ILE:HB | 16:CP:37:GLY:O | 1.94 | 0.68 |
| 13:AM:33:ALA:HB1 | 13:AM:56:LEU:HD21 | 1.74 | 0.68 |
| 28:DF:8:LYS:HD3 | 28:DF:9:ARG:HG3 | 1.74 | 0.68 |
| 23:DA:547:A:C6 | 23:DA:548:A:C6 | 2.81 | 0.68 |
| 23:DA:2210:G:H21 | 23:DA:2211:G:H5' | 1.54 | 0.68 |
| 17:CQ:45:HIS:CD2 | 17:CQ:47:PRO:HD3 | 2.28 | 0.68 |
| 23:DA:1607:C:H4' | 23:DA:1608:A:O5' | 1.94 | 0.68 |
| 36:DN:55:ALA:HA | 36:DN:80:PHE:HE1 | 1.56 | 0.68 |
| 1:CA:1152:A:OP1 | 10:CJ:68:HIS:CD2 | 2.47 | 0.68 |
| 1:AA:833:U:H2' | 1:AA:834:C:C6 | 2.28 | 0.68 |
| 29:DG:30:LYS:HB2 | 29:DG:79:VAL:HA | 1.75 | 0.68 |
| 1:AA:919:A:O2' | 1:AA:920:U:H5' | 1.93 | 0.68 |
| 23:BA:2740:A:H2' | 23:BA:2741:A:C8 | 2.29 | 0.68 |
| 23:DA:1537:C:H2' | 23:DA:1538:G:O4' | 1.94 | 0.68 |
| 33:BK:2:ILE:HG12 | 33:BK:8:LEU:HD11 | 1.73 | 0.68 |
| 10:AJ:96:ILE:HD13 | 10:AJ:96:ILE:H | 1.59 | 0.68 |
| 23:BA:987:G:C2' | 23:BA:988:A:H5' | 2.23 | 0.68 |
| 51:D3:30:THR:HG22 | 51:D3:31:PRO:HD2 | 1.75 | 0.68 |
| 12:CL:74:HIS:HD2 | 12:CL:76:LEU:H | 1.39 | 0.68 |
| 23:DA:2433:A:H5'' | 23:DA:2434:A:P | 2.34 | 0.68 |
| 34:DL:85:LEU:HA | 34:DL:88:LEU:HB2 | 1.74 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BA:918:A:N3 | 24:BB:80:U:O2' | 2.27 | 0.68 |
| 2:CB:163:PHE:HD1 | 2:CB:185:ILE:HG13 | 1.59 | 0.68 |
| 4:CD:51:PRO:HB3 | 4:CD:55:ALA:HB3 | 1.75 | 0.68 |
| 3:AC:113:ALA:HB3 | 3:AC:114:PRO:HD3 | 1.75 | 0.68 |
| 42:DT:30:VAL:HG12 | 42:DT:31:HIS:N | 2.09 | 0.68 |
| 20:AT:71:THR:HG22 | 20:AT:72:LEU:H | 1.59 | 0.68 |
| 3:CC:195:VAL:CG1 | 3:CC:196:LEU:H | 2.07 | 0.68 |
| 1:CA:10:A:H2' | 1:CA:11:G:H8 | 1.59 | 0.68 |
| 1:CA:350:G:O2' | 1:CA:351:G:H5' | 1.94 | 0.68 |
| 23:BA:2209:C:O2 | 23:BA:2216:G:C2 | 2.47 | 0.68 |
| 23:DA:1536:A:H5'' | 23:DA:1537:C:OP2 | 1.94 | 0.68 |
| 1:AA:909:A:H2' | 1:AA:910:C:O4' | 1.94 | 0.68 |
| 23:BA:357:A:H2' | 23:BA:358:U:H6 | 1.58 | 0.68 |
| 1:CA:345:C:OP2 | 38:DP:39:ARG:NH2 | 2.20 | 0.68 |
| 3:AC:23:TYR:CD2 | 3:AC:24:ALA:N | 2.62 | 0.68 |
| 23:BA:1946:U:H2' | 23:BA:1947:C:H6 | 1.59 | 0.68 |
| 25:DC:201:HIS:O | 25:DC:204:ILE:HG13 | 1.93 | 0.68 |
| 23:DA:1862:G:H2' | 23:DA:1863:G:H8 | 1.59 | 0.68 |
| 23:DA:1528:A:C2 | 23:DA:1529:A:C2 | 2.81 | 0.68 |
| 23:BA:1566:A:OP1 | 25:BC:211:ARG:NH1 | 2.27 | 0.68 |
| 42:DT:63:LYS:HZ1 | 42:DT:72:LYS:HB3 | 1.58 | 0.68 |
| 23:DA:1019:U:N3 | 23:DA:114(B):A:N6 | 2.42 | 0.68 |
| 3:CC:18:TRP:HB3 | 3:CC:20:SER:O | 1.93 | 0.68 |
| 42:BT:51:VAL:HG11 | 42:BT:81:VAL:HG12 | 1.76 | 0.68 |
| 23:BA:1343:G:H5' | 23:BA:1343:G:H8 | 1.56 | 0.68 |
| 1:AA:629:G:H2' | 1:AA:630:G:C8 | 2.29 | 0.68 |
| 23:DA:999:U:H5'' | 23:DA:1154:G:O6 | 1.94 | 0.68 |
| 1:AA:106:C:C2' | 1:AA:107:G:H5' | 2.24 | 0.68 |
| 23:BA:2469:A:H2 | 23:BA:2481:G:H21 | 1.42 | 0.68 |
| 5:AE:96:PRO:HA | 5:AE:117:ASP:CG | 2.13 | 0.68 |
| 32:DJ:101:TYR:HB3 | 32:DJ:102:PRO:HD2 | 1.75 | 0.68 |
| 23:DA:2093:G:H1 | 23:DA:2196:C:H42 | 1.39 | 0.68 |
| 1:CA:629:G:H2' | 1:CA:630:G:C8 | 2.29 | 0.68 |
| 3:CC:150:LYS:HB3 | 3:CC:201:TYR:HB2 | 1.76 | 0.68 |
| 10:CJ:45:ARG:HB3 | 10:CJ:47:PHE:CZ | 2.29 | 0.68 |
| 10:CJ:96:ILE:H | 10:CJ:96:ILE:HD13 | 1.59 | 0.68 |
| 23:BA:1310:G:OP2 | 52:B4:9:ARG:NH1 | 2.27 | 0.68 |
| 10:AJ:48:THR:CA | 10:AJ:62:HIS:HB3 | 2.18 | 0.68 |
| 34:BL:146:VAL:HG13 | 34:BL:147:LEU:HD12 | 1.74 | 0.68 |
| 38:BP:54:ARG:HG3 | 38:BP:54:ARG:NH1 | 1.96 | 0.68 |
| 2:CB:185:ILE:CG2 | 2:CB:199:TYR:HB2 | 2.18 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 39:DQ:92:ARG:CB | 39:DQ:92:ARG:HH11 | 2.06 | 0.68 |
| 23:DA:918:A:N3 | 24:DB:80:U:O2' | 2.26 | 0.68 |
| 39:BQ:90:VAL:HG13 | 39:BQ:91:ASP:H | 1.59 | 0.68 |
| 40:BR:40:LEU:C | 40:BR:45:THR:HB | 2.15 | 0.68 |
| 1:CA:89:U:H2' | 1:CA:90:C:C6 | 2.29 | 0.68 |
| 39:DQ:57:PHE:O | 39:DQ:58:ARG:C | 2.32 | 0.68 |
| 36:DN:2:ARG:O | 36:DN:4:LEU:N | 2.27 | 0.68 |
| 23:BA:847:U:OP2 | 23:BA:929:G:O6 | 2.12 | 0.68 |
| 26:BD:120:TRP:CD1 | 26:BD:155:LYS:HB3 | 2.27 | 0.68 |
| 1:AA:987:G:H1 | 1:AA:1218:C:N4 | 1.90 | 0.68 |
| 35:BM:8:LYS:HG3 | 35:BM:9:TYR:H | 1.59 | 0.68 |
| 1:AA:625:G:H4' | 16:AP:16:HIS:CD2 | 2.29 | 0.68 |
| 1:AA:976:G:N2 | 1:AA:136(A):C:H2' | 2.08 | 0.68 |
| 1:AA:1016:A:H2' | 1:AA:1017:G:O4' | 1.94 | 0.68 |
| 1:AA:108:G:H5' | 1:AA:109:A:H5'' | 1.75 | 0.68 |
| 2:AB:115:LEU:HD12 | 2:AB:118:LEU:HD12 | 1.74 | 0.68 |
| 1:CA:108:G:H5' | 1:CA:109:A:H5'' | 1.76 | 0.68 |
| 35:BM:54:MET:HG2 | 35:BM:64:ILE:HD13 | 1.74 | 0.68 |
| 18:AR:66:LEU:O | 18:AR:70:ILE:HG13 | 1.94 | 0.68 |
| 43:BU:17:SER:OG | 43:BU:18:GLY:N | 2.25 | 0.68 |
| 10:AJ:48:THR:HA | 10:AJ:62:HIS:CB | 2.18 | 0.68 |
| 34:BL:126:VAL:HA | 34:BL:145:PRO:HG2 | 1.75 | 0.68 |
| 53:B5:32:LEU:HD23 | 53:B5:33:ASN:N | 2.08 | 0.68 |
| 34:DL:35:HIS:O | 34:DL:36:LYS:CB | 2.41 | 0.68 |
| 38:DP:24:PRO:HA | 38:DP:49:VAL:CG1 | 2.23 | 0.68 |
| 1:CA:376:G:O2' | 1:CA:377:G:H5' | 1.94 | 0.68 |
| 44:DV:29:TYR:HA | 44:DV:33:LEU:O | 1.94 | 0.68 |
| 15:AO:53:HIS:HE1 | 23:BA:715:G:O6 | 1.77 | 0.68 |
| 23:DA:760:G:H2' | 23:DA:761:A:H5' | 1.76 | 0.68 |
| 23:DA:1476:C:H6 | 23:DA:1476:C:H3' | 1.59 | 0.68 |
| 8:AH:97:VAL:O | 8:AH:100:ILE:HG13 | 1.94 | 0.68 |
| 23:DA:2871:C:H5'' | 23:DA:2872:G:OP1 | 1.94 | 0.68 |
| 5:CE:96:PRO:HA | 5:CE:117:ASP:CG | 2.14 | 0.68 |
| 23:BA:273(G):C:H2' | 23:BA:274:G:H5'' | 1.74 | 0.68 |
| 8:CH:64:LYS:HB3 | 8:CH:79:VAL:HG11 | 1.75 | 0.68 |
| 10:CJ:40:LEU:HB2 | 10:CJ:69:ASN:HB3 | 1.74 | 0.68 |
| 38:DP:86:ILE:O | 38:DP:86:ILE:HG12 | 1.94 | 0.68 |
| 35:BM:32:PHE:HZ | 35:BM:111:GLU:HG2 | 1.58 | 0.68 |
| 13:CM:99:ARG:HB2 | 13:CM:101:GLN:NE2 | 2.09 | 0.68 |
| 22:AV:6189:G:O2' | 22:AV:6190:U:H5' | 1.94 | 0.67 |
| 1:CA:552:U:O2' | 1:CA:553:A:H5' | 1.95 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:BR:38:LEU:HD23 | 40:BR:39:LEU:N | 2.09 | 0.67 |
| 23:DA:2335:A:O2' | 23:DA:2336:A:H5'' | 1.94 | 0.67 |
| 13:CM:33:ALA:HB1 | 13:CM:56:LEU:HD21 | 1.75 | 0.67 |
| 23:BA:1654:A:OP1 | 36:BN:2:ARG:N | 2.27 | 0.67 |
| 46:BX:13:ILE:HG12 | 46:BX:63:ALA:CB | 2.23 | 0.67 |
| 1:AA:105:G:H2' | 1:AA:106:C:H6 | 1.59 | 0.67 |
| 8:CH:51:VAL:HG21 | 8:CH:60:ARG:CG | 2.24 | 0.67 |
| 1:AA:1194:U:H2' | 1:AA:1195:C:C6 | 2.28 | 0.67 |
| 26:DD:30:PRO:O | 26:DD:32:PRO:HD3 | 1.94 | 0.67 |
| 1:AA:521:G:O2' | 1:AA:522:C:H5' | 1.94 | 0.67 |
| 1:AA:24:U:H2' | 1:AA:25:C:H6 | 1.57 | 0.67 |
| 32:DJ:80:ALA:O | 32:DJ:82:LYS:N | 2.27 | 0.67 |
| 21:AU:6:ARG:HG3 | 21:AU:15:ARG:HH12 | 1.58 | 0.67 |
| 32:BJ:157:ARG:HG2 | 32:BJ:157:ARG:O | 1.93 | 0.67 |
| 28:BF:86:MET:H | 28:BF:87:PRO:CD | 2.08 | 0.67 |
| 23:DA:1021:A:C3' | 23:DA:1021:A:C8 | 2.76 | 0.67 |
| 26:BD:2:LYS:HE2 | 26:BD:95:ILE:O | 1.95 | 0.67 |
| 3:CC:153:VAL:HG12 | 3:CC:198:VAL:HG22 | 1.76 | 0.67 |
| 28:BF:41:GLN:HG2 | 28:BF:155:MET:HB3 | 1.76 | 0.67 |
| 13:AM:10:PRO:HG3 | 13:AM:22:ILE:HD11 | 1.76 | 0.67 |
| 6:CF:26:ILE:HG22 | 6:CF:30:LEU:CD1 | 2.25 | 0.67 |
| 1:CA:624:C:O3' | 16:CP:10:GLY:HA2 | 1.94 | 0.67 |
| 1:CA:1151:A:O2' | 1:CA:1152:A:H8 | 1.78 | 0.67 |
| 23:DA:227:A:H5' | 23:DA:228:A:C2 | 2.29 | 0.67 |
| 23:BA:2637:U:H5'' | 26:BD:82:ARG:HH21 | 1.57 | 0.67 |
| 1:AA:1051:C:H42 | 1:AA:1207:G:H1 | 1.43 | 0.67 |
| 24:BB:30:C:H2' | 24:BB:31:C:H5' | 1.77 | 0.67 |
| 12:AL:6:ILE:HD12 | 12:AL:6:ILE:H | 1.59 | 0.67 |
| 23:BA:492:A:H2' | 23:BA:493:G:O4' | 1.95 | 0.67 |
| 3:AC:76:VAL:HG21 | 3:AC:103:VAL:HG11 | 1.75 | 0.67 |
| 23:BA:603:A:N6 | 23:BA:655:A:C4' | 2.55 | 0.67 |
| 25:BC:242:ARG:HG2 | 25:BC:242:ARG:HH11 | 1.59 | 0.67 |
| 1:AA:89:U:H2' | 1:AA:90:C:C6 | 2.28 | 0.67 |
| 34:DL:16:ARG:CZ | 34:DL:18:ARG:H | 2.07 | 0.67 |
| 4:CD:100:ARG:HH21 | 4:CD:118:ARG:NH1 | 1.91 | 0.67 |
| 23:DA:528:A:H2 | 23:DA:2043:C:H5' | 1.58 | 0.67 |
| 23:DA:1669:A:O3' | 23:DA:2549:G:H5' | 1.94 | 0.67 |
| 53:B5:50:LEU:O | 53:B5:51:ALA:CB | 2.42 | 0.67 |
| 23:DA:971:C:C2' | 23:DA:972:G:H5' | 2.24 | 0.67 |
| 22:AV:6177:U:H2' | 22:AV:6178:A:H8 | 1.60 | 0.67 |
| 36:BN:99:LYS:H | 36:BN:99:LYS:CD | 2.05 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:255:G:C4 | 1:CA:256:U:C5 | 2.82 | 0.67 |
| 10:AJ:92:THR:HG23 | 10:AJ:93:GLY:H | 1.59 | 0.67 |
| 23:DA:229:A:H5' | 23:DA:230:U:H5' | 1.76 | 0.67 |
| 4:AD:36:ARG:HG2 | 4:AD:38:TYR:OH | 1.94 | 0.67 |
| 15:AO:69:TYR:HD1 | 15:AO:72:ARG:HH21 | 1.40 | 0.67 |
| 23:DA:1007:C:O2' | 32:DJ:131:PRO:HA | 1.93 | 0.67 |
| 38:BP:86:ILE:O | 38:BP:86:ILE:HG12 | 1.93 | 0.67 |
| 6:CF:12:PRO:HG2 | 6:CF:55:ASP:OD2 | 1.94 | 0.67 |
| 23:DA:628:G:H2' | 23:DA:629:G:H8 | 1.58 | 0.67 |
| 43:DU:13:VAL:CG1 | 43:DU:72:VAL:HB | 2.24 | 0.67 |
| 13:CM:107:ALA:O | 13:CM:111:LYS:HG3 | 1.93 | 0.67 |
| 23:BA:1658:C:OP1 | 26:BD:132:HIS:O | 2.13 | 0.67 |
| 23:BA:1141:U:OP2 | 32:BJ:86:THR:CG2 | 2.43 | 0.67 |
| 23:DA:242:G:C5' | 53:D5:63:PRO:HG2 | 2.25 | 0.67 |
| 23:BA:322:A:H3' | 27:BE:169:ASN:HD21 | 1.57 | 0.67 |
| 36:DN:4:LEU:O | 36:DN:6:SER:N | 2.27 | 0.67 |
| 5:AE:51:VAL:O | 5:AE:55:VAL:HG23 | 1.94 | 0.67 |
| 1:CA:1301:U:H3' | 1:CA:1302:U:H5'' | 1.76 | 0.67 |
| 8:AH:21:LYS:O | 8:AH:63:LEU:HD12 | 1.95 | 0.67 |
| 25:BC:132:PRO:O | 25:BC:136:ILE:HD12 | 1.95 | 0.67 |
| 19:CS:19:VAL:O | 19:CS:22:LEU:HB2 | 1.94 | 0.67 |
| 42:DT:52:VAL:HG23 | 42:DT:82:GLN:O | 1.94 | 0.67 |
| 23:DA:2277:G:H5'' | 35:DM:85:LYS:HB2 | 1.74 | 0.67 |
| 23:DA:380:U:C2 | 46:DX:20:ARG:NH2 | 2.61 | 0.67 |
| 33:BK:102:VAL:HG23 | 33:BK:121:VAL:HA | 1.76 | 0.67 |
| 23:DA:357:A:H2' | 23:DA:358:U:C6 | 2.30 | 0.67 |
| 29:DG:102:ALA:HB2 | 29:DG:116:GLU:HA | 1.75 | 0.67 |
| 23:BA:1862:G:H2' | 23:BA:1863:G:H8 | 1.60 | 0.67 |
| 23:DA:565:C:H2' | 23:DA:566:U:O5' | 1.95 | 0.67 |
| 23:DA:314:A:O2' | 23:DA:315:G:H5' | 1.94 | 0.67 |
| 25:BC:70:TRP:CZ3 | 25:BC:146:GLU:OE1 | 2.45 | 0.67 |
| 23:DA:941:A:H4' | 34:DL:35:HIS:CE1 | 2.28 | 0.67 |
| 1:AA:692:U:O2' | 1:AA:694:A:N7 | 2.22 | 0.67 |
| 1:CA:37:U:P | 12:CL:122:LYS:HG3 | 2.34 | 0.67 |
| 9:AI:17:VAL:HG13 | 9:AI:63:ILE:HD11 | 1.77 | 0.67 |
| 23:BA:910:A:H62 | 35:BM:12:GLN:HA | 1.59 | 0.67 |
| 1:AA:625:G:H2' | 1:AA:626:U:C6 | 2.29 | 0.67 |
| 1:CA:66:G:H4' | 1:CA:173:U:C5 | 2.30 | 0.67 |
| 22:CV:6177:U:H2' | 22:CV:6178:A:H8 | 1.60 | 0.67 |
| 23:BA:335:C:H2' | 23:BA:336:C:H6 | 1.59 | 0.67 |
| 1:CA:976:G:C8 | 1:CA:1358:U:H2' | 2.29 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:AH:64:LYS:HB3 | 8:AH:79:VAL:HG11 | 1.76 | 0.67 |
| 3:AC:175:LEU:HD23 | 3:AC:175:LEU:O | 1.94 | 0.67 |
| 23:DA:2631:G:N3 | 23:DA:2810:A:H2 | 1.91 | 0.67 |
| 23:DA:116:C:H2' | 23:DA:117:G:C8 | 2.29 | 0.67 |
| 1:CA:973:G:H3' | 1:CA:974:A:H5'' | 1.74 | 0.67 |
| 36:BN:44:LEU:O | 36:BN:44:LEU:HD13 | 1.95 | 0.67 |
| 23:BA:2275:C:H5' | 23:BA:2275:C:H6 | 1.60 | 0.67 |
| 23:DA:826:U:H4' | 34:DL:55:ARG:HB2 | 1.76 | 0.67 |
| 22:AV:6182:A:C2 | 22:AV:6195:G:C2 | 2.83 | 0.67 |
| 38:BP:51:ARG:HD3 | 38:BP:62:THR:HG23 | 1.77 | 0.67 |
| 23:DA:729:G:OP2 | 25:DC:13:ARG:NH1 | 2.26 | 0.67 |
| 1:AA:438:G:H4' | 4:AD:123:HIS:ND1 | 2.09 | 0.67 |
| 1:AA:397:A:H3' | 1:AA:397:A:N3 | 2.09 | 0.67 |
| 30:DH:111:PRO:HG2 | 30:DH:112:LYS:HE2 | 1.77 | 0.67 |
| 28:BF:129:GLY:HA3 | 28:BF:163:ALA:HB3 | 1.76 | 0.67 |
| 23:DA:94:G:N2 | 47:DY:47:ASN:ND2 | 2.41 | 0.67 |
| 23:DA:1596:A:H2' | 23:DA:1597:A:H5' | 1.76 | 0.67 |
| 44:BV:30:ASN:O | 44:BV:32:HIS:N | 2.27 | 0.67 |
| 1:AA:1368:G:O2' | 1:AA:1369:C:H5' | 1.93 | 0.67 |
| 25:BC:79:VAL:HG12 | 25:BC:113:VAL:HA | 1.77 | 0.67 |
| 40:BR:28:GLU:OE1 | 40:BR:31:ALA:HB2 | 1.95 | 0.67 |
| 23:DA:588:U:H1' | 27:DE:90:PHE:CD1 | 2.30 | 0.67 |
| 1:CA:914:A:H2' | 1:CA:915:A:H5' | 1.76 | 0.67 |
| 21:CU:6:ARG:HG3 | 21:CU:15:ARG:HH12 | 1.58 | 0.67 |
| 3:CC:89:GLU:O | 3:CC:93:LYS:HB2 | 1.94 | 0.67 |
| 4:AD:71:SER:HB2 | 4:AD:74:GLN:HB2 | 1.76 | 0.67 |
| 35:DM:134:ARG:O | 35:DM:136:ALA:N | 2.28 | 0.67 |
| 51:B3:30:THR:HG22 | 51:B3:31:PRO:HD2 | 1.75 | 0.67 |
| 23:DA:1909:C:C2 | 23:DA:1922:G:N2 | 2.63 | 0.67 |
| 6:AF:67:MET:HB2 | 6:AF:68:PRO:HD2 | 1.76 | 0.67 |
| 13:CM:25:ILE:HD11 | 13:CM:66:LEU:HD13 | 1.76 | 0.67 |
| 2:CB:127:ILE:HD13 | 2:CB:127:ILE:N | 2.09 | 0.67 |
| 2:AB:69:LEU:HD13 | 2:AB:91:PRO:HB2 | 1.77 | 0.67 |
| 34:BL:38:GLN:HG3 | 34:BL:39:LYS:N | 2.10 | 0.67 |
| 1:CA:1347:G:N7 | 9:CI:107:ARG:HB3 | 2.08 | 0.67 |
| 12:CL:26:LEU:HB3 | 12:CL:29:ALA:HB3 | 1.77 | 0.67 |
| 39:DQ:108:GLU:HG3 | 40:DR:44:LYS:HG2 | 1.76 | 0.67 |
| 23:DA:1021:A:H2' | 23:DA:1023:U:H5' | 1.76 | 0.67 |
| 30:BH:79:ILE:HG22 | 30:BH:81:VAL:HG23 | 1.74 | 0.67 |
| 23:BA:1158:C:O2' | 23:BA:1159:U:H5' | 1.95 | 0.67 |
| 39:BQ:79:PHE:O | 39:BQ:83:LEU:HD13 | 1.95 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:DO:12:PHE:HE1 | 37:DO:16:ASN:HD21 | 1.43 | 0.67 |
| 4:AD:119:GLN:HG3 | 4:AD:123:HIS:HD2 | 1.57 | 0.67 |
| 26:DD:84:PHE:CZ | 26:DD:86:PRO:HG3 | 2.30 | 0.67 |
| 5:AE:33:VAL:HG11 | 5:AE:109:ILE:HA | 1.77 | 0.67 |
| 2:CB:97:TRP:CH2 | 2:CB:176:GLU:HG3 | 2.30 | 0.67 |
| 42:DT:29:TRP:CZ3 | 42:DT:78:LYS:HG3 | 2.29 | 0.67 |
| 23:BA:1858:G:HO2' | 23:BA:1859:A:H8 | 1.41 | 0.67 |
| 45:DW:72:ARG:HB3 | 45:DW:75:LEU:HD12 | 1.77 | 0.67 |
| 53:B5:57:ARG:HA | 53:B5:57:ARG:NE | 2.10 | 0.67 |
| 1:AA:511:C:H1' | 4:AD:43:HIS:NE2 | 2.10 | 0.67 |
| 32:BJ:160:LYS:HE3 | 32:BJ:161:LEU:N | 2.08 | 0.67 |
| 1:CA:579:G:C5 | 1:CA:580:U:C5 | 2.82 | 0.67 |
| 23:DA:1593:G:H2' | 23:DA:1594:G:C8 | 2.30 | 0.67 |
| 23:BA:2840:C:H4' | 36:BN:53:HIS:CD2 | 2.30 | 0.67 |
| 1:AA:1468:A:H2' | 1:AA:1469:G:O4' | 1.94 | 0.67 |
| 12:CL:22:LYS:O | 12:CL:96:ARG:HD2 | 1.94 | 0.67 |
| 23:BA:2322:A:H3' | 23:BA:2323:G:H8 | 1.60 | 0.67 |
| 51:B3:42:TRP:CE3 | 51:B3:42:TRP:HA | 2.28 | 0.67 |
| 25:DC:95:LEU:HD12 | 25:DC:95:LEU:O | 1.95 | 0.67 |
| 23:BA:2036:C:H6 | 23:BA:2036:C:H5' | 1.60 | 0.67 |
| 1:CA:1229:A:H2' | 1:CA:1230:C:C6 | 2.30 | 0.67 |
| 34:DL:112:LEU:HD23 | 34:DL:113:LYS:N | 2.09 | 0.67 |
| 43:DU:17:SER:OG | 43:DU:18:GLY:N | 2.27 | 0.67 |
| 23:BA:807:U:OP2 | 34:BL:39:LYS:CG | 2.38 | 0.67 |
| 34:DL:33:ARG:H | 34:DL:36:LYS:CE | 2.03 | 0.67 |
| 24:DB:83:G:H5'' | 48:DZ:52:HIS:CE1 | 2.29 | 0.67 |
| 1:AA:411:A:N7 | 1:AA:429:U:H5 | 1.93 | 0.67 |
| 23:DA:2723:C:O3' | 36:DN:2:ARG:NH2 | 2.27 | 0.67 |
| 25:DC:231:HIS:CD2 | 25:DC:232:PRO:HD2 | 2.30 | 0.67 |
| 25:BC:166:GLN:N | 25:BC:166:GLN:HE21 | 1.93 | 0.67 |
| 39:DQ:5:LYS:HG2 | 39:DQ:6:THR:H | 1.58 | 0.67 |
| 43:DU:63:LYS:HG3 | 43:DU:64:GLU:H | 1.58 | 0.67 |
| 1:AA:1512:U:H3 | 1:AA:1523:G:H1 | 1.43 | 0.67 |
| 1:CA:433:C:H2' | 1:CA:434:U:H6 | 1.59 | 0.67 |
| 23:BA:540:G:H2' | 23:BA:541:C:H6 | 1.59 | 0.67 |
| 35:DM:116:GLU:OE1 | 35:DM:116:GLU:HA | 1.94 | 0.67 |
| 7:AG:142:GLU:O | 7:AG:145:ALA:HB3 | 1.94 | 0.67 |
| 1:CA:937:A:H1' | 1:CA:1379:G:N2 | 2.10 | 0.67 |
| 20:AT:90:GLN:O | 20:AT:93:GLU:HB3 | 1.95 | 0.67 |
| 23:DA:1946:U:H2' | 23:DA:1947:C:H6 | 1.59 | 0.67 |
| 53:D5:57:ARG:NE | 53:D5:57:ARG:HA | 2.10 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DA:2415:G:H4' | 34:DL:66:GLY:CA | 2.24 | 0.67 |
| 23:DA:637:A:OP2 | 34:DL:115:LEU:HB2 | 1.94 | 0.67 |
| 23:BA:2389:G:H5'' | 23:BA:2390:U:C5' | 2.11 | 0.67 |
| 25:BC:145:VAL:HG12 | 25:BC:146:GLU:O | 1.94 | 0.67 |
| 9:CI:113:LYS:H | 9:CI:119:ALA:HA | 1.60 | 0.67 |
| 22:CV:6182:A:C2 | 22:CV:6195:G:C2 | 2.83 | 0.67 |
| 1:CA:950:U:H4' | 1:CA:971:G:N2 | 2.10 | 0.67 |
| 1:CA:1250:A:H5' | 9:CI:67:GLY:HA2 | 1.77 | 0.67 |
| 44:BV:94:GLU:CD | 44:BV:94:GLU:H | 1.99 | 0.67 |
| 44:BV:132:ASN:C | 44:BV:134:PRO:HD3 | 2.14 | 0.67 |
| 6:CF:37:VAL:HG12 | 6:CF:38:GLU:O | 1.94 | 0.67 |
| 40:DR:28:GLU:OE1 | 40:DR:31:ALA:HB2 | 1.95 | 0.67 |
| 23:DA:2599:G:C8 | 25:DC:237:GLU:HG3 | 2.30 | 0.67 |
| 37:DO:34:HIS:CE1 | 37:DO:54:LEU:HB3 | 2.29 | 0.67 |
| 23:BA:580:C:H2' | 23:BA:581:C:C6 | 2.30 | 0.67 |
| 11:AK:21:ILE:N | 11:AK:21:ILE:HD12 | 2.10 | 0.67 |
| 35:DM:60:ARG:H | 44:DV:179:ASP:CG | 1.99 | 0.67 |
| 1:CA:300:A:H1' | 1:CA:565:U:O2 | 1.95 | 0.67 |
| 23:BA:2871:C:H5'' | 23:BA:2872:G:OP1 | 1.94 | 0.67 |
| 32:BJ:101:TYR:HB3 | 32:BJ:102:PRO:HD2 | 1.77 | 0.67 |
| 23:DA:2322:A:H3' | 23:DA:2323:G:H8 | 1.60 | 0.67 |
| 23:DA:1683:C:H42 | 23:DA:1705:G:H1 | 1.41 | 0.67 |
| 23:DA:1310:G:OP2 | 52:D4:9:ARG:NH1 | 2.28 | 0.67 |
| 52:B4:11:LYS:HD2 | 52:B4:15:THR:CG2 | 2.25 | 0.67 |
| 3:AC:13:GLY:CA | 14:AN:57:ARG:HE | 2.07 | 0.67 |
| 32:DJ:127:LYS:HB2 | 32:DJ:140:PHE:CE1 | 2.30 | 0.67 |
| 39:BQ:92:ARG:CB | 39:BQ:92:ARG:HH11 | 2.08 | 0.67 |
| 4:AD:94:LEU:HA | 4:AD:97:LEU:HD12 | 1.76 | 0.67 |
| 23:DA:1786:A:H4' | 23:DA:1787:A:OP2 | 1.94 | 0.67 |
| 3:AC:195:VAL:CG1 | 3:AC:196:LEU:H | 2.07 | 0.67 |
| 46:BX:62:VAL:HG22 | 46:BX:63:ALA:N | 2.10 | 0.67 |
| 25:DC:134:ARG:HD3 | 25:DC:135:PHE:CE1 | 2.30 | 0.67 |
| 10:CJ:55:LYS:HD2 | 10:CJ:55:LYS:O | 1.95 | 0.67 |
| 23:BA:971:C:H2' | 23:BA:972:G:C5' | 2.25 | 0.67 |
| 25:DC:77:ALA:CB | 25:DC:97:TYR:HA | 2.25 | 0.67 |
| 23:BA:534:U:O2' | 39:BQ:49:HIS:HD2 | 1.78 | 0.67 |
| 1:AA:24:U:H2' | 1:AA:25:C:C6 | 2.30 | 0.67 |
| 1:CA:346:G:OP1 | 38:DP:41:ARG:NH2 | 2.27 | 0.67 |
| 29:DG:98:LEU:HD12 | 29:DG:99:VAL:N | 2.09 | 0.67 |
| 28:BF:7:LEU:HD23 | 28:BF:10:LYS:HD2 | 1.75 | 0.67 |
| 23:BA:2705:A:H2 | 36:BN:64:ARG:NH1 | 1.93 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:DM:43:THR:OG1 | 35:DM:45:GLN:HG2 | 1.95 | 0.67 |
| 3:AC:40:ARG:O | 3:AC:44:GLU:HG2 | 1.94 | 0.66 |
| 1:AA:1073:U:H2' | 1:AA:1074:G:C8 | 2.30 | 0.66 |
| 9:AI:113:LYS:H | 9:AI:119:ALA:HA | 1.60 | 0.66 |
| 6:AF:63:TYR:N | 6:AF:63:TYR:HD2 | 1.92 | 0.66 |
| 33:DK:103:ALA:HB1 | 33:DK:105:GLU:OE1 | 1.95 | 0.66 |
| 23:BA:7:G:H2' | 23:BA:8:A:C8 | 2.30 | 0.66 |
| 23:DA:971:C:H2' | 23:DA:972:G:C5' | 2.24 | 0.66 |
| 23:DA:389:G:H1 | 34:DL:71:VAL:H | 1.43 | 0.66 |
| 1:AA:105:G:H2' | 1:AA:106:C:C6 | 2.30 | 0.66 |
| 43:DU:76:CYS:SG | 43:DU:77:PRO:HD3 | 2.35 | 0.66 |
| 23:BA:2593:U:H2' | 23:BA:2594:C:H6 | 1.58 | 0.66 |
| 1:CA:532:A:H2 | 1:CA:1207:G:H4' | 1.60 | 0.66 |
| 24:DB:75:G:H21 | 44:DV:85:HIS:HE1 | 1.40 | 0.66 |
| 1:CA:564:C:C2 | 17:CQ:31:LEU:HD11 | 2.30 | 0.66 |
| 1:CA:632:A:C8 | 1:CA:633:G:C8 | 2.83 | 0.66 |
| 12:AL:6:ILE:O | 12:AL:10:VAL:HG23 | 1.95 | 0.66 |
| 19:CS:49:ILE:HD12 | 19:CS:49:ILE:H | 1.60 | 0.66 |
| 15:AO:15:PHE:O | 15:AO:27:VAL:HG22 | 1.95 | 0.66 |
| 23:BA:978:G:C2' | 23:BA:979:G:H5' | 2.25 | 0.66 |
| 8:AH:7:ALA:HB2 | 8:AH:85:ARG:HD3 | 1.76 | 0.66 |
| 22:AV:6188:G:N2 | 22:AV:6216:U:C2 | 2.63 | 0.66 |
| 32:BJ:157:ARG:N | 32:BJ:158:PRO:HD3 | 2.02 | 0.66 |
| 16:AP:20:VAL:HG21 | 16:AP:32:TYR:CD1 | 2.30 | 0.66 |
| 20:CT:71:THR:HG22 | 20:CT:72:LEU:H | 1.60 | 0.66 |
| 28:BF:5:LEU:HD23 | 28:BF:6:ALA:H | 1.60 | 0.66 |
| 8:AH:91:ARG:HG2 | 8:AH:91:ARG:HH11 | 1.59 | 0.66 |
| 41:DS:4:LYS:HD3 | 41:DS:6:ILE:HD11 | 1.77 | 0.66 |
| 36:BN:9:LYS:C | 36:BN:10:LEU:HG | 2.14 | 0.66 |
| 4:CD:126:ILE:HG22 | 4:CD:127:THR:N | 2.09 | 0.66 |
| 23:BA:1858:G:O2' | 23:BA:1859:A:H8 | 1.77 | 0.66 |
| 25:DC:166:GLN:NE2 | 25:DC:166:GLN:HA | 2.10 | 0.66 |
| 23:BA:2758:A:C4 | 29:BG:67:LEU:HD21 | 2.30 | 0.66 |
| 13:AM:99:ARG:HB2 | 13:AM:101:GLN:NE2 | 2.10 | 0.66 |
| 35:BM:134:ARG:O | 35:BM:136:ALA:N | 2.27 | 0.66 |
| 7:CG:27:ILE:HD11 | 7:CG:43:PHE:HD2 | 1.59 | 0.66 |
| 23:BA:2661:G:O2' | 23:BA:2662:A:H5' | 1.95 | 0.66 |
| 1:CA:24:U:H2' | 1:CA:25:C:H6 | 1.59 | 0.66 |
| 1:AA:1111:A:H8 | 1:AA:1111:A:O5' | 1.79 | 0.66 |
| 1:AA:1426:C:H2' | 1:AA:1427:U:C6 | 2.30 | 0.66 |
| 34:DL:91:PHE:HD1 | 34:DL:91:PHE:N | 1.93 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:DL:91:PHE:N | 34:DL:91:PHE:CD1 | 2.63 | 0.66 |
| 23:BA:1546:A:C8 | 23:BA:154(B):C:O2 | 2.48 | 0.66 |
| 1:AA:1229:A:H2' | 1:AA:1230:C:C6 | 2.30 | 0.66 |
| 23:BA:1141:U:OP2 | 32:BJ:86:THR:HG23 | 1.94 | 0.66 |
| 39:DQ:79:PHE:HD1 | 39:DQ:79:PHE:C | 1.98 | 0.66 |
| 16:AP:17:TYR:CD1 | 16:AP:17:TYR:N | 2.63 | 0.66 |
| 23:BA:1813:G:C1' | 25:BC:50:THR:HG21 | 2.22 | 0.66 |
| 3:CC:35:GLU:HA | 3:CC:38:ARG:HG2 | 1.77 | 0.66 |
| 23:DA:1606:G:H5'' | 23:DA:1607:C:OP1 | 1.95 | 0.66 |
| 23:DA:1495:A:N3 | 23:DA:1495:A:H2' | 2.08 | 0.66 |
| 46:BX:10:LYS:O | 46:BX:11:ARG:HG2 | 1.95 | 0.66 |
| 23:BA:2277:G:H5'' | 35:BM:85:LYS:HB2 | 1.76 | 0.66 |
| 35:DM:8:LYS:HG3 | 35:DM:9:TYR:H | 1.59 | 0.66 |
| 24:DB:11:C:H3' | 24:DB:12:C:C6 | 2.30 | 0.66 |
| 23:BA:1683:C:N4 | 23:BA:1705:G:H1 | 1.93 | 0.66 |
| 11:AK:32:ILE:HD12 | 11:AK:72:ALA:HB2 | 1.78 | 0.66 |
| 1:AA:710:G:OP1 | 6:AF:54:LYS:HE2 | 1.94 | 0.66 |
| 40:DR:91:TYR:CD2 | 40:DR:91:TYR:O | 2.48 | 0.66 |
| 1:AA:707:C:H2' | 1:AA:708:C:H6 | 1.60 | 0.66 |
| 23:DA:1386:C:H2' | 23:DA:1387:C:H6 | 1.61 | 0.66 |
| 17:AQ:18:THR:HG23 | 17:AQ:69:LYS:HE3 | 1.77 | 0.66 |
| 23:DA:814:C:H41 | 34:DL:27:HIS:CD2 | 2.13 | 0.66 |
| 16:CP:43:LYS:HG2 | 16:CP:48:TRP:CD2 | 2.29 | 0.66 |
| 1:AA:1410:G:O2' | 1:AA:1411:C:H5' | 1.95 | 0.66 |
| 23:DA:2036:C:H6 | 23:DA:2036:C:H5' | 1.58 | 0.66 |
| 23:BA:227:A:H5' | 23:BA:228:A:C2 | 2.30 | 0.66 |
| 1:AA:433:C:H2' | 1:AA:434:U:H6 | 1.61 | 0.66 |
| 13:CM:96:LEU:HB3 | 13:CM:97:PRO:HD2 | 1.76 | 0.66 |
| 1:AA:1252:A:H61 | 1:AA:1285:A:H61 | 1.44 | 0.66 |
| 23:DA:1828:G:OP2 | 25:DC:239:ARG:NH1 | 2.28 | 0.66 |
| 12:AL:44:PRO:HG3 | 12:AL:52:ARG:HE | 1.61 | 0.66 |
| 1:AA:738:C:H2' | 1:AA:739:C:C6 | 2.30 | 0.66 |
| 37:BO:34:HIS:CE1 | 37:BO:54:LEU:HB3 | 2.30 | 0.66 |
| 23:BA:966:G:C4 | 23:BA:967:C:C5 | 2.83 | 0.66 |
| 1:AA:1010:G:H2' | 1:AA:1011:G:H8 | 1.59 | 0.66 |
| 44:BV:24:LEU:HD11 | 44:BV:86:VAL:HG22 | 1.77 | 0.66 |
| 9:CI:22:GLY:HA3 | 9:CI:60:ASP:OD2 | 1.94 | 0.66 |
| 23:BA:796:C:H2' | 23:BA:797:C:C6 | 2.31 | 0.66 |
| 23:BA:1856:G:N2 | 23:BA:1886:C:O2 | 2.28 | 0.66 |
| 23:BA:1536:A:H5'' | 23:BA:1537:C:OP2 | 1.94 | 0.66 |
| 23:BA:1746:G:C2 | 23:BA:1747:G:C8 | 2.84 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:AH:39:LEU:HB3 | 8:AH:45:ILE:HG23 | 1.78 | 0.66 |
| 23:DA:855:G:H5'' | 23:DA:856:C:OP2 | 1.95 | 0.66 |
| 23:BA:752:A:H3' | 52:B4:1:MET:HE3 | 1.78 | 0.66 |
| 1:CA:498:A:H4' | 1:CA:500:G:OP1 | 1.95 | 0.66 |
| 23:BA:609(B):G:N2 | 23:BA:619:G:H1' | 2.09 | 0.66 |
| 40:BR:7:THR:HG23 | 40:BR:22:VAL:HG11 | 1.76 | 0.66 |
| 1:AA:1226:C:N4 | 13:AM:104:ARG:HD2 | 2.10 | 0.66 |
| 25:BC:108:PRO:HB3 | 25:BC:143:HIS:CE1 | 2.31 | 0.66 |
| 23:DA:2294:C:H2' | 23:DA:2295:C:C6 | 2.30 | 0.66 |
| 25:DC:155:LEU:CD2 | 25:DC:177:LEU:HD21 | 2.23 | 0.66 |
| 5:CE:33:VAL:HG11 | 5:CE:109:ILE:HA | 1.76 | 0.66 |
| 23:DA:1331:A:O2' | 23:DA:1332:G:H8 | 1.78 | 0.66 |
| 2:CB:97:TRP:HH2 | 2:CB:176:GLU:HG3 | 1.60 | 0.66 |
| 28:BF:105:LYS:HZ3 | 49:B1:52:SER:HB2 | 1.61 | 0.66 |
| 1:AA:255:G:C4 | 1:AA:256:U:C5 | 2.84 | 0.66 |
| 46:DX:45:ASN:HD21 | 46:DX:47:GLN:HE21 | 1.41 | 0.66 |
| 6:CF:63:TYR:N | 6:CF:63:TYR:HD2 | 1.94 | 0.66 |
| 1:AA:57:G:C5 | 1:AA:58:C:C4 | 2.84 | 0.66 |
| 23:BA:2785:C:H2' | 23:BA:2786:U:O4' | 1.96 | 0.66 |
| 43:BU:2:ARG:O | 43:BU:4:LYS:N | 2.24 | 0.66 |
| 1:AA:976:G:C8 | 1:AA:1358:U:H2' | 2.31 | 0.66 |
| 23:BA:814:C:H41 | 34:BL:27:HIS:CD2 | 2.14 | 0.66 |
| 10:CJ:92:THR:HG23 | 10:CJ:93:GLY:H | 1.60 | 0.66 |
| 1:CA:862:C:H2' | 1:CA:863:U:H5' | 1.77 | 0.66 |
| 39:DQ:18:LEU:HD11 | 39:DQ:31:SER:H | 1.60 | 0.66 |
| 6:CF:67:MET:HB2 | 6:CF:68:PRO:HD2 | 1.77 | 0.66 |
| 28:BF:94:LEU:HD12 | 28:BF:99:MET:HA | 1.78 | 0.66 |
| 23:BA:481:G:C4 | 23:BA:507:A:C2 | 2.84 | 0.66 |
| 12:CL:6:ILE:O | 12:CL:10:VAL:HG23 | 1.96 | 0.66 |
| 10:CJ:7:LYS:O | 10:CJ:8:LEU:HD12 | 1.95 | 0.66 |
| 1:CA:1016:A:H2' | 1:CA:1017:G:O4' | 1.95 | 0.66 |
| 41:BS:22:ASP:HA | 41:BS:25:ARG:HH12 | 1.61 | 0.66 |
| 23:BA:1019:U:N3 | 23:BA:114(B):A:N6 | 2.43 | 0.66 |
| 28:BF:84:LYS:HG3 | 28:BF:85:GLY:N | 2.07 | 0.66 |
| 40:DR:38:LEU:HD23 | 40:DR:39:LEU:N | 2.11 | 0.66 |
| 23:BA:1614:A:H62 | 41:BS:93:ALA:CB | 2.05 | 0.66 |
| 16:AP:19:ILE:HB | 16:AP:37:GLY:O | 1.96 | 0.66 |
| 13:AM:39:ILE:HD11 | 13:AM:52:GLU:HG2 | 1.76 | 0.66 |
| 28:DF:70:VAL:HG12 | 28:DF:90:LEU:HD22 | 1.77 | 0.66 |
| 49:D1:50:THR:HG22 | 49:D1:51:TYR:H | 1.60 | 0.66 |
| 30:BH:111:PRO:HG2 | 30:BH:112:LYS:HE2 | 1.77 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BA:9:U:C4 | 23:BA:2629:A:C6 | 2.83 | 0.66 |
| 24:BB:21:G:H1 | 24:BB:62:C:N4 | 1.93 | 0.66 |
| 50:B2:40:LYS:HZ3 | 50:B2:49:CYS:HB3 | 1.59 | 0.66 |
| 29:BG:98:LEU:HD12 | 29:BG:99:VAL:H | 1.60 | 0.66 |
| 1:CA:373:A:O2' | 1:CA:374:A:H5' | 1.96 | 0.66 |
| 29:BG:55:PRO:HG2 | 29:BG:61:HIS:CE1 | 2.29 | 0.66 |
| 3:AC:35:GLU:HA | 3:AC:38:ARG:HG2 | 1.76 | 0.66 |
| 6:AF:15:ASP:OD1 | 6:AF:17:SER:HB2 | 1.95 | 0.66 |
| 23:DA:628:G:H2' | 23:DA:629:G:C8 | 2.31 | 0.66 |
| 26:DD:170:LEU:N | 26:DD:170:LEU:HD23 | 2.09 | 0.66 |
| 22:AV:6182:A:C6 | 22:AV:6183:G:C5 | 2.84 | 0.66 |
| 22:CV:6189:G:O2' | 22:CV:6190:U:H5' | 1.96 | 0.66 |
| 23:BA:2729:G:H2' | 23:BA:2730:C:H6 | 1.61 | 0.66 |
| 5:CE:57:LYS:O | 5:CE:61:TYR:CD2 | 2.49 | 0.66 |
| 46:DX:62:VAL:HG22 | 46:DX:63:ALA:N | 2.11 | 0.66 |
| 4:CD:105:VAL:HG13 | 4:CD:110:PHE:HB2 | 1.78 | 0.66 |
| 1:AA:668:G:H1' | 15:AO:46:HIS:HD2 | 1.60 | 0.66 |
| 34:BL:18:ARG:NH1 | 34:BL:18:ARG:HB3 | 2.10 | 0.66 |
| 45:DW:36:ILE:HG23 | 45:DW:58:THR:HG23 | 1.76 | 0.66 |
| 29:DG:94:TYR:H | 29:DG:94:TYR:HD1 | 1.44 | 0.66 |
| 23:DA:912:C:H2' | 23:DA:912:C:O2 | 1.96 | 0.66 |
| 23:DA:1411:C:H2' | 23:DA:1412:A:C8 | 2.30 | 0.66 |
| 51:D3:42:TRP:HA | 51:D3:42:TRP:HE3 | 1.60 | 0.66 |
| 23:BA:2773:C:OP1 | 26:BD:166:THR:OG1 | 2.13 | 0.66 |
| 8:CH:7:ALA:HB2 | 8:CH:85:ARG:HD3 | 1.76 | 0.66 |
| 2:CB:115:LEU:HD12 | 2:CB:118:LEU:HD12 | 1.76 | 0.66 |
| 34:DL:75:ILE:HD12 | 34:DL:75:ILE:H | 1.61 | 0.66 |
| 23:BA:18:C:O3' | 39:BQ:23:GLY:HA2 | 1.96 | 0.66 |
| 23:BA:2780:G:H4' | 23:BA:2781:A:OP2 | 1.95 | 0.66 |
| 32:DJ:114:LEU:HA | 32:DJ:118:PRO:HB3 | 1.77 | 0.66 |
| 16:AP:17:TYR:H | 16:AP:17:TYR:HD1 | 1.42 | 0.66 |
| 23:DA:603:A:C2 | 23:DA:655:A:N3 | 2.64 | 0.66 |
| 3:CC:113:ALA:HB3 | 3:CC:114:PRO:HD3 | 1.77 | 0.66 |
| 23:DA:1813:G:C1' | 25:DC:50:THR:HG21 | 2.24 | 0.66 |
| 42:DT:51:VAL:HG11 | 42:DT:81:VAL:HG12 | 1.76 | 0.66 |
| 44:DV:132:ASN:C | 44:DV:134:PRO:HD3 | 2.16 | 0.66 |
| 44:DV:134:PRO:O | 44:DV:136:PHE:N | 2.28 | 0.66 |
| 46:BX:11:ARG:HH12 | 46:BX:61:ARG:N | 1.94 | 0.66 |
| 16:AP:72:ARG:O | 16:AP:73:LEU:HD23 | 1.96 | 0.66 |
| 25:DC:134:ARG:HG3 | 25:DC:135:PHE:CD1 | 2.31 | 0.66 |
| 52:B4:12:ARG:HG3 | 52:B4:12:ARG:NH1 | 2.10 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BA:2599:G:C8 | 25:BC:237:GLU:HG3 | 2.31 | 0.66 |
| 23:DA:582:G:OP1 | 39:DQ:14:HIS:HD2 | 1.78 | 0.66 |
| 9:CI:97:LYS:HB3 | 9:CI:98:PRO:HD3 | 1.78 | 0.66 |
| 32:DJ:160:LYS:HE3 | 32:DJ:161:LEU:N | 2.10 | 0.66 |
| 8:CH:64:LYS:HG2 | 8:CH:79:VAL:HG21 | 1.78 | 0.66 |
| 23:BA:1248:G:OP1 | 39:BQ:2:PRO:HD2 | 1.96 | 0.66 |
| 23:DA:1794:U:H2' | 23:DA:1795:C:H6 | 1.59 | 0.66 |
| 32:DJ:148:GLY:HA3 | 32:DJ:149:PRO:O | 1.96 | 0.66 |
| 1:CA:444:C:O2' | 1:CA:445:G:H5' | 1.96 | 0.66 |
| 23:DA:2051:A:H4' | 26:DD:141:ILE:HG23 | 1.78 | 0.66 |
| 1:AA:1513:A:H2' | 1:AA:1514:C:C6 | 2.30 | 0.66 |
| 12:AL:74:HIS:HD2 | 12:AL:76:LEU:H | 1.41 | 0.66 |
| 23:BA:328:U:H4' | 43:BU:68:HIS:ND1 | 2.11 | 0.66 |
| 15:CO:15:PHE:O | 15:CO:27:VAL:HG22 | 1.96 | 0.66 |
| 1:CA:222:U:H2' | 1:CA:223:U:H6 | 1.59 | 0.66 |
| 23:DA:651:G:OP1 | 53:D5:19:SER:HB3 | 1.96 | 0.66 |
| 10:AJ:63:PHE:HD1 | 14:AN:58:LYS:HA | 1.60 | 0.66 |
| 1:CA:1346:A:C8 | 7:CG:10:ARG:NH2 | 2.64 | 0.66 |
| 23:DA:2846:G:H2' | 23:DA:2847:U:C6 | 2.31 | 0.66 |
| 39:DQ:90:VAL:HG13 | 39:DQ:91:ASP:H | 1.61 | 0.66 |
| 25:BC:238:GLY:O | 25:BC:239:ARG:O | 2.13 | 0.66 |
| 30:DH:102:SER:HA | 30:DH:107:ILE:O | 1.95 | 0.66 |
| 23:DA:1210:A:C5' | 23:DA:1210:A:C8 | 2.79 | 0.66 |
| 23:DA:2724:C:OP1 | 26:DD:118:LYS:HE3 | 1.96 | 0.66 |
| 26:DD:120:TRP:CD1 | 26:DD:155:LYS:HB3 | 2.31 | 0.66 |
| 23:DA:1156:A:H4' | 23:DA:1157:G:OP2 | 1.96 | 0.66 |
| 16:CP:72:ARG:O | 16:CP:73:LEU:HD23 | 1.96 | 0.66 |
| 8:CH:97:VAL:HG13 | 8:CH:98:LYS:N | 2.11 | 0.66 |
| 1:CA:20:U:C2' | 1:CA:21:G:H5' | 2.26 | 0.66 |
| 1:CA:1081:G:OP1 | 5:CE:18:ARG:HG2 | 1.96 | 0.66 |
| 1:AA:300:A:O5' | 1:AA:300:A:H8 | 1.79 | 0.66 |
| 36:BN:85:PRO:O | 36:BN:87:TYR:N | 2.29 | 0.66 |
| 17:AQ:45:HIS:CD2 | 17:AQ:47:PRO:HD3 | 2.31 | 0.66 |
| 25:BC:257:LEU:HD23 | 25:BC:257:LEU:C | 2.17 | 0.66 |
| 23:BA:737:C:C2' | 23:BA:738:G:H5' | 2.26 | 0.66 |
| 1:AA:1483:A:H5'' | 1:AA:1484:C:OP2 | 1.96 | 0.66 |
| 23:DA:2190:G:H2' | 23:DA:2191:G:H8 | 1.60 | 0.66 |
| 1:AA:1126:U:H2' | 1:AA:1127:G:C8 | 2.31 | 0.66 |
| 23:BA:1218:C:O2' | 23:BA:1219:G:H5' | 1.95 | 0.66 |
| 16:CP:20:VAL:HG21 | 16:CP:32:TYR:CG | 2.31 | 0.66 |
| 30:BH:102:SER:HA | 30:BH:107:ILE:O | 1.95 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 39:BQ:88:ILE:HD12 | 39:BQ:90:VAL:CG1 | 2.26 | 0.66 |
| 44:DV:53:ILE:HG22 | 44:DV:71:VAL:O | 1.96 | 0.66 |
| 49:B1:50:THR:HG22 | 49:B1:51:TYR:H | 1.59 | 0.66 |
| 23:BA:125:G:H4' | 23:BA:126:A:OP2 | 1.95 | 0.66 |
| 2:AB:97:TRP:CH2 | 2:AB:176:GLU:HG3 | 2.31 | 0.66 |
| 6:AF:8:ILE:HD11 | 6:AF:79:LEU:HD13 | 1.78 | 0.66 |
| 36:BN:4:LEU:O | 36:BN:6:SER:N | 2.28 | 0.66 |
| 4:CD:110:PHE:H | 4:CD:110:PHE:HD2 | 1.43 | 0.66 |
| 27:BE:101:LEU:HD12 | 27:BE:102:PRO:CD | 2.27 | 0.66 |
| 1:AA:579:G:C5 | 1:AA:580:U:C5 | 2.84 | 0.66 |
| 1:AA:1446:A:H4' | 1:AA:1446:A:OP1 | 1.96 | 0.66 |
| 2:AB:118:LEU:HD13 | 2:AB:142:LEU:HB2 | 1.77 | 0.66 |
| 3:AC:150:LYS:HB3 | 3:AC:201:TYR:HB2 | 1.76 | 0.66 |
| 8:CH:39:LEU:HB3 | 8:CH:45:ILE:HG23 | 1.76 | 0.66 |
| 33:BK:80:ASP:OD2 | 38:BP:71:GLY:HA3 | 1.94 | 0.66 |
| 1:AA:1306:A:H1' | 1:AA:1332:A:C2 | 2.31 | 0.66 |
| 34:BL:58:THR:O | 34:BL:61:ARG:NE | 2.26 | 0.65 |
| 32:DJ:86:THR:O | 32:DJ:89:LYS:HG2 | 1.95 | 0.65 |
| 39:BQ:57:PHE:O | 39:BQ:58:ARG:C | 2.34 | 0.65 |
| 37:DO:38:GLN:HB3 | 37:DO:47:THR:CG2 | 2.26 | 0.65 |
| 1:AA:551:U:H5' | 12:AL:118:LYS:NZ | 2.10 | 0.65 |
| 28:BF:70:VAL:HG12 | 28:BF:90:LEU:HD22 | 1.77 | 0.65 |
| 5:AE:43:LEU:HD22 | 5:AE:136:MET:CG | 2.24 | 0.65 |
| 1:CA:57:G:C5 | 1:CA:58:C:C4 | 2.84 | 0.65 |
| 9:AI:28:VAL:HG22 | 9:AI:63:ILE:HB | 1.78 | 0.65 |
| 4:AD:126:ILE:HG22 | 4:AD:127:THR:N | 2.10 | 0.65 |
| 23:DA:558:G:OP1 | 32:DJ:134:PRO:HD2 | 1.94 | 0.65 |
| 34:DL:14:LYS:O | 34:DL:15:ARG:HB2 | 1.95 | 0.65 |
| 35:BM:60:ARG:H | 44:BV:179:ASP:CG | 1.99 | 0.65 |
| 23:BA:588:U:H2' | 23:BA:589:C:C6 | 2.31 | 0.65 |
| 1:AA:1298:C:H4' | 1:AA:1299:A:N9 | 2.11 | 0.65 |
| 23:BA:1710:C:O2' | 23:BA:1711:C:H5' | 1.95 | 0.65 |
| 23:DA:1726:G:H2' | 23:DA:1727:U:C6 | 2.31 | 0.65 |
| 24:DB:30:C:H2' | 24:DB:31:C:H5' | 1.78 | 0.65 |
| 43:BU:6:HIS:HD2 | 43:BU:35:TYR:CE1 | 2.14 | 0.65 |
| 39:DQ:79:PHE:O | 39:DQ:83:LEU:HD13 | 1.96 | 0.65 |
| 39:BQ:92:ARG:HD3 | 39:BQ:94:ASN:HB3 | 1.78 | 0.65 |
| 16:AP:4:ILE:HB | 16:AP:66:PRO:HB3 | 1.76 | 0.65 |
| 4:CD:94:LEU:HA | 4:CD:97:LEU:HD12 | 1.78 | 0.65 |
| 1:CA:397:A:N7 | 1:CA:548:G:C8 | 2.65 | 0.65 |
| 23:DA:1493:C:C4 | 23:DA:2210:G:O2' | 2.49 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:DN:2:ARG:C | 36:DN:4:LEU:N | 2.47 | 0.65 |
| 3:AC:130:VAL:HG11 | 3:AC:153:VAL:HG21 | 1.78 | 0.65 |
| 2:AB:97:TRP:HH2 | 2:AB:176:GLU:HG3 | 1.61 | 0.65 |
| 3:AC:15:THR:HG21 | 3:AC:181:ASN:HA | 1.78 | 0.65 |
| 4:AD:155:LEU:HD23 | 4:AD:156:GLU:H | 1.61 | 0.65 |
| 1:CA:622:A:C8 | 1:CA:623:C:C6 | 2.84 | 0.65 |
| 19:AS:6:LYS:CG | 19:AS:7:LYS:HD3 | 2.26 | 0.65 |
| 23:BA:106:C:H1' | 43:BU:2:ARG:HE | 1.60 | 0.65 |
| 23:BA:773:U:H5' | 25:BC:47:GLY:HA3 | 1.78 | 0.65 |
| 1:CA:521:G:O6 | 1:CA:529:G:C2 | 2.50 | 0.65 |
| 23:BA:1153:C:H5' | 39:BQ:76:TYR:HE2 | 1.60 | 0.65 |
| 23:BA:987:G:H2' | 23:BA:988:A:H5' | 1.77 | 0.65 |
| 23:BA:226:G:N2 | 23:BA:228:A:H62 | 1.92 | 0.65 |
| 23:DA:1893:C:C5 | 23:DA:1894:C:C5 | 2.84 | 0.65 |
| 23:DA:2740:A:H2' | 23:DA:2741:A:C8 | 2.32 | 0.65 |
| 23:BA:1754:C:OP1 | 38:BP:96:ARG:NH1 | 2.25 | 0.65 |
| 23:DA:2773:C:OP1 | 26:DD:166:THR:OG1 | 2.14 | 0.65 |
| 41:DS:65:LEU:HB2 | 41:DS:68:ARG:HE | 1.60 | 0.65 |
| 1:AA:1448:C:H2' | 1:AA:1449:C:H6 | 1.59 | 0.65 |
| 23:BA:2093:G:H1 | 23:BA:2196:C:H42 | 1.44 | 0.65 |
| 1:AA:1095:U:H2' | 1:AA:1096:C:C6 | 2.31 | 0.65 |
| 34:BL:61:ARG:HA | 34:BL:62:LEU:HD13 | 1.77 | 0.65 |
| 23:DA:942:G:H5' | 34:DL:35:HIS:HB3 | 1.78 | 0.65 |
| 16:CP:20:VAL:HG21 | 16:CP:32:TYR:CD1 | 2.32 | 0.65 |
| 30:BH:68:LEU:O | 30:BH:138:ILE:HD13 | 1.95 | 0.65 |
| 47:DY:28:LYS:HE3 | 47:DY:56:GLN:NE2 | 2.11 | 0.65 |
| 42:BT:30:VAL:HG11 | 42:BT:39:ILE:CD1 | 2.27 | 0.65 |
| 1:CA:692:U:O2' | 1:CA:694:A:N7 | 2.28 | 0.65 |
| 12:CL:41:THR:HA | 12:CL:52:ARG:O | 1.95 | 0.65 |
| 43:BU:81:LYS:HZ3 | 43:BU:98:VAL:N | 1.93 | 0.65 |
| 4:CD:155:LEU:HD23 | 4:CD:156:GLU:H | 1.61 | 0.65 |
| 42:BT:57:LEU:HD11 | 42:BT:78:LYS:HB2 | 1.78 | 0.65 |
| 9:CI:17:VAL:HG13 | 9:CI:63:ILE:HD11 | 1.77 | 0.65 |
| 23:BA:662:G:P | 34:BL:18:ARG:HD2 | 2.36 | 0.65 |
| 8:CH:97:VAL:HG13 | 8:CH:98:LYS:H | 1.60 | 0.65 |
| 1:CA:457:C:H42 | 1:CA:475:G:H1 | 1.44 | 0.65 |
| 1:CA:106:C:C2' | 1:CA:107:G:H5' | 2.27 | 0.65 |
| 38:BP:27:THR:CG2 | 38:BP:90:GLN:HB3 | 2.26 | 0.65 |
| 23:DA:335:C:H2' | 23:DA:336:C:H6 | 1.61 | 0.65 |
| 1:AA:707:C:H2' | 1:AA:708:C:C6 | 2.32 | 0.65 |
| 40:BR:21:ARG:CZ | 40:BR:91:TYR:HE1 | 2.09 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1411:C:O2' | 1:CA:1412:C:H5' | 1.96 | 0.65 |
| 8:AH:64:LYS:HG2 | 8:AH:79:VAL:HG21 | 1.78 | 0.65 |
| 23:BA:17:G:H4' | 39:BQ:25:TRP:CH2 | 2.31 | 0.65 |
| 26:BD:30:PRO:O | 26:BD:32:PRO:HD3 | 1.96 | 0.65 |
| 23:DA:795:C:H2' | 23:DA:796:C:H6 | 1.60 | 0.65 |
| 1:CA:1306:A:H1' | 1:CA:1332:A:C2 | 2.32 | 0.65 |
| 27:DE:127:GLU:O | 27:DE:129:PHE:N | 2.28 | 0.65 |
| 27:DE:46:ARG:HH11 | 27:DE:46:ARG:HG2 | 1.61 | 0.65 |
| 12:AL:37:THR:O | 12:AL:78:GLU:HG2 | 1.96 | 0.65 |
| 23:BA:1430:C:H2' | 23:BA:1431:U:C6 | 2.31 | 0.65 |
| 23:BA:430:G:H5'' | 23:BA:431:U:OP2 | 1.96 | 0.65 |
| 38:DP:74:ARG:HD3 | 38:DP:76:PHE:CZ | 2.31 | 0.65 |
| 22:AV:6182:A:H2' | 22:AV:6183:G:O4' | 1.97 | 0.65 |
| 32:BJ:74:PHE:CE1 | 32:BJ:142:ARG:HD2 | 2.30 | 0.65 |
| 1:AA:552:U:O2' | 1:AA:553:A:H5' | 1.96 | 0.65 |
| 1:AA:691:G:N1 | 11:AK:52:GLY:HA2 | 2.12 | 0.65 |
| 3:CC:130:VAL:HG11 | 3:CC:153:VAL:HG21 | 1.78 | 0.65 |
| 24:DB:104:A:O4' | 44:DV:29:TYR:HE1 | 1.80 | 0.65 |
| 1:AA:1301:U:H3' | 1:AA:1302:U:H5'' | 1.77 | 0.65 |
| 1:CA:332:G:OP2 | 20:CT:10:LEU:HD23 | 1.97 | 0.65 |
| 46:BX:46:LEU:CD2 | 46:BX:61:ARG:HE | 2.10 | 0.65 |
| 25:DC:79:VAL:HG12 | 25:DC:113:VAL:HA | 1.77 | 0.65 |
| 23:BA:865:C:H4' | 23:BA:866:A:N7 | 2.11 | 0.65 |
| 23:BA:1165:U:H2' | 23:BA:1166:C:C6 | 2.31 | 0.65 |
| 40:BR:21:ARG:CZ | 40:BR:91:TYR:CE1 | 2.79 | 0.65 |
| 23:DA:924:C:H2' | 23:DA:925:C:C6 | 2.31 | 0.65 |
| 1:CA:500:G:N2 | 1:CA:546:G:H1' | 2.10 | 0.65 |
| 39:DQ:30:LYS:O | 39:DQ:31:SER:CB | 2.45 | 0.65 |
| 1:CA:1430:C:H2' | 1:CA:1431:C:C6 | 2.31 | 0.65 |
| 1:CA:411:A:C4 | 1:CA:413:G:O4' | 2.50 | 0.65 |
| 26:BD:158:GLY:O | 26:BD:159:HIS:C | 2.34 | 0.65 |
| 23:DA:2840:C:H4' | 36:DN:53:HIS:CD2 | 2.31 | 0.65 |
| 5:CE:147:ASP:O | 5:CE:151:LEU:HG | 1.96 | 0.65 |
| 23:DA:184:C:H2' | 23:DA:185:U:H6 | 1.60 | 0.65 |
| 7:CG:142:GLU:O | 7:CG:145:ALA:HB3 | 1.96 | 0.65 |
| 52:D4:11:LYS:HD2 | 52:D4:15:THR:HG21 | 1.77 | 0.65 |
| 43:BU:13:VAL:HG11 | 43:BU:72:VAL:HB | 1.79 | 0.65 |
| 23:DA:2780:G:H4' | 23:DA:2781:A:OP2 | 1.96 | 0.65 |
| 10:CJ:48:THR:CA | 10:CJ:62:HIS:HB3 | 2.18 | 0.65 |
| 27:BE:164:ARG:NH1 | 27:BE:164:ARG:HG2 | 2.01 | 0.65 |
| 25:DC:70:TRP:CH2 | 25:DC:150:LYS:HA | 2.31 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 44:BV:134:PRO:O | 44:BV:136:PHE:N | 2.30 | 0.65 |
| 25:DC:172:TYR:HD1 | 25:DC:185:VAL:O | 1.80 | 0.65 |
| 23:DA:2219:G:O2' | 23:DA:2224:G:H5' | 1.96 | 0.65 |
| 25:DC:166:GLN:N | 25:DC:166:GLN:HE21 | 1.94 | 0.65 |
| 9:CI:28:VAL:HG22 | 9:CI:63:ILE:HB | 1.77 | 0.65 |
| 1:CA:707:C:H2' | 1:CA:708:C:C6 | 2.31 | 0.65 |
| 35:BM:58:PHE:O | 35:BM:58:PHE:CD1 | 2.47 | 0.65 |
| 23:BA:2636:U:H4' | 26:BD:80:GLU:OE1 | 1.95 | 0.65 |
| 23:BA:828:U:O2 | 23:BA:828:U:C2' | 2.42 | 0.65 |
| 1:CA:1430:C:H2' | 1:CA:1431:C:H6 | 1.60 | 0.65 |
| 1:CA:1095:U:H2' | 1:CA:1096:C:C6 | 2.31 | 0.65 |
| 1:CA:193:C:H2' | 1:CA:194:C:C6 | 2.31 | 0.65 |
| 27:DE:13:SER:OG | 27:DE:14:PRO:HD2 | 1.96 | 0.65 |
| 23:DA:461:C:O2' | 23:DA:462:C:H5' | 1.96 | 0.65 |
| 23:BA:2889:C:H2' | 23:BA:2891:G:C8 | 2.31 | 0.65 |
| 15:AO:37:ASN:HD22 | 15:AO:37:ASN:H | 1.45 | 0.65 |
| 23:DA:2056:G:N2 | 50:D2:4:HIS:O | 2.30 | 0.65 |
| 38:BP:64:ARG:HD2 | 38:BP:73:GLU:HG2 | 1.78 | 0.65 |
| 1:CA:501:C:OP1 | 12:CL:116:ARG:NH2 | 2.30 | 0.65 |
| 37:BO:38:GLN:HB3 | 37:BO:47:THR:HG21 | 1.79 | 0.65 |
| 34:DL:33:ARG:HG2 | 34:DL:34:GLY:H | 1.60 | 0.65 |
| 53:D5:11:LYS:O | 53:D5:11:LYS:HE2 | 1.96 | 0.65 |
| 23:DA:1141:U:H6 | 32:DJ:86:THR:OG1 | 1.80 | 0.65 |
| 4:CD:63:LYS:HD2 | 4:CD:198:VAL:HG22 | 1.77 | 0.65 |
| 1:AA:323:U:O3' | 20:AT:22:ARG:HG2 | 1.96 | 0.65 |
| 23:DA:140:A:H8 | 23:DA:1408:C:O2' | 1.79 | 0.65 |
| 1:CA:1295:G:N2 | 1:CA:1302:U:H3 | 1.92 | 0.65 |
| 6:CF:63:TYR:N | 6:CF:63:TYR:CD2 | 2.65 | 0.65 |
| 46:BX:32:LYS:HG2 | 46:BX:33:LYS:H | 1.62 | 0.65 |
| 1:CA:339:C:OP2 | 33:DK:97:ARG:NH1 | 2.29 | 0.65 |
| 23:BA:1478:G:HO2' | 23:BA:1558:A:H2 | 1.44 | 0.65 |
| 25:BC:125:ILE:O | 25:BC:125:ILE:CG2 | 2.44 | 0.65 |
| 44:BV:180:VAL:C | 44:BV:182:LYS:H | 2.00 | 0.65 |
| 12:CL:23:VAL:HG13 | 12:CL:97:TYR:CE2 | 2.32 | 0.65 |
| 1:CA:974:A:H8 | 1:CA:974:A:OP1 | 1.80 | 0.65 |
| 7:CG:138:LYS:HE2 | 7:CG:142:GLU:OE2 | 1.97 | 0.65 |
| 19:AS:49:ILE:HD12 | 19:AS:49:ILE:H | 1.61 | 0.65 |
| 52:B4:35:ARG:HG3 | 52:B4:42:LEU:HD11 | 1.79 | 0.65 |
| 15:CO:69:TYR:HD1 | 15:CO:72:ARG:HH21 | 1.43 | 0.65 |
| 43:DU:30:VAL:HG23 | 43:DU:37:VAL:HG12 | 1.79 | 0.65 |
| 45:DW:35:ASN:HD22 | 45:DW:35:ASN:H | 1.44 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:AG:27:ILE:HD11 | 7:AG:43:PHE:HD2 | 1.61 | 0.65 |
| 32:BJ:127:LYS:HB2 | 32:BJ:140:PHE:CE1 | 2.32 | 0.65 |
| 10:CJ:63:PHE:HD1 | 14:CN:58:LYS:HA | 1.61 | 0.65 |
| 2:CB:69:LEU:HD13 | 2:CB:91:PRO:HB2 | 1.78 | 0.65 |
| 23:DA:1899:G:N2 | 23:DA:1902:C:C5 | 2.65 | 0.65 |
| 23:BA:197:A:C5' | 23:BA:197:A:H8 | 2.06 | 0.65 |
| 23:BA:1210:A:H8 | 23:BA:1210:A:H5' | 1.62 | 0.65 |
| 23:BA:1596:A:H2' | 23:BA:1597:A:H5' | 1.77 | 0.65 |
| 35:BM:48:GLU:O | 35:BM:52:VAL:HG12 | 1.96 | 0.65 |
| 2:CB:173:ALA:HA | 2:CB:176:GLU:HG3 | 1.77 | 0.65 |
| 36:BN:9:LYS:HE2 | 36:BN:43:GLU:OE2 | 1.97 | 0.65 |
| 23:DA:528:A:C2 | 23:DA:2043:C:C5' | 2.80 | 0.65 |
| 1:CA:1010:G:H2' | 1:CA:1011:G:H8 | 1.58 | 0.65 |
| 23:DA:226:G:N2 | 23:DA:228:A:N6 | 2.45 | 0.65 |
| 2:AB:135:GLN:O | 2:AB:139:LYS:HG2 | 1.96 | 0.65 |
| 23:DA:17:G:H4' | 39:DQ:25:TRP:CZ3 | 2.32 | 0.65 |
| 23:BA:912:C:H2' | 23:BA:912:C:O2 | 1.96 | 0.65 |
| 23:BA:828:U:C3' | 23:BA:828:U:O2 | 2.45 | 0.65 |
| 51:B3:42:TRP:HA | 51:B3:42:TRP:HE3 | 1.61 | 0.65 |
| 23:DA:992:C:O3' | 40:DR:72:VAL:HG11 | 1.96 | 0.65 |
| 23:DA:222:A:H5'' | 23:DA:421:U:OP1 | 1.97 | 0.65 |
| 23:BA:2846:G:H2' | 23:BA:2847:U:C6 | 2.31 | 0.65 |
| 32:BJ:90:LEU:O | 32:BJ:111:GLU:HG3 | 1.97 | 0.65 |
| 40:DR:47:VAL:O | 40:DR:49:THR:O | 2.14 | 0.65 |
| 42:DT:30:VAL:HG11 | 42:DT:39:ILE:CD1 | 2.26 | 0.65 |
| 26:BD:52:LEU:O | 26:BD:76:ARG:N | 2.30 | 0.65 |
| 3:CC:15:THR:HG21 | 3:CC:181:ASN:HA | 1.79 | 0.65 |
| 2:AB:80:ILE:HD12 | 2:AB:211:ILE:HB | 1.78 | 0.65 |
| 23:DA:322:A:OP2 | 27:DE:169:ASN:HB2 | 1.97 | 0.65 |
| 46:BX:27:GLU:CB | 46:BX:33:LYS:HG3 | 2.26 | 0.65 |
| 1:AA:350:G:O2' | 1:AA:351:G:H5' | 1.97 | 0.65 |
| 23:BA:1434:A:H61 | 23:BA:1558:A:H62 | 1.44 | 0.65 |
| 27:DE:31:HIS:CG | 34:DL:13:ASN:HB2 | 2.32 | 0.65 |
| 23:DA:277:C:H5' | 23:DA:278:A:OP2 | 1.96 | 0.65 |
| 1:CA:579:G:C4 | 1:CA:580:U:C5 | 2.84 | 0.65 |
| 23:BA:277:C:H5' | 23:BA:278:A:OP2 | 1.97 | 0.65 |
| 1:AA:754:C:H6 | 15:AO:69:TYR:CE2 | 2.14 | 0.65 |
| 35:DM:32:PHE:HZ | 35:DM:111:GLU:HG2 | 1.60 | 0.65 |
| 23:BA:979:G:H3' | 23:BA:980:A:H5'' | 1.79 | 0.65 |
| 24:DB:31:C:O2 | 24:DB:31:C:H2' | 1.97 | 0.65 |
| 44:DV:5:LEU:HG | 44:DV:47:VAL:HG21 | 1.79 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 44:DV:5:LEU:HD23 | 44:DV:6:LYS:N | 2.11 | 0.65 |
| 25:BC:244:ARG:HB2 | 25:BC:245:PRO:CD | 2.26 | 0.65 |
| 8:AH:119:LEU:HB2 | 8:AH:124:ALA:HB2 | 1.77 | 0.65 |
| 12:AL:5:THR:HG23 | 12:AL:8:GLN:HG3 | 1.78 | 0.65 |
| 1:CA:1298:C:H4' | 1:CA:1299:A:N9 | 2.11 | 0.65 |
| 32:BJ:80:ALA:O | 32:BJ:83:ILE:HG12 | 1.97 | 0.65 |
| 32:BJ:80:ALA:O | 32:BJ:83:ILE:CG1 | 2.45 | 0.65 |
| 46:BX:30:VAL:O | 46:BX:30:VAL:HG12 | 1.97 | 0.65 |
| 34:BL:75:ILE:HD12 | 34:BL:75:ILE:H | 1.61 | 0.65 |
| 24:DB:2:C:H2' | 24:DB:3:C:C6 | 2.32 | 0.65 |
| 27:DE:39:TRP:O | 27:DE:43:LYS:HG2 | 1.96 | 0.65 |
| 47:DY:2:LYS:HA | 47:DY:5:GLU:CD | 2.17 | 0.65 |
| 1:CA:965:A:H2 | 1:CA:969:A:C2 | 2.14 | 0.65 |
| 40:DR:41:GLY:HA3 | 40:DR:45:THR:OG1 | 1.97 | 0.65 |
| 23:DA:1141:U:OP2 | 32:DJ:86:THR:HG23 | 1.97 | 0.65 |
| 37:DO:89:ARG:O | 37:DO:90:GLY:O | 2.14 | 0.65 |
| 1:AA:377:G:OP1 | 16:AP:3:LYS:HD2 | 1.97 | 0.65 |
| 44:DV:51:ALA:HB1 | 44:DV:57:ILE:HD11 | 1.77 | 0.65 |
| 42:BT:39:ILE:O | 42:BT:43:VAL:HG12 | 1.96 | 0.65 |
| 25:BC:172:TYR:HD1 | 25:BC:186:HIS:HA | 1.57 | 0.65 |
| 25:DC:186:HIS:CD2 | 25:DC:188:GLU:H | 2.15 | 0.65 |
| 36:BN:38:VAL:HB | 36:BN:39:PRO:CD | 2.26 | 0.65 |
| 36:BN:100:LEU:HD21 | 36:BN:113:LEU:HB2 | 1.79 | 0.65 |
| 23:BA:2476:A:C2 | 23:BA:2477:C:C6 | 2.85 | 0.65 |
| 10:CJ:4:ILE:HB | 10:CJ:74:ILE:HD11 | 1.79 | 0.65 |
| 8:CH:77:GLU:HG3 | 8:CH:78:GLN:N | 2.12 | 0.65 |
| 23:DA:1973:G:H2' | 23:DA:1974:C:H6 | 1.62 | 0.65 |
| 23:DA:1710:C:O2' | 23:DA:1711:C:H5' | 1.97 | 0.65 |
| 1:CA:382:A:H2' | 1:CA:383:A:C8 | 2.32 | 0.65 |
| 14:AN:44:LEU:HD12 | 14:AN:44:LEU:O | 1.96 | 0.65 |
| 32:BJ:68:ASN:ND2 | 32:BJ:68:ASN:H | 1.95 | 0.65 |
| 53:D5:50:LEU:O | 53:D5:51:ALA:CB | 2.44 | 0.65 |
| 28:DF:161:THR:HG21 | 28:DF:172:LEU:HD23 | 1.79 | 0.65 |
| 1:AA:386:C:H2' | 1:AA:387:U:C5' | 2.27 | 0.65 |
| 3:CC:134:ILE:CG2 | 3:CC:151:VAL:HB | 2.26 | 0.65 |
| 3:CC:91:LEU:HB3 | 3:CC:99:VAL:HG11 | 1.79 | 0.65 |
| 41:DS:73:ALA:O | 41:DS:106:ILE:HG12 | 1.97 | 0.65 |
| 5:CE:51:VAL:O | 5:CE:55:VAL:HG23 | 1.95 | 0.65 |
| 1:AA:457:C:H42 | 1:AA:475:G:H1 | 1.45 | 0.65 |
| 23:DA:557:U:H2' | 23:DA:558:G:C8 | 2.31 | 0.65 |
| 23:BA:1288:U:C2 | 23:BA:1327:C:O2 | 2.50 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:DO:36:TYR:CD1 | 37:DO:36:TYR:N | 2.65 | 0.65 |
| 27:BE:31:HIS:CG | 34:BL:13:ASN:HB2 | 2.32 | 0.65 |
| 33:BK:87:ILE:HG13 | 33:BK:91:LEU:HD12 | 1.78 | 0.65 |
| 38:DP:27:THR:CG2 | 38:DP:90:GLN:HB3 | 2.27 | 0.65 |
| 23:DA:2637:U:H5'' | 26:DD:82:ARG:NH2 | 2.11 | 0.65 |
| 9:AI:97:LYS:HB3 | 9:AI:98:PRO:HD3 | 1.78 | 0.65 |
| 1:AA:1448:C:H2' | 1:AA:1449:C:C6 | 2.32 | 0.65 |
| 26:BD:32:PRO:HA | 26:BD:90:THR:HG22 | 1.78 | 0.65 |
| 6:AF:44:GLY:HA2 | 6:AF:59:TYR:CZ | 2.32 | 0.65 |
| 1:AA:968:A:OP1 | 1:AA:968:A:H8 | 1.80 | 0.65 |
| 23:DA:1857:G:N2 | 23:DA:1886:C:N4 | 2.45 | 0.65 |
| 22:CV:6182:A:H2' | 22:CV:6183:G:O4' | 1.96 | 0.64 |
| 39:DQ:83:LEU:HD12 | 39:DQ:113:ALA:CB | 2.27 | 0.64 |
| 23:BA:1614:A:H61 | 41:BS:88:ARG:H | 1.45 | 0.64 |
| 23:BA:2219:G:O2' | 23:BA:2224:G:H5' | 1.96 | 0.64 |
| 24:BB:103:U:O2' | 24:BB:104:A:H5' | 1.96 | 0.64 |
| 3:AC:134:ILE:HG21 | 3:AC:168:ALA:HB3 | 1.79 | 0.64 |
| 25:BC:172:TYR:HD1 | 25:BC:185:VAL:O | 1.79 | 0.64 |
| 23:DA:380:U:O2' | 46:DX:20:ARG:HB3 | 1.97 | 0.64 |
| 23:BA:2815:C:O2' | 50:B2:43:HIS:CD2 | 2.50 | 0.64 |
| 30:DH:66:GLU:HG2 | 30:DH:67:ARG:CZ | 2.27 | 0.64 |
| 28:DF:36:LYS:HD3 | 28:DF:160:VAL:HG21 | 1.79 | 0.64 |
| 27:DE:117:ARG:NH2 | 27:DE:187:VAL:HA | 2.12 | 0.64 |
| 23:BA:1006:C:H1' | 32:BJ:129:MET:HB3 | 1.79 | 0.64 |
| 1:CA:1446:A:OP1 | 1:CA:1446:A:H4' | 1.97 | 0.64 |
| 25:DC:80:ALA:HB3 | 25:DC:94:LEU:HD13 | 1.78 | 0.64 |
| 23:DA:1268:A:H2' | 23:DA:1269:A:O5' | 1.97 | 0.64 |
| 23:DA:2364:C:C2' | 23:DA:2365:G:H5' | 2.27 | 0.64 |
| 26:DD:16:ARG:O | 26:DD:18:ASP:N | 2.29 | 0.64 |
| 15:CO:44:LYS:HZ3 | 15:CO:44:LYS:HB2 | 1.61 | 0.64 |
| 1:AA:334:C:H2' | 1:AA:335:C:H6 | 1.63 | 0.64 |
| 23:DA:626:U:O2 | 34:DL:105:LEU:HB3 | 1.97 | 0.64 |
| 34:DL:109:GLY:O | 34:DL:111:ARG:N | 2.30 | 0.64 |
| 23:DA:2262:U:H2' | 23:DA:2263:C:H6 | 1.62 | 0.64 |
| 23:BA:1971:A:C2 | 25:BC:241:PRO:HD3 | 2.31 | 0.64 |
| 23:BA:114(B):A:H4' | 32:BJ:48:ARG:NH2 | 2.11 | 0.64 |
| 25:DC:35:LYS:HE2 | 25:DC:103:ARG:HA | 1.79 | 0.64 |
| 4:CD:49:ARG:NE | 4:CD:50:ARG:H | 1.95 | 0.64 |
| 43:BU:29:GLU:HB3 | 43:BU:38:ILE:CB | 2.26 | 0.64 |
| 23:BA:2698:U:H2' | 23:BA:2699:C:C6 | 2.33 | 0.64 |
| 44:BV:51:ALA:HB1 | 44:BV:57:ILE:HD11 | 1.77 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 37:DO:51:ALA:HB1 | 37:DO:72:ALA:CB | 2.26 | 0.64 |
| 23:DA:2758:A:C4 | 29:DG:67:LEU:HD21 | 2.32 | 0.64 |
| 11:CK:95:ILE:HG21 | 11:CK:108:ILE:HD13 | 1.79 | 0.64 |
| 23:DA:847:U:OP2 | 23:DA:929:G:O6 | 2.15 | 0.64 |
| 23:DA:2892:A:H2' | 23:DA:2893:G:H5' | 1.79 | 0.64 |
| 25:DC:25:THR:HG21 | 25:DC:81:ALA:HA | 1.77 | 0.64 |
| 1:AA:1180:A:H5' | 9:AI:103:THR:HG23 | 1.78 | 0.64 |
| 23:DA:2209:C:O2 | 23:DA:2216:G:C2 | 2.51 | 0.64 |
| 38:BP:90:GLN:NE2 | 38:BP:90:GLN:HA | 2.12 | 0.64 |
| 23:BA:2346:A:H5'' | 23:BA:2383:G:C1' | 2.27 | 0.64 |
| 1:AA:579:G:C4 | 1:AA:580:U:C5 | 2.84 | 0.64 |
| 23:BA:1162:G:C2' | 23:BA:1163:G:H5' | 2.28 | 0.64 |
| 12:CL:6:ILE:H | 12:CL:6:ILE:HD12 | 1.61 | 0.64 |
| 23:BA:2394:C:OP1 | 34:BL:63:PRO:HD2 | 1.97 | 0.64 |
| 23:BA:2852:G:O2' | 23:BA:2853:C:H5' | 1.97 | 0.64 |
| 19:AS:5:LEU:HD12 | 19:AS:8:GLY:O | 1.97 | 0.64 |
| 1:AA:222:U:H2' | 1:AA:223:U:H6 | 1.62 | 0.64 |
| 1:CA:1311:G:H1 | 1:CA:1326:C:H42 | 1.43 | 0.64 |
| 34:DL:95:VAL:HG23 | 34:DL:125:VAL:HG23 | 1.79 | 0.64 |
| 34:DL:62:LEU:CD2 | 53:D5:25:MET:HB2 | 2.27 | 0.64 |
| 23:DA:2275:C:H5' | 23:DA:2275:C:H6 | 1.62 | 0.64 |
| 53:D5:11:LYS:HD2 | 53:D5:64:TYR:CZ | 2.33 | 0.64 |
| 4:CD:21:LEU:HD12 | 4:CD:21:LEU:H | 1.63 | 0.64 |
| 4:AD:21:LEU:HD12 | 4:AD:21:LEU:H | 1.61 | 0.64 |
| 20:CT:26:ASN:N | 20:CT:26:ASN:HD22 | 1.91 | 0.64 |
| 26:DD:1:MET:HB3 | 26:DD:84:PHE:HB2 | 1.79 | 0.64 |
| 23:DA:1654:A:OP1 | 36:DN:2:ARG:N | 2.30 | 0.64 |
| 1:CA:738:C:H2' | 1:CA:739:C:H6 | 1.59 | 0.64 |
| 1:AA:781:A:C2' | 1:AA:782:A:H5' | 2.28 | 0.64 |
| 23:DA:2593:U:H2' | 23:DA:2594:C:H6 | 1.60 | 0.64 |
| 10:AJ:45:ARG:HH12 | 14:AN:36:PHE:HD2 | 1.45 | 0.64 |
| 27:BE:127:GLU:O | 27:BE:129:PHE:N | 2.28 | 0.64 |
| 38:BP:84:GLN:HA | 38:BP:84:GLN:HE21 | 1.62 | 0.64 |
| 23:BA:565:C:H2' | 23:BA:566:U:O5' | 1.95 | 0.64 |
| 5:AE:140:ARG:O | 5:AE:140:ARG:HG2 | 1.96 | 0.64 |
| 1:AA:444:C:O2' | 1:AA:445:G:H5' | 1.96 | 0.64 |
| 1:AA:186(D):G:C6 | 1:AA:191(E):G:N1 | 2.65 | 0.64 |
| 53:D5:23:VAL:CG1 | 53:D5:47:LYS:HB3 | 2.27 | 0.64 |
| 53:D5:22:VAL:HG12 | 53:D5:50:LEU:HD12 | 1.79 | 0.64 |
| 23:DA:960:A:H61 | 35:DM:82:ARG:NH2 | 1.96 | 0.64 |
| 34:BL:95:VAL:HG23 | 34:BL:125:VAL:HG23 | 1.78 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:979:C:H5'' | 1:CA:980:C:OP2 | 1.96 | 0.64 |
| 16:CP:28:ARG:HH11 | 16:CP:28:ARG:CG | 2.09 | 0.64 |
| 12:AL:85:ARG:HB2 | 12:AL:100:VAL:HG23 | 1.80 | 0.64 |
| 12:AL:103:VAL:O | 12:AL:106:ALA:HB3 | 1.96 | 0.64 |
| 30:DH:82:ARG:C | 30:DH:89:TYR:HB2 | 2.18 | 0.64 |
| 28:DF:71:THR:HG22 | 28:DF:89:GLY:O | 1.98 | 0.64 |
| 23:BA:1411:C:H2' | 23:BA:1412:A:C8 | 2.32 | 0.64 |
| 1:CA:397:A:N6 | 1:CA:548:G:C5 | 2.66 | 0.64 |
| 25:BC:223:GLY:HA3 | 25:BC:231:HIS:CE1 | 2.32 | 0.64 |
| 26:DD:52:LEU:O | 26:DD:76:ARG:N | 2.31 | 0.64 |
| 12:AL:44:PRO:HG3 | 12:AL:52:ARG:NE | 2.12 | 0.64 |
| 29:BG:140:LYS:O | 29:BG:144:VAL:HG23 | 1.96 | 0.64 |
| 23:BA:1486:A:N6 | 23:BA:1504:C:H42 | 1.95 | 0.64 |
| 24:DB:13:A:C8 | 45:DW:74:ARG:NH2 | 2.65 | 0.64 |
| 36:DN:100:LEU:HD21 | 36:DN:113:LEU:HB2 | 1.80 | 0.64 |
| 24:DB:21:G:H1 | 24:DB:62:C:N4 | 1.94 | 0.64 |
| 23:DA:2820:A:O4' | 36:DN:5:LYS:HG3 | 1.97 | 0.64 |
| 1:CA:17:U:H1' | 1:CA:1080:A:N3 | 2.12 | 0.64 |
| 2:CB:118:LEU:HD13 | 2:CB:142:LEU:HB2 | 1.78 | 0.64 |
| 23:DA:2365:G:H4' | 45:DW:60:PHE:CZ | 2.33 | 0.64 |
| 44:BV:5:LEU:HG | 44:BV:47:VAL:HG21 | 1.78 | 0.64 |
| 36:DN:85:PRO:O | 36:DN:87:TYR:N | 2.30 | 0.64 |
| 23:DA:2212:A:H1' | 23:DA:2215:G:C4 | 2.33 | 0.64 |
| 32:DJ:53:ILE:O | 32:DJ:57:LEU:HD22 | 1.96 | 0.64 |
| 37:BO:12:PHE:HE1 | 37:BO:16:ASN:HD21 | 1.45 | 0.64 |
| 32:BJ:157:ARG:N | 32:BJ:158:PRO:CD | 2.51 | 0.64 |
| 28:DF:84:LYS:O | 28:DF:86:MET:HG3 | 1.96 | 0.64 |
| 1:AA:411:A:C5 | 1:AA:429:U:C5 | 2.86 | 0.64 |
| 1:CA:1252:A:H61 | 1:CA:1285:A:H61 | 1.45 | 0.64 |
| 46:DX:11:ARG:HB3 | 46:DX:12:PRO:HD2 | 1.80 | 0.64 |
| 23:DA:1510:A:H2' | 23:DA:1511:A:H8 | 1.61 | 0.64 |
| 1:CA:987:G:H1 | 1:CA:1218:C:N4 | 1.94 | 0.64 |
| 1:CA:625:G:H2' | 1:CA:626:U:C6 | 2.31 | 0.64 |
| 35:DM:22:LYS:HD3 | 35:DM:22:LYS:O | 1.98 | 0.64 |
| 29:DG:54:ARG:HB3 | 29:DG:65:HIS:CD2 | 2.32 | 0.64 |
| 23:BA:990:A:H5'' | 23:BA:991:C:OP2 | 1.96 | 0.64 |
| 8:AH:77:GLU:HG3 | 8:AH:78:GLN:H | 1.61 | 0.64 |
| 23:DA:1006:C:H1' | 32:DJ:129:MET:HB3 | 1.79 | 0.64 |
| 23:DA:2036:C:C6 | 23:DA:2036:C:H5' | 2.32 | 0.64 |
| 50:D2:4:HIS:HB3 | 50:D2:5:PRO:HD3 | 1.79 | 0.64 |
| 29:BG:54:ARG:HB3 | 29:BG:65:HIS:CD2 | 2.33 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:DA:176:G:C2' | 23:DA:177:G:H5' | 2.27 | 0.64 |
| 1:CA:1448:C:H2' | 1:CA:1449:C:H6 | 1.63 | 0.64 |
| 4:AD:173:TRP:CD1 | 4:AD:174:LEU:HG | 2.33 | 0.64 |
| 23:DA:2828:C:O2' | 23:DA:2829:C:H5' | 1.98 | 0.64 |
| 39:BQ:114:LYS:O | 39:BQ:117:GLN:HB2 | 1.97 | 0.64 |
| 22:CV:6198:U:H2' | 22:CV:6199:G:H8 | 1.63 | 0.64 |
| 23:BA:855:G:H5'' | 23:BA:856:C:OP2 | 1.97 | 0.64 |
| 23:DA:492:A:H2' | 23:DA:493:G:O4' | 1.96 | 0.64 |
| 43:BU:89:PHE:H | 43:BU:90:LEU:HD23 | 1.62 | 0.64 |
| 1:AA:950:U:H4' | 1:AA:971:G:N2 | 2.12 | 0.64 |
| 38:DP:57:PHE:O | 38:DP:59:THR:N | 2.31 | 0.64 |
| 25:DC:182:LEU:H | 25:DC:272:ALA:HB3 | 1.62 | 0.64 |
| 16:AP:28:ARG:NH1 | 16:AP:29:ASP:OD1 | 2.30 | 0.64 |
| 25:DC:242:ARG:HG2 | 25:DC:242:ARG:NH1 | 2.11 | 0.64 |
| 23:BA:2886:G:O2' | 23:BA:2887:U:H5' | 1.98 | 0.64 |
| 5:CE:109:ILE:HG22 | 5:CE:110:LEU:HD23 | 1.80 | 0.64 |
| 27:BE:9:ILE:HD11 | 27:BE:125:LEU:CG | 2.28 | 0.64 |
| 46:BX:13:ILE:HG23 | 46:BX:14:VAL:H | 1.63 | 0.64 |
| 46:BX:45:ASN:HD21 | 46:BX:47:GLN:HE21 | 1.45 | 0.64 |
| 25:BC:134:ARG:HG3 | 25:BC:135:PHE:CD1 | 2.32 | 0.64 |
| 23:BA:952:G:P | 35:BM:16:ARG:HH22 | 2.21 | 0.64 |
| 1:CA:781:A:C2' | 1:CA:782:A:H5' | 2.27 | 0.64 |
| 23:DA:1475:G:N2 | 23:DA:1519:G:C5 | 2.66 | 0.64 |
| 35:BM:37:LEU:HG | 35:BM:128:LYS:O | 1.97 | 0.64 |
| 35:BM:22:LYS:O | 35:BM:22:LYS:HD3 | 1.98 | 0.64 |
| 4:CD:79:PHE:CG | 4:CD:207:TYR:HD1 | 2.16 | 0.64 |
| 24:BB:31:C:H2' | 24:BB:31:C:O2 | 1.98 | 0.64 |
| 1:AA:1111:A:C2 | 3:AC:177:THR:HG23 | 2.33 | 0.64 |
| 1:AA:937:A:H1' | 1:AA:1379:G:N2 | 2.12 | 0.64 |
| 23:BA:1833:U:C2 | 23:BA:1834:U:C5 | 2.86 | 0.64 |
| 1:CA:638:G:O2' | 1:CA:639:G:H5' | 1.96 | 0.64 |
| 23:BA:2190:G:H2' | 23:BA:2191:G:H8 | 1.61 | 0.64 |
| 26:BD:47:VAL:HG21 | 26:BD:86:PRO:HD3 | 1.78 | 0.64 |
| 23:DA:1187:G:H5'' | 40:DR:81:TYR:CE2 | 2.33 | 0.64 |
| 1:CA:622:A:C8 | 1:CA:623:C:C5 | 2.85 | 0.64 |
| 32:DJ:69:VAL:HG13 | 32:DJ:71:MET:HG3 | 1.79 | 0.64 |
| 28:BF:174:GLU:HG2 | 28:BF:180:PHE:CD1 | 2.33 | 0.64 |
| 23:DA:2655:G:N2 | 23:DA:2664:G:C5 | 2.66 | 0.64 |
| 1:CA:255:G:H4' | 17:CQ:17:LYS:HD3 | 1.79 | 0.64 |
| 10:CJ:45:ARG:HH12 | 14:CN:36:PHE:HD2 | 1.46 | 0.64 |
| 1:AA:1411:C:O2' | 1:AA:1412:C:H5' | 1.97 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BE:13:SER:OG | 27:BE:14:PRO:HD2 | 1.97 | 0.64 |
| 1:CA:1126:U:H2' | 1:CA:1127:G:C8 | 2.32 | 0.64 |
| 24:BB:2:C:H2' | 24:BB:3:C:C6 | 2.33 | 0.64 |
| 11:CK:48:ILE:HD11 | 11:CK:64:ALA:HA | 1.80 | 0.64 |
| 51:D3:38:LYS:HG2 | 51:D3:39:TYR:H | 1.63 | 0.64 |
| 1:CA:1512:U:H3 | 1:CA:1523:G:H1 | 1.46 | 0.64 |
| 23:DA:83:G:H1 | 23:DA:102:G:HO2' | 0.66 | 0.64 |
| 42:DT:63:LYS:NZ | 42:DT:72:LYS:HB3 | 2.13 | 0.64 |
| 32:DJ:157:ARG:HG2 | 32:DJ:157:ARG:O | 1.96 | 0.64 |
| 26:DD:59:VAL:O | 26:DD:59:VAL:HG12 | 1.98 | 0.64 |
| 2:AB:97:TRP:HZ2 | 2:AB:102:LEU:CD1 | 2.11 | 0.64 |
| 25:DC:172:TYR:HD1 | 25:DC:186:HIS:HA | 1.60 | 0.64 |
| 23:BA:588:U:H1' | 27:BE:90:PHE:CD1 | 2.33 | 0.64 |
| 1:CA:1443:G:H3' | 1:CA:1446:A:H5'' | 1.79 | 0.64 |
| 23:DA:2401:U:H2' | 23:DA:2402:C:H5'' | 1.80 | 0.64 |
| 1:AA:862:C:H2' | 1:AA:863:U:H5' | 1.80 | 0.64 |
| 1:AA:922:G:C6 | 1:AA:923:A:C6 | 2.85 | 0.64 |
| 7:AG:50:ILE:HD12 | 7:AG:61:VAL:HG11 | 1.80 | 0.64 |
| 29:BG:54:ARG:HB3 | 29:BG:65:HIS:HD2 | 1.63 | 0.64 |
| 44:BV:9:TYR:CZ | 44:BV:61:LEU:HD13 | 2.33 | 0.64 |
| 23:BA:60:G:H4' | 23:BA:61:G:P | 2.37 | 0.64 |
| 1:CA:1111:A:O5' | 1:CA:1111:A:H8 | 1.80 | 0.64 |
| 27:BE:181:LEU:HD21 | 27:BE:186:ILE:HD11 | 1.80 | 0.64 |
| 2:AB:158:LEU:H | 2:AB:158:LEU:HD12 | 1.63 | 0.64 |
| 15:CO:76:GLU:OE2 | 15:CO:76:GLU:HA | 1.98 | 0.64 |
| 32:BJ:148:GLY:HA3 | 32:BJ:149:PRO:O | 1.98 | 0.64 |
| 36:BN:11:ASN:O | 36:BN:12:ARG:HB2 | 1.98 | 0.64 |
| 40:BR:41:GLY:HA3 | 40:BR:45:THR:OG1 | 1.98 | 0.64 |
| 37:DO:12:PHE:O | 37:DO:15:ARG:HG3 | 1.97 | 0.64 |
| 30:DH:92:VAL:CG2 | 30:DH:97:ILE:HG12 | 2.27 | 0.64 |
| 23:BA:1493:C:C4 | 23:BA:2210:G:O2' | 2.51 | 0.64 |
| 23:DA:1786:A:H1' | 23:DA:1938:A:N6 | 2.13 | 0.64 |
| 25:DC:85:ASP:OD2 | 25:DC:86:PRO:HD2 | 1.98 | 0.64 |
| 36:DN:50:HIS:O | 36:DN:54:LEU:HB2 | 1.97 | 0.64 |
| 46:DX:27:GLU:CG | 46:DX:33:LYS:HG3 | 2.28 | 0.64 |
| 23:BA:2892:A:H2' | 23:BA:2893:G:H5' | 1.80 | 0.64 |
| 23:DA:2785:C:H2' | 23:DA:2786:U:O4' | 1.98 | 0.64 |
| 23:BA:1669:A:O3' | 23:BA:2549:G:H5' | 1.98 | 0.64 |
| 43:BU:76:CYS:SG | 43:BU:77:PRO:HD3 | 2.38 | 0.64 |
| 23:DA:65:C:H2' | 23:DA:66:C:H6 | 1.60 | 0.64 |
| 29:DG:98:LEU:HD12 | 29:DG:99:VAL:H | 1.62 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:382:A:H2' | 1:AA:383:A:C8 | 2.33 | 0.64 |
| 40:DR:7:THR:HG23 | 40:DR:22:VAL:HG11 | 1.79 | 0.64 |
| 1:CA:775:G:C2' | 1:CA:776:G:H5' | 2.27 | 0.64 |
| 35:BM:80:GLU:HA | 35:BM:80:GLU:OE2 | 1.97 | 0.64 |
| 6:CF:18:GLN:HA | 6:CF:21:LEU:HD23 | 1.80 | 0.64 |
| 44:BV:120:ILE:HD13 | 44:BV:120:ILE:N | 2.12 | 0.64 |
| 26:DD:21:VAL:HG12 | 26:DD:23:VAL:HG13 | 1.80 | 0.64 |
| 5:AE:102:ALA:HB2 | 5:AE:120:THR:CG2 | 2.28 | 0.64 |
| 23:BA:2846:G:C5 | 23:BA:2847:U:C5 | 2.85 | 0.64 |
| 36:DN:38:VAL:CB | 36:DN:39:PRO:HD3 | 2.24 | 0.64 |
| 42:BT:44:GLU:OE2 | 42:BT:50:LYS:HG2 | 1.97 | 0.64 |
| 6:AF:53:ALA:HB3 | 6:AF:86:ARG:NH1 | 2.13 | 0.64 |
| 53:B5:11:LYS:HD2 | 53:B5:64:TYR:CZ | 2.33 | 0.64 |
| 23:BA:242:G:C5' | 53:B5:63:PRO:HG2 | 2.27 | 0.64 |
| 34:BL:45:LEU:HD23 | 34:BL:46:LYS:H | 1.61 | 0.64 |
| 23:DA:2723:C:H4' | 36:DN:2:ARG:NH2 | 2.12 | 0.64 |
| 3:AC:152:ILE:HD11 | 3:AC:167:TRP:HD1 | 1.60 | 0.64 |
| 19:AS:63:THR:N | 19:AS:66:MET:HE3 | 2.13 | 0.64 |
| 1:CA:53:A:N1 | 1:CA:54:C:C2 | 2.67 | 0.64 |
| 6:AF:26:ILE:HG22 | 6:AF:30:LEU:CD1 | 2.28 | 0.64 |
| 23:BA:1495:A:H2' | 23:BA:1495:A:N3 | 2.13 | 0.64 |
| 8:CH:21:LYS:O | 8:CH:63:LEU:HD12 | 1.98 | 0.64 |
| 1:AA:632:A:C8 | 1:AA:633:G:C8 | 2.85 | 0.64 |
| 23:DA:2842:G:H1 | 23:DA:2875:C:H42 | 1.43 | 0.64 |
| 40:DR:21:ARG:CZ | 40:DR:91:TYR:CE1 | 2.81 | 0.64 |
| 23:BA:992:C:O3' | 40:BR:72:VAL:HG11 | 1.98 | 0.64 |
| 25:DC:260:ARG:O | 25:DC:261:LYS:O | 2.15 | 0.64 |
| 23:BA:626:U:O2 | 34:BL:105:LEU:HB3 | 1.98 | 0.64 |
| 1:AA:160:A:H2' | 1:AA:161:A:O4' | 1.98 | 0.64 |
| 34:BL:62:LEU:CD2 | 53:B5:25:MET:HB2 | 2.28 | 0.63 |
| 34:BL:58:THR:C | 34:BL:61:ARG:HE | 2.01 | 0.63 |
| 2:AB:162:ILE:O | 2:AB:162:ILE:HD12 | 1.97 | 0.63 |
| 22:CV:6182:A:C6 | 22:CV:6183:G:C5 | 2.85 | 0.63 |
| 2:CB:162:ILE:HD12 | 2:CB:162:ILE:O | 1.97 | 0.63 |
| 30:BH:82:ARG:C | 30:BH:89:TYR:HB2 | 2.19 | 0.63 |
| 1:CA:674:G:H2' | 1:CA:675:A:H8 | 1.63 | 0.63 |
| 1:AA:688:G:H2' | 1:AA:689:C:C6 | 2.33 | 0.63 |
| 26:BD:1:MET:HB3 | 26:BD:84:PHE:HB2 | 1.80 | 0.63 |
| 28:BF:71:THR:HG22 | 28:BF:89:GLY:O | 1.98 | 0.63 |
| 44:DV:72:ARG:HG2 | 44:DV:89:PHE:HB2 | 1.80 | 0.63 |
| 1:CA:735:C:H2' | 1:CA:736:C:C6 | 2.34 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:AH:89:PRO:HA | 8:AH:92:ARG:NH1 | 2.11 | 0.63 |
| 2:AB:173:ALA:HA | 2:AB:176:GLU:HG3 | 1.80 | 0.63 |
| 10:AJ:42:THR:HG23 | 10:AJ:68:HIS:HA | 1.79 | 0.63 |
| 1:AA:735:C:H2' | 1:AA:736:C:C6 | 2.32 | 0.63 |
| 19:CS:6:LYS:CG | 19:CS:7:LYS:HD3 | 2.28 | 0.63 |
| 1:AA:976:G:H21 | 1:AA:136(A):C:H2' | 1.62 | 0.63 |
| 26:DD:26:ILE:N | 26:DD:26:ILE:HD13 | 2.14 | 0.63 |
| 3:AC:77:ILE:C | 3:AC:83:ARG:HB3 | 2.18 | 0.63 |
| 23:DA:2365:G:O6 | 53:D5:39:LYS:HE3 | 1.98 | 0.63 |
| 27:DE:53:THR:HG23 | 27:DE:56:GLU:OE1 | 1.98 | 0.63 |
| 23:DA:1870:C:H2' | 23:DA:1870:C:O2 | 1.97 | 0.63 |
| 22:AV:6198:U:H2' | 22:AV:6199:G:H8 | 1.63 | 0.63 |
| 23:DA:1546:A:C8 | 23:DA:154(B):C:O2 | 2.51 | 0.63 |
| 2:AB:163:PHE:HD1 | 2:AB:185:ILE:HG13 | 1.63 | 0.63 |
| 1:CA:980:C:O2 | 14:CN:21:TYR:HD1 | 1.81 | 0.63 |
| 1:CA:551:U:O2' | 12:CL:85:ARG:HD2 | 1.99 | 0.63 |
| 25:DC:33:LEU:HD23 | 25:DC:33:LEU:N | 2.13 | 0.63 |
| 16:CP:28:ARG:NH1 | 16:CP:29:ASP:OD1 | 2.31 | 0.63 |
| 23:DA:2335:A:C8 | 23:DA:2337:G:C5 | 2.86 | 0.63 |
| 34:DL:18:ARG:HB3 | 34:DL:18:ARG:CZ | 2.27 | 0.63 |
| 36:DN:9:LYS:HE2 | 36:DN:43:GLU:OE2 | 1.98 | 0.63 |
| 1:AA:1352:C:C2 | 1:AA:1371:G:C2 | 2.86 | 0.63 |
| 8:AH:20:TYR:HD1 | 8:AH:65:TYR:CD2 | 2.16 | 0.63 |
| 46:BX:46:LEU:HD21 | 46:BX:61:ARG:HE | 1.62 | 0.63 |
| 34:BL:16:ARG:CZ | 34:BL:18:ARG:H | 2.10 | 0.63 |
| 1:CA:626:U:H2' | 1:CA:627:G:C8 | 2.34 | 0.63 |
| 23:DA:226:G:H21 | 23:DA:228:A:H62 | 1.46 | 0.63 |
| 23:DA:966:G:C6 | 23:DA:967:C:N4 | 2.67 | 0.63 |
| 18:CR:47:THR:OG1 | 18:CR:49:LYS:HG2 | 1.98 | 0.63 |
| 2:CB:135:GLN:O | 2:CB:139:LYS:HG2 | 1.96 | 0.63 |
| 23:DA:1856:G:N2 | 23:DA:1886:C:O2 | 2.32 | 0.63 |
| 23:DA:1162:G:C2' | 23:DA:1163:G:H5' | 2.28 | 0.63 |
| 35:BM:10:ARG:HB3 | 35:BM:11:LYS:HG2 | 1.79 | 0.63 |
| 23:DA:903:C:H2' | 23:DA:904:C:H6 | 1.64 | 0.63 |
| 38:DP:42:ILE:HD12 | 38:DP:42:ILE:O | 1.98 | 0.63 |
| 2:CB:22:LYS:HZ3 | 2:CB:22:LYS:H | 1.46 | 0.63 |
| 12:CL:103:VAL:O | 12:CL:106:ALA:HB3 | 1.97 | 0.63 |
| 23:BA:222:A:H5'' | 23:BA:421:U:OP1 | 1.98 | 0.63 |
| 29:DG:109:PHE:CE2 | 29:DG:152:ARG:NH1 | 2.66 | 0.63 |
| 23:DA:1218:C:O2' | 23:DA:1219:G:H5' | 1.98 | 0.63 |
| 32:BJ:57:LEU:O | 32:BJ:72:GLY:HA3 | 1.97 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:AB:162:ILE:HD11 | 2:AB:184:VAL:HG13 | 1.79 | 0.63 |
| 25:BC:143:HIS:HD2 | 25:BC:144:ALA:CB | 2.12 | 0.63 |
| 53:D5:60:LEU:O | 53:D5:62:LEU:HB2 | 1.99 | 0.63 |
| 23:DA:114(B):A:H4' | 32:DJ:48:ARG:NH2 | 2.13 | 0.63 |
| 16:CP:4:ILE:HB | 16:CP:66:PRO:HB3 | 1.80 | 0.63 |
| 23:DA:603:A:N6 | 23:DA:655:A:C4' | 2.58 | 0.63 |
| 47:DY:35:LEU:CD1 | 47:DY:53:LEU:HD12 | 2.28 | 0.63 |
| 41:BS:4:LYS:HD3 | 41:BS:6:ILE:HD11 | 1.80 | 0.63 |
| 4:AD:64:LEU:HD12 | 4:AD:64:LEU:O | 1.99 | 0.63 |
| 23:BA:528:A:C2 | 23:BA:2043:C:C5' | 2.80 | 0.63 |
| 6:AF:37:VAL:HG12 | 6:AF:38:GLU:O | 1.98 | 0.63 |
| 23:BA:2820:A:O4' | 36:BN:5:LYS:HG3 | 1.97 | 0.63 |
| 2:CB:24:TRP:CE3 | 2:CB:25:ASN:O | 2.52 | 0.63 |
| 53:B5:52:LYS:HD3 | 53:B5:52:LYS:N | 2.12 | 0.63 |
| 23:DA:1152:C:H5'' | 39:DQ:80:ILE:HG22 | 1.80 | 0.63 |
| 25:BC:25:THR:HG23 | 25:BC:25:THR:O | 1.99 | 0.63 |
| 23:DA:966:G:H2' | 23:DA:967:C:C6 | 2.32 | 0.63 |
| 1:AA:677:U:H3 | 1:AA:713:G:H22 | 1.45 | 0.63 |
| 29:DG:54:ARG:HB3 | 29:DG:65:HIS:HD2 | 1.62 | 0.63 |
| 23:BA:302:C:H2' | 23:BA:303:U:C6 | 2.34 | 0.63 |
| 23:DA:571:A:C8 | 23:DA:2030:A:N6 | 2.66 | 0.63 |
| 38:DP:48:ILE:H | 38:DP:48:ILE:HD12 | 1.62 | 0.63 |
| 23:BA:2461:C:O2 | 23:BA:2461:C:H2' | 1.99 | 0.63 |
| 44:BV:121:HIS:HB3 | 44:BV:123:ASP:O | 1.98 | 0.63 |
| 4:AD:99:SER:O | 4:AD:140:VAL:HG23 | 1.99 | 0.63 |
| 23:DA:1541:U:H2' | 23:DA:1541:U:O2 | 1.97 | 0.63 |
| 23:BA:2185:C:H2' | 23:BA:2186:G:H8 | 1.63 | 0.63 |
| 34:BL:50:ARG:HB2 | 53:B5:60:LEU:HD11 | 1.81 | 0.63 |
| 16:AP:20:VAL:HG23 | 16:AP:34:GLU:O | 1.98 | 0.63 |
| 3:CC:173:VAL:N | 3:CC:174:PRO:HD3 | 2.13 | 0.63 |
| 3:CC:152:ILE:HD11 | 3:CC:167:TRP:HD1 | 1.60 | 0.63 |
| 23:BA:1439:A:C2 | 23:BA:1553:A:C5 | 2.86 | 0.63 |
| 9:AI:17:VAL:HA | 9:AI:63:ILE:HG13 | 1.81 | 0.63 |
| 1:AA:10:A:H2' | 1:AA:11:G:H8 | 1.63 | 0.63 |
| 29:DG:23:ARG:N | 29:DG:23:ARG:HD3 | 2.14 | 0.63 |
| 27:DE:101:LEU:O | 27:DE:106:ARG:NH1 | 2.24 | 0.63 |
| 37:BO:36:TYR:CD1 | 37:BO:36:TYR:N | 2.66 | 0.63 |
| 23:DA:954:G:H5'' | 35:DM:13:GLN:CG | 2.28 | 0.63 |
| 1:CA:677:U:H3 | 1:CA:713:G:H22 | 1.46 | 0.63 |
| 10:AJ:4:ILE:HB | 10:AJ:74:ILE:HD11 | 1.78 | 0.63 |
| 46:BX:23:LYS:HG3 | 46:BX:23:LYS:O | 1.98 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DA:828:U:H3' | 23:DA:828:U:O2 | 1.96 | 0.63 |
| 6:AF:14:LEU:HD23 | 6:AF:15:ASP:O | 1.98 | 0.63 |
| 23:BA:2655:G:N2 | 23:BA:2664:G:C5 | 2.67 | 0.63 |
| 23:BA:2849:U:H4' | 23:BA:2868:A:C2 | 2.33 | 0.63 |
| 1:CA:186(D):G:C6 | 1:CA:191(E):G:N1 | 2.67 | 0.63 |
| 2:CB:30:ARG:HG3 | 2:CB:31:TYR:CD2 | 2.33 | 0.63 |
| 50:B2:36:CYS:SG | 50:B2:37:LYS:N | 2.72 | 0.63 |
| 13:CM:34:LEU:HD13 | 13:CM:41:PRO:HG3 | 1.80 | 0.63 |
| 1:CA:1040:U:H2' | 1:CA:1041:A:C8 | 2.34 | 0.63 |
| 1:AA:1123:A:H4' | 10:AJ:36:GLY:CA | 2.17 | 0.63 |
| 45:DW:23:VAL:HB | 45:DW:26:TYR:CE2 | 2.34 | 0.63 |
| 25:DC:143:HIS:HD2 | 25:DC:144:ALA:CB | 2.11 | 0.63 |
| 25:DC:267:SER:O | 25:DC:269:PHE:N | 2.32 | 0.63 |
| 13:CM:33:ALA:HA | 13:CM:59:TYR:HE2 | 1.64 | 0.63 |
| 23:BA:140:A:C8 | 23:BA:1408:C:O2' | 2.49 | 0.63 |
| 27:DE:155:LEU:HD12 | 27:DE:174:VAL:HB | 1.80 | 0.63 |
| 33:DK:87:ILE:HG13 | 33:DK:91:LEU:HD12 | 1.79 | 0.63 |
| 8:CH:87:SER:HA | 8:CH:93:VAL:HG23 | 1.79 | 0.63 |
| 44:DV:37:VAL:HG23 | 44:DV:38:TYR:N | 2.13 | 0.63 |
| 1:AA:1053:G:C4 | 1:AA:1199:U:C5 | 2.87 | 0.63 |
| 10:CJ:45:ARG:NH1 | 14:CN:36:PHE:CD2 | 2.67 | 0.63 |
| 18:AR:70:ILE:O | 18:AR:74:ARG:HG3 | 1.99 | 0.63 |
| 12:AL:6:ILE:CD1 | 12:AL:6:ILE:H | 2.11 | 0.63 |
| 35:DM:43:THR:HG23 | 35:DM:46:GLN:OE1 | 1.97 | 0.63 |
| 1:CA:222:U:H2' | 1:CA:223:U:C6 | 2.33 | 0.63 |
| 32:BJ:80:ALA:O | 32:BJ:82:LYS:N | 2.32 | 0.63 |
| 1:AA:186(D):G:C4 | 1:AA:191(E):G:N2 | 2.66 | 0.63 |
| 44:DV:104:PHE:HB3 | 44:DV:141:VAL:HG11 | 1.79 | 0.63 |
| 7:CG:99:LEU:HB3 | 7:CG:103:TRP:CZ3 | 2.33 | 0.63 |
| 23:BA:1930:G:N2 | 23:BA:1968:G:H2' | 2.14 | 0.63 |
| 23:DA:990:A:H5'' | 23:DA:991:C:P | 2.38 | 0.63 |
| 26:BD:117:MET:CE | 26:BD:124:GLY:HA3 | 2.28 | 0.63 |
| 53:B5:26:LYS:HA | 53:B5:48:PHE:HE2 | 1.64 | 0.63 |
| 34:DL:62:LEU:CD2 | 34:DL:62:LEU:N | 2.52 | 0.63 |
| 37:BO:11:LYS:O | 37:BO:12:PHE:HB3 | 1.99 | 0.63 |
| 23:BA:1899:G:N2 | 23:BA:1902:C:C5 | 2.66 | 0.63 |
| 40:DR:40:LEU:C | 40:DR:45:THR:HB | 2.18 | 0.63 |
| 47:BY:14:ARG:HA | 47:BY:17:SER:CB | 2.23 | 0.63 |
| 2:CB:80:ILE:HD12 | 2:CB:211:ILE:HB | 1.79 | 0.63 |
| 1:CA:40:C:H2' | 1:CA:41:G:O4' | 1.99 | 0.63 |
| 1:AA:1151:A:O2' | 1:AA:1152:A:H8 | 1.81 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 37:DO:33:LYS:O | 37:DO:54:LEU:HG | 1.98 | 0.63 |
| 39:DQ:62:ILE:O | 39:DQ:63:VAL:C | 2.37 | 0.63 |
| 2:CB:11:LEU:HD12 | 2:CB:217:ARG:NH2 | 2.14 | 0.63 |
| 1:AA:511:C:H1' | 4:AD:43:HIS:HE2 | 1.63 | 0.63 |
| 25:BC:237:GLU:O | 25:BC:237:GLU:OE2 | 2.17 | 0.63 |
| 44:BV:24:LEU:CB | 44:BV:41:LEU:HG | 2.28 | 0.63 |
| 50:D2:40:LYS:HZ1 | 50:D2:49:CYS:HB3 | 1.64 | 0.63 |
| 1:CA:1051:C:H42 | 1:CA:1207:G:H1 | 1.47 | 0.63 |
| 1:CA:648:A:H2' | 1:CA:649:G:H8 | 1.64 | 0.63 |
| 23:BA:2432:A:H2' | 23:BA:2433:A:C8 | 2.33 | 0.63 |
| 23:DA:185:U:H2' | 23:DA:186:G:C8 | 2.33 | 0.63 |
| 1:CA:186(D):G:C4 | 1:CA:191(E):G:N2 | 2.67 | 0.63 |
| 32:DJ:94:ILE:CG2 | 32:DJ:107:LYS:HB3 | 2.28 | 0.63 |
| 33:DK:11:ALA:HB3 | 33:DK:85:VAL:HG23 | 1.80 | 0.63 |
| 12:CL:5:THR:HG23 | 12:CL:8:GLN:HG3 | 1.80 | 0.63 |
| 15:AO:76:GLU:OE2 | 15:AO:76:GLU:HA | 1.98 | 0.63 |
| 39:BQ:30:LYS:O | 39:BQ:31:SER:CB | 2.46 | 0.63 |
| 34:BL:91:PHE:CD1 | 34:BL:91:PHE:N | 2.66 | 0.63 |
| 39:DQ:92:ARG:CG | 40:DR:11:GLN:NE2 | 2.57 | 0.63 |
| 28:DF:86:MET:H | 28:DF:87:PRO:CD | 2.11 | 0.63 |
| 25:BC:35:LYS:CE | 25:BC:103:ARG:HA | 2.29 | 0.63 |
| 25:DC:244:ARG:HB2 | 25:DC:245:PRO:CD | 2.29 | 0.63 |
| 26:BD:51:PHE:HB3 | 26:BD:77:ILE:HD12 | 1.80 | 0.63 |
| 28:BF:105:LYS:NZ | 49:B1:52:SER:HB2 | 2.13 | 0.63 |
| 28:BF:8:LYS:HD3 | 28:BF:9:ARG:HG3 | 1.80 | 0.63 |
| 45:BW:50:ASN:C | 45:BW:62:LEU:HB2 | 2.19 | 0.63 |
| 36:DN:67:LEU:HD22 | 36:DN:76:VAL:HG11 | 1.81 | 0.63 |
| 23:DA:296:C:O2' | 23:DA:297:C:H5' | 1.99 | 0.63 |
| 29:BG:94:TYR:H | 29:BG:94:TYR:HD1 | 1.44 | 0.63 |
| 23:BA:2036:C:H5' | 23:BA:2036:C:C6 | 2.34 | 0.63 |
| 40:BR:22:VAL:HG12 | 40:BR:23:GLU:N | 2.13 | 0.63 |
| 26:DD:176:ILE:O | 26:DD:176:ILE:HG22 | 1.96 | 0.63 |
| 10:AJ:7:LYS:O | 10:AJ:8:LEU:HD12 | 1.98 | 0.63 |
| 23:BA:1726:G:H2' | 23:BA:1727:U:C6 | 2.34 | 0.63 |
| 28:DF:55:LYS:HD2 | 28:DF:58:GLN:HE21 | 1.63 | 0.63 |
| 35:BM:43:THR:HG23 | 35:BM:46:GLN:OE1 | 1.98 | 0.63 |
| 36:DN:44:LEU:O | 36:DN:44:LEU:HD13 | 1.99 | 0.63 |
| 35:DM:80:GLU:OE2 | 35:DM:80:GLU:HA | 1.98 | 0.63 |
| 23:BA:1132:A:O2' | 23:BA:1133:U:H5' | 1.98 | 0.63 |
| 1:AA:643:C:H5' | 8:AH:31:PHE:CE1 | 2.33 | 0.63 |
| 1:AA:805:C:H2' | 1:AA:806:C:H6 | 1.64 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:DL:61:ARG:C | 34:DL:62:LEU:HD13 | 2.18 | 0.63 |
| 47:BY:2:LYS:HA | 47:BY:5:GLU:CD | 2.19 | 0.63 |
| 23:DA:1139:G:OP1 | 32:DJ:125:ALA:HB2 | 1.99 | 0.63 |
| 1:CA:1347:G:C6 | 9:CI:107:ARG:NH2 | 2.61 | 0.63 |
| 7:CG:9:VAL:HG22 | 7:CG:94:ARG:HH11 | 1.63 | 0.63 |
| 1:AA:364:A:C2 | 1:AA:365:U:O4 | 2.51 | 0.63 |
| 39:DQ:92:ARG:HD3 | 39:DQ:94:ASN:HB3 | 1.79 | 0.63 |
| 23:DA:1022:G:H8 | 32:DJ:92:GLN:HE22 | 1.45 | 0.63 |
| 23:BA:2541:A:H5'' | 23:BA:2542:A:OP2 | 1.99 | 0.63 |
| 23:BA:2543:G:H2' | 23:BA:2544:G:C8 | 2.34 | 0.63 |
| 7:AG:9:VAL:HG22 | 7:AG:94:ARG:HH11 | 1.62 | 0.63 |
| 35:DM:48:GLU:O | 35:DM:52:VAL:HG12 | 1.99 | 0.63 |
| 23:BA:379:G:H1 | 46:BX:20:ARG:HH22 | 1.45 | 0.63 |
| 23:BA:1558:A:H1' | 23:BA:1559:G:OP2 | 1.98 | 0.63 |
| 23:DA:2531:A:H5' | 29:DG:157:TYR:CE1 | 2.34 | 0.63 |
| 1:CA:781:A:H2' | 1:CA:782:A:H5' | 1.80 | 0.63 |
| 17:CQ:18:THR:HG23 | 17:CQ:69:LYS:HE3 | 1.79 | 0.63 |
| 23:DA:336:C:H2' | 23:DA:336:C:O2 | 1.98 | 0.63 |
| 7:AG:138:LYS:HE2 | 7:AG:142:GLU:OE2 | 1.98 | 0.63 |
| 23:DA:2485:G:H5'' | 35:DM:46:GLN:HE21 | 1.64 | 0.63 |
| 6:AF:18:GLN:HA | 6:AF:21:LEU:HD23 | 1.80 | 0.63 |
| 35:BM:43:THR:HG23 | 35:BM:46:GLN:CD | 2.19 | 0.63 |
| 2:AB:106:LYS:HE2 | 2:AB:110:GLN:NE2 | 2.14 | 0.63 |
| 29:DG:168:PRO:O | 29:DG:170:ARG:HG3 | 1.97 | 0.63 |
| 23:DA:628:G:H5'' | 53:D5:18:ALA:CB | 2.29 | 0.63 |
| 53:D5:50:LEU:O | 53:D5:51:ALA:HB2 | 1.99 | 0.63 |
| 53:D5:51:ALA:H | 53:D5:54:GLU:HB2 | 1.63 | 0.63 |
| 34:DL:58:THR:C | 34:DL:61:ARG:HE | 2.02 | 0.63 |
| 23:BA:310:A:OP1 | 43:BU:18:GLY:HA2 | 1.99 | 0.63 |
| 9:CI:10:ARG:HD3 | 9:CI:11:LYS:HG3 | 1.81 | 0.63 |
| 23:DA:2846:G:C5 | 23:DA:2847:U:C5 | 2.86 | 0.63 |
| 23:BA:1141:U:H6 | 32:BJ:86:THR:OG1 | 1.80 | 0.63 |
| 34:DL:49:ARG:CG | 34:DL:50:ARG:N | 2.59 | 0.63 |
| 1:CA:386:C:H2' | 1:CA:387:U:C5' | 2.27 | 0.63 |
| 4:CD:109:GLY:C | 4:CD:111:ALA:H | 2.01 | 0.63 |
| 23:BA:2712:U:H1' | 23:BA:712(B):A:H8 | 1.64 | 0.63 |
| 6:CF:90:VAL:CG1 | 6:CF:91:VAL:N | 2.61 | 0.63 |
| 26:BD:37:ARG:O | 26:BD:45:THR:HA | 1.99 | 0.63 |
| 23:DA:2808:U:C2' | 23:DA:2809:A:H5' | 2.29 | 0.63 |
| 23:DA:1010:A:H1' | 23:DA:1153:C:H1' | 1.81 | 0.63 |
| 23:BA:1476:C:H3' | 23:BA:1476:C:H6 | 1.63 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 38:DP:89:VAL:HG22 | 38:DP:89:VAL:O | 1.98 | 0.63 |
| 38:DP:90:GLN:HA | 38:DP:90:GLN:NE2 | 2.13 | 0.63 |
| 23:DA:2476:A:C2 | 23:DA:2477:C:C6 | 2.87 | 0.63 |
| 28:DF:174:GLU:HG2 | 28:DF:180:PHE:CD1 | 2.34 | 0.63 |
| 10:AJ:45:ARG:NH1 | 14:AN:36:PHE:CD2 | 2.67 | 0.63 |
| 44:BV:5:LEU:HD23 | 44:BV:6:LYS:N | 2.12 | 0.63 |
| 6:CF:15:ASP:OD1 | 6:CF:17:SER:HB2 | 1.97 | 0.63 |
| 23:DA:1162:G:H2' | 23:DA:1163:G:H5' | 1.81 | 0.63 |
| 23:DA:1165:U:H2' | 23:DA:1166:C:C6 | 2.34 | 0.63 |
| 32:DJ:94:ILE:HG21 | 32:DJ:107:LYS:HB3 | 1.81 | 0.63 |
| 2:AB:30:ARG:HG3 | 2:AB:31:TYR:CD2 | 2.33 | 0.63 |
| 23:DA:270(J):G:HO2' | 23:DA:270(K):G:H8 | 1.44 | 0.63 |
| 44:BV:104:PHE:HB3 | 44:BV:141:VAL:HG11 | 1.81 | 0.63 |
| 44:BV:108:PRO:HA | 44:BV:142:SER:O | 1.99 | 0.63 |
| 51:B3:38:LYS:HG2 | 51:B3:39:TYR:H | 1.63 | 0.63 |
| 38:BP:48:ILE:HD12 | 38:BP:48:ILE:H | 1.63 | 0.63 |
| 34:DL:128:HIS:CA | 34:DL:147:LEU:HB3 | 2.10 | 0.62 |
| 34:BL:138:LEU:HD11 | 34:BL:144:GLU:HB3 | 1.81 | 0.62 |
| 23:BA:2335:A:O2' | 23:BA:2336:A:H5'' | 1.98 | 0.62 |
| 23:DA:1900:A:N1 | 23:DA:1970:A:C6 | 2.68 | 0.62 |
| 23:BA:114(B):A:C4 | 23:BA:1144:G:C8 | 2.87 | 0.62 |
| 32:BJ:93:LYS:CE | 32:BJ:95:TYR:HE1 | 2.12 | 0.62 |
| 25:DC:267:SER:O | 25:DC:270:ILE:HG13 | 1.99 | 0.62 |
| 28:BF:32:PRO:HB2 | 28:BF:172:LEU:HD22 | 1.80 | 0.62 |
| 3:AC:91:LEU:HB3 | 3:AC:99:VAL:HG11 | 1.79 | 0.62 |
| 1:CA:736:C:H2' | 1:CA:737:A:C8 | 2.34 | 0.62 |
| 23:DA:2378:A:O2' | 37:DO:21:THR:HG21 | 1.99 | 0.62 |
| 46:DX:13:ILE:HD12 | 46:DX:13:ILE:C | 2.19 | 0.62 |
| 1:AA:1152:A:OP1 | 10:AJ:68:HIS:CD2 | 2.52 | 0.62 |
| 3:AC:195:VAL:O | 3:AC:196:LEU:HB2 | 1.98 | 0.62 |
| 23:BA:2747:G:C6 | 23:BA:2754:U:C5 | 2.86 | 0.62 |
| 37:BO:72:ALA:O | 37:BO:76:LYS:HG3 | 1.99 | 0.62 |
| 40:BR:66:ARG:HD2 | 40:BR:88:ARG:NH1 | 2.13 | 0.62 |
| 1:CA:1083:U:C5 | 1:CA:1084:G:C5 | 2.88 | 0.62 |
| 25:BC:235:GLY:O | 25:BC:237:GLU:N | 2.32 | 0.62 |
| 30:DH:15:VAL:O | 30:DH:17:GLN:N | 2.32 | 0.62 |
| 23:DA:1434:A:H61 | 23:DA:1558:A:H62 | 1.46 | 0.62 |
| 23:BA:1794:U:H2' | 23:BA:1795:C:C6 | 2.34 | 0.62 |
| 23:BA:336:C:O2 | 23:BA:336:C:H2' | 1.98 | 0.62 |
| 1:AA:1328:C:OP1 | 13:AM:28:ALA:HB2 | 1.99 | 0.62 |
| 23:BA:229:A:H5' | 23:BA:230:U:H5' | 1.80 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:BB:93:C:H2' | 24:BB:94:C:H6 | 1.65 | 0.62 |
| 23:DA:628:G:H5'' | 53:D5:18:ALA:HB2 | 1.82 | 0.62 |
| 1:CA:1352:C:C2 | 1:CA:1371:G:C2 | 2.87 | 0.62 |
| 23:DA:2185:C:H2' | 23:DA:2186:G:H8 | 1.63 | 0.62 |
| 40:DR:40:LEU:H | 40:DR:47:VAL:CG2 | 2.10 | 0.62 |
| 42:BT:49:VAL:HG23 | 42:BT:50:LYS:N | 2.13 | 0.62 |
| 25:DC:145:VAL:HG12 | 25:DC:146:GLU:O | 1.99 | 0.62 |
| 30:DH:79:ILE:HB | 30:DH:144:VAL:HA | 1.81 | 0.62 |
| 30:DH:88:ILE:CG2 | 30:DH:90:GLY:H | 2.12 | 0.62 |
| 2:AB:215:LEU:O | 2:AB:219:VAL:HG23 | 1.99 | 0.62 |
| 29:DG:43:VAL:HG12 | 29:DG:52:VAL:HG22 | 1.81 | 0.62 |
| 46:DX:32:LYS:HG2 | 46:DX:33:LYS:H | 1.64 | 0.62 |
| 6:AF:63:TYR:N | 6:AF:63:TYR:CD2 | 2.63 | 0.62 |
| 23:DA:1486:A:N6 | 23:DA:1504:C:H42 | 1.97 | 0.62 |
| 33:DK:102:VAL:HG23 | 33:DK:121:VAL:HA | 1.80 | 0.62 |
| 27:BE:53:THR:N | 27:BE:56:GLU:OE1 | 2.32 | 0.62 |
| 23:BA:2597:G:O2' | 23:BA:2598:A:H5' | 1.98 | 0.62 |
| 23:DA:270(I):C:O2 | 23:DA:270(I):C:H2' | 1.97 | 0.62 |
| 36:BN:54:LEU:HD23 | 36:BN:62:ALA:HB1 | 1.80 | 0.62 |
| 23:BA:483:A:H4' | 43:BU:49:VAL:HG23 | 1.81 | 0.62 |
| 1:CA:509:A:H5' | 4:CD:54:TYR:HD2 | 1.64 | 0.62 |
| 23:BA:795:C:H2' | 23:BA:796:C:H6 | 1.64 | 0.62 |
| 1:CA:24:U:H2' | 1:CA:25:C:C6 | 2.33 | 0.62 |
| 23:BA:1449:G:H2' | 23:BA:1450:C:C6 | 2.34 | 0.62 |
| 35:DM:69:PHE:CD1 | 35:DM:70:PRO:HD2 | 2.33 | 0.62 |
| 15:AO:7:GLU:O | 15:AO:11:VAL:HG23 | 1.99 | 0.62 |
| 1:AA:505:G:H2' | 1:AA:506:G:H8 | 1.64 | 0.62 |
| 3:AC:126:ARG:O | 3:AC:127:ARG:HB2 | 1.99 | 0.62 |
| 25:DC:40:THR:HG22 | 25:DC:41:GLY:N | 2.14 | 0.62 |
| 15:CO:7:GLU:O | 15:CO:11:VAL:HG23 | 1.99 | 0.62 |
| 43:BU:13:VAL:CG1 | 43:BU:72:VAL:HB | 2.28 | 0.62 |
| 27:DE:66:PRO:HB3 | 27:DE:68:LYS:NZ | 2.15 | 0.62 |
| 23:DA:1899:G:N2 | 23:DA:1902:C:N4 | 2.35 | 0.62 |
| 40:DR:55:ALA:HA | 40:DR:101:GLY:O | 1.99 | 0.62 |
| 24:DB:16:G:C6 | 24:DB:69:G:C2 | 2.87 | 0.62 |
| 5:CE:14:ARG:NH1 | 5:CE:129:ILE:HD11 | 2.14 | 0.62 |
| 5:CE:43:LEU:HD11 | 5:CE:132:ALA:HB1 | 1.81 | 0.62 |
| 1:AA:1201:A:C1' | 1:AA:1202:G:OP2 | 2.47 | 0.62 |
| 30:BH:130:TYR:O | 30:BH:132:PRO:HD3 | 1.99 | 0.62 |
| 32:DJ:142:ARG:HG3 | 32:DJ:142:ARG:NH1 | 2.07 | 0.62 |
| 23:DA:2329:G:H2' | 23:DA:2330:G:C8 | 2.34 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:CH:119:LEU:HB2 | 8:CH:124:ALA:HB2 | 1.80 | 0.62 |
| 23:BA:1156:A:H4' | 23:BA:1157:G:OP2 | 1.98 | 0.62 |
| 23:DA:1592:C:H2' | 23:DA:1593:G:H8 | 1.64 | 0.62 |
| 1:AA:648:A:H2' | 1:AA:649:G:H8 | 1.63 | 0.62 |
| 1:CA:1111:A:C2 | 3:CC:177:THR:HG23 | 2.34 | 0.62 |
| 2:CB:32:ILE:HD11 | 2:CB:190:THR:HG21 | 1.81 | 0.62 |
| 23:DA:1051:G:C6 | 23:DA:1052:C:N3 | 2.67 | 0.62 |
| 1:CA:160:A:H2' | 1:CA:161:A:O4' | 1.99 | 0.62 |
| 1:AA:1430:C:H2' | 1:AA:1431:C:H6 | 1.64 | 0.62 |
| 34:DL:140:ALA:O | 34:DL:141:ALA:HB2 | 1.99 | 0.62 |
| 34:BL:91:PHE:HD1 | 34:BL:91:PHE:N | 1.96 | 0.62 |
| 32:DJ:143:LEU:HD13 | 32:DJ:143:LEU:C | 2.18 | 0.62 |
| 1:AA:963:G:H2' | 1:AA:964:A:C8 | 2.34 | 0.62 |
| 1:CA:950:U:H2' | 1:CA:951:G:H8 | 1.63 | 0.62 |
| 32:BJ:94:ILE:HG21 | 32:BJ:107:LYS:HB3 | 1.82 | 0.62 |
| 34:BL:49:ARG:HG3 | 34:BL:50:ARG:H | 1.63 | 0.62 |
| 25:BC:31:LYS:O | 25:BC:35:LYS:CB | 2.46 | 0.62 |
| 25:DC:158:ALA:O | 25:DC:161:THR:HG23 | 2.00 | 0.62 |
| 3:CC:173:VAL:CG1 | 3:CC:173:VAL:O | 2.41 | 0.62 |
| 26:DD:111:ARG:HD2 | 26:DD:160:TYR:CE1 | 2.31 | 0.62 |
| 5:AE:41:VAL:HG11 | 5:AE:113:ALA:CB | 2.28 | 0.62 |
| 1:AA:1083:U:C5 | 1:AA:1084:G:C5 | 2.87 | 0.62 |
| 1:AA:1124:G:H4' | 10:AJ:38:ILE:HD11 | 1.80 | 0.62 |
| 1:CA:878:G:H5' | 8:CH:89:PRO:HG2 | 1.81 | 0.62 |
| 46:BX:19:GLN:CG | 46:BX:41:ARG:HE | 2.10 | 0.62 |
| 46:BX:19:GLN:HG3 | 46:BX:41:ARG:NE | 2.13 | 0.62 |
| 1:AA:349:A:O2' | 1:AA:350:G:H5' | 1.99 | 0.62 |
| 1:AA:1179:A:H4' | 9:AI:103:THR:HA | 1.81 | 0.62 |
| 2:AB:11:LEU:HD12 | 2:AB:217:ARG:NH2 | 2.13 | 0.62 |
| 2:AB:63:MET:CG | 2:AB:225:ALA:HB1 | 2.30 | 0.62 |
| 36:BN:50:HIS:O | 36:BN:54:LEU:HB2 | 1.99 | 0.62 |
| 1:AA:920:U:H2' | 1:AA:921:U:H6 | 1.64 | 0.62 |
| 7:CG:47:CYS:O | 7:CG:50:ILE:HB | 1.99 | 0.62 |
| 6:CF:14:LEU:HD23 | 6:CF:15:ASP:O | 1.98 | 0.62 |
| 1:AA:505:G:C6 | 1:AA:535:A:C2 | 2.87 | 0.62 |
| 1:AA:1430:C:H2' | 1:AA:1431:C:C6 | 2.35 | 0.62 |
| 5:AE:145:LYS:HE3 | 5:AE:149:GLU:OE1 | 1.99 | 0.62 |
| 1:CA:799:G:H2' | 1:CA:800:G:O5' | 1.99 | 0.62 |
| 41:BS:36:LEU:HD12 | 41:BS:48:ALA:HA | 1.80 | 0.62 |
| 43:DU:89:PHE:H | 43:DU:90:LEU:HD23 | 1.64 | 0.62 |
| 23:DA:1449:G:H2' | 23:DA:1450:C:C6 | 2.35 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:BA:2371:G:O2' | 51:B3:45:LYS:HB3 | 2.00 | 0.62 |
| 33:DK:80:ASP:OD2 | 38:DP:71:GLY:HA3 | 1.99 | 0.62 |
| 38:DP:84:GLN:HA | 38:DP:84:GLN:HE21 | 1.64 | 0.62 |
| 5:CE:15:ARG:HG2 | 5:CE:15:ARG:O | 1.98 | 0.62 |
| 34:DL:58:THR:O | 34:DL:61:ARG:NE | 2.29 | 0.62 |
| 34:BL:59:LEU:HA | 34:BL:61:ARG:HD2 | 1.80 | 0.62 |
| 22:CV:6195:G:N2 | 22:CV:6196:A:C4 | 2.67 | 0.62 |
| 50:B2:20:ARG:CA | 50:B2:23:HIS:HD2 | 2.08 | 0.62 |
| 32:DJ:113:MET:O | 32:DJ:116:THR:O | 2.17 | 0.62 |
| 40:BR:5:VAL:HG21 | 40:BR:35:LEU:HG | 1.80 | 0.62 |
| 40:BR:6:LYS:HG3 | 40:BR:11:GLN:HG2 | 1.80 | 0.62 |
| 1:AA:376:G:OP1 | 16:AP:5:ARG:HB2 | 1.99 | 0.62 |
| 25:DC:108:PRO:HB3 | 25:DC:143:HIS:CE1 | 2.34 | 0.62 |
| 3:AC:11:ARG:HH21 | 3:AC:180:ALA:HB3 | 1.64 | 0.62 |
| 35:BM:47:ILE:CG2 | 35:BM:48:GLU:N | 2.56 | 0.62 |
| 3:AC:173:VAL:N | 3:AC:174:PRO:HD3 | 2.15 | 0.62 |
| 24:BB:13:A:C8 | 45:BW:74:ARG:NH2 | 2.68 | 0.62 |
| 9:CI:17:VAL:HA | 9:CI:63:ILE:HG13 | 1.81 | 0.62 |
| 10:CJ:42:THR:HG23 | 10:CJ:68:HIS:HA | 1.80 | 0.62 |
| 23:BA:257:A:H2' | 23:BA:258:G:O5' | 1.99 | 0.62 |
| 43:DU:76:CYS:HB3 | 43:DU:77:PRO:CD | 2.29 | 0.62 |
| 1:AA:300:A:H1' | 1:AA:565:U:O2 | 1.99 | 0.62 |
| 23:DA:991:C:C5 | 23:DA:1185:C:C4 | 2.88 | 0.62 |
| 23:BA:2485:G:H5'' | 35:BM:46:GLN:HE21 | 1.63 | 0.62 |
| 2:AB:95:GLN:HG3 | 2:AB:147:LYS:O | 2.00 | 0.62 |
| 6:CF:74:ASP:HB3 | 6:CF:77:ARG:HH22 | 1.64 | 0.62 |
| 9:AI:69:GLY:O | 9:AI:73:GLN:HG3 | 1.99 | 0.62 |
| 23:BA:2212:A:H1' | 23:BA:2215:G:C4 | 2.34 | 0.62 |
| 2:CB:177:ALA:HB1 | 2:CB:182:ILE:HB | 1.82 | 0.62 |
| 23:DA:2718:G:H2' | 23:DA:2719:G:H8 | 1.64 | 0.62 |
| 25:BC:155:LEU:HD23 | 25:BC:177:LEU:CD2 | 2.20 | 0.62 |
| 28:BF:76:SER:HB2 | 28:BF:83:ARG:C | 2.19 | 0.62 |
| 39:BQ:83:LEU:HA | 39:BQ:86:ALA:HB3 | 1.82 | 0.62 |
| 28:DF:129:GLY:HA3 | 28:DF:163:ALA:HB3 | 1.80 | 0.62 |
| 37:DO:90:GLY:O | 37:DO:92:TYR:N | 2.33 | 0.62 |
| 1:AA:405:U:H5'' | 1:AA:406:G:O4' | 2.00 | 0.62 |
| 4:AD:100:ARG:HH21 | 4:AD:118:ARG:NH1 | 1.95 | 0.62 |
| 1:AA:193:C:H2' | 1:AA:194:C:C6 | 2.34 | 0.62 |
| 23:BA:2090:G:H21 | 46:BX:45:ASN:HD21 | 1.46 | 0.62 |
| 6:CF:8:ILE:HD11 | 6:CF:79:LEU:HD13 | 1.82 | 0.62 |
| 23:BA:1055:G:H2' | 23:BA:1056:G:H8 | 1.63 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:324:G:OP1 | 20:CT:70:SER:HB2 | 2.00 | 0.62 |
| 23:DA:7:G:H2' | 23:DA:8:A:C8 | 2.34 | 0.62 |
| 23:BA:2101:G:C2' | 23:BA:2102:U:H5' | 2.30 | 0.62 |
| 12:AL:23:VAL:HG13 | 12:AL:97:TYR:CE2 | 2.35 | 0.62 |
| 1:AA:1311:G:H1 | 1:AA:1326:C:H42 | 1.45 | 0.62 |
| 1:CA:137:C:O4' | 16:CP:63:GLY:HA3 | 1.99 | 0.62 |
| 1:AA:1040:U:H2' | 1:AA:1041:A:C8 | 2.34 | 0.62 |
| 29:DG:89:ILE:O | 29:DG:89:ILE:HG22 | 1.99 | 0.62 |
| 6:AF:74:ASP:HB3 | 6:AF:77:ARG:HH22 | 1.64 | 0.62 |
| 32:BJ:114:LEU:HA | 32:BJ:118:PRO:HB3 | 1.81 | 0.62 |
| 23:DA:1018:C:N3 | 23:DA:1019:U:C5 | 2.68 | 0.62 |
| 23:DA:1142:U:H5'' | 23:DA:114(B):A:H5' | 1.80 | 0.62 |
| 23:BA:2218:G:O2' | 23:BA:2219:G:H5' | 2.00 | 0.62 |
| 26:DD:36:ARG:HD3 | 26:DD:85:ASN:ND2 | 2.10 | 0.62 |
| 23:DA:1586:A:N6 | 23:DA:1587:A:C2 | 2.68 | 0.62 |
| 12:AL:41:THR:HA | 12:AL:52:ARG:O | 1.99 | 0.62 |
| 23:DA:556:G:H2' | 23:DA:557:U:C6 | 2.34 | 0.62 |
| 8:AH:86:ILE:HG21 | 8:AH:133:LEU:HD13 | 1.82 | 0.62 |
| 11:AK:95:ILE:HG21 | 11:AK:108:ILE:HD13 | 1.81 | 0.62 |
| 23:DA:2273:A:O2' | 23:DA:2274:A:H5' | 2.00 | 0.62 |
| 1:AA:102:G:H2' | 1:AA:103:C:C6 | 2.35 | 0.62 |
| 35:BM:21:THR:O | 35:BM:23:GLY:N | 2.33 | 0.62 |
| 39:BQ:30:LYS:O | 39:BQ:31:SER:HB3 | 1.99 | 0.62 |
| 23:DA:978:G:C2' | 23:DA:979:G:H5' | 2.30 | 0.62 |
| 26:BD:149:ARG:HG3 | 26:BD:150:VAL:N | 2.15 | 0.62 |
| 24:DB:93:C:H2' | 24:DB:94:C:H6 | 1.64 | 0.62 |
| 15:CO:78:TYR:O | 15:CO:82:ILE:HG22 | 2.00 | 0.62 |
| 1:CA:836:G:C6 | 1:CA:851:G:C6 | 2.88 | 0.62 |
| 53:D5:33:ASN:HA | 53:D5:36:LYS:HD3 | 1.81 | 0.62 |
| 22:AV:6191:A:H2' | 22:AV:6192:G:C8 | 2.34 | 0.62 |
| 23:BA:2847:U:OP1 | 38:BP:98:LYS:HD3 | 2.00 | 0.62 |
| 30:BH:79:ILE:HB | 30:BH:144:VAL:HA | 1.82 | 0.62 |
| 40:BR:39:LEU:CB | 40:BR:47:VAL:HG21 | 2.30 | 0.62 |
| 23:DA:2729:G:H1' | 26:DD:187:ALA:CB | 2.26 | 0.62 |
| 16:AP:20:VAL:HG21 | 16:AP:32:TYR:CG | 2.35 | 0.62 |
| 25:DC:155:LEU:HD23 | 25:DC:177:LEU:CD2 | 2.26 | 0.62 |
| 52:D4:19:ARG:NH1 | 52:D4:19:ARG:HG3 | 2.03 | 0.62 |
| 4:AD:93:PHE:O | 4:AD:97:LEU:HG | 1.99 | 0.62 |
| 1:AA:1347:G:H22 | 1:AA:1373:G:H2' | 1.64 | 0.62 |
| 26:BD:111:ARG:HD2 | 26:BD:160:TYR:CE1 | 2.30 | 0.62 |
| 23:BA:1586:A:N6 | 23:BA:1587:A:C2 | 2.67 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DA:1858:G:O2' | 23:DA:1859:A:H8 | 1.82 | 0.62 |
| 23:DA:244:A:C2 | 23:DA:255:A:C4 | 2.88 | 0.62 |
| 40:DR:21:ARG:CZ | 40:DR:91:TYR:HE1 | 2.12 | 0.62 |
| 1:CA:919:A:O2' | 1:CA:920:U:H5' | 1.99 | 0.62 |
| 1:AA:1443:G:H3' | 1:AA:1446:A:H5'' | 1.80 | 0.62 |
| 7:AG:47:CYS:O | 7:AG:50:ILE:HB | 1.99 | 0.62 |
| 1:AA:152:A:H62 | 1:AA:169:C:N4 | 1.97 | 0.62 |
| 23:BA:903:C:H2' | 23:BA:904:C:H6 | 1.65 | 0.62 |
| 23:DA:245:G:H2' | 23:DA:246:C:H6 | 1.63 | 0.62 |
| 14:AN:26:ARG:NH1 | 14:AN:47:LEU:HD21 | 2.15 | 0.62 |
| 9:CI:79:LEU:HD23 | 9:CI:101:PHE:O | 1.99 | 0.62 |
| 51:B3:34:LEU:HD22 | 51:B3:34:LEU:O | 2.00 | 0.62 |
| 23:BA:2262:U:H2' | 23:BA:2263:C:H6 | 1.65 | 0.62 |
| 30:BH:88:ILE:HG12 | 30:BH:123:LEU:HA | 1.82 | 0.62 |
| 25:DC:142:VAL:HG23 | 25:DC:193:VAL:HA | 1.82 | 0.62 |
| 30:DH:88:ILE:HG22 | 30:DH:90:GLY:H | 1.65 | 0.62 |
| 24:DB:45:A:H1' | 28:DF:95:ARG:NH2 | 2.15 | 0.62 |
| 2:CB:215:LEU:O | 2:CB:219:VAL:HG23 | 1.99 | 0.62 |
| 1:CA:405:U:H5'' | 1:CA:406:G:O4' | 1.99 | 0.62 |
| 4:CD:3:ARG:HH21 | 4:CD:118:ARG:HD3 | 1.65 | 0.62 |
| 9:AI:10:ARG:HD3 | 9:AI:11:LYS:HG3 | 1.81 | 0.62 |
| 36:DN:54:LEU:HD23 | 36:DN:62:ALA:HB1 | 1.81 | 0.62 |
| 23:DA:1343:G:H8 | 23:DA:1343:G:C5' | 2.13 | 0.62 |
| 1:AA:736:C:H2' | 1:AA:737:A:C8 | 2.35 | 0.62 |
| 1:CA:623:C:C4 | 1:CA:624:C:C5 | 2.88 | 0.62 |
| 15:CO:30:ALA:CA | 15:CO:85:LEU:HD11 | 2.29 | 0.62 |
| 40:DR:20:LEU:HD23 | 40:DR:20:LEU:O | 2.00 | 0.62 |
| 1:CA:1053:G:C4 | 1:CA:1199:U:C5 | 2.87 | 0.62 |
| 36:BN:52:ILE:CD1 | 36:BN:79:LEU:HD21 | 2.29 | 0.62 |
| 1:AA:920:U:H2' | 1:AA:921:U:C6 | 2.35 | 0.62 |
| 5:AE:147:ASP:O | 5:AE:151:LEU:HG | 1.99 | 0.62 |
| 23:BA:2401:U:H2' | 23:BA:2402:C:H5'' | 1.81 | 0.62 |
| 23:BA:1010:A:H1' | 23:BA:1153:C:H1' | 1.82 | 0.62 |
| 40:BR:22:VAL:CG1 | 40:BR:23:GLU:N | 2.62 | 0.62 |
| 7:CG:69:VAL:O | 7:CG:71:PRO:HD3 | 2.00 | 0.62 |
| 7:CG:71:PRO:HG3 | 7:CG:103:TRP:HZ3 | 1.65 | 0.62 |
| 1:AA:1391:U:H2' | 1:AA:1392:G:C8 | 2.35 | 0.62 |
| 23:BA:924:C:H2' | 23:BA:925:C:C6 | 2.35 | 0.62 |
| 44:BV:117:LEU:O | 44:BV:117:LEU:HG | 2.00 | 0.62 |
| 2:CB:158:LEU:H | 2:CB:158:LEU:HD12 | 1.65 | 0.62 |
| 1:AA:1516:G:H2' | 1:AA:1518:A:OP2 | 2.00 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 34:DL:59:LEU:HA | 34:DL:61:ARG:HD2 | 1.79 | 0.62 |
| 53:B5:23:VAL:CG1 | 53:B5:47:LYS:HB3 | 2.30 | 0.62 |
| 36:DN:11:ASN:O | 36:DN:12:ARG:HB2 | 1.98 | 0.62 |
| 12:CL:85:ARG:HB2 | 12:CL:100:VAL:HG23 | 1.81 | 0.62 |
| 42:DT:49:VAL:HG23 | 42:DT:50:LYS:N | 2.15 | 0.62 |
| 30:DH:88:ILE:HG12 | 30:DH:123:LEU:HA | 1.81 | 0.62 |
| 36:BN:55:ALA:HA | 36:BN:80:PHE:HE1 | 1.59 | 0.62 |
| 23:BA:558:G:OP1 | 32:BJ:134:PRO:HD2 | 2.00 | 0.62 |
| 23:BA:1331:A:O2' | 23:BA:1332:G:H8 | 1.82 | 0.62 |
| 23:DA:1153:C:H5' | 39:DQ:76:TYR:HE2 | 1.65 | 0.62 |
| 1:CA:1117:G:O3' | 9:CI:104:ARG:HG3 | 1.99 | 0.62 |
| 1:CA:781:A:H4' | 1:CA:1522:U:O2' | 2.00 | 0.62 |
| 38:BP:26:ASP:HB3 | 38:BP:92:GLY:H | 1.64 | 0.62 |
| 35:BM:119:ARG:HG2 | 35:BM:120:ILE:HD13 | 1.82 | 0.62 |
| 23:DA:1558:A:H1' | 23:DA:1559:G:OP2 | 2.00 | 0.62 |
| 1:CA:109:A:N6 | 1:CA:326:G:C5 | 2.68 | 0.62 |
| 2:CB:126:GLU:C | 2:CB:127:ILE:HD13 | 2.20 | 0.62 |
| 27:DE:108:LYS:O | 27:DE:112:MET:HG3 | 2.00 | 0.62 |
| 1:CA:304:U:H2' | 1:CA:305:G:C8 | 2.35 | 0.62 |
| 34:BL:30:THR:HG22 | 34:BL:31:ALA:N | 2.15 | 0.62 |
| 23:DA:573:G:O2' | 23:DA:574:C:H3' | 1.99 | 0.62 |
| 21:CU:24:ARG:HG3 | 21:CU:25:LYS:H | 1.65 | 0.62 |
| 29:BG:109:PHE:CE2 | 29:BG:152:ARG:NH1 | 2.68 | 0.62 |
| 19:CS:5:LEU:HD12 | 19:CS:8:GLY:O | 1.99 | 0.62 |
| 2:CB:106:LYS:HE2 | 2:CB:110:GLN:NE2 | 2.15 | 0.62 |
| 39:BQ:16:LYS:O | 39:BQ:20:LEU:HD22 | 2.00 | 0.62 |
| 4:CD:57:ARG:HB3 | 4:CD:206:PHE:HB2 | 1.82 | 0.62 |
| 5:CE:102:ALA:HB2 | 5:CE:120:THR:CG2 | 2.28 | 0.61 |
| 16:CP:67:THR:HG22 | 16:CP:68:ASP:H | 1.64 | 0.61 |
| 42:BT:14:SER:O | 42:BT:17:ALA:N | 2.33 | 0.61 |
| 1:AA:406:G:N2 | 1:AA:437:U:C2 | 2.68 | 0.61 |
| 30:DH:88:ILE:HD11 | 30:DH:123:LEU:HG | 1.82 | 0.61 |
| 20:AT:71:THR:HG22 | 20:AT:72:LEU:N | 2.15 | 0.61 |
| 13:AM:33:ALA:HA | 13:AM:59:TYR:HE2 | 1.64 | 0.61 |
| 5:AE:31:LEU:HD21 | 5:AE:43:LEU:CD1 | 2.29 | 0.61 |
| 3:AC:134:ILE:CG2 | 3:AC:168:ALA:HB3 | 2.30 | 0.61 |
| 1:AA:193:C:O4' | 20:AT:60:GLU:OE2 | 2.17 | 0.61 |
| 11:AK:59:TYR:CZ | 11:AK:63:LEU:HD11 | 2.35 | 0.61 |
| 2:AB:25:ASN:HB3 | 2:AB:26:PRO:HD2 | 1.82 | 0.61 |
| 11:CK:92:GLU:HA | 11:CK:95:ILE:HG13 | 1.81 | 0.61 |
| 23:DA:1487:G:N3 | 23:DA:1488:G:C8 | 2.68 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:BR:64:HIS:CD2 | 40:BR:92:THR:CG2 | 2.83 | 0.61 |
| 18:CR:54:ARG:HD2 | 18:CR:54:ARG:N | 2.14 | 0.61 |
| 40:DR:58:VAL:HG12 | 40:DR:97:LYS:HB2 | 1.82 | 0.61 |
| 25:BC:166:GLN:NE2 | 25:BC:166:GLN:HA | 2.15 | 0.61 |
| 36:BN:99:LYS:HA | 36:BN:112:ALA:CB | 2.30 | 0.61 |
| 23:DA:356:G:H2' | 23:DA:357:A:H8 | 1.64 | 0.61 |
| 26:BD:117:MET:HE2 | 26:BD:124:GLY:HA3 | 1.82 | 0.61 |
| 23:BA:1981:A:H5'' | 23:BA:1982:C:OP2 | 2.00 | 0.61 |
| 23:DA:188:G:H2' | 23:DA:189:G:H5' | 1.81 | 0.61 |
| 37:BO:41:ASP:OD2 | 37:BO:44:LYS:HD3 | 2.00 | 0.61 |
| 25:BC:95:LEU:O | 25:BC:95:LEU:HD12 | 2.00 | 0.61 |
| 23:DA:2705:A:H2 | 36:DN:64:ARG:NH1 | 1.98 | 0.61 |
| 17:AQ:7:THR:O | 17:AQ:23:VAL:HG13 | 2.00 | 0.61 |
| 23:DA:310:A:OP1 | 43:DU:18:GLY:HA2 | 1.99 | 0.61 |
| 23:DA:860:U:HO2' | 23:DA:861:A:H5' | 1.65 | 0.61 |
| 39:BQ:92:ARG:NH2 | 40:BR:11:GLN:N | 2.44 | 0.61 |
| 34:BL:50:ARG:HG3 | 53:B5:7:HIS:CD2 | 2.35 | 0.61 |
| 3:CC:40:ARG:O | 3:CC:44:GLU:HG2 | 1.98 | 0.61 |
| 23:DA:2542:A:OP1 | 23:DA:2542:A:H4' | 1.97 | 0.61 |
| 11:CK:63:LEU:N | 11:CK:63:LEU:HD23 | 2.15 | 0.61 |
| 19:CS:63:THR:N | 19:CS:66:MET:HE3 | 2.16 | 0.61 |
| 40:DR:66:ARG:HD2 | 40:DR:88:ARG:NH1 | 2.15 | 0.61 |
| 29:DG:144:VAL:HA | 29:DG:147:ASN:HB2 | 1.82 | 0.61 |
| 43:BU:81:LYS:NZ | 43:BU:97:ARG:HD3 | 2.14 | 0.61 |
| 37:BO:39:ILE:HG13 | 37:BO:73:LEU:HD13 | 1.81 | 0.61 |
| 23:BA:2273:A:O2' | 23:BA:2274:A:H5' | 1.99 | 0.61 |
| 1:AA:781:A:H2' | 1:AA:782:A:H5' | 1.82 | 0.61 |
| 23:DA:1046:A:H3' | 23:DA:1047:G:C5' | 2.30 | 0.61 |
| 29:DG:73:ALA:O | 29:DG:77:LYS:HG2 | 2.00 | 0.61 |
| 23:DA:2531:A:C5' | 29:DG:157:TYR:CZ | 2.83 | 0.61 |
| 27:BE:117:ARG:NH2 | 27:BE:187:VAL:HA | 2.14 | 0.61 |
| 44:BV:39:VAL:HG23 | 44:BV:40:ASP:N | 2.14 | 0.61 |
| 8:AH:48:TYR:HA | 8:AH:60:ARG:O | 2.00 | 0.61 |
| 23:DA:1389:G:H2' | 23:DA:1390:U:C6 | 2.35 | 0.61 |
| 44:DV:39:VAL:HG23 | 44:DV:40:ASP:N | 2.14 | 0.61 |
| 23:BA:357:A:H2' | 23:BA:358:U:C6 | 2.35 | 0.61 |
| 14:CN:36:PHE:CD1 | 14:CN:36:PHE:O | 2.54 | 0.61 |
| 35:DM:43:THR:HG23 | 35:DM:46:GLN:CD | 2.20 | 0.61 |
| 5:CE:151:LEU:HD13 | 8:CH:77:GLU:HG2 | 1.82 | 0.61 |
| 39:DQ:15:LYS:O | 39:DQ:19:LYS:HG3 | 1.99 | 0.61 |
| 18:AR:19:LYS:O | 18:AR:20:ALA:HB2 | 1.99 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BA:2086:U:OP2 | 25:BC:263:ARG:HD3 | 2.01 | 0.61 |
| 1:AA:114:U:H2' | 1:AA:115:G:C8 | 2.35 | 0.61 |
| 5:CE:140:ARG:HG2 | 5:CE:140:ARG:O | 2.00 | 0.61 |
| 23:BA:1216:G:OP1 | 39:BQ:8:VAL:HG12 | 2.00 | 0.61 |
| 23:BA:2064:C:H2' | 23:BA:2065:C:C6 | 2.36 | 0.61 |
| 44:DV:127:LYS:HD3 | 44:DV:162:GLU:OE1 | 1.99 | 0.61 |
| 6:CF:16:GLN:H | 6:CF:16:GLN:CD | 2.03 | 0.61 |
| 39:BQ:15:LYS:O | 39:BQ:19:LYS:HG3 | 2.00 | 0.61 |
| 45:DW:23:VAL:HB | 45:DW:26:TYR:HE2 | 1.65 | 0.61 |
| 38:DP:64:ARG:HD2 | 38:DP:73:GLU:OE2 | 1.99 | 0.61 |
| 1:AA:1223:C:P | 1:AA:1224:G:H2' | 2.40 | 0.61 |
| 1:AA:950:U:H2' | 1:AA:951:G:H8 | 1.66 | 0.61 |
| 23:BA:942:G:H5' | 34:BL:35:HIS:HB3 | 1.81 | 0.61 |
| 1:CA:1324:A:H4' | 1:CA:136(A):C:O3' | 2.00 | 0.61 |
| 1:CA:552:U:H4' | 12:CL:85:ARG:HG2 | 1.82 | 0.61 |
| 34:DL:32:THR:HG21 | 34:DL:37:GLY:HA2 | 1.82 | 0.61 |
| 23:BA:1141:U:H6 | 32:BJ:86:THR:HG1 | 1.45 | 0.61 |
| 42:BT:50:LYS:H | 42:BT:87:GLN:NE2 | 1.89 | 0.61 |
| 1:AA:373:A:O2' | 1:AA:374:A:H5' | 1.99 | 0.61 |
| 23:BA:1812:A:C2' | 23:BA:1813:G:H5' | 2.30 | 0.61 |
| 24:DB:103:U:O2' | 44:DV:72:ARG:HG3 | 2.00 | 0.61 |
| 26:DD:47:VAL:HG21 | 26:DD:86:PRO:HD3 | 1.81 | 0.61 |
| 24:BB:104:A:O4' | 44:BV:29:TYR:HE1 | 1.83 | 0.61 |
| 44:BV:29:TYR:HA | 44:BV:33:LEU:O | 2.00 | 0.61 |
| 32:DJ:74:PHE:CE1 | 32:DJ:142:ARG:HD2 | 2.35 | 0.61 |
| 36:BN:4:LEU:O | 36:BN:4:LEU:HD23 | 1.99 | 0.61 |
| 23:BA:2808:U:C2' | 23:BA:2809:A:H5' | 2.30 | 0.61 |
| 6:CF:44:GLY:HA2 | 6:CF:59:TYR:CZ | 2.35 | 0.61 |
| 1:AA:625:G:C5 | 1:AA:626:U:C5 | 2.88 | 0.61 |
| 23:BA:2531:A:H5' | 29:BG:157:TYR:CE1 | 2.35 | 0.61 |
| 1:CA:1130:A:H5' | 1:CA:1131:G:OP2 | 1.99 | 0.61 |
| 11:CK:21:ILE:HD12 | 11:CK:21:ILE:N | 2.15 | 0.61 |
| 38:BP:26:ASP:HB3 | 38:BP:92:GLY:N | 2.15 | 0.61 |
| 21:AU:18:TYR:HD2 | 21:AU:22:ARG:CG | 2.13 | 0.61 |
| 37:DO:41:ASP:OD2 | 37:DO:44:LYS:HD3 | 2.01 | 0.61 |
| 13:AM:34:LEU:HD13 | 13:AM:41:PRO:HG3 | 1.81 | 0.61 |
| 25:BC:40:THR:HG22 | 25:BC:41:GLY:N | 2.14 | 0.61 |
| 1:AA:1257:U:O4' | 1:AA:1257:U:OP2 | 2.18 | 0.61 |
| 7:AG:69:VAL:O | 7:AG:71:PRO:HD3 | 1.99 | 0.61 |
| 7:AG:99:LEU:HB3 | 7:AG:103:TRP:CZ3 | 2.34 | 0.61 |
| 4:CD:62:GLN:O | 4:CD:66:ARG:HG3 | 2.01 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BA:1541:U:O2 | 23:BA:1541:U:H2' | 1.98 | 0.61 |
| 2:AB:82:ARG:HA | 2:AB:92:TYR:CE1 | 2.36 | 0.61 |
| 32:BJ:77:VAL:HB | 32:BJ:145:VAL:HG22 | 1.82 | 0.61 |
| 26:BD:132:HIS:CG | 26:BD:135:HIS:NE2 | 2.68 | 0.61 |
| 34:DL:48:PRO:O | 34:DL:49:ARG:O | 2.18 | 0.61 |
| 1:CA:376:G:C4 | 1:CA:389:A:C2 | 2.89 | 0.61 |
| 30:BH:92:VAL:O | 30:BH:120:ILE:HD12 | 2.01 | 0.61 |
| 37:DO:11:LYS:O | 37:DO:12:PHE:HB3 | 2.00 | 0.61 |
| 1:AA:501:C:OP1 | 12:AL:116:ARG:NH2 | 2.33 | 0.61 |
| 1:CA:265:G:C2' | 1:CA:266:G:H5'' | 2.28 | 0.61 |
| 1:CA:1201:A:C1' | 1:CA:1202:G:OP2 | 2.46 | 0.61 |
| 1:AA:1083:U:H5 | 1:AA:1084:G:C6 | 2.19 | 0.61 |
| 48:DZ:43:ILE:N | 48:DZ:43:ILE:CD1 | 2.63 | 0.61 |
| 23:BA:1264:G:C5' | 50:B2:11:THR:HG21 | 2.31 | 0.61 |
| 2:AB:24:TRP:C | 2:AB:25:ASN:HD22 | 2.03 | 0.61 |
| 23:DA:2746:U:H2' | 23:DA:2747:G:O5' | 2.01 | 0.61 |
| 1:CA:599:C:H2' | 1:CA:600:C:C6 | 2.36 | 0.61 |
| 1:CA:707:C:H2' | 1:CA:708:C:H6 | 1.64 | 0.61 |
| 23:BA:783:A:H2' | 23:BA:785:G:OP1 | 2.00 | 0.61 |
| 1:AA:1130:A:H5' | 1:AA:1131:G:OP2 | 1.99 | 0.61 |
| 21:CU:18:TYR:HD2 | 21:CU:22:ARG:CG | 2.12 | 0.61 |
| 35:DM:119:ARG:HG2 | 35:DM:120:ILE:HD13 | 1.81 | 0.61 |
| 3:CC:17:ASP:HB3 | 3:CC:21:ARG:NH2 | 2.15 | 0.61 |
| 17:AQ:5:VAL:HG22 | 17:AQ:60:ILE:HG13 | 1.81 | 0.61 |
| 18:AR:47:THR:OG1 | 18:AR:49:LYS:HG2 | 2.00 | 0.61 |
| 1:AA:222:U:H2' | 1:AA:223:U:C6 | 2.35 | 0.61 |
| 23:DA:991:C:C5 | 23:DA:1185:C:N4 | 2.69 | 0.61 |
| 23:DA:2233:U:H2' | 23:DA:2234:G:C8 | 2.35 | 0.61 |
| 23:BA:1024:G:O5' | 23:BA:1024:G:H8 | 1.83 | 0.61 |
| 37:BO:14:VAL:HG12 | 37:BO:18:ILE:HD11 | 1.82 | 0.61 |
| 1:AA:1057:G:H2' | 1:AA:1058:G:O4' | 2.01 | 0.61 |
| 1:CA:968:A:OP1 | 1:CA:968:A:H8 | 1.82 | 0.61 |
| 43:DU:8:LYS:NZ | 43:DU:8:LYS:H | 1.98 | 0.61 |
| 22:AV:6192:G:C2 | 22:AV:6193:U:C2 | 2.89 | 0.61 |
| 1:AA:365:U:C5' | 1:AA:366:C:OP1 | 2.40 | 0.61 |
| 40:DR:5:VAL:HG21 | 40:DR:35:LEU:HG | 1.83 | 0.61 |
| 39:BQ:83:LEU:HD12 | 39:BQ:113:ALA:CB | 2.28 | 0.61 |
| 23:BA:2728:U:O2 | 23:BA:2729:G:C8 | 2.54 | 0.61 |
| 34:BL:47:ASP:OD1 | 34:BL:49:ARG:HG2 | 2.01 | 0.61 |
| 24:DB:66:A:C5 | 24:DB:108:C:C5 | 2.88 | 0.61 |
| 46:BX:13:ILE:C | 46:BX:13:ILE:HD12 | 2.21 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:476:G:H2' | 1:AA:477:G:C8 | 2.34 | 0.61 |
| 29:BG:139:GLN:HG3 | 29:BG:140:LYS:N | 2.14 | 0.61 |
| 18:AR:54:ARG:N | 18:AR:54:ARG:HD2 | 2.14 | 0.61 |
| 23:DA:910:A:C6 | 23:DA:911:A:C6 | 2.88 | 0.61 |
| 15:CO:81:LEU:O | 15:CO:85:LEU:HB2 | 2.00 | 0.61 |
| 1:AA:624:C:O3' | 16:AP:10:GLY:HA2 | 2.00 | 0.61 |
| 1:CA:1513:A:H2' | 1:CA:1514:C:H6 | 1.63 | 0.61 |
| 23:BA:628:G:H5'' | 53:B5:18:ALA:CB | 2.30 | 0.61 |
| 1:CA:1418:A:C2 | 1:CA:1483:A:C2 | 2.88 | 0.61 |
| 23:BA:2365:G:O6 | 53:B5:39:LYS:HE3 | 2.01 | 0.61 |
| 23:BA:2854:G:H2' | 23:BA:2855:C:H6 | 1.65 | 0.61 |
| 23:DA:979:G:H3' | 23:DA:980:A:H5'' | 1.83 | 0.61 |
| 23:DA:2461:C:O2 | 23:DA:2461:C:H2' | 2.01 | 0.61 |
| 44:DV:121:HIS:HB3 | 44:DV:123:ASP:O | 1.99 | 0.61 |
| 27:DE:11:VAL:O | 27:DE:12:LEU:HD12 | 2.00 | 0.61 |
| 23:DA:2774:C:H2' | 23:DA:2775:A:O4' | 2.00 | 0.61 |
| 1:CA:1257:U:O4' | 1:CA:1257:U:OP2 | 2.19 | 0.61 |
| 23:BA:1336:A:OP1 | 42:BT:64:LYS:HD3 | 2.01 | 0.61 |
| 34:DL:62:LEU:HD23 | 53:D5:25:MET:HB2 | 1.82 | 0.61 |
| 22:AV:6195:G:N2 | 22:AV:6196:A:C4 | 2.68 | 0.61 |
| 1:CA:551:U:H5' | 12:CL:118:LYS:NZ | 2.15 | 0.61 |
| 42:BT:14:SER:O | 42:BT:15:GLU:C | 2.39 | 0.61 |
| 23:DA:2727:G:C4 | 23:DA:2728:U:C5 | 2.89 | 0.61 |
| 28:BF:32:PRO:CB | 28:BF:172:LEU:HD22 | 2.30 | 0.61 |
| 20:CT:56:MET:O | 20:CT:59:ALA:HB3 | 2.01 | 0.61 |
| 19:AS:63:THR:HG23 | 19:AS:65:ASN:H | 1.65 | 0.61 |
| 25:BC:134:ARG:HD3 | 25:BC:135:PHE:CE1 | 2.36 | 0.61 |
| 29:BG:144:VAL:HA | 29:BG:147:ASN:HB2 | 1.81 | 0.61 |
| 25:DC:25:THR:CG2 | 25:DC:82:ILE:N | 2.64 | 0.61 |
| 25:DC:25:THR:HG22 | 25:DC:82:ILE:O | 2.00 | 0.61 |
| 23:DA:105:C:H2' | 23:DA:106:C:C6 | 2.35 | 0.61 |
| 1:AA:623:C:C4 | 1:AA:624:C:C5 | 2.89 | 0.61 |
| 11:AK:21:ILE:HB | 11:AK:84:VAL:HG12 | 1.82 | 0.61 |
| 26:BD:46:ALA:CB | 26:BD:82:ARG:HA | 2.30 | 0.61 |
| 1:CA:1057:G:H2' | 1:CA:1058:G:O4' | 1.99 | 0.61 |
| 23:DA:2100:G:N2 | 23:DA:2101:G:H1' | 2.15 | 0.61 |
| 32:BJ:65:TRP:O | 39:BQ:64:ARG:NH1 | 2.33 | 0.61 |
| 23:DA:302:C:H2' | 23:DA:303:U:C6 | 2.36 | 0.61 |
| 1:CA:1483:A:H2 | 23:DA:1959:G:N3 | 1.99 | 0.61 |
| 3:CC:175:LEU:O | 3:CC:175:LEU:HD23 | 1.99 | 0.61 |
| 44:DV:108:PRO:HA | 44:DV:142:SER:O | 2.01 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:DA:1164:G:C6 | 23:DA:1165:U:C4 | 2.88 | 0.61 |
| 26:BD:176:ILE:HB | 26:BD:181:LEU:HB2 | 1.82 | 0.61 |
| 3:AC:17:ASP:HB3 | 3:AC:21:ARG:NH2 | 2.15 | 0.61 |
| 44:BV:127:LYS:HD3 | 44:BV:162:GLU:OE1 | 2.01 | 0.61 |
| 6:AF:12:PRO:HG2 | 6:AF:55:ASP:OD2 | 2.00 | 0.61 |
| 1:AA:775:G:C2' | 1:AA:776:G:H5' | 2.31 | 0.61 |
| 23:DA:484:C:H2' | 23:DA:485:C:C6 | 2.36 | 0.61 |
| 43:BU:59:GLY:HA3 | 43:BU:61:ILE:HG12 | 1.83 | 0.61 |
| 3:CC:34:LEU:HG | 14:CN:25:VAL:HG11 | 1.83 | 0.61 |
| 53:D5:57:ARG:HH11 | 53:D5:57:ARG:HB2 | 1.65 | 0.61 |
| 33:DK:76:ALA:HB3 | 38:DP:75:ILE:HB | 1.83 | 0.61 |
| 34:DL:33:ARG:O | 34:DL:35:HIS:O | 2.17 | 0.61 |
| 23:BA:1018:C:N3 | 23:BA:1019:U:C5 | 2.69 | 0.61 |
| 25:DC:31:LYS:O | 25:DC:35:LYS:CB | 2.47 | 0.61 |
| 34:DL:45:LEU:HD23 | 34:DL:46:LYS:H | 1.66 | 0.61 |
| 23:DA:114(B):A:C4 | 23:DA:1144:G:C8 | 2.88 | 0.61 |
| 2:CB:174:VAL:O | 2:CB:178:ARG:CB | 2.46 | 0.61 |
| 1:CA:404:U:H2' | 1:CA:405:U:H6 | 1.66 | 0.61 |
| 46:DX:46:LEU:HD23 | 46:DX:46:LEU:C | 2.21 | 0.61 |
| 43:DU:81:LYS:NZ | 43:DU:97:ARG:HD3 | 2.15 | 0.61 |
| 8:CH:91:ARG:HG2 | 8:CH:91:ARG:HH11 | 1.64 | 0.61 |
| 8:CH:20:TYR:HD1 | 8:CH:65:TYR:CD2 | 2.19 | 0.61 |
| 23:BA:2758:A:C5 | 29:BG:67:LEU:HD21 | 2.36 | 0.61 |
| 37:BO:51:ALA:HB1 | 37:BO:72:ALA:CB | 2.31 | 0.61 |
| 33:BK:19:ILE:N | 33:BK:19:ILE:HD13 | 2.15 | 0.61 |
| 23:BA:966:G:C6 | 23:BA:967:C:N4 | 2.69 | 0.61 |
| 35:BM:8:LYS:CG | 35:BM:9:TYR:H | 2.13 | 0.61 |
| 1:AA:175:C:H2' | 1:AA:176:C:C6 | 2.34 | 0.61 |
| 23:DA:483:A:H4' | 43:DU:49:VAL:HG23 | 1.82 | 0.61 |
| 44:DV:180:VAL:C | 44:DV:182:LYS:H | 2.03 | 0.61 |
| 23:DA:2101:G:C2' | 23:DA:2102:U:H5' | 2.29 | 0.61 |
| 25:DC:30:GLU:HG3 | 25:DC:63:ARG:NH2 | 2.14 | 0.61 |
| 23:DA:2639:A:C2' | 23:DA:2640:G:H5' | 2.30 | 0.61 |
| 5:AE:151:LEU:HD13 | 8:AH:77:GLU:HG2 | 1.81 | 0.61 |
| 7:CG:50:ILE:HD12 | 7:CG:61:VAL:HG11 | 1.83 | 0.61 |
| 23:BA:737:C:H2' | 23:BA:738:G:H5' | 1.83 | 0.61 |
| 1:CA:411:A:N7 | 1:CA:429:U:H5 | 1.97 | 0.61 |
| 36:DN:52:ILE:HG21 | 36:DN:94:TYR:CG | 2.35 | 0.61 |
| 3:AC:34:LEU:HG | 14:AN:25:VAL:HG11 | 1.83 | 0.61 |
| 38:BP:29:ARG:HD2 | 38:BP:44:ASP:OD2 | 2.01 | 0.61 |
| 23:BA:1232:G:H2' | 23:BA:1233:C:H6 | 1.65 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 36:BN:103:ARG:NH1 | 36:BN:110:PRO:HG3 | 2.15 | 0.61 |
| 23:BA:249:C:O2 | 53:B5:12:LYS:HE3 | 2.00 | 0.61 |
| 21:AU:24:ARG:HG3 | 21:AU:25:LYS:H | 1.65 | 0.61 |
| 1:AA:638:G:O2' | 1:AA:639:G:H5' | 2.01 | 0.61 |
| 23:DA:2392:A:OP2 | 53:D5:31:HIS:CE1 | 2.54 | 0.61 |
| 34:BL:61:ARG:CA | 34:BL:62:LEU:HD13 | 2.30 | 0.61 |
| 23:BA:2329:G:H2' | 23:BA:2330:G:C8 | 2.35 | 0.61 |
| 10:AJ:63:PHE:HA | 14:AN:59:ALA:H | 1.65 | 0.61 |
| 23:BA:1448:G:N3 | 23:BA:1529:A:H2 | 1.98 | 0.61 |
| 25:BC:155:LEU:N | 25:BC:155:LEU:CD1 | 2.63 | 0.61 |
| 12:CL:26:LEU:HD12 | 12:CL:29:ALA:HB2 | 1.83 | 0.61 |
| 23:DA:1657:C:H2' | 23:DA:1658:C:H6 | 1.63 | 0.61 |
| 28:BF:84:LYS:CG | 28:BF:85:GLY:H | 2.09 | 0.61 |
| 23:BA:2731:G:C6 | 23:BA:2732:G:C6 | 2.88 | 0.61 |
| 37:DO:12:PHE:CD1 | 37:DO:12:PHE:C | 2.74 | 0.61 |
| 25:BC:158:ALA:O | 25:BC:161:THR:HG23 | 2.01 | 0.61 |
| 23:BA:2712:U:O2' | 23:BA:712(B):A:H5'' | 2.01 | 0.61 |
| 26:DD:2:LYS:HD3 | 26:DD:95:ILE:HB | 1.83 | 0.61 |
| 23:DA:2723:C:C2' | 23:DA:2724:C:O5' | 2.48 | 0.61 |
| 10:AJ:75:ILE:HG13 | 10:AJ:76:ASN:N | 2.15 | 0.61 |
| 2:AB:24:TRP:CE3 | 2:AB:25:ASN:O | 2.54 | 0.61 |
| 23:BA:528:A:C2 | 23:BA:2043:C:H4' | 2.36 | 0.61 |
| 25:DC:133:LEU:C | 25:DC:135:PHE:N | 2.54 | 0.61 |
| 36:BN:67:LEU:HD22 | 36:BN:76:VAL:HG11 | 1.81 | 0.61 |
| 39:DQ:98:LEU:O | 39:DQ:101:ARG:O | 2.19 | 0.61 |
| 17:CQ:5:VAL:HG22 | 17:CQ:60:ILE:HG13 | 1.82 | 0.61 |
| 24:BB:75:G:H21 | 44:BV:85:HIS:CE1 | 2.18 | 0.61 |
| 8:CH:48:TYR:HA | 8:CH:60:ARG:O | 2.00 | 0.61 |
| 23:DA:115:C:C2' | 23:DA:116:C:H5' | 2.31 | 0.61 |
| 23:BA:1162:G:H2' | 23:BA:1163:G:H5' | 1.82 | 0.61 |
| 51:D3:38:LYS:HD3 | 51:D3:46:HIS:ND1 | 2.16 | 0.61 |
| 33:BK:11:ALA:HB3 | 33:BK:85:VAL:HG23 | 1.81 | 0.61 |
| 24:BB:28:C:H2' | 24:BB:29:A:H8 | 1.66 | 0.61 |
| 1:CA:356:A:O2' | 1:CA:357:G:H5' | 2.00 | 0.61 |
| 23:DA:1430:C:H2' | 23:DA:1431:U:C6 | 2.36 | 0.61 |
| 7:AG:86:GLN:HB2 | 7:AG:148:ASN:HD22 | 1.65 | 0.61 |
| 23:DA:1216:G:OP1 | 39:DQ:8:VAL:HG12 | 2.00 | 0.61 |
| 1:CA:563:A:N7 | 1:CA:567:G:H1' | 2.15 | 0.61 |
| 23:DA:2853:C:H2' | 23:DA:2854:G:H8 | 1.64 | 0.61 |
| 3:CC:191:THR:HB | 3:CC:193:TYR:CE2 | 2.35 | 0.61 |
| 23:BA:1973:G:H2' | 23:BA:1974:C:H6 | 1.65 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:CA:963:G:H2' | 1:CA:964:A:H8 | 1.66 | 0.61 |
| 23:DA:2416:C:H2' | 23:DA:2417:C:H6 | 1.66 | 0.61 |
| 34:DL:126:VAL:HA | 34:DL:145:PRO:HG2 | 1.82 | 0.61 |
| 23:BA:858:U:C2 | 23:BA:2268:A:C2 | 2.88 | 0.61 |
| 23:BA:861:A:H2' | 23:BA:862:G:C5' | 2.31 | 0.61 |
| 23:BA:1899:G:HO2' | 23:BA:1900:A:P | 2.23 | 0.61 |
| 23:BA:1142:U:H5'' | 23:BA:114(B):A:H5' | 1.82 | 0.61 |
| 23:DA:994:C:O2' | 23:DA:996:A:OP1 | 2.19 | 0.61 |
| 30:BH:92:VAL:CG2 | 30:BH:97:ILE:HG12 | 2.31 | 0.61 |
| 4:AD:3:ARG:HH21 | 4:AD:118:ARG:HD3 | 1.64 | 0.61 |
| 42:DT:28:PHE:HD1 | 42:DT:28:PHE:N | 1.99 | 0.61 |
| 23:DA:2712:U:O2' | 23:DA:712(B):A:H5'' | 2.00 | 0.61 |
| 28:DF:105:LYS:NZ | 49:D1:52:SER:HB2 | 2.16 | 0.61 |
| 24:DB:103:U:O2' | 24:DB:104:A:H5' | 2.00 | 0.61 |
| 42:BT:30:VAL:CG1 | 42:BT:31:HIS:N | 2.64 | 0.61 |
| 46:BX:86:SER:O | 46:BX:90:ILE:HG12 | 2.00 | 0.61 |
| 1:CA:1291:G:H4' | 9:CI:38:GLN:O | 2.00 | 0.61 |
| 23:DA:1495:A:C5' | 23:DA:1496:A:OP2 | 2.48 | 0.61 |
| 40:BR:64:HIS:HD2 | 40:BR:92:THR:HG22 | 1.65 | 0.61 |
| 6:AF:90:VAL:HG12 | 6:AF:91:VAL:N | 2.16 | 0.61 |
| 1:AA:622:A:C8 | 1:AA:623:C:C5 | 2.89 | 0.61 |
| 25:DC:136:ILE:HG23 | 25:DC:137:PRO:HD2 | 1.83 | 0.61 |
| 23:DA:865:C:H4' | 23:DA:866:A:N7 | 2.15 | 0.61 |
| 25:DC:75:ILE:O | 25:DC:118:VAL:HG23 | 2.01 | 0.61 |
| 23:BA:628:G:H5'' | 53:B5:18:ALA:HB2 | 1.83 | 0.61 |
| 23:DA:2432:A:H5'' | 23:DA:2433:A:OP2 | 2.01 | 0.61 |
| 8:CH:77:GLU:HG3 | 8:CH:78:GLN:H | 1.66 | 0.61 |
| 19:AS:53:ASN:HD21 | 19:AS:55:LYS:HB3 | 1.66 | 0.61 |
| 24:BB:45:A:H1' | 28:BF:95:ARG:NH2 | 2.15 | 0.61 |
| 23:DA:1916:A:H2' | 23:DA:1917:U:O4' | 2.01 | 0.61 |
| 4:CD:173:TRP:CD1 | 4:CD:174:LEU:HG | 2.35 | 0.61 |
| 1:AA:540:G:H2' | 1:AA:541:G:O4' | 2.01 | 0.61 |
| 24:BB:111:U:O2 | 24:BB:112:G:C8 | 2.54 | 0.61 |
| 37:DO:93:LYS:NZ | 37:DO:93:LYS:HB2 | 2.15 | 0.61 |
| 44:BV:177:PRO:O | 44:BV:178:GLU:HB3 | 2.01 | 0.61 |
| 24:DB:56:G:H4' | 24:DB:57:A:C8 | 2.36 | 0.61 |
| 14:CN:26:ARG:NH1 | 14:CN:47:LEU:HD21 | 2.15 | 0.61 |
| 7:CG:26:PHE:CE2 | 7:CG:30:ILE:HD11 | 2.36 | 0.61 |
| 32:BJ:113:MET:O | 32:BJ:116:THR:O | 2.19 | 0.61 |
| 39:DQ:88:ILE:HG13 | 39:DQ:88:ILE:O | 2.01 | 0.61 |
| 39:DQ:95:LEU:HD13 | 40:DR:4:ILE:HG23 | 1.83 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:BH:82:ARG:HB3 | 30:BH:89:TYR:CD1 | 2.35 | 0.61 |
| 39:BQ:102:GLU:HG3 | 40:BR:2:PHE:CD1 | 2.36 | 0.61 |
| 36:DN:9:LYS:C | 36:DN:10:LEU:HG | 2.21 | 0.61 |
| 23:BA:2723:C:H4' | 36:BN:2:ARG:NH2 | 2.16 | 0.61 |
| 42:BT:57:LEU:N | 42:BT:57:LEU:HD12 | 2.16 | 0.61 |
| 23:DA:528:A:C3' | 23:DA:528:A:C8 | 2.83 | 0.61 |
| 25:DC:133:LEU:O | 25:DC:135:PHE:N | 2.33 | 0.61 |
| 1:CA:555:C:H2' | 1:CA:556:C:C6 | 2.36 | 0.61 |
| 29:DG:94:TYR:OH | 29:DG:160:LYS:HD3 | 2.00 | 0.61 |
| 45:BW:56:ASP:O | 45:BW:57:PHE:CB | 2.48 | 0.61 |
| 44:BV:74:VAL:HG22 | 44:BV:86:VAL:HG13 | 1.83 | 0.61 |
| 18:CR:66:LEU:HG | 18:CR:70:ILE:HD11 | 1.83 | 0.61 |
| 23:DA:2637:U:H5'' | 26:DD:82:ARG:HH21 | 1.66 | 0.61 |
| 23:BA:637:A:OP2 | 34:BL:115:LEU:HB2 | 1.99 | 0.61 |
| 1:CA:920:U:H2' | 1:CA:921:U:C6 | 2.35 | 0.61 |
| 32:DJ:80:ALA:O | 32:DJ:83:ILE:CG1 | 2.49 | 0.61 |
| 7:CG:27:ILE:HD11 | 7:CG:43:PHE:CD2 | 2.36 | 0.61 |
| 23:DA:639:U:H2' | 23:DA:640:C:C6 | 2.35 | 0.61 |
| 2:AB:32:ILE:HD11 | 2:AB:190:THR:CG2 | 2.31 | 0.61 |
| 14:AN:25:VAL:HG23 | 14:AN:38:GLY:O | 2.00 | 0.61 |
| 6:AF:96:PRO:HB3 | 18:AR:30:ASP:CG | 2.21 | 0.61 |
| 30:DH:87:LYS:HA | 30:DH:122:GLU:HA | 1.83 | 0.61 |
| 26:DD:158:GLY:O | 26:DD:159:HIS:C | 2.39 | 0.61 |
| 30:DH:118:LYS:HG2 | 30:DH:119:PRO:N | 2.16 | 0.61 |
| 35:BM:116:GLU:HA | 35:BM:116:GLU:OE1 | 1.99 | 0.61 |
| 11:CK:125:PHE:CD1 | 11:CK:125:PHE:N | 2.66 | 0.61 |
| 23:BA:706:A:H2' | 23:BA:707:G:O4' | 2.01 | 0.61 |
| 23:DA:83:G:N1 | 23:DA:102:G:O2' | 1.96 | 0.60 |
| 23:DA:1178:C:O2' | 23:DA:1179:C:H5' | 2.00 | 0.60 |
| 1:AA:965:A:H2 | 1:AA:969:A:C2 | 2.15 | 0.60 |
| 22:CV:6192:G:C2 | 22:CV:6193:U:C2 | 2.89 | 0.60 |
| 25:DC:35:LYS:CE | 25:DC:103:ARG:HA | 2.31 | 0.60 |
| 25:BC:242:ARG:HG2 | 25:BC:242:ARG:NH1 | 2.15 | 0.60 |
| 32:DJ:93:LYS:CE | 32:DJ:95:TYR:HE1 | 2.14 | 0.60 |
| 53:B5:11:LYS:HE2 | 53:B5:11:LYS:O | 2.00 | 0.60 |
| 24:DB:7:G:H5'' | 37:DO:29:PHE:CE2 | 2.35 | 0.60 |
| 3:CC:11:ARG:HH21 | 3:CC:180:ALA:HB3 | 1.65 | 0.60 |
| 23:BA:1208:C:C4 | 23:BA:1209:G:N7 | 2.69 | 0.60 |
| 37:DO:72:ALA:O | 37:DO:76:LYS:HG3 | 2.01 | 0.60 |
| 41:DS:29:LEU:O | 41:DS:33:ARG:HD2 | 2.01 | 0.60 |
| 1:CA:1320:C:H2' | 1:CA:1321:C:O4' | 2.00 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DA:1503:U:C2 | 23:DA:1504:C:C5 | 2.89 | 0.60 |
| 23:DA:686:G:O6 | 52:D4:12:ARG:HG3 | 2.01 | 0.60 |
| 23:BA:966:G:H2' | 23:BA:967:C:C6 | 2.34 | 0.60 |
| 25:DC:25:THR:HG23 | 25:DC:25:THR:O | 2.01 | 0.60 |
| 1:AA:799:G:H2' | 1:AA:800:G:O5' | 2.00 | 0.60 |
| 19:AS:6:LYS:HD2 | 19:AS:6:LYS:H | 1.64 | 0.60 |
| 23:BA:2531:A:C5' | 29:BG:157:TYR:CZ | 2.84 | 0.60 |
| 23:DA:379:G:H1 | 46:DX:20:ARG:HH22 | 1.47 | 0.60 |
| 1:AA:102:G:H2' | 1:AA:103:C:H6 | 1.66 | 0.60 |
| 1:AA:599:C:H2' | 1:AA:600:C:C6 | 2.36 | 0.60 |
| 19:CS:6:LYS:HD3 | 19:CS:7:LYS:HD3 | 1.83 | 0.60 |
| 1:AA:622:A:C8 | 1:AA:623:C:C6 | 2.89 | 0.60 |
| 38:DP:1:MET:C | 38:DP:3:ARG:N | 2.54 | 0.60 |
| 23:DA:184:C:H2' | 23:DA:185:U:C6 | 2.36 | 0.60 |
| 23:BA:2279:G:O6 | 45:BW:14:ARG:HD2 | 2.01 | 0.60 |
| 23:DA:1451:C:N3 | 23:DA:1459:G:O6 | 2.34 | 0.60 |
| 5:AE:68:GLU:O | 5:AE:68:GLU:HG3 | 2.01 | 0.60 |
| 47:BY:2:LYS:HA | 47:BY:5:GLU:OE2 | 2.00 | 0.60 |
| 23:BA:1178:C:O2' | 23:BA:1179:C:H5' | 2.00 | 0.60 |
| 9:CI:69:GLY:O | 9:CI:73:GLN:HG3 | 2.01 | 0.60 |
| 1:AA:960:U:C5 | 1:AA:1225:A:H1' | 2.36 | 0.60 |
| 5:CE:101:ILE:O | 5:CE:120:THR:HG23 | 2.01 | 0.60 |
| 32:BJ:94:ILE:CG2 | 32:BJ:107:LYS:HB3 | 2.30 | 0.60 |
| 34:DL:46:LYS:HG2 | 34:DL:52:GLU:OE1 | 2.01 | 0.60 |
| 39:BQ:88:ILE:HG13 | 39:BQ:88:ILE:O | 1.99 | 0.60 |
| 1:AA:501:C:H2' | 1:AA:502:G:H8 | 1.67 | 0.60 |
| 26:BD:59:VAL:O | 26:BD:59:VAL:HG12 | 1.99 | 0.60 |
| 3:CC:57:ILE:CD1 | 3:CC:66:VAL:HG22 | 2.30 | 0.60 |
| 4:AD:63:LYS:HD2 | 4:AD:198:VAL:HG22 | 1.83 | 0.60 |
| 41:DS:36:LEU:HD12 | 41:DS:48:ALA:HA | 1.83 | 0.60 |
| 1:CA:59:A:H5" | 1:CA:60:A:H5" | 1.83 | 0.60 |
| 23:BA:558:G:P | 32:BJ:134:PRO:HD2 | 2.42 | 0.60 |
| 17:AQ:10:VAL:HG11 | 17:AQ:52:LYS:O | 2.00 | 0.60 |
| 11:CK:32:ILE:HD12 | 11:CK:72:ALA:HB2 | 1.82 | 0.60 |
| 3:CC:47:LEU:HD21 | 3:CC:68:VAL:HG11 | 1.83 | 0.60 |
| 1:CA:1083:U:H5 | 1:CA:1084:G:C5 | 2.19 | 0.60 |
| 23:DA:257:A:C2' | 23:DA:258:G:O5' | 2.48 | 0.60 |
| 25:DC:132:PRO:O | 25:DC:136:ILE:HD12 | 2.01 | 0.60 |
| 1:AA:40:C:H2' | 1:AA:41:G:O4' | 2.01 | 0.60 |
| 7:CG:131:LYS:HE3 | 7:CG:136:LYS:HZ2 | 1.66 | 0.60 |
| 44:DV:41:LEU:HD21 | 44:DV:83:PRO:HG2 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BA:1152:C:H5'' | 39:BQ:80:ILE:HG22 | 1.82 | 0.60 |
| 23:DA:2485:G:C5' | 35:DM:46:GLN:HE21 | 2.14 | 0.60 |
| 23:BA:2485:G:C5' | 35:BM:46:GLN:HE21 | 2.14 | 0.60 |
| 23:BA:2233:U:H2' | 23:BA:2234:G:C8 | 2.35 | 0.60 |
| 23:DA:692:C:O2' | 23:DA:693:C:H5' | 2.01 | 0.60 |
| 1:CA:334:C:H2' | 1:CA:335:C:H6 | 1.65 | 0.60 |
| 1:CA:805:C:H2' | 1:CA:806:C:H6 | 1.65 | 0.60 |
| 23:DA:2739:U:O2 | 23:DA:2739:U:H2' | 1.99 | 0.60 |
| 41:BS:45:TYR:HD2 | 41:BS:46:PHE:CD1 | 2.19 | 0.60 |
| 1:AA:868:C:H2' | 1:AA:869:G:O4' | 2.01 | 0.60 |
| 19:CS:53:ASN:HD21 | 19:CS:55:LYS:HB3 | 1.66 | 0.60 |
| 28:BF:148:MET:HA | 28:BF:148:MET:HE3 | 1.82 | 0.60 |
| 23:BA:692:C:O2' | 23:BA:693:C:H5' | 2.01 | 0.60 |
| 23:DA:1543:A:H5' | 23:DA:1544:C:O5' | 2.01 | 0.60 |
| 23:BA:943:U:OP2 | 34:BL:38:GLN:CD | 2.39 | 0.60 |
| 23:DA:2847:U:OP1 | 38:DP:98:LYS:HD3 | 2.01 | 0.60 |
| 37:BO:12:PHE:CD1 | 37:BO:12:PHE:C | 2.74 | 0.60 |
| 6:AF:87:ARG:NH1 | 6:AF:87:ARG:HG3 | 2.15 | 0.60 |
| 32:DJ:88:LYS:O | 32:DJ:89:LYS:C | 2.40 | 0.60 |
| 47:BY:18:PRO:O | 47:BY:22:GLU:HG3 | 2.02 | 0.60 |
| 25:DC:70:TRP:CZ3 | 25:DC:146:GLU:OE1 | 2.51 | 0.60 |
| 28:BF:128:ARG:NH2 | 28:BF:161:THR:O | 2.34 | 0.60 |
| 1:AA:1083:U:H5 | 1:AA:1084:G:C5 | 2.19 | 0.60 |
| 25:BC:186:HIS:CD2 | 25:BC:188:GLU:H | 2.20 | 0.60 |
| 1:CA:53:A:C2 | 1:CA:54:C:H1' | 2.36 | 0.60 |
| 23:BA:2842:G:H1 | 23:BA:2875:C:H42 | 1.47 | 0.60 |
| 1:CA:318:G:N2 | 1:CA:319:G:C4 | 2.69 | 0.60 |
| 4:CD:105:VAL:HG12 | 4:CD:105:VAL:O | 2.01 | 0.60 |
| 32:DJ:81:ASP:OD2 | 32:DJ:147:ALA:HB1 | 2.01 | 0.60 |
| 23:BA:1963:U:C2' | 23:BA:1963:U:O2 | 2.50 | 0.60 |
| 23:DA:9:U:N3 | 23:DA:2629:A:N6 | 2.49 | 0.60 |
| 1:CA:102:G:H2' | 1:CA:103:C:C6 | 2.36 | 0.60 |
| 1:CA:1422:G:H5'' | 33:DK:48:PRO:HB3 | 1.82 | 0.60 |
| 1:CA:15:G:H4' | 5:CE:24:ARG:HH12 | 1.66 | 0.60 |
| 25:BC:227:ASN:N | 25:BC:227:ASN:HD22 | 1.98 | 0.60 |
| 40:DR:22:VAL:HG12 | 40:DR:23:GLU:N | 2.15 | 0.60 |
| 7:AG:71:PRO:HG3 | 7:AG:103:TRP:HZ3 | 1.64 | 0.60 |
| 23:BA:448:U:H1' | 27:BE:84:VAL:HG21 | 1.83 | 0.60 |
| 26:BD:16:ARG:O | 26:BD:18:ASP:N | 2.34 | 0.60 |
| 23:DA:1547:C:H2' | 23:DA:1548:C:H6 | 1.67 | 0.60 |
| 12:CL:37:THR:O | 12:CL:78:GLU:HG2 | 2.00 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 36:BN:30:THR:HG22 | 36:BN:31:HIS:ND1 | 2.16 | 0.60 |
| 29:BG:168:PRO:O | 29:BG:170:ARG:HG3 | 2.01 | 0.60 |
| 37:BO:93:LYS:NZ | 37:BO:93:LYS:HB2 | 2.16 | 0.60 |
| 7:AG:26:PHE:CE2 | 7:AG:30:ILE:HD11 | 2.36 | 0.60 |
| 24:BB:83:G:H5' | 48:BZ:52:HIS:CE1 | 2.36 | 0.60 |
| 1:AA:1320:C:H2' | 1:AA:1321:C:O4' | 2.01 | 0.60 |
| 32:BJ:85:VAL:CG2 | 32:BJ:89:LYS:HG3 | 2.30 | 0.60 |
| 24:DB:81:G:C6 | 24:DB:82:G:C5 | 2.89 | 0.60 |
| 4:AD:49:ARG:NE | 4:AD:50:ARG:H | 1.98 | 0.60 |
| 23:BA:2727:G:C4 | 23:BA:2728:U:C5 | 2.90 | 0.60 |
| 53:B5:60:LEU:O | 53:B5:62:LEU:HB2 | 2.01 | 0.60 |
| 1:AA:411:A:C4 | 1:AA:413:G:O4' | 2.54 | 0.60 |
| 30:DH:88:ILE:HG12 | 30:DH:123:LEU:CA | 2.31 | 0.60 |
| 24:BB:46:A:H2' | 24:BB:47:C:C6 | 2.36 | 0.60 |
| 23:BA:322:A:O4' | 23:BA:340:A:H1' | 2.01 | 0.60 |
| 36:DN:4:LEU:O | 36:DN:4:LEU:HD23 | 2.01 | 0.60 |
| 10:CJ:75:ILE:HG13 | 10:CJ:76:ASN:N | 2.15 | 0.60 |
| 1:CA:691:G:O6 | 11:CK:52:GLY:HA2 | 2.00 | 0.60 |
| 23:BA:2090:G:H21 | 46:BX:45:ASN:ND2 | 2.00 | 0.60 |
| 23:BA:1510:A:H2' | 23:BA:1511:A:H8 | 1.64 | 0.60 |
| 29:BG:43:VAL:HG12 | 29:BG:52:VAL:HG22 | 1.83 | 0.60 |
| 37:DO:36:TYR:N | 37:DO:36:TYR:HD1 | 1.99 | 0.60 |
| 23:DA:380:U:O2 | 23:DA:381:G:C8 | 2.53 | 0.60 |
| 23:DA:389:G:H22 | 34:DL:72:PRO:HD3 | 1.66 | 0.60 |
| 23:BA:282:A:C5 | 23:BA:359:A:C2 | 2.89 | 0.60 |
| 1:CA:522:C:C2' | 1:CA:523:A:H5' | 2.31 | 0.60 |
| 1:CA:521:G:O2' | 1:CA:522:C:H5' | 2.00 | 0.60 |
| 1:CA:1443:G:H3' | 1:CA:1446:A:C5' | 2.30 | 0.60 |
| 23:BA:2365:G:H4' | 45:BW:60:PHE:CZ | 2.36 | 0.60 |
| 23:DA:461:C:C2' | 23:DA:462:C:H5' | 2.31 | 0.60 |
| 24:BB:2:C:H2' | 24:BB:3:C:H6 | 1.67 | 0.60 |
| 2:AB:31:TYR:O | 2:AB:32:ILE:HD12 | 2.01 | 0.60 |
| 25:DC:226:MET:C | 25:DC:227:ASN:HD22 | 2.05 | 0.60 |
| 3:AC:191:THR:HB | 3:AC:193:TYR:CE2 | 2.36 | 0.60 |
| 23:DA:270(Q):C:HO2' | 23:DA:270(R):C:H6 | 1.48 | 0.60 |
| 23:DA:643:A:C2 | 23:DA:644:A:C4 | 2.90 | 0.60 |
| 33:DK:25:LEU:HB2 | 33:DK:38:VAL:O | 2.00 | 0.60 |
| 51:D3:34:LEU:HD22 | 51:D3:34:LEU:O | 2.01 | 0.60 |
| 46:DX:30:VAL:HG12 | 46:DX:30:VAL:O | 2.01 | 0.60 |
| 3:AC:107:GLN:CD | 3:AC:107:GLN:H | 2.04 | 0.60 |
| 1:CA:44:G:OP2 | 16:CP:12:LYS:HB2 | 2.02 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:715:A:O2' | 1:AA:716:A:H5' | 2.01 | 0.60 |
| 23:BA:2739:U:H2' | 23:BA:2739:U:O2 | 2.00 | 0.60 |
| 27:DE:110:LEU:HD11 | 27:DE:181:LEU:HD13 | 1.84 | 0.60 |
| 23:BA:1526:G:C6 | 23:BA:1527:G:C2 | 2.90 | 0.60 |
| 2:AB:177:ALA:HB1 | 2:AB:182:ILE:HB | 1.82 | 0.60 |
| 38:BP:74:ARG:HD3 | 38:BP:76:PHE:CE2 | 2.36 | 0.60 |
| 32:BJ:86:THR:O | 32:BJ:89:LYS:HG2 | 2.01 | 0.60 |
| 42:BT:63:LYS:NZ | 42:BT:72:LYS:HB3 | 2.16 | 0.60 |
| 23:DA:1159:U:H2' | 23:DA:1160:G:H8 | 1.67 | 0.60 |
| 42:BT:28:PHE:N | 42:BT:28:PHE:HD1 | 1.97 | 0.60 |
| 34:BL:49:ARG:CG | 34:BL:50:ARG:N | 2.62 | 0.60 |
| 30:DH:109:ILE:N | 30:DH:109:ILE:HD13 | 2.16 | 0.60 |
| 23:BA:1210:A:H5'' | 23:BA:1210:A:C8 | 2.29 | 0.60 |
| 44:BV:33:LEU:HD23 | 44:BV:90:VAL:HG21 | 1.84 | 0.60 |
| 1:AA:1084:G:OP1 | 1:AA:1086:U:C2 | 2.54 | 0.60 |
| 46:DX:45:ASN:HD22 | 46:DX:46:LEU:N | 1.99 | 0.60 |
| 36:BN:9:LYS:O | 36:BN:10:LEU:HD23 | 2.02 | 0.60 |
| 1:CA:505:G:H2' | 1:CA:506:G:H8 | 1.66 | 0.60 |
| 23:DA:2577:A:H5'' | 23:DA:2578:G:C5' | 2.32 | 0.60 |
| 23:BA:1105:U:O2' | 23:BA:1106:G:H5' | 2.02 | 0.60 |
| 1:CA:1279:A:H5'' | 1:CA:1280:A:OP1 | 2.00 | 0.60 |
| 1:CA:66:G:C2 | 1:CA:67:C:C6 | 2.88 | 0.60 |
| 38:DP:26:ASP:HB3 | 38:DP:92:GLY:H | 1.67 | 0.60 |
| 23:DA:1433:U:O2' | 23:DA:1434:A:H5' | 2.02 | 0.60 |
| 46:DX:23:LYS:HG3 | 46:DX:23:LYS:O | 2.01 | 0.60 |
| 34:BL:84:ASN:HA | 34:BL:115:LEU:O | 2.00 | 0.60 |
| 36:BN:79:LEU:HD23 | 36:BN:83:ILE:HB | 1.84 | 0.60 |
| 1:CA:1076:C:C2 | 1:CA:1082:G:N2 | 2.69 | 0.60 |
| 1:AA:500:G:N2 | 1:AA:546:G:H1' | 2.17 | 0.60 |
| 4:AD:62:GLN:O | 4:AD:66:ARG:HG3 | 2.01 | 0.60 |
| 10:AJ:45:ARG:NH1 | 14:AN:36:PHE:HD2 | 1.98 | 0.60 |
| 23:DA:1794:U:H2' | 23:DA:1795:C:C6 | 2.35 | 0.60 |
| 25:BC:246:PRO:HD2 | 25:BC:255:LYS:HB3 | 1.84 | 0.60 |
| 23:BA:924:C:H2' | 23:BA:925:C:H6 | 1.66 | 0.60 |
| 44:DV:177:PRO:O | 44:DV:178:GLU:HB3 | 2.01 | 0.60 |
| 44:DV:120:ILE:N | 44:DV:120:ILE:HD13 | 2.16 | 0.60 |
| 26:BD:7:VAL:HA | 26:BD:194:GLY:O | 2.02 | 0.60 |
| 26:DD:11:MET:HE3 | 26:DD:24:THR:HB | 1.84 | 0.60 |
| 23:BA:860:U:O2' | 23:BA:861:A:C5' | 2.48 | 0.60 |
| 34:BL:38:GLN:CG | 34:BL:39:LYS:H | 2.11 | 0.60 |
| 38:DP:54:ARG:NH1 | 38:DP:54:ARG:HG3 | 1.95 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:BO:38:GLN:HB3 | 37:BO:47:THR:CG2 | 2.31 | 0.60 |
| 23:BA:1121:C:H6 | 23:BA:1121:C:O5' | 1.85 | 0.60 |
| 30:BH:88:ILE:CG2 | 30:BH:90:GLY:H | 2.14 | 0.60 |
| 6:CF:53:ALA:HB3 | 6:CF:86:ARG:NH1 | 2.17 | 0.60 |
| 30:DH:92:VAL:O | 30:DH:120:ILE:HD12 | 2.01 | 0.60 |
| 23:BA:1209:G:N2 | 23:BA:1210:A:H62 | 1.95 | 0.60 |
| 47:DY:60:LEU:C | 47:DY:62:THR:H | 2.04 | 0.60 |
| 3:AC:134:ILE:CG2 | 3:AC:151:VAL:HB | 2.30 | 0.60 |
| 19:CS:63:THR:HG23 | 19:CS:65:ASN:H | 1.66 | 0.60 |
| 23:BA:1046:A:H3' | 23:BA:1047:G:C5' | 2.31 | 0.60 |
| 37:BO:33:LYS:O | 37:BO:54:LEU:HG | 2.02 | 0.60 |
| 11:AK:92:GLU:HA | 11:AK:95:ILE:HG13 | 1.82 | 0.60 |
| 23:BA:783:A:H3' | 23:BA:783:A:C8 | 2.36 | 0.60 |
| 1:AA:509:A:H5' | 4:AD:54:TYR:CD2 | 2.33 | 0.60 |
| 43:BU:2:ARG:N | 43:BU:4:LYS:HZ2 | 1.99 | 0.60 |
| 17:CQ:40:LYS:HD2 | 17:CQ:42:TYR:CZ | 2.37 | 0.60 |
| 44:DV:24:LEU:CD1 | 44:DV:85:HIS:HA | 2.32 | 0.60 |
| 23:DA:356:G:H2' | 23:DA:357:A:C8 | 2.35 | 0.60 |
| 1:CA:537:G:H5'' | 12:CL:112:ARG:NH2 | 2.16 | 0.60 |
| 1:AA:522:C:C2' | 1:AA:523:A:H5' | 2.30 | 0.60 |
| 23:DA:1946:U:H2' | 23:DA:1947:C:C6 | 2.37 | 0.60 |
| 23:DA:1268:A:C2' | 23:DA:1269:A:O5' | 2.50 | 0.60 |
| 23:DA:2852:G:O2' | 23:DA:2853:C:H5' | 2.01 | 0.60 |
| 28:BF:143:GLU:CD | 28:BF:143:GLU:H | 2.04 | 0.60 |
| 27:BE:50:SER:HA | 27:BE:92:PRO:O | 2.00 | 0.60 |
| 23:DA:1169:G:H1 | 23:DA:1180:C:H42 | 1.49 | 0.60 |
| 1:CA:1159:U:H4' | 1:CA:1160:G:OP1 | 2.01 | 0.60 |
| 24:BB:56:G:H4' | 24:BB:57:A:C8 | 2.36 | 0.60 |
| 3:CC:107:GLN:CD | 3:CC:107:GLN:H | 2.03 | 0.60 |
| 11:CK:67:ASP:OD1 | 11:CK:71:LYS:HE3 | 2.02 | 0.60 |
| 23:DA:631:A:H2' | 23:DA:632:A:O4' | 2.01 | 0.60 |
| 23:BA:631:A:H2' | 23:BA:632:A:O4' | 2.01 | 0.60 |
| 32:BJ:143:LEU:C | 32:BJ:143:LEU:HD13 | 2.22 | 0.60 |
| 37:BO:90:GLY:O | 37:BO:92:TYR:N | 2.35 | 0.60 |
| 23:BA:1019:U:H2' | 23:BA:1020:A:C8 | 2.36 | 0.60 |
| 28:DF:76:SER:HB2 | 28:DF:83:ARG:C | 2.21 | 0.60 |
| 23:DA:1141:U:H6 | 32:DJ:86:THR:HG1 | 1.45 | 0.60 |
| 6:CF:87:ARG:HG3 | 6:CF:87:ARG:NH1 | 2.13 | 0.60 |
| 34:BL:50:ARG:HB2 | 53:B5:60:LEU:CD1 | 2.32 | 0.60 |
| 23:BA:1812:A:O2' | 23:BA:1813:G:H5' | 2.02 | 0.60 |
| 28:BF:161:THR:HG21 | 28:BF:172:LEU:HD23 | 1.82 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DA:1208:C:C4 | 23:DA:1209:G:N7 | 2.70 | 0.60 |
| 5:CE:12:LEU:C | 5:CE:12:LEU:HD22 | 2.22 | 0.60 |
| 5:AE:10:MET:CB | 5:AE:32:VAL:HG22 | 2.31 | 0.60 |
| 20:AT:56:MET:O | 20:AT:59:ALA:HB3 | 2.02 | 0.60 |
| 45:BW:31:VAL:HG23 | 45:BW:32:ARG:O | 2.02 | 0.60 |
| 23:DA:2681:C:C5 | 23:DA:2725:A:N6 | 2.58 | 0.60 |
| 1:AA:1279:A:H5'' | 1:AA:1280:A:OP1 | 2.02 | 0.60 |
| 23:DA:1343:G:C5' | 23:DA:1343:G:C8 | 2.82 | 0.60 |
| 25:DC:237:GLU:O | 25:DC:237:GLU:OE2 | 2.18 | 0.60 |
| 23:BA:1328:G:H2' | 23:BA:1330:C:C5 | 2.37 | 0.60 |
| 16:AP:7:ALA:O | 16:AP:9:PHE:HD2 | 1.85 | 0.60 |
| 23:DA:954:G:C5 | 23:DA:955:C:C5 | 2.89 | 0.60 |
| 2:AB:8:LYS:HA | 2:AB:217:ARG:NH1 | 2.16 | 0.60 |
| 25:BC:166:GLN:NE2 | 25:BC:166:GLN:CA | 2.65 | 0.60 |
| 36:DN:99:LYS:HA | 36:DN:112:ALA:CB | 2.32 | 0.60 |
| 23:DA:286:C:H2' | 23:DA:287:C:C6 | 2.34 | 0.60 |
| 23:DA:1778:U:H2' | 23:DA:1784:A:H62 | 1.66 | 0.60 |
| 26:DD:117:MET:HE2 | 26:DD:124:GLY:HA3 | 1.81 | 0.60 |
| 23:BA:2284:C:H1' | 23:BA:2325:G:C2 | 2.37 | 0.60 |
| 35:BM:37:LEU:HD23 | 35:BM:37:LEU:N | 2.16 | 0.60 |
| 1:AA:1443:G:H3' | 1:AA:1446:A:C5' | 2.32 | 0.60 |
| 23:BA:639:U:H2' | 23:BA:640:C:C6 | 2.36 | 0.60 |
| 23:BA:997:G:C2' | 23:BA:998:C:H5' | 2.32 | 0.60 |
| 23:BA:1153:C:H5' | 39:BQ:76:TYR:CE2 | 2.37 | 0.60 |
| 26:DD:32:PRO:HA | 26:DD:90:THR:HG22 | 1.82 | 0.60 |
| 1:CA:1448:C:H2' | 1:CA:1449:C:C6 | 2.35 | 0.60 |
| 27:DE:53:THR:N | 27:DE:56:GLU:OE1 | 2.35 | 0.60 |
| 26:DD:181:LEU:HD21 | 38:DP:7:ILE:CG2 | 2.30 | 0.60 |
| 23:BA:1335:U:O2' | 23:BA:1336:A:H5' | 2.02 | 0.60 |
| 1:CA:152:A:H62 | 1:CA:169:C:N4 | 2.00 | 0.60 |
| 23:BA:1356:G:C5 | 23:BA:1357:U:C5 | 2.89 | 0.60 |
| 23:DA:886:C:O2' | 23:DA:887:A:H4' | 2.01 | 0.60 |
| 23:DA:1981:A:H5'' | 23:DA:1982:C:OP2 | 2.01 | 0.60 |
| 53:D5:26:LYS:HA | 53:D5:48:PHE:HE2 | 1.66 | 0.60 |
| 53:D5:14:VAL:CG1 | 53:D5:22:VAL:HG13 | 2.32 | 0.60 |
| 34:DL:80:TYR:CD1 | 34:DL:111:ARG:HB3 | 2.37 | 0.60 |
| 34:DL:111:ARG:HG3 | 34:DL:128:HIS:CB | 2.32 | 0.60 |
| 23:DA:747:U:C4 | 50:D2:2:ALA:N | 2.70 | 0.60 |
| 23:BA:1543:A:N7 | 23:BA:1545:A:H5'' | 2.16 | 0.60 |
| 1:CA:1251:A:H5'' | 9:CI:12:GLU:OE1 | 2.02 | 0.60 |
| 53:B5:33:ASN:HA | 53:B5:36:LYS:HD3 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:BJ:38:LEU:HD12 | 32:BJ:39:ILE:H | 1.66 | 0.60 |
| 23:BA:568:U:O4 | 40:BR:78:LYS:CE | 2.50 | 0.60 |
| 32:DJ:38:LEU:HD12 | 32:DJ:39:ILE:H | 1.65 | 0.60 |
| 23:DA:861:A:H2' | 23:DA:862:G:C5' | 2.32 | 0.60 |
| 28:DF:32:PRO:HB2 | 28:DF:172:LEU:HD22 | 1.83 | 0.60 |
| 5:AE:51:VAL:HB | 5:AE:52:PRO:CD | 2.25 | 0.60 |
| 28:BF:9:ARG:HD3 | 28:BF:13:GLU:OE1 | 2.01 | 0.60 |
| 23:DA:226:G:H21 | 23:DA:228:A:N6 | 1.98 | 0.60 |
| 23:DA:225:A:N6 | 23:DA:226:G:N1 | 2.50 | 0.60 |
| 44:DV:24:LEU:CB | 44:DV:41:LEU:HG | 2.32 | 0.60 |
| 23:BA:1946:U:H2' | 23:BA:1947:C:C6 | 2.36 | 0.60 |
| 23:DA:2879:C:H4' | 23:DA:2880:C:OP1 | 2.02 | 0.60 |
| 39:BQ:18:LEU:HD11 | 39:BQ:31:SER:H | 1.67 | 0.60 |
| 41:BS:24:ILE:HG21 | 41:BS:36:LEU:HD21 | 1.81 | 0.60 |
| 14:CN:25:VAL:HG23 | 14:CN:38:GLY:O | 2.01 | 0.60 |
| 36:DN:52:ILE:CD1 | 36:DN:79:LEU:HD21 | 2.32 | 0.60 |
| 1:AA:44:G:OP2 | 16:AP:12:LYS:HB2 | 2.01 | 0.60 |
| 39:DQ:34:LYS:HA | 39:DQ:34:LYS:HE3 | 1.83 | 0.60 |
| 23:DA:1996:C:H4' | 23:DA:1997:G:OP1 | 2.02 | 0.60 |
| 23:BA:958:U:OP2 | 35:BM:14:ARG:NH1 | 2.35 | 0.60 |
| 23:BA:886:C:O2' | 23:BA:887:A:H4' | 2.02 | 0.60 |
| 25:BC:124:PRO:HG2 | 25:BC:129:ASN:ND2 | 2.17 | 0.60 |
| 23:BA:2621:A:OP1 | 26:BD:119:ARG:NH2 | 2.35 | 0.60 |
| 23:BA:1514:U:H2' | 23:BA:1515:C:H6 | 1.67 | 0.60 |
| 41:DS:59:VAL:HG12 | 41:DS:60:ASN:OD1 | 2.02 | 0.60 |
| 22:CV:6191:A:H2' | 22:CV:6192:G:C8 | 2.37 | 0.60 |
| 4:CD:111:ALA:HA | 4:CD:161:ASN:ND2 | 2.17 | 0.60 |
| 47:BY:35:LEU:HD12 | 47:BY:53:LEU:CD1 | 2.28 | 0.60 |
| 47:BY:57:ILE:HG22 | 47:BY:61:LEU:HD22 | 1.83 | 0.60 |
| 23:BA:1593:G:H2' | 23:BA:1594:G:C8 | 2.37 | 0.60 |
| 49:B1:59:VAL:HG12 | 49:B1:60:GLU:N | 2.14 | 0.60 |
| 1:AA:190:G:H4' | 1:AA:191(A):G:OP2 | 2.01 | 0.60 |
| 1:AA:1372:U:H2' | 1:AA:1373:G:O4' | 1.99 | 0.60 |
| 5:CE:53:LEU:HD23 | 5:CE:53:LEU:H | 1.67 | 0.60 |
| 23:BA:1503:U:C2 | 23:BA:1504:C:C5 | 2.89 | 0.60 |
| 27:BE:192:LEU:HD22 | 27:BE:194:MET:HG2 | 1.82 | 0.60 |
| 45:DW:72:ARG:CZ | 45:DW:75:LEU:HD13 | 2.32 | 0.60 |
| 32:DJ:65:TRP:O | 39:DQ:64:ARG:NH1 | 2.35 | 0.60 |
| 23:DA:241:A:H5' | 23:DA:243:U:H1' | 1.83 | 0.60 |
| 3:AC:105:GLU:HG2 | 3:AC:106:VAL:N | 2.16 | 0.60 |
| 43:BU:42:VAL:HG23 | 43:BU:67:LEU:HD11 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:BP:89:VAL:O | 38:BP:89:VAL:HG22 | 2.01 | 0.60 |
| 23:BA:1953:A:H2 | 23:BA:2549:G:N3 | 2.00 | 0.60 |
| 23:DA:2655:G:N2 | 23:DA:2664:G:C4 | 2.69 | 0.60 |
| 23:BA:753:C:OP1 | 52:B4:1:MET:HE3 | 2.01 | 0.60 |
| 35:BM:43:THR:OG1 | 35:BM:45:GLN:HG2 | 2.02 | 0.60 |
| 4:CD:71:SER:HB2 | 4:CD:74:GLN:HB2 | 1.84 | 0.60 |
| 20:AT:42:GLN:HG3 | 20:AT:43:LEU:HD23 | 1.84 | 0.60 |
| 23:BA:2718:G:H2' | 23:BA:2719:G:H8 | 1.67 | 0.60 |
| 5:CE:145:LYS:HE3 | 5:CE:149:GLU:OE1 | 2.01 | 0.60 |
| 28:DF:94:LEU:HD12 | 28:DF:99:MET:HA | 1.83 | 0.60 |
| 27:DE:150:GLY:HA2 | 27:DE:172:TRP:CD2 | 2.37 | 0.60 |
| 23:BA:1893:C:C5 | 23:BA:1894:C:C5 | 2.89 | 0.60 |
| 23:BA:630:G:N2 | 23:BA:632:A:H3' | 2.17 | 0.60 |
| 26:DD:106:GLY:HA3 | 26:DD:189:PRO:HB2 | 1.84 | 0.60 |
| 26:DD:11:MET:CB | 26:DD:24:THR:HA | 2.32 | 0.60 |
| 10:CJ:63:PHE:HA | 14:CN:59:ALA:H | 1.67 | 0.60 |
| 34:BL:35:HIS:O | 34:BL:36:LYS:CB | 2.49 | 0.60 |
| 1:CA:1225:A:H2' | 1:CA:1225:A:N3 | 2.17 | 0.60 |
| 12:CL:33:ARG:O | 12:CL:60:THR:HG23 | 2.01 | 0.60 |
| 25:BC:108:PRO:HB3 | 25:BC:143:HIS:HE1 | 1.67 | 0.60 |
| 23:DA:1141:U:OP2 | 32:DJ:86:THR:CG2 | 2.50 | 0.60 |
| 37:DO:14:VAL:HG12 | 37:DO:18:ILE:HD11 | 1.84 | 0.60 |
| 52:D4:19:ARG:NH1 | 52:D4:19:ARG:HB3 | 2.17 | 0.60 |
| 35:BM:75:THR:HA | 35:BM:88:GLY:HA3 | 1.81 | 0.60 |
| 30:DH:130:TYR:O | 30:DH:132:PRO:HD3 | 2.01 | 0.60 |
| 26:BD:2:LYS:HD3 | 26:BD:95:ILE:HB | 1.82 | 0.60 |
| 5:AE:41:VAL:HG11 | 5:AE:113:ALA:HB2 | 1.82 | 0.60 |
| 24:DB:50:G:C5 | 24:DB:51:G:C8 | 2.89 | 0.60 |
| 2:AB:187:LEU:HD11 | 2:AB:204:ASN:O | 2.02 | 0.60 |
| 6:AF:62:TRP:CE3 | 6:AF:62:TRP:O | 2.55 | 0.60 |
| 47:DY:46:GLN:HB2 | 47:DY:49:LYS:HZ1 | 1.64 | 0.60 |
| 23:DA:528:A:C2 | 23:DA:2043:C:H4' | 2.36 | 0.60 |
| 23:DA:2277:G:H5'' | 35:DM:85:LYS:CB | 2.32 | 0.60 |
| 3:CC:105:GLU:HG2 | 3:CC:106:VAL:N | 2.15 | 0.60 |
| 1:CA:1083:U:H5 | 1:CA:1084:G:C6 | 2.19 | 0.60 |
| 43:BU:20:TYR:CE1 | 43:BU:42:VAL:HA | 2.37 | 0.60 |
| 29:DG:86:GLU:O | 29:DG:86:GLU:HG2 | 2.01 | 0.60 |
| 15:AO:30:ALA:CA | 15:AO:85:LEU:HD11 | 2.32 | 0.60 |
| 23:BA:773:U:C5' | 25:BC:47:GLY:HA3 | 2.31 | 0.60 |
| 27:BE:117:ARG:HD2 | 27:BE:190:GLU:O | 2.02 | 0.60 |
| 43:BU:30:VAL:CG2 | 43:BU:37:VAL:HG12 | 2.32 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:CH:86:ILE:HG21 | 8:CH:133:LEU:HD13 | 1.84 | 0.60 |
| 1:CA:540:G:H2' | 1:CA:541:G:O4' | 2.00 | 0.60 |
| 23:DA:828:U:C2' | 23:DA:828:U:O2 | 2.49 | 0.60 |
| 7:AG:27:ILE:HD11 | 7:AG:43:PHE:CD2 | 2.37 | 0.60 |
| 2:CB:31:TYR:O | 2:CB:32:ILE:HD12 | 2.01 | 0.60 |
| 1:CA:44:G:N3 | 1:CA:399:G:C2 | 2.70 | 0.60 |
| 23:DA:415:A:H2' | 23:DA:416:C:H6 | 1.66 | 0.60 |
| 6:AF:16:GLN:CD | 6:AF:16:GLN:H | 2.04 | 0.60 |
| 23:DA:2394:C:OP1 | 34:DL:63:PRO:HD2 | 2.02 | 0.60 |
| 38:DP:23:ARG:HH11 | 38:DP:23:ARG:CG | 2.15 | 0.60 |
| 14:CN:44:LEU:HD12 | 14:CN:44:LEU:O | 2.01 | 0.60 |
| 34:BL:62:LEU:N | 34:BL:62:LEU:HD13 | 2.17 | 0.59 |
| 23:BA:1543:A:C8 | 23:BA:1545:A:O4' | 2.55 | 0.59 |
| 1:CA:1372:U:H2' | 1:CA:1373:G:O4' | 2.01 | 0.59 |
| 48:DZ:52:HIS:CD2 | 48:DZ:52:HIS:H | 2.18 | 0.59 |
| 30:BH:123:LEU:HD23 | 30:BH:124:GLY:N | 2.17 | 0.59 |
| 25:BC:34:VAL:O | 25:BC:35:LYS:HD3 | 2.02 | 0.59 |
| 5:CE:43:LEU:CD1 | 5:CE:132:ALA:HB1 | 2.32 | 0.59 |
| 29:DG:67:LEU:O | 29:DG:71:LEU:HD23 | 2.01 | 0.59 |
| 28:BF:134:GLY:C | 28:BF:135:LEU:HD12 | 2.22 | 0.59 |
| 23:BA:1343:G:C5' | 23:BA:1343:G:C8 | 2.84 | 0.59 |
| 1:AA:1238:A:C8 | 1:AA:1303:C:H1' | 2.37 | 0.59 |
| 1:AA:781:A:H4' | 1:AA:1522:U:O2' | 2.02 | 0.59 |
| 23:DA:2346:A:H5'' | 23:DA:2383:G:C1' | 2.32 | 0.59 |
| 38:DP:26:ASP:HB3 | 38:DP:92:GLY:N | 2.17 | 0.59 |
| 23:BA:1386:C:OP2 | 23:BA:1396:U:C5 | 2.55 | 0.59 |
| 3:CC:77:ILE:C | 3:CC:83:ARG:HB3 | 2.22 | 0.59 |
| 23:DA:229:A:H5' | 23:DA:230:U:C5' | 2.31 | 0.59 |
| 23:BA:1711:C:O2' | 23:BA:1712:C:H5' | 2.02 | 0.59 |
| 23:DA:796:C:H2' | 23:DA:797:C:C6 | 2.37 | 0.59 |
| 23:DA:2347:C:OP1 | 51:D3:39:TYR:HE1 | 1.84 | 0.59 |
| 1:CA:1112:C:H42 | 3:CC:177:THR:HA | 1.66 | 0.59 |
| 26:BD:181:LEU:HD21 | 38:BP:7:ILE:CG2 | 2.32 | 0.59 |
| 26:DD:100:GLU:O | 26:DD:172:VAL:HG23 | 2.02 | 0.59 |
| 12:AL:33:ARG:O | 12:AL:60:THR:HG23 | 2.02 | 0.59 |
| 25:BC:43:ARG:HB2 | 25:BC:49:ILE:HA | 1.84 | 0.59 |
| 23:DA:496:G:H1' | 41:DS:61:ASN:HD21 | 1.67 | 0.59 |
| 23:DA:1773:A:H2' | 23:DA:1774:C:H5' | 1.84 | 0.59 |
| 23:BA:2056:G:N2 | 50:B2:4:HIS:O | 2.35 | 0.59 |
| 38:DP:64:ARG:HA | 38:DP:72:VAL:O | 2.02 | 0.59 |
| 2:AB:61:LEU:HD21 | 2:AB:161:ALA:HB3 | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:136(A):C:O2' | 1:CA:136(B):C:H5'' | 2.02 | 0.59 |
| 38:BP:57:PHE:O | 38:BP:59:THR:N | 2.36 | 0.59 |
| 23:DA:1657:C:H2' | 23:DA:1658:C:C6 | 2.37 | 0.59 |
| 25:DC:71:ASP:OD2 | 25:DC:103:ARG:NH2 | 2.35 | 0.59 |
| 23:DA:142:G:H1' | 42:DT:37:THR:HG21 | 1.84 | 0.59 |
| 30:DH:123:LEU:HD23 | 30:DH:124:GLY:N | 2.17 | 0.59 |
| 20:CT:71:THR:HG22 | 20:CT:72:LEU:N | 2.17 | 0.59 |
| 5:CE:10:MET:CB | 5:CE:32:VAL:HG22 | 2.32 | 0.59 |
| 26:DD:50:GLY:HA2 | 26:DD:78:LEU:HB3 | 1.84 | 0.59 |
| 1:AA:1076:C:C2 | 1:AA:1082:G:N2 | 2.71 | 0.59 |
| 46:DX:11:ARG:HH12 | 46:DX:61:ARG:H | 1.50 | 0.59 |
| 1:AA:1348:U:H4' | 9:AI:120:ARG:HD2 | 1.83 | 0.59 |
| 29:DG:52:VAL:O | 29:DG:52:VAL:HG12 | 2.02 | 0.59 |
| 5:CE:51:VAL:HB | 5:CE:52:PRO:CD | 2.31 | 0.59 |
| 1:AA:623:C:O5' | 1:AA:623:C:H6 | 1.84 | 0.59 |
| 23:DA:282:A:C5 | 23:DA:359:A:C2 | 2.90 | 0.59 |
| 44:DV:25:PRO:O | 44:DV:85:HIS:HB2 | 2.02 | 0.59 |
| 23:DA:2401:U:C2' | 23:DA:2402:C:H5'' | 2.32 | 0.59 |
| 23:BA:2655:G:N2 | 23:BA:2664:G:C4 | 2.70 | 0.59 |
| 25:BC:80:ALA:HB3 | 25:BC:94:LEU:HD13 | 1.82 | 0.59 |
| 7:AG:74:GLU:O | 7:AG:88:PRO:HA | 2.02 | 0.59 |
| 23:DA:49:A:H4' | 23:DA:50:U:H5'' | 1.84 | 0.59 |
| 23:DA:1149:G:H2' | 23:DA:1150:C:C6 | 2.36 | 0.59 |
| 1:CA:715:A:O2' | 1:CA:716:A:H5' | 2.02 | 0.59 |
| 10:AJ:6:ILE:HG22 | 10:AJ:98:ILE:HG23 | 1.84 | 0.59 |
| 9:AI:79:LEU:HD23 | 9:AI:101:PHE:O | 2.02 | 0.59 |
| 5:AE:36:ASP:O | 5:AE:37:ARG:HB2 | 2.02 | 0.59 |
| 23:BA:1870:C:H2' | 23:BA:1870:C:O2 | 2.01 | 0.59 |
| 23:BA:136:G:C5 | 23:BA:137(A):C:C5 | 2.90 | 0.59 |
| 33:DK:14:THR:HG22 | 33:DK:52:VAL:HB | 1.83 | 0.59 |
| 1:AA:1423:G:H2' | 1:AA:1424:C:H6 | 1.67 | 0.59 |
| 1:AA:20:U:C2' | 1:AA:21:G:H5' | 2.31 | 0.59 |
| 23:DA:2436:G:C5 | 23:DA:2437:U:C5 | 2.90 | 0.59 |
| 52:D4:8:ASN:ND2 | 52:D4:9:ARG:N | 2.46 | 0.59 |
| 22:CV:6189:G:H2' | 22:CV:6190:U:H6 | 1.67 | 0.59 |
| 23:DA:2272:U:H6 | 23:DA:2272:U:C5' | 2.07 | 0.59 |
| 23:BA:1188:U:H4' | 40:BR:79:VAL:HG22 | 1.84 | 0.59 |
| 32:DJ:157:ARG:N | 32:DJ:158:PRO:HD3 | 2.05 | 0.59 |
| 25:BC:85:ASP:OD2 | 25:BC:86:PRO:HD2 | 2.03 | 0.59 |
| 1:AA:376:G:C4 | 1:AA:389:A:C2 | 2.89 | 0.59 |
| 25:BC:33:LEU:HD23 | 25:BC:33:LEU:N | 2.16 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DA:1639:U:H2' | 23:DA:1640:C:H5'' | 1.83 | 0.59 |
| 24:DB:45:A:N3 | 24:DB:45:A:H2' | 2.17 | 0.59 |
| 23:DA:661:C:O3' | 34:DL:18:ARG:HG2 | 2.03 | 0.59 |
| 3:CC:57:ILE:HD13 | 3:CC:66:VAL:HG22 | 1.84 | 0.59 |
| 44:BV:72:ARG:HG2 | 44:BV:89:PHE:HB2 | 1.84 | 0.59 |
| 5:AE:109:ILE:HG22 | 5:AE:110:LEU:HD23 | 1.84 | 0.59 |
| 5:AE:10:MET:HB2 | 5:AE:32:VAL:HG22 | 1.82 | 0.59 |
| 43:DU:29:GLU:HA | 43:DU:29:GLU:OE2 | 2.03 | 0.59 |
| 48:BZ:40:THR:CG2 | 48:BZ:43:ILE:HG12 | 2.28 | 0.59 |
| 23:BA:557:U:H2' | 23:BA:558:G:C8 | 2.32 | 0.59 |
| 19:CS:6:LYS:H | 19:CS:6:LYS:HD2 | 1.68 | 0.59 |
| 15:AO:81:LEU:O | 15:AO:85:LEU:HB2 | 2.01 | 0.59 |
| 17:CQ:59:ILE:HG23 | 17:CQ:71:PHE:CD1 | 2.38 | 0.59 |
| 44:BV:24:LEU:CD1 | 44:BV:85:HIS:HA | 2.32 | 0.59 |
| 35:DM:37:LEU:HG | 35:DM:128:LYS:O | 2.02 | 0.59 |
| 28:BF:36:LYS:HD3 | 28:BF:160:VAL:HG21 | 1.83 | 0.59 |
| 23:BA:781:A:H2 | 23:BA:1776:G:N3 | 2.01 | 0.59 |
| 44:BV:13:GLU:HB3 | 44:BV:18:LEU:CD1 | 2.33 | 0.59 |
| 45:DW:50:ASN:C | 45:DW:62:LEU:HB2 | 2.22 | 0.59 |
| 6:CF:47:ARG:HG2 | 6:CF:47:ARG:HH11 | 1.66 | 0.59 |
| 23:DA:565:C:C2' | 23:DA:566:U:O5' | 2.51 | 0.59 |
| 23:DA:828:U:C3' | 23:DA:828:U:O2 | 2.51 | 0.59 |
| 2:AB:32:ILE:HD11 | 2:AB:190:THR:HG21 | 1.82 | 0.59 |
| 46:BX:53:VAL:HG22 | 46:BX:74:VAL:HG13 | 1.85 | 0.59 |
| 23:BA:2051:A:H4' | 26:BD:141:ILE:HG23 | 1.83 | 0.59 |
| 25:DC:218:ARG:HB3 | 25:DC:219:PRO:HD2 | 1.83 | 0.59 |
| 23:BA:184:C:H2' | 23:BA:185:U:H6 | 1.66 | 0.59 |
| 23:DA:1514:U:H2' | 23:DA:1515:C:H6 | 1.66 | 0.59 |
| 17:CQ:7:THR:HA | 17:CQ:57:VAL:O | 2.02 | 0.59 |
| 27:DE:158:THR:HG23 | 27:DE:160:ASN:N | 2.17 | 0.59 |
| 8:AH:50:ARG:HG2 | 8:AH:50:ARG:HH11 | 1.68 | 0.59 |
| 50:D2:36:CYS:SG | 50:D2:37:LYS:N | 2.75 | 0.59 |
| 34:BL:140:ALA:O | 34:BL:141:ALA:HB2 | 2.02 | 0.59 |
| 34:DL:84:ASN:HA | 34:DL:115:LEU:O | 2.02 | 0.59 |
| 34:DL:59:LEU:O | 34:DL:59:LEU:HD23 | 2.03 | 0.59 |
| 23:DA:1448:G:N3 | 23:DA:1529:A:H2 | 1.99 | 0.59 |
| 38:BP:51:ARG:O | 38:BP:61:PHE:HA | 2.02 | 0.59 |
| 23:DA:1971:A:N3 | 25:DC:240:ALA:HA | 2.17 | 0.59 |
| 23:BA:1187:G:H5'' | 40:BR:81:TYR:CE2 | 2.37 | 0.59 |
| 23:BA:1159:U:H2' | 23:BA:1160:G:H8 | 1.67 | 0.59 |
| 40:BR:55:ALA:HA | 40:BR:101:GLY:O | 2.02 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:AP:55:ARG:NH1 | 16:AP:55:ARG:HB3 | 2.18 | 0.59 |
| 16:AP:55:ARG:O | 16:AP:58:TYR:HB3 | 2.01 | 0.59 |
| 4:CD:109:GLY:O | 4:CD:111:ALA:N | 2.35 | 0.59 |
| 1:AA:391:G:C6 | 1:AA:392:G:C5 | 2.91 | 0.59 |
| 5:CE:10:MET:HB2 | 5:CE:32:VAL:HG22 | 1.83 | 0.59 |
| 5:AE:43:LEU:CD1 | 5:AE:132:ALA:HB1 | 2.33 | 0.59 |
| 46:DX:12:PRO:O | 46:DX:14:VAL:HG23 | 2.03 | 0.59 |
| 23:DA:1495:A:C2 | 23:DA:1496:A:C2 | 2.91 | 0.59 |
| 46:BX:45:ASN:O | 46:BX:63:ALA:HA | 2.01 | 0.59 |
| 23:DA:528:A:C2 | 23:DA:2042:A:H2' | 2.37 | 0.59 |
| 23:BA:1475:G:N2 | 23:BA:1519:G:C5 | 2.69 | 0.59 |
| 1:CA:625:G:C5 | 1:CA:626:U:C5 | 2.89 | 0.59 |
| 44:BV:41:LEU:HD21 | 44:BV:83:PRO:HG2 | 1.83 | 0.59 |
| 1:CA:750:G:C2 | 1:CA:751:U:C6 | 2.90 | 0.59 |
| 43:DU:20:TYR:CE1 | 43:DU:42:VAL:HA | 2.38 | 0.59 |
| 23:DA:534:U:O2' | 39:DQ:49:HIS:HD2 | 1.81 | 0.59 |
| 23:DA:1396:U:C2' | 23:DA:1396:U:O2 | 2.50 | 0.59 |
| 4:CD:79:PHE:CZ | 4:CD:204:ILE:HA | 2.37 | 0.59 |
| 2:CB:223:ILE:C | 2:CB:225:ALA:H | 2.06 | 0.59 |
| 3:CC:22:TRP:HE3 | 3:CC:23:TYR:O | 1.84 | 0.59 |
| 26:DD:46:ALA:CB | 26:DD:82:ARG:HA | 2.32 | 0.59 |
| 27:DE:181:LEU:HD21 | 27:DE:186:ILE:HD11 | 1.83 | 0.59 |
| 17:CQ:7:THR:O | 17:CQ:23:VAL:HG13 | 2.02 | 0.59 |
| 15:CO:5:LYS:HD3 | 15:CO:6:GLU:H | 1.67 | 0.59 |
| 37:BO:20:ARG:HH12 | 45:BW:47:PRO:HB2 | 1.68 | 0.59 |
| 6:CF:96:PRO:HB3 | 18:CR:30:ASP:CG | 2.23 | 0.59 |
| 1:CA:868:C:H2' | 1:CA:869:G:O4' | 2.01 | 0.59 |
| 5:AE:15:ARG:O | 5:AE:15:ARG:HG2 | 2.01 | 0.59 |
| 23:BA:1516:U:H2' | 23:BA:1517:G:C8 | 2.37 | 0.59 |
| 1:AA:1333:A:C8 | 1:AA:1334:G:C8 | 2.90 | 0.59 |
| 23:DA:2889:C:H2' | 23:DA:2891:G:C8 | 2.37 | 0.59 |
| 23:BA:2393:A:H5' | 34:BL:60:MET:O | 2.02 | 0.59 |
| 23:BA:1268:A:H2' | 23:BA:1269:A:O5' | 2.03 | 0.59 |
| 23:BA:919:G:N2 | 23:BA:2269:A:OP2 | 2.36 | 0.59 |
| 1:CA:1351:U:O2' | 1:CA:1352:C:H5' | 2.02 | 0.59 |
| 1:CA:1353:G:H1 | 1:CA:1369:C:H42 | 1.49 | 0.59 |
| 22:CV:6213:A:C6 | 22:CV:6214:C:N4 | 2.70 | 0.59 |
| 1:CA:1234:C:O2' | 1:CA:1235:U:H5' | 2.02 | 0.59 |
| 37:BO:27:SER:HA | 37:BO:88:ASP:HB3 | 1.84 | 0.59 |
| 39:DQ:92:ARG:NH2 | 40:DR:11:GLN:N | 2.48 | 0.59 |
| 30:BH:87:LYS:HA | 30:BH:122:GLU:HA | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:BB:103:U:O2' | 44:BV:72:ARG:HG3 | 2.03 | 0.59 |
| 5:AE:43:LEU:HD11 | 5:AE:132:ALA:HB1 | 1.83 | 0.59 |
| 35:DM:47:ILE:CG2 | 35:DM:48:GLU:N | 2.61 | 0.59 |
| 23:BA:528:A:C2 | 23:BA:2042:A:H2' | 2.37 | 0.59 |
| 1:CA:447:G:H2' | 1:CA:485:G:N2 | 2.18 | 0.59 |
| 3:CC:131:ARG:HE | 5:CE:50:GLU:HG2 | 1.67 | 0.59 |
| 8:AH:87:SER:HA | 8:AH:93:VAL:HG23 | 1.83 | 0.59 |
| 1:AA:555:C:H2' | 1:AA:556:C:C6 | 2.35 | 0.59 |
| 53:B5:22:VAL:CG1 | 53:B5:50:LEU:HD12 | 2.32 | 0.59 |
| 23:BA:1478:G:C2 | 23:BA:1479:G:C8 | 2.90 | 0.59 |
| 23:BA:389:G:H1 | 34:BL:71:VAL:H | 1.50 | 0.59 |
| 44:DV:13:GLU:HB3 | 44:DV:18:LEU:CD1 | 2.33 | 0.59 |
| 50:B2:48:GLU:O | 50:B2:49:CYS:HB2 | 2.03 | 0.59 |
| 1:CA:1442:G:N7 | 1:CA:1446:A:C2 | 2.70 | 0.59 |
| 23:BA:825:C:O2 | 34:BL:55:ARG:NH2 | 2.34 | 0.59 |
| 1:AA:1442:G:N7 | 1:AA:1446:A:C2 | 2.71 | 0.59 |
| 1:AA:1095:U:H2' | 1:AA:1096:C:H6 | 1.67 | 0.59 |
| 23:DA:1973:G:H2' | 23:DA:1974:C:C6 | 2.37 | 0.59 |
| 1:CA:1326:C:O2 | 1:CA:1326:C:H2' | 2.03 | 0.59 |
| 1:AA:113:G:O2' | 1:AA:114:U:H5' | 2.02 | 0.59 |
| 1:CA:355:C:C4 | 1:CA:356:A:N7 | 2.71 | 0.59 |
| 23:BA:1817:G:OP1 | 25:BC:88:ARG:NH2 | 2.31 | 0.59 |
| 1:AA:1394:A:H4' | 1:AA:1395:C:OP2 | 2.01 | 0.59 |
| 1:AA:186(A):C:H5' | 20:AT:78:ALA:HB1 | 1.82 | 0.59 |
| 33:BK:86:ILE:HD12 | 33:BK:86:ILE:H | 1.68 | 0.59 |
| 49:B1:38:ALA:HA | 49:B1:55:PRO:HA | 1.84 | 0.59 |
| 45:DW:14:ARG:CZ | 45:DW:14:ARG:HB2 | 2.32 | 0.59 |
| 1:CA:685:G:C2 | 1:CA:686:U:C4 | 2.90 | 0.59 |
| 28:BF:55:LYS:HD2 | 28:BF:58:GLN:HE21 | 1.65 | 0.59 |
| 23:BA:1188:U:C2' | 23:BA:1189:A:H5' | 2.32 | 0.59 |
| 47:DY:13:ALA:O | 47:DY:17:SER:OG | 2.05 | 0.59 |
| 30:BH:88:ILE:HG12 | 30:BH:123:LEU:CA | 2.32 | 0.59 |
| 25:BC:86:PRO:HD2 | 25:BC:87:ASN:ND2 | 2.18 | 0.59 |
| 25:DC:108:PRO:HG3 | 25:DC:143:HIS:CE1 | 2.38 | 0.59 |
| 47:BY:28:LYS:HE3 | 47:BY:56:GLN:NE2 | 2.17 | 0.59 |
| 1:AA:1253:G:H1 | 1:AA:1284:C:N4 | 1.94 | 0.59 |
| 23:DA:819:A:OP2 | 23:DA:1187:G:N2 | 2.24 | 0.59 |
| 41:BS:75:TYR:CE2 | 41:BS:104:THR:CB | 2.84 | 0.59 |
| 24:BB:16:G:C6 | 24:BB:69:G:C2 | 2.91 | 0.59 |
| 23:BA:1786:A:H1' | 23:BA:1938:A:N6 | 2.18 | 0.59 |
| 48:BZ:40:THR:HG23 | 48:BZ:43:ILE:CG1 | 2.28 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:AA:265:G:C2' | 1:AA:266:G:H5'' | 2.28 | 0.59 |
| 24:BB:66:A:C5 | 24:BB:108:C:C5 | 2.91 | 0.59 |
| 17:AQ:83:ASP:O | 17:AQ:86:GLU:HB2 | 2.03 | 0.59 |
| 23:BA:1332:G:N2 | 23:BA:1609:A:O2' | 2.34 | 0.59 |
| 1:AA:630:G:O2' | 1:AA:631:G:H5' | 2.03 | 0.59 |
| 1:AA:667:G:H4' | 15:AO:51:HIS:ND1 | 2.17 | 0.59 |
| 23:DA:2565:A:H5'' | 23:DA:2566:A:OP2 | 2.03 | 0.59 |
| 23:BA:270(I):C:O2 | 23:BA:270(I):C:H2' | 2.01 | 0.59 |
| 1:CA:527:G:C2' | 1:CA:528:C:H5' | 2.33 | 0.59 |
| 23:BA:1218:C:C2' | 23:BA:1219:G:H5' | 2.33 | 0.59 |
| 1:AA:1239:A:H4' | 1:AA:1240:U:C5' | 2.33 | 0.59 |
| 45:DW:35:ASN:N | 45:DW:35:ASN:HD22 | 2.01 | 0.59 |
| 1:AA:1326:C:O2 | 1:AA:1326:C:H2' | 2.03 | 0.59 |
| 23:BA:184:C:H2' | 23:BA:185:U:C6 | 2.38 | 0.59 |
| 39:BQ:65:ILE:O | 39:BQ:66:ASN:C | 2.40 | 0.59 |
| 23:DA:1526:G:C6 | 23:DA:1527:G:C2 | 2.91 | 0.59 |
| 23:BA:2774:C:H2' | 23:BA:2775:A:O4' | 2.03 | 0.59 |
| 23:DA:2836:U:C4 | 23:DA:2883:A:N6 | 2.69 | 0.59 |
| 23:DA:270(M):U:H3' | 23:DA:270(N):U:H5'' | 1.85 | 0.59 |
| 26:BD:175:VAL:O | 26:BD:177:PRO:HD3 | 2.03 | 0.59 |
| 33:DK:26:LYS:O | 33:DK:27:GLY:O | 2.21 | 0.59 |
| 23:DA:191:A:H2' | 23:DA:192:C:C6 | 2.38 | 0.59 |
| 5:CE:68:GLU:O | 5:CE:68:GLU:HG3 | 2.02 | 0.59 |
| 41:BS:52:GLU:OE2 | 41:BS:52:GLU:HA | 2.02 | 0.59 |
| 15:CO:37:ASN:HD22 | 15:CO:37:ASN:H | 1.49 | 0.59 |
| 10:CJ:6:ILE:HG22 | 10:CJ:98:ILE:HG23 | 1.84 | 0.59 |
| 23:DA:2317:C:H2' | 23:DA:2318:G:H5' | 1.85 | 0.59 |
| 32:BJ:141:LYS:O | 32:BJ:144:LYS:HE3 | 2.02 | 0.59 |
| 1:CA:1349:A:H2' | 1:CA:1350:A:O4' | 2.02 | 0.59 |
| 23:BA:2438:U:O3' | 23:BA:2439:A:H3' | 2.02 | 0.59 |
| 37:BO:12:PHE:O | 37:BO:15:ARG:HG3 | 2.03 | 0.59 |
| 39:DQ:102:GLU:HG3 | 40:DR:2:PHE:CD1 | 2.38 | 0.59 |
| 34:BL:46:LYS:HG2 | 34:BL:52:GLU:OE1 | 2.03 | 0.59 |
| 1:AA:428:G:O4' | 1:AA:430:A:C8 | 2.56 | 0.59 |
| 47:DY:6:VAL:CG1 | 47:DY:10:LEU:HD11 | 2.28 | 0.59 |
| 28:DF:43:LEU:O | 28:DF:88:ILE:HG23 | 2.02 | 0.59 |
| 26:DD:57:LYS:HG3 | 26:DD:58:ARG:H | 1.68 | 0.59 |
| 23:BA:2542:A:H4' | 23:BA:2542:A:OP1 | 2.02 | 0.59 |
| 3:CC:195:VAL:O | 3:CC:196:LEU:HB2 | 2.02 | 0.59 |
| 23:BA:83:G:N1 | 23:BA:102:G:O2' | 1.97 | 0.59 |
| 25:DC:24:ILE:CD1 | 25:DC:84:TYR:HB2 | 2.32 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1503:A:OP1 | 1:CA:1531:A:O2' | 2.20 | 0.59 |
| 34:BL:18:ARG:CZ | 34:BL:18:ARG:HB3 | 2.32 | 0.59 |
| 23:DA:753:C:OP1 | 52:D4:1:MET:HE3 | 2.02 | 0.59 |
| 7:AG:131:LYS:HE3 | 7:AG:136:LYS:HZ2 | 1.67 | 0.59 |
| 18:CR:70:ILE:O | 18:CR:74:ARG:HG3 | 2.02 | 0.59 |
| 1:AA:136(A):C:H2' | 1:AA:136(B):C:H5'' | 1.83 | 0.59 |
| 2:CB:63:MET:CG | 2:CB:225:ALA:HB1 | 2.31 | 0.59 |
| 23:DA:2036:C:H6 | 23:DA:2036:C:C5' | 2.16 | 0.59 |
| 34:BL:105:LEU:HD12 | 34:BL:105:LEU:H | 1.66 | 0.59 |
| 23:DA:2716:U:O2' | 23:DA:2717:G:H5' | 2.02 | 0.59 |
| 23:BA:207:A:H2' | 23:BA:208:C:O4' | 2.02 | 0.59 |
| 13:AM:29:ARG:HB3 | 13:AM:64:TRP:CZ2 | 2.38 | 0.59 |
| 23:BA:2879:C:H4' | 23:BA:2880:C:OP1 | 2.01 | 0.59 |
| 23:BA:2443:C:O2' | 23:BA:2444:G:H5' | 2.03 | 0.59 |
| 1:CA:55:A:C4 | 1:CA:56:U:C6 | 2.91 | 0.59 |
| 29:BG:89:ILE:O | 29:BG:89:ILE:HG22 | 2.03 | 0.59 |
| 38:DP:64:ARG:HD2 | 38:DP:73:GLU:HG2 | 1.85 | 0.59 |
| 1:AA:1225:A:N3 | 1:AA:1225:A:H2' | 2.16 | 0.59 |
| 34:BL:33:ARG:CG | 34:BL:34:GLY:N | 2.65 | 0.59 |
| 2:CB:163:PHE:CD1 | 2:CB:185:ILE:HG13 | 2.37 | 0.59 |
| 23:DA:993:G:C4 | 23:DA:994:C:H5 | 2.20 | 0.59 |
| 28:DF:128:ARG:NH2 | 28:DF:161:THR:O | 2.34 | 0.59 |
| 23:DA:71:A:C2 | 42:DT:31:HIS:CE1 | 2.89 | 0.59 |
| 30:DH:68:LEU:C | 30:DH:138:ILE:HD13 | 2.23 | 0.59 |
| 3:AC:57:ILE:CD1 | 3:AC:66:VAL:HG22 | 2.32 | 0.59 |
| 25:DC:96:HIS:HD2 | 25:DC:102:LYS:HD3 | 1.63 | 0.59 |
| 5:AE:12:LEU:HD22 | 5:AE:12:LEU:C | 2.23 | 0.59 |
| 48:DZ:40:THR:HG23 | 48:DZ:43:ILE:CG1 | 2.31 | 0.59 |
| 44:DV:102:LEU:HD21 | 44:DV:124:ILE:CD1 | 2.33 | 0.59 |
| 6:CF:62:TRP:CE3 | 6:CF:62:TRP:O | 2.55 | 0.59 |
| 46:BX:11:ARG:HB3 | 46:BX:12:PRO:HD2 | 1.83 | 0.59 |
| 46:BX:45:ASN:HD22 | 46:BX:46:LEU:N | 2.01 | 0.59 |
| 23:DA:61:G:H5' | 47:DY:50:ILE:HG21 | 1.85 | 0.59 |
| 1:AA:318:G:N2 | 1:AA:319:G:C4 | 2.71 | 0.59 |
| 37:BO:36:TYR:HD1 | 37:BO:36:TYR:N | 2.00 | 0.59 |
| 23:BA:2469:A:H2 | 23:BA:2481:G:N2 | 2.00 | 0.59 |
| 23:BA:2100:G:N2 | 23:BA:2101:G:H1' | 2.17 | 0.59 |
| 15:CO:8:LYS:O | 15:CO:12:ILE:HG13 | 2.03 | 0.59 |
| 27:DE:36:VAL:O | 27:DE:40:GLN:HG3 | 2.03 | 0.59 |
| 29:BG:86:GLU:HG2 | 29:BG:164:TYR:O | 2.02 | 0.59 |
| 17:AQ:59:ILE:HG23 | 17:AQ:71:PHE:CD1 | 2.38 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:863:U:H2' | 1:CA:865:A:OP2 | 2.03 | 0.59 |
| 24:BB:30:C:OP2 | 37:BO:32:LEU:HD11 | 2.03 | 0.59 |
| 40:DR:22:VAL:CG1 | 40:DR:23:GLU:N | 2.64 | 0.59 |
| 9:AI:52:ALA:HB1 | 9:AI:95:LYS:NZ | 2.18 | 0.59 |
| 11:AK:48:ILE:HD11 | 11:AK:64:ALA:HA | 1.83 | 0.59 |
| 1:CA:179:A:H2' | 1:CA:180:U:C6 | 2.38 | 0.59 |
| 1:AA:224:C:H2' | 1:AA:225:C:C6 | 2.38 | 0.59 |
| 23:DA:1901:A:N3 | 23:DA:1901:A:H2' | 2.16 | 0.59 |
| 1:AA:1159:U:H4' | 1:AA:1160:G:OP1 | 2.02 | 0.59 |
| 9:CI:52:ALA:HB1 | 9:CI:95:LYS:NZ | 2.18 | 0.59 |
| 23:DA:958:U:OP2 | 35:DM:14:ARG:NH1 | 2.36 | 0.59 |
| 23:BA:747:U:OP2 | 50:B2:3:LYS:HD3 | 2.03 | 0.59 |
| 24:BB:81:G:C6 | 24:BB:82:G:C5 | 2.91 | 0.59 |
| 1:AA:1234:C:O2' | 1:AA:1235:U:H5' | 2.03 | 0.59 |
| 26:BD:167:VAL:HG11 | 26:BD:189:PRO:HD3 | 1.84 | 0.59 |
| 1:CA:1223:C:P | 1:CA:1224:G:H2' | 2.42 | 0.59 |
| 23:DA:727:A:C2 | 25:DC:9:TYR:CD2 | 2.90 | 0.59 |
| 39:DQ:92:ARG:HD2 | 39:DQ:95:LEU:HG | 1.85 | 0.59 |
| 32:DJ:89:LYS:O | 32:DJ:90:LEU:C | 2.41 | 0.59 |
| 40:BR:49:THR:HB | 40:BR:50:PRO:HD2 | 1.83 | 0.59 |
| 1:AA:362:G:O2' | 12:AL:32:ARG:NH2 | 2.36 | 0.59 |
| 25:BC:75:ILE:O | 25:BC:118:VAL:HG23 | 2.02 | 0.59 |
| 1:CA:391:G:C6 | 1:CA:392:G:C5 | 2.91 | 0.59 |
| 2:CB:187:LEU:HD11 | 2:CB:204:ASN:O | 2.03 | 0.59 |
| 44:BV:92:SER:HB2 | 44:BV:94:GLU:OE2 | 2.03 | 0.59 |
| 23:DA:1288:U:C2 | 23:DA:1327:C:O2 | 2.55 | 0.59 |
| 2:CB:102:LEU:HD12 | 2:CB:102:LEU:N | 2.18 | 0.59 |
| 42:BT:29:TRP:CZ3 | 42:BT:78:LYS:HG3 | 2.38 | 0.59 |
| 29:BG:23:ARG:N | 29:BG:23:ARG:HD3 | 2.18 | 0.59 |
| 24:BB:33:G:C2 | 24:BB:50:G:C2 | 2.91 | 0.59 |
| 23:BA:910:A:C6 | 23:BA:911:A:C6 | 2.91 | 0.59 |
| 28:BF:133:LEU:HD23 | 28:BF:133:LEU:N | 2.18 | 0.59 |
| 23:BA:1433:U:O2' | 23:BA:1434:A:H5' | 2.03 | 0.59 |
| 28:DF:7:LEU:HA | 28:DF:10:LYS:HB2 | 1.85 | 0.59 |
| 35:DM:134:ARG:HA | 35:DM:134:ARG:NE | 2.18 | 0.59 |
| 23:BA:2705:A:C2 | 36:BN:64:ARG:NH1 | 2.71 | 0.59 |
| 1:CA:178:C:O2' | 1:CA:179:A:H5' | 2.03 | 0.59 |
| 38:BP:109:GLU:O | 38:BP:112:ARG:HG3 | 2.03 | 0.59 |
| 1:CA:458:C:H2' | 1:CA:464:G:O4' | 2.03 | 0.59 |
| 1:AA:685:G:C2 | 1:AA:686:U:C4 | 2.91 | 0.59 |
| 23:DA:1833:U:C2' | 23:DA:1834:U:H5' | 2.33 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:DC:43:ARG:HB2 | 25:DC:49:ILE:HA | 1.83 | 0.59 |
| 24:BB:82:G:C2' | 24:BB:83:G:H5' | 2.33 | 0.59 |
| 23:DA:84:A:H2 | 23:DA:98:G:N3 | 2.01 | 0.59 |
| 38:BP:74:ARG:HD3 | 38:BP:76:PHE:CZ | 2.37 | 0.59 |
| 32:BJ:89:LYS:O | 32:BJ:90:LEU:C | 2.39 | 0.59 |
| 23:DA:1019:U:O2' | 23:DA:1021:A:C2 | 2.55 | 0.59 |
| 23:BA:94:G:N2 | 47:BY:47:ASN:HD22 | 1.97 | 0.59 |
| 20:CT:76:ALA:O | 20:CT:80:ARG:HG2 | 2.03 | 0.59 |
| 5:CE:33:VAL:HG13 | 5:CE:109:ILE:HD13 | 1.85 | 0.59 |
| 5:CE:11:ILE:HB | 5:CE:31:LEU:HB3 | 1.85 | 0.59 |
| 23:BA:2378:A:O2' | 37:BO:21:THR:HG21 | 2.03 | 0.59 |
| 1:AA:1281:U:C5' | 1:AA:1282:C:H5 | 2.15 | 0.59 |
| 41:DS:24:ILE:HG21 | 41:DS:36:LEU:HD21 | 1.84 | 0.59 |
| 41:BS:29:LEU:HD21 | 41:BS:33:ARG:NE | 2.16 | 0.59 |
| 23:BA:1858:G:O2' | 23:BA:1859:A:C8 | 2.53 | 0.59 |
| 23:DA:1105:U:O2' | 23:DA:1106:G:H5' | 2.03 | 0.59 |
| 6:AF:91:VAL:HG13 | 18:AR:72:ARG:NH2 | 2.17 | 0.59 |
| 28:BF:131:TYR:HE2 | 28:BF:133:LEU:HB3 | 1.68 | 0.59 |
| 1:CA:782:A:H2' | 1:CA:783:C:H5' | 1.84 | 0.59 |
| 18:CR:63:GLN:O | 18:CR:66:LEU:HB3 | 2.03 | 0.59 |
| 23:BA:971:C:C2' | 23:BA:972:G:H5' | 2.32 | 0.59 |
| 23:DA:185:U:H2' | 23:DA:186:G:H8 | 1.68 | 0.59 |
| 2:CB:32:ILE:HD11 | 2:CB:190:THR:CG2 | 2.33 | 0.59 |
| 35:DM:62:GLY:O | 44:DV:178:GLU:HG2 | 2.02 | 0.59 |
| 39:BQ:65:ILE:O | 39:BQ:68:ALA:N | 2.35 | 0.59 |
| 25:BC:260:ARG:O | 25:BC:261:LYS:O | 2.21 | 0.59 |
| 27:DE:59:TYR:HB3 | 27:DE:78:ILE:HD12 | 1.84 | 0.59 |
| 28:DF:143:GLU:CD | 28:DF:143:GLU:H | 2.05 | 0.59 |
| 23:BA:2506:U:H5 | 23:BA:2507:C:C5 | 2.21 | 0.59 |
| 41:BS:62:HIS:C | 41:BS:64:MET:H | 2.06 | 0.59 |
| 23:BA:1850:G:C6 | 23:BA:1851:U:C4 | 2.91 | 0.59 |
| 40:DR:1:MET:H2 | 40:DR:16:PRO:HD3 | 1.67 | 0.59 |
| 32:DJ:146:TYR:CD1 | 32:DJ:146:TYR:N | 2.70 | 0.59 |
| 3:CC:126:ARG:O | 3:CC:127:ARG:HB2 | 2.01 | 0.59 |
| 32:BJ:114:LEU:HD21 | 32:BJ:121:VAL:HG21 | 1.83 | 0.58 |
| 10:AJ:62:HIS:O | 14:AN:59:ALA:HB3 | 2.03 | 0.58 |
| 26:BD:11:MET:CB | 26:BD:24:THR:HA | 2.33 | 0.58 |
| 34:BL:33:ARG:O | 34:BL:35:HIS:O | 2.20 | 0.58 |
| 1:CA:960:U:C5 | 1:CA:1225:A:H1' | 2.37 | 0.58 |
| 27:BE:63:LYS:HZ3 | 27:BE:67:GLN:NE2 | 2.01 | 0.58 |
| 37:BO:89:ARG:O | 37:BO:90:GLY:O | 2.21 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 26:DD:132:HIS:CG | 26:DD:135:HIS:NE2 | 2.70 | 0.58 |
| 25:BC:108:PRO:CG | 25:BC:143:HIS:HE1 | 2.15 | 0.58 |
| 23:BA:1826:G:H4' | 25:BC:242:ARG:NE | 2.08 | 0.58 |
| 32:DJ:90:LEU:O | 32:DJ:111:GLU:HG3 | 2.02 | 0.58 |
| 23:BA:2729:G:H2' | 23:BA:2730:C:C6 | 2.37 | 0.58 |
| 23:DA:2730:C:O2' | 23:DA:2731:G:H5' | 2.02 | 0.58 |
| 12:AL:26:LEU:HD12 | 12:AL:29:ALA:HB2 | 1.84 | 0.58 |
| 30:DH:82:ARG:HB3 | 30:DH:89:TYR:CD1 | 2.38 | 0.58 |
| 20:AT:26:ASN:O | 20:AT:30:LYS:HB2 | 2.03 | 0.58 |
| 23:DA:1771:C:H1' | 23:DA:1786:A:C8 | 2.38 | 0.58 |
| 43:DU:29:GLU:CB | 43:DU:38:ILE:HB | 2.31 | 0.58 |
| 48:BZ:17:LYS:C | 48:BZ:17:LYS:HD3 | 2.23 | 0.58 |
| 1:AA:1349:A:P | 9:AI:118:LYS:NZ | 2.76 | 0.58 |
| 12:CL:40:ARG:HG2 | 12:CL:41:THR:N | 2.16 | 0.58 |
| 23:DA:2808:U:H2' | 23:DA:2809:A:C5' | 2.32 | 0.58 |
| 1:AA:749:C:OP2 | 1:AA:750:G:OP2 | 2.21 | 0.58 |
| 53:B5:14:VAL:CG1 | 53:B5:22:VAL:HG13 | 2.33 | 0.58 |
| 25:BC:25:THR:HG22 | 25:BC:82:ILE:O | 2.02 | 0.58 |
| 1:CA:1084:G:OP1 | 1:CA:1086:U:C2 | 2.56 | 0.58 |
| 1:CA:663:A:O2' | 1:CA:664:G:H5' | 2.02 | 0.58 |
| 23:BA:1778:U:H2' | 23:BA:1784:A:H62 | 1.66 | 0.58 |
| 1:CA:920:U:H2' | 1:CA:921:U:H6 | 1.66 | 0.58 |
| 8:AH:114:THR:HG22 | 8:AH:130:GLY:O | 2.02 | 0.58 |
| 6:AF:47:ARG:HH11 | 6:AF:47:ARG:HG2 | 1.67 | 0.58 |
| 7:CG:120:ILE:HG22 | 7:CG:124:LEU:HD12 | 1.85 | 0.58 |
| 1:CA:342:C:C2' | 1:CA:343:U:H5' | 2.33 | 0.58 |
| 1:AA:663:A:O2' | 1:AA:664:G:H5' | 2.03 | 0.58 |
| 38:BP:124:ASP:O | 38:BP:128:GLU:HB2 | 2.02 | 0.58 |
| 1:CA:1360:A:H8 | 1:CA:1360:A:OP1 | 1.86 | 0.58 |
| 23:BA:2038:G:H2' | 23:BA:2039:C:H6 | 1.68 | 0.58 |
| 11:AK:109:VAL:CG1 | 18:AR:84:LYS:HB2 | 2.33 | 0.58 |
| 27:BE:158:THR:HG23 | 27:BE:160:ASN:N | 2.17 | 0.58 |
| 23:DA:2058:A:N6 | 23:DA:2059:A:N6 | 2.51 | 0.58 |
| 16:AP:54:GLU:O | 16:AP:57:ARG:HB2 | 2.03 | 0.58 |
| 53:D5:57:ARG:CZ | 53:D5:57:ARG:CA | 2.81 | 0.58 |
| 45:BW:23:VAL:HB | 45:BW:26:TYR:CE2 | 2.38 | 0.58 |
| 34:BL:33:ARG:CG | 34:BL:34:GLY:H | 2.16 | 0.58 |
| 27:DE:65:TRP:CZ3 | 27:DE:72:ARG:HB3 | 2.39 | 0.58 |
| 23:BA:1971:A:N3 | 25:BC:241:PRO:HD3 | 2.18 | 0.58 |
| 23:BA:1266:G:O5' | 41:BS:15:ARG:NH2 | 2.36 | 0.58 |
| 41:BS:12:ILE:HG12 | 41:BS:13:SER:N | 2.18 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:DF:84:LYS:CG | 28:DF:85:GLY:H | 2.07 | 0.58 |
| 16:CP:55:ARG:NH1 | 16:CP:55:ARG:HB3 | 2.19 | 0.58 |
| 23:DA:1266:G:O5' | 41:DS:15:ARG:NH2 | 2.36 | 0.58 |
| 12:AL:116:ARG:O | 12:AL:118:LYS:N | 2.36 | 0.58 |
| 3:CC:130:VAL:O | 3:CC:134:ILE:HG13 | 2.03 | 0.58 |
| 26:BD:57:LYS:HG3 | 26:BD:58:ARG:N | 2.18 | 0.58 |
| 1:AA:191(G):G:H2' | 1:AA:192:U:H6 | 1.68 | 0.58 |
| 23:DA:2787:C:H1' | 26:DD:62:PRO:CB | 2.33 | 0.58 |
| 36:DN:57:ARG:HD2 | 36:DN:59:ASP:OD2 | 2.03 | 0.58 |
| 1:AA:1292:U:H2' | 1:AA:1293:G:C8 | 2.38 | 0.58 |
| 23:BA:2808:U:H2' | 23:BA:2809:A:C5' | 2.33 | 0.58 |
| 1:CA:349:A:O2' | 1:CA:350:G:H5' | 2.03 | 0.58 |
| 23:BA:953:A:OP2 | 35:BM:16:ARG:NH2 | 2.35 | 0.58 |
| 18:CR:26:LEU:HD21 | 18:CR:42:ARG:NH1 | 2.17 | 0.58 |
| 32:BJ:81:ASP:OD2 | 32:BJ:147:ALA:HB1 | 2.02 | 0.58 |
| 23:DA:2287:A:O2' | 23:DA:2288:A:O5' | 2.20 | 0.58 |
| 11:CK:21:ILE:HB | 11:CK:84:VAL:HG12 | 1.84 | 0.58 |
| 1:CA:664:G:P | 18:CR:64:ARG:HH21 | 2.25 | 0.58 |
| 23:DA:1746:G:C2 | 23:DA:1747:G:N7 | 2.71 | 0.58 |
| 1:CA:1411:C:H2' | 1:CA:1412:C:H6 | 1.67 | 0.58 |
| 1:CA:632:A:N7 | 1:CA:633:G:C5 | 2.70 | 0.58 |
| 10:CJ:45:ARG:NH1 | 14:CN:36:PHE:HD2 | 2.00 | 0.58 |
| 35:BM:134:ARG:HA | 35:BM:134:ARG:NE | 2.18 | 0.58 |
| 39:DQ:30:LYS:O | 39:DQ:31:SER:HB3 | 2.03 | 0.58 |
| 1:CA:1095:U:H2' | 1:CA:1096:C:H6 | 1.68 | 0.58 |
| 23:DA:903:C:H2' | 23:DA:904:C:C6 | 2.38 | 0.58 |
| 35:BM:43:THR:OG1 | 35:BM:46:GLN:HG3 | 2.03 | 0.58 |
| 2:AB:20:GLU:HB2 | 2:AB:190:THR:OG1 | 2.02 | 0.58 |
| 23:DA:207:A:H2' | 23:DA:208:C:O4' | 2.02 | 0.58 |
| 18:CR:19:LYS:O | 18:CR:20:ALA:HB2 | 2.03 | 0.58 |
| 1:CA:816:A:OP2 | 1:CA:1527:C:H4' | 2.04 | 0.58 |
| 23:BA:2317:C:H2' | 23:BA:2318:G:C5' | 2.32 | 0.58 |
| 44:DV:11:GLU:HG3 | 44:DV:12:GLY:N | 2.18 | 0.58 |
| 29:DG:13:LYS:O | 29:DG:15:VAL:HG13 | 2.03 | 0.58 |
| 34:DL:61:ARG:CD | 53:D5:13:ARG:HD2 | 2.32 | 0.58 |
| 23:BA:2272:U:H6 | 23:BA:2272:U:C5' | 2.03 | 0.58 |
| 1:AA:979:C:H42 | 14:AN:18:VAL:HG12 | 1.67 | 0.58 |
| 1:CA:1333:A:C8 | 1:CA:1334:G:C8 | 2.90 | 0.58 |
| 1:CA:1316:G:O2' | 14:CN:18:VAL:HG21 | 2.02 | 0.58 |
| 24:BB:7:G:H5'' | 37:BO:29:PHE:CE2 | 2.38 | 0.58 |
| 23:BA:1141:U:P | 32:BJ:86:THR:HG21 | 2.44 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 26:DD:132:HIS:HA | 26:DD:135:HIS:CE1 | 2.38 | 0.58 |
| 23:DA:1158:C:C2' | 23:DA:1159:U:H5' | 2.33 | 0.58 |
| 40:DR:39:LEU:CB | 40:DR:47:VAL:HG21 | 2.32 | 0.58 |
| 24:DB:81:G:C5 | 24:DB:82:G:C8 | 2.91 | 0.58 |
| 1:CA:377:G:O2' | 1:CA:378:G:H5' | 2.01 | 0.58 |
| 34:BL:49:ARG:HG3 | 53:B5:60:LEU:HD21 | 1.84 | 0.58 |
| 1:AA:404:U:H2' | 1:AA:405:U:H6 | 1.67 | 0.58 |
| 36:DN:107:ASP:OD2 | 36:DN:107:ASP:C | 2.40 | 0.58 |
| 28:BF:43:LEU:O | 28:BF:88:ILE:HG23 | 2.03 | 0.58 |
| 35:BM:140:ALA:HB3 | 44:BV:53:ILE:HG12 | 1.85 | 0.58 |
| 45:BW:70:GLN:OE1 | 45:BW:72:ARG:HD3 | 2.03 | 0.58 |
| 23:BA:142:G:H1' | 42:BT:37:THR:CG2 | 2.33 | 0.58 |
| 23:BA:528:A:C8 | 23:BA:528:A:C3' | 2.87 | 0.58 |
| 23:BA:556:G:H2' | 23:BA:557:U:C6 | 2.38 | 0.58 |
| 23:DA:2755:C:O2' | 23:DA:2756:U:H2' | 2.03 | 0.58 |
| 3:AC:47:LEU:HD23 | 3:AC:52:LEU:HD13 | 1.85 | 0.58 |
| 30:BH:15:VAL:HG12 | 30:BH:16:GLY:H | 1.68 | 0.58 |
| 23:DA:270(H):C:H2' | 23:DA:270(I):C:C6 | 2.36 | 0.58 |
| 23:BA:270(H):C:H2' | 23:BA:270(I):C:C6 | 2.35 | 0.58 |
| 23:BA:1389:G:H2' | 23:BA:1390:U:C6 | 2.38 | 0.58 |
| 23:DA:1389:G:O2' | 23:DA:1390:U:H5' | 2.04 | 0.58 |
| 23:BA:830:G:H4' | 23:BA:831:G:OP2 | 2.04 | 0.58 |
| 1:AA:921:U:O2 | 5:AE:19:MET:HB2 | 2.04 | 0.58 |
| 18:AR:63:GLN:O | 18:AR:66:LEU:HB3 | 2.04 | 0.58 |
| 1:AA:1426:C:H2' | 1:AA:1427:U:H6 | 1.67 | 0.58 |
| 23:DA:1793:C:H2' | 23:DA:1794:U:C6 | 2.39 | 0.58 |
| 23:BA:1845:G:OP1 | 25:BC:258:LYS:HE3 | 2.04 | 0.58 |
| 1:AA:1418:A:C2 | 1:AA:1483:A:C2 | 2.92 | 0.58 |
| 1:CA:411:A:C5 | 1:CA:429:U:C5 | 2.91 | 0.58 |
| 27:BE:14:PRO:HD3 | 27:BE:128:ALA:HB2 | 1.86 | 0.58 |
| 23:BA:185:U:H2' | 23:BA:186:G:C8 | 2.37 | 0.58 |
| 23:BA:188:G:H2' | 23:BA:189:G:H5' | 1.85 | 0.58 |
| 1:AA:1464:G:O2' | 1:AA:1465:C:H5' | 2.03 | 0.58 |
| 44:DV:9:TYR:CZ | 44:DV:61:LEU:HD13 | 2.37 | 0.58 |
| 23:BA:1459:G:N3 | 23:BA:1459:G:H2' | 2.18 | 0.58 |
| 23:BA:1916:A:H2' | 23:BA:1917:U:O4' | 2.02 | 0.58 |
| 23:DA:706:A:H2' | 23:DA:707:G:O4' | 2.03 | 0.58 |
| 1:CA:826:C:H2' | 8:CH:15:ASN:HD22 | 1.68 | 0.58 |
| 12:CL:54:VAL:HG12 | 12:CL:55:ALA:H | 1.68 | 0.58 |
| 28:BF:165:THR:OG1 | 28:BF:168:GLU:HG3 | 2.02 | 0.58 |
| 38:DP:124:ASP:O | 38:DP:128:GLU:HB2 | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:BB:116:G:H4' | 37:BO:55:ALA:O | 2.03 | 0.58 |
| 38:DP:80:SER:C | 38:DP:82:LEU:H | 2.06 | 0.58 |
| 1:AA:42:G:H8 | 1:AA:42:G:OP2 | 1.86 | 0.58 |
| 19:AS:16:LEU:O | 19:AS:20:LEU:HG | 2.04 | 0.58 |
| 1:CA:247:G:OP2 | 17:CQ:100:LYS:N | 2.36 | 0.58 |
| 34:DL:81:GLN:HG2 | 34:DL:106:LEU:HD22 | 1.85 | 0.58 |
| 50:B2:4:HIS:HB3 | 50:B2:5:PRO:HD3 | 1.84 | 0.58 |
| 32:BJ:118:PRO:HD2 | 32:BJ:119:GLU:OE1 | 2.04 | 0.58 |
| 1:CA:1349:A:OP1 | 9:CI:120:ARG:HB2 | 2.03 | 0.58 |
| 1:AA:946:A:H2' | 1:AA:947:G:H8 | 1.68 | 0.58 |
| 22:AV:6189:G:H2' | 22:AV:6190:U:H6 | 1.69 | 0.58 |
| 23:BA:1190:G:H5'' | 34:BL:35:HIS:HA | 1.84 | 0.58 |
| 23:DA:1158:C:O2' | 23:DA:1159:U:H5' | 2.03 | 0.58 |
| 25:BC:108:PRO:HG3 | 25:BC:143:HIS:CE1 | 2.38 | 0.58 |
| 34:DL:49:ARG:HG3 | 53:D5:60:LEU:HD21 | 1.84 | 0.58 |
| 12:AL:116:ARG:NH2 | 12:AL:123:LYS:HB2 | 2.18 | 0.58 |
| 23:DA:2698:U:H2' | 23:DA:2699:C:C6 | 2.38 | 0.58 |
| 28:DF:88:ILE:HD11 | 28:DF:90:LEU:CD2 | 2.33 | 0.58 |
| 8:AH:123:GLU:O | 8:AH:127:LEU:HB2 | 2.04 | 0.58 |
| 23:DA:661:C:C4' | 34:DL:18:ARG:HG2 | 2.32 | 0.58 |
| 1:CA:266:G:C5' | 1:CA:267:C:H5 | 2.16 | 0.58 |
| 26:DD:111:ARG:CD | 26:DD:160:TYR:HE1 | 2.14 | 0.58 |
| 1:AA:1080:A:H5'' | 1:AA:1081:G:OP2 | 2.03 | 0.58 |
| 1:CA:409:G:H2' | 1:CA:410:G:O5' | 2.03 | 0.58 |
| 19:AS:63:THR:HG22 | 19:AS:66:MET:CG | 2.32 | 0.58 |
| 33:BK:24:VAL:HB | 33:BK:33:ALA:HB2 | 1.86 | 0.58 |
| 25:BC:133:LEU:C | 25:BC:135:PHE:N | 2.57 | 0.58 |
| 23:DA:952:G:OP1 | 35:DM:16:ARG:NH2 | 2.33 | 0.58 |
| 23:DA:226:G:C2 | 23:DA:228:A:N6 | 2.72 | 0.58 |
| 7:AG:136:LYS:O | 7:AG:140:ASP:HB2 | 2.04 | 0.58 |
| 23:DA:1478:G:C2 | 23:DA:1479:G:C8 | 2.92 | 0.58 |
| 24:DB:48:A:H4' | 37:DO:95:HIS:CD2 | 2.38 | 0.58 |
| 32:BJ:66:THR:O | 32:BJ:69:VAL:HG12 | 2.03 | 0.58 |
| 17:AQ:4:LYS:HG3 | 17:AQ:5:VAL:N | 2.18 | 0.58 |
| 1:AA:109:A:N6 | 1:AA:326:G:C5 | 2.72 | 0.58 |
| 1:AA:521:G:O6 | 1:AA:529:G:C2 | 2.57 | 0.58 |
| 1:CA:972:C:H4' | 10:CJ:57:LYS:HG3 | 1.84 | 0.58 |
| 23:BA:225:A:N6 | 23:BA:226:G:N1 | 2.50 | 0.58 |
| 1:CA:491:G:H2' | 1:CA:492:G:H8 | 1.67 | 0.58 |
| 5:AE:79:GLU:CD | 5:AE:79:GLU:H | 2.06 | 0.58 |
| 23:BA:2511:U:O3' | 26:BD:123:ALA:HB3 | 2.04 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 12:AL:63:TYR:O | 12:AL:64:GLU:HB2 | 2.01 | 0.58 |
| 23:BA:1991:U:H2' | 23:BA:1992:G:H5' | 1.85 | 0.58 |
| 34:DL:136:GLU:O | 34:DL:137:LYS:C | 2.42 | 0.58 |
| 1:CA:136(A):C:H2' | 1:CA:136(B):C:H5'' | 1.84 | 0.58 |
| 23:BA:2335:A:C8 | 23:BA:2337:G:C5 | 2.91 | 0.58 |
| 23:DA:2320:A:N3 | 23:DA:2320:A:H2' | 2.19 | 0.58 |
| 1:CA:262:A:C6 | 1:CA:263:A:C6 | 2.92 | 0.58 |
| 4:AD:67:ILE:HG22 | 4:AD:68:TYR:CD1 | 2.38 | 0.58 |
| 26:BD:57:LYS:HG3 | 26:BD:58:ARG:H | 1.67 | 0.58 |
| 26:DD:6:GLY:HA2 | 26:DD:51:PHE:HE2 | 1.69 | 0.58 |
| 48:BZ:40:THR:OG1 | 48:BZ:41:PRO:HD2 | 2.04 | 0.58 |
| 48:DZ:43:ILE:HD13 | 48:DZ:43:ILE:H | 1.64 | 0.58 |
| 45:DW:70:GLN:OE1 | 45:DW:72:ARG:HD3 | 2.03 | 0.58 |
| 24:DB:78:A:C2 | 24:DB:99:A:C5 | 2.91 | 0.58 |
| 1:AA:232:G:H1' | 1:AA:262:A:N1 | 2.19 | 0.58 |
| 2:AB:223:ILE:C | 2:AB:225:ALA:H | 2.06 | 0.58 |
| 21:CU:22:ARG:HD2 | 21:CU:23:PRO:HD2 | 1.84 | 0.58 |
| 20:CT:13:LEU:CD1 | 20:CT:13:LEU:H | 2.15 | 0.58 |
| 1:CA:630:G:O2' | 1:CA:631:G:H5' | 2.03 | 0.58 |
| 1:AA:1411:C:H2' | 1:AA:1412:C:H6 | 1.68 | 0.58 |
| 23:DA:640:C:H2' | 23:DA:641:C:C6 | 2.37 | 0.58 |
| 23:BA:61:G:H5' | 47:BY:50:ILE:HG21 | 1.86 | 0.58 |
| 2:CB:20:GLU:HB2 | 2:CB:190:THR:OG1 | 2.03 | 0.58 |
| 1:AA:1057:G:C2 | 1:AA:1204:A:C2 | 2.92 | 0.58 |
| 24:BB:28:C:H2' | 24:BB:29:A:C8 | 2.39 | 0.58 |
| 16:CP:54:GLU:O | 16:CP:57:ARG:HB2 | 2.04 | 0.58 |
| 53:D5:29:LYS:NZ | 53:D5:29:LYS:HB3 | 2.19 | 0.58 |
| 38:DP:29:ARG:HD2 | 38:DP:44:ASP:OD2 | 2.03 | 0.58 |
| 23:BA:2183:C:O2 | 23:BA:2183:C:H2' | 2.04 | 0.58 |
| 23:BA:1901:A:N3 | 23:BA:1901:A:H2' | 2.19 | 0.58 |
| 1:AA:991:U:O2' | 1:AA:993:G:C8 | 2.56 | 0.58 |
| 12:AL:22:LYS:O | 12:AL:96:ARG:HD2 | 2.04 | 0.58 |
| 23:BA:1996:C:H4' | 23:BA:1997:G:OP1 | 2.03 | 0.58 |
| 34:BL:111:ARG:HG3 | 34:BL:128:HIS:CB | 2.33 | 0.58 |
| 26:BD:23:VAL:HA | 26:BD:184:VAL:O | 2.03 | 0.58 |
| 38:BP:64:ARG:HA | 38:BP:72:VAL:O | 2.03 | 0.58 |
| 41:BS:86:LEU:HD12 | 41:BS:87:PRO:HD2 | 1.86 | 0.58 |
| 23:DA:819:A:C4 | 23:DA:1189:A:C2 | 2.91 | 0.58 |
| 28:BF:88:ILE:HD11 | 28:BF:90:LEU:CD2 | 2.33 | 0.58 |
| 26:DD:6:GLY:HA2 | 26:DD:51:PHE:CE2 | 2.37 | 0.58 |
| 26:DD:51:PHE:HB3 | 26:DD:77:ILE:HD12 | 1.84 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:DX:11:ARG:HH12 | 46:DX:61:ARG:N | 2.01 | 0.58 |
| 1:AA:1349:A:OP2 | 9:AI:118:LYS:NZ | 2.36 | 0.58 |
| 23:DA:2758:A:C5 | 29:DG:67:LEU:HD21 | 2.38 | 0.58 |
| 23:BA:1858:G:H1' | 23:BA:1884:A:H62 | 1.68 | 0.58 |
| 23:DA:1055:G:H2' | 23:DA:1056:G:H8 | 1.63 | 0.58 |
| 23:DA:558:G:P | 32:DJ:134:PRO:HD2 | 2.44 | 0.58 |
| 8:AH:86:ILE:CB | 8:AH:133:LEU:HD22 | 2.32 | 0.58 |
| 25:DC:25:THR:HG21 | 25:DC:82:ILE:H | 1.68 | 0.58 |
| 25:DC:25:THR:O | 25:DC:27:THR:HB | 2.04 | 0.58 |
| 1:CA:643:C:H5' | 8:CH:31:PHE:CD1 | 2.38 | 0.58 |
| 24:BB:48:A:H4' | 37:BO:95:HIS:CD2 | 2.38 | 0.58 |
| 23:BA:389:G:H22 | 34:BL:72:PRO:HD3 | 1.69 | 0.58 |
| 2:CB:72:GLY:HA3 | 2:CB:165:VAL:CG1 | 2.34 | 0.58 |
| 23:BA:1006:C:C2 | 23:BA:1138:G:N2 | 2.71 | 0.58 |
| 34:BL:55:ARG:CG | 34:BL:56:SER:N | 2.63 | 0.58 |
| 18:AR:66:LEU:HG | 18:AR:70:ILE:HD11 | 1.85 | 0.58 |
| 1:AA:1298:C:H4' | 1:AA:1299:A:C8 | 2.38 | 0.58 |
| 43:DU:59:GLY:HA3 | 43:DU:61:ILE:HG12 | 1.84 | 0.58 |
| 23:DA:2709:G:C2' | 23:DA:2710:C:H5' | 2.34 | 0.58 |
| 1:AA:465:A:N7 | 1:AA:467:G:C6 | 2.72 | 0.58 |
| 19:CS:16:LEU:O | 19:CS:20:LEU:HG | 2.03 | 0.58 |
| 7:AG:70:LYS:HE2 | 7:AG:96:GLN:NE2 | 2.19 | 0.58 |
| 35:DM:40:ALA:HB2 | 35:DM:127:ILE:HD12 | 1.85 | 0.58 |
| 14:AN:12:ARG:HG2 | 14:AN:14:PRO:HD3 | 1.86 | 0.58 |
| 23:DA:530:G:C5 | 23:DA:2022:U:H5'' | 2.39 | 0.58 |
| 23:DA:46:C:H42 | 23:DA:179:G:H1 | 1.52 | 0.58 |
| 23:DA:399:G:H2' | 23:DA:400:G:H5' | 1.85 | 0.58 |
| 1:AA:273:A:N6 | 1:AA:274:A:N6 | 2.52 | 0.58 |
| 26:DD:24:THR:HB | 26:DD:186:GLY:HA2 | 1.85 | 0.58 |
| 23:BA:1529:A:C8 | 23:BA:1530:G:C8 | 2.91 | 0.58 |
| 23:BA:727:A:C2 | 25:BC:9:TYR:CD2 | 2.92 | 0.58 |
| 1:CA:365:U:C5' | 1:CA:366:C:OP1 | 2.42 | 0.58 |
| 23:BA:2392:A:OP1 | 53:B5:32:LEU:HB3 | 2.04 | 0.58 |
| 39:DQ:69:CYS:CB | 39:DQ:79:PHE:HD2 | 2.17 | 0.58 |
| 50:D2:20:ARG:CA | 50:D2:23:HIS:HD2 | 2.10 | 0.58 |
| 39:BQ:95:LEU:HD13 | 40:BR:4:ILE:HG23 | 1.85 | 0.58 |
| 28:DF:105:LYS:HZ3 | 49:D1:52:SER:HB2 | 1.69 | 0.58 |
| 23:DA:2723:C:H2' | 23:DA:2724:C:O5' | 2.03 | 0.58 |
| 5:AE:48:ALA:O | 5:AE:50:GLU:N | 2.37 | 0.58 |
| 2:AB:207:ALA:O | 2:AB:211:ILE:HG13 | 2.04 | 0.58 |
| 1:AA:1151:A:O2' | 1:AA:1152:A:C8 | 2.55 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BA:1343:G:C5' | 23:BA:1343:G:H8 | 2.16 | 0.58 |
| 1:CA:723:U:H5'' | 1:CA:724:G:OP2 | 2.03 | 0.58 |
| 33:BK:35:VAL:HG11 | 33:BK:103:ALA:HB3 | 1.85 | 0.58 |
| 40:BR:64:HIS:HD2 | 40:BR:92:THR:CG2 | 2.17 | 0.58 |
| 8:AH:111:ILE:O | 8:AH:112:LEU:HB3 | 2.04 | 0.58 |
| 1:AA:723:U:H5'' | 1:AA:724:G:OP2 | 2.04 | 0.58 |
| 23:BA:954:G:H5'' | 35:BM:13:GLN:CG | 2.34 | 0.58 |
| 23:BA:661:C:C4' | 34:BL:18:ARG:HG2 | 2.33 | 0.58 |
| 1:AA:626:U:H2' | 1:AA:627:G:C8 | 2.37 | 0.58 |
| 23:DA:953:A:OP2 | 35:DM:16:ARG:NH2 | 2.36 | 0.58 |
| 23:DA:997:G:O2' | 23:DA:998:C:H5' | 2.04 | 0.58 |
| 1:CA:104:G:C2 | 1:CA:105:G:C8 | 2.91 | 0.58 |
| 1:CA:102:G:H2' | 1:CA:103:C:H6 | 1.68 | 0.58 |
| 29:DG:86:GLU:HG2 | 29:DG:164:TYR:O | 2.04 | 0.58 |
| 38:DP:88:ILE:HD12 | 38:DP:89:VAL:H | 1.67 | 0.58 |
| 23:BA:2188:C:H2' | 23:BA:2189:U:O4' | 2.04 | 0.58 |
| 1:CA:538:G:OP1 | 12:CL:112:ARG:HG3 | 2.04 | 0.58 |
| 1:AA:590:C:H2' | 1:AA:591:U:H6 | 1.68 | 0.58 |
| 23:BA:997:G:O2' | 23:BA:998:C:H5' | 2.04 | 0.58 |
| 14:AN:36:PHE:O | 14:AN:36:PHE:CD1 | 2.57 | 0.58 |
| 39:BQ:25:TRP:C | 39:BQ:25:TRP:CD1 | 2.76 | 0.58 |
| 1:CA:1298:C:H4' | 1:CA:1299:A:C8 | 2.38 | 0.58 |
| 23:BA:903:C:H2' | 23:BA:904:C:C6 | 2.38 | 0.58 |
| 39:BQ:20:LEU:HB2 | 39:BQ:39:LEU:HD11 | 1.85 | 0.58 |
| 1:CA:356:A:H2' | 1:CA:357:G:H8 | 1.68 | 0.58 |
| 11:CK:109:VAL:CG1 | 18:CR:84:LYS:HB2 | 2.34 | 0.58 |
| 42:DT:40:LYS:O | 42:DT:42:ALA:N | 2.36 | 0.58 |
| 26:DD:175:VAL:O | 26:DD:177:PRO:HD3 | 2.03 | 0.58 |
| 23:DA:851:U:O2 | 23:DA:928:G:C2 | 2.57 | 0.58 |
| 4:AD:57:ARG:HB3 | 4:AD:206:PHE:HB2 | 1.85 | 0.58 |
| 32:BJ:146:TYR:N | 32:BJ:146:TYR:CD1 | 2.71 | 0.58 |
| 23:DA:2604:U:O2 | 23:DA:2604:U:H2' | 2.02 | 0.58 |
| 23:BA:2828:C:O2' | 23:BA:2829:C:H5' | 2.03 | 0.58 |
| 24:DB:111:U:O2 | 24:DB:112:G:C8 | 2.56 | 0.58 |
| 1:CA:1347:G:H22 | 1:CA:1373:G:H2' | 1.66 | 0.58 |
| 9:AI:114:TYR:HD1 | 10:AJ:60:ARG:CG | 2.17 | 0.58 |
| 5:CE:90:VAL:O | 5:CE:120:THR:HA | 2.04 | 0.58 |
| 42:DT:44:GLU:OE2 | 42:DT:50:LYS:HG2 | 2.04 | 0.58 |
| 47:DY:14:ARG:HA | 47:DY:17:SER:CB | 2.25 | 0.58 |
| 24:DB:84:C:O2 | 24:DB:84:C:H2' | 2.02 | 0.58 |
| 16:CP:55:ARG:O | 16:CP:58:TYR:HB3 | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 40:BR:52:VAL:HG13 | 40:BR:55:ALA:HB3 | 1.84 | 0.58 |
| 26:DD:54:GLN:OE1 | 26:DD:55:ASN:N | 2.36 | 0.58 |
| 1:AA:878:G:H5' | 8:AH:89:PRO:HG2 | 1.86 | 0.58 |
| 43:DU:81:LYS:CG | 43:DU:97:ARG:HB3 | 2.34 | 0.58 |
| 1:AA:1351:U:O2' | 1:AA:1352:C:H5' | 2.04 | 0.58 |
| 44:DV:137:ILE:HD12 | 44:DV:137:ILE:N | 2.18 | 0.58 |
| 1:AA:630:G:C2' | 1:AA:631:G:H5' | 2.33 | 0.58 |
| 23:BA:2531:A:H4' | 29:BG:157:TYR:CD2 | 2.39 | 0.58 |
| 25:BC:25:THR:CG2 | 25:BC:82:ILE:N | 2.66 | 0.58 |
| 23:DA:2815:C:O2' | 50:D2:43:HIS:CD2 | 2.56 | 0.58 |
| 11:AK:36:ASP:HB2 | 11:AK:38:ASN:OD1 | 2.04 | 0.58 |
| 23:DA:773:U:H5' | 25:DC:47:GLY:HA3 | 1.85 | 0.58 |
| 12:CL:24:PRO:HD2 | 12:CL:97:TYR:OH | 2.04 | 0.58 |
| 1:CA:921:U:O2 | 5:CE:19:MET:HB2 | 2.04 | 0.58 |
| 45:DW:28:GLY:HA2 | 45:DW:66:VAL:CG1 | 2.34 | 0.58 |
| 23:BA:991:C:C5 | 23:BA:1185:C:C4 | 2.92 | 0.58 |
| 23:BA:991:C:C5 | 23:BA:1185:C:N4 | 2.72 | 0.58 |
| 1:AA:649:G:H2' | 1:AA:650:G:H8 | 1.67 | 0.58 |
| 1:AA:542:G:O2' | 1:AA:543:C:H5' | 2.03 | 0.58 |
| 5:CE:70:PRO:HB3 | 5:CE:144:THR:HG22 | 1.86 | 0.58 |
| 15:AO:36:ILE:HG22 | 15:AO:37:ASN:N | 2.18 | 0.58 |
| 23:DA:1711:C:O2' | 23:DA:1712:C:H5' | 2.03 | 0.58 |
| 23:BA:2853:C:H2' | 23:BA:2854:G:H8 | 1.69 | 0.58 |
| 23:BA:1449:G:H2' | 23:BA:1450:C:H6 | 1.69 | 0.58 |
| 23:DA:1429:G:H2' | 23:DA:1430:C:C6 | 2.39 | 0.58 |
| 24:BB:45:A:N3 | 24:BB:45:A:H2' | 2.19 | 0.58 |
| 1:AA:458:C:H2' | 1:AA:464:G:O4' | 2.03 | 0.58 |
| 23:BA:530:G:N1 | 23:BA:2022:U:OP1 | 2.36 | 0.58 |
| 49:D1:38:ALA:HA | 49:D1:55:PRO:HA | 1.85 | 0.58 |
| 1:CA:525:C:OP1 | 12:CL:90:LYS:HG2 | 2.03 | 0.58 |
| 24:DB:113:C:O2' | 37:DO:46:VAL:HG13 | 2.04 | 0.58 |
| 4:AD:103:ASN:OD1 | 4:AD:114:ARG:NH2 | 2.36 | 0.58 |
| 23:DA:1403:C:H5'' | 23:DA:1471:A:H1' | 1.85 | 0.58 |
| 1:AA:178:C:O2' | 1:AA:179:A:H5' | 2.03 | 0.58 |
| 34:DL:50:ARG:HG3 | 53:D5:7:HIS:CD2 | 2.38 | 0.58 |
| 23:DA:126:A:O5' | 52:D4:19:ARG:HG2 | 2.03 | 0.58 |
| 42:DT:35:THR:HG22 | 42:DT:36:LYS:H | 1.69 | 0.58 |
| 26:BD:84:PHE:CZ | 26:BD:86:PRO:HG3 | 2.38 | 0.58 |
| 40:DR:77:ALA:O | 40:DR:79:VAL:N | 2.37 | 0.58 |
| 23:BA:322:A:OP2 | 27:BE:169:ASN:HB2 | 2.04 | 0.58 |
| 1:CA:1070:U:C2 | 1:CA:1071:C:C5 | 2.92 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:CA:1292:U:H2' | 1:CA:1293:G:C8 | 2.37 | 0.58 |
| 25:DC:172:TYR:HD1 | 25:DC:185:VAL:C | 2.06 | 0.58 |
| 41:DS:29:LEU:HD21 | 41:DS:33:ARG:NE | 2.15 | 0.58 |
| 23:BA:1859:A:C6 | 23:BA:1884:A:C8 | 2.92 | 0.58 |
| 23:DA:848:G:O6 | 23:DA:929:G:H2' | 2.04 | 0.58 |
| 1:CA:328:C:H4' | 1:CA:329:A:H5' | 1.85 | 0.58 |
| 23:DA:952:G:P | 35:DM:16:ARG:HH22 | 2.26 | 0.58 |
| 39:DQ:61:TRP:O | 39:DQ:64:ARG:N | 2.37 | 0.58 |
| 23:DA:2842:G:H1 | 23:DA:2875:C:N4 | 2.02 | 0.58 |
| 23:DA:2284:C:H1' | 23:DA:2325:G:C2 | 2.39 | 0.58 |
| 23:BA:2287:A:O2' | 23:BA:2288:A:O5' | 2.22 | 0.58 |
| 17:CQ:10:VAL:HG11 | 17:CQ:52:LYS:O | 2.04 | 0.58 |
| 17:CQ:33:GLY:O | 17:CQ:34:LYS:C | 2.41 | 0.58 |
| 2:AB:22:LYS:HZ3 | 2:AB:22:LYS:H | 1.49 | 0.58 |
| 23:BA:356:G:H2' | 23:BA:357:A:C8 | 2.39 | 0.58 |
| 32:DJ:101:TYR:HB3 | 32:DJ:102:PRO:CD | 2.33 | 0.58 |
| 36:DN:44:LEU:C | 36:DN:44:LEU:HD13 | 2.23 | 0.58 |
| 23:BA:270(M):U:H3' | 23:BA:270(N):U:H5'' | 1.84 | 0.58 |
| 2:CB:15:VAL:C | 2:CB:16:HIS:CG | 2.77 | 0.58 |
| 23:BA:907:U:O2' | 35:BM:101:ARG:NH2 | 2.36 | 0.58 |
| 1:AA:342:C:C2' | 1:AA:343:U:H5' | 2.34 | 0.58 |
| 32:BJ:57:LEU:HD21 | 32:BJ:143:LEU:HB2 | 1.85 | 0.58 |
| 32:DJ:127:LYS:HB2 | 32:DJ:140:PHE:HE1 | 1.68 | 0.58 |
| 34:DL:33:ARG:CB | 34:DL:36:LYS:HD3 | 2.33 | 0.58 |
| 26:BD:132:HIS:HA | 26:BD:135:HIS:CE1 | 2.37 | 0.58 |
| 34:DL:41:ARG:NH2 | 34:DL:45:LEU:HD12 | 2.19 | 0.58 |
| 40:BR:40:LEU:H | 40:BR:47:VAL:CG2 | 2.15 | 0.58 |
| 1:AA:37:U:H2' | 1:AA:38:G:H8 | 1.69 | 0.58 |
| 4:AD:30:LYS:C | 4:AD:32:ALA:H | 2.06 | 0.58 |
| 23:DA:142:G:H1' | 42:DT:37:THR:CG2 | 2.34 | 0.58 |
| 26:DD:57:LYS:HG3 | 26:DD:58:ARG:N | 2.19 | 0.58 |
| 23:DA:1332:G:N2 | 23:DA:1609:A:O2' | 2.36 | 0.58 |
| 46:BX:11:ARG:HB3 | 46:BX:12:PRO:HD3 | 1.85 | 0.58 |
| 23:BA:952:G:OP1 | 35:BM:16:ARG:NH2 | 2.35 | 0.58 |
| 1:AA:59:A:H5'' | 1:AA:60:A:H5'' | 1.86 | 0.58 |
| 35:DM:8:LYS:CG | 35:DM:9:TYR:H | 2.16 | 0.58 |
| 46:DX:19:GLN:CG | 46:DX:41:ARG:HE | 2.17 | 0.58 |
| 1:CA:1130:A:N1 | 1:CA:1146:A:N1 | 2.51 | 0.58 |
| 25:BC:166:GLN:HA | 25:BC:166:GLN:HE21 | 1.68 | 0.58 |
| 13:CM:27:LYS:CE | 13:CM:31:LYS:HE3 | 2.33 | 0.58 |
| 43:BU:2:ARG:C | 43:BU:4:LYS:H | 2.06 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1288:A:C6 | 1:AA:1289:A:C6 | 2.92 | 0.58 |
| 35:BM:37:LEU:O | 35:BM:99:PRO:HB3 | 2.03 | 0.58 |
| 1:CA:1423:G:C5' | 33:DK:49:ARG:HH22 | 2.16 | 0.58 |
| 27:BE:46:ARG:HH11 | 27:BE:46:ARG:CG | 2.17 | 0.58 |
| 1:CA:1239:A:H4' | 1:CA:1240:U:C5' | 2.33 | 0.58 |
| 23:BA:2485:G:H5'' | 35:BM:46:GLN:NE2 | 2.19 | 0.58 |
| 25:DC:227:ASN:N | 25:DC:227:ASN:HD22 | 2.02 | 0.58 |
| 23:DA:2317:C:H2' | 23:DA:2318:G:C5' | 2.34 | 0.58 |
| 23:BA:1547:C:H2' | 23:BA:1548:C:H6 | 1.68 | 0.58 |
| 11:CK:102:GLY:O | 11:CK:103:LEU:HD13 | 2.04 | 0.58 |
| 48:BZ:23:LEU:N | 48:BZ:23:LEU:HD12 | 2.19 | 0.58 |
| 44:BV:11:GLU:HG3 | 44:BV:12:GLY:N | 2.19 | 0.58 |
| 1:CA:1386:G:O2' | 1:CA:1387:G:H5' | 2.04 | 0.58 |
| 1:CA:478:A:H2' | 1:CA:479:C:H6 | 1.69 | 0.58 |
| 1:AA:1316:G:N2 | 1:AA:1319:A:OP2 | 2.37 | 0.58 |
| 23:DA:553:U:C2' | 23:DA:554:U:H5' | 2.34 | 0.58 |
| 39:DQ:65:ILE:O | 39:DQ:68:ALA:N | 2.34 | 0.58 |
| 23:BA:2604:U:H2' | 23:BA:2604:U:O2 | 2.03 | 0.58 |
| 29:BG:38:SER:HB3 | 29:BG:41:MET:HG2 | 1.86 | 0.58 |
| 1:AA:816:A:OP2 | 1:AA:1527:C:H4' | 2.04 | 0.58 |
| 53:D5:31:HIS:C | 53:D5:33:ASN:N | 2.49 | 0.57 |
| 23:BA:1448:G:H2' | 23:BA:149(B):A:C8 | 2.39 | 0.57 |
| 23:BA:1543:A:H5' | 23:BA:1544:C:O5' | 2.02 | 0.57 |
| 13:AM:106:ASN:O | 13:AM:107:ALA:HB3 | 2.04 | 0.57 |
| 23:BA:587:C:N4 | 34:BL:33:ARG:HB2 | 2.19 | 0.57 |
| 1:CA:979:C:N4 | 14:CN:18:VAL:HG12 | 2.16 | 0.57 |
| 27:DE:66:PRO:HB3 | 27:DE:68:LYS:HZ3 | 1.68 | 0.57 |
| 23:BA:603:A:N1 | 23:BA:655:A:N3 | 2.52 | 0.57 |
| 34:DL:50:ARG:HB2 | 53:D5:60:LEU:HD11 | 1.86 | 0.57 |
| 1:CA:376:G:OP1 | 16:CP:5:ARG:HB2 | 2.03 | 0.57 |
| 4:AD:161:ASN:O | 4:AD:165:MET:HB2 | 2.03 | 0.57 |
| 20:AT:76:ALA:O | 20:AT:80:ARG:HG2 | 2.04 | 0.57 |
| 23:DA:1487:G:C4 | 23:DA:1488:G:C8 | 2.91 | 0.57 |
| 1:AA:750:G:C2 | 1:AA:751:U:C6 | 2.92 | 0.57 |
| 1:CA:618:C:N3 | 1:CA:622:A:N6 | 2.52 | 0.57 |
| 24:BB:50:G:C5 | 24:BB:51:G:C8 | 2.91 | 0.57 |
| 1:CA:1281:U:C5' | 1:CA:1282:C:H5 | 2.16 | 0.57 |
| 1:AA:782:A:H2' | 1:AA:783:C:H5' | 1.86 | 0.57 |
| 43:DU:2:ARG:C | 43:DU:4:LYS:H | 2.07 | 0.57 |
| 1:CA:1014:A:H5' | 19:CS:14:HIS:CD2 | 2.39 | 0.57 |
| 24:BB:78:A:C2 | 24:BB:99:A:C5 | 2.91 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 17:AQ:33:GLY:O | 17:AQ:34:LYS:C | 2.42 | 0.57 |
| 39:BQ:5:LYS:HG2 | 39:BQ:6:THR:H | 1.68 | 0.57 |
| 1:CA:522:C:N4 | 1:CA:528:C:H42 | 2.01 | 0.57 |
| 1:CA:542:G:O2' | 1:CA:543:C:H5' | 2.04 | 0.57 |
| 25:BC:253:GLN:OE1 | 25:BC:255:LYS:HD3 | 2.04 | 0.57 |
| 2:CB:22:LYS:HZ2 | 2:CB:22:LYS:HA | 1.69 | 0.57 |
| 23:DA:1218:C:C2' | 23:DA:1219:G:H5' | 2.34 | 0.57 |
| 1:AA:506:G:C5 | 1:AA:507:C:C5 | 2.92 | 0.57 |
| 20:CT:97:ALA:O | 20:CT:99:LEU:N | 2.37 | 0.57 |
| 1:AA:563:A:N7 | 1:AA:567:G:H1' | 2.18 | 0.57 |
| 15:CO:61:GLY:O | 15:CO:64:ARG:HB3 | 2.04 | 0.57 |
| 23:DA:880:G:H2' | 23:DA:881:G:C8 | 2.39 | 0.57 |
| 23:DA:2371:G:O2' | 51:D3:45:LYS:HB3 | 2.04 | 0.57 |
| 1:CA:1288:A:C6 | 1:CA:1289:A:C6 | 2.92 | 0.57 |
| 46:DX:53:VAL:HG22 | 46:DX:74:VAL:HG13 | 1.85 | 0.57 |
| 13:CM:15:VAL:O | 13:CM:19:LEU:HD23 | 2.04 | 0.57 |
| 23:BA:2058:A:N6 | 23:BA:2059:A:N6 | 2.52 | 0.57 |
| 1:AA:123:C:OP1 | 1:AA:312:C:H5' | 2.04 | 0.57 |
| 23:BA:1051:G:C6 | 23:BA:1052:C:N3 | 2.72 | 0.57 |
| 27:BE:179:GLU:CD | 27:BE:179:GLU:H | 2.06 | 0.57 |
| 28:DF:148:MET:HE3 | 28:DF:148:MET:HA | 1.86 | 0.57 |
| 1:CA:114:U:H2' | 1:CA:115:G:C8 | 2.38 | 0.57 |
| 12:CL:63:TYR:O | 12:CL:64:GLU:HB2 | 2.04 | 0.57 |
| 23:DA:2780:G:OP2 | 32:DJ:141:LYS:HD3 | 2.03 | 0.57 |
| 32:DJ:118:PRO:HD2 | 32:DJ:119:GLU:OE1 | 2.04 | 0.57 |
| 22:AV:6191:A:H2' | 22:AV:6192:G:O4' | 2.04 | 0.57 |
| 36:BN:11:ASN:O | 36:BN:12:ARG:NH1 | 2.32 | 0.57 |
| 23:DA:2261:C:O2' | 23:DA:2262:U:H5' | 2.04 | 0.57 |
| 1:CA:364:A:C2 | 1:CA:365:U:O4 | 2.57 | 0.57 |
| 23:BA:1899:G:N2 | 23:BA:1902:C:N4 | 2.37 | 0.57 |
| 1:CA:375:U:C4 | 1:CA:376:G:N7 | 2.72 | 0.57 |
| 16:CP:34:GLU:HG2 | 16:CP:35:LYS:N | 2.19 | 0.57 |
| 30:BH:88:ILE:HD11 | 30:BH:123:LEU:HG | 1.87 | 0.57 |
| 53:B5:62:LEU:C | 53:B5:64:TYR:H | 2.08 | 0.57 |
| 28:DF:32:PRO:CB | 28:DF:172:LEU:HD22 | 2.34 | 0.57 |
| 1:AA:377:G:O2' | 1:AA:378:G:H5' | 2.04 | 0.57 |
| 4:CD:161:ASN:O | 4:CD:165:MET:HB2 | 2.03 | 0.57 |
| 2:CB:219:VAL:HA | 2:CB:222:ILE:HG12 | 1.86 | 0.57 |
| 1:CA:1202:G:H4' | 14:CN:29:ARG:CD | 2.34 | 0.57 |
| 5:CE:31:LEU:HD21 | 5:CE:43:LEU:CD1 | 2.34 | 0.57 |
| 37:DO:39:ILE:HG13 | 37:DO:73:LEU:HD13 | 1.85 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BA:72:U:O4 | 23:BA:112:U:H4' | 2.03 | 0.57 |
| 1:AA:265:G:H5' | 17:AQ:64:PRO:O | 2.03 | 0.57 |
| 45:BW:31:VAL:O | 45:BW:64:ASP:HA | 2.04 | 0.57 |
| 1:AA:1353:G:H1 | 1:AA:1369:C:H42 | 1.50 | 0.57 |
| 9:AI:9:ARG:HG3 | 9:AI:14:VAL:HG13 | 1.86 | 0.57 |
| 1:CA:506:G:C5 | 1:CA:507:C:C5 | 2.91 | 0.57 |
| 36:BN:63:ARG:NH1 | 36:BN:63:ARG:HB2 | 2.18 | 0.57 |
| 23:DA:2747:G:C6 | 23:DA:2754:U:C5 | 2.91 | 0.57 |
| 23:BA:2755:C:O2' | 23:BA:2756:U:H2' | 2.05 | 0.57 |
| 29:BG:67:LEU:O | 29:BG:71:LEU:HD23 | 2.04 | 0.57 |
| 42:BT:52:VAL:HG23 | 42:BT:82:GLN:O | 2.03 | 0.57 |
| 1:CA:476:G:H2' | 1:CA:477:G:C8 | 2.35 | 0.57 |
| 1:AA:1130:A:N1 | 1:AA:1146:A:N1 | 2.52 | 0.57 |
| 25:BC:268:ARG:HD2 | 25:BC:269:PHE:CE1 | 2.38 | 0.57 |
| 25:BC:267:SER:O | 25:BC:269:PHE:N | 2.36 | 0.57 |
| 43:DU:76:CYS:CB | 43:DU:77:PRO:CD | 2.81 | 0.57 |
| 23:BA:1680:U:O2 | 23:BA:1763:G:H3' | 2.04 | 0.57 |
| 9:CI:114:TYR:HD1 | 10:CJ:60:ARG:CG | 2.16 | 0.57 |
| 23:BA:2850:A:OP2 | 23:BA:2866:U:C5 | 2.54 | 0.57 |
| 20:AT:13:LEU:CD1 | 20:AT:13:LEU:H | 2.18 | 0.57 |
| 1:AA:1051:C:N4 | 1:AA:1207:G:H1 | 2.02 | 0.57 |
| 23:DA:1414:G:H2' | 23:DA:1415:U:H6 | 1.69 | 0.57 |
| 23:BA:2401:U:C2' | 23:BA:2402:C:H5'' | 2.33 | 0.57 |
| 23:BA:311:A:C6 | 23:BA:328:U:C4 | 2.93 | 0.57 |
| 34:DL:105:LEU:H | 34:DL:105:LEU:HD12 | 1.69 | 0.57 |
| 1:CA:638:G:C2' | 1:CA:639:G:H5' | 2.35 | 0.57 |
| 23:DA:571:A:H4' | 23:DA:572:A:OP1 | 2.03 | 0.57 |
| 23:BA:1028:A:N6 | 23:BA:1125:G:H2' | 2.19 | 0.57 |
| 23:DA:871:U:H4' | 35:DM:69:PHE:CE2 | 2.38 | 0.57 |
| 9:CI:99:LEU:O | 9:CI:99:LEU:HD13 | 2.04 | 0.57 |
| 23:BA:1973:G:H2' | 23:BA:1974:C:C6 | 2.39 | 0.57 |
| 1:CA:1288:A:N6 | 1:CA:1289:A:C6 | 2.72 | 0.57 |
| 23:DA:511:U:C5 | 23:DA:512:G:C5 | 2.92 | 0.57 |
| 30:BH:118:LYS:HG2 | 30:BH:119:PRO:N | 2.18 | 0.57 |
| 1:AA:836:G:C6 | 1:AA:851:G:C6 | 2.91 | 0.57 |
| 44:DV:17:ALA:HA | 44:DV:20:ARG:NH1 | 2.19 | 0.57 |
| 7:CG:86:GLN:HB2 | 7:CG:148:ASN:HD22 | 1.70 | 0.57 |
| 41:DS:45:TYR:HD2 | 41:DS:46:PHE:CD1 | 2.22 | 0.57 |
| 23:BA:1149:G:H2' | 23:BA:1150:C:C6 | 2.40 | 0.57 |
| 25:BC:218:ARG:HB3 | 25:BC:219:PRO:HD2 | 1.86 | 0.57 |
| 26:BD:73:GLU:OE2 | 26:BD:74:PRO:HD2 | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DA:781:A:H2 | 23:DA:1776:G:N3 | 2.02 | 0.57 |
| 23:DA:1543:A:C8 | 23:DA:1545:A:O4' | 2.57 | 0.57 |
| 32:DJ:141:LYS:O | 32:DJ:144:LYS:HE3 | 2.04 | 0.57 |
| 25:DC:11:PRO:O | 25:DC:13:ARG:N | 2.37 | 0.57 |
| 34:DL:52:GLU:OE1 | 34:DL:52:GLU:HA | 2.04 | 0.57 |
| 16:AP:67:THR:HG22 | 16:AP:68:ASP:H | 1.68 | 0.57 |
| 20:AT:56:MET:HG3 | 20:AT:88:VAL:HG21 | 1.85 | 0.57 |
| 1:AA:1065:U:C5 | 1:AA:1190:G:H1' | 2.40 | 0.57 |
| 36:BN:10:LEU:HB3 | 36:BN:17:ARG:CD | 2.35 | 0.57 |
| 23:BA:83:G:H1 | 23:BA:102:G:HO2' | 0.59 | 0.57 |
| 23:BA:2723:C:O3' | 36:BN:2:ARG:NH2 | 2.34 | 0.57 |
| 2:CB:24:TRP:C | 2:CB:25:ASN:HD22 | 2.08 | 0.57 |
| 25:BC:133:LEU:HD13 | 25:BC:173:VAL:HG11 | 1.85 | 0.57 |
| 23:DA:1104:C:O2' | 23:DA:1105:U:H5' | 2.04 | 0.57 |
| 40:DR:64:HIS:CD2 | 40:DR:92:THR:CG2 | 2.86 | 0.57 |
| 23:BA:1104:C:O2' | 23:BA:1105:U:H5' | 2.05 | 0.57 |
| 30:BH:8:PRO:HB3 | 30:BH:14:ASP:OD1 | 2.03 | 0.57 |
| 2:CB:8:LYS:HA | 2:CB:217:ARG:NH1 | 2.17 | 0.57 |
| 33:DK:24:VAL:HB | 33:DK:33:ALA:HB2 | 1.84 | 0.57 |
| 23:DA:1516:U:H2' | 23:DA:1517:G:C8 | 2.39 | 0.57 |
| 43:DU:42:VAL:HG23 | 43:DU:67:LEU:HD11 | 1.87 | 0.57 |
| 44:BV:179:ASP:CG | 44:BV:180:VAL:HG13 | 2.24 | 0.57 |
| 23:DA:582:G:OP1 | 39:DQ:14:HIS:CD2 | 2.58 | 0.57 |
| 5:AE:144:THR:O | 5:AE:148:VAL:HG23 | 2.05 | 0.57 |
| 1:CA:630:G:C2' | 1:CA:631:G:H5' | 2.34 | 0.57 |
| 32:DJ:80:ALA:O | 32:DJ:83:ILE:HG12 | 2.04 | 0.57 |
| 2:CB:127:ILE:HG22 | 2:CB:135:GLN:HE21 | 1.69 | 0.57 |
| 26:DD:181:LEU:HD13 | 26:DD:181:LEU:N | 2.18 | 0.57 |
| 51:B3:38:LYS:HD3 | 51:B3:46:HIS:ND1 | 2.18 | 0.57 |
| 7:AG:71:PRO:HG3 | 7:AG:103:TRP:CZ3 | 2.39 | 0.57 |
| 23:BA:2716:U:O2' | 23:BA:2717:G:H5' | 2.03 | 0.57 |
| 1:AA:179:A:H2' | 1:AA:180:U:C6 | 2.39 | 0.57 |
| 35:DM:78:PRO:O | 35:DM:79:LEU:HB2 | 2.04 | 0.57 |
| 7:CG:70:LYS:HE2 | 7:CG:96:GLN:NE2 | 2.19 | 0.57 |
| 23:BA:484:C:H2' | 23:BA:485:C:C6 | 2.39 | 0.57 |
| 23:DA:2572:A:H62 | 26:DD:145:LYS:HG3 | 1.69 | 0.57 |
| 1:CA:224:C:H2' | 1:CA:225:C:C6 | 2.39 | 0.57 |
| 1:AA:1360:A:H8 | 1:AA:1360:A:OP1 | 1.87 | 0.57 |
| 43:BU:14:LEU:HD23 | 43:BU:15:VAL:C | 2.25 | 0.57 |
| 43:DU:14:LEU:HD23 | 43:DU:15:VAL:C | 2.24 | 0.57 |
| 43:DU:8:LYS:CA | 43:DU:8:LYS:NZ | 2.68 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:DJ:143:LEU:O | 32:DJ:144:LYS:HD2 | 2.04 | 0.57 |
| 34:DL:32:THR:HG21 | 34:DL:37:GLY:H | 1.67 | 0.57 |
| 30:BH:88:ILE:HG22 | 30:BH:90:GLY:H | 1.69 | 0.57 |
| 39:BQ:105:VAL:HG11 | 40:BR:40:LEU:HD13 | 1.87 | 0.57 |
| 1:AA:375:U:C4 | 1:AA:376:G:N7 | 2.72 | 0.57 |
| 1:AA:397:A:N7 | 1:AA:548:G:C8 | 2.73 | 0.57 |
| 25:BC:32:SER:O | 25:BC:33:LEU:O | 2.22 | 0.57 |
| 2:CB:175:ARG:O | 2:CB:178:ARG:HB3 | 2.05 | 0.57 |
| 42:DT:43:VAL:HG23 | 42:DT:47:PHE:CD1 | 2.39 | 0.57 |
| 28:DF:9:ARG:HD3 | 28:DF:13:GLU:OE1 | 2.04 | 0.57 |
| 24:BB:43:C:H4' | 28:BF:98:ARG:HH12 | 1.70 | 0.57 |
| 26:BD:54:GLN:OE1 | 26:BD:55:ASN:N | 2.37 | 0.57 |
| 3:AC:172:ARG:HB3 | 3:AC:174:PRO:HD3 | 1.87 | 0.57 |
| 23:DA:1439:A:C2 | 23:DA:1553:A:C5 | 2.93 | 0.57 |
| 1:AA:1366:C:H2' | 1:AA:1367:C:C6 | 2.40 | 0.57 |
| 8:AH:63:LEU:HB2 | 8:AH:65:TYR:CE1 | 2.39 | 0.57 |
| 6:CF:60:PHE:C | 6:CF:61:LEU:HD12 | 2.25 | 0.57 |
| 23:BA:1326:U:O2' | 23:BA:2010:G:H1' | 2.03 | 0.57 |
| 11:CK:34:ASP:H | 11:CK:40:ILE:HD11 | 1.68 | 0.57 |
| 38:BP:53:ARG:HH11 | 38:BP:53:ARG:CG | 2.17 | 0.57 |
| 1:AA:53:A:N1 | 1:AA:54:C:C2 | 2.72 | 0.57 |
| 53:B5:57:ARG:HB2 | 53:B5:57:ARG:HH11 | 1.68 | 0.57 |
| 23:BA:686:G:O6 | 52:B4:12:ARG:HG3 | 2.04 | 0.57 |
| 23:DA:2563:U:H4' | 33:DK:28:SER:HA | 1.85 | 0.57 |
| 1:AA:104:G:C2 | 1:AA:105:G:C8 | 2.92 | 0.57 |
| 23:DA:784:A:C5 | 25:DC:229:VAL:HG21 | 2.40 | 0.57 |
| 23:DA:739:G:H4' | 23:DA:740:U:OP1 | 2.05 | 0.57 |
| 21:AU:22:ARG:HD2 | 21:AU:23:PRO:HD2 | 1.87 | 0.57 |
| 23:DA:1386:C:OP2 | 23:DA:1396:U:C5 | 2.58 | 0.57 |
| 26:DD:4:ILE:CG1 | 26:DD:28:ALA:HB1 | 2.34 | 0.57 |
| 38:BP:1:MET:C | 38:BP:3:ARG:N | 2.57 | 0.57 |
| 41:BS:55:ALA:O | 41:BS:58:ALA:HB3 | 2.05 | 0.57 |
| 3:AC:150:LYS:HG3 | 3:AC:169:ALA:HB2 | 1.86 | 0.57 |
| 23:DA:1893:C:C6 | 23:DA:1894:C:C5 | 2.92 | 0.57 |
| 41:DS:55:ALA:O | 41:DS:58:ALA:HB3 | 2.05 | 0.57 |
| 1:AA:684:A:H2' | 1:AA:685:G:C8 | 2.38 | 0.57 |
| 1:AA:1387:G:H2' | 1:AA:1388:C:C6 | 2.40 | 0.57 |
| 1:AA:110:C:H2' | 1:AA:111:G:O4' | 2.03 | 0.57 |
| 23:DA:812:C:H5' | 34:DL:25:SER:O | 2.03 | 0.57 |
| 23:DA:914:C:H5 | 23:DA:915:C:C6 | 2.21 | 0.57 |
| 23:BA:415:A:H2' | 23:BA:416:C:H6 | 1.70 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:DD:7:VAL:HA | 26:DD:194:GLY:O | 2.04 | 0.57 |
| 23:DA:328:U:H4' | 43:DU:68:HIS:ND1 | 2.20 | 0.57 |
| 38:DP:51:ARG:O | 38:DP:61:PHE:HA | 2.05 | 0.57 |
| 23:BA:1275:A:C4 | 36:BN:16:HIS:CE1 | 2.93 | 0.57 |
| 22:CV:6191:A:H2' | 22:CV:6192:G:O4' | 2.04 | 0.57 |
| 23:DA:807:U:OP2 | 34:DL:39:LYS:CG | 2.42 | 0.57 |
| 24:BB:7:G:H1' | 37:BO:38:GLN:NE2 | 2.19 | 0.57 |
| 23:DA:729:G:C8 | 25:DC:208:LYS:HD3 | 2.39 | 0.57 |
| 43:BU:29:GLU:OE2 | 43:BU:29:GLU:HA | 2.03 | 0.57 |
| 3:CC:182:ILE:HG23 | 3:CC:202:ILE:C | 2.25 | 0.57 |
| 3:CC:134:ILE:HG21 | 3:CC:168:ALA:HB3 | 1.85 | 0.57 |
| 35:BM:68:ILE:HD13 | 35:BM:103:MET:CG | 2.32 | 0.57 |
| 1:CA:190:G:H4' | 1:CA:191(A):G:OP2 | 2.02 | 0.57 |
| 4:CD:9:CYS:SG | 4:CD:31:CYS:C | 2.83 | 0.57 |
| 24:DB:33:G:C2 | 24:DB:50:G:C2 | 2.93 | 0.57 |
| 36:DN:63:ARG:NH1 | 36:DN:63:ARG:HB2 | 2.17 | 0.57 |
| 1:CA:1220:G:H2' | 1:CA:1221:G:C8 | 2.38 | 0.57 |
| 27:BE:65:TRP:CZ3 | 27:BE:72:ARG:HB3 | 2.39 | 0.57 |
| 15:AO:39:LEU:CD1 | 15:AO:56:LEU:HB2 | 2.35 | 0.57 |
| 23:DA:997:G:C2' | 23:DA:998:C:H5' | 2.34 | 0.57 |
| 29:DG:94:TYR:CZ | 29:DG:160:LYS:HD3 | 2.40 | 0.57 |
| 23:DA:2531:A:H4' | 29:DG:157:TYR:CD2 | 2.38 | 0.57 |
| 25:DC:76:PRO:CB | 25:DC:116:GLN:HE21 | 2.17 | 0.57 |
| 8:CH:86:ILE:CB | 8:CH:133:LEU:HD22 | 2.33 | 0.57 |
| 23:BA:2639:A:C2' | 23:BA:2640:G:H5' | 2.35 | 0.57 |
| 23:BA:774:A:H2 | 23:BA:787:U:O2' | 1.88 | 0.57 |
| 8:AH:97:VAL:C | 8:AH:99:GLU:H | 2.08 | 0.57 |
| 23:BA:1857:G:N2 | 23:BA:1886:C:C4 | 2.72 | 0.57 |
| 23:DA:1538:G:H2' | 23:DA:1539:G:C8 | 2.40 | 0.57 |
| 23:DA:2093:G:H1 | 23:DA:2196:C:N4 | 2.03 | 0.57 |
| 18:AR:45:SER:H | 18:AR:51:LEU:HD11 | 1.68 | 0.57 |
| 23:BA:2036:C:H6 | 23:BA:2036:C:C5' | 2.18 | 0.57 |
| 12:CL:6:ILE:H | 12:CL:6:ILE:CD1 | 2.15 | 0.57 |
| 15:CO:44:LYS:NZ | 15:CO:44:LYS:HB2 | 2.19 | 0.57 |
| 23:BA:2854:G:H2' | 23:BA:2855:C:C6 | 2.39 | 0.57 |
| 15:AO:5:LYS:HD3 | 15:AO:6:GLU:H | 1.69 | 0.57 |
| 9:AI:99:LEU:O | 9:AI:99:LEU:HD13 | 2.04 | 0.57 |
| 1:AA:1159:U:C6 | 1:AA:1182:G:C2 | 2.92 | 0.57 |
| 23:DA:24:G:O2' | 41:DS:77:ASP:HB3 | 2.04 | 0.57 |
| 23:BA:173:G:H2' | 23:BA:174:C:C6 | 2.40 | 0.57 |
| 23:DA:1797:C:O2' | 25:DC:259:THR:HG23 | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:304:U:H2' | 1:AA:305:G:C8 | 2.40 | 0.57 |
| 23:BA:399:G:H2' | 23:BA:400:G:H5' | 1.86 | 0.57 |
| 23:BA:496:G:H1' | 41:BS:61:ASN:HD21 | 1.68 | 0.57 |
| 23:BA:1773:A:H2' | 23:BA:1774:C:H5' | 1.87 | 0.57 |
| 47:BY:36:ARG:HA | 47:BY:39:ALA:CB | 2.34 | 0.57 |
| 8:CH:80:ILE:H | 8:CH:80:ILE:HD12 | 1.68 | 0.57 |
| 25:BC:141:VAL:HG23 | 25:BC:162:SER:OG | 2.04 | 0.57 |
| 23:DA:2393:A:H5' | 34:DL:60:MET:O | 2.04 | 0.57 |
| 23:DA:1171:G:H2' | 23:DA:1173:G:O4' | 2.05 | 0.57 |
| 1:AA:1220:G:H2' | 1:AA:1221:G:C8 | 2.37 | 0.57 |
| 26:BD:11:MET:HB2 | 26:BD:24:THR:HA | 1.87 | 0.57 |
| 22:CV:6188:G:N2 | 22:CV:6216:U:N3 | 2.52 | 0.57 |
| 1:CA:950:U:OP2 | 13:CM:102:ARG:HG3 | 2.04 | 0.57 |
| 23:DA:919:G:N2 | 23:DA:2269:A:OP2 | 2.38 | 0.57 |
| 23:BA:244:A:C2 | 23:BA:255:A:C4 | 2.93 | 0.57 |
| 23:DA:1826:G:H4' | 25:DC:242:ARG:NE | 2.13 | 0.57 |
| 25:DC:238:GLY:O | 25:DC:239:ARG:O | 2.22 | 0.57 |
| 3:AC:57:ILE:HD13 | 3:AC:66:VAL:HG22 | 1.87 | 0.57 |
| 5:AE:11:ILE:HB | 5:AE:31:LEU:HB3 | 1.86 | 0.57 |
| 48:BZ:26:LEU:HD21 | 48:BZ:46:ASN:HB2 | 1.86 | 0.57 |
| 36:DN:63:ARG:HA | 36:DN:80:PHE:CE2 | 2.39 | 0.57 |
| 25:BC:186:HIS:HD2 | 25:BC:188:GLU:HB2 | 1.70 | 0.57 |
| 36:BN:57:ARG:HD2 | 36:BN:59:ASP:OD2 | 2.05 | 0.57 |
| 29:DG:20:ALA:HB3 | 29:DG:23:ARG:O | 2.04 | 0.57 |
| 1:CA:10:A:H2' | 1:CA:11:G:C8 | 2.37 | 0.57 |
| 23:BA:2565:A:H5'' | 23:BA:2566:A:OP2 | 2.04 | 0.57 |
| 46:BX:9:GLY:O | 46:BX:13:ILE:HG21 | 2.05 | 0.57 |
| 8:CH:63:LEU:HB2 | 8:CH:65:TYR:CE1 | 2.40 | 0.57 |
| 1:CA:1238:A:C8 | 1:CA:1303:C:H1' | 2.39 | 0.57 |
| 1:AA:53:A:C2 | 1:AA:54:C:H1' | 2.39 | 0.57 |
| 19:AS:6:LYS:HD3 | 19:AS:7:LYS:HD3 | 1.87 | 0.57 |
| 23:BA:390:A:C5 | 34:BL:71:VAL:HG21 | 2.40 | 0.57 |
| 25:BC:182:LEU:H | 25:BC:272:ALA:CB | 2.16 | 0.57 |
| 1:CA:278:G:OP2 | 17:CQ:41:LYS:HE2 | 2.05 | 0.57 |
| 23:DA:1568:G:P | 25:DC:63:ARG:HH22 | 2.27 | 0.57 |
| 23:DA:2636:U:H4' | 26:DD:80:GLU:CD | 2.25 | 0.57 |
| 41:DS:25:ARG:HH11 | 41:DS:25:ARG:HB2 | 1.69 | 0.57 |
| 41:DS:22:ASP:HA | 41:DS:25:ARG:NH1 | 2.19 | 0.57 |
| 23:BA:1788:C:OP1 | 25:BC:222:ARG:NH2 | 2.37 | 0.57 |
| 1:CA:300:A:C8 | 1:CA:300:A:H3' | 2.40 | 0.57 |
| 24:DB:2:C:H2' | 24:DB:3:C:H6 | 1.67 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 41:BS:43:GLY:O | 41:BS:47:VAL:HG23 | 2.03 | 0.57 |
| 23:DA:1459:G:H2' | 23:DA:1459:G:N3 | 2.19 | 0.57 |
| 38:BP:126:ALA:O | 38:BP:128:GLU:N | 2.37 | 0.57 |
| 23:BA:1550:C:H2' | 23:BA:1551:C:H6 | 1.70 | 0.57 |
| 13:AM:15:VAL:O | 13:AM:19:LEU:HD23 | 2.04 | 0.57 |
| 23:BA:289:A:H2' | 23:BA:290:G:O4' | 2.05 | 0.57 |
| 23:DA:1991:U:H2' | 23:DA:1992:G:H5' | 1.87 | 0.57 |
| 9:CI:46:ALA:O | 9:CI:49:PRO:HD2 | 2.04 | 0.57 |
| 20:CT:64:ASP:O | 20:CT:67:ALA:HB3 | 2.05 | 0.57 |
| 24:DB:28:C:H2' | 24:DB:29:A:H8 | 1.70 | 0.57 |
| 3:AC:16:ARG:NH1 | 3:AC:16:ARG:HB2 | 2.20 | 0.57 |
| 23:DA:2183:C:H2' | 23:DA:2183:C:O2 | 2.04 | 0.57 |
| 5:AE:53:LEU:H | 5:AE:53:LEU:HD23 | 1.68 | 0.57 |
| 34:BL:101:VAL:HG23 | 34:BL:107:LYS:H | 1.70 | 0.57 |
| 38:DP:55:ASN:H | 38:DP:59:THR:HB | 1.69 | 0.57 |
| 13:CM:106:ASN:O | 13:CM:107:ALA:HB3 | 2.04 | 0.57 |
| 1:CA:363:A:C8 | 12:CL:32:ARG:NH2 | 2.72 | 0.57 |
| 27:BE:63:LYS:NZ | 27:BE:67:GLN:NE2 | 2.53 | 0.57 |
| 2:CB:82:ARG:HA | 2:CB:92:TYR:CE1 | 2.39 | 0.57 |
| 34:DL:50:ARG:HD2 | 34:DL:51:PHE:CA | 2.35 | 0.57 |
| 23:BA:1158:C:C2' | 23:BA:1159:U:H5' | 2.35 | 0.57 |
| 12:AL:116:ARG:O | 12:AL:117:SER:C | 2.43 | 0.57 |
| 25:BC:71:ASP:OD2 | 25:BC:103:ARG:NH2 | 2.37 | 0.57 |
| 52:D4:19:ARG:HH11 | 52:D4:19:ARG:CB | 2.17 | 0.57 |
| 1:AA:1435:G:H2' | 1:AA:1436:U:C5 | 2.39 | 0.57 |
| 23:DA:1188:U:C2' | 23:DA:1189:A:H5' | 2.34 | 0.57 |
| 2:CB:207:ALA:O | 2:CB:211:ILE:HG13 | 2.03 | 0.57 |
| 4:AD:105:VAL:HG13 | 4:AD:110:PHE:HB2 | 1.87 | 0.57 |
| 3:CC:35:GLU:HA | 3:CC:38:ARG:CG | 2.35 | 0.57 |
| 23:DA:2543:G:H2' | 23:DA:2544:G:C8 | 2.39 | 0.57 |
| 46:DX:13:ILE:HG23 | 46:DX:14:VAL:H | 1.68 | 0.57 |
| 8:CH:11:THR:HA | 8:CH:14:ARG:NH1 | 2.19 | 0.57 |
| 29:BG:151:ILE:HD13 | 29:BG:151:ILE:N | 2.20 | 0.57 |
| 23:BA:1312:U:H4' | 23:BA:1313:U:O5' | 2.04 | 0.57 |
| 1:CA:1151:A:O2' | 1:CA:1152:A:C8 | 2.52 | 0.57 |
| 23:DA:1046:A:H2 | 31:DI:8:GLU:OE1 | 1.88 | 0.57 |
| 28:DF:131:TYR:HE2 | 28:DF:133:LEU:HB3 | 1.70 | 0.57 |
| 36:DN:99:LYS:HD2 | 36:DN:99:LYS:H | 1.69 | 0.57 |
| 35:DM:37:LEU:O | 35:DM:99:PRO:HB3 | 2.04 | 0.57 |
| 16:CP:7:ALA:O | 16:CP:9:PHE:HD2 | 1.88 | 0.57 |
| 1:CA:254:G:H2' | 1:CA:255:G:H8 | 1.69 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:865:A:C2 | 1:AA:918:A:H4' | 2.39 | 0.57 |
| 23:BA:356:G:H2' | 23:BA:357:A:H8 | 1.69 | 0.57 |
| 3:AC:22:TRP:HE3 | 3:AC:23:TYR:O | 1.88 | 0.57 |
| 23:BA:226:G:N2 | 23:BA:228:A:N6 | 2.52 | 0.57 |
| 1:CA:754:C:H6 | 15:CO:69:TYR:CE2 | 2.23 | 0.57 |
| 22:AV:6198:U:H2' | 22:AV:6199:G:C8 | 2.40 | 0.57 |
| 23:DA:270(K):G:H2' | 23:DA:270(L):C:O4' | 2.05 | 0.57 |
| 7:AG:120:ILE:HG22 | 7:AG:124:LEU:HD12 | 1.87 | 0.57 |
| 1:AA:1386:G:O2' | 1:AA:1387:G:H5' | 2.05 | 0.57 |
| 15:CO:53:HIS:HE1 | 23:DA:715:G:O6 | 1.86 | 0.57 |
| 38:BP:80:SER:C | 38:BP:82:LEU:H | 2.08 | 0.57 |
| 33:BK:49:ARG:HA | 33:BK:53:LYS:NZ | 2.20 | 0.57 |
| 23:BA:1027:A:N6 | 23:BA:1126:A:C4 | 2.73 | 0.57 |
| 23:DA:1204:A:N1 | 23:DA:1241:A:H2 | 2.03 | 0.57 |
| 27:BE:59:TYR:HB3 | 27:BE:78:ILE:HD12 | 1.87 | 0.57 |
| 23:DA:1115:G:O2' | 23:DA:1116:C:H5' | 2.04 | 0.57 |
| 28:DF:165:THR:OG1 | 28:DF:168:GLU:HG3 | 2.04 | 0.57 |
| 23:DA:127:A:H5'' | 23:DA:128:C:C6 | 2.39 | 0.57 |
| 23:BA:165:U:N3 | 23:BA:171:G:C8 | 2.72 | 0.57 |
| 23:DA:631:A:OP1 | 34:DL:64:LYS:HE3 | 2.04 | 0.57 |
| 23:BA:1171:G:H2' | 23:BA:1173:G:O4' | 2.05 | 0.57 |
| 10:AJ:49:VAL:HG21 | 14:AN:41:ARG:HB3 | 1.87 | 0.57 |
| 23:BA:1828:G:OP2 | 25:BC:239:ARG:NH1 | 2.38 | 0.57 |
| 39:BQ:69:CYS:CB | 39:BQ:79:PHE:HD2 | 2.18 | 0.57 |
| 30:DH:142:VAL:HG12 | 30:DH:143:SER:H | 1.69 | 0.57 |
| 23:DA:1187:G:H8 | 23:DA:1187:G:O5' | 1.88 | 0.57 |
| 3:CC:172:ARG:HB3 | 3:CC:174:PRO:HD3 | 1.86 | 0.57 |
| 20:CT:26:ASN:O | 20:CT:30:LYS:HB2 | 2.04 | 0.57 |
| 3:AC:130:VAL:CG1 | 3:AC:153:VAL:HG21 | 2.35 | 0.57 |
| 23:BA:2517:C:C6 | 23:BA:2542:A:C2 | 2.92 | 0.57 |
| 1:AA:1068:G:N3 | 1:AA:1191:A:C2 | 2.72 | 0.57 |
| 46:DX:45:ASN:O | 46:DX:63:ALA:HA | 2.04 | 0.57 |
| 1:AA:1368:G:OP2 | 9:AI:112:LYS:HD3 | 2.05 | 0.57 |
| 9:AI:28:VAL:HG13 | 9:AI:63:ILE:O | 2.05 | 0.57 |
| 41:BS:29:LEU:O | 41:BS:33:ARG:HD2 | 2.04 | 0.57 |
| 1:CA:642:A:N3 | 8:CH:113:SER:OG | 2.26 | 0.57 |
| 33:DK:88:ASN:ND2 | 33:DK:90:GLN:HB3 | 2.20 | 0.57 |
| 36:BN:47:PHE:CE2 | 36:BN:51:LEU:HD11 | 2.40 | 0.57 |
| 43:DU:47:LYS:HA | 43:DU:60:PHE:CZ | 2.40 | 0.57 |
| 23:BA:1856:G:H2' | 23:BA:1857:G:O4' | 2.05 | 0.57 |
| 23:DA:2243:U:H2' | 23:DA:2244:U:C6 | 2.39 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:527:G:C2' | 1:AA:528:C:H5' | 2.34 | 0.57 |
| 35:DM:133:ARG:O | 35:DM:134:ARG:HB2 | 2.04 | 0.57 |
| 12:AL:78:GLU:O | 12:AL:79:HIS:CD2 | 2.58 | 0.57 |
| 23:BA:564:C:O2' | 23:BA:565:C:H5' | 2.05 | 0.57 |
| 1:CA:465:A:N7 | 1:CA:467:G:C6 | 2.72 | 0.57 |
| 2:CB:95:GLN:HG3 | 2:CB:147:LYS:O | 2.04 | 0.57 |
| 23:BA:2023:G:H5' | 23:BA:2617:C:H4' | 1.87 | 0.57 |
| 52:B4:5:TRP:NE1 | 52:B4:7:PRO:HG3 | 2.20 | 0.57 |
| 23:BA:1193:G:O2' | 23:BA:1194:A:H5' | 2.05 | 0.57 |
| 28:DF:137:GLU:HG2 | 28:DF:152:LEU:HD22 | 1.85 | 0.57 |
| 1:CA:1492:A:H2' | 23:DA:1913:A:C2 | 2.40 | 0.57 |
| 23:DA:289:A:H2' | 23:DA:290:G:O4' | 2.04 | 0.57 |
| 23:DA:749:C:O2 | 23:DA:1618:A:H2' | 2.05 | 0.57 |
| 3:CC:119:ARG:O | 3:CC:123:GLN:HG3 | 2.05 | 0.57 |
| 32:DJ:49:LEU:O | 32:DJ:53:ILE:HG13 | 2.05 | 0.57 |
| 26:BD:101:ARG:HB3 | 26:BD:169:ASN:ND2 | 2.20 | 0.57 |
| 22:AV:6181:C:O2' | 22:AV:6182:A:H8 | 1.88 | 0.57 |
| 1:CA:501:C:H2' | 1:CA:502:G:H8 | 1.69 | 0.57 |
| 23:BA:2392:A:OP2 | 53:B5:31:HIS:CE1 | 2.58 | 0.57 |
| 23:BA:2320:A:H2' | 23:BA:2320:A:N3 | 2.19 | 0.57 |
| 2:CB:91:PRO:HG3 | 2:CB:154:LEU:HD21 | 1.87 | 0.57 |
| 16:CP:67:THR:HG22 | 16:CP:68:ASP:N | 2.20 | 0.57 |
| 30:BH:109:ILE:HD13 | 30:BH:109:ILE:N | 2.20 | 0.57 |
| 30:BH:82:ARG:HB3 | 30:BH:89:TYR:CG | 2.39 | 0.57 |
| 23:BA:993:G:C4 | 23:BA:994:C:H5 | 2.22 | 0.57 |
| 39:BQ:92:ARG:HD2 | 39:BQ:95:LEU:HG | 1.86 | 0.57 |
| 34:BL:41:ARG:NH2 | 34:BL:45:LEU:HD12 | 2.20 | 0.57 |
| 1:AA:409:G:H2' | 1:AA:410:G:O5' | 2.05 | 0.57 |
| 52:D4:19:ARG:NH1 | 52:D4:19:ARG:CG | 2.56 | 0.57 |
| 1:CA:232:G:H1' | 1:CA:262:A:N1 | 2.20 | 0.57 |
| 25:DC:253:GLN:OE1 | 25:DC:255:LYS:HD3 | 2.04 | 0.57 |
| 45:BW:28:GLY:HA2 | 45:BW:66:VAL:CG1 | 2.35 | 0.57 |
| 23:DA:1587:A:H2' | 23:DA:1588:C:H6 | 1.62 | 0.57 |
| 20:CT:56:MET:HG3 | 20:CT:88:VAL:HG21 | 1.87 | 0.57 |
| 37:BO:36:TYR:H | 37:BO:36:TYR:HD1 | 1.52 | 0.57 |
| 1:AA:632:A:N7 | 1:AA:633:G:C5 | 2.72 | 0.57 |
| 23:BA:2531:A:H2 | 23:BA:2658:C:O2 | 1.88 | 0.57 |
| 30:BH:15:VAL:O | 30:BH:17:GLN:N | 2.37 | 0.57 |
| 23:BA:1478:G:O2' | 23:BA:1558:A:H2 | 1.88 | 0.57 |
| 23:BA:2476:A:N3 | 23:BA:2476:A:H2' | 2.20 | 0.57 |
| 9:CI:114:TYR:HD1 | 10:CJ:60:ARG:HG3 | 1.70 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:DM:19:GLY:O | 35:DM:98:LYS:HD3 | 2.04 | 0.57 |
| 23:DA:2469:A:H2 | 23:DA:2481:G:N2 | 2.00 | 0.57 |
| 23:DA:18:C:OP1 | 39:DQ:26:GLY:HA2 | 2.05 | 0.57 |
| 1:AA:535:A:H4' | 1:AA:536:C:OP2 | 2.05 | 0.57 |
| 1:AA:562:C:N4 | 1:AA:884:U:C6 | 2.73 | 0.57 |
| 23:BA:296:C:O2' | 23:BA:297:C:H5' | 2.04 | 0.57 |
| 26:DD:149:ARG:HG3 | 26:DD:150:VAL:N | 2.19 | 0.57 |
| 1:CA:928:G:C2 | 1:CA:1390:U:O2 | 2.58 | 0.57 |
| 1:CA:1394:A:H4' | 1:CA:1395:C:OP2 | 2.04 | 0.57 |
| 3:AC:120:VAL:HG21 | 3:AC:137:ALA:HB2 | 1.87 | 0.57 |
| 35:BM:26:TYR:CD1 | 35:BM:26:TYR:O | 2.58 | 0.57 |
| 1:CA:1043:C:H2' | 1:CA:1044:A:H8 | 1.70 | 0.57 |
| 47:BY:38:GLN:HB3 | 47:BY:44:LEU:O | 2.05 | 0.57 |
| 1:AA:355:C:C4 | 1:AA:356:A:N7 | 2.73 | 0.57 |
| 23:BA:2197:U:O3' | 23:BA:2198:A:H8 | 1.88 | 0.57 |
| 1:AA:636:U:C5' | 17:AQ:2:PRO:HG3 | 2.35 | 0.57 |
| 43:BU:15:VAL:HG13 | 43:BU:17:SER:HB3 | 1.87 | 0.57 |
| 23:BA:1139:G:OP1 | 32:BJ:125:ALA:HB2 | 2.05 | 0.57 |
| 32:BJ:49:LEU:O | 32:BJ:53:ILE:HG13 | 2.05 | 0.57 |
| 23:DA:1530:G:N1 | 23:DA:1542:G:N2 | 2.53 | 0.57 |
| 32:BJ:74:PHE:CZ | 32:BJ:142:ARG:HD2 | 2.40 | 0.57 |
| 32:DJ:90:LEU:HA | 32:DJ:110:LEU:HD13 | 1.87 | 0.57 |
| 16:CP:22:THR:HG22 | 16:CP:32:TYR:CB | 2.33 | 0.57 |
| 40:BR:2:PHE:O | 40:BR:41:GLY:HA2 | 2.04 | 0.57 |
| 23:DA:2727:G:C5 | 23:DA:2728:U:C5 | 2.93 | 0.57 |
| 26:DD:134:ILE:HA | 26:DD:137:HIS:CD2 | 2.39 | 0.57 |
| 25:BC:35:LYS:HZ1 | 25:BC:104:TYR:H | 1.53 | 0.57 |
| 30:DH:92:VAL:CG2 | 30:DH:96:ASP:HB2 | 2.34 | 0.57 |
| 3:AC:173:VAL:CG1 | 3:AC:173:VAL:O | 2.53 | 0.57 |
| 1:CA:1253:G:H1 | 1:CA:1284:C:N4 | 1.94 | 0.57 |
| 6:CF:91:VAL:HG13 | 18:CR:72:ARG:NH2 | 2.20 | 0.57 |
| 2:AB:219:VAL:HA | 2:AB:222:ILE:HG12 | 1.86 | 0.57 |
| 23:BA:84:A:C5' | 43:BU:9:LYS:HD2 | 2.31 | 0.57 |
| 33:DK:97:ARG:N | 33:DK:117:LEU:HD22 | 2.20 | 0.57 |
| 23:BA:1504:C:O2' | 23:BA:1505:C:O5' | 2.23 | 0.57 |
| 8:CH:114:THR:HG22 | 8:CH:130:GLY:O | 2.05 | 0.57 |
| 1:CA:1145:C:H4' | 1:CA:1146:A:H8 | 1.70 | 0.57 |
| 23:BA:2688:U:C5 | 23:BA:2720:U:OP2 | 2.57 | 0.57 |
| 30:DH:15:VAL:HG12 | 30:DH:16:GLY:H | 1.70 | 0.57 |
| 27:DE:206:ILE:O | 27:DE:206:ILE:HD12 | 2.04 | 0.57 |
| 19:CS:6:LYS:CD | 19:CS:7:LYS:HD3 | 2.35 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:BG:73:ALA:O | 29:BG:77:LYS:HG2 | 2.05 | 0.57 |
| 1:AA:136(A):C:O2' | 1:AA:136(B):C:H5'' | 2.05 | 0.57 |
| 23:DA:2188:C:H2' | 23:DA:2189:U:O4' | 2.05 | 0.57 |
| 23:DA:2476:A:N1 | 23:DA:2477:C:C4 | 2.73 | 0.57 |
| 40:BR:20:LEU:HD23 | 40:BR:20:LEU:O | 2.05 | 0.57 |
| 33:DK:49:ARG:HA | 33:DK:53:LYS:NZ | 2.20 | 0.57 |
| 16:AP:43:LYS:HA | 16:AP:48:TRP:HB3 | 1.87 | 0.57 |
| 8:AH:80:ILE:HD12 | 8:AH:80:ILE:H | 1.70 | 0.57 |
| 23:BA:2347:C:OP1 | 51:B3:39:TYR:HE1 | 1.88 | 0.57 |
| 23:DA:1831:G:C5 | 23:DA:1832:C:C5 | 2.92 | 0.57 |
| 38:DP:126:ALA:O | 38:DP:128:GLU:N | 2.38 | 0.57 |
| 35:DM:29:PHE:O | 35:DM:30:GLY:O | 2.23 | 0.57 |
| 2:AB:37:ASN:O | 2:AB:39:ILE:HD12 | 2.05 | 0.57 |
| 23:BA:2464:C:C2 | 23:BA:2487:G:N2 | 2.73 | 0.57 |
| 1:CA:927:G:C2 | 1:CA:1391:U:O2 | 2.58 | 0.57 |
| 23:BA:219:G:N3 | 23:BA:234:C:O2' | 2.36 | 0.57 |
| 23:BA:880:G:H2' | 23:BA:881:G:C8 | 2.39 | 0.57 |
| 4:CD:103:ASN:OD1 | 4:CD:114:ARG:NH2 | 2.38 | 0.57 |
| 34:BL:62:LEU:HD23 | 53:B5:25:MET:HB2 | 1.87 | 0.56 |
| 26:DD:23:VAL:HA | 26:DD:184:VAL:O | 2.04 | 0.56 |
| 23:DA:1543:A:N7 | 23:DA:1545:A:H5'' | 2.19 | 0.56 |
| 7:CG:115:ARG:HB2 | 7:CG:118:VAL:CG1 | 2.35 | 0.56 |
| 32:DJ:114:LEU:HD21 | 32:DJ:121:VAL:HG21 | 1.86 | 0.56 |
| 1:CA:1348:U:H4' | 9:CI:120:ARG:HD2 | 1.87 | 0.56 |
| 26:BD:21:VAL:HG12 | 26:BD:23:VAL:HG13 | 1.85 | 0.56 |
| 34:BL:33:ARG:H | 34:BL:36:LYS:CE | 2.06 | 0.56 |
| 42:DT:50:LYS:H | 42:DT:87:GLN:NE2 | 1.90 | 0.56 |
| 28:BF:86:MET:N | 28:BF:87:PRO:CD | 2.66 | 0.56 |
| 30:BH:68:LEU:HD21 | 30:BH:107:ILE:HD11 | 1.87 | 0.56 |
| 39:BQ:98:LEU:O | 39:BQ:101:ARG:O | 2.23 | 0.56 |
| 34:BL:52:GLU:HA | 34:BL:52:GLU:OE1 | 2.04 | 0.56 |
| 16:AP:34:GLU:HG2 | 16:AP:35:LYS:N | 2.19 | 0.56 |
| 1:CA:1103:C:H5'' | 2:CB:98:LEU:HD22 | 1.85 | 0.56 |
| 11:AK:59:TYR:CE2 | 11:AK:63:LEU:HD11 | 2.40 | 0.56 |
| 43:DU:95:LYS:HD3 | 43:DU:99:CYS:O | 2.05 | 0.56 |
| 43:BU:81:LYS:CG | 43:BU:97:ARG:HB3 | 2.34 | 0.56 |
| 23:BA:380:U:O2 | 46:BX:20:ARG:NH2 | 2.38 | 0.56 |
| 1:AA:66:G:C2 | 1:AA:67:C:C6 | 2.93 | 0.56 |
| 27:DE:192:LEU:HD22 | 27:DE:194:MET:HG2 | 1.85 | 0.56 |
| 1:CA:173:U:C6 | 1:CA:197:A:C2 | 2.93 | 0.56 |
| 1:CA:236:G:H1' | 17:CQ:4:LYS:HE3 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:CQ:54:GLY:HA3 | 17:CQ:82:MET:SD | 2.45 | 0.56 |
| 23:DA:1326:U:O2' | 23:DA:2010:G:H1' | 2.05 | 0.56 |
| 27:BE:89:VAL:HG12 | 27:BE:90:PHE:H | 1.68 | 0.56 |
| 23:BA:627:A:C6 | 23:BA:637:A:C8 | 2.93 | 0.56 |
| 1:CA:962:C:H42 | 1:CA:973:G:H1 | 1.53 | 0.56 |
| 1:CA:963:G:H2' | 1:CA:964:A:C8 | 2.39 | 0.56 |
| 12:CL:78:GLU:O | 12:CL:79:HIS:CD2 | 2.58 | 0.56 |
| 1:CA:342:C:O2' | 1:CA:343:U:H5' | 2.04 | 0.56 |
| 23:DA:2078:C:O2' | 23:DA:2079:U:H5' | 2.05 | 0.56 |
| 26:DD:128:SER:OG | 26:DD:129:HIS:N | 2.37 | 0.56 |
| 23:BA:974(B):C:H4' | 23:BA:974(B):C:OP2 | 2.05 | 0.56 |
| 23:DA:1028:A:N6 | 23:DA:1125:G:H2' | 2.20 | 0.56 |
| 26:DD:101:ARG:HB3 | 26:DD:169:ASN:ND2 | 2.20 | 0.56 |
| 25:BC:70:TRP:CH2 | 25:BC:150:LYS:HA | 2.41 | 0.56 |
| 1:CA:1226:C:C5 | 13:CM:104:ARG:HB2 | 2.39 | 0.56 |
| 1:CA:1224:G:H4' | 13:CM:102:ARG:HH22 | 1.68 | 0.56 |
| 40:DR:49:THR:HB | 40:DR:50:PRO:HD2 | 1.87 | 0.56 |
| 35:DM:140:ALA:HB3 | 44:DV:53:ILE:HG12 | 1.87 | 0.56 |
| 49:B1:40:ILE:HG23 | 49:B1:59:VAL:HG21 | 1.86 | 0.56 |
| 36:DN:10:LEU:HB3 | 36:DN:17:ARG:CD | 2.35 | 0.56 |
| 23:BA:142:G:H1' | 42:BT:37:THR:HG21 | 1.86 | 0.56 |
| 19:CS:63:THR:HG22 | 19:CS:66:MET:CG | 2.32 | 0.56 |
| 48:DZ:17:LYS:HD3 | 48:DZ:17:LYS:C | 2.26 | 0.56 |
| 3:CC:70:VAL:HG12 | 3:CC:71:ALA:N | 2.21 | 0.56 |
| 46:DX:19:GLN:O | 46:DX:20:ARG:HG3 | 2.06 | 0.56 |
| 14:CN:17:LYS:C | 14:CN:19:ARG:H | 2.09 | 0.56 |
| 1:CA:626:U:H2' | 1:CA:627:G:H8 | 1.68 | 0.56 |
| 30:DH:7:GLU:CD | 30:DH:8:PRO:HD2 | 2.26 | 0.56 |
| 13:AM:27:LYS:CE | 13:AM:31:LYS:HE3 | 2.33 | 0.56 |
| 18:AR:26:LEU:HD21 | 18:AR:42:ARG:NH1 | 2.17 | 0.56 |
| 23:BA:1388:G:H4' | 23:BA:1525:G:O2' | 2.05 | 0.56 |
| 23:BA:284:U:H2' | 23:BA:285:C:C6 | 2.40 | 0.56 |
| 1:AA:1288:A:N6 | 1:AA:1289:A:C6 | 2.73 | 0.56 |
| 23:DA:988:A:C2' | 23:DA:989:G:O5' | 2.53 | 0.56 |
| 23:BA:1607:C:N4 | 23:BA:1621:U:H3' | 2.20 | 0.56 |
| 23:DA:115:C:O2' | 23:DA:116:C:H5' | 2.05 | 0.56 |
| 43:BU:68:HIS:O | 43:BU:70:SER:N | 2.37 | 0.56 |
| 36:DN:93:GLY:O | 36:DN:117:VAL:HG11 | 2.05 | 0.56 |
| 35:BM:62:GLY:O | 44:BV:178:GLU:HG2 | 2.05 | 0.56 |
| 1:CA:525:C:H5'' | 12:CL:90:LYS:HE3 | 1.86 | 0.56 |
| 1:AA:814:A:N7 | 1:AA:816:A:C4 | 2.73 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BA:1797:C:O2' | 25:BC:259:THR:HG23 | 2.04 | 0.56 |
| 1:CA:273:A:N6 | 1:CA:274:A:N6 | 2.53 | 0.56 |
| 44:BV:17:ALA:HA | 44:BV:20:ARG:NH1 | 2.20 | 0.56 |
| 23:BA:1757:U:C2' | 23:BA:1758:G:OP1 | 2.53 | 0.56 |
| 18:CR:45:SER:H | 18:CR:51:LEU:HD11 | 1.70 | 0.56 |
| 33:BK:14:THR:HG22 | 33:BK:14:THR:O | 2.05 | 0.56 |
| 1:CA:294:U:H2' | 1:CA:295:C:H6 | 1.69 | 0.56 |
| 52:D4:5:TRP:NE1 | 52:D4:7:PRO:HG3 | 2.19 | 0.56 |
| 35:DM:97:VAL:HG12 | 35:DM:97:VAL:O | 2.05 | 0.56 |
| 45:BW:35:ASN:HD22 | 45:BW:35:ASN:H | 1.53 | 0.56 |
| 2:AB:15:VAL:C | 2:AB:16:HIS:CG | 2.78 | 0.56 |
| 23:BA:747:U:C4 | 50:B2:2:ALA:N | 2.73 | 0.56 |
| 25:BC:68:LYS:O | 25:BC:70:TRP:CE3 | 2.57 | 0.56 |
| 23:DA:1175:U:H2' | 23:DA:1176:G:H8 | 1.70 | 0.56 |
| 9:AI:114:TYR:HD1 | 10:AJ:60:ARG:HG3 | 1.69 | 0.56 |
| 1:AA:1226:C:H2' | 13:AM:103:THR:HB | 1.87 | 0.56 |
| 9:CI:10:ARG:CZ | 9:CI:11:LYS:HE3 | 2.35 | 0.56 |
| 1:CA:950:U:O4 | 13:CM:105:THR:HG21 | 2.05 | 0.56 |
| 23:DA:1899:G:O2' | 23:DA:1900:A:OP2 | 2.20 | 0.56 |
| 28:DF:86:MET:N | 28:DF:87:PRO:CD | 2.68 | 0.56 |
| 1:AA:376:G:N3 | 1:AA:389:A:C2 | 2.73 | 0.56 |
| 25:DC:108:PRO:HB3 | 25:DC:143:HIS:HE1 | 1.69 | 0.56 |
| 3:AC:180:ALA:HB1 | 3:AC:182:ILE:HG13 | 1.87 | 0.56 |
| 4:AD:111:ALA:HB1 | 4:AD:116:GLN:HG2 | 1.87 | 0.56 |
| 12:AL:26:LEU:HD13 | 12:AL:27:LYS:N | 2.20 | 0.56 |
| 23:DA:1812:A:O2' | 25:DC:45:ASN:HB3 | 2.05 | 0.56 |
| 35:BM:47:ILE:HD11 | 35:BM:68:ILE:HD12 | 1.87 | 0.56 |
| 23:DA:1210:A:H5'' | 23:DA:1210:A:C8 | 2.37 | 0.56 |
| 23:DA:2886:G:O2' | 23:DA:2887:U:H5' | 2.05 | 0.56 |
| 5:AE:64:ARG:HG3 | 5:AE:65:ASN:N | 2.20 | 0.56 |
| 4:AD:64:LEU:HD23 | 4:AD:203:VAL:HG21 | 1.87 | 0.56 |
| 26:DD:52:LEU:HB2 | 26:DD:76:ARG:HB2 | 1.87 | 0.56 |
| 12:AL:69:ILE:HG23 | 12:AL:99:ILE:CG2 | 2.31 | 0.56 |
| 3:AC:131:ARG:HE | 5:AE:50:GLU:HG2 | 1.71 | 0.56 |
| 2:CB:97:TRP:HH2 | 2:CB:176:GLU:CG | 2.19 | 0.56 |
| 1:CA:1292:U:C2 | 1:CA:1293:G:C8 | 2.93 | 0.56 |
| 1:CA:520:A:OP2 | 12:CL:50:ALA:O | 2.23 | 0.56 |
| 23:DA:2755:C:HO2' | 23:DA:2756:U:H6 | 1.53 | 0.56 |
| 28:DF:134:GLY:C | 28:DF:135:LEU:HD12 | 2.26 | 0.56 |
| 43:BU:95:LYS:HD3 | 43:BU:99:CYS:O | 2.05 | 0.56 |
| 1:CA:724:G:C2 | 1:CA:725:G:C8 | 2.93 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BA:1495:A:C2 | 23:BA:1496:A:C2 | 2.93 | 0.56 |
| 40:BR:61:VAL:O | 40:BR:61:VAL:HG23 | 2.04 | 0.56 |
| 25:BC:24:ILE:CD1 | 25:BC:84:TYR:HB2 | 2.35 | 0.56 |
| 40:DR:64:HIS:HD2 | 40:DR:92:THR:HG22 | 1.66 | 0.56 |
| 33:BK:19:ILE:HB | 33:BK:41:ALA:HB1 | 1.87 | 0.56 |
| 1:CA:817:C:H4' | 1:CA:818:G:OP1 | 2.05 | 0.56 |
| 8:CH:97:VAL:C | 8:CH:99:GLU:H | 2.09 | 0.56 |
| 1:CA:327:A:C4 | 1:CA:329:A:C8 | 2.93 | 0.56 |
| 23:DA:954:G:H5'' | 35:DM:13:GLN:HG3 | 1.87 | 0.56 |
| 3:CC:47:LEU:HD23 | 3:CC:52:LEU:HD13 | 1.86 | 0.56 |
| 1:AA:173:U:C6 | 1:AA:197:A:C2 | 2.93 | 0.56 |
| 30:BH:6:LEU:O | 30:BH:7:GLU:HB2 | 2.05 | 0.56 |
| 4:AD:79:PHE:CG | 4:AD:207:TYR:HD1 | 2.23 | 0.56 |
| 11:AK:84:VAL:HG23 | 11:AK:110:ASP:OD1 | 2.05 | 0.56 |
| 23:BA:2476:A:N1 | 23:BA:2477:C:C4 | 2.73 | 0.56 |
| 23:BA:2476:A:H2 | 23:BA:2477:C:C6 | 2.24 | 0.56 |
| 23:BA:2287:A:C4 | 23:BA:2289:G:C8 | 2.93 | 0.56 |
| 29:BG:94:TYR:OH | 29:BG:160:LYS:HD3 | 2.05 | 0.56 |
| 1:CA:590:C:H2' | 1:CA:591:U:H6 | 1.69 | 0.56 |
| 24:DB:75:G:N1 | 24:DB:102:G:N2 | 2.53 | 0.56 |
| 23:BA:1793:C:H2' | 23:BA:1794:U:C6 | 2.40 | 0.56 |
| 1:AA:942:G:N2 | 1:AA:943:U:C2 | 2.73 | 0.56 |
| 44:BV:38:TYR:O | 44:BV:38:TYR:CD1 | 2.59 | 0.56 |
| 1:AA:863:U:H2' | 1:AA:865:A:OP2 | 2.05 | 0.56 |
| 23:BA:270(K):G:H2' | 23:BA:270(L):C:O4' | 2.04 | 0.56 |
| 1:AA:542:G:P | 4:AD:10:ARG:HH21 | 2.28 | 0.56 |
| 6:CF:12:PRO:HG3 | 6:CF:57:GLN:O | 2.05 | 0.56 |
| 34:DL:55:ARG:CG | 34:DL:56:SER:N | 2.66 | 0.56 |
| 1:CA:428:G:O4' | 1:CA:430:A:C8 | 2.58 | 0.56 |
| 50:D2:4:HIS:HB3 | 50:D2:5:PRO:CD | 2.34 | 0.56 |
| 44:BV:5:LEU:HD23 | 44:BV:6:LYS:H | 1.69 | 0.56 |
| 27:BE:181:LEU:CD2 | 27:BE:186:ILE:HD11 | 2.35 | 0.56 |
| 27:DE:52:LYS:HB3 | 27:DE:56:GLU:HB2 | 1.87 | 0.56 |
| 26:DD:181:LEU:HD21 | 38:DP:7:ILE:HG23 | 1.88 | 0.56 |
| 23:BA:229:A:H5' | 23:BA:230:U:C5' | 2.35 | 0.56 |
| 36:BN:30:THR:HG22 | 36:BN:31:HIS:CE1 | 2.41 | 0.56 |
| 26:BD:100:GLU:O | 26:BD:172:VAL:HG23 | 2.05 | 0.56 |
| 1:AA:683:G:C6 | 1:AA:684:A:C5 | 2.93 | 0.56 |
| 23:BA:2038:G:H2' | 23:BA:2039:C:C6 | 2.39 | 0.56 |
| 23:BA:2317:C:H2' | 23:BA:2318:G:H5' | 1.85 | 0.56 |
| 23:DA:2709:G:O2' | 23:DA:2710:C:H5' | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:CH:80:ILE:N | 8:CH:80:ILE:HD12 | 2.21 | 0.56 |
| 1:AA:478:A:H2' | 1:AA:479:C:H6 | 1.70 | 0.56 |
| 1:AA:294:U:H2' | 1:AA:295:C:H6 | 1.71 | 0.56 |
| 23:BA:461:C:C2' | 23:BA:462:C:H5' | 2.36 | 0.56 |
| 2:CB:17:PHE:CD1 | 2:CB:44:LEU:HD21 | 2.40 | 0.56 |
| 30:DH:58:LEU:C | 30:DH:60:GLU:H | 2.08 | 0.56 |
| 13:CM:29:ARG:HB3 | 13:CM:64:TRP:CZ2 | 2.40 | 0.56 |
| 23:DA:974(B):C:OP2 | 23:DA:974(B):C:H4' | 2.05 | 0.56 |
| 8:CH:50:ARG:HG2 | 8:CH:50:ARG:HH11 | 1.70 | 0.56 |
| 27:BE:108:LYS:O | 27:BE:112:MET:HG3 | 2.04 | 0.56 |
| 23:BA:459:U:H4' | 52:B4:40:TRP:CZ3 | 2.41 | 0.56 |
| 23:BA:1015:G:C2' | 23:BA:1016:G:H5' | 2.34 | 0.56 |
| 1:AA:1047:G:C2' | 1:AA:1048:G:H5' | 2.34 | 0.56 |
| 44:DV:117:LEU:O | 44:DV:117:LEU:HG | 2.05 | 0.56 |
| 1:AA:497:U:H2' | 1:AA:497:U:O2 | 2.06 | 0.56 |
| 9:CI:83:ARG:HA | 9:CI:86:VAL:HG12 | 1.87 | 0.56 |
| 23:DA:2427:C:H5'' | 23:DA:2428:G:OP1 | 2.06 | 0.56 |
| 53:D5:52:LYS:N | 53:D5:53:PRO:HD2 | 2.19 | 0.56 |
| 34:DL:61:ARG:HA | 34:DL:62:LEU:HD13 | 1.87 | 0.56 |
| 34:BL:81:GLN:HG2 | 34:BL:106:LEU:HD22 | 1.87 | 0.56 |
| 9:CI:112:LYS:HA | 9:CI:119:ALA:HB2 | 1.87 | 0.56 |
| 5:AE:90:VAL:O | 5:AE:120:THR:HA | 2.05 | 0.56 |
| 23:BA:2846:G:OP2 | 38:BP:54:ARG:HB2 | 2.06 | 0.56 |
| 12:CL:82:VAL:HG13 | 12:CL:83:LEU:N | 2.21 | 0.56 |
| 40:DR:38:LEU:C | 40:DR:39:LEU:HD13 | 2.25 | 0.56 |
| 53:D5:7:HIS:HB2 | 53:D5:60:LEU:HB3 | 1.86 | 0.56 |
| 34:DL:50:ARG:HB3 | 34:DL:50:ARG:HH11 | 1.69 | 0.56 |
| 23:BA:2730:C:O2' | 23:BA:2731:G:H5' | 2.04 | 0.56 |
| 23:DA:2729:G:H2' | 23:DA:2730:C:H6 | 1.70 | 0.56 |
| 16:AP:19:ILE:HG22 | 16:AP:19:ILE:O | 2.05 | 0.56 |
| 12:AL:116:ARG:O | 12:AL:119:TYR:N | 2.37 | 0.56 |
| 3:CC:120:VAL:HG21 | 3:CC:137:ALA:HB2 | 1.87 | 0.56 |
| 20:CT:26:ASN:N | 20:CT:26:ASN:ND2 | 2.52 | 0.56 |
| 3:CC:36:ASP:OD2 | 3:CC:57:ILE:HG21 | 2.06 | 0.56 |
| 27:BE:155:LEU:HD12 | 27:BE:174:VAL:HB | 1.87 | 0.56 |
| 1:AA:1309:G:H22 | 1:AA:1329:A:H1' | 1.70 | 0.56 |
| 23:DA:1858:G:O2' | 23:DA:1859:A:C8 | 2.57 | 0.56 |
| 1:CA:324:G:N1 | 1:CA:327:A:OP2 | 2.39 | 0.56 |
| 53:B5:51:ALA:C | 53:B5:52:LYS:HD3 | 2.26 | 0.56 |
| 1:CA:1068:G:N3 | 1:CA:1191:A:C2 | 2.73 | 0.56 |
| 2:AB:127:ILE:HG22 | 2:AB:135:GLN:HE21 | 1.70 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:DM:37:LEU:N | 35:DM:37:LEU:HD23 | 2.20 | 0.56 |
| 35:BM:40:ALA:HB2 | 35:BM:127:ILE:HD12 | 1.88 | 0.56 |
| 44:BV:179:ASP:CG | 44:BV:180:VAL:H | 2.08 | 0.56 |
| 27:BE:88:VAL:HG13 | 27:BE:89:VAL:O | 2.05 | 0.56 |
| 5:CE:98:THR:HG22 | 5:CE:99:GLY:N | 2.20 | 0.56 |
| 23:BA:2641:G:OP1 | 32:BJ:97:ARG:HD3 | 2.05 | 0.56 |
| 23:BA:1164:G:C6 | 23:BA:1165:U:C4 | 2.94 | 0.56 |
| 3:CC:149:ALA:HA | 3:CC:201:TYR:O | 2.06 | 0.56 |
| 23:DA:1683:C:N4 | 23:DA:1705:G:H1 | 2.01 | 0.56 |
| 38:DP:36:GLU:OE2 | 38:DP:41:ARG:HD3 | 2.05 | 0.56 |
| 1:AA:1040:U:H2' | 1:AA:1041:A:H8 | 1.71 | 0.56 |
| 36:DN:79:LEU:HD23 | 36:DN:83:ILE:HB | 1.87 | 0.56 |
| 41:BS:62:HIS:O | 41:BS:64:MET:N | 2.38 | 0.56 |
| 1:CA:113:G:O2' | 1:CA:114:U:H5' | 2.05 | 0.56 |
| 23:BA:24:G:O2' | 41:BS:77:ASP:HB3 | 2.05 | 0.56 |
| 1:CA:991:U:O2' | 1:CA:993:G:C8 | 2.58 | 0.56 |
| 23:BA:2020:A:OP1 | 39:BQ:27:LEU:HB2 | 2.06 | 0.56 |
| 23:DA:165:U:N3 | 23:DA:171:G:C8 | 2.73 | 0.56 |
| 12:AL:75:ASN:OD1 | 12:AL:107:ALA:HB3 | 2.06 | 0.56 |
| 48:DZ:8:LEU:HD13 | 48:DZ:31:LEU:HD12 | 1.85 | 0.56 |
| 1:AA:137:C:O4' | 16:AP:63:GLY:HA3 | 2.05 | 0.56 |
| 38:BP:23:ARG:HH11 | 38:BP:23:ARG:CG | 2.19 | 0.56 |
| 9:AI:24:GLY:O | 9:AI:26:VAL:HG23 | 2.05 | 0.56 |
| 20:CT:82:SER:O | 20:CT:86:ARG:HB2 | 2.06 | 0.56 |
| 34:DL:85:LEU:CD2 | 34:DL:85:LEU:H | 2.18 | 0.56 |
| 23:DA:1265:A:H5' | 23:DA:1267:U:H1' | 1.86 | 0.56 |
| 26:DD:24:THR:HG21 | 26:DD:188:VAL:HG12 | 1.87 | 0.56 |
| 23:BA:1169:G:H1 | 23:BA:1180:C:H42 | 1.54 | 0.56 |
| 32:BJ:53:ILE:O | 32:BJ:57:LEU:HD22 | 2.04 | 0.56 |
| 12:CL:26:LEU:HD13 | 12:CL:27:LYS:N | 2.21 | 0.56 |
| 23:BA:2338:G:O2' | 23:BA:2339:G:H5' | 2.05 | 0.56 |
| 42:DT:39:ILE:O | 42:DT:43:VAL:HG12 | 2.04 | 0.56 |
| 35:BM:68:ILE:HG21 | 35:BM:103:MET:HG3 | 1.88 | 0.56 |
| 26:BD:4:ILE:CG1 | 26:BD:28:ALA:HB1 | 2.36 | 0.56 |
| 23:BA:2681:C:C5 | 23:BA:2725:A:N6 | 2.63 | 0.56 |
| 24:DB:50:G:OP2 | 37:DO:62:LYS:HD3 | 2.04 | 0.56 |
| 23:BA:1771:C:H1' | 23:BA:1786:A:C8 | 2.41 | 0.56 |
| 48:DZ:40:THR:CG2 | 48:DZ:43:ILE:HG12 | 2.34 | 0.56 |
| 46:DX:65:SER:OG | 46:DX:66:HIS:CD2 | 2.58 | 0.56 |
| 12:CL:53:LYS:HB3 | 12:CL:69:ILE:HG13 | 1.88 | 0.56 |
| 25:BC:172:TYR:HD1 | 25:BC:185:VAL:C | 2.08 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:BN:55:ALA:O | 36:BN:57:ARG:O | 2.24 | 0.56 |
| 23:DA:2309:A:N6 | 23:DA:2310:A:N1 | 2.54 | 0.56 |
| 6:AF:60:PHE:C | 6:AF:61:LEU:HD12 | 2.26 | 0.56 |
| 25:DC:25:THR:HG22 | 25:DC:82:ILE:H | 1.69 | 0.56 |
| 6:AF:90:VAL:CG1 | 6:AF:91:VAL:N | 2.68 | 0.56 |
| 1:CA:327:A:C2 | 1:CA:329:A:C4 | 2.93 | 0.56 |
| 1:AA:1118:C:P | 9:AI:104:ARG:HG3 | 2.45 | 0.56 |
| 23:BA:2598:A:H2' | 23:BA:2599:G:O5' | 2.05 | 0.56 |
| 23:DA:966:G:C4 | 23:DA:967:C:H5 | 2.21 | 0.56 |
| 23:DA:966:G:C5 | 23:DA:967:C:C5 | 2.94 | 0.56 |
| 34:BL:136:GLU:O | 34:BL:137:LYS:C | 2.44 | 0.56 |
| 44:DV:38:TYR:CD1 | 44:DV:38:TYR:O | 2.59 | 0.56 |
| 1:CA:865:A:C2 | 1:CA:918:A:H4' | 2.40 | 0.56 |
| 1:AA:652:U:O4 | 1:AA:752:G:O2' | 2.15 | 0.56 |
| 5:AE:70:PRO:HB3 | 5:AE:144:THR:HG22 | 1.87 | 0.56 |
| 19:CS:28:LYS:HB3 | 19:CS:29:ARG:NH1 | 2.21 | 0.56 |
| 3:AC:35:GLU:HA | 3:AC:38:ARG:CG | 2.36 | 0.56 |
| 50:D2:4:HIS:CB | 50:D2:5:PRO:HD3 | 2.35 | 0.56 |
| 23:BA:565:C:C2' | 23:BA:566:U:O5' | 2.53 | 0.56 |
| 23:DA:1773:A:C2' | 23:DA:1774:C:H5' | 2.35 | 0.56 |
| 23:DA:2356:C:O3' | 45:DW:20:ARG:HD3 | 2.04 | 0.56 |
| 23:DA:1338:G:C2' | 23:DA:1339:G:H5' | 2.35 | 0.56 |
| 48:DZ:50:VAL:O | 48:DZ:54:VAL:HG22 | 2.04 | 0.56 |
| 1:AA:55:A:C4 | 1:AA:56:U:C6 | 2.93 | 0.56 |
| 1:CA:177:C:OP1 | 20:CT:65:LYS:NZ | 2.30 | 0.56 |
| 25:BC:52:ARG:HB3 | 25:BC:53:PHE:CD2 | 2.40 | 0.56 |
| 35:DM:26:TYR:CD1 | 35:DM:26:TYR:O | 2.59 | 0.56 |
| 40:DR:87:HIS:CD2 | 40:DR:87:HIS:O | 2.59 | 0.56 |
| 2:CB:235:SER:O | 2:CB:239:VAL:HG23 | 2.05 | 0.56 |
| 23:DA:89:G:C4 | 23:DA:90:U:C5 | 2.94 | 0.56 |
| 26:BD:134:ILE:HA | 26:BD:137:HIS:CD2 | 2.40 | 0.56 |
| 23:BA:241:A:H5' | 23:BA:243:U:H1' | 1.86 | 0.56 |
| 25:DC:44:ASN:CG | 25:DC:45:ASN:N | 2.58 | 0.56 |
| 42:DT:14:SER:O | 42:DT:15:GLU:C | 2.42 | 0.56 |
| 42:DT:30:VAL:HG11 | 42:DT:39:ILE:HD13 | 1.86 | 0.56 |
| 30:DH:68:LEU:HD21 | 30:DH:107:ILE:HD11 | 1.86 | 0.56 |
| 3:CC:134:ILE:CG2 | 3:CC:168:ALA:HB3 | 2.35 | 0.56 |
| 44:DV:94:GLU:HB2 | 44:DV:95:PRO:HD2 | 1.88 | 0.56 |
| 23:BA:2681:C:H5 | 23:BA:2725:A:N6 | 1.82 | 0.56 |
| 3:AC:33:LEU:HD21 | 14:AN:53:LEU:CD2 | 2.32 | 0.56 |
| 1:AA:15:G:C4 | 1:AA:16:A:C8 | 2.93 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 43:DU:81:LYS:HD2 | 43:DU:96:ILE:CD1 | 2.35 | 0.56 |
| 35:DM:68:ILE:HD13 | 35:DM:103:MET:CG | 2.33 | 0.56 |
| 35:DM:68:ILE:HG21 | 35:DM:103:MET:HG3 | 1.87 | 0.56 |
| 1:AA:57:G:C8 | 1:AA:58:C:C5 | 2.93 | 0.56 |
| 23:DA:322:A:OP1 | 27:DE:168:ARG:HD3 | 2.06 | 0.56 |
| 9:CI:28:VAL:HG13 | 9:CI:63:ILE:O | 2.06 | 0.56 |
| 1:AA:781:A:O2' | 1:AA:1522:U:O2 | 2.23 | 0.56 |
| 23:DA:1153:C:H5' | 39:DQ:76:TYR:CE2 | 2.40 | 0.56 |
| 23:DA:1152:C:H5'' | 39:DQ:80:ILE:CG2 | 2.35 | 0.56 |
| 1:CA:1065:U:C5 | 1:CA:1190:G:H1' | 2.39 | 0.56 |
| 44:BV:24:LEU:O | 44:BV:24:LEU:HG | 2.04 | 0.56 |
| 1:AA:913:A:C1' | 1:AA:914:A:OP2 | 2.54 | 0.56 |
| 9:CI:25:LYS:O | 9:CI:60:ASP:HA | 2.05 | 0.56 |
| 1:CA:749:C:OP2 | 1:CA:750:G:OP2 | 2.23 | 0.56 |
| 25:BC:30:GLU:HG3 | 25:BC:63:ARG:NH2 | 2.20 | 0.56 |
| 23:DA:2480:C:H2' | 23:DA:2481:G:H5' | 1.88 | 0.56 |
| 34:BL:132:LYS:N | 34:BL:132:LYS:HD3 | 2.20 | 0.56 |
| 23:BA:640:C:H2' | 23:BA:641:C:C6 | 2.41 | 0.56 |
| 13:AM:66:LEU:O | 13:AM:69:GLU:HG2 | 2.05 | 0.56 |
| 1:CA:109:A:N7 | 1:CA:326:G:C4 | 2.74 | 0.56 |
| 3:AC:77:ILE:O | 3:AC:83:ARG:HB3 | 2.06 | 0.56 |
| 23:DA:830:G:H4' | 23:DA:831:G:OP2 | 2.04 | 0.56 |
| 6:AF:14:LEU:HD21 | 6:AF:18:GLN:HB2 | 1.87 | 0.56 |
| 50:D2:3:LYS:O | 50:D2:4:HIS:C | 2.43 | 0.56 |
| 23:DA:2228:G:OP2 | 25:DC:263:ARG:NH2 | 2.39 | 0.56 |
| 12:CL:78:GLU:O | 12:CL:79:HIS:CG | 2.59 | 0.56 |
| 33:BK:14:THR:HG22 | 33:BK:52:VAL:HB | 1.87 | 0.56 |
| 23:BA:914:C:H3' | 23:BA:914:C:H6 | 1.71 | 0.56 |
| 23:DA:2511:U:O3' | 26:DD:123:ALA:HB3 | 2.06 | 0.56 |
| 1:CA:110:C:H2' | 1:CA:111:G:O4' | 2.05 | 0.56 |
| 23:DA:1850:G:C6 | 23:DA:1851:U:C4 | 2.93 | 0.56 |
| 23:DA:1762:A:H8 | 23:DA:1762:A:O5' | 1.88 | 0.56 |
| 1:AA:1167:A:N7 | 1:AA:1169:A:C6 | 2.74 | 0.56 |
| 39:DQ:16:LYS:O | 39:DQ:20:LEU:HD22 | 2.05 | 0.56 |
| 9:AI:46:ALA:O | 9:AI:49:PRO:HD2 | 2.05 | 0.56 |
| 51:D3:25:LYS:HD3 | 53:D5:34:TRP:CZ3 | 2.41 | 0.56 |
| 34:BL:59:LEU:CA | 34:BL:61:ARG:HE | 2.13 | 0.56 |
| 34:BL:61:ARG:CD | 53:B5:13:ARG:HD2 | 2.36 | 0.56 |
| 38:DP:50:ILE:HA | 38:DP:99:LEU:HD11 | 1.87 | 0.56 |
| 1:AA:46:G:O2' | 1:AA:365:U:H1' | 2.06 | 0.56 |
| 23:BA:729:G:C8 | 25:BC:208:LYS:HD3 | 2.41 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BA:1266:G:C6 | 41:BS:16:LYS:HD2 | 2.40 | 0.56 |
| 25:DC:31:LYS:O | 25:DC:36:PRO:HD3 | 2.06 | 0.56 |
| 35:DM:75:THR:HA | 35:DM:88:GLY:HA3 | 1.86 | 0.56 |
| 23:DA:1121:C:O5' | 23:DA:1121:C:H6 | 1.88 | 0.56 |
| 30:BH:97:ILE:O | 30:BH:101:LEU:HB2 | 2.05 | 0.56 |
| 1:AA:411:A:N7 | 1:AA:429:U:C5 | 2.74 | 0.56 |
| 4:CD:109:GLY:C | 4:CD:111:ALA:N | 2.59 | 0.56 |
| 24:BB:40:U:O2' | 24:BB:41:U:H5' | 2.06 | 0.56 |
| 23:DA:662:G:OP1 | 34:DL:18:ARG:NH1 | 2.39 | 0.56 |
| 5:AE:32:VAL:O | 5:AE:43:LEU:HA | 2.06 | 0.56 |
| 37:DO:39:ILE:HG22 | 37:DO:39:ILE:O | 2.06 | 0.56 |
| 9:AI:112:LYS:HA | 9:AI:119:ALA:HB2 | 1.88 | 0.56 |
| 25:DC:186:HIS:HD2 | 25:DC:188:GLU:HB2 | 1.70 | 0.56 |
| 32:DJ:74:PHE:CZ | 32:DJ:142:ARG:HD2 | 2.39 | 0.56 |
| 1:AA:832:C:N4 | 1:AA:854:G:H1 | 2.01 | 0.56 |
| 1:AA:618:C:N3 | 1:AA:622:A:N6 | 2.53 | 0.56 |
| 10:AJ:34:VAL:HG13 | 10:AJ:74:ILE:HG22 | 1.88 | 0.56 |
| 47:BY:46:GLN:HB2 | 47:BY:49:LYS:HZ3 | 1.70 | 0.56 |
| 20:CT:11:SER:HA | 20:CT:13:LEU:HD13 | 1.88 | 0.56 |
| 23:DA:1414:G:C5 | 23:DA:1415:U:C5 | 2.94 | 0.56 |
| 23:DA:814:C:O2' | 23:DA:815:C:H5' | 2.05 | 0.56 |
| 1:CA:1254:C:OP1 | 10:CJ:45:ARG:HA | 2.06 | 0.56 |
| 4:AD:70:ILE:HG12 | 4:AD:71:SER:N | 2.20 | 0.56 |
| 28:BF:7:LEU:HA | 28:BF:10:LYS:HB2 | 1.86 | 0.56 |
| 35:DM:43:THR:OG1 | 35:DM:46:GLN:HG3 | 2.06 | 0.56 |
| 1:AA:300:A:C8 | 1:AA:300:A:H3' | 2.41 | 0.56 |
| 1:CA:1428:A:H2' | 1:CA:1429:C:O4' | 2.05 | 0.56 |
| 26:DD:176:ILE:HB | 26:DD:181:LEU:HB2 | 1.88 | 0.56 |
| 23:BA:880:G:H2' | 23:BA:881:G:H8 | 1.71 | 0.56 |
| 23:BA:2836:U:C4 | 23:BA:2883:A:N6 | 2.74 | 0.56 |
| 23:BA:176:G:C2' | 23:BA:177:G:H5' | 2.36 | 0.56 |
| 23:DA:718:A:H8 | 23:DA:718:A:O5' | 1.89 | 0.56 |
| 23:DA:533:G:N3 | 39:DQ:45:TYR:CE1 | 2.74 | 0.56 |
| 20:AT:64:ASP:O | 20:AT:67:ALA:HB3 | 2.06 | 0.56 |
| 23:BA:1317:A:C6 | 23:BA:1318:C:C4 | 2.93 | 0.56 |
| 33:DK:86:ILE:HD12 | 33:DK:86:ILE:H | 1.71 | 0.56 |
| 24:BB:115:G:H5' | 37:BO:50:SER:OG | 2.05 | 0.56 |
| 53:B5:29:LYS:HB2 | 53:B5:44:LYS:HB3 | 1.86 | 0.56 |
| 15:AO:78:TYR:O | 15:AO:82:ILE:HG22 | 2.05 | 0.56 |
| 22:AV:6182:A:N1 | 22:AV:6183:G:C5 | 2.74 | 0.56 |
| 40:DR:13:ARG:HG3 | 40:DR:13:ARG:HH11 | 1.70 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:DJ:85:VAL:CG2 | 32:DJ:89:LYS:HG3 | 2.32 | 0.56 |
| 47:BY:60:LEU:C | 47:BY:62:THR:H | 2.09 | 0.56 |
| 49:D1:59:VAL:HG12 | 49:D1:60:GLU:N | 2.13 | 0.56 |
| 23:BA:142:G:H4' | 42:BT:35:THR:HG21 | 1.87 | 0.56 |
| 43:DU:81:LYS:CE | 43:DU:97:ARG:HB3 | 2.36 | 0.56 |
| 9:AI:10:ARG:CZ | 9:AI:11:LYS:HE3 | 2.35 | 0.56 |
| 23:BA:84:A:H2 | 23:BA:98:G:N3 | 2.03 | 0.56 |
| 1:AA:456:C:H42 | 1:AA:476:G:H1 | 1.54 | 0.56 |
| 37:DO:36:TYR:H | 37:DO:36:TYR:HD1 | 1.53 | 0.56 |
| 3:AC:47:LEU:HD21 | 3:AC:68:VAL:HG11 | 1.87 | 0.56 |
| 23:BA:1478:G:N3 | 23:BA:1479:G:C8 | 2.74 | 0.56 |
| 23:DA:243:U:C2' | 23:DA:244:A:H5' | 2.36 | 0.56 |
| 1:AA:262:A:C6 | 1:AA:263:A:C6 | 2.94 | 0.56 |
| 7:CG:136:LYS:O | 7:CG:140:ASP:HB2 | 2.06 | 0.56 |
| 25:DC:61:LEU:CB | 25:DC:63:ARG:NH1 | 2.69 | 0.56 |
| 1:CA:1207:G:H2' | 1:CA:1208:C:H6 | 1.71 | 0.56 |
| 29:BG:85:LYS:O | 29:BG:132:ARG:HA | 2.06 | 0.56 |
| 29:DG:54:ARG:NH2 | 29:DG:62:LYS:HE2 | 2.19 | 0.56 |
| 1:AA:729:A:H2' | 1:AA:730:G:C8 | 2.40 | 0.56 |
| 3:AC:149:ALA:HA | 3:AC:201:TYR:O | 2.06 | 0.56 |
| 1:AA:300:A:H2' | 1:AA:301:G:H5' | 1.88 | 0.56 |
| 1:AA:1239:A:H4' | 1:AA:1240:U:H5' | 1.88 | 0.56 |
| 27:DE:14:PRO:HD3 | 27:DE:128:ALA:HB2 | 1.87 | 0.56 |
| 26:BD:149:ARG:CG | 26:BD:150:VAL:N | 2.69 | 0.56 |
| 1:CA:1494:G:N2 | 23:DA:1912:A:N3 | 2.53 | 0.56 |
| 1:CA:1501:C:C5 | 1:CA:1504:G:C5 | 2.94 | 0.56 |
| 1:AA:342:C:O2' | 1:AA:343:U:H5' | 2.05 | 0.56 |
| 23:DA:1204:A:N1 | 23:DA:1241:A:C2 | 2.74 | 0.56 |
| 23:BA:1168:G:C2 | 23:BA:1182:A:C2 | 2.94 | 0.56 |
| 23:DA:173:G:H2' | 23:DA:174:C:C6 | 2.41 | 0.56 |
| 13:CM:14:ARG:HG2 | 13:CM:44:ARG:NH1 | 2.21 | 0.56 |
| 1:AA:1043:C:H2' | 1:AA:1044:A:H8 | 1.70 | 0.56 |
| 3:CC:55:VAL:HG22 | 3:CC:55:VAL:O | 2.06 | 0.56 |
| 25:DC:198:ASN:C | 25:DC:198:ASN:HD22 | 2.09 | 0.56 |
| 1:AA:439:A:H2' | 1:AA:440:A:H5' | 1.88 | 0.56 |
| 1:AA:270:A:C6 | 1:AA:271:C:C4 | 2.94 | 0.56 |
| 23:DA:2392:A:H2 | 23:DA:2424:C:N4 | 1.95 | 0.56 |
| 23:BA:2415:G:O3' | 34:BL:66:GLY:HA3 | 2.06 | 0.56 |
| 26:DD:11:MET:HB2 | 26:DD:24:THR:HA | 1.86 | 0.56 |
| 23:DA:1448:G:H2' | 23:DA:149(B):A:C8 | 2.40 | 0.56 |
| 3:CC:13:GLY:HA2 | 14:CN:57:ARG:HE | 1.71 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BA:973:A:O4' | 23:BA:1188:U:C6 | 2.58 | 0.56 |
| 23:DA:1263:U:O2' | 50:D2:11:THR:HG23 | 2.06 | 0.56 |
| 39:DQ:88:ILE:HG22 | 40:DR:47:VAL:O | 2.05 | 0.56 |
| 23:DA:666:G:H5'' | 34:DL:47:ASP:O | 2.06 | 0.56 |
| 23:DA:1022:G:H22 | 23:DA:114(B):A:H2 | 1.53 | 0.56 |
| 39:BQ:102:GLU:HG3 | 40:BR:2:PHE:CE1 | 2.41 | 0.56 |
| 1:CA:37:U:H2' | 1:CA:38:G:H8 | 1.71 | 0.56 |
| 1:CA:1101:A:N3 | 1:CA:1102:A:H1' | 2.21 | 0.56 |
| 48:DZ:26:LEU:HD21 | 48:DZ:46:ASN:HB2 | 1.86 | 0.56 |
| 46:DX:10:LYS:O | 46:DX:11:ARG:CB | 2.54 | 0.56 |
| 10:AJ:33:GLN:HB2 | 10:AJ:75:ILE:HD11 | 1.88 | 0.56 |
| 1:CA:1124:G:H4' | 10:CJ:38:ILE:HD11 | 1.88 | 0.56 |
| 23:BA:83:G:C4 | 23:BA:102:G:N2 | 2.74 | 0.56 |
| 23:DA:1495:A:H2' | 23:DA:1496:A:N3 | 2.21 | 0.56 |
| 43:BU:81:LYS:HZ1 | 43:BU:98:VAL:HG12 | 1.70 | 0.56 |
| 46:BX:65:SER:OG | 46:BX:66:HIS:CD2 | 2.59 | 0.56 |
| 1:CA:1084:G:C5 | 1:CA:1085:U:C4 | 2.94 | 0.56 |
| 23:BA:2688:U:C3' | 23:BA:2688:U:O2 | 2.54 | 0.56 |
| 23:BA:2599:G:N7 | 25:BC:237:GLU:HG3 | 2.20 | 0.56 |
| 23:BA:300:A:P | 43:BU:84:ARG:NH2 | 2.78 | 0.56 |
| 43:BU:76:CYS:HB3 | 43:BU:77:PRO:CD | 2.35 | 0.56 |
| 44:DV:23:LYS:HB3 | 44:DV:38:TYR:CD1 | 2.40 | 0.56 |
| 44:DV:39:VAL:CG2 | 44:DV:44:PHE:HB2 | 2.36 | 0.56 |
| 23:BA:637:A:P | 34:BL:116:GLY:HA2 | 2.46 | 0.56 |
| 1:AA:1231:G:H2' | 1:AA:1232:U:H6 | 1.71 | 0.56 |
| 23:BA:1538:G:H2' | 23:BA:1539:G:C8 | 2.41 | 0.56 |
| 3:CC:150:LYS:HG3 | 3:CC:169:ALA:HB2 | 1.88 | 0.56 |
| 34:DL:75:ILE:CD1 | 34:DL:75:ILE:H | 2.17 | 0.56 |
| 23:BA:871:U:H4' | 35:BM:69:PHE:CE2 | 2.41 | 0.56 |
| 45:DW:11:LYS:O | 45:DW:14:ARG:NH2 | 2.37 | 0.56 |
| 23:DA:1833:U:C2 | 23:DA:1834:U:C5 | 2.93 | 0.56 |
| 1:CA:577:G:H1' | 1:CA:816:A:N3 | 2.20 | 0.56 |
| 1:AA:42:G:C8 | 1:AA:42:G:OP2 | 2.58 | 0.56 |
| 23:DA:530:G:N1 | 23:DA:2022:U:OP1 | 2.39 | 0.56 |
| 1:CA:1387:G:H2' | 1:CA:1388:C:C6 | 2.40 | 0.56 |
| 1:CA:285:G:O2' | 1:CA:286:G:H5' | 2.05 | 0.56 |
| 17:AQ:99:SER:O | 17:AQ:100:LYS:HD3 | 2.05 | 0.56 |
| 23:BA:2709:G:O2' | 23:BA:2710:C:H5' | 2.04 | 0.56 |
| 1:CA:1167:A:N7 | 1:CA:1169:A:C6 | 2.74 | 0.56 |
| 47:DY:36:ARG:HA | 47:DY:39:ALA:CB | 2.35 | 0.56 |
| 23:BA:191:A:H2' | 23:BA:192:C:C6 | 2.40 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 23:BA:2301:C:H2' | 23:BA:2302:G:H8 | 1.70 | 0.56 |
| 5:CE:36:ASP:O | 5:CE:37:ARG:HB2 | 2.06 | 0.56 |
| 23:DA:2064:C:H2' | 23:DA:2065:C:C6 | 2.40 | 0.56 |
| 26:DD:8:LYS:HG2 | 26:DD:192:ASN:HD22 | 1.70 | 0.56 |
| 23:DA:2392:A:OP1 | 53:D5:32:LEU:HB3 | 2.06 | 0.56 |
| 26:DD:11:MET:HE3 | 26:DD:186:GLY:HA2 | 1.87 | 0.56 |
| 43:DU:11:ASP:OD1 | 43:DU:12:THR:N | 2.39 | 0.56 |
| 9:CI:9:ARG:HG3 | 9:CI:14:VAL:HG13 | 1.87 | 0.56 |
| 1:AA:951:G:H1' | 1:AA:970:C:O2' | 2.05 | 0.56 |
| 3:CC:13:GLY:HA3 | 14:CN:57:ARG:HE | 1.70 | 0.56 |
| 1:CA:1226:C:C4 | 13:CM:104:ARG:HB2 | 2.41 | 0.56 |
| 23:BA:1900:A:N1 | 23:BA:1970:A:C6 | 2.74 | 0.56 |
| 23:BA:1022:G:O2' | 23:BA:1023:U:OP2 | 2.15 | 0.56 |
| 23:BA:2727:G:C5 | 23:BA:2728:U:H5 | 2.23 | 0.56 |
| 4:AD:9:CYS:SG | 4:AD:31:CYS:C | 2.85 | 0.56 |
| 3:CC:180:ALA:HB1 | 3:CC:182:ILE:HG13 | 1.88 | 0.56 |
| 42:DT:12:VAL:HG12 | 42:DT:28:PHE:HA | 1.86 | 0.56 |
| 30:DH:77:LEU:HD12 | 30:DH:101:LEU:HD13 | 1.88 | 0.56 |
| 23:DA:568:U:O4 | 40:DR:78:LYS:NZ | 2.39 | 0.56 |
| 23:BA:1592:C:H2' | 23:BA:1593:G:H8 | 1.71 | 0.56 |
| 49:D1:40:ILE:HG23 | 49:D1:59:VAL:HG21 | 1.87 | 0.56 |
| 2:CB:205:ASP:C | 2:CB:207:ALA:H | 2.09 | 0.56 |
| 23:BA:2787:C:H1' | 26:BD:62:PRO:CB | 2.36 | 0.56 |
| 23:DA:363(C):G:H2' | 23:DA:363(D):G:H8 | 1.71 | 0.56 |
| 23:BA:363(C):G:H2' | 23:BA:363(D):G:H8 | 1.70 | 0.56 |
| 23:BA:712(B):A:H5'' | 23:BA:2713:A:OP2 | 2.06 | 0.56 |
| 48:BZ:43:ILE:CD1 | 48:BZ:43:ILE:N | 2.69 | 0.56 |
| 1:AA:254:G:H2' | 1:AA:255:G:H8 | 1.70 | 0.56 |
| 29:DG:151:ILE:N | 29:DG:151:ILE:HD13 | 2.20 | 0.56 |
| 23:BA:2307:G:O5' | 23:BA:2307:G:H8 | 1.89 | 0.56 |
| 6:AF:61:LEU:HB3 | 6:AF:63:TYR:HE2 | 1.71 | 0.56 |
| 1:AA:456:C:N4 | 1:AA:476:G:H1 | 2.03 | 0.56 |
| 23:BA:1587:A:H2' | 23:BA:1588:C:H6 | 1.66 | 0.56 |
| 23:BA:1512:G:C6 | 23:BA:1513:C:N3 | 2.73 | 0.56 |
| 24:DB:90:C:OP2 | 35:DM:16:ARG:HD2 | 2.05 | 0.56 |
| 19:AS:6:LYS:CD | 19:AS:7:LYS:HD3 | 2.36 | 0.56 |
| 1:AA:1128:C:H42 | 1:AA:1143:G:H1 | 1.53 | 0.56 |
| 25:BC:265:PRO:C | 25:BC:267:SER:H | 2.08 | 0.56 |
| 25:BC:61:LEU:CB | 25:BC:63:ARG:NH1 | 2.69 | 0.56 |
| 23:DA:1820:U:O2 | 25:DC:201:HIS:HB3 | 2.05 | 0.56 |
| 13:CM:66:LEU:O | 13:CM:69:GLU:HG2 | 2.06 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:CE:144:THR:O | 5:CE:148:VAL:HG23 | 2.06 | 0.56 |
| 44:DV:5:LEU:HD23 | 44:DV:6:LYS:H | 1.71 | 0.56 |
| 1:CA:1239:A:H4' | 1:CA:1240:U:H5' | 1.88 | 0.56 |
| 22:CV:6198:U:H2' | 22:CV:6199:G:C8 | 2.40 | 0.56 |
| 4:CD:4:TYR:HE1 | 4:CD:11:LEU:HD11 | 1.71 | 0.56 |
| 1:AA:638:G:C2' | 1:AA:639:G:H5' | 2.36 | 0.56 |
| 23:DA:914:C:H6 | 23:DA:914:C:H3' | 1.70 | 0.56 |
| 23:BA:270(O):G:O2' | 23:BA:270(Q):C:H5' | 2.06 | 0.56 |
| 23:DA:1252:G:C2 | 23:DA:1253:A:C2 | 2.94 | 0.56 |
| 23:DA:1757:U:C2' | 23:DA:1758:G:OP1 | 2.54 | 0.56 |
| 23:DA:1368:G:C2 | 23:DA:1369:G:C8 | 2.94 | 0.56 |
| 41:BS:95:ILE:O | 41:BS:95:ILE:HG13 | 2.06 | 0.56 |
| 12:AL:19:LYS:HD3 | 12:AL:19:LYS:H | 1.71 | 0.56 |
| 32:DJ:53:ILE:HD12 | 32:DJ:122:LEU:HD11 | 1.88 | 0.55 |
| 1:AA:974:A:OP1 | 1:AA:974:A:H8 | 1.88 | 0.55 |
| 13:CM:91:ARG:HH11 | 19:CS:81:ARG:NH2 | 2.02 | 0.55 |
| 28:BF:76:SER:HB2 | 28:BF:83:ARG:N | 2.21 | 0.55 |
| 32:DJ:90:LEU:H | 32:DJ:90:LEU:HD12 | 1.72 | 0.55 |
| 1:AA:397:A:N6 | 1:AA:548:G:C5 | 2.74 | 0.55 |
| 3:CC:182:ILE:HG23 | 3:CC:202:ILE:O | 2.06 | 0.55 |
| 25:BC:44:ASN:CG | 25:BC:45:ASN:N | 2.59 | 0.55 |
| 47:DY:60:LEU:O | 47:DY:62:THR:N | 2.38 | 0.55 |
| 11:AK:63:LEU:HD23 | 11:AK:63:LEU:N | 2.20 | 0.55 |
| 1:AA:1075:C:OP1 | 2:AB:103:THR:HG21 | 2.06 | 0.55 |
| 23:BA:848:G:N9 | 23:BA:933:A:H8 | 2.05 | 0.55 |
| 29:DG:139:GLN:HG3 | 29:DG:140:LYS:N | 2.20 | 0.55 |
| 23:BA:2309:A:N6 | 23:BA:2310:A:N1 | 2.54 | 0.55 |
| 43:BU:81:LYS:CE | 43:BU:97:ARG:HB3 | 2.35 | 0.55 |
| 26:BD:26:ILE:N | 26:BD:26:ILE:HD13 | 2.21 | 0.55 |
| 6:CF:8:ILE:HG22 | 6:CF:10:LEU:HD12 | 1.87 | 0.55 |
| 47:DY:9:GLN:HG3 | 47:DY:12:GLU:OE1 | 2.05 | 0.55 |
| 25:DC:24:ILE:HD11 | 25:DC:84:TYR:HB2 | 1.87 | 0.55 |
| 23:BA:1487:G:C4 | 23:BA:1488:G:C8 | 2.95 | 0.55 |
| 29:BG:19:VAL:CG1 | 29:BG:20:ALA:H | 2.17 | 0.55 |
| 23:BA:9:U:N3 | 23:BA:2629:A:N6 | 2.53 | 0.55 |
| 1:AA:632:A:H2' | 1:AA:633:G:H5' | 1.89 | 0.55 |
| 32:DJ:62:ARG:HH21 | 32:DJ:64:ASP:CG | 2.10 | 0.55 |
| 23:DA:2284:C:C2' | 23:DA:2285:C:H5' | 2.36 | 0.55 |
| 1:AA:712:A:N6 | 1:AA:713:G:C6 | 2.74 | 0.55 |
| 32:BJ:62:ARG:HH21 | 32:BJ:64:ASP:CG | 2.10 | 0.55 |
| 50:B2:33:CYS:SG | 50:B2:40:LYS:HE3 | 2.47 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DA:2480:C:N4 | 23:DA:2481:G:C6 | 2.74 | 0.55 |
| 17:AQ:40:LYS:HD2 | 17:AQ:42:TYR:CZ | 2.40 | 0.55 |
| 19:CS:31:ILE:HG23 | 19:CS:49:ILE:HA | 1.88 | 0.55 |
| 1:CA:414:A:H2' | 1:CA:415:A:H8 | 1.70 | 0.55 |
| 19:AS:28:LYS:HB3 | 19:AS:29:ARG:NH1 | 2.21 | 0.55 |
| 7:CG:71:PRO:HG3 | 7:CG:103:TRP:CZ3 | 2.41 | 0.55 |
| 23:BA:1028:A:N3 | 23:BA:2486:G:O2' | 2.30 | 0.55 |
| 1:AA:1057:G:H4' | 3:AC:197:GLY:H | 1.71 | 0.55 |
| 23:DA:1918:A:O2' | 23:DA:1920:C:N4 | 2.39 | 0.55 |
| 1:CA:1159:U:C6 | 1:CA:1182:G:C2 | 2.94 | 0.55 |
| 23:DA:2279:G:O6 | 45:DW:14:ARG:HD2 | 2.05 | 0.55 |
| 1:CA:814:A:N7 | 1:CA:816:A:C4 | 2.73 | 0.55 |
| 23:BA:530:G:C5 | 23:BA:2022:U:H5'' | 2.41 | 0.55 |
| 23:DA:553:U:O2' | 23:DA:554:U:H5' | 2.05 | 0.55 |
| 23:BA:533:G:N3 | 39:BQ:45:TYR:CE1 | 2.74 | 0.55 |
| 23:DA:1335:U:O2' | 23:DA:1336:A:H5' | 2.06 | 0.55 |
| 1:CA:1187:G:H2' | 1:CA:1188:A:H8 | 1.71 | 0.55 |
| 32:BJ:51:THR:HG22 | 32:BJ:52:LYS:N | 2.21 | 0.55 |
| 23:DA:1394:U:C5 | 23:DA:1395:A:C5 | 2.94 | 0.55 |
| 29:DG:118:PRO:O | 29:DG:121:ILE:HG22 | 2.06 | 0.55 |
| 32:DJ:68:ASN:ND2 | 32:DJ:68:ASN:H | 2.04 | 0.55 |
| 23:BA:2098:U:O2' | 23:BA:2099:U:O5' | 2.24 | 0.55 |
| 9:AI:39:GLY:O | 9:AI:40:LEU:HD23 | 2.06 | 0.55 |
| 23:BA:2416:C:H2' | 23:BA:2417:C:H6 | 1.72 | 0.55 |
| 48:BZ:52:HIS:H | 48:BZ:52:HIS:CD2 | 2.23 | 0.55 |
| 23:BA:1530:G:N1 | 23:BA:1542:G:N2 | 2.55 | 0.55 |
| 41:DS:18:ARG:HH11 | 41:DS:18:ARG:HG2 | 1.72 | 0.55 |
| 25:DC:108:PRO:CG | 25:DC:143:HIS:HE1 | 2.19 | 0.55 |
| 1:AA:491:G:H2' | 1:AA:492:G:H8 | 1.72 | 0.55 |
| 3:CC:182:ILE:HG12 | 3:CC:203:PHE:CA | 2.29 | 0.55 |
| 20:AT:26:ASN:HB2 | 20:AT:71:THR:CG2 | 2.31 | 0.55 |
| 28:DF:40:ASN:O | 28:DF:155:MET:HB2 | 2.05 | 0.55 |
| 23:BA:1210:A:C8 | 23:BA:1210:A:H5' | 2.40 | 0.55 |
| 17:CQ:63:ARG:HG2 | 17:CQ:64:PRO:HD2 | 1.88 | 0.55 |
| 12:AL:53:LYS:HB3 | 12:AL:69:ILE:HG13 | 1.89 | 0.55 |
| 45:BW:50:ASN:O | 45:BW:62:LEU:HB2 | 2.05 | 0.55 |
| 1:AA:1349:A:H2' | 1:AA:1350:A:O4' | 2.05 | 0.55 |
| 29:DG:19:VAL:CG1 | 29:DG:20:ALA:H | 2.17 | 0.55 |
| 29:DG:84:SER:CA | 29:DG:133:VAL:O | 2.51 | 0.55 |
| 6:CF:88:VAL:HG12 | 6:CF:89:MET:N | 2.22 | 0.55 |
| 25:DC:25:THR:HG21 | 25:DC:82:ILE:N | 2.22 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:781:A:H3' | 1:AA:782:A:H5' | 1.86 | 0.55 |
| 8:AH:11:THR:HA | 8:AH:14:ARG:NH1 | 2.20 | 0.55 |
| 18:CR:22:VAL:HG11 | 18:CR:42:ARG:O | 2.06 | 0.55 |
| 1:AA:601:C:H2' | 1:AA:602:A:H8 | 1.70 | 0.55 |
| 5:AE:98:THR:HG22 | 5:AE:99:GLY:N | 2.21 | 0.55 |
| 38:DP:89:VAL:CG2 | 38:DP:89:VAL:O | 2.53 | 0.55 |
| 1:CA:1194:U:H4' | 5:CE:22:GLY:O | 2.05 | 0.55 |
| 1:CA:649:G:H2' | 1:CA:650:G:H8 | 1.70 | 0.55 |
| 1:AA:590:C:H2' | 1:AA:591:U:C6 | 2.41 | 0.55 |
| 6:CF:14:LEU:HD21 | 6:CF:18:GLN:HB2 | 1.88 | 0.55 |
| 35:BM:43:THR:O | 35:BM:46:GLN:HB2 | 2.07 | 0.55 |
| 41:BS:24:ILE:HG21 | 41:BS:36:LEU:CD2 | 2.35 | 0.55 |
| 23:BA:1130:U:O2 | 26:BD:149:ARG:NH2 | 2.39 | 0.55 |
| 23:DA:2086:U:OP2 | 25:DC:263:ARG:HD3 | 2.06 | 0.55 |
| 11:CK:124:LYS:HD2 | 11:CK:125:PHE:HE1 | 1.70 | 0.55 |
| 1:AA:851:G:O2' | 1:AA:852:G:H5' | 2.06 | 0.55 |
| 23:BA:2097:C:O2' | 23:BA:2098:U:H5' | 2.06 | 0.55 |
| 1:AA:1005:A:H2' | 1:AA:1006:C:H5' | 1.88 | 0.55 |
| 30:BH:58:LEU:C | 30:BH:60:GLU:H | 2.09 | 0.55 |
| 23:BA:49:A:H4' | 23:BA:50:U:H5' | 1.87 | 0.55 |
| 27:BE:122:LYS:HD2 | 27:BE:122:LYS:N | 2.20 | 0.55 |
| 38:BP:36:GLU:OE2 | 38:BP:41:ARG:HD3 | 2.06 | 0.55 |
| 23:BA:1204:A:N1 | 23:BA:1241:A:H2 | 2.03 | 0.55 |
| 35:BM:78:PRO:O | 35:BM:79:LEU:HB2 | 2.05 | 0.55 |
| 1:CA:142:G:N2 | 1:CA:143:A:C4 | 2.74 | 0.55 |
| 23:DA:637:A:P | 34:DL:116:GLY:HA2 | 2.46 | 0.55 |
| 23:DA:2250:G:C6 | 35:DM:82:ARG:HD2 | 2.41 | 0.55 |
| 3:AC:13:GLY:HA2 | 14:AN:57:ARG:HE | 1.71 | 0.55 |
| 23:BA:1543:A:C8 | 23:BA:1543:A:C3' | 2.88 | 0.55 |
| 23:BA:806:C:OP2 | 34:BL:39:LYS:HD3 | 2.06 | 0.55 |
| 1:AA:960:U:H5 | 1:AA:1225:A:H1' | 1.71 | 0.55 |
| 35:DM:89:ASN:C | 35:DM:92:GLY:H | 2.09 | 0.55 |
| 41:BS:86:LEU:HD12 | 41:BS:87:PRO:CD | 2.36 | 0.55 |
| 4:AD:111:ALA:HB1 | 4:AD:116:GLN:OE1 | 2.06 | 0.55 |
| 4:AD:3:ARG:HG2 | 4:AD:5:ILE:HD13 | 1.88 | 0.55 |
| 30:DH:88:ILE:HG22 | 30:DH:90:GLY:N | 2.21 | 0.55 |
| 23:DA:330:A:O2' | 23:DA:331:A:C8 | 2.50 | 0.55 |
| 47:DY:57:ILE:HG22 | 47:DY:61:LEU:HD22 | 1.88 | 0.55 |
| 36:DN:8:ARG:HD3 | 36:DN:43:GLU:OE1 | 2.06 | 0.55 |
| 25:BC:231:HIS:HD2 | 25:BC:249:PRO:CA | 2.13 | 0.55 |
| 23:BA:71:A:C2 | 42:BT:31:HIS:CE1 | 2.92 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:266:G:C5' | 1:AA:267:C:H5 | 2.19 | 0.55 |
| 46:BX:40:ARG:HG2 | 46:BX:41:ARG:N | 2.22 | 0.55 |
| 42:BT:23:GLU:HA | 42:BT:23:GLU:OE1 | 2.05 | 0.55 |
| 1:AA:626:U:H2' | 1:AA:627:G:H8 | 1.71 | 0.55 |
| 6:AF:98:LEU:CD1 | 6:AF:101:ALA:HB2 | 2.36 | 0.55 |
| 23:DA:2287:A:C4 | 23:DA:2289:G:C8 | 2.95 | 0.55 |
| 44:DV:38:TYR:CG | 44:DV:38:TYR:O | 2.59 | 0.55 |
| 1:CA:515:G:C2 | 1:CA:537:G:C2 | 2.94 | 0.55 |
| 32:BJ:101:TYR:HB3 | 32:BJ:102:PRO:CD | 2.36 | 0.55 |
| 39:DQ:50:ARG:HH12 | 40:DR:72:VAL:HG12 | 1.72 | 0.55 |
| 43:BU:90:LEU:HG | 43:BU:91:GLU:N | 2.21 | 0.55 |
| 27:DE:181:LEU:CD2 | 27:DE:186:ILE:HD11 | 2.37 | 0.55 |
| 20:AT:97:ALA:O | 20:AT:99:LEU:N | 2.37 | 0.55 |
| 23:DA:1445:C:C2 | 23:DA:1446:C:C5 | 2.95 | 0.55 |
| 1:CA:562:C:H1' | 12:CL:14:ARG:HB3 | 1.87 | 0.55 |
| 38:DP:109:GLU:O | 38:DP:112:ARG:HG3 | 2.05 | 0.55 |
| 11:AK:67:ASP:OD1 | 11:AK:71:LYS:HE3 | 2.07 | 0.55 |
| 20:CT:42:GLN:HG3 | 20:CT:43:LEU:HD23 | 1.87 | 0.55 |
| 1:AA:1399:C:C4 | 1:AA:1502:A:N1 | 2.75 | 0.55 |
| 23:DA:2038:G:H2' | 23:DA:2039:C:C6 | 2.41 | 0.55 |
| 46:BX:17:SER:HA | 46:BX:44:PRO:HD3 | 1.88 | 0.55 |
| 34:DL:80:TYR:CE1 | 34:DL:111:ARG:HG2 | 2.42 | 0.55 |
| 1:CA:1333:A:H2' | 1:CA:1334:G:O4' | 2.06 | 0.55 |
| 27:BE:63:LYS:HZ1 | 27:BE:67:GLN:HE21 | 1.51 | 0.55 |
| 1:AA:671:G:H2' | 1:AA:672:U:H6 | 1.71 | 0.55 |
| 23:BA:2727:G:C5 | 23:BA:2728:U:C5 | 2.94 | 0.55 |
| 23:DA:2727:G:C5 | 23:DA:2728:U:H5 | 2.24 | 0.55 |
| 53:B5:62:LEU:C | 53:B5:64:TYR:N | 2.60 | 0.55 |
| 1:AA:62:U:O2' | 1:AA:379:C:H1' | 2.06 | 0.55 |
| 4:AD:104:VAL:C | 4:AD:106:TYR:H | 2.09 | 0.55 |
| 23:DA:1812:A:O2' | 23:DA:1813:G:H5' | 2.06 | 0.55 |
| 42:DT:12:VAL:HG13 | 42:DT:27:THR:O | 2.06 | 0.55 |
| 4:AD:105:VAL:O | 4:AD:105:VAL:HG12 | 2.05 | 0.55 |
| 5:CE:64:ARG:HG3 | 5:CE:65:ASN:N | 2.21 | 0.55 |
| 23:BA:125:G:OP2 | 52:B4:19:ARG:NH1 | 2.38 | 0.55 |
| 1:AA:1072:G:H2' | 1:AA:1073:U:C6 | 2.41 | 0.55 |
| 1:CA:406:G:N2 | 1:CA:437:U:C2 | 2.74 | 0.55 |
| 23:DA:1789:A:OP1 | 25:DC:222:ARG:HG3 | 2.07 | 0.55 |
| 1:AA:255:G:H2' | 1:AA:256:U:C6 | 2.40 | 0.55 |
| 1:AA:256:U:H2' | 1:AA:257:G:C8 | 2.41 | 0.55 |
| 46:DX:14:VAL:HG12 | 46:DX:14:VAL:O | 2.07 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DA:2218:G:O2' | 23:DA:2219:G:H5' | 2.05 | 0.55 |
| 46:BX:11:ARG:O | 46:BX:12:PRO:C | 2.44 | 0.55 |
| 23:BA:1495:A:C5' | 23:BA:1496:A:OP2 | 2.51 | 0.55 |
| 23:BA:2746:U:O3' | 29:BG:138:LYS:HD3 | 2.06 | 0.55 |
| 23:DA:1858:G:H1' | 23:DA:1884:A:H61 | 1.71 | 0.55 |
| 23:BA:1046:A:H2 | 31:BI:8:GLU:OE1 | 1.90 | 0.55 |
| 1:AA:1179:A:H2' | 1:AA:1180:A:O4' | 2.07 | 0.55 |
| 19:AS:6:LYS:HD2 | 19:AS:6:LYS:N | 2.22 | 0.55 |
| 3:AC:70:VAL:HG12 | 3:AC:71:ALA:N | 2.21 | 0.55 |
| 1:CA:1128:C:H42 | 1:CA:1143:G:H1 | 1.55 | 0.55 |
| 30:DH:6:LEU:O | 30:DH:7:GLU:HB2 | 2.06 | 0.55 |
| 43:DU:19:LYS:HB3 | 43:DU:20:TYR:CD1 | 2.40 | 0.55 |
| 32:BJ:59:GLY:O | 32:BJ:65:TRP:HE3 | 1.89 | 0.55 |
| 1:CA:255:G:H2' | 1:CA:256:U:C6 | 2.40 | 0.55 |
| 5:CE:18:ARG:HH21 | 5:CE:25:ARG:CB | 2.20 | 0.55 |
| 1:CA:632:A:H2' | 1:CA:633:G:H5' | 1.88 | 0.55 |
| 23:BA:328:U:H4' | 43:BU:68:HIS:CE1 | 2.40 | 0.55 |
| 23:DA:1726:G:H2' | 23:DA:1727:U:H6 | 1.70 | 0.55 |
| 23:DA:1184:G:C5 | 23:DA:1185:C:C5 | 2.94 | 0.55 |
| 8:AH:31:PHE:O | 8:AH:35:ILE:HG12 | 2.07 | 0.55 |
| 19:CS:53:ASN:ND2 | 19:CS:55:LYS:HB3 | 2.21 | 0.55 |
| 1:AA:44:G:N3 | 1:AA:399:G:C2 | 2.75 | 0.55 |
| 46:BX:67:ILE:HB | 46:BX:68:PRO:HD3 | 1.87 | 0.55 |
| 1:AA:247:G:OP2 | 17:AQ:100:LYS:N | 2.38 | 0.55 |
| 18:AR:53:ARG:C | 18:AR:55:ARG:H | 2.09 | 0.55 |
| 3:AC:188:LEU:O | 3:AC:189:ALA:HB2 | 2.07 | 0.55 |
| 4:CD:99:SER:O | 4:CD:140:VAL:HG23 | 2.06 | 0.55 |
| 2:AB:52:GLU:O | 2:AB:56:ARG:HG3 | 2.05 | 0.55 |
| 12:AL:46:LYS:HB3 | 12:AL:47:PRO:HD3 | 1.89 | 0.55 |
| 23:DA:2032:G:H21 | 26:DD:146:THR:HG23 | 1.72 | 0.55 |
| 3:CC:186:PHE:HZ | 3:CC:188:LEU:HD13 | 1.71 | 0.55 |
| 34:DL:97:PRO:HA | 34:DL:112:LEU:HD12 | 1.87 | 0.55 |
| 1:CA:1372:U:H5'' | 9:CI:71:SER:HB3 | 1.88 | 0.55 |
| 26:BD:24:THR:HB | 26:BD:186:GLY:HA2 | 1.88 | 0.55 |
| 22:AV:6182:A:N1 | 22:AV:6183:G:C4 | 2.74 | 0.55 |
| 22:CV:6182:A:N1 | 22:CV:6183:G:C5 | 2.75 | 0.55 |
| 1:CA:1225:A:H5'' | 1:CA:1226:C:OP2 | 2.05 | 0.55 |
| 1:CA:503:C:C2 | 1:CA:504:C:C5 | 2.94 | 0.55 |
| 32:BJ:37:VAL:HG12 | 32:BJ:38:LEU:H | 1.72 | 0.55 |
| 23:BA:114(B):A:C5 | 23:BA:1144:G:C5 | 2.95 | 0.55 |
| 32:BJ:88:LYS:O | 32:BJ:89:LYS:C | 2.44 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:DQ:79:PHE:CD1 | 39:DQ:83:LEU:HD13 | 2.41 | 0.55 |
| 3:AC:182:ILE:HG23 | 3:AC:202:ILE:C | 2.27 | 0.55 |
| 4:AD:111:ALA:HA | 4:AD:161:ASN:ND2 | 2.21 | 0.55 |
| 23:DA:1188:U:H4' | 40:DR:79:VAL:HG22 | 1.87 | 0.55 |
| 3:CC:14:ILE:HG12 | 3:CC:15:THR:N | 2.21 | 0.55 |
| 1:CA:187:C:O2 | 1:CA:191(A):G:C6 | 2.59 | 0.55 |
| 23:BA:848:G:C4 | 23:BA:933:A:H8 | 2.25 | 0.55 |
| 48:DZ:28:LEU:N | 48:DZ:28:LEU:HD12 | 2.20 | 0.55 |
| 23:BA:2723:C:C2' | 23:BA:2724:C:O5' | 2.54 | 0.55 |
| 23:DA:528:A:C2 | 23:DA:2043:C:O5' | 2.60 | 0.55 |
| 1:AA:339:C:OP2 | 33:BK:97:ARG:NH1 | 2.39 | 0.55 |
| 23:BA:1332:G:N2 | 23:BA:1610:A:H8 | 2.03 | 0.55 |
| 23:DA:2284:C:H2' | 23:DA:2285:C:H5' | 1.89 | 0.55 |
| 38:BP:27:THR:HG22 | 38:BP:90:GLN:HB3 | 1.88 | 0.55 |
| 44:DV:24:LEU:HD11 | 44:DV:86:VAL:HG22 | 1.89 | 0.55 |
| 23:BA:115:C:C2' | 23:BA:116:C:H5' | 2.36 | 0.55 |
| 1:AA:592:G:C2 | 1:AA:593:G:N7 | 2.74 | 0.55 |
| 23:BA:2364:C:O2' | 23:BA:2365:G:H5' | 2.07 | 0.55 |
| 23:DA:1538:G:H2' | 23:DA:1539:G:H8 | 1.71 | 0.55 |
| 7:CG:69:VAL:O | 7:CG:69:VAL:HG12 | 2.07 | 0.55 |
| 23:BA:1336:A:H2' | 23:BA:1337:G:C8 | 2.42 | 0.55 |
| 53:B5:29:LYS:HB3 | 53:B5:29:LYS:NZ | 2.21 | 0.55 |
| 23:DA:2097:C:C2' | 23:DA:2098:U:H5' | 2.36 | 0.55 |
| 35:DM:73:PRO:HB3 | 35:DM:93:TYR:CE2 | 2.41 | 0.55 |
| 23:DA:2399:G:H2' | 23:DA:2400:G:O4' | 2.06 | 0.55 |
| 1:CA:1480:G:C5 | 1:CA:1481:U:C5 | 2.95 | 0.55 |
| 3:AC:55:VAL:HG22 | 3:AC:55:VAL:O | 2.06 | 0.55 |
| 42:DT:75:ASP:O | 42:DT:76:ARG:HG3 | 2.06 | 0.55 |
| 34:DL:111:ARG:HD2 | 34:DL:128:HIS:CD2 | 2.41 | 0.55 |
| 45:BW:23:VAL:HB | 45:BW:26:TYR:HE2 | 1.71 | 0.55 |
| 1:AA:1225:A:H5'' | 1:AA:1226:C:OP2 | 2.07 | 0.55 |
| 22:AV:6192:G:H2' | 22:AV:6193:U:O4' | 2.07 | 0.55 |
| 5:CE:102:ALA:HB2 | 5:CE:120:THR:HG23 | 1.88 | 0.55 |
| 22:CV:6192:G:H2' | 22:CV:6193:U:O4' | 2.07 | 0.55 |
| 1:AA:1228:C:N4 | 1:AA:1229:A:H62 | 2.04 | 0.55 |
| 1:CA:46:G:O2' | 1:CA:365:U:H1' | 2.07 | 0.55 |
| 34:DL:32:THR:HG21 | 34:DL:37:GLY:CA | 2.36 | 0.55 |
| 25:DC:33:LEU:HD23 | 25:DC:33:LEU:H | 1.72 | 0.55 |
| 23:DA:860:U:O2 | 23:DA:860:U:O4' | 2.22 | 0.55 |
| 50:B2:17:ASP:O | 50:B2:20:ARG:HB2 | 2.07 | 0.55 |
| 23:DA:1022:G:O2' | 23:DA:1023:U:OP2 | 2.21 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BA:242:G:N7 | 53:B5:5:LYS:HG2 | 2.22 | 0.55 |
| 30:DH:82:ARG:HB3 | 30:DH:89:TYR:CG | 2.41 | 0.55 |
| 23:BA:1414:G:H2' | 23:BA:1415:U:H6 | 1.70 | 0.55 |
| 27:DE:124:LEU:HD12 | 27:DE:125:LEU:O | 2.06 | 0.55 |
| 1:CA:38:G:H22 | 1:CA:397:A:C5' | 2.16 | 0.55 |
| 1:CA:1071:C:H5'' | 5:CE:49:PRO:HG2 | 1.89 | 0.55 |
| 23:BA:848:G:O6 | 23:BA:929:G:H2' | 2.07 | 0.55 |
| 1:CA:689:C:H2' | 1:CA:690:G:O4' | 2.07 | 0.55 |
| 36:BN:8:ARG:HD3 | 36:BN:43:GLU:OE1 | 2.06 | 0.55 |
| 1:CA:62:U:O2' | 1:CA:379:C:H1' | 2.06 | 0.55 |
| 23:BA:1506:C:H2' | 23:BA:1508:A:C8 | 2.42 | 0.55 |
| 23:BA:2277:G:H5'' | 35:BM:85:LYS:CB | 2.35 | 0.55 |
| 1:AA:853:G:C2' | 1:AA:854:G:H5' | 2.36 | 0.55 |
| 43:BU:2:ARG:HG2 | 43:BU:3:VAL:N | 2.22 | 0.55 |
| 38:BP:28:VAL:HA | 38:BP:89:VAL:HG12 | 1.89 | 0.55 |
| 1:AA:712:A:C2' | 1:AA:713:G:H5' | 2.37 | 0.55 |
| 50:D2:48:GLU:O | 50:D2:49:CYS:HB2 | 2.06 | 0.55 |
| 23:BA:1270:C:H5'' | 23:BA:1271:G:C5' | 2.37 | 0.55 |
| 23:BA:1138:G:O2' | 32:BJ:128:GLY:HA3 | 2.06 | 0.55 |
| 27:BE:206:ILE:O | 27:BE:206:ILE:HD12 | 2.06 | 0.55 |
| 43:BU:76:CYS:CB | 43:BU:77:PRO:CD | 2.85 | 0.55 |
| 8:AH:80:ILE:HD12 | 8:AH:80:ILE:N | 2.21 | 0.55 |
| 1:CA:300:A:H8 | 1:CA:300:A:O5' | 1.88 | 0.55 |
| 7:CG:40:ALA:O | 7:CG:44:TYR:CD1 | 2.60 | 0.55 |
| 23:BA:18:C:OP1 | 39:BQ:26:GLY:HA2 | 2.05 | 0.55 |
| 24:DB:30:C:OP2 | 37:DO:32:LEU:HD11 | 2.06 | 0.55 |
| 1:AA:191(D):U:H2' | 1:AA:191(E):G:C8 | 2.42 | 0.55 |
| 53:B5:26:LYS:HA | 53:B5:48:PHE:CE2 | 2.41 | 0.55 |
| 23:DA:2279:G:N2 | 23:DA:2280:G:H1' | 2.21 | 0.55 |
| 9:AI:95:LYS:HD3 | 9:AI:96:LEU:N | 2.22 | 0.55 |
| 1:CA:577:G:H1' | 1:CA:816:A:C4 | 2.42 | 0.55 |
| 23:DA:898:C:H2' | 23:DA:899:A:O4' | 2.06 | 0.55 |
| 23:BA:461:C:O2' | 23:BA:462:C:H5' | 2.07 | 0.55 |
| 23:DA:2097:C:O2' | 23:DA:2098:U:H5' | 2.07 | 0.55 |
| 23:DA:482:A:C2 | 23:DA:506:G:C5 | 2.95 | 0.55 |
| 28:BF:137:GLU:HG2 | 28:BF:152:LEU:HD22 | 1.87 | 0.55 |
| 23:DA:2301:C:H2' | 23:DA:2302:G:H8 | 1.71 | 0.55 |
| 23:DA:1448:G:N2 | 23:DA:149(B):A:N6 | 2.54 | 0.55 |
| 33:BK:76:ALA:HB3 | 38:BP:75:ILE:HB | 1.88 | 0.55 |
| 51:B3:25:LYS:HD3 | 53:B5:34:TRP:CZ3 | 2.41 | 0.55 |
| 2:CB:61:LEU:HD21 | 2:CB:161:ALA:HB3 | 1.87 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:DQ:90:VAL:O | 39:DQ:92:ARG:N | 2.39 | 0.55 |
| 53:D5:6:THR:HG21 | 53:D5:64:TYR:HD1 | 1.72 | 0.55 |
| 30:BH:142:VAL:HG12 | 30:BH:143:SER:H | 1.72 | 0.55 |
| 4:CD:64:LEU:HD23 | 4:CD:203:VAL:HG21 | 1.87 | 0.55 |
| 5:CE:75:THR:HG23 | 5:CE:76:ILE:N | 2.22 | 0.55 |
| 5:CE:79:GLU:H | 5:CE:79:GLU:CD | 2.08 | 0.55 |
| 5:AE:11:ILE:CB | 5:AE:31:LEU:HD13 | 2.37 | 0.55 |
| 23:DA:2541:A:H5'' | 23:DA:2542:A:OP2 | 2.06 | 0.55 |
| 1:AA:447:G:H2' | 1:AA:485:G:N2 | 2.21 | 0.55 |
| 23:DA:2599:G:N7 | 25:DC:237:GLU:HG3 | 2.22 | 0.55 |
| 1:AA:659:U:C2 | 1:AA:660:G:C8 | 2.94 | 0.55 |
| 23:DA:1884:A:C2 | 23:DA:1885:A:C8 | 2.94 | 0.55 |
| 24:BB:90:C:OP2 | 35:BM:16:ARG:HD2 | 2.07 | 0.55 |
| 23:DA:1952:A:C6 | 33:DK:22:ILE:CD1 | 2.89 | 0.55 |
| 25:DC:15:PHE:O | 25:DC:205:VAL:HG11 | 2.06 | 0.55 |
| 1:AA:1145:C:H4' | 1:AA:1146:A:H8 | 1.71 | 0.55 |
| 44:BV:44:PHE:CE2 | 44:BV:86:VAL:HG11 | 2.41 | 0.55 |
| 23:BA:2284:C:C2' | 23:BA:2285:C:H5' | 2.36 | 0.55 |
| 23:BA:2284:C:H2' | 23:BA:2285:C:H5' | 1.89 | 0.55 |
| 1:CA:590:C:H2' | 1:CA:591:U:C6 | 2.42 | 0.55 |
| 1:CA:337:C:H2' | 1:CA:338:A:C8 | 2.40 | 0.55 |
| 1:CA:1357:A:C6 | 1:CA:1358:U:N3 | 2.75 | 0.55 |
| 1:AA:1112:C:C5 | 3:AC:178:LEU:HD23 | 2.41 | 0.55 |
| 15:CO:24:SER:O | 15:CO:28:GLN:HG3 | 2.07 | 0.55 |
| 27:DE:46:ARG:HH11 | 27:DE:46:ARG:CG | 2.19 | 0.55 |
| 23:DA:270(O):G:O2' | 23:DA:270(Q):C:H5' | 2.06 | 0.55 |
| 8:AH:50:ARG:HG2 | 8:AH:50:ARG:NH1 | 2.21 | 0.55 |
| 23:BA:2037:G:C6 | 23:BA:2038:G:C6 | 2.95 | 0.55 |
| 48:DZ:23:LEU:N | 48:DZ:23:LEU:HD12 | 2.20 | 0.55 |
| 23:DA:969:U:H2' | 23:DA:970:C:C6 | 2.41 | 0.55 |
| 23:DA:1382:G:O2' | 23:DA:1383:C:H5' | 2.06 | 0.55 |
| 46:DX:52:ARG:O | 46:DX:56:GLN:O | 2.25 | 0.55 |
| 41:BS:54:ALA:HB1 | 41:BS:107:LEU:HD22 | 1.88 | 0.55 |
| 46:BX:48:LYS:NZ | 46:BX:50:ARG:NH1 | 2.55 | 0.55 |
| 34:DL:101:VAL:HG23 | 34:DL:107:LYS:H | 1.72 | 0.55 |
| 34:DL:132:LYS:N | 34:DL:132:LYS:HD3 | 2.18 | 0.55 |
| 23:DA:1540:G:H3' | 23:DA:1541:U:H6 | 1.72 | 0.55 |
| 13:AM:91:ARG:HH11 | 19:AS:81:ARG:NH2 | 2.02 | 0.55 |
| 7:AG:115:ARG:HB2 | 7:AG:118:VAL:CG1 | 2.36 | 0.55 |
| 23:BA:810:U:O5' | 23:BA:810:U:H6 | 1.89 | 0.55 |
| 23:BA:1276:A:H1' | 36:BN:16:HIS:HE1 | 1.71 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DA:993:G:C5 | 23:DA:994:C:C5 | 2.95 | 0.55 |
| 23:DA:1614:A:N6 | 41:DS:93:ALA:HB2 | 2.08 | 0.55 |
| 30:BH:77:LEU:HD12 | 30:BH:101:LEU:HD13 | 1.88 | 0.55 |
| 1:CA:671:G:H2' | 1:CA:672:U:H6 | 1.72 | 0.55 |
| 28:DF:161:THR:C | 28:DF:163:ALA:H | 2.10 | 0.55 |
| 1:AA:1435:G:H2' | 1:AA:1436:U:H6 | 1.67 | 0.55 |
| 24:DB:43:C:H4' | 28:DF:98:ARG:HH12 | 1.70 | 0.55 |
| 23:BA:1414:G:C5 | 23:BA:1415:U:C5 | 2.95 | 0.55 |
| 26:BD:52:LEU:HB2 | 26:BD:76:ARG:HB2 | 1.88 | 0.55 |
| 36:DN:10:LEU:CB | 36:DN:17:ARG:NE | 2.67 | 0.55 |
| 23:DA:2633:G:O2' | 26:DD:61:ARG:HD3 | 2.07 | 0.55 |
| 23:DA:2090:G:H21 | 46:DX:45:ASN:ND2 | 2.05 | 0.55 |
| 10:CJ:33:GLN:HB2 | 10:CJ:75:ILE:HD11 | 1.89 | 0.55 |
| 1:CA:535:A:H4' | 1:CA:536:C:OP2 | 2.07 | 0.55 |
| 1:CA:318:G:O2' | 1:CA:319:G:H5' | 2.07 | 0.55 |
| 8:CH:10:LEU:HB3 | 8:CH:83:ILE:HD13 | 1.89 | 0.55 |
| 8:CH:111:ILE:O | 8:CH:112:LEU:HB3 | 2.07 | 0.55 |
| 53:B5:52:LYS:N | 53:B5:53:PRO:HD2 | 2.21 | 0.55 |
| 23:BA:1476:C:C5 | 23:BA:1477:A:N7 | 2.75 | 0.55 |
| 1:CA:781:A:O2' | 1:CA:1522:U:O2 | 2.24 | 0.55 |
| 1:CA:101:A:C4 | 1:CA:102:G:C8 | 2.95 | 0.55 |
| 23:DA:1777:U:O2' | 23:DA:1778:U:H5' | 2.05 | 0.55 |
| 36:BN:100:LEU:HD23 | 36:BN:100:LEU:N | 2.21 | 0.55 |
| 1:AA:1286:A:N7 | 21:AU:22:ARG:NH2 | 2.53 | 0.55 |
| 23:BA:864:G:O2' | 23:BA:865:C:H5' | 2.06 | 0.55 |
| 45:DW:31:VAL:O | 45:DW:64:ASP:HA | 2.07 | 0.55 |
| 1:CA:1080:A:H5' | 1:CA:1081:G:OP2 | 2.07 | 0.55 |
| 1:AA:728:A:H2' | 1:AA:729:A:C8 | 2.42 | 0.55 |
| 23:BA:1152:C:HO2' | 39:BQ:76:TYR:HE2 | 1.55 | 0.55 |
| 7:AG:138:LYS:O | 7:AG:142:GLU:HG3 | 2.06 | 0.55 |
| 23:DA:634:C:H2' | 23:DA:635:C:C6 | 2.41 | 0.55 |
| 26:BD:181:LEU:HD21 | 38:BP:7:ILE:HG23 | 1.88 | 0.55 |
| 36:BN:31:HIS:O | 36:BN:33:ARG:N | 2.39 | 0.55 |
| 23:BA:1917:U:C2' | 23:BA:1918:A:H5' | 2.36 | 0.55 |
| 26:BD:114:ALA:O | 26:BD:157:ALA:HB1 | 2.07 | 0.55 |
| 1:AA:1480:G:C5 | 1:AA:1481:U:C5 | 2.95 | 0.55 |
| 1:CA:1005:A:H2' | 1:CA:1006:C:H5' | 1.88 | 0.55 |
| 23:BA:2356:C:O3' | 45:BW:20:ARG:HD3 | 2.07 | 0.55 |
| 1:AA:503:C:H2' | 1:AA:504:C:H6 | 1.72 | 0.55 |
| 11:AK:125:PHE:N | 11:AK:125:PHE:CD1 | 2.70 | 0.55 |
| 23:BA:1338:G:C2' | 23:BA:1339:G:H5' | 2.36 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 34:DL:61:ARG:HD3 | 53:D5:13:ARG:HD2 | 1.89 | 0.55 |
| 32:BJ:127:LYS:HB2 | 32:BJ:140:PHE:HE1 | 1.71 | 0.55 |
| 23:DA:1141:U:H4' | 23:DA:114(B):A:O4' | 2.07 | 0.55 |
| 4:CD:63:LYS:HD2 | 4:CD:198:VAL:CG2 | 2.37 | 0.55 |
| 23:DA:142:G:H4' | 42:DT:35:THR:HG21 | 1.88 | 0.55 |
| 42:DT:28:PHE:H | 42:DT:28:PHE:HD1 | 1.53 | 0.55 |
| 1:AA:324:G:N1 | 1:AA:327:A:OP2 | 2.40 | 0.55 |
| 24:DB:71:C:C2 | 24:DB:72:G:C8 | 2.95 | 0.55 |
| 23:DA:1407:C:H2' | 23:DA:1408:C:H6 | 1.72 | 0.55 |
| 1:CA:266:G:C5' | 1:CA:267:C:C5 | 2.90 | 0.55 |
| 5:CE:41:VAL:HG11 | 5:CE:113:ALA:CB | 2.36 | 0.55 |
| 5:AE:11:ILE:HG12 | 5:AE:33:VAL:HG23 | 1.89 | 0.55 |
| 23:BA:72:U:C4 | 23:BA:112:U:H4' | 2.42 | 0.55 |
| 48:DZ:26:LEU:HB2 | 48:DZ:28:LEU:CD1 | 2.36 | 0.55 |
| 17:AQ:63:ARG:HG2 | 17:AQ:64:PRO:HD2 | 1.89 | 0.55 |
| 23:DA:2307:G:O5' | 23:DA:2307:G:H8 | 1.90 | 0.55 |
| 29:DG:123:PHE:HB3 | 29:DG:133:VAL:HG13 | 1.88 | 0.55 |
| 25:BC:25:THR:O | 25:BC:27:THR:HB | 2.07 | 0.55 |
| 27:DE:31:HIS:O | 27:DE:34:TRP:HB3 | 2.07 | 0.55 |
| 23:BA:2636:U:H4' | 26:BD:80:GLU:OE2 | 2.07 | 0.55 |
| 23:BA:2468:G:O2' | 23:BA:2476:A:N7 | 2.40 | 0.55 |
| 23:DA:1476:C:C2' | 23:DA:1477:A:H5' | 2.37 | 0.55 |
| 23:DA:1478:G:N3 | 23:DA:1479:G:C8 | 2.75 | 0.55 |
| 44:DV:37:VAL:O | 44:DV:38:TYR:HB3 | 2.07 | 0.55 |
| 1:CA:729:A:H2' | 1:CA:730:G:C8 | 2.38 | 0.55 |
| 12:AL:74:HIS:HB2 | 12:AL:76:LEU:CD2 | 2.36 | 0.55 |
| 19:AS:31:ILE:HG23 | 19:AS:49:ILE:HA | 1.88 | 0.55 |
| 19:AS:53:ASN:ND2 | 19:AS:55:LYS:HB3 | 2.22 | 0.55 |
| 23:DA:1920:C:H2' | 23:DA:1920:C:O2 | 2.07 | 0.55 |
| 53:D5:26:LYS:HG2 | 53:D5:48:PHE:CD2 | 2.42 | 0.55 |
| 23:DA:399:G:C2' | 23:DA:400:G:H5' | 2.36 | 0.55 |
| 23:BA:1757:U:H2' | 23:BA:1758:G:OP1 | 2.07 | 0.55 |
| 23:BA:1445:C:C2 | 23:BA:1446:C:C5 | 2.95 | 0.55 |
| 33:BK:26:LYS:O | 33:BK:27:GLY:O | 2.24 | 0.55 |
| 14:AN:17:LYS:C | 14:AN:19:ARG:H | 2.10 | 0.55 |
| 1:CA:1089:G:C5 | 1:CA:1090:U:C5 | 2.94 | 0.55 |
| 1:AA:118:U:O4 | 1:AA:288:A:H2' | 2.07 | 0.55 |
| 35:DM:137:TYR:HB3 | 44:DV:76:LEU:HD21 | 1.89 | 0.55 |
| 7:CG:74:GLU:O | 7:CG:88:PRO:HA | 2.07 | 0.55 |
| 2:CB:75:LYS:C | 2:CB:75:LYS:HD3 | 2.27 | 0.55 |
| 27:DE:28:ILE:O | 27:DE:28:ILE:HG13 | 2.07 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DA:1275:A:C4 | 36:DN:16:HIS:CE1 | 2.95 | 0.55 |
| 23:BA:1175:U:H2' | 23:BA:1176:G:H8 | 1.72 | 0.55 |
| 32:BJ:143:LEU:O | 32:BJ:144:LYS:HD2 | 2.06 | 0.55 |
| 23:DA:83:G:C4 | 23:DA:102:G:N2 | 2.75 | 0.55 |
| 43:DU:15:VAL:HG13 | 43:DU:17:SER:HB3 | 1.88 | 0.55 |
| 2:AB:163:PHE:CD1 | 2:AB:185:ILE:HG13 | 2.41 | 0.55 |
| 1:CA:1346:A:H61 | 1:CA:1374:A:H3' | 1.72 | 0.55 |
| 1:CA:1369:C:OP1 | 9:CI:111:ARG:HG3 | 2.07 | 0.55 |
| 25:BC:15:PHE:O | 25:BC:205:VAL:HG11 | 2.07 | 0.55 |
| 1:CA:1316:G:N2 | 1:CA:1319:A:OP2 | 2.39 | 0.55 |
| 12:CL:116:ARG:O | 12:CL:119:TYR:N | 2.35 | 0.55 |
| 3:AC:18:TRP:HD1 | 14:AN:54:PRO:HA | 1.72 | 0.55 |
| 23:BA:666:G:H5'' | 34:BL:47:ASP:O | 2.07 | 0.55 |
| 25:DC:108:PRO:HG3 | 25:DC:143:HIS:HE1 | 1.72 | 0.55 |
| 25:BC:76:PRO:CB | 25:BC:116:GLN:HE21 | 2.19 | 0.55 |
| 1:CA:392:G:C4 | 1:CA:393:A:C8 | 2.95 | 0.55 |
| 4:CD:111:ALA:HB1 | 4:CD:116:GLN:OE1 | 2.07 | 0.55 |
| 47:BY:53:LEU:O | 47:BY:57:ILE:HG13 | 2.07 | 0.55 |
| 24:DB:40:U:O2' | 24:DB:41:U:H5' | 2.06 | 0.55 |
| 1:CA:92:G:C2' | 1:CA:93:U:H5' | 2.37 | 0.55 |
| 1:AA:92:G:C6 | 1:AA:93:U:C2 | 2.95 | 0.55 |
| 24:BB:71:C:C2 | 24:BB:72:G:C8 | 2.95 | 0.55 |
| 44:BV:3:TYR:CD1 | 44:BV:3:TYR:N | 2.74 | 0.55 |
| 23:DA:1607:C:N4 | 23:DA:1621:U:H3' | 2.22 | 0.55 |
| 23:BA:932:G:H4' | 23:BA:933:A:O5' | 2.06 | 0.55 |
| 1:AA:187:C:O2 | 1:AA:191(A):G:C6 | 2.60 | 0.55 |
| 1:CA:1309:G:C6 | 1:CA:1329:A:C2 | 2.95 | 0.55 |
| 1:AA:1375:A:C2 | 1:AA:1376:U:C2 | 2.95 | 0.55 |
| 26:BD:111:ARG:CD | 26:BD:160:TYR:HE1 | 2.15 | 0.55 |
| 46:BX:10:LYS:O | 46:BX:11:ARG:CB | 2.55 | 0.55 |
| 46:BX:11:ARG:NH1 | 46:BX:61:ARG:N | 2.55 | 0.55 |
| 23:BA:1487:G:N3 | 23:BA:1488:G:C8 | 2.74 | 0.55 |
| 1:CA:623:C:H6 | 1:CA:623:C:O5' | 1.89 | 0.55 |
| 42:DT:23:GLU:HG3 | 42:DT:24:GLY:H | 1.72 | 0.55 |
| 33:DK:35:VAL:HG11 | 33:DK:103:ALA:HB3 | 1.87 | 0.55 |
| 9:CI:17:VAL:HG21 | 9:CI:80:GLY:HA3 | 1.88 | 0.55 |
| 8:CH:31:PHE:O | 8:CH:35:ILE:HG12 | 2.07 | 0.55 |
| 44:BV:24:LEU:HB3 | 44:BV:41:LEU:HG | 1.88 | 0.55 |
| 25:DC:131:LEU:HD11 | 25:DC:136:ILE:HG13 | 1.88 | 0.55 |
| 20:AT:13:LEU:HD12 | 20:AT:13:LEU:N | 2.21 | 0.55 |
| 7:CG:40:ALA:O | 7:CG:44:TYR:HD1 | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BA:481:G:OP1 | 23:BA:481:G:H4' | 2.06 | 0.55 |
| 12:AL:78:GLU:O | 12:AL:79:HIS:CG | 2.60 | 0.55 |
| 1:AA:927:G:C2 | 1:AA:1391:U:O2 | 2.60 | 0.55 |
| 36:DN:79:LEU:HD23 | 36:DN:83:ILE:HG13 | 1.89 | 0.55 |
| 23:DA:2854:G:H2' | 23:DA:2855:C:H6 | 1.71 | 0.55 |
| 7:CG:67:GLU:OE1 | 7:CG:70:LYS:HD2 | 2.06 | 0.55 |
| 1:AA:636:U:H5' | 17:AQ:2:PRO:HG3 | 1.88 | 0.55 |
| 47:DY:36:ARG:HA | 47:DY:39:ALA:HB3 | 1.89 | 0.55 |
| 23:DA:2038:G:C5 | 23:DA:2039:C:C5 | 2.94 | 0.55 |
| 23:DA:231:C:N4 | 23:DA:232:G:N1 | 2.55 | 0.55 |
| 23:DA:263:C:H2' | 23:DA:264:C:O4' | 2.07 | 0.55 |
| 18:CR:53:ARG:C | 18:CR:55:ARG:H | 2.11 | 0.55 |
| 23:DA:2771:C:H2' | 23:DA:2771:C:O2 | 2.07 | 0.55 |
| 2:CB:52:GLU:O | 2:CB:56:ARG:HG3 | 2.06 | 0.55 |
| 1:CA:1047:G:C2' | 1:CA:1048:G:H5' | 2.37 | 0.55 |
| 11:CK:123:LYS:O | 11:CK:126:ARG:HB2 | 2.07 | 0.55 |
| 40:BR:1:MET:H2 | 40:BR:16:PRO:HD3 | 1.72 | 0.55 |
| 18:AR:36:ASN:HB2 | 18:AR:39:VAL:HG23 | 1.87 | 0.55 |
| 34:BL:135:LEU:HD13 | 34:BL:139:LYS:HB2 | 1.89 | 0.55 |
| 34:DL:125:VAL:O | 34:DL:145:PRO:HD2 | 2.06 | 0.54 |
| 24:BB:83:G:C2 | 24:BB:84:C:C6 | 2.95 | 0.54 |
| 24:BB:84:C:H2' | 24:BB:84:C:O2 | 2.06 | 0.54 |
| 22:CV:6181:C:O2' | 22:CV:6182:A:H8 | 1.89 | 0.54 |
| 23:DA:2846:G:OP2 | 38:DP:54:ARG:HB2 | 2.07 | 0.54 |
| 38:DP:56:GLY:O | 38:DP:59:THR:CG2 | 2.50 | 0.54 |
| 23:DA:587:C:N4 | 34:DL:33:ARG:HB2 | 2.22 | 0.54 |
| 23:BA:1022:G:H22 | 23:BA:114(B):A:H2 | 1.54 | 0.54 |
| 40:DR:52:VAL:HG13 | 40:DR:55:ALA:HB3 | 1.89 | 0.54 |
| 41:DS:14:PRO:O | 41:DS:16:LYS:N | 2.39 | 0.54 |
| 39:BQ:92:ARG:HD2 | 39:BQ:95:LEU:H | 1.72 | 0.54 |
| 3:AC:182:ILE:HG12 | 3:AC:203:PHE:CA | 2.29 | 0.54 |
| 42:DT:14:SER:O | 42:DT:17:ALA:N | 2.39 | 0.54 |
| 3:CC:130:VAL:CG1 | 3:CC:153:VAL:HG21 | 2.37 | 0.54 |
| 24:DB:73:A:C4 | 24:DB:74:U:C6 | 2.95 | 0.54 |
| 37:DO:69:VAL:O | 37:DO:72:ALA:CB | 2.52 | 0.54 |
| 41:DS:24:ILE:HG21 | 41:DS:36:LEU:CD2 | 2.37 | 0.54 |
| 23:DA:2219:G:C2' | 23:DA:2224:G:C5' | 2.81 | 0.54 |
| 1:AA:1309:G:C6 | 1:AA:1329:A:C2 | 2.95 | 0.54 |
| 33:DK:97:ARG:H | 33:DK:117:LEU:HD22 | 1.73 | 0.54 |
| 1:AA:748:C:H4' | 1:AA:749:C:O5' | 2.07 | 0.54 |
| 1:CA:682:G:C6 | 1:CA:709:G:C6 | 2.95 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DA:9:U:C4 | 23:DA:2629:A:N6 | 2.75 | 0.54 |
| 9:AI:25:LYS:O | 9:AI:60:ASP:HA | 2.07 | 0.54 |
| 1:CA:518:C:C5 | 1:CA:530:G:C4 | 2.95 | 0.54 |
| 23:DA:2476:A:N3 | 23:DA:2476:A:H2' | 2.22 | 0.54 |
| 23:BA:1777:U:C2' | 23:BA:1778:U:H5' | 2.37 | 0.54 |
| 23:BA:628:G:H2' | 23:BA:629:G:C8 | 2.42 | 0.54 |
| 1:AA:648:A:H2' | 1:AA:649:G:C8 | 2.41 | 0.54 |
| 23:DA:2850:A:OP2 | 23:DA:2866:U:C5 | 2.58 | 0.54 |
| 10:CJ:49:VAL:HG21 | 14:CN:41:ARG:HB3 | 1.88 | 0.54 |
| 1:CA:974:A:OP2 | 14:CN:41:ARG:NH1 | 2.40 | 0.54 |
| 1:AA:1333:A:H2' | 1:AA:1334:G:O4' | 2.07 | 0.54 |
| 10:CJ:6:ILE:O | 10:CJ:71:LEU:HD12 | 2.07 | 0.54 |
| 46:DX:70:VAL:O | 46:DX:74:VAL:HG23 | 2.07 | 0.54 |
| 23:DA:1993:U:H4' | 26:DD:128:SER:CB | 2.37 | 0.54 |
| 3:AC:186:PHE:CZ | 3:AC:188:LEU:HD13 | 2.43 | 0.54 |
| 29:BG:118:PRO:O | 29:BG:121:ILE:HG22 | 2.07 | 0.54 |
| 23:BA:2399:G:H2' | 23:BA:2400:G:O4' | 2.07 | 0.54 |
| 3:AC:139:GLN:OE1 | 3:AC:139:GLN:HA | 2.07 | 0.54 |
| 31:DI:14:LYS:HE2 | 31:DI:14:LYS:HA | 1.89 | 0.54 |
| 33:DK:7:TYR:HE1 | 33:DK:20:MET:HE3 | 1.72 | 0.54 |
| 23:DA:2527:C:C4 | 23:DA:2528:U:C5 | 2.95 | 0.54 |
| 26:DD:167:VAL:HG11 | 26:DD:189:PRO:HD3 | 1.88 | 0.54 |
| 1:CA:1371:G:H5'' | 9:CI:69:GLY:H | 1.72 | 0.54 |
| 1:AA:962:C:H42 | 1:AA:973:G:H1 | 1.53 | 0.54 |
| 26:BD:11:MET:HE3 | 26:BD:24:THR:HB | 1.90 | 0.54 |
| 23:BA:1657:C:H2' | 23:BA:1658:C:H6 | 1.72 | 0.54 |
| 39:DQ:105:VAL:HG11 | 40:DR:40:LEU:HD13 | 1.89 | 0.54 |
| 30:BH:88:ILE:HG12 | 30:BH:123:LEU:N | 2.22 | 0.54 |
| 40:BR:2:PHE:HE2 | 40:BR:13:ARG:CD | 2.18 | 0.54 |
| 12:AL:31:PHE:HD2 | 12:AL:85:ARG:HA | 1.72 | 0.54 |
| 35:BM:75:THR:C | 35:BM:88:GLY:HA2 | 2.28 | 0.54 |
| 42:DT:11:PRO:HG2 | 42:DT:13:LEU:HD21 | 1.89 | 0.54 |
| 23:BA:2711:A:OP1 | 23:BA:712(B):A:OP1 | 2.25 | 0.54 |
| 3:AC:130:VAL:O | 3:AC:134:ILE:HG13 | 2.07 | 0.54 |
| 11:CK:59:TYR:CZ | 11:CK:63:LEU:HD11 | 2.42 | 0.54 |
| 1:CA:57:G:C8 | 1:CA:58:C:C5 | 2.95 | 0.54 |
| 38:BP:24:PRO:HA | 38:BP:49:VAL:CG1 | 2.33 | 0.54 |
| 23:BA:2842:G:H1 | 23:BA:2875:C:N4 | 2.05 | 0.54 |
| 8:CH:89:PRO:HA | 8:CH:92:ARG:NH1 | 2.22 | 0.54 |
| 25:BC:136:ILE:HG23 | 25:BC:137:PRO:HD2 | 1.88 | 0.54 |
| 37:BO:65:VAL:O | 37:BO:69:VAL:HG12 | 2.06 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:724:G:C2 | 1:AA:725:G:C8 | 2.95 | 0.54 |
| 1:AA:99:C:C2 | 1:AA:101:A:C8 | 2.95 | 0.54 |
| 23:DA:480:A:OP2 | 43:DU:46:LYS:HE2 | 2.07 | 0.54 |
| 50:D2:52:TYR:C | 50:D2:52:TYR:CD1 | 2.80 | 0.54 |
| 25:BC:148:GLU:HB2 | 25:BC:151:LYS:HD2 | 1.89 | 0.54 |
| 38:DP:105:LEU:O | 38:DP:107:ASP:CG | 2.46 | 0.54 |
| 23:DA:1963:U:C2' | 23:DA:1963:U:O2 | 2.54 | 0.54 |
| 23:BA:1348:G:C2' | 23:BA:1349:A:H5'' | 2.35 | 0.54 |
| 44:DV:24:LEU:O | 44:DV:24:LEU:HG | 2.07 | 0.54 |
| 44:DV:85:HIS:ND1 | 44:DV:85:HIS:C | 2.61 | 0.54 |
| 44:DV:24:LEU:HD11 | 44:DV:85:HIS:HA | 1.90 | 0.54 |
| 23:BA:2346:A:C2 | 23:BA:2383:G:C2 | 2.95 | 0.54 |
| 17:AQ:40:LYS:HG2 | 17:AQ:41:LYS:N | 2.23 | 0.54 |
| 1:AA:579:G:C4 | 1:AA:580:U:C6 | 2.95 | 0.54 |
| 44:BV:37:VAL:O | 44:BV:38:TYR:HB3 | 2.07 | 0.54 |
| 23:BA:2243:U:H2' | 23:BA:2244:U:C6 | 2.42 | 0.54 |
| 23:DA:1449:G:H2' | 23:DA:1450:C:H6 | 1.71 | 0.54 |
| 7:CG:26:PHE:HB2 | 7:CG:62:PHE:HZ | 1.72 | 0.54 |
| 1:AA:1423:G:H2' | 1:AA:1424:C:C6 | 2.42 | 0.54 |
| 23:DA:2023:G:H5' | 23:DA:2617:C:H4' | 1.90 | 0.54 |
| 9:CI:86:VAL:HG23 | 9:CI:93:ARG:HB2 | 1.90 | 0.54 |
| 23:BA:1638:C:H4' | 23:BA:2710:C:O2 | 2.07 | 0.54 |
| 3:CC:186:PHE:CZ | 3:CC:188:LEU:HD13 | 2.43 | 0.54 |
| 3:CC:121:ALA:HB1 | 3:CC:188:LEU:O | 2.07 | 0.54 |
| 11:AK:124:LYS:HD2 | 11:AK:125:PHE:HE1 | 1.73 | 0.54 |
| 23:DA:907:U:O2' | 35:DM:101:ARG:NH2 | 2.40 | 0.54 |
| 26:DD:73:GLU:OE2 | 26:DD:74:PRO:HD2 | 2.08 | 0.54 |
| 47:DY:38:GLN:HB3 | 47:DY:44:LEU:O | 2.07 | 0.54 |
| 23:BA:749:C:O2 | 23:BA:1618:A:H2' | 2.07 | 0.54 |
| 1:CA:1296:C:C5 | 1:CA:1297:C:H5 | 2.24 | 0.54 |
| 3:AC:13:GLY:HA3 | 14:AN:57:ARG:HE | 1.70 | 0.54 |
| 32:BJ:112:LYS:O | 32:BJ:116:THR:HG23 | 2.07 | 0.54 |
| 23:DA:993:G:C4 | 23:DA:994:C:C5 | 2.95 | 0.54 |
| 30:BH:88:ILE:HG22 | 30:BH:90:GLY:N | 2.22 | 0.54 |
| 23:BA:994:C:O2' | 23:BA:996:A:OP1 | 2.25 | 0.54 |
| 25:DC:126:GLN:HG2 | 25:DC:127:VAL:N | 2.22 | 0.54 |
| 23:DA:603:A:N1 | 23:DA:655:A:N3 | 2.55 | 0.54 |
| 44:DV:3:TYR:CD1 | 44:DV:3:TYR:N | 2.74 | 0.54 |
| 5:AE:139:LEU:HA | 5:AE:142:LEU:HD12 | 1.89 | 0.54 |
| 1:AA:1068:G:N7 | 1:AA:1094:G:C8 | 2.75 | 0.54 |
| 48:DZ:26:LEU:HD21 | 48:DZ:46:ASN:CB | 2.37 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:AB:24:TRP:CZ3 | 2:AB:29:ALA:HB2 | 2.42 | 0.54 |
| 46:BX:62:VAL:CG2 | 46:BX:63:ALA:N | 2.70 | 0.54 |
| 40:BR:28:GLU:O | 40:BR:61:VAL:HG21 | 2.07 | 0.54 |
| 42:DT:23:GLU:OE1 | 42:DT:23:GLU:HA | 2.06 | 0.54 |
| 25:DC:133:LEU:HD13 | 25:DC:173:VAL:HG11 | 1.89 | 0.54 |
| 40:BR:58:VAL:HG12 | 40:BR:97:LYS:HB2 | 1.88 | 0.54 |
| 1:CA:712:A:N6 | 1:CA:713:G:C6 | 2.75 | 0.54 |
| 28:DF:133:LEU:HD23 | 28:DF:133:LEU:N | 2.22 | 0.54 |
| 23:BA:784:A:C5 | 25:BC:229:VAL:HG21 | 2.43 | 0.54 |
| 30:BH:7:GLU:CD | 30:BH:8:PRO:HD2 | 2.28 | 0.54 |
| 23:DA:1777:U:C2' | 23:DA:1778:U:H5' | 2.36 | 0.54 |
| 1:AA:564:C:C2 | 17:AQ:31:LEU:HD11 | 2.42 | 0.54 |
| 32:BJ:65:TRP:HA | 32:BJ:71:MET:HE1 | 1.89 | 0.54 |
| 23:DA:1390:U:O2' | 23:DA:1391:U:H5' | 2.06 | 0.54 |
| 23:DA:1388:G:H4' | 23:DA:1525:G:O2' | 2.06 | 0.54 |
| 1:CA:20:U:O2' | 1:CA:21:G:H5' | 2.07 | 0.54 |
| 29:BG:86:GLU:O | 29:BG:86:GLU:HG2 | 2.07 | 0.54 |
| 23:BA:1921:G:O2' | 23:BA:1922:G:H5' | 2.08 | 0.54 |
| 39:BQ:62:ILE:HD12 | 39:BQ:76:TYR:CE1 | 2.42 | 0.54 |
| 23:DA:1845:G:OP1 | 25:DC:258:LYS:HE3 | 2.07 | 0.54 |
| 16:CP:43:LYS:HA | 16:CP:48:TRP:HB3 | 1.88 | 0.54 |
| 23:DA:271(C):G:N7 | 23:DA:421:U:H2' | 2.23 | 0.54 |
| 8:AH:119:LEU:N | 8:AH:119:LEU:HD23 | 2.22 | 0.54 |
| 23:DA:1856:G:H2' | 23:DA:1857:G:O4' | 2.07 | 0.54 |
| 23:DA:1856:G:C2 | 23:DA:1887:C:N3 | 2.76 | 0.54 |
| 23:DA:2364:C:H2' | 23:DA:2365:G:O4' | 2.08 | 0.54 |
| 1:CA:1040:U:H2' | 1:CA:1041:A:H8 | 1.70 | 0.54 |
| 1:AA:20:U:O2' | 1:AA:21:G:H5' | 2.07 | 0.54 |
| 23:BA:1918:A:O2' | 23:BA:1920:C:N4 | 2.40 | 0.54 |
| 48:BZ:23:LEU:CD1 | 48:BZ:23:LEU:N | 2.70 | 0.54 |
| 1:AA:1387:G:H2' | 1:AA:1388:C:H6 | 1.71 | 0.54 |
| 23:BA:464:U:H4' | 52:B4:5:TRP:CZ3 | 2.43 | 0.54 |
| 1:AA:1381:U:O2' | 1:AA:1382:C:H5' | 2.07 | 0.54 |
| 2:AB:235:SER:O | 2:AB:239:VAL:HG23 | 2.07 | 0.54 |
| 2:CB:37:ASN:O | 2:CB:39:ILE:HD12 | 2.07 | 0.54 |
| 23:BA:1115:G:O2' | 23:BA:1116:C:H5' | 2.07 | 0.54 |
| 23:BA:1762:A:O5' | 23:BA:1762:A:H8 | 1.91 | 0.54 |
| 26:DD:114:ALA:O | 26:DD:157:ALA:HB1 | 2.06 | 0.54 |
| 23:BA:2079:U:H2' | 23:BA:2080:G:O5' | 2.06 | 0.54 |
| 1:AA:258:G:H2' | 1:AA:259:G:H8 | 1.72 | 0.54 |
| 53:D5:22:VAL:CG1 | 53:D5:50:LEU:HD12 | 2.37 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1366:C:C4 | 1:CA:1367:C:C4 | 2.96 | 0.54 |
| 34:BL:32:THR:HB | 34:BL:36:LYS:HB2 | 1.89 | 0.54 |
| 23:DA:1257:C:OP1 | 27:DE:72:ARG:NH1 | 2.40 | 0.54 |
| 2:CB:154:LEU:HD13 | 2:CB:155:LEU:N | 2.22 | 0.54 |
| 34:DL:49:ARG:O | 34:DL:50:ARG:C | 2.46 | 0.54 |
| 23:DA:114(B):A:C5 | 23:DA:1144:G:C5 | 2.95 | 0.54 |
| 23:BA:195:A:OP1 | 34:BL:46:LYS:HE2 | 2.07 | 0.54 |
| 16:AP:22:THR:HG22 | 16:AP:32:TYR:CB | 2.37 | 0.54 |
| 12:AL:31:PHE:HB3 | 12:AL:84:ILE:O | 2.06 | 0.54 |
| 44:DV:48:PHE:CZ | 44:DV:52:SER:HA | 2.42 | 0.54 |
| 3:AC:36:ASP:OD2 | 3:AC:57:ILE:HG21 | 2.07 | 0.54 |
| 1:AA:17:U:H2' | 1:AA:18:C:C6 | 2.42 | 0.54 |
| 1:AA:1366:C:C4 | 1:AA:1367:C:C4 | 2.95 | 0.54 |
| 1:CA:506:G:C6 | 1:CA:507:C:C4 | 2.95 | 0.54 |
| 23:DA:2330:G:O2' | 45:DW:41:ARG:HB2 | 2.08 | 0.54 |
| 23:BA:1257:C:OP1 | 27:BE:72:ARG:NH1 | 2.40 | 0.54 |
| 1:AA:859:A:H2' | 1:AA:860:A:O4' | 2.07 | 0.54 |
| 23:BA:783:A:C3' | 23:BA:783:A:C8 | 2.89 | 0.54 |
| 23:DA:390:A:C5 | 34:DL:71:VAL:HG21 | 2.43 | 0.54 |
| 4:AD:79:PHE:CZ | 4:AD:204:ILE:HA | 2.43 | 0.54 |
| 23:BA:1670:C:OP2 | 23:BA:2550:G:OP1 | 2.25 | 0.54 |
| 38:DP:1:MET:O | 38:DP:3:ARG:N | 2.41 | 0.54 |
| 26:DD:110:GLY:O | 36:DN:5:LYS:NZ | 2.39 | 0.54 |
| 2:AB:22:LYS:HA | 2:AB:22:LYS:NZ | 2.22 | 0.54 |
| 28:BF:10:LYS:O | 28:BF:14:GLU:HB3 | 2.08 | 0.54 |
| 41:BS:22:ASP:HA | 41:BS:25:ARG:NH1 | 2.21 | 0.54 |
| 23:DA:176:G:O2' | 23:DA:177:G:H5' | 2.07 | 0.54 |
| 35:BM:69:PHE:CD1 | 35:BM:70:PRO:HD2 | 2.42 | 0.54 |
| 23:DA:1451:C:H42 | 23:DA:1459:G:H1 | 1.56 | 0.54 |
| 23:DA:2572:A:H2' | 26:DD:144:ARG:HG3 | 1.89 | 0.54 |
| 1:CA:667:G:H4' | 15:CO:51:HIS:ND1 | 2.22 | 0.54 |
| 23:BA:914:C:H5 | 23:BA:915:C:C6 | 2.25 | 0.54 |
| 23:DA:611:C:C2 | 23:DA:612:G:C8 | 2.95 | 0.54 |
| 36:DN:14:SER:O | 36:DN:15:SER:C | 2.44 | 0.54 |
| 24:DB:35:U:O2' | 24:DB:36:C:H5' | 2.08 | 0.54 |
| 2:CB:96:ARG:H | 2:CB:96:ARG:HD2 | 1.72 | 0.54 |
| 3:AC:12:LEU:O | 3:AC:12:LEU:HD13 | 2.06 | 0.54 |
| 23:DA:544:C:H6 | 23:DA:544:C:O5' | 1.90 | 0.54 |
| 1:AA:285:G:O2' | 1:AA:286:G:H5' | 2.08 | 0.54 |
| 23:BA:1268:A:C2' | 23:BA:1269:A:O5' | 2.56 | 0.54 |
| 1:CA:1366:C:H2' | 1:CA:1367:C:C6 | 2.42 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:946:A:H2' | 1:CA:947:G:H8 | 1.72 | 0.54 |
| 25:BC:108:PRO:HG3 | 25:BC:143:HIS:HE1 | 1.73 | 0.54 |
| 16:AP:21:VAL:HG23 | 16:AP:33:ILE:HB | 1.90 | 0.54 |
| 4:AD:9:CYS:SG | 4:AD:31:CYS:O | 2.66 | 0.54 |
| 23:DA:125:G:OP2 | 52:D4:19:ARG:NH1 | 2.40 | 0.54 |
| 23:BA:1813:G:O2' | 25:BC:50:THR:HG21 | 2.07 | 0.54 |
| 24:DB:46:A:H2' | 24:DB:47:C:C6 | 2.43 | 0.54 |
| 44:DV:33:LEU:HD23 | 44:DV:90:VAL:HG21 | 1.89 | 0.54 |
| 1:AA:392:G:C4 | 1:AA:393:A:C8 | 2.95 | 0.54 |
| 5:AE:10:MET:HG3 | 5:AE:13:ILE:HD11 | 1.90 | 0.54 |
| 1:CA:1309:G:H22 | 1:CA:1329:A:H1' | 1.72 | 0.54 |
| 41:DS:23:LEU:HD22 | 50:D2:25:LEU:HD13 | 1.88 | 0.54 |
| 1:CA:332:G:O2' | 1:CA:333:G:H5' | 2.07 | 0.54 |
| 29:DG:46:GLU:O | 29:DG:49:VAL:HG22 | 2.08 | 0.54 |
| 23:DA:2894:G:H2' | 23:DA:2894:G:N3 | 2.22 | 0.54 |
| 23:DA:1953:A:H2 | 23:DA:2549:G:N3 | 2.04 | 0.54 |
| 53:B5:57:ARG:CZ | 53:B5:57:ARG:CA | 2.84 | 0.54 |
| 18:AR:56:THR:HB | 18:AR:58:LEU:CD1 | 2.38 | 0.54 |
| 25:BC:25:THR:HG22 | 25:BC:82:ILE:H | 1.73 | 0.54 |
| 1:CA:1179:A:H2' | 1:CA:1180:A:O4' | 2.07 | 0.54 |
| 43:BU:47:LYS:HA | 43:BU:60:PHE:CZ | 2.42 | 0.54 |
| 38:DP:27:THR:HG22 | 38:DP:90:GLN:HB3 | 1.89 | 0.54 |
| 23:DA:334:C:O2' | 23:DA:335:C:P | 2.66 | 0.54 |
| 1:AA:1357:A:C6 | 1:AA:1358:U:N3 | 2.75 | 0.54 |
| 35:BM:38:GLU:HB2 | 35:BM:127:ILE:CG1 | 2.38 | 0.54 |
| 23:DA:1414:G:C4 | 23:DA:1415:U:C5 | 2.96 | 0.54 |
| 36:BN:93:GLY:O | 36:BN:117:VAL:HG11 | 2.07 | 0.54 |
| 1:AA:518:C:C5 | 1:AA:530:G:C4 | 2.96 | 0.54 |
| 1:CA:565:U:C6 | 1:CA:566:G:C8 | 2.95 | 0.54 |
| 8:CH:38:ILE:HD11 | 8:CH:118:VAL:O | 2.07 | 0.54 |
| 1:CA:160:A:H4' | 1:CA:344:A:C6 | 2.43 | 0.54 |
| 6:AF:12:PRO:HG3 | 6:AF:57:GLN:O | 2.08 | 0.54 |
| 23:BA:1231:G:O2' | 23:BA:1232:G:H5' | 2.08 | 0.54 |
| 1:AA:1262:C:OP2 | 21:AU:25:LYS:HD3 | 2.08 | 0.54 |
| 1:CA:356:A:H2' | 1:CA:357:G:C8 | 2.43 | 0.54 |
| 19:CS:53:ASN:HD22 | 19:CS:55:LYS:H | 1.53 | 0.54 |
| 23:BA:399:G:C2' | 23:BA:400:G:H5' | 2.38 | 0.54 |
| 23:BA:1027:A:C2 | 23:BA:2488:A:H5' | 2.43 | 0.54 |
| 1:AA:356:A:O2' | 1:AA:357:G:H5' | 2.08 | 0.54 |
| 23:BA:898:C:H2' | 23:BA:899:A:O4' | 2.07 | 0.54 |
| 23:BA:2097:C:C2' | 23:BA:2098:U:H5' | 2.37 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:DA:2098:U:O2' | 23:DA:2099:U:O5' | 2.24 | 0.54 |
| 1:CA:1516:G:H2' | 1:CA:1518:A:OP2 | 2.07 | 0.54 |
| 23:BA:263:C:H2' | 23:BA:264:C:O4' | 2.07 | 0.54 |
| 34:DL:30:THR:HG22 | 34:DL:31:ALA:N | 2.22 | 0.54 |
| 1:CA:127:G:C2 | 1:CA:128:G:C8 | 2.96 | 0.54 |
| 1:CA:1217:C:H5'' | 14:CN:9:LYS:HZ1 | 1.72 | 0.54 |
| 1:CA:744:C:H3' | 1:CA:744:C:C6 | 2.42 | 0.54 |
| 3:CC:16:ARG:NH1 | 3:CC:16:ARG:HB2 | 2.22 | 0.54 |
| 42:BT:75:ASP:O | 42:BT:76:ARG:HG3 | 2.07 | 0.54 |
| 2:AB:154:LEU:HD13 | 2:AB:155:LEU:N | 2.23 | 0.54 |
| 2:AB:70:PHE:O | 2:AB:71:VAL:HG13 | 2.07 | 0.54 |
| 34:BL:33:ARG:CB | 34:BL:36:LYS:HD3 | 2.38 | 0.54 |
| 12:CL:31:PHE:HB3 | 12:CL:84:ILE:O | 2.08 | 0.54 |
| 39:BQ:88:ILE:HG22 | 40:BR:47:VAL:O | 2.07 | 0.54 |
| 1:AA:386:C:C3' | 1:AA:387:U:H5'' | 2.37 | 0.54 |
| 46:DX:10:LYS:O | 46:DX:11:ARG:CG | 2.55 | 0.54 |
| 40:DR:61:VAL:O | 40:DR:61:VAL:HG23 | 2.07 | 0.54 |
| 2:CB:8:LYS:HG2 | 2:CB:217:ARG:NH1 | 2.22 | 0.54 |
| 11:AK:20:TYR:O | 11:AK:30:VAL:HA | 2.08 | 0.54 |
| 1:CA:592:G:C2 | 1:CA:593:G:N7 | 2.75 | 0.54 |
| 12:AL:23:VAL:HG12 | 12:AL:23:VAL:O | 2.06 | 0.54 |
| 3:AC:86:VAL:O | 3:AC:90:GLU:HG2 | 2.07 | 0.54 |
| 3:AC:150:LYS:O | 3:AC:200:ALA:HA | 2.07 | 0.54 |
| 23:BA:1746:G:C2 | 23:BA:1747:G:N7 | 2.76 | 0.54 |
| 7:AG:40:ALA:O | 7:AG:44:TYR:HD1 | 1.90 | 0.54 |
| 14:AN:43:CYS:SG | 14:AN:44:LEU:N | 2.81 | 0.54 |
| 23:BA:573:G:O2' | 23:BA:574:C:H3' | 2.07 | 0.54 |
| 23:DA:205:G:HO2' | 23:DA:206:U:P | 2.28 | 0.54 |
| 53:D5:29:LYS:HB2 | 53:D5:44:LYS:HB3 | 1.89 | 0.54 |
| 24:DB:28:C:H2' | 24:DB:29:A:O4' | 2.08 | 0.54 |
| 33:DK:60:ALA:HB2 | 33:DK:86:ILE:HA | 1.87 | 0.54 |
| 23:DA:1015:G:C2' | 23:DA:1016:G:H5' | 2.37 | 0.54 |
| 1:CA:439:A:H2' | 1:CA:440:A:H5' | 1.89 | 0.54 |
| 1:AA:1389:C:H2' | 1:AA:1390:U:O4' | 2.08 | 0.54 |
| 23:BA:57:C:H2' | 23:BA:58:G:O4' | 2.08 | 0.54 |
| 27:DE:126:VAL:O | 27:DE:196:LEU:HG | 2.07 | 0.54 |
| 3:AC:111:LEU:HD23 | 3:AC:146:ALA:HB2 | 1.89 | 0.54 |
| 30:DH:12:LEU:HD22 | 30:DH:12:LEU:N | 2.23 | 0.54 |
| 8:CH:123:GLU:O | 8:CH:127:LEU:HB2 | 2.08 | 0.54 |
| 45:BW:27:GLU:HB2 | 45:BW:69:PHE:HD1 | 1.72 | 0.54 |
| 1:AA:1305:G:C8 | 1:AA:1305:G:OP2 | 2.61 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 43:BU:8:LYS:HZ3 | 43:BU:8:LYS:C | 2.09 | 0.54 |
| 26:DD:24:THR:HG21 | 26:DD:188:VAL:CG1 | 2.38 | 0.54 |
| 23:DA:858:U:C2 | 23:DA:2268:A:C2 | 2.95 | 0.54 |
| 23:DA:307:G:N1 | 23:DA:310:A:OP2 | 2.41 | 0.54 |
| 43:DU:68:HIS:O | 43:DU:70:SER:N | 2.41 | 0.54 |
| 2:AB:181:PHE:O | 2:AB:183:PRO:HD3 | 2.07 | 0.54 |
| 7:AG:113:GLU:CB | 7:AG:119:ARG:HG2 | 2.23 | 0.54 |
| 23:DA:806:C:OP2 | 34:DL:39:LYS:HD3 | 2.08 | 0.54 |
| 38:BP:56:GLY:C | 38:BP:57:PHE:O | 2.45 | 0.54 |
| 25:BC:126:GLN:HG2 | 25:BC:127:VAL:N | 2.22 | 0.54 |
| 1:CA:386:C:C3' | 1:CA:387:U:H5'' | 2.37 | 0.54 |
| 23:DA:1266:G:C6 | 41:DS:16:LYS:HD2 | 2.43 | 0.54 |
| 1:AA:328:C:H4' | 1:AA:329:A:H5' | 1.88 | 0.54 |
| 28:BF:40:ASN:O | 28:BF:155:MET:HB2 | 2.08 | 0.54 |
| 23:DA:140:A:C8 | 23:DA:1408:C:O2' | 2.55 | 0.54 |
| 5:CE:110:LEU:O | 5:CE:113:ALA:HB3 | 2.08 | 0.54 |
| 1:CA:199:G:H1 | 1:CA:218:C:N4 | 1.98 | 0.54 |
| 43:DU:81:LYS:CD | 43:DU:96:ILE:HG13 | 2.37 | 0.54 |
| 1:AA:10:A:H2' | 1:AA:11:G:C8 | 2.42 | 0.54 |
| 1:AA:11:G:C5 | 1:AA:12:U:C5 | 2.95 | 0.54 |
| 1:AA:1292:U:C2 | 1:AA:1293:G:C8 | 2.96 | 0.54 |
| 23:DA:752:A:H3' | 52:D4:1:MET:CE | 2.37 | 0.54 |
| 1:CA:616:G:H1' | 1:CA:625:G:N2 | 2.22 | 0.54 |
| 23:DA:7:G:N2 | 23:DA:2897:U:C4 | 2.76 | 0.54 |
| 10:CJ:34:VAL:HG13 | 10:CJ:74:ILE:HG22 | 1.90 | 0.54 |
| 23:BA:1568:G:OP2 | 25:BC:63:ARG:NH2 | 2.38 | 0.54 |
| 44:DV:44:PHE:CE2 | 44:DV:86:VAL:HG11 | 2.43 | 0.54 |
| 4:AD:4:TYR:HE1 | 4:AD:11:LEU:HD11 | 1.72 | 0.54 |
| 23:DA:2432:A:H2' | 23:DA:2433:A:C8 | 2.43 | 0.54 |
| 23:BA:752:A:H3' | 52:B4:1:MET:CE | 2.37 | 0.54 |
| 1:AA:1429:C:H2' | 1:AA:1430:C:C6 | 2.43 | 0.54 |
| 23:DA:2705:A:C2 | 36:DN:64:ARG:NH1 | 2.76 | 0.54 |
| 1:AA:716:A:N3 | 11:AK:118:GLY:HA2 | 2.23 | 0.54 |
| 23:BA:185:U:H2' | 23:BA:186:G:H8 | 1.73 | 0.54 |
| 23:DA:880:G:H2' | 23:DA:881:G:H8 | 1.72 | 0.54 |
| 24:DB:116:G:H4' | 37:DO:55:ALA:O | 2.07 | 0.54 |
| 23:BA:1241:A:N6 | 23:BA:1242:A:C6 | 2.76 | 0.54 |
| 5:CE:103:GLY:O | 5:CE:104:ALA:C | 2.46 | 0.54 |
| 23:DA:430:G:H5'' | 23:DA:431:U:OP2 | 2.08 | 0.54 |
| 27:BE:150:GLY:HA2 | 27:BE:172:TRP:CD2 | 2.41 | 0.54 |
| 19:CS:40:ILE:HD13 | 19:CS:62:ILE:HD11 | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:AI:83:ARG:HA | 9:AI:86:VAL:HG12 | 1.88 | 0.54 |
| 9:AI:85:LEU:O | 9:AI:89:ASN:HB2 | 2.07 | 0.54 |
| 23:BA:2607:G:H2' | 23:BA:2608:G:O4' | 2.06 | 0.54 |
| 23:DA:1465:G:C2 | 23:DA:1466:G:C8 | 2.96 | 0.54 |
| 1:CA:497:U:O2 | 1:CA:497:U:H2' | 2.07 | 0.54 |
| 3:CC:12:LEU:HD13 | 3:CC:12:LEU:O | 2.08 | 0.54 |
| 25:BC:210:GLY:HA2 | 25:BC:213:ARG:HG3 | 1.89 | 0.54 |
| 23:DA:2419:U:O4 | 53:D5:30:ARG:NH1 | 2.40 | 0.54 |
| 10:AJ:63:PHE:HB3 | 14:AN:57:ARG:O | 2.08 | 0.54 |
| 23:BA:1543:A:C8 | 23:BA:1545:A:H5'' | 2.42 | 0.54 |
| 22:AV:6213:A:C6 | 22:AV:6214:C:N4 | 2.76 | 0.54 |
| 10:CJ:62:HIS:O | 14:CN:59:ALA:HB3 | 2.08 | 0.54 |
| 12:CL:31:PHE:HD2 | 12:CL:85:ARG:HA | 1.71 | 0.54 |
| 23:BA:1022:G:H8 | 32:BJ:92:GLN:NE2 | 2.05 | 0.54 |
| 23:BA:1141:U:H4' | 23:BA:114(B):A:O4' | 2.06 | 0.54 |
| 23:BA:2579:C:O4' | 26:BD:134:ILE:HG12 | 2.08 | 0.54 |
| 36:BN:107:ASP:OD2 | 36:BN:107:ASP:C | 2.44 | 0.54 |
| 23:BA:1414:G:C4 | 23:BA:1415:U:C5 | 2.96 | 0.54 |
| 25:DC:246:PRO:HD2 | 25:DC:255:LYS:HB3 | 1.90 | 0.54 |
| 44:DV:97:GLU:HB3 | 44:DV:125:LEU:HD21 | 1.89 | 0.54 |
| 5:CE:111:GLU:C | 5:CE:113:ALA:H | 2.12 | 0.54 |
| 1:AA:191(F):U:H2' | 1:AA:191(G):G:H8 | 1.72 | 0.54 |
| 25:DC:86:PRO:HD2 | 25:DC:87:ASN:ND2 | 2.23 | 0.54 |
| 4:AD:129:ASN:N | 4:AD:129:ASN:OD1 | 2.41 | 0.54 |
| 41:BS:29:LEU:HD21 | 41:BS:33:ARG:HH21 | 1.73 | 0.54 |
| 23:BA:528:A:OP2 | 32:BJ:134:PRO:HB3 | 2.08 | 0.54 |
| 12:AL:52:ARG:NH1 | 12:AL:52:ARG:CG | 2.61 | 0.54 |
| 29:BG:84:SER:CA | 29:BG:133:VAL:O | 2.53 | 0.54 |
| 23:BA:2894:G:H2' | 23:BA:2894:G:N3 | 2.23 | 0.54 |
| 23:BA:1496:A:N7 | 23:BA:1498:C:N3 | 2.55 | 0.54 |
| 2:CB:24:TRP:CZ3 | 2:CB:29:ALA:HB2 | 2.42 | 0.54 |
| 1:AA:832:C:N4 | 1:AA:855:G:C6 | 2.76 | 0.54 |
| 23:DA:2562:U:H2' | 23:DA:2563:U:H5' | 1.89 | 0.54 |
| 23:BA:81:G:H21 | 43:BU:2:ARG:NH2 | 2.05 | 0.54 |
| 17:CQ:4:LYS:HG3 | 17:CQ:5:VAL:N | 2.22 | 0.54 |
| 26:DD:117:MET:HE1 | 26:DD:124:GLY:HA3 | 1.89 | 0.54 |
| 13:CM:3:ARG:HG2 | 13:CM:9:ILE:CD1 | 2.37 | 0.54 |
| 44:DV:179:ASP:CG | 44:DV:180:VAL:HG13 | 2.27 | 0.54 |
| 50:D2:40:LYS:CD | 50:D2:46:CYS:HB3 | 2.38 | 0.54 |
| 23:DA:1478:G:O2' | 23:DA:1558:A:H2 | 1.91 | 0.54 |
| 44:DV:74:VAL:HG22 | 44:DV:86:VAL:HG13 | 1.88 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 45:DW:51:VAL:HG21 | 45:DW:80:HIS:HA | 1.89 | 0.54 |
| 1:CA:728:A:H2' | 1:CA:729:A:C8 | 2.43 | 0.54 |
| 1:AA:546:G:P | 4:AD:72:GLU:HB2 | 2.47 | 0.54 |
| 3:AC:175:LEU:HD11 | 3:AC:201:TYR:HE2 | 1.72 | 0.54 |
| 15:AO:24:SER:O | 15:AO:28:GLN:HG3 | 2.07 | 0.54 |
| 23:BA:1726:G:C2 | 23:BA:1735:U:O2 | 2.61 | 0.54 |
| 19:AS:53:ASN:HD22 | 19:AS:55:LYS:H | 1.54 | 0.54 |
| 7:AG:26:PHE:HB2 | 7:AG:62:PHE:HZ | 1.73 | 0.54 |
| 1:AA:145:G:C2 | 1:AA:178:C:N3 | 2.76 | 0.54 |
| 23:BA:1204:A:N1 | 23:BA:1241:A:C2 | 2.75 | 0.54 |
| 23:DA:2038:G:H2' | 23:DA:2039:C:H6 | 1.72 | 0.54 |
| 1:CA:258:G:H2' | 1:CA:259:G:H8 | 1.73 | 0.54 |
| 48:BZ:10:LYS:HB3 | 48:BZ:53:LEU:HD23 | 1.89 | 0.54 |
| 36:BN:96:ARG:HD3 | 36:BN:98:LEU:HD21 | 1.90 | 0.54 |
| 23:DA:298:G:OP2 | 43:DU:85:VAL:HG22 | 2.07 | 0.54 |
| 1:CA:270:A:C6 | 1:CA:271:C:C4 | 2.95 | 0.54 |
| 23:BA:1403:C:H5'' | 23:BA:1471:A:H1' | 1.90 | 0.54 |
| 27:DE:93:LYS:HB3 | 27:DE:94:PRO:HD2 | 1.89 | 0.54 |
| 3:CC:139:GLN:HA | 3:CC:139:GLN:OE1 | 2.07 | 0.54 |
| 30:DH:57:ARG:O | 30:DH:57:ARG:HG2 | 2.08 | 0.54 |
| 34:DL:115:LEU:HA | 34:DL:134:ALA:CB | 2.38 | 0.54 |
| 22:CV:6182:A:N1 | 22:CV:6183:G:C4 | 2.75 | 0.54 |
| 1:CA:1364:U:O2' | 1:CA:1365:G:H5' | 2.08 | 0.54 |
| 42:DT:63:LYS:HE3 | 42:DT:72:LYS:HG2 | 1.89 | 0.54 |
| 2:CB:181:PHE:O | 2:CB:183:PRO:HD3 | 2.08 | 0.54 |
| 23:BA:1971:A:C5 | 25:BC:241:PRO:HG3 | 2.43 | 0.54 |
| 39:DQ:102:GLU:HG3 | 40:DR:2:PHE:CE1 | 2.43 | 0.54 |
| 25:DC:34:VAL:O | 25:DC:35:LYS:HD3 | 2.07 | 0.54 |
| 23:DA:748:G:C8 | 23:DA:750:A:C8 | 2.96 | 0.54 |
| 1:CA:376:G:N3 | 1:CA:389:A:C2 | 2.75 | 0.54 |
| 23:DA:2731:G:C6 | 23:DA:2732:G:O6 | 2.61 | 0.54 |
| 47:BY:28:LYS:HG3 | 47:BY:60:LEU:HD12 | 1.90 | 0.54 |
| 23:BA:1407:C:H2' | 23:BA:1408:C:C6 | 2.43 | 0.54 |
| 23:BA:1589:C:O2 | 23:BA:1589:C:H2' | 2.08 | 0.54 |
| 23:BA:1408:C:H42 | 23:BA:1594:G:H1 | 1.55 | 0.54 |
| 4:CD:31:CYS:O | 4:CD:32:ALA:HB3 | 2.08 | 0.54 |
| 1:AA:15:G:H2' | 1:AA:16:A:H8 | 1.71 | 0.54 |
| 4:CD:100:ARG:NH2 | 4:CD:118:ARG:HH12 | 2.03 | 0.54 |
| 10:AJ:13:HIS:CE1 | 10:AJ:14:LYS:HG3 | 2.43 | 0.54 |
| 41:DS:29:LEU:HD22 | 41:DS:69:LEU:HD11 | 1.90 | 0.54 |
| 1:CA:9:G:H2' | 1:CA:10:A:H8 | 1.73 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:CH:9:MET:O | 8:CH:12:ARG:HB2 | 2.08 | 0.54 |
| 1:AA:616:G:H1' | 1:AA:625:G:N2 | 2.23 | 0.54 |
| 1:CA:456:C:N4 | 1:CA:476:G:H1 | 2.06 | 0.54 |
| 38:BP:89:VAL:O | 38:BP:90:GLN:CB | 2.55 | 0.54 |
| 23:BA:282:A:N6 | 23:BA:284:U:C2 | 2.76 | 0.54 |
| 20:AT:11:SER:HA | 20:AT:13:LEU:HD13 | 1.89 | 0.54 |
| 1:CA:862:C:H2' | 1:CA:863:U:C5' | 2.38 | 0.54 |
| 3:CC:150:LYS:O | 3:CC:200:ALA:HA | 2.08 | 0.54 |
| 1:CA:1378:C:H3' | 1:CA:1379:G:H5'' | 1.90 | 0.54 |
| 1:AA:1089:G:C5 | 1:AA:1090:U:C5 | 2.96 | 0.54 |
| 1:CA:414:A:H2' | 1:CA:415:A:C8 | 2.43 | 0.54 |
| 23:BA:2852:G:H2' | 23:BA:2853:C:C6 | 2.43 | 0.54 |
| 1:AA:1428:A:H2' | 1:AA:1429:C:O4' | 2.08 | 0.54 |
| 9:CI:99:LEU:HD12 | 9:CI:101:PHE:CE2 | 2.43 | 0.54 |
| 23:DA:205:G:O2' | 23:DA:206:U:OP2 | 2.19 | 0.54 |
| 26:BD:176:ILE:O | 26:BD:176:ILE:HG22 | 2.06 | 0.54 |
| 41:BS:45:TYR:CD2 | 41:BS:45:TYR:C | 2.81 | 0.54 |
| 5:AE:79:GLU:HB3 | 5:AE:92:LYS:HA | 1.89 | 0.54 |
| 23:DA:1336:A:OP1 | 42:DT:64:LYS:HD3 | 2.08 | 0.54 |
| 1:AA:926:G:C6 | 1:AA:1505:G:C5 | 2.96 | 0.54 |
| 3:CC:125:GLU:OE2 | 3:CC:189:ALA:HA | 2.08 | 0.54 |
| 35:DM:73:PRO:HA | 35:DM:93:TYR:CD2 | 2.43 | 0.54 |
| 3:AC:81:GLY:O | 3:AC:85:ARG:HD3 | 2.08 | 0.54 |
| 39:BQ:47:TYR:C | 39:BQ:47:TYR:CD2 | 2.80 | 0.54 |
| 48:DZ:10:LYS:HB3 | 48:DZ:53:LEU:HD23 | 1.89 | 0.54 |
| 13:AM:14:ARG:HG2 | 13:AM:44:ARG:NH1 | 2.21 | 0.54 |
| 23:DA:2564:A:OP1 | 23:DA:2648:C:H4' | 2.08 | 0.54 |
| 23:DA:433:C:H2' | 23:DA:434:U:C6 | 2.43 | 0.54 |
| 23:BA:482:A:C2 | 23:BA:506:G:C5 | 2.96 | 0.54 |
| 14:CN:12:ARG:HG2 | 14:CN:14:PRO:HD3 | 1.89 | 0.54 |
| 7:AG:49:ILE:HG22 | 7:AG:49:ILE:O | 2.08 | 0.54 |
| 23:BA:2602:A:OP2 | 23:BA:2602:A:H4' | 2.08 | 0.54 |
| 42:DT:4:ALA:C | 42:DT:6:ASP:H | 2.11 | 0.54 |
| 23:BA:1689:A:H62 | 23:BA:1698:A:H2 | 1.56 | 0.54 |
| 2:AB:183:PRO:HA | 2:AB:198:ASP:OD1 | 2.08 | 0.54 |
| 1:CA:1353:G:H8 | 1:CA:1353:G:OP2 | 1.91 | 0.54 |
| 34:DL:33:ARG:CG | 34:DL:34:GLY:N | 2.71 | 0.54 |
| 32:BJ:90:LEU:H | 32:BJ:90:LEU:HD12 | 1.73 | 0.54 |
| 42:BT:71:GLY:C | 42:BT:72:LYS:HG3 | 2.28 | 0.54 |
| 28:BF:86:MET:N | 28:BF:87:PRO:HD3 | 2.23 | 0.54 |
| 25:BC:142:VAL:HG23 | 25:BC:193:VAL:HA | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:BH:68:LEU:C | 30:BH:138:ILE:HD13 | 2.27 | 0.54 |
| 39:BQ:92:ARG:NE | 39:BQ:94:ASN:HB3 | 2.23 | 0.54 |
| 23:BA:253:C:H2' | 23:BA:254:G:O4' | 2.08 | 0.54 |
| 23:BA:1812:A:O2' | 25:BC:45:ASN:HB3 | 2.08 | 0.54 |
| 1:CA:92:G:C6 | 1:CA:93:U:C2 | 2.95 | 0.54 |
| 26:BD:50:GLY:HA2 | 26:BD:78:LEU:HB3 | 1.89 | 0.54 |
| 23:DA:1493:C:O2 | 23:DA:1493:C:H2' | 2.08 | 0.54 |
| 5:CE:41:VAL:HG11 | 5:CE:113:ALA:HB2 | 1.90 | 0.54 |
| 44:BV:102:LEU:HD21 | 44:BV:124:ILE:CD1 | 2.38 | 0.54 |
| 1:AA:17:U:O4' | 1:AA:1080:A:H1' | 2.07 | 0.54 |
| 46:DX:45:ASN:ND2 | 46:DX:47:GLN:HE21 | 2.06 | 0.54 |
| 25:DC:186:HIS:CD2 | 25:DC:188:GLU:HB2 | 2.42 | 0.54 |
| 29:DG:44:VAL:HG12 | 29:DG:45:VAL:N | 2.18 | 0.54 |
| 25:BC:133:LEU:O | 25:BC:135:PHE:N | 2.40 | 0.54 |
| 35:DM:16:ARG:C | 35:DM:17:LEU:HD23 | 2.28 | 0.54 |
| 23:BA:2658:C:H4' | 29:BG:158:HIS:NE2 | 2.23 | 0.54 |
| 1:CA:781:A:H3' | 1:CA:782:A:H5' | 1.91 | 0.54 |
| 23:DA:909:A:C2 | 23:DA:912:C:C6 | 2.96 | 0.54 |
| 43:DU:36:ALA:HA | 43:DU:67:LEU:O | 2.08 | 0.54 |
| 35:BM:21:THR:C | 35:BM:23:GLY:N | 2.60 | 0.54 |
| 1:CA:841:U:C2' | 1:CA:842:C:H5'' | 2.38 | 0.54 |
| 23:DA:2443:C:C2' | 23:DA:2444:G:H5' | 2.38 | 0.54 |
| 33:BK:63:VAL:HB | 33:BK:102:VAL:HG12 | 1.90 | 0.54 |
| 1:CA:1231:G:H2' | 1:CA:1232:U:H6 | 1.72 | 0.54 |
| 23:DA:564:C:O2' | 23:DA:565:C:H5' | 2.08 | 0.54 |
| 23:BA:226:G:C2 | 23:BA:228:A:N6 | 2.76 | 0.54 |
| 3:AC:31:HIS:O | 3:AC:35:GLU:HG2 | 2.08 | 0.54 |
| 1:AA:1513:A:H2' | 1:AA:1514:C:H6 | 1.71 | 0.54 |
| 7:CG:138:LYS:O | 7:CG:142:GLU:HG3 | 2.08 | 0.54 |
| 7:AG:69:VAL:HG12 | 7:AG:69:VAL:O | 2.08 | 0.54 |
| 1:CA:44:G:C2 | 1:CA:399:G:C2 | 2.96 | 0.54 |
| 10:AJ:6:ILE:O | 10:AJ:71:LEU:HD12 | 2.08 | 0.54 |
| 18:CR:84:LYS:HB3 | 18:CR:84:LYS:NZ | 2.23 | 0.54 |
| 23:DA:1403:C:H5'' | 23:DA:1471:A:C1' | 2.37 | 0.54 |
| 1:CA:1167:A:N7 | 1:CA:1169:A:C5 | 2.76 | 0.54 |
| 42:DT:64:LYS:HG2 | 42:DT:65:ARG:HH21 | 1.73 | 0.54 |
| 23:DA:2038:G:C6 | 23:DA:2039:C:C4 | 2.96 | 0.54 |
| 9:CI:24:GLY:O | 9:CI:26:VAL:HG23 | 2.08 | 0.54 |
| 7:AG:38:LEU:O | 7:AG:42:ILE:HG13 | 2.08 | 0.54 |
| 23:BA:1717:G:C6 | 23:BA:1743:G:C6 | 2.96 | 0.54 |
| 1:AA:698:G:C6 | 1:AA:699:C:C4 | 2.96 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:DA:370:G:H4' | 23:DA:371:A:OP2 | 2.08 | 0.54 |
| 11:AK:86:GLY:C | 11:AK:88:GLY:H | 2.11 | 0.54 |
| 29:BG:13:LYS:O | 29:BG:15:VAL:HG13 | 2.08 | 0.54 |
| 31:DI:57:THR:HG23 | 31:DI:60:ARG:HH12 | 1.73 | 0.54 |
| 35:BM:83:MET:O | 35:BM:83:MET:HG3 | 2.08 | 0.54 |
| 41:DS:62:HIS:C | 41:DS:64:MET:H | 2.12 | 0.54 |
| 1:AA:419:C:O2 | 1:AA:425:G:C2 | 2.61 | 0.54 |
| 45:DW:27:GLU:HB2 | 45:DW:69:PHE:HD1 | 1.71 | 0.54 |
| 46:DX:17:SER:HA | 46:DX:44:PRO:HD3 | 1.90 | 0.54 |
| 36:DN:30:THR:HG22 | 36:DN:31:HIS:ND1 | 2.23 | 0.54 |
| 23:DA:627:A:C6 | 23:DA:637:A:C8 | 2.95 | 0.53 |
| 47:BY:3:LEU:O | 47:BY:4:SER:C | 2.47 | 0.53 |
| 26:DD:171:GLU:HG2 | 26:DD:185:LYS:HG2 | 1.90 | 0.53 |
| 26:DD:102:VAL:HA | 26:DD:199:ARG:O | 2.08 | 0.53 |
| 25:DC:208:LYS:HG3 | 25:DC:211:ARG:H | 1.73 | 0.53 |
| 39:DQ:92:ARG:NE | 39:DQ:94:ASN:HB3 | 2.22 | 0.53 |
| 35:DM:88:GLY:C | 35:DM:89:ASN:CG | 2.67 | 0.53 |
| 23:DA:1615:C:C2 | 41:DS:87:PRO:HG2 | 2.43 | 0.53 |
| 39:BQ:92:ARG:HH22 | 40:BR:11:GLN:H | 1.53 | 0.53 |
| 23:DA:2729:G:H2' | 23:DA:2730:C:C6 | 2.43 | 0.53 |
| 3:AC:116:VAL:HG21 | 3:AC:202:ILE:HD11 | 1.90 | 0.53 |
| 4:CD:93:PHE:O | 4:CD:97:LEU:HG | 2.07 | 0.53 |
| 3:CC:29:TYR:HD1 | 3:CC:29:TYR:O | 1.90 | 0.53 |
| 44:BV:94:GLU:HB2 | 44:BV:95:PRO:HD2 | 1.89 | 0.53 |
| 2:AB:97:TRP:CZ2 | 2:AB:102:LEU:HD13 | 2.37 | 0.53 |
| 1:AA:1346:A:H5'' | 9:AI:120:ARG:HH12 | 1.74 | 0.53 |
| 25:BC:186:HIS:CD2 | 25:BC:188:GLU:HB2 | 2.43 | 0.53 |
| 33:BK:103:ALA:HB1 | 33:BK:105:GLU:OE1 | 2.08 | 0.53 |
| 23:DA:1504:C:O2' | 23:DA:1505:C:O5' | 2.26 | 0.53 |
| 23:BA:1329:U:H5'' | 23:BA:1330:C:C5 | 2.40 | 0.53 |
| 1:AA:1118:C:C5' | 9:AI:104:ARG:HG3 | 2.38 | 0.53 |
| 1:AA:101:A:C4 | 1:AA:102:G:C8 | 2.96 | 0.53 |
| 1:AA:620:C:H2' | 1:AA:621:A:O4' | 2.07 | 0.53 |
| 28:DF:111:LEU:HB2 | 28:DF:112:PRO:HD3 | 1.90 | 0.53 |
| 23:BA:2478:A:H2' | 23:BA:2479:G:O4' | 2.07 | 0.53 |
| 27:DE:153:SER:OG | 27:DE:190:GLU:HG3 | 2.08 | 0.53 |
| 23:DA:276:A:N7 | 23:DA:278:A:H8 | 2.06 | 0.53 |
| 1:AA:1207:G:H2' | 1:AA:1208:C:H6 | 1.72 | 0.53 |
| 17:CQ:29:HIS:CE1 | 17:CQ:32:TYR:CD1 | 2.96 | 0.53 |
| 23:BA:1538:G:H2' | 23:BA:1539:G:H8 | 1.73 | 0.53 |
| 7:AG:40:ALA:O | 7:AG:44:TYR:CD1 | 2.60 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DA:492:A:C2' | 23:DA:493:G:H5' | 2.38 | 0.53 |
| 1:AA:160:A:H4' | 1:AA:344:A:C6 | 2.42 | 0.53 |
| 2:CB:22:LYS:NZ | 2:CB:22:LYS:HA | 2.23 | 0.53 |
| 23:DA:2079:U:H2' | 23:DA:2080:G:O5' | 2.09 | 0.53 |
| 23:BA:531:C:H4' | 23:BA:532:A:H5'' | 1.89 | 0.53 |
| 23:DA:444:C:H4' | 27:DE:49:ALA:HB2 | 1.91 | 0.53 |
| 19:CS:25:LYS:HB3 | 19:CS:27:GLU:OE1 | 2.08 | 0.53 |
| 23:BA:2771:C:O2 | 23:BA:2771:C:H2' | 2.07 | 0.53 |
| 23:DA:1356:G:C5 | 23:DA:1357:U:C5 | 2.96 | 0.53 |
| 2:AB:74:LYS:HZ2 | 2:AB:74:LYS:CB | 2.20 | 0.53 |
| 23:BA:89:G:C4 | 23:BA:90:U:C5 | 2.96 | 0.53 |
| 23:DA:2602:A:OP2 | 23:DA:2602:A:H4' | 2.09 | 0.53 |
| 23:BA:1647:G:OP2 | 23:BA:1647:G:H3' | 2.09 | 0.53 |
| 23:DA:2607:G:H2' | 23:DA:2608:G:O4' | 2.08 | 0.53 |
| 35:BM:55:VAL:HG22 | 35:BM:56:ARG:N | 2.23 | 0.53 |
| 53:D5:51:ALA:C | 53:D5:52:LYS:HD3 | 2.29 | 0.53 |
| 34:DL:132:LYS:O | 34:DL:136:GLU:HG2 | 2.08 | 0.53 |
| 23:DA:1529:A:C8 | 23:DA:1530:G:C8 | 2.96 | 0.53 |
| 24:BB:81:G:C5 | 24:BB:82:G:C8 | 2.96 | 0.53 |
| 12:CL:116:ARG:O | 12:CL:118:LYS:N | 2.42 | 0.53 |
| 23:BA:819:A:C4 | 23:BA:1189:A:C2 | 2.95 | 0.53 |
| 23:DA:2338:G:O2' | 23:DA:2339:G:H5' | 2.08 | 0.53 |
| 1:AA:408:A:H2' | 1:AA:409:G:H8 | 1.73 | 0.53 |
| 12:AL:26:LEU:HB3 | 12:AL:29:ALA:CB | 2.38 | 0.53 |
| 25:BC:33:LEU:C | 25:BC:35:LYS:N | 2.61 | 0.53 |
| 42:DT:35:THR:HG22 | 42:DT:36:LYS:N | 2.24 | 0.53 |
| 3:CC:33:LEU:HD21 | 14:CN:53:LEU:CD2 | 2.32 | 0.53 |
| 1:CA:1252:A:O2' | 1:CA:1253:G:H5' | 2.08 | 0.53 |
| 49:B1:51:TYR:O | 49:B1:52:SER:HB2 | 2.07 | 0.53 |
| 23:BA:2352:A:H2' | 23:BA:2353:G:H5' | 1.90 | 0.53 |
| 1:AA:1202:G:H4' | 14:AN:29:ARG:CD | 2.38 | 0.53 |
| 19:AS:40:ILE:HD13 | 19:AS:62:ILE:HD11 | 1.89 | 0.53 |
| 5:AE:126:ARG:NH1 | 5:AE:126:ARG:CG | 2.60 | 0.53 |
| 23:BA:2723:C:OP2 | 26:BD:109:LYS:NZ | 2.40 | 0.53 |
| 29:BG:12:PRO:HB2 | 29:BG:49:VAL:HA | 1.91 | 0.53 |
| 23:DA:1511:A:H2' | 23:DA:1512:G:C8 | 2.42 | 0.53 |
| 25:DC:58:HIS:HD2 | 25:DC:59:LYS:O | 1.91 | 0.53 |
| 41:DS:43:GLY:O | 41:DS:47:VAL:HG23 | 2.07 | 0.53 |
| 52:D4:1:MET:O | 52:D4:2:LYS:C | 2.46 | 0.53 |
| 1:CA:859:A:H2' | 1:CA:860:A:O4' | 2.07 | 0.53 |
| 27:BE:132:VAL:HG23 | 27:BE:133:ASN:N | 2.22 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:CK:20:TYR:O | 11:CK:30:VAL:HA | 2.07 | 0.53 |
| 23:BA:2598:A:C2' | 23:BA:2599:G:O5' | 2.56 | 0.53 |
| 36:DN:99:LYS:HD2 | 36:DN:99:LYS:N | 2.23 | 0.53 |
| 28:BF:111:LEU:HB2 | 28:BF:112:PRO:HD3 | 1.89 | 0.53 |
| 25:DC:131:LEU:HG | 25:DC:136:ILE:HD11 | 1.91 | 0.53 |
| 1:CA:659:U:C2 | 1:CA:660:G:C8 | 2.95 | 0.53 |
| 1:CA:748:C:H4' | 1:CA:749:C:O5' | 2.08 | 0.53 |
| 12:AL:24:PRO:HD2 | 12:AL:97:TYR:OH | 2.08 | 0.53 |
| 1:AA:938:A:C6 | 1:AA:939:G:C5 | 2.96 | 0.53 |
| 45:DW:31:VAL:HG23 | 45:DW:32:ARG:O | 2.07 | 0.53 |
| 16:AP:43:LYS:HG2 | 16:AP:48:TRP:CG | 2.43 | 0.53 |
| 23:BA:988:A:C2' | 23:BA:989:G:O5' | 2.56 | 0.53 |
| 12:CL:74:HIS:HD2 | 12:CL:76:LEU:N | 2.06 | 0.53 |
| 23:DA:1862:G:H2' | 23:DA:1863:G:C8 | 2.41 | 0.53 |
| 38:DP:41:ARG:HB3 | 38:DP:41:ARG:HH11 | 1.73 | 0.53 |
| 23:BA:1025:G:C4 | 23:BA:1135:C:H1' | 2.43 | 0.53 |
| 23:DA:2058:A:C6 | 23:DA:2059:A:N6 | 2.76 | 0.53 |
| 1:CA:814:A:C8 | 1:CA:816:A:C8 | 2.96 | 0.53 |
| 38:DP:81:PRO:C | 38:DP:82:LEU:HD23 | 2.28 | 0.53 |
| 23:BA:49:A:H5'' | 23:BA:51:G:O4' | 2.07 | 0.53 |
| 4:CD:120:LEU:O | 4:CD:125:HIS:HB2 | 2.08 | 0.53 |
| 23:DA:2822:G:H2' | 23:DA:2823:A:H5'' | 1.88 | 0.53 |
| 7:CG:80:VAL:HG23 | 7:CG:83:ALA:HB3 | 1.90 | 0.53 |
| 1:CA:191(G):G:H2' | 1:CA:192:U:H6 | 1.73 | 0.53 |
| 33:DK:9:GLU:OE1 | 33:DK:18:LYS:HE2 | 2.08 | 0.53 |
| 23:DA:833:U:H2' | 23:DA:834:C:C6 | 2.42 | 0.53 |
| 23:BA:2527:C:C4 | 23:BA:2528:U:C5 | 2.96 | 0.53 |
| 12:CL:19:LYS:H | 12:CL:19:LYS:HD3 | 1.74 | 0.53 |
| 29:DG:105:LEU:N | 29:DG:105:LEU:HD23 | 2.23 | 0.53 |
| 34:BL:125:VAL:HG11 | 34:BL:138:LEU:HD22 | 1.89 | 0.53 |
| 34:BL:125:VAL:O | 34:BL:145:PRO:HD2 | 2.09 | 0.53 |
| 23:BA:943:U:OP2 | 34:BL:38:GLN:OE1 | 2.26 | 0.53 |
| 23:BA:2420:C:OP1 | 53:B5:34:TRP:HA | 2.08 | 0.53 |
| 23:BA:2296:U:O2 | 23:BA:2333:A:N3 | 2.42 | 0.53 |
| 39:DQ:79:PHE:HE2 | 39:DQ:106:PHE:CZ | 2.25 | 0.53 |
| 35:DM:89:ASN:O | 35:DM:92:GLY:N | 2.40 | 0.53 |
| 28:DF:25:TYR:OH | 28:DF:32:PRO:HD3 | 2.08 | 0.53 |
| 24:DB:7:G:H5'' | 37:DO:29:PHE:CD2 | 2.43 | 0.53 |
| 16:AP:67:THR:HG22 | 16:AP:68:ASP:N | 2.22 | 0.53 |
| 1:AA:362:G:O3' | 12:AL:32:ARG:NH2 | 2.42 | 0.53 |
| 1:AA:413:G:H21 | 1:AA:428:G:H1' | 1.74 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BA:1209:G:N2 | 23:BA:1210:A:N6 | 2.52 | 0.53 |
| 23:DA:1407:C:H2' | 23:DA:1408:C:C6 | 2.43 | 0.53 |
| 23:BA:275:G:OP2 | 23:BA:363(A):G:N2 | 2.42 | 0.53 |
| 24:BB:73:A:C4 | 24:BB:104:A:C2 | 2.96 | 0.53 |
| 5:AE:41:VAL:CG1 | 5:AE:113:ALA:HA | 2.37 | 0.53 |
| 3:AC:151:VAL:O | 3:AC:152:ILE:HG13 | 2.09 | 0.53 |
| 46:DX:13:ILE:HA | 46:DX:66:HIS:ND1 | 2.23 | 0.53 |
| 18:CR:56:THR:HB | 18:CR:58:LEU:CD1 | 2.38 | 0.53 |
| 46:DX:31:GLY:O | 46:DX:32:LYS:CB | 2.57 | 0.53 |
| 46:BX:27:GLU:HB2 | 46:BX:33:LYS:CA | 2.37 | 0.53 |
| 17:AQ:53:LEU:HD12 | 17:AQ:54:GLY:H | 1.74 | 0.53 |
| 43:DU:2:ARG:N | 43:DU:4:LYS:HZ2 | 2.06 | 0.53 |
| 4:CD:121:VAL:O | 4:CD:134:ASP:HA | 2.08 | 0.53 |
| 23:BA:2592:G:C5 | 23:BA:2593:U:C5 | 2.97 | 0.53 |
| 1:AA:841:U:C2' | 1:AA:842:C:H5'' | 2.38 | 0.53 |
| 23:BA:1389:G:O2' | 23:BA:1390:U:H5' | 2.08 | 0.53 |
| 35:BM:20:ALA:O | 35:BM:21:THR:O | 2.26 | 0.53 |
| 23:DA:1467:C:H42 | 23:DA:1525:G:H1 | 1.55 | 0.53 |
| 1:CA:648:A:H2' | 1:CA:649:G:C8 | 2.43 | 0.53 |
| 1:CA:509:A:C6 | 1:CA:510:A:N1 | 2.77 | 0.53 |
| 23:DA:988:A:H2' | 23:DA:989:G:O5' | 2.08 | 0.53 |
| 12:CL:10:VAL:HG11 | 17:CQ:36:ILE:HG21 | 1.90 | 0.53 |
| 23:BA:575:A:H2' | 23:BA:575:A:N3 | 2.23 | 0.53 |
| 23:BA:2213:U:H5'' | 23:BA:2215:G:OP2 | 2.08 | 0.53 |
| 23:DA:2854:G:H2' | 23:DA:2855:C:C6 | 2.43 | 0.53 |
| 1:CA:145:G:C2 | 1:CA:178:C:N3 | 2.76 | 0.53 |
| 23:BA:2039:C:H2' | 23:BA:2040:C:H6 | 1.72 | 0.53 |
| 1:CA:224:C:C2 | 1:CA:225:C:C5 | 2.97 | 0.53 |
| 8:CH:50:ARG:HG2 | 8:CH:50:ARG:NH1 | 2.23 | 0.53 |
| 1:AA:741:G:H2' | 1:AA:742:G:O4' | 2.08 | 0.53 |
| 1:AA:1296:C:C5 | 1:AA:1297:C:H5 | 2.27 | 0.53 |
| 1:CA:933:G:N7 | 7:CG:3:ARG:NH2 | 2.56 | 0.53 |
| 23:BA:2493:U:C4 | 23:BA:2494:G:C8 | 2.95 | 0.53 |
| 18:CR:36:ASN:HB2 | 18:CR:39:VAL:HG23 | 1.90 | 0.53 |
| 3:AC:119:ARG:O | 3:AC:123:GLN:HG3 | 2.07 | 0.53 |
| 41:DS:52:GLU:OE2 | 41:DS:52:GLU:HA | 2.08 | 0.53 |
| 23:DA:1647:G:H3' | 23:DA:1647:G:OP2 | 2.07 | 0.53 |
| 1:CA:785:G:N2 | 1:CA:798:G:C4 | 2.76 | 0.53 |
| 23:DA:219:G:N3 | 23:DA:234:C:O2' | 2.37 | 0.53 |
| 23:DA:1543:A:H5' | 23:DA:1544:C:P | 2.48 | 0.53 |
| 34:BL:113:LYS:HA | 34:BL:129:ALA:O | 2.08 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 34:BL:80:TYR:CD1 | 34:BL:111:ARG:HB3 | 2.43 | 0.53 |
| 25:BC:11:PRO:O | 25:BC:13:ARG:N | 2.40 | 0.53 |
| 23:BA:1252:G:C2 | 23:BA:1253:A:C2 | 2.96 | 0.53 |
| 23:BA:2338:G:C2' | 23:BA:2339:G:H5' | 2.38 | 0.53 |
| 23:DA:1614:A:H61 | 41:DS:88:ARG:H | 1.56 | 0.53 |
| 24:DB:83:G:C2 | 24:DB:84:C:C6 | 2.96 | 0.53 |
| 53:D5:62:LEU:C | 53:D5:64:TYR:H | 2.12 | 0.53 |
| 23:DA:195:A:H4' | 23:DA:251:A:O2' | 2.08 | 0.53 |
| 39:BQ:90:VAL:HG13 | 39:BQ:91:ASP:N | 2.22 | 0.53 |
| 39:BQ:98:LEU:O | 39:BQ:99:ALA:C | 2.47 | 0.53 |
| 25:BC:86:PRO:HD2 | 25:BC:87:ASN:HD21 | 1.73 | 0.53 |
| 35:BM:89:ASN:C | 35:BM:92:GLY:H | 2.12 | 0.53 |
| 2:CB:80:ILE:HD11 | 2:CB:208:ILE:CG2 | 2.38 | 0.53 |
| 1:CA:1202:G:H4' | 14:CN:29:ARG:HD3 | 1.90 | 0.53 |
| 44:BV:97:GLU:HB3 | 44:BV:125:LEU:HD21 | 1.89 | 0.53 |
| 43:DU:29:GLU:HB3 | 43:DU:38:ILE:CB | 2.33 | 0.53 |
| 2:AB:97:TRP:HH2 | 2:AB:176:GLU:CG | 2.20 | 0.53 |
| 1:CA:42:G:C8 | 1:CA:42:G:OP2 | 2.62 | 0.53 |
| 1:CA:689:C:H2' | 1:CA:689:C:O2 | 2.09 | 0.53 |
| 20:CT:53:LEU:HD13 | 20:CT:102:GLY:HA3 | 1.91 | 0.53 |
| 45:DW:56:ASP:O | 45:DW:57:PHE:CB | 2.56 | 0.53 |
| 1:CA:878:G:H1' | 8:CH:3:THR:HG21 | 1.90 | 0.53 |
| 46:DX:27:GLU:CB | 46:DX:33:LYS:HA | 2.35 | 0.53 |
| 23:BA:2821:A:OP2 | 36:BN:5:LYS:NZ | 2.37 | 0.53 |
| 23:BA:379:G:N1 | 46:BX:20:ARG:NH2 | 2.55 | 0.53 |
| 23:DA:556:G:H2' | 23:DA:557:U:H6 | 1.72 | 0.53 |
| 29:BG:21:PRO:HB2 | 29:BG:23:ARG:NH1 | 2.24 | 0.53 |
| 8:CH:119:LEU:N | 8:CH:119:LEU:HD23 | 2.24 | 0.53 |
| 23:DA:2531:A:H2 | 23:DA:2658:C:O2 | 1.92 | 0.53 |
| 23:DA:8:A:H2' | 23:DA:9:U:C6 | 2.44 | 0.53 |
| 23:BA:2638:G:OP2 | 26:BD:82:ARG:NH2 | 2.42 | 0.53 |
| 18:CR:44:LEU:HA | 18:CR:49:LYS:O | 2.09 | 0.53 |
| 1:CA:658:G:C5 | 1:CA:659:U:C5 | 2.96 | 0.53 |
| 25:DC:72:LYS:HE2 | 25:DC:101:GLU:HG2 | 1.90 | 0.53 |
| 23:BA:2862:G:C6 | 23:BA:2863:C:C4 | 2.96 | 0.53 |
| 1:CA:913:A:C1' | 1:CA:914:A:OP2 | 2.57 | 0.53 |
| 45:DW:66:VAL:O | 45:DW:81:VAL:HA | 2.09 | 0.53 |
| 1:CA:942:G:N2 | 1:CA:943:U:C2 | 2.76 | 0.53 |
| 1:CA:15:G:C4 | 1:CA:16:A:C8 | 2.97 | 0.53 |
| 1:AA:545:C:O2' | 1:AA:546:G:O5' | 2.26 | 0.53 |
| 1:CA:413:G:H21 | 1:CA:428:G:H1' | 1.73 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:AF:9:VAL:HA | 6:AF:59:TYR:O | 2.08 | 0.53 |
| 1:AA:506:G:C6 | 1:AA:507:C:C4 | 2.97 | 0.53 |
| 17:AQ:7:THR:HA | 17:AQ:57:VAL:O | 2.08 | 0.53 |
| 23:BA:2279:G:N2 | 23:BA:2280:G:H1' | 2.23 | 0.53 |
| 23:DA:2831:G:O4' | 23:DA:2883:A:C2 | 2.62 | 0.53 |
| 23:BA:1451:C:N3 | 23:BA:1459:G:O6 | 2.42 | 0.53 |
| 1:CA:1386:G:C2 | 1:CA:1387:G:C8 | 2.96 | 0.53 |
| 1:CA:123:C:OP1 | 1:CA:312:C:H5' | 2.09 | 0.53 |
| 23:BA:553:U:O2' | 23:BA:554:U:H5' | 2.08 | 0.53 |
| 24:BB:35:U:O2' | 24:BB:36:C:H5' | 2.09 | 0.53 |
| 8:CH:109:ILE:HG12 | 8:CH:110:ALA:N | 2.23 | 0.53 |
| 11:AK:102:GLY:O | 11:AK:103:LEU:HD13 | 2.08 | 0.53 |
| 39:DQ:46:ALA:O | 39:DQ:47:TYR:C | 2.47 | 0.53 |
| 1:CA:8:A:N7 | 4:CD:208:SER:OG | 2.40 | 0.53 |
| 1:AA:515:G:C2 | 1:AA:537:G:C2 | 2.97 | 0.53 |
| 23:BA:2564:A:OP1 | 23:BA:2648:C:H4' | 2.09 | 0.53 |
| 53:D5:57:ARG:NE | 53:D5:57:ARG:CA | 2.70 | 0.53 |
| 50:B2:4:HIS:HB3 | 50:B2:5:PRO:CD | 2.39 | 0.53 |
| 23:DA:84:A:C2 | 23:DA:98:G:N3 | 2.76 | 0.53 |
| 32:DJ:57:LEU:HD21 | 32:DJ:143:LEU:HB2 | 1.88 | 0.53 |
| 1:AA:1221:G:H1' | 19:AS:54:GLY:HA3 | 1.88 | 0.53 |
| 23:BA:1190:G:H2' | 23:BA:1191:G:C8 | 2.43 | 0.53 |
| 23:BA:2419:U:O4 | 53:B5:30:ARG:NH1 | 2.42 | 0.53 |
| 2:CB:163:PHE:HA | 2:CB:185:ILE:O | 2.08 | 0.53 |
| 25:DC:33:LEU:C | 25:DC:35:LYS:N | 2.61 | 0.53 |
| 34:DL:50:ARG:HB2 | 53:D5:60:LEU:CD1 | 2.39 | 0.53 |
| 23:BA:993:G:C5 | 23:BA:994:C:C5 | 2.94 | 0.53 |
| 23:DA:2338:G:C2' | 23:DA:2339:G:H5' | 2.39 | 0.53 |
| 23:DA:1813:G:H1' | 25:DC:50:THR:CG2 | 2.30 | 0.53 |
| 42:DT:12:VAL:CG1 | 42:DT:28:PHE:HA | 2.38 | 0.53 |
| 42:DT:30:VAL:CG1 | 42:DT:31:HIS:N | 2.71 | 0.53 |
| 30:DH:132:PRO:O | 30:DH:134:PRO:HD3 | 2.08 | 0.53 |
| 28:BF:19:LEU:HD11 | 28:BF:172:LEU:HD13 | 1.90 | 0.53 |
| 23:BA:2633:G:O2' | 26:BD:61:ARG:HD3 | 2.08 | 0.53 |
| 17:CQ:45:HIS:HB3 | 17:CQ:72:ARG:HG2 | 1.90 | 0.53 |
| 5:CE:139:LEU:HA | 5:CE:142:LEU:HD12 | 1.89 | 0.53 |
| 52:B4:19:ARG:HB3 | 52:B4:19:ARG:NH1 | 2.23 | 0.53 |
| 8:AH:19:VAL:HG23 | 8:AH:21:LYS:HG2 | 1.91 | 0.53 |
| 46:BX:27:GLU:CB | 46:BX:33:LYS:HA | 2.34 | 0.53 |
| 47:BY:9:GLN:HG3 | 47:BY:12:GLU:OE1 | 2.08 | 0.53 |
| 1:AA:1503:A:OP1 | 1:AA:1531:A:O2' | 2.26 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:CB:83:MET:O | 2:CB:87:ARG:HB2 | 2.09 | 0.53 |
| 23:BA:2746:U:H2' | 23:BA:2747:G:O5' | 2.09 | 0.53 |
| 23:BA:1486:A:H2' | 23:BA:1487:G:H8 | 1.73 | 0.53 |
| 23:BA:9:U:C4 | 23:BA:2629:A:N6 | 2.77 | 0.53 |
| 23:DA:1046:A:H8 | 23:DA:1046:A:O5' | 1.92 | 0.53 |
| 24:DB:78:A:H61 | 24:DB:98:G:H1' | 1.74 | 0.53 |
| 11:AK:34:ASP:HB2 | 11:AK:35:PRO:CD | 2.39 | 0.53 |
| 25:BC:267:SER:O | 25:BC:270:ILE:HG13 | 2.08 | 0.53 |
| 25:BC:148:GLU:HB2 | 25:BC:151:LYS:CD | 2.38 | 0.53 |
| 35:DM:22:LYS:HD3 | 35:DM:22:LYS:C | 2.29 | 0.53 |
| 12:CL:46:LYS:HB3 | 12:CL:47:PRO:HD3 | 1.90 | 0.53 |
| 23:DA:580:C:O2' | 23:DA:581:C:H5' | 2.09 | 0.53 |
| 23:BA:276:A:N7 | 23:BA:278:A:H8 | 2.06 | 0.53 |
| 39:BQ:62:ILE:HD11 | 39:BQ:93:LYS:HG2 | 1.91 | 0.53 |
| 23:DA:1921:G:O2' | 23:DA:1922:G:H5' | 2.08 | 0.53 |
| 20:AT:82:SER:O | 20:AT:86:ARG:HB2 | 2.08 | 0.53 |
| 1:CA:498:A:H4' | 1:CA:500:G:H5' | 1.91 | 0.53 |
| 23:DA:1726:G:C2 | 23:DA:1735:U:O2 | 2.61 | 0.53 |
| 23:DA:1857:G:N2 | 23:DA:1886:C:C4 | 2.76 | 0.53 |
| 1:CA:851:G:O2' | 1:CA:852:G:H5' | 2.08 | 0.53 |
| 15:CO:36:ILE:HG22 | 15:CO:37:ASN:N | 2.22 | 0.53 |
| 24:DB:28:C:H2' | 24:DB:29:A:C8 | 2.42 | 0.53 |
| 47:BY:42:GLY:O | 47:BY:44:LEU:N | 2.32 | 0.53 |
| 1:AA:1167:A:N7 | 1:AA:1169:A:C5 | 2.76 | 0.53 |
| 23:BA:812:C:H5' | 34:BL:25:SER:O | 2.08 | 0.53 |
| 35:BM:29:PHE:O | 35:BM:30:GLY:O | 2.27 | 0.53 |
| 12:AL:125:LYS:HE2 | 12:AL:127:ALA:H | 1.73 | 0.53 |
| 23:DA:2506:U:H5 | 23:DA:2507:C:C5 | 2.26 | 0.53 |
| 31:DI:9:LEU:HD23 | 31:DI:9:LEU:O | 2.09 | 0.53 |
| 15:AO:61:GLY:O | 15:AO:64:ARG:HB3 | 2.08 | 0.53 |
| 23:DA:772:C:H2' | 23:DA:772:C:O2 | 2.08 | 0.53 |
| 23:DA:681:G:C2' | 23:DA:682:G:O5' | 2.56 | 0.53 |
| 53:D5:52:LYS:HD3 | 53:D5:52:LYS:N | 2.22 | 0.53 |
| 13:AM:96:LEU:HD22 | 13:AM:103:THR:HG21 | 1.89 | 0.53 |
| 26:BD:170:LEU:CD2 | 26:BD:170:LEU:N | 2.72 | 0.53 |
| 38:DP:98:LYS:HB3 | 38:DP:100:TYR:CE1 | 2.43 | 0.53 |
| 23:DA:673:C:H5' | 27:DE:81:PRO:HD2 | 1.89 | 0.53 |
| 37:BO:28:VAL:HG21 | 37:BO:87:PHE:CE1 | 2.44 | 0.53 |
| 27:BE:164:ARG:NH1 | 27:BE:164:ARG:CG | 2.70 | 0.53 |
| 32:DJ:112:LYS:O | 32:DJ:116:THR:HG23 | 2.08 | 0.53 |
| 39:BQ:92:ARG:HG2 | 40:BR:11:GLN:HE21 | 1.70 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:DC:268:ARG:HD2 | 25:DC:269:PHE:CE1 | 2.43 | 0.53 |
| 30:DH:129:THR:HA | 30:DH:138:ILE:O | 2.09 | 0.53 |
| 1:AA:327:A:C2 | 1:AA:329:A:C4 | 2.96 | 0.53 |
| 25:DC:141:VAL:HG23 | 25:DC:162:SER:OG | 2.08 | 0.53 |
| 4:CD:28:SER:HB3 | 4:CD:29:PRO:CD | 2.36 | 0.53 |
| 5:CE:10:MET:HG3 | 5:CE:13:ILE:HD11 | 1.91 | 0.53 |
| 44:BV:48:PHE:CZ | 44:BV:52:SER:HA | 2.43 | 0.53 |
| 1:AA:586:C:H1' | 1:AA:878:G:O2' | 2.09 | 0.53 |
| 9:AI:17:VAL:HG21 | 9:AI:80:GLY:HA3 | 1.89 | 0.53 |
| 35:DM:55:VAL:HG22 | 35:DM:56:ARG:N | 2.23 | 0.53 |
| 13:AM:84:ILE:CG2 | 19:AS:74:PHE:HE1 | 2.21 | 0.53 |
| 6:AF:8:ILE:HG22 | 6:AF:10:LEU:HD12 | 1.90 | 0.53 |
| 6:AF:63:TYR:O | 6:AF:65:VAL:HG12 | 2.09 | 0.53 |
| 47:DY:9:GLN:HA | 47:DY:12:GLU:HB3 | 1.91 | 0.53 |
| 37:BO:52:SER:O | 37:BO:53:SER:HB2 | 2.08 | 0.53 |
| 33:BK:97:ARG:N | 33:BK:117:LEU:HD22 | 2.23 | 0.53 |
| 8:AH:28:ALA:HA | 8:AH:59:LEU:HD21 | 1.88 | 0.53 |
| 23:DA:1003:G:O2' | 23:DA:1010:A:N1 | 2.36 | 0.53 |
| 23:DA:598:G:H5' | 34:DL:15:ARG:HG2 | 1.89 | 0.53 |
| 1:CA:105:G:C4 | 1:CA:106:C:C5 | 2.96 | 0.53 |
| 36:BN:66:VAL:HG13 | 36:BN:70:LEU:HD12 | 1.91 | 0.53 |
| 2:AB:72:GLY:HA3 | 2:AB:165:VAL:CG1 | 2.38 | 0.53 |
| 1:AA:337:C:H2' | 1:AA:338:A:C8 | 2.38 | 0.53 |
| 50:D2:40:LYS:HZ3 | 50:D2:49:CYS:HB3 | 1.74 | 0.53 |
| 12:CL:21:SER:O | 12:CL:23:VAL:N | 2.42 | 0.53 |
| 23:BA:628:G:H2' | 23:BA:629:G:H8 | 1.73 | 0.53 |
| 23:BA:828:U:H4' | 23:BA:831:G:N1 | 2.24 | 0.53 |
| 1:CA:579:G:C4 | 1:CA:580:U:C6 | 2.96 | 0.53 |
| 1:AA:1446:A:N1 | 38:BP:118:ARG:CZ | 2.71 | 0.53 |
| 12:CL:74:HIS:CD2 | 12:CL:76:LEU:H | 2.25 | 0.53 |
| 23:BA:492:A:C2' | 23:BA:493:G:H5' | 2.39 | 0.53 |
| 52:B4:1:MET:O | 52:B4:2:LYS:C | 2.47 | 0.53 |
| 23:DA:2739:U:C2' | 23:DA:2739:U:O2 | 2.55 | 0.53 |
| 1:CA:44:G:N2 | 1:CA:399:G:C4 | 2.76 | 0.53 |
| 4:CD:70:ILE:HG12 | 4:CD:71:SER:N | 2.22 | 0.53 |
| 23:DA:2572:A:P | 26:DD:144:ARG:HB2 | 2.49 | 0.53 |
| 15:CO:50:HIS:O | 15:CO:53:HIS:HB3 | 2.07 | 0.53 |
| 7:AG:80:VAL:HG23 | 7:AG:83:ALA:HB3 | 1.90 | 0.53 |
| 23:DA:2641:G:OP1 | 32:DJ:97:ARG:HD3 | 2.08 | 0.53 |
| 26:BD:173:VAL:HG12 | 26:BD:174:ASP:H | 1.73 | 0.53 |
| 23:DA:532:A:C8 | 23:DA:2021:C:C5 | 2.97 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 20:CT:37:SER:O | 20:CT:40:ALA:HB3 | 2.09 | 0.53 |
| 23:BA:2436:G:C5 | 23:BA:2437:U:C5 | 2.97 | 0.53 |
| 2:AB:96:ARG:H | 2:AB:96:ARG:HD2 | 1.73 | 0.53 |
| 43:BU:75:ILE:HG13 | 43:BU:79:CYS:HA | 1.91 | 0.53 |
| 42:DT:66:LEU:HD23 | 42:DT:67:GLY:N | 2.24 | 0.53 |
| 2:AB:17:PHE:CD1 | 2:AB:44:LEU:HD21 | 2.44 | 0.53 |
| 23:DA:2416:C:C2 | 23:DA:2417:C:C5 | 2.96 | 0.53 |
| 23:DA:2415:G:O3' | 34:DL:66:GLY:HA3 | 2.08 | 0.53 |
| 32:BJ:119:GLU:N | 32:BJ:119:GLU:OE1 | 2.29 | 0.53 |
| 23:DA:1543:A:C8 | 23:DA:1543:A:C3' | 2.88 | 0.53 |
| 2:AB:69:LEU:HD12 | 2:AB:70:PHE:N | 2.24 | 0.53 |
| 1:CA:960:U:H5 | 1:CA:1225:A:H1' | 1.73 | 0.53 |
| 23:BA:2334:G:H4' | 23:BA:2335:A:OP2 | 2.09 | 0.53 |
| 39:DQ:83:LEU:HA | 39:DQ:86:ALA:HB3 | 1.89 | 0.53 |
| 34:DL:47:ASP:CB | 34:DL:51:PHE:HB2 | 2.38 | 0.53 |
| 28:DF:76:SER:HB2 | 28:DF:83:ARG:N | 2.24 | 0.53 |
| 41:DS:14:PRO:C | 41:DS:16:LYS:N | 2.62 | 0.53 |
| 41:BS:86:LEU:C | 41:BS:86:LEU:HD12 | 2.27 | 0.53 |
| 30:DH:77:LEU:HD21 | 30:DH:104:GLN:HB2 | 1.91 | 0.53 |
| 44:DV:92:SER:HB2 | 44:DV:94:GLU:OE2 | 2.09 | 0.53 |
| 1:AA:92:G:C2' | 1:AA:93:U:H5' | 2.38 | 0.53 |
| 26:BD:6:GLY:HA2 | 26:BD:51:PHE:CE2 | 2.43 | 0.53 |
| 11:CK:59:TYR:CE2 | 11:CK:63:LEU:HD11 | 2.44 | 0.53 |
| 1:CA:42:G:H8 | 1:CA:42:G:OP2 | 1.90 | 0.53 |
| 46:DX:46:LEU:HD21 | 46:DX:61:ARG:HG3 | 1.90 | 0.53 |
| 1:AA:1369:C:H2' | 1:AA:1370:G:O4' | 2.09 | 0.53 |
| 1:AA:57:G:C5 | 1:AA:58:C:C5 | 2.97 | 0.53 |
| 12:AL:40:ARG:HG2 | 12:AL:41:THR:N | 2.24 | 0.53 |
| 23:DA:319:C:H2' | 23:DA:320:A:C8 | 2.44 | 0.53 |
| 1:CA:644:G:C5' | 8:CH:92:ARG:HH21 | 2.22 | 0.53 |
| 29:BG:123:PHE:HB3 | 29:BG:133:VAL:HG13 | 1.91 | 0.53 |
| 46:BX:12:PRO:O | 46:BX:14:VAL:HG23 | 2.08 | 0.53 |
| 1:AA:738:C:H2' | 1:AA:739:C:H6 | 1.70 | 0.53 |
| 23:DA:773:U:C5' | 25:DC:47:GLY:HA3 | 2.38 | 0.53 |
| 1:AA:841:U:O2 | 1:AA:841:U:H3' | 2.09 | 0.53 |
| 13:AM:3:ARG:HG2 | 13:AM:9:ILE:CD1 | 2.38 | 0.53 |
| 1:CA:1423:G:H2' | 1:CA:1424:C:H6 | 1.73 | 0.53 |
| 23:DA:2364:C:O2' | 23:DA:2365:G:H5' | 2.09 | 0.53 |
| 35:BM:43:THR:HG1 | 35:BM:45:GLN:HG2 | 1.72 | 0.53 |
| 23:BA:2228:G:OP2 | 25:BC:263:ARG:NH2 | 2.41 | 0.53 |
| 45:DW:14:ARG:CB | 45:DW:14:ARG:CZ | 2.86 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:AC:186:PHE:HZ | 3:AC:188:LEU:HD13 | 1.72 | 0.53 |
| 7:CG:80:VAL:CG2 | 7:CG:83:ALA:HB3 | 2.39 | 0.53 |
| 10:CJ:17:ASP:O | 10:CJ:21:GLN:HB2 | 2.09 | 0.53 |
| 46:DX:48:LYS:NZ | 46:DX:50:ARG:CZ | 2.72 | 0.53 |
| 34:DL:135:LEU:HD13 | 34:DL:139:LYS:HB2 | 1.90 | 0.53 |
| 39:BQ:73:GLY:O | 39:BQ:74:LEU:HB3 | 2.09 | 0.53 |
| 23:DA:351:G:H5'' | 23:DA:352:G:OP1 | 2.09 | 0.53 |
| 11:AK:123:LYS:O | 11:AK:126:ARG:HB2 | 2.09 | 0.53 |
| 12:CL:75:ASN:OD1 | 12:CL:107:ALA:HB3 | 2.09 | 0.53 |
| 9:CI:85:LEU:O | 9:CI:89:ASN:HB2 | 2.09 | 0.53 |
| 34:DL:125:VAL:HG11 | 34:DL:138:LEU:HD22 | 1.90 | 0.53 |
| 23:DA:2267:A:H5'' | 23:DA:2268:A:H5'' | 1.91 | 0.53 |
| 32:DJ:119:GLU:OE1 | 32:DJ:119:GLU:N | 2.33 | 0.53 |
| 1:AA:1364:U:O2' | 1:AA:1365:G:H5' | 2.08 | 0.53 |
| 42:DT:71:GLY:C | 42:DT:72:LYS:HG3 | 2.29 | 0.53 |
| 23:DA:114(B):A:C4' | 32:DJ:48:ARG:HH22 | 2.20 | 0.53 |
| 23:DA:518:G:H4' | 41:DS:18:ARG:NH1 | 2.23 | 0.53 |
| 42:BT:12:VAL:CG1 | 42:BT:28:PHE:HA | 2.39 | 0.53 |
| 24:DB:7:G:H1' | 37:DO:38:GLN:NE2 | 2.23 | 0.53 |
| 3:AC:182:ILE:HG23 | 3:AC:202:ILE:O | 2.09 | 0.53 |
| 23:BA:1493:C:O2 | 23:BA:1493:C:H2' | 2.08 | 0.53 |
| 29:BG:35:VAL:HG21 | 29:BG:75:ALA:HB2 | 1.90 | 0.53 |
| 4:CD:31:CYS:C | 4:CD:33:MET:H | 2.11 | 0.53 |
| 5:AE:11:ILE:HG22 | 5:AE:12:LEU:N | 2.24 | 0.53 |
| 1:AA:1070:U:C2 | 1:AA:1071:C:C5 | 2.97 | 0.53 |
| 2:AB:173:ALA:O | 2:AB:176:GLU:N | 2.42 | 0.53 |
| 48:BZ:26:LEU:HB2 | 48:BZ:28:LEU:HD13 | 1.91 | 0.53 |
| 1:CA:57:G:C5 | 1:CA:58:C:C5 | 2.97 | 0.53 |
| 1:AA:1346:A:C8 | 7:AG:10:ARG:NH2 | 2.77 | 0.53 |
| 46:DX:27:GLU:HB2 | 46:DX:33:LYS:CA | 2.36 | 0.53 |
| 46:BX:11:ARG:CG | 46:BX:61:ARG:O | 2.56 | 0.53 |
| 47:DY:46:GLN:HB2 | 47:DY:49:LYS:HZ3 | 1.71 | 0.53 |
| 23:DA:848:G:C4 | 23:DA:933:A:H8 | 2.26 | 0.53 |
| 23:BA:2755:C:HO2' | 23:BA:2756:U:H6 | 1.57 | 0.53 |
| 33:BK:19:ILE:HG22 | 33:BK:43:VAL:HA | 1.89 | 0.53 |
| 23:BA:1684:C:C2 | 23:BA:1705:G:N2 | 2.77 | 0.53 |
| 23:DA:270(H):C:C5 | 23:DA:270(I):C:H5 | 2.27 | 0.53 |
| 18:AR:22:VAL:HG11 | 18:AR:42:ARG:O | 2.08 | 0.53 |
| 38:BP:89:VAL:O | 38:BP:89:VAL:CG2 | 2.57 | 0.53 |
| 27:DE:132:VAL:HG23 | 27:DE:133:ASN:N | 2.23 | 0.53 |
| 1:AA:677:U:H2' | 1:AA:678:U:C6 | 2.43 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:841:U:H3' | 1:CA:841:U:O2 | 2.08 | 0.53 |
| 23:BA:336:C:C2' | 23:BA:336:C:O2 | 2.57 | 0.53 |
| 23:BA:681:G:C2' | 23:BA:682:G:O5' | 2.56 | 0.53 |
| 1:CA:939:G:H2' | 1:CA:940:C:C6 | 2.44 | 0.53 |
| 23:BA:270(J):G:O2' | 23:BA:270(K):G:H8 | 1.91 | 0.53 |
| 1:CA:373:A:C2 | 1:CA:482:A:N6 | 2.77 | 0.53 |
| 36:BN:44:LEU:HD13 | 36:BN:44:LEU:C | 2.28 | 0.53 |
| 23:DA:2485:G:H5'' | 35:DM:46:GLN:NE2 | 2.23 | 0.53 |
| 23:BA:226:G:H21 | 23:BA:228:A:N6 | 2.07 | 0.53 |
| 1:AA:433:C:H2' | 1:AA:434:U:C6 | 2.43 | 0.53 |
| 23:BA:1336:A:H2' | 23:BA:1337:G:H8 | 1.73 | 0.53 |
| 23:DA:270(Q):C:O2' | 23:DA:270(R):C:H6 | 1.91 | 0.53 |
| 9:AI:99:LEU:HD12 | 9:AI:101:PHE:CE2 | 2.44 | 0.53 |
| 1:AA:664:G:P | 18:AR:64:ARG:HH21 | 2.32 | 0.53 |
| 1:CA:142:G:C2 | 1:CA:143:A:C5 | 2.97 | 0.53 |
| 37:BO:67:ARG:HG3 | 37:BO:100:ALA:HB1 | 1.90 | 0.53 |
| 23:BA:2026:C:C2 | 23:BA:2027:G:C8 | 2.97 | 0.53 |
| 46:BX:77:ALA:HA | 46:BX:80:LEU:HB2 | 1.91 | 0.53 |
| 23:BA:833:U:H2' | 23:BA:834:C:C6 | 2.44 | 0.53 |
| 23:DA:1281:G:C5 | 23:DA:1282:U:C5 | 2.97 | 0.53 |
| 1:CA:1489:G:C6 | 1:CA:1490:C:N4 | 2.77 | 0.53 |
| 23:BA:2557:G:H2' | 23:BA:2558:C:C6 | 2.44 | 0.53 |
| 34:DL:62:LEU:N | 34:DL:62:LEU:HD13 | 2.23 | 0.53 |
| 7:CG:113:GLU:CB | 7:CG:119:ARG:HG2 | 2.23 | 0.53 |
| 28:DF:60:LEU:O | 28:DF:64:THR:HG22 | 2.09 | 0.53 |
| 7:AG:115:ARG:HB2 | 7:AG:118:VAL:HG11 | 1.90 | 0.53 |
| 1:CA:951:G:H1' | 1:CA:970:C:O2' | 2.09 | 0.53 |
| 5:AE:102:ALA:HB2 | 5:AE:120:THR:HG23 | 1.90 | 0.53 |
| 25:DC:35:LYS:HZ1 | 25:DC:104:TYR:H | 1.57 | 0.53 |
| 23:DA:1144:G:C4 | 23:DA:1145:C:C5 | 2.97 | 0.53 |
| 1:CA:376:G:C2 | 1:CA:377:G:C8 | 2.97 | 0.53 |
| 41:DS:12:ILE:HG12 | 41:DS:13:SER:N | 2.23 | 0.53 |
| 25:DC:265:PRO:C | 25:DC:267:SER:H | 2.11 | 0.53 |
| 1:AA:327:A:C4 | 1:AA:329:A:C8 | 2.96 | 0.53 |
| 23:BA:197:A:C8 | 23:BA:197:A:C5' | 2.87 | 0.53 |
| 24:BB:71:C:C4 | 24:BB:72:G:N7 | 2.77 | 0.53 |
| 5:AE:75:THR:HG23 | 5:AE:76:ILE:N | 2.24 | 0.53 |
| 48:BZ:26:LEU:HD21 | 48:BZ:46:ASN:CB | 2.38 | 0.53 |
| 2:AB:80:ILE:HD11 | 2:AB:208:ILE:CG2 | 2.39 | 0.53 |
| 1:CA:506:G:C4 | 1:CA:507:C:C5 | 2.97 | 0.53 |
| 23:BA:2562:U:H2' | 23:BA:2563:U:H5' | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 46:BX:11:ARG:HG3 | 46:BX:61:ARG:O | 2.09 | 0.53 |
| 46:BX:27:GLU:CG | 46:BX:33:LYS:HG3 | 2.38 | 0.53 |
| 4:CD:152:SER:O | 4:CD:155:LEU:HB2 | 2.09 | 0.53 |
| 46:DX:19:GLN:HG3 | 46:DX:41:ARG:NE | 2.20 | 0.53 |
| 1:CA:197:A:C5 | 1:CA:221:C:H4' | 2.44 | 0.53 |
| 17:CQ:40:LYS:HG2 | 17:CQ:41:LYS:N | 2.24 | 0.53 |
| 23:BA:582:G:OP1 | 39:BQ:14:HIS:HD2 | 1.92 | 0.53 |
| 1:CA:832:C:N4 | 1:CA:855:G:C6 | 2.77 | 0.53 |
| 1:AA:682:G:C6 | 1:AA:709:G:C6 | 2.96 | 0.53 |
| 34:BL:85:LEU:CD2 | 34:BL:85:LEU:H | 2.22 | 0.53 |
| 23:DA:1746:G:N3 | 23:DA:1747:G:C8 | 2.77 | 0.53 |
| 23:BA:634:C:H2' | 23:BA:635:C:C6 | 2.44 | 0.53 |
| 1:AA:518:C:O2 | 1:AA:529:G:C6 | 2.62 | 0.53 |
| 1:AA:560:U:H5' | 1:AA:566:G:N2 | 2.24 | 0.53 |
| 23:DA:2345:G:OP2 | 51:D3:39:TYR:HA | 2.09 | 0.53 |
| 1:AA:180:U:H2' | 1:AA:181:G:H5' | 1.89 | 0.53 |
| 12:CL:61:SER:C | 12:CL:63:TYR:H | 2.12 | 0.53 |
| 23:BA:1798:U:H5'' | 25:BC:259:THR:O | 2.09 | 0.53 |
| 23:DA:681:G:H2' | 23:DA:682:G:O5' | 2.09 | 0.53 |
| 23:DA:1937:A:N7 | 23:DA:1939:U:H2' | 2.23 | 0.53 |
| 1:AA:1037:C:H2' | 1:AA:1038:C:H6 | 1.73 | 0.53 |
| 49:B1:43:GLY:O | 49:B1:44:CYS:HB3 | 2.08 | 0.53 |
| 1:CA:380:G:C2 | 1:CA:384:G:C6 | 2.96 | 0.53 |
| 23:DA:2582:G:C2 | 23:DA:2583:G:C8 | 2.96 | 0.53 |
| 31:BI:9:LEU:HD23 | 31:BI:9:LEU:O | 2.09 | 0.53 |
| 23:DA:527:C:O4' | 23:DA:527:C:O2 | 2.23 | 0.53 |
| 28:BF:49:ASP:HB3 | 28:BF:52:ILE:HG12 | 1.91 | 0.53 |
| 23:BA:860:U:C4 | 23:BA:2268:A:C8 | 2.96 | 0.53 |
| 7:CG:113:GLU:O | 7:CG:119:ARG:HD3 | 2.09 | 0.53 |
| 27:DE:74:ARG:O | 27:DE:74:ARG:HG2 | 2.08 | 0.53 |
| 1:AA:1228:C:N4 | 1:AA:1229:A:N6 | 2.57 | 0.53 |
| 34:DL:33:ARG:CG | 34:DL:34:GLY:H | 2.20 | 0.53 |
| 23:BA:114(B):A:O2' | 23:BA:1143:A:H3' | 2.08 | 0.53 |
| 23:DA:1658:C:H2' | 23:DA:1659:U:C6 | 2.44 | 0.53 |
| 39:DQ:92:ARG:HD2 | 39:DQ:95:LEU:N | 2.24 | 0.53 |
| 28:DF:83:ARG:HG3 | 28:DF:84:LYS:N | 2.24 | 0.53 |
| 39:BQ:102:GLU:N | 39:BQ:103:PRO:CD | 2.72 | 0.53 |
| 37:DO:12:PHE:HD1 | 37:DO:12:PHE:C | 2.12 | 0.53 |
| 37:DO:28:VAL:HG21 | 37:DO:87:PHE:CE1 | 2.44 | 0.53 |
| 35:BM:89:ASN:O | 35:BM:92:GLY:N | 2.40 | 0.53 |
| 1:CA:1072:G:H2' | 1:CA:1073:U:C6 | 2.44 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:408:A:H2' | 1:CA:409:G:H8 | 1.74 | 0.53 |
| 6:CF:9:VAL:HA | 6:CF:59:TYR:O | 2.09 | 0.53 |
| 15:AO:8:LYS:O | 15:AO:12:ILE:HG13 | 2.09 | 0.53 |
| 23:DA:1884:A:C4 | 23:DA:1885:A:C8 | 2.97 | 0.53 |
| 23:BA:7:G:N2 | 23:BA:2897:U:C4 | 2.77 | 0.53 |
| 32:DJ:59:GLY:O | 32:DJ:65:TRP:HE3 | 1.91 | 0.53 |
| 23:DA:389:G:H1 | 34:DL:71:VAL:HG23 | 1.74 | 0.53 |
| 23:DA:2289:G:N3 | 23:DA:2289:G:H2' | 2.23 | 0.53 |
| 23:DA:270(H):C:C4 | 23:DA:270(I):C:H5 | 2.25 | 0.53 |
| 23:BA:270(H):C:C4 | 23:BA:270(I):C:H5 | 2.26 | 0.53 |
| 1:CA:236:G:OP1 | 17:CQ:40:LYS:NZ | 2.42 | 0.53 |
| 1:CA:1057:G:C2 | 1:CA:1204:A:C2 | 2.97 | 0.53 |
| 29:BG:94:TYR:CD1 | 29:BG:94:TYR:N | 2.77 | 0.53 |
| 23:DA:786:C:C2' | 23:DA:787:U:H5' | 2.39 | 0.53 |
| 34:BL:132:LYS:O | 34:BL:136:GLU:HG2 | 2.09 | 0.53 |
| 1:AA:1446:A:H61 | 38:BP:118:ARG:HH21 | 1.54 | 0.53 |
| 35:DM:134:ARG:NH1 | 35:DM:138:ASP:OD1 | 2.39 | 0.53 |
| 1:CA:1228:C:N4 | 1:CA:1229:A:H62 | 2.07 | 0.53 |
| 1:CA:1378:C:H5 | 1:CA:1379:G:N9 | 2.07 | 0.53 |
| 12:AL:74:HIS:HD2 | 12:AL:76:LEU:N | 2.07 | 0.53 |
| 29:BG:54:ARG:NH2 | 29:BG:62:LYS:HE2 | 2.24 | 0.53 |
| 23:BA:2459:A:C2 | 23:BA:2460:U:H1' | 2.44 | 0.53 |
| 45:BW:35:ASN:N | 45:BW:35:ASN:HD22 | 2.07 | 0.53 |
| 23:BA:2709:G:C2' | 23:BA:2710:C:H5' | 2.39 | 0.53 |
| 27:BE:139:PHE:HB2 | 27:BE:166:ALA:HB1 | 1.90 | 0.53 |
| 24:DB:115:G:H5' | 37:DO:50:SER:OG | 2.09 | 0.53 |
| 23:DA:1904:G:O2' | 23:DA:1905:C:H5' | 2.08 | 0.53 |
| 11:CK:36:ASP:HB2 | 11:CK:38:ASN:OD1 | 2.08 | 0.53 |
| 15:AO:44:LYS:HB2 | 15:AO:44:LYS:HZ3 | 1.74 | 0.53 |
| 23:DA:685:A:H1' | 23:DA:688:U:O4 | 2.09 | 0.53 |
| 38:DP:56:GLY:C | 38:DP:57:PHE:O | 2.43 | 0.52 |
| 38:BP:55:ASN:H | 38:BP:59:THR:HB | 1.73 | 0.52 |
| 30:BH:81:VAL:HG11 | 30:BH:90:GLY:HA3 | 1.90 | 0.52 |
| 42:BT:11:PRO:HG2 | 42:BT:13:LEU:HD21 | 1.92 | 0.52 |
| 42:BT:28:PHE:HD1 | 42:BT:28:PHE:H | 1.56 | 0.52 |
| 30:DH:113:ARG:HB2 | 30:DH:130:TYR:CE1 | 2.44 | 0.52 |
| 30:DH:88:ILE:HG12 | 30:DH:123:LEU:N | 2.24 | 0.52 |
| 36:DN:103:ARG:NH1 | 36:DN:110:PRO:HG3 | 2.24 | 0.52 |
| 25:DC:242:ARG:HD3 | 25:DC:242:ARG:N | 2.24 | 0.52 |
| 34:DL:18:ARG:C | 34:DL:19:VAL:HG22 | 2.29 | 0.52 |
| 23:DA:1312:U:H4' | 23:DA:1313:U:O5' | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:DX:46:LEU:HD23 | 46:DX:46:LEU:O | 2.07 | 0.52 |
| 4:AD:152:SER:O | 4:AD:155:LEU:HB2 | 2.09 | 0.52 |
| 8:AH:63:LEU:HB2 | 8:AH:65:TYR:HE1 | 1.74 | 0.52 |
| 6:AF:62:TRP:CG | 18:AR:35:ARG:NH1 | 2.77 | 0.52 |
| 29:BG:52:VAL:O | 29:BG:52:VAL:HG12 | 2.06 | 0.52 |
| 25:DC:27:THR:CG2 | 25:DC:27:THR:O | 2.51 | 0.52 |
| 30:DH:133:HIS:HD2 | 30:DH:135:GLU:HG2 | 1.73 | 0.52 |
| 1:AA:1117:G:N2 | 1:AA:1180:A:H1' | 2.21 | 0.52 |
| 23:DA:2276:G:O2' | 23:DA:2277:G:H5' | 2.09 | 0.52 |
| 45:DW:36:ILE:HG23 | 45:DW:58:THR:CG2 | 2.39 | 0.52 |
| 25:DC:148:GLU:HB2 | 25:DC:151:LYS:CD | 2.39 | 0.52 |
| 25:BC:27:THR:O | 25:BC:27:THR:CG2 | 2.54 | 0.52 |
| 23:DA:2657:A:H5'' | 23:DA:2658:C:OP2 | 2.09 | 0.52 |
| 24:BB:21:G:H2' | 24:BB:22:U:H6 | 1.74 | 0.52 |
| 23:BA:2636:U:H2' | 23:BA:2637:U:H6 | 1.74 | 0.52 |
| 33:BK:1:MET:HE2 | 33:BK:32:TYR:CG | 2.44 | 0.52 |
| 1:CA:740:U:O2' | 1:CA:741:G:H5' | 2.08 | 0.52 |
| 23:DA:912:C:C2 | 23:DA:913:U:C5 | 2.97 | 0.52 |
| 35:BM:38:GLU:HB2 | 35:BM:127:ILE:HG12 | 1.91 | 0.52 |
| 29:BG:94:TYR:CZ | 29:BG:160:LYS:HD3 | 2.44 | 0.52 |
| 23:DA:1387:C:C2 | 23:DA:1388:G:C8 | 2.97 | 0.52 |
| 23:DA:2476:A:H2 | 23:DA:2477:C:C6 | 2.27 | 0.52 |
| 23:DA:1270:C:H5'' | 23:DA:1271:G:C5' | 2.38 | 0.52 |
| 1:AA:579:G:H2' | 1:AA:580:U:C6 | 2.42 | 0.52 |
| 1:CA:1076:C:C2 | 1:CA:1082:G:C2 | 2.97 | 0.52 |
| 1:CA:15:G:H2' | 1:CA:16:A:H8 | 1.74 | 0.52 |
| 1:CA:632:A:H8 | 1:CA:633:G:C8 | 2.27 | 0.52 |
| 1:CA:973:G:OP1 | 10:CJ:57:LYS:NZ | 2.41 | 0.52 |
| 23:DA:2213:U:H5'' | 23:DA:2215:G:OP2 | 2.08 | 0.52 |
| 1:AA:1378:C:H5 | 1:AA:1379:G:N9 | 2.07 | 0.52 |
| 40:BR:72:VAL:O | 40:BR:72:VAL:HG23 | 2.09 | 0.52 |
| 34:BL:105:LEU:N | 34:BL:105:LEU:HD12 | 2.24 | 0.52 |
| 23:DA:975:G:H1' | 23:DA:990:A:C2 | 2.43 | 0.52 |
| 1:AA:1328:C:H5'' | 13:AM:28:ALA:CB | 2.39 | 0.52 |
| 1:AA:775:G:O2' | 1:AA:776:G:H5' | 2.09 | 0.52 |
| 33:DK:7:TYR:CZ | 33:DK:44:LYS:HG3 | 2.43 | 0.52 |
| 15:AO:44:LYS:NZ | 15:AO:44:LYS:HB2 | 2.23 | 0.52 |
| 23:BA:466:A:O3' | 52:B4:33:ARG:NH1 | 2.43 | 0.52 |
| 12:CL:92:LEU:HB2 | 12:CL:95:VAL:HG21 | 1.91 | 0.52 |
| 25:DC:212:SER:O | 25:DC:217:ARG:HG3 | 2.09 | 0.52 |
| 23:DA:841:A:C2 | 23:DA:938:G:C2 | 2.96 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 42:BT:66:LEU:HD23 | 42:BT:67:GLY:N | 2.24 | 0.52 |
| 11:CK:85:ARG:HA | 11:CK:112:THR:OG1 | 2.09 | 0.52 |
| 14:AN:2:ALA:HB1 | 14:AN:6:LEU:HD12 | 1.92 | 0.52 |
| 4:AD:23:GLY:CA | 4:AD:112:VAL:HG22 | 2.39 | 0.52 |
| 12:AL:92:LEU:HB2 | 12:AL:95:VAL:HG21 | 1.90 | 0.52 |
| 24:BB:113:C:O2' | 37:BO:46:VAL:HG13 | 2.09 | 0.52 |
| 1:AA:1187:G:H2' | 1:AA:1188:A:H8 | 1.74 | 0.52 |
| 1:AA:977:A:N3 | 1:AA:977:A:H5'' | 2.24 | 0.52 |
| 22:CV:6189:G:C6 | 22:CV:6190:U:C4 | 2.97 | 0.52 |
| 1:AA:8:A:N7 | 4:AD:208:SER:OG | 2.42 | 0.52 |
| 23:DA:1190:G:H5'' | 34:DL:35:HIS:HA | 1.90 | 0.52 |
| 53:D5:62:LEU:C | 53:D5:64:TYR:N | 2.61 | 0.52 |
| 30:BH:92:VAL:CG2 | 30:BH:96:ASP:HB2 | 2.36 | 0.52 |
| 23:BA:993:G:C4 | 23:BA:994:C:C5 | 2.96 | 0.52 |
| 39:BQ:79:PHE:CD1 | 39:BQ:83:LEU:HD13 | 2.45 | 0.52 |
| 40:BR:5:VAL:HG12 | 40:BR:14:VAL:HG21 | 1.92 | 0.52 |
| 25:DC:68:LYS:O | 25:DC:70:TRP:CE3 | 2.63 | 0.52 |
| 4:CD:49:ARG:CZ | 4:CD:50:ARG:H | 2.21 | 0.52 |
| 26:DD:137:HIS:HB3 | 26:DD:138:PRO:HD2 | 1.90 | 0.52 |
| 4:AD:100:ARG:NH2 | 4:AD:118:ARG:HH12 | 2.06 | 0.52 |
| 1:AA:38:G:H22 | 1:AA:397:A:C5' | 2.16 | 0.52 |
| 4:CD:68:TYR:CE2 | 4:CD:97:LEU:HB3 | 2.43 | 0.52 |
| 4:CD:111:ALA:HB1 | 4:CD:116:GLN:HG2 | 1.90 | 0.52 |
| 1:CA:92:G:H2' | 1:CA:93:U:H5' | 1.91 | 0.52 |
| 26:BD:6:GLY:HA2 | 26:BD:51:PHE:HE2 | 1.74 | 0.52 |
| 26:DD:111:ARG:CD | 26:DD:160:TYR:CE1 | 2.92 | 0.52 |
| 42:BT:43:VAL:HG23 | 42:BT:47:PHE:CD1 | 2.44 | 0.52 |
| 11:CK:59:TYR:O | 11:CK:63:LEU:HG | 2.10 | 0.52 |
| 1:AA:1076:C:C2 | 1:AA:1082:G:C2 | 2.97 | 0.52 |
| 43:DU:81:LYS:HZ1 | 43:DU:98:VAL:HG12 | 1.72 | 0.52 |
| 1:AA:1347:G:H8 | 9:AI:107:ARG:HB3 | 1.70 | 0.52 |
| 41:BS:32:ALA:O | 41:BS:33:ARG:C | 2.46 | 0.52 |
| 29:DG:43:VAL:HG12 | 29:DG:52:VAL:CG2 | 2.39 | 0.52 |
| 23:DA:2756:U:H4' | 23:DA:2757:A:OP1 | 2.08 | 0.52 |
| 23:DA:322:A:O4' | 23:DA:340:A:H1' | 2.09 | 0.52 |
| 23:BA:2723:C:H2' | 23:BA:2724:C:O5' | 2.09 | 0.52 |
| 23:DA:2598:A:H2' | 23:DA:2599:G:O5' | 2.09 | 0.52 |
| 6:CF:22:GLU:OE1 | 6:CF:84:ASN:HB2 | 2.09 | 0.52 |
| 20:AT:10:LEU:HD12 | 20:AT:10:LEU:C | 2.30 | 0.52 |
| 23:BA:2756:U:H4' | 23:BA:2757:A:OP1 | 2.09 | 0.52 |
| 23:BA:1105:U:C2 | 23:BA:1106:G:C8 | 2.97 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1148:U:C2 | 9:CI:16:ARG:NH2 | 2.77 | 0.52 |
| 1:AA:197:A:C5 | 1:AA:221:C:H4' | 2.43 | 0.52 |
| 23:DA:909:A:C4 | 23:DA:912:C:C5 | 2.96 | 0.52 |
| 23:DA:301:G:H4' | 23:DA:301:G:OP1 | 2.09 | 0.52 |
| 3:CC:23:TYR:CG | 3:CC:24:ALA:N | 2.77 | 0.52 |
| 35:BM:134:ARG:NH1 | 35:BM:138:ASP:OD1 | 2.38 | 0.52 |
| 35:DM:43:THR:O | 35:DM:46:GLN:HB2 | 2.10 | 0.52 |
| 34:DL:75:ILE:HD12 | 34:DL:75:ILE:N | 2.25 | 0.52 |
| 23:BA:1429:G:H2' | 23:BA:1430:C:C6 | 2.44 | 0.52 |
| 19:AS:5:LEU:HG | 19:AS:10:PHE:HB3 | 1.91 | 0.52 |
| 7:CG:70:LYS:CG | 7:CG:96:GLN:HB3 | 2.39 | 0.52 |
| 23:BA:1773:A:C2' | 23:BA:1774:C:H5' | 2.40 | 0.52 |
| 23:BA:1027:A:C6 | 23:BA:1126:A:C4 | 2.97 | 0.52 |
| 23:BA:1015:G:H2' | 23:BA:1016:G:H5' | 1.91 | 0.52 |
| 13:AM:14:ARG:HB3 | 13:AM:16:ASP:OD2 | 2.09 | 0.52 |
| 23:BA:238:C:O2' | 23:BA:608:A:H1' | 2.08 | 0.52 |
| 44:DV:68:PRO:O | 44:DV:91:LEU:HB2 | 2.08 | 0.52 |
| 1:AA:380:G:C2 | 1:AA:384:G:C6 | 2.96 | 0.52 |
| 23:BA:2315:G:H2' | 23:BA:2316:C:C6 | 2.43 | 0.52 |
| 23:BA:1235:G:C6 | 23:BA:1236:G:N1 | 2.76 | 0.52 |
| 35:DM:10:ARG:HB3 | 35:DM:11:LYS:HG2 | 1.90 | 0.52 |
| 26:BD:128:SER:OG | 26:BD:129:HIS:N | 2.38 | 0.52 |
| 36:DN:11:ASN:O | 36:DN:12:ARG:NH1 | 2.38 | 0.52 |
| 22:AV:6191:A:H2' | 22:AV:6192:G:H8 | 1.73 | 0.52 |
| 37:BO:28:VAL:O | 37:BO:92:TYR:HE1 | 1.92 | 0.52 |
| 23:BA:568:U:O4 | 40:BR:78:LYS:NZ | 2.42 | 0.52 |
| 23:BA:1615:C:C2 | 41:BS:87:PRO:HG2 | 2.44 | 0.52 |
| 34:BL:48:PRO:O | 34:BL:49:ARG:O | 2.28 | 0.52 |
| 4:AD:3:ARG:H | 4:AD:3:ARG:HD2 | 1.73 | 0.52 |
| 1:AA:1252:A:O2' | 1:AA:1253:G:H5' | 2.10 | 0.52 |
| 3:CC:134:ILE:HG23 | 3:CC:151:VAL:CB | 2.33 | 0.52 |
| 47:DY:29:LYS:HD3 | 47:DY:57:ILE:HG21 | 1.92 | 0.52 |
| 5:AE:11:ILE:HB | 5:AE:31:LEU:HD13 | 1.92 | 0.52 |
| 23:DA:1324:G:N2 | 23:DA:1331:A:C4 | 2.78 | 0.52 |
| 48:DZ:26:LEU:HB2 | 48:DZ:28:LEU:HD13 | 1.92 | 0.52 |
| 12:AL:49:SER:O | 12:AL:50:ALA:HB2 | 2.07 | 0.52 |
| 46:BX:9:GLY:O | 46:BX:13:ILE:CG2 | 2.57 | 0.52 |
| 2:AB:83:MET:O | 2:AB:87:ARG:HB2 | 2.09 | 0.52 |
| 23:BA:1858:G:H1' | 23:BA:1884:A:H61 | 1.69 | 0.52 |
| 23:DA:2598:A:C2' | 23:DA:2599:G:O5' | 2.58 | 0.52 |
| 1:AA:1237:C:OP1 | 1:AA:1238:A:H1' | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BA:1505:C:H2' | 23:BA:1506:C:C6 | 2.44 | 0.52 |
| 25:DC:25:THR:HG21 | 25:DC:81:ALA:CB | 2.38 | 0.52 |
| 23:DA:955:C:H5'' | 35:DM:85:LYS:HE2 | 1.92 | 0.52 |
| 35:DM:16:ARG:O | 35:DM:17:LEU:HD23 | 2.09 | 0.52 |
| 1:CA:712:A:C2' | 1:CA:713:G:H5' | 2.39 | 0.52 |
| 39:DQ:62:ILE:N | 39:DQ:62:ILE:HD13 | 2.24 | 0.52 |
| 29:DG:94:TYR:CD1 | 29:DG:94:TYR:N | 2.76 | 0.52 |
| 23:DA:783:A:H2' | 23:DA:785:G:OP1 | 2.10 | 0.52 |
| 33:BK:115:VAL:O | 33:BK:118:ALA:HB3 | 2.09 | 0.52 |
| 1:CA:741:G:H2' | 1:CA:742:G:O4' | 2.10 | 0.52 |
| 23:BA:908:C:OP1 | 35:BM:22:LYS:HD2 | 2.09 | 0.52 |
| 25:DC:74:GLY:O | 25:DC:76:PRO:HD3 | 2.09 | 0.52 |
| 39:BQ:76:TYR:CZ | 39:BQ:80:ILE:HG12 | 2.44 | 0.52 |
| 1:AA:527:G:O2' | 1:AA:528:C:H5' | 2.09 | 0.52 |
| 41:BS:25:ARG:HH11 | 41:BS:25:ARG:HB2 | 1.75 | 0.52 |
| 1:CA:411:A:N7 | 1:CA:429:U:C5 | 2.77 | 0.52 |
| 23:BA:271(C):G:N7 | 23:BA:421:U:H2' | 2.25 | 0.52 |
| 2:CB:31:TYR:O | 2:CB:42:ILE:HD12 | 2.09 | 0.52 |
| 7:AG:86:GLN:HB2 | 7:AG:148:ASN:ND2 | 2.23 | 0.52 |
| 1:CA:1408:A:H4' | 23:DA:1912:A:N6 | 2.25 | 0.52 |
| 23:DA:1917:U:C2' | 23:DA:1918:A:H5' | 2.40 | 0.52 |
| 23:DA:1130:U:O2 | 26:DD:149:ARG:NH2 | 2.41 | 0.52 |
| 23:DA:1027:A:C2 | 23:DA:2488:A:H5' | 2.44 | 0.52 |
| 23:DA:464:U:H4' | 52:D4:5:TRP:CZ3 | 2.44 | 0.52 |
| 23:BA:151:C:C2 | 23:BA:176:G:N2 | 2.77 | 0.52 |
| 3:CC:188:LEU:O | 3:CC:189:ALA:HB2 | 2.09 | 0.52 |
| 8:CH:42:GLU:HG3 | 8:CH:109:ILE:HD12 | 1.92 | 0.52 |
| 1:CA:420:U:O2 | 1:CA:424:G:N1 | 2.42 | 0.52 |
| 23:BA:2584:U:H5'' | 23:BA:2585:U:OP2 | 2.08 | 0.52 |
| 1:CA:1305:G:C8 | 1:CA:1305:G:OP2 | 2.62 | 0.52 |
| 1:AA:761:G:H2' | 1:AA:762:C:H6 | 1.75 | 0.52 |
| 5:AE:69:VAL:HG12 | 5:AE:71:LEU:HG | 1.92 | 0.52 |
| 52:B4:11:LYS:HD2 | 52:B4:15:THR:HG21 | 1.91 | 0.52 |
| 23:BA:2780:G:OP2 | 32:BJ:141:LYS:HD3 | 2.08 | 0.52 |
| 2:AB:182:ILE:O | 2:AB:182:ILE:HG22 | 2.08 | 0.52 |
| 28:BF:83:ARG:HG3 | 28:BF:84:LYS:N | 2.25 | 0.52 |
| 23:DA:861:A:N3 | 24:DB:79:C:O2' | 2.38 | 0.52 |
| 1:AA:674:G:H2' | 1:AA:675:A:C8 | 2.43 | 0.52 |
| 1:CA:376:G:O3' | 16:CP:5:ARG:HD2 | 2.09 | 0.52 |
| 40:BR:38:LEU:C | 40:BR:39:LEU:HD13 | 2.29 | 0.52 |
| 47:BY:6:VAL:CG1 | 47:BY:10:LEU:HD11 | 2.30 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:DC:181:GLU:HA | 25:DC:272:ALA:HB3 | 1.90 | 0.52 |
| 23:BA:1813:G:H1' | 25:BC:50:THR:CG2 | 2.31 | 0.52 |
| 28:DF:8:LYS:HD3 | 28:DF:9:ARG:CG | 2.40 | 0.52 |
| 23:BA:1589:C:C2 | 23:BA:1590:U:C5 | 2.97 | 0.52 |
| 3:CC:130:VAL:HA | 3:CC:133:ALA:HB3 | 1.90 | 0.52 |
| 23:BA:363(C):G:O2' | 23:BA:363(D):G:H5' | 2.10 | 0.52 |
| 23:BA:2886:G:N2 | 23:BA:2887:U:C2 | 2.78 | 0.52 |
| 26:DD:5:LEU:CB | 26:DD:51:PHE:HD2 | 2.17 | 0.52 |
| 23:BA:1785:A:O2' | 23:BA:1786:A:H2' | 2.10 | 0.52 |
| 1:AA:1107:C:C4 | 1:AA:1108:G:C8 | 2.97 | 0.52 |
| 1:AA:1346:A:H61 | 1:AA:1374:A:H3' | 1.74 | 0.52 |
| 23:BA:103:A:O5' | 23:BA:103:A:H8 | 1.92 | 0.52 |
| 46:BX:14:VAL:O | 46:BX:14:VAL:HG12 | 2.10 | 0.52 |
| 29:BG:46:GLU:O | 29:BG:49:VAL:HG22 | 2.09 | 0.52 |
| 23:DA:1506:C:H2' | 23:DA:1508:A:C8 | 2.44 | 0.52 |
| 25:BC:58:HIS:HD2 | 25:BC:59:LYS:O | 1.92 | 0.52 |
| 1:CA:620:C:H2' | 1:CA:621:A:O4' | 2.09 | 0.52 |
| 33:DK:63:VAL:HB | 33:DK:102:VAL:HG12 | 1.89 | 0.52 |
| 23:DA:598:G:H5' | 34:DL:15:ARG:HB3 | 1.91 | 0.52 |
| 23:BA:270(H):C:C5 | 23:BA:270(I):C:H5 | 2.28 | 0.52 |
| 1:CA:99:C:C2 | 1:CA:101:A:C8 | 2.97 | 0.52 |
| 15:AO:29:VAL:HG12 | 15:AO:85:LEU:CD1 | 2.39 | 0.52 |
| 23:DA:1476:C:C6 | 23:DA:1476:C:H3' | 2.42 | 0.52 |
| 23:DA:2100:G:H21 | 23:DA:2101:G:H1' | 1.74 | 0.52 |
| 23:DA:277:C:H3' | 23:DA:278:A:C5' | 2.39 | 0.52 |
| 1:CA:1051:C:N4 | 1:CA:1207:G:H1 | 2.06 | 0.52 |
| 23:BA:1184:G:C5 | 23:BA:1185:C:C5 | 2.98 | 0.52 |
| 3:CC:86:VAL:O | 3:CC:90:GLU:HG2 | 2.08 | 0.52 |
| 23:BA:1922:G:H2' | 23:BA:1923:U:O4' | 2.10 | 0.52 |
| 1:CA:1357:A:N7 | 1:CA:1358:U:C4 | 2.78 | 0.52 |
| 26:DD:25:VAL:C | 26:DD:26:ILE:HD13 | 2.29 | 0.52 |
| 35:BM:133:ARG:O | 35:BM:134:ARG:HB2 | 2.08 | 0.52 |
| 35:DM:43:THR:HG1 | 35:DM:45:GLN:HG2 | 1.74 | 0.52 |
| 23:BA:1709:U:H2' | 23:BA:1710:C:C6 | 2.44 | 0.52 |
| 23:BA:2093:G:H1 | 23:BA:2196:C:N4 | 2.08 | 0.52 |
| 23:DA:795:C:H2' | 23:DA:796:C:C6 | 2.43 | 0.52 |
| 41:BS:45:TYR:CG | 41:BS:45:TYR:O | 2.62 | 0.52 |
| 23:DA:415:A:H2' | 23:DA:416:C:C6 | 2.44 | 0.52 |
| 23:BA:2443:C:C2' | 23:BA:2444:G:H5' | 2.39 | 0.52 |
| 9:CI:95:LYS:HD3 | 9:CI:96:LEU:N | 2.25 | 0.52 |
| 7:AG:67:GLU:OE1 | 7:AG:70:LYS:HD2 | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 46:DX:67:ILE:HB | 46:DX:68:PRO:HD3 | 1.92 | 0.52 |
| 23:DA:1757:U:H2' | 23:DA:1758:G:OP1 | 2.09 | 0.52 |
| 1:CA:1246:C:H2' | 1:CA:1247:U:C6 | 2.44 | 0.52 |
| 8:AH:109:ILE:HG12 | 8:AH:110:ALA:N | 2.24 | 0.52 |
| 23:DA:459:U:H4' | 52:D4:40:TRP:CZ3 | 2.45 | 0.52 |
| 6:CF:97:PHE:CD2 | 18:CR:31:LEU:HD21 | 2.45 | 0.52 |
| 23:DA:2584:U:O5' | 23:DA:2584:U:H6 | 1.92 | 0.52 |
| 23:BA:77:C:O3' | 47:BY:7:ARG:NH1 | 2.43 | 0.52 |
| 50:B2:4:HIS:CB | 50:B2:5:PRO:HD3 | 2.39 | 0.52 |
| 23:BA:1543:A:H5' | 23:BA:1544:C:P | 2.49 | 0.52 |
| 25:BC:108:PRO:CB | 25:BC:143:HIS:HE1 | 2.23 | 0.52 |
| 40:BR:2:PHE:CE2 | 40:BR:13:ARG:CD | 2.85 | 0.52 |
| 23:DA:2296:U:O2 | 23:DA:2333:A:N3 | 2.43 | 0.52 |
| 25:BC:77:ALA:HB1 | 25:BC:96:HIS:O | 2.09 | 0.52 |
| 30:DH:142:VAL:O | 30:DH:143:SER:HB2 | 2.09 | 0.52 |
| 28:BF:25:TYR:OH | 28:BF:32:PRO:HD3 | 2.10 | 0.52 |
| 2:AB:174:VAL:O | 2:AB:178:ARG:CB | 2.50 | 0.52 |
| 23:BA:2713:A:H3' | 23:BA:2714:G:C5' | 2.39 | 0.52 |
| 20:AT:53:LEU:HD13 | 20:AT:102:GLY:HA3 | 1.91 | 0.52 |
| 37:DO:52:SER:O | 37:DO:53:SER:HB2 | 2.09 | 0.52 |
| 37:DO:65:VAL:O | 37:DO:69:VAL:HG12 | 2.08 | 0.52 |
| 11:AK:59:TYR:O | 11:AK:63:LEU:HG | 2.09 | 0.52 |
| 13:CM:84:ILE:CG2 | 19:CS:74:PHE:HE1 | 2.21 | 0.52 |
| 46:DX:13:ILE:O | 46:DX:14:VAL:HB | 2.10 | 0.52 |
| 1:AA:1351:U:H4' | 7:AG:33:ASP:OD2 | 2.09 | 0.52 |
| 23:DA:2396:G:H4' | 46:DX:31:GLY:HA2 | 1.92 | 0.52 |
| 30:BH:133:HIS:HD2 | 30:BH:135:GLU:HG2 | 1.72 | 0.52 |
| 23:BA:1104:C:C4 | 23:BA:1105:U:H5 | 2.28 | 0.52 |
| 23:BA:1109:C:N4 | 23:BA:1110:G:C2 | 2.78 | 0.52 |
| 25:DC:25:THR:HG21 | 25:DC:81:ALA:HB1 | 1.92 | 0.52 |
| 1:AA:617:G:H5' | 16:AP:45:THR:HG22 | 1.92 | 0.52 |
| 29:BG:44:VAL:HG12 | 29:BG:45:VAL:N | 2.20 | 0.52 |
| 30:BH:66:GLU:HB3 | 30:BH:67:ARG:NH1 | 2.23 | 0.52 |
| 43:DU:2:ARG:HG2 | 43:DU:3:VAL:N | 2.24 | 0.52 |
| 1:AA:1128:C:O2 | 1:AA:1130:A:N6 | 2.43 | 0.52 |
| 6:CF:78:GLU:HA | 6:CF:81:ILE:HD11 | 1.89 | 0.52 |
| 23:BA:389:G:H1 | 34:BL:71:VAL:HG23 | 1.75 | 0.52 |
| 11:AK:34:ASP:H | 11:AK:40:ILE:HD11 | 1.74 | 0.52 |
| 1:CA:1313:U:OP1 | 19:CS:6:LYS:HG3 | 2.10 | 0.52 |
| 1:AA:712:A:C6 | 1:AA:713:G:C6 | 2.98 | 0.52 |
| 23:DA:480:A:H2' | 23:DA:480:A:N3 | 2.24 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DA:336:C:O2 | 23:DA:336:C:C2' | 2.57 | 0.52 |
| 50:D2:52:TYR:O | 50:D2:52:TYR:CD1 | 2.62 | 0.52 |
| 23:BA:1952:A:C6 | 33:BK:22:ILE:CD1 | 2.93 | 0.52 |
| 23:DA:908:C:OP1 | 35:DM:22:LYS:HD2 | 2.08 | 0.52 |
| 2:CB:72:GLY:HA3 | 2:CB:165:VAL:HG11 | 1.91 | 0.52 |
| 1:CA:1412:C:H2' | 1:CA:1413:A:H8 | 1.75 | 0.52 |
| 1:AA:1411:C:H2' | 1:AA:1412:C:C6 | 2.44 | 0.52 |
| 23:BA:2460:U:C4 | 23:BA:2461:C:C5 | 2.97 | 0.52 |
| 23:DA:991:C:C6 | 23:DA:1185:C:N3 | 2.78 | 0.52 |
| 43:DU:90:LEU:HG | 43:DU:91:GLU:N | 2.23 | 0.52 |
| 1:CA:1387:G:H2' | 1:CA:1388:C:H6 | 1.73 | 0.52 |
| 46:DX:68:PRO:O | 46:DX:71:TYR:N | 2.42 | 0.52 |
| 9:CI:39:GLY:O | 9:CI:40:LEU:HD23 | 2.09 | 0.52 |
| 37:DO:67:ARG:HG3 | 37:DO:100:ALA:HB1 | 1.92 | 0.52 |
| 11:AK:85:ARG:HA | 11:AK:112:THR:OG1 | 2.09 | 0.52 |
| 23:BA:544:C:O5' | 23:BA:544:C:H6 | 1.93 | 0.52 |
| 44:BV:68:PRO:O | 44:BV:91:LEU:HB2 | 2.09 | 0.52 |
| 6:AF:97:PHE:CD2 | 18:AR:31:LEU:HD21 | 2.45 | 0.52 |
| 8:AH:54:ASP:O | 8:AH:56:LYS:HG3 | 2.10 | 0.52 |
| 34:DL:59:LEU:HD23 | 34:DL:59:LEU:C | 2.30 | 0.52 |
| 26:BD:201:THR:C | 26:BD:202:LYS:HD3 | 2.29 | 0.52 |
| 1:CA:977:A:N3 | 1:CA:977:A:H5'' | 2.24 | 0.52 |
| 53:B5:33:ASN:O | 53:B5:34:TRP:HB3 | 2.09 | 0.52 |
| 37:BO:12:PHE:C | 37:BO:12:PHE:HD1 | 2.12 | 0.52 |
| 2:CB:69:LEU:HD12 | 2:CB:70:PHE:N | 2.23 | 0.52 |
| 32:DJ:95:TYR:HB2 | 32:DJ:108:ILE:O | 2.10 | 0.52 |
| 12:AL:100:VAL:HG12 | 12:AL:100:VAL:O | 2.09 | 0.52 |
| 1:AA:551:U:H5' | 12:AL:118:LYS:HZ2 | 1.73 | 0.52 |
| 24:DB:103:U:C2' | 24:DB:104:A:H5' | 2.39 | 0.52 |
| 23:DA:1493:C:H4' | 23:DA:1494:A:OP1 | 2.09 | 0.52 |
| 23:DA:275:G:OP2 | 23:DA:363(A):G:N2 | 2.41 | 0.52 |
| 14:CN:24:CYS:HG | 14:CN:27:CYS:HG | 1.55 | 0.52 |
| 5:CE:11:ILE:HG12 | 5:CE:33:VAL:HG23 | 1.91 | 0.52 |
| 23:DA:2886:G:H2' | 23:DA:2887:U:H6 | 1.73 | 0.52 |
| 1:AA:1084:G:C5 | 1:AA:1085:U:C4 | 2.98 | 0.52 |
| 2:AB:205:ASP:C | 2:AB:207:ALA:H | 2.12 | 0.52 |
| 46:DX:11:ARG:HG3 | 46:DX:11:ARG:NH1 | 2.24 | 0.52 |
| 29:DG:21:PRO:HB2 | 29:DG:23:ARG:NH1 | 2.24 | 0.52 |
| 6:AF:22:GLU:OE1 | 6:AF:84:ASN:HB2 | 2.10 | 0.52 |
| 4:CD:105:VAL:CG1 | 4:CD:105:VAL:O | 2.57 | 0.52 |
| 23:DA:932:G:H4' | 23:DA:933:A:O5' | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:658:G:C5 | 1:AA:659:U:C5 | 2.98 | 0.52 |
| 23:BA:966:G:C5 | 23:BA:967:C:C5 | 2.98 | 0.52 |
| 23:BA:1324:G:C5 | 23:BA:1328:G:O6 | 2.63 | 0.52 |
| 53:B5:57:ARG:CZ | 53:B5:57:ARG:CB | 2.87 | 0.52 |
| 23:DA:379:G:N1 | 46:DX:20:ARG:NH2 | 2.56 | 0.52 |
| 32:DJ:70:ALA:HB2 | 32:DJ:135:LEU:HD11 | 1.90 | 0.52 |
| 2:AB:8:LYS:HG2 | 2:AB:217:ARG:NH1 | 2.24 | 0.52 |
| 25:BC:174:ILE:CD1 | 25:BC:174:ILE:N | 2.72 | 0.52 |
| 43:BU:19:LYS:HB3 | 43:BU:20:TYR:CD1 | 2.44 | 0.52 |
| 34:BL:10:PRO:CD | 34:BL:11:GLY:N | 2.69 | 0.52 |
| 23:BA:598:G:H5' | 34:BL:15:ARG:HB3 | 1.91 | 0.52 |
| 23:BA:773:U:H4' | 25:BC:47:GLY:CA | 2.39 | 0.52 |
| 23:DA:481:G:H4' | 23:DA:481:G:OP1 | 2.09 | 0.52 |
| 23:BA:1467:C:H42 | 23:BA:1525:G:H1 | 1.58 | 0.52 |
| 25:DC:30:GLU:CG | 25:DC:63:ARG:NH2 | 2.73 | 0.52 |
| 29:BG:88:LEU:O | 29:BG:162:ILE:HA | 2.09 | 0.52 |
| 1:CA:1055:A:N7 | 1:CA:1200:C:N4 | 2.53 | 0.52 |
| 1:CA:1056:U:H5 | 1:CA:1200:C:N4 | 2.08 | 0.52 |
| 23:BA:2865:U:C5 | 23:BA:2866:U:C4 | 2.98 | 0.52 |
| 23:DA:1590:U:O2 | 23:DA:1591:G:C8 | 2.63 | 0.52 |
| 23:DA:2352:A:H2' | 23:DA:2353:G:H5' | 1.90 | 0.52 |
| 1:CA:942:G:H21 | 9:CI:124:GLN:NE2 | 2.07 | 0.52 |
| 1:CA:1411:C:H2' | 1:CA:1412:C:C6 | 2.43 | 0.52 |
| 23:BA:988:A:H2' | 23:BA:989:G:O5' | 2.10 | 0.52 |
| 1:CA:632:A:N7 | 1:CA:633:G:C4 | 2.77 | 0.52 |
| 1:AA:1112:C:C4 | 3:AC:178:LEU:HD23 | 2.45 | 0.52 |
| 7:AG:47:CYS:O | 7:AG:58:PRO:HG3 | 2.10 | 0.52 |
| 1:CA:1494:G:N2 | 23:DA:1912:A:C2 | 2.78 | 0.52 |
| 44:DV:9:TYR:CG | 44:DV:35:ARG:NH1 | 2.78 | 0.52 |
| 13:CM:14:ARG:HB3 | 13:CM:16:ASP:OD2 | 2.09 | 0.52 |
| 46:BX:48:LYS:NZ | 46:BX:50:ARG:CZ | 2.72 | 0.52 |
| 30:DH:12:LEU:HD22 | 30:DH:12:LEU:H | 1.75 | 0.52 |
| 7:CG:79:ARG:HA | 7:CG:83:ALA:O | 2.10 | 0.52 |
| 23:BA:370:G:H4' | 23:BA:371:A:OP2 | 2.09 | 0.52 |
| 23:BA:811:U:OP2 | 34:BL:24:GLY:HA2 | 2.10 | 0.52 |
| 23:DA:270(S):G:H2' | 23:DA:270(T):G:C8 | 2.45 | 0.52 |
| 23:BA:491:G:O6 | 41:BS:49:LYS:HD3 | 2.10 | 0.52 |
| 4:CD:199:ASN:ND2 | 4:CD:202:LEU:HG | 2.24 | 0.52 |
| 31:BI:14:LYS:HE2 | 31:BI:14:LYS:HA | 1.91 | 0.52 |
| 50:B2:3:LYS:O | 50:B2:4:HIS:C | 2.48 | 0.52 |
| 7:CG:115:ARG:HB2 | 7:CG:118:VAL:HG11 | 1.90 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1346:A:C2 | 1:CA:1348:U:O4 | 2.63 | 0.52 |
| 1:CA:1352:C:H2' | 1:CA:1353:G:C8 | 2.45 | 0.52 |
| 23:DA:806:C:H6 | 23:DA:806:C:O5' | 1.93 | 0.52 |
| 1:CA:1226:C:H42 | 13:CM:104:ARG:HD2 | 1.73 | 0.52 |
| 23:BA:114(B):A:C4' | 32:BJ:48:ARG:HH22 | 2.21 | 0.52 |
| 32:BJ:95:TYR:HB2 | 32:BJ:108:ILE:O | 2.10 | 0.52 |
| 1:CA:376:G:H1 | 1:CA:387:U:H3 | 1.57 | 0.52 |
| 4:AD:51:PRO:HB3 | 4:AD:55:ALA:CB | 2.40 | 0.52 |
| 28:DF:19:LEU:HD11 | 28:DF:172:LEU:HD13 | 1.92 | 0.52 |
| 4:CD:21:LEU:HD12 | 4:CD:22:LYS:H | 1.73 | 0.52 |
| 23:DA:72:U:O4 | 23:DA:112:U:H4' | 2.09 | 0.52 |
| 1:CA:1107:C:C4 | 1:CA:1108:G:C8 | 2.98 | 0.52 |
| 45:BW:66:VAL:HG12 | 45:BW:67:VAL:N | 2.25 | 0.52 |
| 23:BA:1439:A:C8 | 23:BA:1440:G:C8 | 2.98 | 0.52 |
| 6:AF:88:VAL:HG12 | 6:AF:89:MET:N | 2.25 | 0.52 |
| 1:AA:332:G:O2' | 1:AA:333:G:H5' | 2.10 | 0.52 |
| 52:D4:12:ARG:HH11 | 52:D4:12:ARG:CG | 2.15 | 0.52 |
| 11:CK:34:ASP:HB2 | 11:CK:35:PRO:CD | 2.40 | 0.52 |
| 1:CA:819:A:N6 | 1:CA:1529:G:C5 | 2.78 | 0.52 |
| 10:CJ:13:HIS:CE1 | 10:CJ:14:LYS:HG3 | 2.44 | 0.52 |
| 1:CA:1237:C:OP1 | 1:CA:1238:A:H1' | 2.10 | 0.52 |
| 1:AA:353:A:C2' | 1:AA:354:G:OP2 | 2.57 | 0.52 |
| 23:DA:81:G:H21 | 43:DU:2:ARG:NH2 | 2.07 | 0.52 |
| 33:DK:28:SER:O | 33:DK:29:ASN:HB3 | 2.10 | 0.52 |
| 32:BJ:69:VAL:O | 32:BJ:70:ALA:HB3 | 2.10 | 0.52 |
| 1:AA:1052:U:H2' | 1:AA:1055:A:OP1 | 2.09 | 0.52 |
| 1:CA:512:U:O2' | 1:CA:513:C:H5' | 2.10 | 0.52 |
| 34:BL:86:LYS:HB3 | 34:BL:118:GLY:HA3 | 1.91 | 0.52 |
| 1:AA:1233:G:OP2 | 9:AI:124:GLN:HB2 | 2.09 | 0.52 |
| 23:DA:1414:G:C6 | 23:DA:1415:U:C4 | 2.97 | 0.52 |
| 23:DA:2352:A:C2' | 23:DA:2353:G:H5' | 2.39 | 0.52 |
| 1:AA:522:C:H2' | 1:AA:523:A:H5' | 1.90 | 0.52 |
| 7:CG:47:CYS:O | 7:CG:58:PRO:HG3 | 2.09 | 0.52 |
| 1:AA:334:C:O2' | 1:AA:335:C:H5' | 2.10 | 0.52 |
| 43:BU:59:GLY:C | 43:BU:61:ILE:H | 2.12 | 0.52 |
| 45:BW:14:ARG:CZ | 45:BW:14:ARG:CB | 2.86 | 0.52 |
| 1:AA:224:C:C2 | 1:AA:225:C:C5 | 2.98 | 0.52 |
| 23:BA:2058:A:C6 | 23:BA:2059:A:N6 | 2.78 | 0.52 |
| 38:BP:81:PRO:C | 38:BP:82:LEU:HD23 | 2.29 | 0.52 |
| 1:AA:356:A:H2' | 1:AA:357:G:H8 | 1.73 | 0.52 |
| 1:CA:294:U:C2 | 1:CA:295:C:C5 | 2.98 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:AG:80:VAL:CG2 | 7:AG:83:ALA:HB3 | 2.40 | 0.52 |
| 46:DX:48:LYS:NZ | 46:DX:50:ARG:NH1 | 2.57 | 0.52 |
| 1:CA:156:G:C2 | 1:CA:166:G:C2 | 2.98 | 0.52 |
| 26:DD:173:VAL:HG12 | 26:DD:174:ASP:H | 1.74 | 0.52 |
| 23:BA:527:C:O2 | 23:BA:527:C:O4' | 2.28 | 0.52 |
| 49:D1:43:GLY:O | 49:D1:44:CYS:HB3 | 2.08 | 0.52 |
| 23:BA:948:G:N2 | 23:BA:970:C:O2 | 2.42 | 0.52 |
| 30:BH:29:TYR:C | 30:BH:32:PRO:HD2 | 2.30 | 0.52 |
| 1:AA:1246:C:H2' | 1:AA:1247:U:C6 | 2.45 | 0.52 |
| 23:DA:2415:G:H1' | 34:DL:67:MET:CE | 2.37 | 0.52 |
| 22:AV:6189:G:C6 | 22:AV:6190:U:C4 | 2.98 | 0.52 |
| 34:BL:47:ASP:OD1 | 34:BL:49:ARG:N | 2.42 | 0.52 |
| 23:DA:568:U:O4 | 40:DR:78:LYS:CE | 2.58 | 0.52 |
| 2:AB:102:LEU:N | 2:AB:102:LEU:HD12 | 2.24 | 0.52 |
| 46:BX:73:LEU:HG | 46:BX:73:LEU:O | 2.08 | 0.52 |
| 36:DN:66:VAL:HG13 | 36:DN:70:LEU:HD12 | 1.92 | 0.52 |
| 36:BN:10:LEU:CB | 36:BN:17:ARG:NE | 2.70 | 0.52 |
| 1:CA:878:G:C5' | 8:CH:89:PRO:HG2 | 2.40 | 0.52 |
| 23:BA:1344:G:H5' | 23:BA:1384:A:C6 | 2.44 | 0.52 |
| 46:BX:19:GLN:O | 46:BX:20:ARG:HG3 | 2.10 | 0.52 |
| 40:DR:64:HIS:HD2 | 40:DR:92:THR:CG2 | 2.21 | 0.52 |
| 25:DC:25:THR:HG22 | 25:DC:82:ILE:N | 2.25 | 0.52 |
| 23:DA:1047:G:H1' | 23:DA:1110:G:N2 | 2.24 | 0.52 |
| 23:BA:780:G:H21 | 23:BA:783:A:N6 | 2.03 | 0.52 |
| 1:AA:68:G:C6 | 1:AA:69:G:N7 | 2.78 | 0.52 |
| 23:BA:389:G:C6 | 34:BL:71:VAL:HG23 | 2.44 | 0.52 |
| 23:DA:284:U:H2' | 23:DA:285:C:C6 | 2.45 | 0.52 |
| 38:BP:88:ILE:HG13 | 38:BP:89:VAL:N | 2.24 | 0.52 |
| 27:DE:36:VAL:HG11 | 27:DE:183:VAL:HG11 | 1.90 | 0.52 |
| 1:CA:527:G:O2' | 1:CA:528:C:H5' | 2.10 | 0.52 |
| 32:BJ:59:GLY:O | 32:BJ:65:TRP:CE3 | 2.63 | 0.52 |
| 45:DW:50:ASN:O | 45:DW:62:LEU:HB2 | 2.10 | 0.52 |
| 45:DW:31:VAL:HG11 | 45:DW:67:VAL:HG23 | 1.92 | 0.52 |
| 48:DZ:11:SER:OG | 48:DZ:13:ILE:HG13 | 2.10 | 0.52 |
| 28:DF:10:LYS:O | 28:DF:14:GLU:HB3 | 2.09 | 0.52 |
| 1:AA:862:C:H2' | 1:AA:863:U:C5' | 2.40 | 0.52 |
| 23:BA:277:C:H3' | 23:BA:278:A:C5' | 2.40 | 0.52 |
| 1:AA:109:A:N7 | 1:AA:326:G:C4 | 2.78 | 0.52 |
| 23:DA:2461:C:O2 | 23:DA:2461:C:C2' | 2.55 | 0.52 |
| 26:BD:179:GLU:HB3 | 26:BD:181:LEU:HD22 | 1.92 | 0.52 |
| 45:BW:14:ARG:CZ | 45:BW:14:ARG:HB2 | 2.40 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DA:2317:C:C2' | 23:DA:2318:G:H5' | 2.40 | 0.52 |
| 23:BA:2317:C:C2' | 23:BA:2318:G:H5' | 2.40 | 0.52 |
| 43:DU:59:GLY:C | 43:DU:61:ILE:H | 2.12 | 0.52 |
| 23:DA:1028:A:N3 | 23:DA:2486:G:O2' | 2.29 | 0.52 |
| 1:AA:137:C:O2' | 1:AA:138:G:H5' | 2.10 | 0.52 |
| 3:AC:121:ALA:HB1 | 3:AC:188:LEU:O | 2.10 | 0.52 |
| 23:BA:2028:U:O4 | 23:BA:2033:A:OP1 | 2.27 | 0.52 |
| 23:DA:1235:G:C6 | 23:DA:1236:G:N1 | 2.78 | 0.52 |
| 30:DH:29:TYR:C | 30:DH:32:PRO:HD2 | 2.29 | 0.52 |
| 23:DA:1301:A:N3 | 23:DA:1301:A:H2' | 2.24 | 0.52 |
| 23:DA:900:A:C4 | 23:DA:901:A:C8 | 2.97 | 0.52 |
| 23:DA:1636:C:H2' | 23:DA:1637:A:C8 | 2.43 | 0.52 |
| 28:BF:18:GLU:HG2 | 28:BF:175:LEU:HD22 | 1.91 | 0.52 |
| 17:AQ:11:VAL:O | 17:AQ:11:VAL:HG13 | 2.10 | 0.52 |
| 23:DA:2342:C:O2' | 23:DA:2374:C:H5'' | 2.08 | 0.52 |
| 26:DD:201:THR:C | 26:DD:202:LYS:HD3 | 2.27 | 0.52 |
| 1:CA:1369:C:H2' | 1:CA:1370:G:O4' | 2.10 | 0.52 |
| 10:CJ:63:PHE:HB3 | 14:CN:57:ARG:O | 2.10 | 0.52 |
| 38:BP:75:ILE:O | 38:BP:75:ILE:HG22 | 2.10 | 0.52 |
| 23:BA:568:U:O4 | 40:BR:78:LYS:HE2 | 2.09 | 0.52 |
| 26:BD:137:HIS:HB3 | 26:BD:138:PRO:HD2 | 1.90 | 0.52 |
| 34:DL:47:ASP:OD1 | 34:DL:49:ARG:N | 2.43 | 0.52 |
| 6:AF:86:ARG:O | 6:AF:87:ARG:CB | 2.50 | 0.52 |
| 1:AA:673:G:H5'' | 6:AF:87:ARG:NH1 | 2.24 | 0.52 |
| 47:BY:16:LEU:HB2 | 47:BY:20:GLU:HG3 | 1.92 | 0.52 |
| 23:DA:1210:A:H5' | 23:DA:1210:A:H8 | 1.73 | 0.52 |
| 4:CD:30:LYS:C | 4:CD:32:ALA:H | 2.13 | 0.52 |
| 4:CD:9:CYS:SG | 4:CD:32:ALA:HB2 | 2.50 | 0.52 |
| 5:CE:41:VAL:HG12 | 5:CE:112:LEU:O | 2.09 | 0.52 |
| 23:DA:2723:C:OP2 | 26:DD:109:LYS:NZ | 2.42 | 0.52 |
| 41:BS:19:LEU:HB3 | 50:B2:25:LEU:HD11 | 1.90 | 0.52 |
| 30:BH:113:ARG:HB2 | 30:BH:130:TYR:CE1 | 2.42 | 0.52 |
| 23:BA:84:A:C2 | 23:BA:98:G:N3 | 2.78 | 0.52 |
| 2:CB:25:ASN:HB3 | 2:CB:26:PRO:HD2 | 1.91 | 0.52 |
| 6:CF:22:GLU:O | 6:CF:26:ILE:HG13 | 2.10 | 0.52 |
| 1:AA:318:G:O2' | 1:AA:319:G:H5' | 2.09 | 0.52 |
| 33:DK:97:ARG:H | 33:DK:117:LEU:CD2 | 2.23 | 0.52 |
| 35:BM:8:LYS:HG3 | 35:BM:9:TYR:N | 2.24 | 0.52 |
| 16:CP:39:TYR:CD2 | 16:CP:40:ASP:N | 2.78 | 0.52 |
| 9:AI:103:THR:HG22 | 9:AI:105:ASP:H | 1.75 | 0.52 |
| 25:DC:120:GLY:HA2 | 25:DC:190:TYR:OH | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DA:1478:G:N2 | 23:DA:1479:G:C4 | 2.77 | 0.52 |
| 23:BA:1952:A:C5 | 33:BK:22:ILE:CD1 | 2.93 | 0.52 |
| 20:CT:13:LEU:N | 20:CT:13:LEU:HD12 | 2.22 | 0.52 |
| 23:BA:2287:A:C6 | 23:BA:2289:G:C4 | 2.98 | 0.52 |
| 44:DV:58:VAL:HG11 | 44:DV:66:SER:HB2 | 1.92 | 0.52 |
| 1:AA:1022:G:H2' | 1:AA:1023:G:C8 | 2.43 | 0.52 |
| 12:AL:6:ILE:HD12 | 12:AL:6:ILE:N | 2.25 | 0.52 |
| 6:CF:18:GLN:O | 6:CF:21:LEU:HB2 | 2.09 | 0.52 |
| 23:DA:2862:G:C6 | 23:DA:2863:C:C4 | 2.98 | 0.52 |
| 24:DB:55:U:O2' | 24:DB:56:G:H5' | 2.10 | 0.52 |
| 44:DV:68:PRO:HG2 | 44:DV:91:LEU:O | 2.09 | 0.52 |
| 23:BA:1993:U:H4' | 26:BD:128:SER:CB | 2.40 | 0.52 |
| 23:BA:1636:C:H2' | 23:BA:1637:A:C8 | 2.45 | 0.52 |
| 35:DM:84:GLY:HA3 | 45:DW:10:THR:CG2 | 2.39 | 0.52 |
| 1:CA:1381:U:O2' | 1:CA:1382:C:H5' | 2.10 | 0.52 |
| 23:DA:2020:A:OP1 | 39:DQ:27:LEU:HB2 | 2.09 | 0.52 |
| 25:DC:168:ARG:O | 25:DC:169:GLU:HB2 | 2.10 | 0.52 |
| 4:CD:23:GLY:CA | 4:CD:112:VAL:HG22 | 2.40 | 0.52 |
| 1:AA:1508:G:H2' | 1:AA:1509:C:O4' | 2.09 | 0.52 |
| 27:DE:179:GLU:CD | 27:DE:179:GLU:H | 2.12 | 0.52 |
| 46:BX:52:ARG:O | 46:BX:56:GLN:O | 2.27 | 0.52 |
| 34:DL:86:LYS:HB3 | 34:DL:118:GLY:HA3 | 1.91 | 0.52 |
| 34:BL:128:HIS:CA | 34:BL:147:LEU:HB3 | 2.10 | 0.52 |
| 28:BF:92:VAL:O | 28:BF:92:VAL:HG13 | 2.09 | 0.52 |
| 53:D5:60:LEU:HD23 | 53:D5:60:LEU:N | 2.25 | 0.52 |
| 23:DA:253:C:H2' | 23:DA:254:G:O4' | 2.10 | 0.52 |
| 39:BQ:90:VAL:O | 39:BQ:92:ARG:N | 2.43 | 0.52 |
| 23:DA:2731:G:C6 | 23:DA:2732:G:C6 | 2.98 | 0.52 |
| 23:DA:2335:A:N7 | 23:DA:2337:G:C5 | 2.78 | 0.52 |
| 25:DC:127:VAL:HA | 25:DC:193:VAL:HG12 | 1.92 | 0.52 |
| 23:DA:1799:G:H8 | 25:DC:181:GLU:CD | 2.14 | 0.52 |
| 1:AA:414:A:H2' | 1:AA:415:A:H8 | 1.75 | 0.52 |
| 1:AA:689:C:OP1 | 11:AK:27:ASN:ND2 | 2.43 | 0.52 |
| 28:BF:161:THR:C | 28:BF:163:ALA:H | 2.11 | 0.52 |
| 23:BA:322:A:OP1 | 27:BE:168:ARG:HD3 | 2.10 | 0.52 |
| 5:CE:10:MET:HA | 5:CE:32:VAL:HA | 1.91 | 0.52 |
| 24:BB:73:A:C4 | 24:BB:74:U:C6 | 2.98 | 0.52 |
| 1:AA:1068:G:H8 | 1:AA:1068:G:OP2 | 1.92 | 0.52 |
| 5:AE:18:ARG:HH21 | 5:AE:25:ARG:CB | 2.23 | 0.52 |
| 1:CA:406:G:H2' | 1:CA:407:G:H8 | 1.75 | 0.52 |
| 46:BX:86:SER:HB3 | 46:BX:89:GLU:HB2 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:1151:A:HO2' | 1:AA:1152:A:H8 | 1.51 | 0.52 |
| 1:AA:11:G:C6 | 1:AA:12:U:C4 | 2.98 | 0.52 |
| 36:BN:63:ARG:HA | 36:BN:80:PHE:CE2 | 2.45 | 0.52 |
| 23:DA:1105:U:C2 | 23:DA:1106:G:C8 | 2.98 | 0.52 |
| 40:DR:98:GLU:HG2 | 40:DR:100:ARG:CD | 2.39 | 0.52 |
| 32:DJ:62:ARG:NH2 | 32:DJ:64:ASP:OD2 | 2.38 | 0.52 |
| 1:AA:600:C:H2' | 1:AA:601:C:H6 | 1.73 | 0.52 |
| 1:AA:105:G:C4 | 1:AA:106:C:C5 | 2.98 | 0.52 |
| 23:BA:1680:U:C2' | 23:BA:1681:G:O5' | 2.58 | 0.52 |
| 35:BM:20:ALA:HB2 | 35:BM:99:PRO:HB2 | 1.91 | 0.52 |
| 50:B2:52:TYR:O | 50:B2:52:TYR:CD1 | 2.63 | 0.52 |
| 24:DB:75:G:H21 | 44:DV:85:HIS:CE1 | 2.27 | 0.52 |
| 1:AA:939:G:H2' | 1:AA:940:C:C6 | 2.44 | 0.52 |
| 23:DA:2721:A:H1' | 23:DA:2873:A:O2' | 2.08 | 0.52 |
| 1:AA:754:C:O5' | 15:AO:72:ARG:NH2 | 2.43 | 0.52 |
| 23:DA:1922:G:H2' | 23:DA:1923:U:O4' | 2.10 | 0.52 |
| 23:BA:2215:G:OP2 | 23:BA:2215:G:H8 | 1.93 | 0.52 |
| 1:CA:563:A:C8 | 1:CA:567:G:H1' | 2.44 | 0.52 |
| 23:DA:779:U:P | 25:DC:49:ILE:HD12 | 2.50 | 0.52 |
| 23:BA:2506:U:C5 | 23:BA:2507:C:H5 | 2.27 | 0.52 |
| 1:CA:577:G:C5 | 1:CA:578:C:C5 | 2.99 | 0.52 |
| 12:AL:61:SER:C | 12:AL:63:TYR:H | 2.12 | 0.52 |
| 1:CA:1389:C:H2' | 1:CA:1390:U:O4' | 2.09 | 0.52 |
| 23:DA:1850:G:C5 | 23:DA:1851:U:C5 | 2.98 | 0.52 |
| 51:D3:11:LEU:O | 51:D3:24:GLU:HB2 | 2.10 | 0.52 |
| 1:CA:1325:C:O3' | 21:CU:17:THR:HG21 | 2.10 | 0.52 |
| 23:BA:2046:G:O5' | 50:B2:19:ARG:HA | 2.09 | 0.52 |
| 23:DA:36:G:C5 | 23:DA:37:C:C5 | 2.98 | 0.52 |
| 44:DV:152:ALA:C | 44:DV:154:ASP:H | 2.13 | 0.52 |
| 23:DA:466:A:H5'' | 23:DA:467:G:OP2 | 2.10 | 0.52 |
| 10:CJ:30:SER:HB2 | 10:CJ:80:LYS:CG | 2.40 | 0.52 |
| 30:BH:1:MET:HG3 | 30:BH:23:PRO:HG3 | 1.92 | 0.52 |
| 1:AA:801:U:H2' | 1:AA:802:A:C8 | 2.45 | 0.52 |
| 43:BU:8:LYS:NZ | 43:BU:8:LYS:H | 2.02 | 0.51 |
| 43:BU:8:LYS:HD2 | 43:BU:13:VAL:CG2 | 2.40 | 0.51 |
| 1:CA:790:A:H5' | 22:CV:6192:G:H4' | 1.91 | 0.51 |
| 23:DA:943:U:OP2 | 34:DL:38:GLN:CD | 2.48 | 0.51 |
| 34:BL:114:ILE:H | 34:BL:114:ILE:CD1 | 2.01 | 0.51 |
| 39:DQ:102:GLU:N | 39:DQ:103:PRO:CD | 2.74 | 0.51 |
| 39:DQ:92:ARG:HH22 | 40:DR:11:GLN:H | 1.55 | 0.51 |
| 23:DA:593:G:H4' | 53:D5:62:LEU:CD1 | 2.40 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:DF:86:MET:N | 28:DF:87:PRO:HD3 | 2.25 | 0.51 |
| 32:DJ:93:LYS:HE3 | 32:DJ:95:TYR:CE1 | 2.35 | 0.51 |
| 1:AA:407:G:H4' | 4:AD:116:GLN:HA | 1.92 | 0.51 |
| 4:CD:64:LEU:HD12 | 4:CD:64:LEU:O | 2.10 | 0.51 |
| 25:BC:31:LYS:O | 25:BC:36:PRO:HD3 | 2.11 | 0.51 |
| 52:D4:19:ARG:NH1 | 52:D4:19:ARG:CB | 2.73 | 0.51 |
| 30:DH:97:ILE:O | 30:DH:101:LEU:HB2 | 2.11 | 0.51 |
| 4:AD:21:LEU:HD12 | 4:AD:22:LYS:H | 1.75 | 0.51 |
| 24:DB:45:A:H1' | 28:DF:95:ARG:CZ | 2.40 | 0.51 |
| 49:D1:51:TYR:O | 49:D1:52:SER:HB2 | 2.09 | 0.51 |
| 28:BF:69:ALA:O | 28:BF:90:LEU:HD13 | 2.10 | 0.51 |
| 5:CE:41:VAL:CG1 | 5:CE:113:ALA:HA | 2.39 | 0.51 |
| 23:DA:2688:U:O2 | 23:DA:2688:U:C3' | 2.57 | 0.51 |
| 1:AA:1353:G:OP2 | 1:AA:1353:G:H8 | 1.92 | 0.51 |
| 9:AI:10:ARG:CD | 9:AI:11:LYS:HG3 | 2.39 | 0.51 |
| 36:DN:47:PHE:CE2 | 36:DN:51:LEU:HD11 | 2.45 | 0.51 |
| 36:DN:48:VAL:O | 36:DN:51:LEU:N | 2.43 | 0.51 |
| 6:CF:63:TYR:O | 6:CF:65:VAL:HG12 | 2.09 | 0.51 |
| 18:AR:76:LEU:HD22 | 18:AR:76:LEU:N | 2.24 | 0.51 |
| 43:BU:95:LYS:HE2 | 43:BU:100:ALA:HB2 | 1.91 | 0.51 |
| 10:CJ:13:HIS:HB3 | 10:CJ:68:HIS:NE2 | 2.25 | 0.51 |
| 23:DA:379:G:C2 | 46:DX:20:ARG:NH2 | 2.77 | 0.51 |
| 23:DA:389:G:C6 | 34:DL:71:VAL:HG23 | 2.45 | 0.51 |
| 1:CA:782:A:C2 | 1:CA:801:U:O2 | 2.63 | 0.51 |
| 25:BC:265:PRO:C | 25:BC:267:SER:N | 2.62 | 0.51 |
| 38:DP:88:ILE:HG13 | 38:DP:89:VAL:N | 2.25 | 0.51 |
| 23:BA:2480:C:N4 | 23:BA:2481:G:C6 | 2.78 | 0.51 |
| 43:BU:63:LYS:HG3 | 43:BU:64:GLU:N | 2.23 | 0.51 |
| 9:CI:114:TYR:HD2 | 9:CI:114:TYR:N | 2.08 | 0.51 |
| 23:BA:286:C:H2' | 23:BA:287:C:C6 | 2.39 | 0.51 |
| 23:BA:909:A:C2 | 23:BA:912:C:C6 | 2.98 | 0.51 |
| 23:DA:774:A:H2 | 23:DA:787:U:O2' | 1.92 | 0.51 |
| 23:BA:2432:A:H5" | 23:BA:2433:A:OP2 | 2.09 | 0.51 |
| 3:AC:23:TYR:HB2 | 10:AJ:93:GLY:O | 2.10 | 0.51 |
| 3:CC:175:LEU:HD11 | 3:CC:201:TYR:HE2 | 1.75 | 0.51 |
| 3:AC:76:VAL:HG23 | 3:AC:77:ILE:HG13 | 1.92 | 0.51 |
| 19:CS:31:ILE:CG2 | 19:CS:49:ILE:HA | 2.39 | 0.51 |
| 1:AA:1112:C:H42 | 3:AC:177:THR:HA | 1.75 | 0.51 |
| 23:BA:480:A:OP2 | 43:BU:46:LYS:HE2 | 2.09 | 0.51 |
| 1:CA:1112:C:O2 | 3:CC:179:ARG:HD3 | 2.11 | 0.51 |
| 1:CA:780:A:C2 | 1:CA:803:G:N1 | 2.78 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:BA:1893:C:C6 | 23:BA:1894:C:C5 | 2.99 | 0.51 |
| 1:CA:1502:A:C8 | 1:CA:1505:G:N2 | 2.77 | 0.51 |
| 41:DS:45:TYR:CD2 | 41:DS:45:TYR:C | 2.84 | 0.51 |
| 9:AI:86:VAL:HG23 | 9:AI:93:ARG:HB2 | 1.90 | 0.51 |
| 28:BF:18:GLU:HG2 | 28:BF:175:LEU:CD2 | 2.40 | 0.51 |
| 23:BA:699:A:H2' | 23:BA:700:G:O4' | 2.09 | 0.51 |
| 1:AA:575:G:OP1 | 1:AA:575:G:H4' | 2.11 | 0.51 |
| 23:DA:449:A:C2' | 23:DA:450:G:H5' | 2.40 | 0.51 |
| 1:CA:1037:C:H2' | 1:CA:1038:C:H6 | 1.75 | 0.51 |
| 44:DV:165:VAL:HG23 | 44:DV:166:SER:O | 2.10 | 0.51 |
| 7:CG:38:LEU:O | 7:CG:42:ILE:HG13 | 2.09 | 0.51 |
| 26:DD:24:THR:HG22 | 26:DD:186:GLY:H | 1.74 | 0.51 |
| 1:AA:1061:G:O4' | 10:AJ:56:HIS:CE1 | 2.63 | 0.51 |
| 38:DP:54:ARG:CG | 38:DP:54:ARG:NH1 | 2.60 | 0.51 |
| 38:BP:64:ARG:HD2 | 38:BP:73:GLU:CG | 2.40 | 0.51 |
| 26:BD:132:HIS:CD2 | 26:BD:135:HIS:CE1 | 2.97 | 0.51 |
| 28:BF:76:SER:HB2 | 28:BF:83:ARG:CA | 2.40 | 0.51 |
| 25:BC:127:VAL:HA | 25:BC:193:VAL:CG1 | 2.40 | 0.51 |
| 24:DB:81:G:C6 | 24:DB:82:G:N7 | 2.78 | 0.51 |
| 1:AA:376:G:O2' | 1:AA:377:G:C5' | 2.59 | 0.51 |
| 3:AC:182:ILE:HD11 | 3:AC:203:PHE:CD1 | 2.45 | 0.51 |
| 4:AD:109:GLY:C | 4:AD:111:ALA:H | 2.13 | 0.51 |
| 4:AD:144:ASP:O | 4:AD:146:ILE:HG13 | 2.10 | 0.51 |
| 12:AL:31:PHE:CB | 12:AL:83:LEU:HD11 | 2.40 | 0.51 |
| 3:CC:172:ARG:HE | 3:CC:174:PRO:HG2 | 1.75 | 0.51 |
| 24:DB:40:U:O2 | 24:DB:43:C:C6 | 2.63 | 0.51 |
| 29:BG:35:VAL:HG21 | 29:BG:75:ALA:CB | 2.41 | 0.51 |
| 23:DA:141(A):A:N6 | 23:DA:1596:A:H5' | 2.26 | 0.51 |
| 5:CE:11:ILE:CB | 5:CE:31:LEU:HD13 | 2.39 | 0.51 |
| 20:AT:57:ARG:HH12 | 20:AT:102:GLY:HA2 | 1.71 | 0.51 |
| 1:AA:1101:A:N3 | 1:AA:1102:A:H1' | 2.25 | 0.51 |
| 1:CA:408:A:C4 | 1:CA:409:G:C8 | 2.98 | 0.51 |
| 23:BA:2352:A:C2' | 23:BA:2353:G:H5' | 2.40 | 0.51 |
| 23:DA:2090:G:H21 | 46:DX:45:ASN:HD21 | 1.59 | 0.51 |
| 46:DX:62:VAL:CG2 | 46:DX:63:ALA:N | 2.73 | 0.51 |
| 23:BA:95:G:N2 | 23:BA:96:G:H1' | 2.25 | 0.51 |
| 10:AJ:13:HIS:HB3 | 10:AJ:68:HIS:NE2 | 2.24 | 0.51 |
| 8:AH:20:TYR:HD1 | 8:AH:65:TYR:CE2 | 2.28 | 0.51 |
| 12:AL:52:ARG:HH11 | 12:AL:52:ARG:HG2 | 1.71 | 0.51 |
| 23:DA:2305:A:H3' | 23:DA:2306:C:H5'' | 1.92 | 0.51 |
| 5:CE:48:ALA:O | 5:CE:50:GLU:N | 2.43 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:AS:25:LYS:HB3 | 19:AS:27:GLU:OE1 | 2.10 | 0.51 |
| 23:BA:1567:A:H5'' | 25:BC:58:HIS:CD2 | 2.45 | 0.51 |
| 23:BA:1487:G:O2' | 23:BA:1488:G:H5' | 2.10 | 0.51 |
| 25:BC:25:THR:HG21 | 25:BC:82:ILE:N | 2.26 | 0.51 |
| 1:CA:1068:G:N7 | 1:CA:1094:G:C8 | 2.78 | 0.51 |
| 23:BA:2482:G:H2' | 23:BA:2483:C:O4' | 2.11 | 0.51 |
| 50:D2:40:LYS:HZ1 | 50:D2:49:CYS:CB | 2.22 | 0.51 |
| 4:CD:13:ARG:CD | 4:CD:38:TYR:O | 2.59 | 0.51 |
| 23:BA:1390:U:O2' | 23:BA:1391:U:H5' | 2.10 | 0.51 |
| 23:BA:1568:G:H5'' | 25:BC:61:LEU:HD22 | 1.92 | 0.51 |
| 4:CD:79:PHE:CE1 | 4:CD:204:ILE:HA | 2.45 | 0.51 |
| 10:CJ:10:GLY:HA3 | 10:CJ:16:LEU:HD21 | 1.92 | 0.51 |
| 23:DA:1680:U:O2 | 23:DA:1763:G:H3' | 2.10 | 0.51 |
| 23:BA:975:G:H1' | 23:BA:990:A:C2 | 2.45 | 0.51 |
| 23:BA:1862:G:H2' | 23:BA:1863:G:C8 | 2.43 | 0.51 |
| 1:CA:433:C:H2' | 1:CA:434:U:C6 | 2.41 | 0.51 |
| 23:BA:480:A:N3 | 23:BA:480:A:H2' | 2.25 | 0.51 |
| 23:BA:17:G:H4' | 39:BQ:25:TRP:CZ3 | 2.45 | 0.51 |
| 1:AA:1298:C:N4 | 7:AG:114:ARG:HD3 | 2.25 | 0.51 |
| 23:DA:1894:C:H2' | 23:DA:1895:C:H6 | 1.75 | 0.51 |
| 27:BE:110:LEU:HD11 | 27:BE:181:LEU:HD13 | 1.92 | 0.51 |
| 1:CA:191(D):U:H2' | 1:CA:191(E):G:C8 | 2.44 | 0.51 |
| 23:BA:2345:G:OP2 | 51:B3:39:TYR:HA | 2.09 | 0.51 |
| 23:DA:2718:G:H2' | 23:DA:2719:G:C8 | 2.45 | 0.51 |
| 23:BA:1232:G:C5 | 23:BA:1233:C:C5 | 2.98 | 0.51 |
| 23:BA:2689:U:P | 23:BA:2719:G:H22 | 2.34 | 0.51 |
| 7:AG:70:LYS:CG | 7:AG:96:GLN:HB3 | 2.39 | 0.51 |
| 23:DA:1993:U:H4' | 26:DD:128:SER:HB3 | 1.92 | 0.51 |
| 1:CA:128:G:O2' | 17:CQ:3:LYS:HE2 | 2.09 | 0.51 |
| 23:DA:769:G:C2' | 23:DA:770:G:H5' | 2.40 | 0.51 |
| 23:DA:771:G:H2' | 23:DA:772:C:H6 | 1.75 | 0.51 |
| 2:AB:17:PHE:CB | 2:AB:44:LEU:HD21 | 2.39 | 0.51 |
| 23:BA:2027:G:H2' | 23:BA:2028:U:O4' | 2.10 | 0.51 |
| 43:BU:11:ASP:OD1 | 43:BU:12:THR:N | 2.43 | 0.51 |
| 23:DA:2473:U:C4 | 23:DA:2474:C:C4 | 2.98 | 0.51 |
| 23:DA:537:C:H2' | 23:DA:539:G:H8 | 1.75 | 0.51 |
| 23:BA:1932:A:H2' | 23:BA:1933:G:O4' | 2.11 | 0.51 |
| 23:BA:851:U:O2 | 23:BA:928:G:C2 | 2.63 | 0.51 |
| 23:BA:771:G:H2' | 23:BA:772:C:H6 | 1.76 | 0.51 |
| 23:BA:2734:A:H2' | 23:BA:2735:G:H5' | 1.93 | 0.51 |
| 53:D5:57:ARG:CB | 53:D5:57:ARG:CZ | 2.87 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BA:2330:G:O2' | 45:BW:41:ARG:HB2 | 2.09 | 0.51 |
| 43:DU:9:LYS:O | 43:DU:27:VAL:HG21 | 2.09 | 0.51 |
| 34:DL:32:THR:HG21 | 34:DL:37:GLY:N | 2.25 | 0.51 |
| 23:DA:197:A:H8 | 23:DA:197:A:C5' | 2.14 | 0.51 |
| 28:DF:82:LEU:HD22 | 28:DF:87:PRO:HG3 | 1.92 | 0.51 |
| 16:CP:19:ILE:HG22 | 16:CP:19:ILE:O | 2.08 | 0.51 |
| 39:BQ:106:PHE:O | 39:BQ:110:VAL:HG23 | 2.11 | 0.51 |
| 16:AP:18:ARG:HD3 | 16:AP:35:LYS:HE3 | 1.91 | 0.51 |
| 3:CC:18:TRP:HD1 | 14:CN:54:PRO:HA | 1.72 | 0.51 |
| 12:AL:26:LEU:O | 12:AL:28:GLY:N | 2.43 | 0.51 |
| 4:CD:104:VAL:C | 4:CD:106:TYR:H | 2.14 | 0.51 |
| 25:DC:44:ASN:CG | 25:DC:45:ASN:H | 2.12 | 0.51 |
| 2:AB:175:ARG:O | 2:AB:178:ARG:HB3 | 2.10 | 0.51 |
| 1:CA:37:U:OP2 | 12:CL:122:LYS:HE3 | 2.09 | 0.51 |
| 3:CC:14:ILE:HG23 | 3:CC:15:THR:N | 2.14 | 0.51 |
| 34:DL:16:ARG:NH2 | 34:DL:18:ARG:N | 2.57 | 0.51 |
| 5:AE:111:GLU:C | 5:AE:113:ALA:H | 2.13 | 0.51 |
| 5:AE:14:ARG:NH1 | 5:AE:129:ILE:HD11 | 2.25 | 0.51 |
| 23:BA:142:G:H2' | 23:BA:143:C:C6 | 2.46 | 0.51 |
| 8:AH:91:ARG:HG3 | 8:AH:91:ARG:NH1 | 2.24 | 0.51 |
| 12:CL:69:ILE:HG23 | 12:CL:99:ILE:CG2 | 2.35 | 0.51 |
| 23:BA:1439:A:H2' | 23:BA:1440:G:H5' | 1.92 | 0.51 |
| 1:AA:1349:A:C2 | 1:AA:1350:A:H1' | 2.46 | 0.51 |
| 25:BC:185:VAL:HG12 | 25:BC:186:HIS:N | 2.25 | 0.51 |
| 1:AA:9:G:H2' | 1:AA:10:A:H8 | 1.75 | 0.51 |
| 44:DV:102:LEU:HD21 | 44:DV:124:ILE:HD11 | 1.93 | 0.51 |
| 41:DS:29:LEU:CG | 41:DS:33:ARG:HE | 2.22 | 0.51 |
| 43:BU:9:LYS:O | 43:BU:27:VAL:HG21 | 2.10 | 0.51 |
| 40:BR:28:GLU:HB2 | 40:BR:31:ALA:CB | 2.40 | 0.51 |
| 25:BC:168:ARG:O | 25:BC:169:GLU:HB2 | 2.10 | 0.51 |
| 20:AT:10:LEU:O | 20:AT:12:ALA:N | 2.37 | 0.51 |
| 47:BY:9:GLN:HA | 47:BY:12:GLU:HB3 | 1.92 | 0.51 |
| 23:DA:1104:C:C4 | 23:DA:1105:U:H5 | 2.28 | 0.51 |
| 23:BA:2745:C:C4 | 23:BA:2746:U:C4 | 2.98 | 0.51 |
| 37:DO:34:HIS:ND1 | 37:DO:54:LEU:HB3 | 2.26 | 0.51 |
| 1:AA:1270:C:O2' | 1:AA:1314:C:H5' | 2.10 | 0.51 |
| 1:CA:1128:C:O2 | 1:CA:1130:A:N6 | 2.43 | 0.51 |
| 27:BE:31:HIS:O | 27:BE:34:TRP:HB3 | 2.10 | 0.51 |
| 1:CA:175:C:H2' | 1:CA:176:C:C6 | 2.39 | 0.51 |
| 24:DB:60:C:C2 | 24:DB:61:G:C8 | 2.98 | 0.51 |
| 35:DM:20:ALA:O | 35:DM:21:THR:O | 2.28 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:518:C:O2 | 1:CA:529:G:C6 | 2.63 | 0.51 |
| 23:BA:2850:A:C4 | 23:BA:2851:A:C8 | 2.99 | 0.51 |
| 23:BA:2862:G:C5 | 23:BA:2863:C:C5 | 2.98 | 0.51 |
| 35:DM:111:GLU:O | 35:DM:115:MET:HB2 | 2.10 | 0.51 |
| 1:CA:444:C:H2' | 1:CA:445:G:H8 | 1.75 | 0.51 |
| 2:CB:22:LYS:HZ3 | 2:CB:22:LYS:N | 2.09 | 0.51 |
| 2:CB:32:ILE:HG12 | 2:CB:40:HIS:HD2 | 1.74 | 0.51 |
| 23:BA:1131:G:N2 | 23:BA:1132:A:C4 | 2.79 | 0.51 |
| 23:BA:2065:C:H2' | 23:BA:2066:C:C6 | 2.44 | 0.51 |
| 12:CL:37:THR:OG1 | 12:CL:38:VAL:N | 2.42 | 0.51 |
| 23:DA:1241:A:N6 | 23:DA:1242:A:C6 | 2.79 | 0.51 |
| 39:DQ:20:LEU:HB2 | 39:DQ:39:LEU:HD11 | 1.90 | 0.51 |
| 1:CA:1038:C:H2' | 1:CA:1039:C:C6 | 2.46 | 0.51 |
| 3:CC:81:GLY:O | 3:CC:85:ARG:HD3 | 2.10 | 0.51 |
| 23:BA:270(S):G:H2' | 23:BA:270(T):G:C8 | 2.45 | 0.51 |
| 1:CA:1171:G:H2' | 1:CA:1172:C:C6 | 2.45 | 0.51 |
| 23:BA:643:A:C2 | 23:BA:644:A:C4 | 2.98 | 0.51 |
| 1:CA:1464:G:O2' | 1:CA:1465:C:H5' | 2.11 | 0.51 |
| 2:AB:75:LYS:C | 2:AB:75:LYS:HD3 | 2.31 | 0.51 |
| 1:AA:19:C:H5'' | 5:AE:86:ALA:HB1 | 1.91 | 0.51 |
| 23:BA:616:A:C4 | 27:BE:180:GLY:HA2 | 2.45 | 0.51 |
| 35:BM:84:GLY:HA3 | 45:BW:10:THR:CG2 | 2.41 | 0.51 |
| 34:DL:113:LYS:HA | 34:DL:129:ALA:O | 2.10 | 0.51 |
| 23:DA:747:U:O2 | 23:DA:2014:A:H1' | 2.10 | 0.51 |
| 1:CA:1375:A:C2 | 1:CA:1376:U:C2 | 2.99 | 0.51 |
| 27:DE:64:ILE:HG23 | 27:DE:65:TRP:NE1 | 2.25 | 0.51 |
| 2:CB:184:VAL:O | 2:CB:198:ASP:HB2 | 2.11 | 0.51 |
| 23:BA:2727:G:C4 | 23:BA:2728:U:H5 | 2.29 | 0.51 |
| 1:AA:402:G:O5' | 1:AA:402:G:H8 | 1.93 | 0.51 |
| 4:CD:61:LYS:HA | 4:CD:203:VAL:HG22 | 1.92 | 0.51 |
| 3:CC:137:ALA:O | 3:CC:141:VAL:HG23 | 2.11 | 0.51 |
| 26:BD:1:MET:O | 26:BD:2:LYS:O | 2.28 | 0.51 |
| 23:DA:548:A:H2' | 23:DA:549:G:H5' | 1.91 | 0.51 |
| 23:BA:1414:G:C6 | 23:BA:1415:U:C4 | 2.98 | 0.51 |
| 26:DD:49:LEU:CD2 | 26:DD:49:LEU:H | 2.16 | 0.51 |
| 1:CA:1435:G:H2' | 1:CA:1436:U:C5 | 2.45 | 0.51 |
| 5:AE:139:LEU:O | 5:AE:141:GLN:N | 2.43 | 0.51 |
| 45:BW:51:VAL:HG21 | 45:BW:80:HIS:HA | 1.91 | 0.51 |
| 3:AC:14:ILE:HG12 | 3:AC:15:THR:N | 2.26 | 0.51 |
| 3:AC:14:ILE:HG23 | 3:AC:15:THR:N | 2.17 | 0.51 |
| 36:DN:73:VAL:O | 36:DN:76:VAL:HG22 | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:CF:35:ALA:O | 6:CF:37:VAL:N | 2.43 | 0.51 |
| 23:DA:95:G:HO2' | 47:DY:48:HIS:CE1 | 2.24 | 0.51 |
| 47:DY:48:HIS:O | 47:DY:49:LYS:C | 2.46 | 0.51 |
| 23:BA:1047:G:H1' | 23:BA:1110:G:N2 | 2.25 | 0.51 |
| 23:DA:2776:A:H4' | 23:DA:2777:G:H5'' | 1.92 | 0.51 |
| 23:DA:2277:G:C5' | 35:DM:85:LYS:HB2 | 2.40 | 0.51 |
| 15:AO:50:HIS:O | 15:AO:53:HIS:HB3 | 2.11 | 0.51 |
| 1:AA:197:A:N7 | 1:AA:221:C:H4' | 2.25 | 0.51 |
| 19:CS:6:LYS:N | 19:CS:6:LYS:HD2 | 2.24 | 0.51 |
| 1:CA:750:G:C6 | 1:CA:751:U:C5 | 2.99 | 0.51 |
| 1:CA:1052:U:H2' | 1:CA:1055:A:OP1 | 2.10 | 0.51 |
| 12:AL:21:SER:O | 12:AL:23:VAL:N | 2.43 | 0.51 |
| 23:BA:335:C:C2 | 23:BA:336:C:C5 | 2.98 | 0.51 |
| 44:BV:38:TYR:O | 44:BV:38:TYR:CG | 2.63 | 0.51 |
| 32:DJ:80:ALA:O | 32:DJ:83:ILE:HG13 | 2.09 | 0.51 |
| 1:CA:640:A:N3 | 8:CH:115:SER:CB | 2.74 | 0.51 |
| 2:AB:32:ILE:HG12 | 2:AB:40:HIS:HD2 | 1.75 | 0.51 |
| 1:CA:836:G:OP1 | 18:CR:61:LYS:HE2 | 2.10 | 0.51 |
| 23:BA:2065:C:H2' | 23:BA:2066:C:H6 | 1.74 | 0.51 |
| 1:AA:512:U:O2' | 1:AA:513:C:H5' | 2.10 | 0.51 |
| 46:BX:67:ILE:N | 46:BX:68:PRO:HD2 | 2.25 | 0.51 |
| 18:AR:84:LYS:NZ | 18:AR:84:LYS:HB3 | 2.25 | 0.51 |
| 46:DX:51:VAL:HG13 | 46:DX:53:VAL:HG23 | 1.92 | 0.51 |
| 5:CE:36:ASP:OD2 | 5:CE:38:GLN:HB3 | 2.10 | 0.51 |
| 1:AA:797:C:OP1 | 11:AK:124:LYS:HE2 | 2.09 | 0.51 |
| 9:CI:26:VAL:O | 9:CI:26:VAL:HG12 | 2.09 | 0.51 |
| 1:AA:1525:G:OP1 | 11:AK:120:ARG:NH2 | 2.43 | 0.51 |
| 23:BA:2026:C:C4 | 23:BA:2027:G:N7 | 2.79 | 0.51 |
| 23:BA:273(B):G:C2 | 23:BA:364:C:N3 | 2.78 | 0.51 |
| 23:BA:1376:C:N4 | 23:BA:1377:G:C6 | 2.79 | 0.51 |
| 23:BA:1839:G:C8 | 23:BA:1927:A:H1' | 2.46 | 0.51 |
| 5:AE:28:PHE:CD1 | 5:AE:28:PHE:N | 2.78 | 0.51 |
| 23:BA:1759:A:C8 | 23:BA:2696:U:H1' | 2.45 | 0.51 |
| 1:AA:966:G:H2' | 1:AA:967:C:C6 | 2.45 | 0.51 |
| 23:BA:1017:G:C2 | 23:BA:1146:C:O2 | 2.63 | 0.51 |
| 15:CO:48:LYS:HA | 15:CO:48:LYS:HE2 | 1.92 | 0.51 |
| 49:D1:47:VAL:HG12 | 49:D1:49:GLU:OE1 | 2.11 | 0.51 |
| 1:CA:261:U:OP2 | 20:CT:79:ARG:NH2 | 2.42 | 0.51 |
| 1:AA:1176:A:H2' | 1:AA:1177:G:C8 | 2.46 | 0.51 |
| 23:BA:2822:G:H2' | 23:BA:2823:A:H5'' | 1.92 | 0.51 |
| 28:DF:171:ALA:O | 28:DF:175:LEU:HG | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:DY:16:LEU:HB2 | 47:DY:20:GLU:HG3 | 1.91 | 0.51 |
| 43:DU:14:LEU:HD23 | 43:DU:14:LEU:C | 2.31 | 0.51 |
| 1:AA:1224:G:H4' | 13:AM:102:ARG:HH22 | 1.76 | 0.51 |
| 1:CA:503:C:H2' | 1:CA:504:C:H6 | 1.75 | 0.51 |
| 32:BJ:90:LEU:HA | 32:BJ:110:LEU:HD13 | 1.92 | 0.51 |
| 39:DQ:90:VAL:HG13 | 39:DQ:91:ASP:N | 2.24 | 0.51 |
| 39:DQ:92:ARG:HD2 | 39:DQ:95:LEU:H | 1.74 | 0.51 |
| 40:DR:5:VAL:HG12 | 40:DR:14:VAL:HG21 | 1.93 | 0.51 |
| 23:DA:242:G:P | 53:D5:3:LYS:HZ1 | 2.33 | 0.51 |
| 28:DF:83:ARG:HG3 | 28:DF:84:LYS:H | 1.75 | 0.51 |
| 25:DC:150:LYS:HE3 | 25:DC:150:LYS:HA | 1.92 | 0.51 |
| 1:AA:552:U:C2' | 1:AA:553:A:H5' | 2.41 | 0.51 |
| 4:AD:21:LEU:CD1 | 4:AD:21:LEU:H | 2.22 | 0.51 |
| 23:BA:137(B):G:H2' | 23:BA:139:G:N7 | 2.25 | 0.51 |
| 23:DA:1404:C:C2' | 23:DA:1404:C:O2 | 2.55 | 0.51 |
| 23:DA:2605:U:H2' | 23:DA:2606:C:C6 | 2.45 | 0.51 |
| 1:AA:199:G:H1 | 1:AA:218:C:N4 | 1.98 | 0.51 |
| 27:BE:124:LEU:HD12 | 27:BE:125:LEU:O | 2.11 | 0.51 |
| 46:DX:11:ARG:O | 46:DX:12:PRO:C | 2.48 | 0.51 |
| 1:CA:59:A:H3' | 1:CA:331:G:H22 | 1.75 | 0.51 |
| 45:DW:42:GLY:CA | 45:DW:57:PHE:CD2 | 2.90 | 0.51 |
| 46:DX:27:GLU:OE2 | 46:DX:33:LYS:HE3 | 2.10 | 0.51 |
| 23:BA:1495:A:H2' | 23:BA:1496:A:N3 | 2.26 | 0.51 |
| 6:CF:26:ILE:C | 6:CF:30:LEU:HD12 | 2.31 | 0.51 |
| 23:BA:2776:A:H4' | 23:BA:2777:G:H5'' | 1.91 | 0.51 |
| 29:BG:20:ALA:HB3 | 29:BG:23:ARG:O | 2.10 | 0.51 |
| 35:BM:16:ARG:C | 35:BM:17:LEU:HD23 | 2.31 | 0.51 |
| 34:BL:16:ARG:NH2 | 34:BL:18:ARG:N | 2.57 | 0.51 |
| 8:AH:9:MET:O | 8:AH:12:ARG:HB2 | 2.11 | 0.51 |
| 27:DE:88:VAL:HG13 | 27:DE:89:VAL:O | 2.11 | 0.51 |
| 31:DI:4:LYS:O | 31:DI:4:LYS:HG2 | 2.11 | 0.51 |
| 23:DA:998:C:H2' | 23:DA:999:U:O5' | 2.11 | 0.51 |
| 1:AA:1147:C:H6 | 1:AA:1147:C:O5' | 1.93 | 0.51 |
| 1:CA:197:A:N6 | 1:CA:221:C:C5' | 2.74 | 0.51 |
| 23:BA:2287:A:O2' | 23:BA:2288:A:P | 2.69 | 0.51 |
| 23:BA:2289:G:H2' | 23:BA:2289:G:N3 | 2.25 | 0.51 |
| 23:DA:2101:G:H2' | 23:DA:2102:U:C5' | 2.40 | 0.51 |
| 23:DA:2477:C:O2' | 23:DA:2478:A:P | 2.69 | 0.51 |
| 1:CA:509:A:H5' | 4:CD:54:TYR:CD2 | 2.45 | 0.51 |
| 1:CA:938:A:C6 | 1:CA:939:G:C5 | 2.98 | 0.51 |
| 23:DA:1348:G:C2' | 23:DA:1349:A:H5'' | 2.39 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:BA:2364:C:H2' | 23:BA:2365:G:O4' | 2.09 | 0.51 |
| 12:CL:74:HIS:HB2 | 12:CL:76:LEU:CD2 | 2.41 | 0.51 |
| 1:CA:1379:G:O2' | 1:CA:1380:U:H5' | 2.10 | 0.51 |
| 36:BN:84:ALA:O | 36:BN:85:PRO:C | 2.47 | 0.51 |
| 23:BA:2459:A:C4 | 23:BA:2460:U:C6 | 2.99 | 0.51 |
| 23:DA:270(J):G:O2' | 23:DA:270(K):G:H8 | 1.92 | 0.51 |
| 41:BS:45:TYR:CD2 | 41:BS:45:TYR:O | 2.63 | 0.51 |
| 5:AE:36:ASP:OD2 | 5:AE:38:GLN:HB3 | 2.10 | 0.51 |
| 1:CA:927:G:C2 | 1:CA:1391:U:C2 | 2.98 | 0.51 |
| 2:CB:17:PHE:CB | 2:CB:44:LEU:HD21 | 2.40 | 0.51 |
| 23:BA:270(Q):C:O2' | 23:BA:270(R):C:C6 | 2.64 | 0.51 |
| 23:BA:270(Q):C:O2' | 23:BA:270(R):C:H6 | 1.93 | 0.51 |
| 37:BO:79:ALA:O | 37:BO:80:LEU:HD23 | 2.11 | 0.51 |
| 44:BV:152:ALA:C | 44:BV:154:ASP:H | 2.14 | 0.51 |
| 23:DA:443:A:H1' | 23:DA:1201:C:O4' | 2.09 | 0.51 |
| 47:DY:7:ARG:NE | 47:DY:11:GLU:OE2 | 2.44 | 0.51 |
| 23:DA:1796:U:H4' | 25:DC:256:GLY:HA2 | 1.92 | 0.51 |
| 23:BA:1127:A:H2' | 23:BA:1128:A:H5'' | 1.91 | 0.51 |
| 36:DN:18:LEU:HD11 | 36:DN:22:ARG:NE | 2.26 | 0.51 |
| 1:CA:1270:C:O2' | 1:CA:1314:C:H5' | 2.11 | 0.51 |
| 1:CA:874:G:C5 | 1:CA:875:C:C5 | 2.99 | 0.51 |
| 34:DL:136:GLU:O | 34:DL:138:LEU:N | 2.44 | 0.51 |
| 23:BA:1173:G:H3' | 23:BA:1174:A:C5' | 2.41 | 0.51 |
| 32:BJ:119:GLU:CD | 32:BJ:119:GLU:H | 2.08 | 0.51 |
| 2:AB:163:PHE:HA | 2:AB:185:ILE:O | 2.11 | 0.51 |
| 38:BP:98:LYS:HB3 | 38:BP:100:TYR:CE1 | 2.46 | 0.51 |
| 12:CL:116:ARG:O | 12:CL:117:SER:C | 2.49 | 0.51 |
| 23:BA:577:G:OP1 | 23:BA:2502:G:H2' | 2.11 | 0.51 |
| 28:BF:85:GLY:C | 28:BF:86:MET:HG3 | 2.30 | 0.51 |
| 40:DR:47:VAL:HG11 | 40:DR:50:PRO:O | 2.11 | 0.51 |
| 23:DA:1141:U:P | 32:DJ:86:THR:HG21 | 2.50 | 0.51 |
| 53:B5:6:THR:HG21 | 53:B5:64:TYR:HD1 | 1.75 | 0.51 |
| 23:DA:94:G:N2 | 47:DY:47:ASN:HD22 | 1.98 | 0.51 |
| 23:BA:2219:G:C2' | 23:BA:2224:G:C5' | 2.77 | 0.51 |
| 3:CC:33:LEU:O | 3:CC:36:ASP:HB3 | 2.11 | 0.51 |
| 3:AC:29:TYR:O | 3:AC:29:TYR:HD1 | 1.93 | 0.51 |
| 1:CA:735:C:H1' | 18:CR:75:ILE:HD11 | 1.93 | 0.51 |
| 5:AE:34:VAL:O | 5:AE:41:VAL:HA | 2.11 | 0.51 |
| 23:BA:142:G:C1' | 42:BT:37:THR:HG21 | 2.40 | 0.51 |
| 36:DN:60:LEU:HA | 36:DN:63:ARG:HB3 | 1.93 | 0.51 |
| 23:DA:2744:G:H1' | 23:DA:2761:G:H22 | 1.75 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:DG:67:LEU:HG | 29:DG:71:LEU:HD23 | 1.92 | 0.51 |
| 23:DA:1496:A:N7 | 23:DA:1498:C:N3 | 2.59 | 0.51 |
| 23:DA:1859:A:C6 | 23:DA:1884:A:C8 | 2.98 | 0.51 |
| 23:BA:954:G:H5'' | 35:BM:13:GLN:HG3 | 1.91 | 0.51 |
| 1:CA:830:G:C2 | 1:CA:831:U:C2 | 2.99 | 0.51 |
| 28:DF:120:LEU:HD13 | 28:DF:133:LEU:HD13 | 1.93 | 0.51 |
| 27:BE:53:THR:HG23 | 27:BE:56:GLU:CD | 2.30 | 0.51 |
| 32:DJ:66:THR:O | 32:DJ:69:VAL:HG12 | 2.11 | 0.51 |
| 1:AA:599:C:H2' | 1:AA:600:C:H6 | 1.76 | 0.51 |
| 1:AA:1054:C:H3' | 1:AA:1054:C:O2 | 2.10 | 0.51 |
| 1:AA:592:G:N1 | 1:AA:648:A:C6 | 2.79 | 0.51 |
| 1:CA:16:A:C2 | 1:CA:17:U:C6 | 2.99 | 0.51 |
| 1:CA:373:A:C8 | 1:CA:482:A:C8 | 2.98 | 0.51 |
| 1:CA:445:G:H2' | 1:CA:446:G:H8 | 1.75 | 0.51 |
| 23:DA:2773:C:P | 26:DD:166:THR:HG1 | 2.34 | 0.51 |
| 1:AA:444:C:H2' | 1:AA:445:G:H8 | 1.76 | 0.51 |
| 46:BX:51:VAL:HG13 | 46:BX:53:VAL:HG23 | 1.93 | 0.51 |
| 1:CA:180:U:H2' | 1:CA:181:G:H5' | 1.91 | 0.51 |
| 1:AA:562:C:C4 | 1:AA:884:U:C5 | 2.98 | 0.51 |
| 47:BY:38:GLN:HB3 | 47:BY:44:LEU:HB3 | 1.92 | 0.51 |
| 23:BA:2648:C:H2' | 23:BA:2649:U:C6 | 2.45 | 0.51 |
| 23:DA:699:A:H2' | 23:DA:700:G:O4' | 2.11 | 0.51 |
| 25:BC:198:ASN:HD22 | 25:BC:198:ASN:C | 2.13 | 0.51 |
| 23:DA:107:C:C2' | 23:DA:108:U:H5' | 2.41 | 0.51 |
| 1:CA:1176:A:H2' | 1:CA:1177:G:C8 | 2.46 | 0.51 |
| 23:DA:2197:U:O3' | 23:DA:2198:A:H8 | 1.93 | 0.51 |
| 23:BA:1677:A:H2' | 23:BA:1678:G:O4' | 2.10 | 0.51 |
| 1:CA:767:A:H2' | 1:CA:768:A:O4' | 2.10 | 0.51 |
| 13:CM:49:THR:O | 13:CM:53:VAL:HG23 | 2.11 | 0.51 |
| 23:DA:1173:G:H3' | 23:DA:1174:A:C5' | 2.40 | 0.51 |
| 34:BL:126:VAL:CA | 34:BL:145:PRO:HG2 | 2.41 | 0.51 |
| 1:CA:1349:A:C2 | 1:CA:1350:A:H1' | 2.45 | 0.51 |
| 26:BD:24:THR:HG21 | 26:BD:188:VAL:CG1 | 2.41 | 0.51 |
| 39:DQ:113:ALA:HA | 39:DQ:116:ALA:HB3 | 1.91 | 0.51 |
| 6:CF:86:ARG:O | 6:CF:87:ARG:CB | 2.49 | 0.51 |
| 12:AL:82:VAL:HG13 | 12:AL:83:LEU:N | 2.24 | 0.51 |
| 25:BC:76:PRO:HA | 25:BC:118:VAL:HG23 | 1.92 | 0.51 |
| 1:CA:394:G:C2 | 1:CA:395:C:C5 | 2.99 | 0.51 |
| 3:CC:172:ARG:HE | 3:CC:174:PRO:CG | 2.24 | 0.51 |
| 23:BA:330:A:O2' | 23:BA:331:A:C8 | 2.55 | 0.51 |
| 24:BB:40:U:O2 | 24:BB:43:C:C6 | 2.63 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:AC:91:LEU:CD1 | 3:AC:101:LEU:HD21 | 2.41 | 0.51 |
| 47:DY:53:LEU:O | 47:DY:57:ILE:HG13 | 2.11 | 0.51 |
| 24:BB:103:U:C2' | 24:BB:104:A:H5' | 2.41 | 0.51 |
| 25:DC:223:GLY:O | 25:DC:224:ALA:C | 2.49 | 0.51 |
| 46:DX:11:ARG:CG | 46:DX:61:ARG:O | 2.59 | 0.51 |
| 4:AD:155:LEU:HD23 | 4:AD:156:GLU:OE2 | 2.11 | 0.51 |
| 4:AD:127:THR:OG1 | 4:AD:128:VAL:N | 2.43 | 0.51 |
| 46:DX:73:LEU:HG | 46:DX:73:LEU:O | 2.10 | 0.51 |
| 8:CH:63:LEU:HB2 | 8:CH:65:TYR:HE1 | 1.75 | 0.51 |
| 1:AA:1014:A:H4' | 19:AS:14:HIS:CE1 | 2.46 | 0.51 |
| 8:CH:11:THR:O | 8:CH:12:ARG:C | 2.49 | 0.51 |
| 17:AQ:54:GLY:HA3 | 17:AQ:82:MET:SD | 2.51 | 0.51 |
| 23:BA:955:C:OP1 | 35:BM:85:LYS:HE2 | 2.10 | 0.51 |
| 40:BR:98:GLU:HG2 | 40:BR:100:ARG:CD | 2.38 | 0.51 |
| 3:AC:68:VAL:HG12 | 3:AC:70:VAL:HG23 | 1.93 | 0.51 |
| 23:DA:379:G:C5 | 23:DA:380:U:C5 | 2.99 | 0.51 |
| 23:BA:1478:G:O2' | 23:BA:1558:A:C2 | 2.64 | 0.51 |
| 6:CF:50:TYR:CE1 | 18:CR:74:ARG:O | 2.64 | 0.51 |
| 50:B2:52:TYR:CD1 | 50:B2:52:TYR:C | 2.82 | 0.51 |
| 4:CD:82:ALA:HB1 | 4:CD:89:THR:HG23 | 1.92 | 0.51 |
| 27:BE:199:TRP:CZ2 | 27:BE:203:GLN:NE2 | 2.79 | 0.51 |
| 23:BA:2225:A:H1' | 23:BA:2226:C:OP2 | 2.11 | 0.51 |
| 23:DA:1025:G:C4 | 23:DA:1135:C:H1' | 2.46 | 0.51 |
| 23:DA:198:C:H5' | 23:DA:2244:U:OP1 | 2.10 | 0.51 |
| 10:CJ:40:LEU:HB2 | 10:CJ:69:ASN:CB | 2.41 | 0.51 |
| 3:AC:76:VAL:CG2 | 3:AC:77:ILE:HG13 | 2.40 | 0.51 |
| 1:AA:754:C:C6 | 15:AO:69:TYR:CE2 | 2.99 | 0.51 |
| 10:CJ:50:ILE:CG2 | 14:CN:41:ARG:HH21 | 2.24 | 0.51 |
| 23:DA:2190:G:H2' | 23:DA:2191:G:C8 | 2.44 | 0.51 |
| 25:BC:94:LEU:HD22 | 25:BC:94:LEU:C | 2.31 | 0.51 |
| 36:DN:79:LEU:CD2 | 36:DN:83:ILE:HB | 2.41 | 0.51 |
| 1:CA:684:A:H2' | 1:CA:685:G:C8 | 2.45 | 0.51 |
| 1:CA:685:G:N2 | 1:CA:686:U:C4 | 2.79 | 0.51 |
| 41:DS:45:TYR:O | 41:DS:45:TYR:CG | 2.63 | 0.51 |
| 26:DD:149:ARG:CG | 26:DD:150:VAL:N | 2.72 | 0.51 |
| 1:AA:294:U:C2 | 1:AA:295:C:C5 | 2.98 | 0.51 |
| 23:BA:2302:G:C2' | 23:BA:2303:G:H5' | 2.41 | 0.51 |
| 1:AA:1504:G:OP1 | 1:AA:1507:A:H4' | 2.11 | 0.51 |
| 47:DY:42:GLY:O | 47:DY:44:LEU:N | 2.36 | 0.51 |
| 1:CA:1296:C:C6 | 1:CA:1297:C:H5 | 2.28 | 0.51 |
| 23:BA:2078:C:O2' | 23:BA:2079:U:H5' | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:BA:510:C:H2' | 23:BA:511:U:O4' | 2.11 | 0.51 |
| 23:BA:900:A:C4 | 23:BA:901:A:C8 | 2.98 | 0.51 |
| 28:BF:121:ASN:ND2 | 28:BF:122:PRO:HD2 | 2.26 | 0.51 |
| 40:BR:75:PHE:C | 40:BR:75:PHE:CD1 | 2.84 | 0.51 |
| 1:CA:575:G:C5 | 1:CA:881:G:N2 | 2.78 | 0.51 |
| 53:D5:33:ASN:O | 53:D5:34:TRP:HB3 | 2.10 | 0.51 |
| 53:D5:22:VAL:CG2 | 53:D5:54:GLU:HG3 | 2.40 | 0.51 |
| 34:DL:85:LEU:HD22 | 34:DL:85:LEU:H | 1.74 | 0.51 |
| 23:BA:2415:G:H1' | 34:BL:67:MET:CE | 2.41 | 0.51 |
| 26:DD:170:LEU:HB3 | 26:DD:185:LYS:HB2 | 1.93 | 0.51 |
| 23:BA:861:A:N3 | 24:BB:79:C:O2' | 2.38 | 0.51 |
| 1:CA:1226:C:H6 | 13:CM:103:THR:OG1 | 1.93 | 0.51 |
| 37:BO:11:LYS:CG | 37:BO:12:PHE:N | 2.65 | 0.51 |
| 23:BA:1971:A:N3 | 25:BC:240:ALA:HA | 2.25 | 0.51 |
| 1:AA:671:G:H2' | 1:AA:672:U:C6 | 2.46 | 0.51 |
| 23:DA:2728:U:H2' | 23:DA:2728:U:O2 | 2.10 | 0.51 |
| 23:BA:243:U:C2' | 23:BA:244:A:H5' | 2.41 | 0.51 |
| 23:DA:2335:A:C8 | 23:DA:2337:G:N7 | 2.79 | 0.51 |
| 1:CA:392:G:N3 | 1:CA:393:A:C8 | 2.78 | 0.51 |
| 44:DV:94:GLU:CD | 44:DV:94:GLU:N | 2.63 | 0.51 |
| 1:AA:95:G:H2' | 1:AA:96:G:O4' | 2.11 | 0.51 |
| 23:BA:2886:G:H2' | 23:BA:2887:U:H6 | 1.75 | 0.51 |
| 5:AE:10:MET:HA | 5:AE:32:VAL:HA | 1.92 | 0.51 |
| 44:BV:137:ILE:HD12 | 44:BV:137:ILE:N | 2.26 | 0.51 |
| 1:CA:401:C:H3' | 1:CA:401:C:C6 | 2.46 | 0.51 |
| 1:AA:487:A:H2' | 1:AA:488:C:O4' | 2.10 | 0.51 |
| 40:DR:66:ARG:HD2 | 40:DR:88:ARG:NE | 2.26 | 0.51 |
| 36:BN:59:ASP:OD1 | 36:BN:61:HIS:HB3 | 2.11 | 0.51 |
| 1:CA:321:A:C2 | 1:CA:333:G:C2 | 2.99 | 0.51 |
| 4:CD:126:ILE:CG2 | 4:CD:127:THR:H | 2.19 | 0.51 |
| 23:DA:1486:A:H2' | 23:DA:1487:G:H8 | 1.75 | 0.51 |
| 23:BA:1046:A:O5' | 23:BA:1046:A:H8 | 1.93 | 0.51 |
| 24:BB:50:G:OP2 | 37:BO:62:LYS:HD3 | 2.10 | 0.51 |
| 30:DH:135:GLU:O | 30:DH:135:GLU:HG3 | 2.11 | 0.51 |
| 23:DA:1109:C:N4 | 23:DA:1110:G:N2 | 2.59 | 0.51 |
| 1:CA:302:G:N3 | 1:CA:556:C:H4' | 2.25 | 0.51 |
| 25:BC:25:THR:HG22 | 25:BC:82:ILE:N | 2.26 | 0.51 |
| 9:CI:103:THR:HG22 | 9:CI:105:ASP:H | 1.75 | 0.51 |
| 23:DA:2287:A:C2 | 23:DA:2289:G:C8 | 2.99 | 0.51 |
| 1:CA:801:U:H2' | 1:CA:802:A:H8 | 1.76 | 0.51 |
| 1:CA:68:G:N1 | 1:CA:69:G:C5 | 2.79 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DA:282:A:N6 | 23:DA:284:U:C2 | 2.78 | 0.51 |
| 29:DG:85:LYS:O | 29:DG:132:ARG:HA | 2.11 | 0.51 |
| 23:BA:1952:A:C6 | 23:BA:1953:A:C6 | 2.98 | 0.51 |
| 23:BA:2287:A:C5 | 23:BA:2289:G:N7 | 2.79 | 0.51 |
| 23:DA:1568:G:OP2 | 25:DC:63:ARG:NH2 | 2.35 | 0.51 |
| 11:AK:29:ILE:HB | 11:AK:44:SER:HB3 | 1.93 | 0.51 |
| 23:DA:1389:G:C2 | 23:DA:1390:U:C2 | 2.99 | 0.51 |
| 33:DK:19:ILE:HG22 | 33:DK:43:VAL:HA | 1.92 | 0.51 |
| 24:DB:75:G:H1 | 24:DB:102:G:N2 | 2.09 | 0.51 |
| 44:DV:24:LEU:HB2 | 44:DV:41:LEU:HG | 1.93 | 0.51 |
| 33:BK:100:GLY:O | 33:BK:101:PRO:O | 2.29 | 0.51 |
| 1:CA:579:G:H2' | 1:CA:580:U:C6 | 2.43 | 0.51 |
| 1:AA:513:C:C2 | 1:AA:539:A:C2 | 2.98 | 0.51 |
| 41:BS:45:TYR:CD2 | 41:BS:46:PHE:CD1 | 2.99 | 0.51 |
| 23:DA:2837:G:C5 | 23:DA:2838:G:N7 | 2.78 | 0.51 |
| 23:BA:1451:C:H42 | 23:BA:1459:G:H1 | 1.57 | 0.51 |
| 23:DA:510:C:H2' | 23:DA:511:U:O4' | 2.10 | 0.51 |
| 23:DA:962:G:H2' | 23:DA:963:U:O4' | 2.11 | 0.51 |
| 23:BA:2744:G:N2 | 23:BA:2761:G:C4 | 2.79 | 0.51 |
| 32:BJ:32:VAL:HG12 | 32:BJ:33:GLU:N | 2.26 | 0.51 |
| 29:DG:38:SER:HB3 | 29:DG:41:MET:HG2 | 1.92 | 0.51 |
| 23:DA:844:C:C2' | 23:DA:845:G:H5' | 2.40 | 0.51 |
| 1:AA:238:G:P | 17:AQ:25:ARG:HH22 | 2.33 | 0.51 |
| 23:BA:298:G:OP2 | 43:BU:85:VAL:HG22 | 2.11 | 0.51 |
| 34:BL:64:LYS:HB2 | 53:B5:25:MET:HG3 | 1.93 | 0.51 |
| 23:BA:2361:A:OP1 | 53:B5:27:THR:OG1 | 2.25 | 0.51 |
| 23:BA:1173:G:H1' | 23:BA:1177:A:H61 | 1.75 | 0.51 |
| 32:BJ:53:ILE:HD12 | 32:BJ:122:LEU:HD11 | 1.93 | 0.51 |
| 28:DF:92:VAL:O | 28:DF:92:VAL:HG13 | 2.10 | 0.51 |
| 23:DA:1005:C:O2' | 32:DJ:51:THR:HG21 | 2.11 | 0.51 |
| 26:BD:106:GLY:HA3 | 26:BD:189:PRO:HB2 | 1.91 | 0.51 |
| 22:AV:6191:A:O2' | 22:AV:6192:G:H5' | 2.10 | 0.51 |
| 40:DR:6:LYS:CG | 40:DR:11:GLN:HG2 | 2.41 | 0.51 |
| 16:CP:18:ARG:HD3 | 16:CP:35:LYS:HE3 | 1.93 | 0.51 |
| 30:BH:101:LEU:O | 30:BH:107:ILE:HG22 | 2.11 | 0.51 |
| 1:AA:692:U:H5 | 11:AK:26:ASN:ND2 | 2.09 | 0.51 |
| 20:CT:32:ALA:O | 20:CT:36:LEU:HD23 | 2.10 | 0.51 |
| 20:CT:72:LEU:HD21 | 20:CT:76:ALA:C | 2.30 | 0.51 |
| 1:AA:92:G:H2' | 1:AA:93:U:H5' | 1.92 | 0.51 |
| 5:CE:11:ILE:HB | 5:CE:31:LEU:HD13 | 1.93 | 0.51 |
| 23:DA:2688:U:C5 | 23:DA:2720:U:OP2 | 2.64 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:AE:61:TYR:HA | 5:AE:64:ARG:HB3 | 1.93 | 0.51 |
| 1:AA:1103:C:C2 | 1:AA:1104:G:C8 | 2.98 | 0.51 |
| 41:DS:29:LEU:HD21 | 41:DS:33:ARG:HH21 | 1.76 | 0.51 |
| 23:BA:2305:A:C4 | 28:BF:154:GLY:HA3 | 2.46 | 0.51 |
| 29:DG:46:GLU:HG3 | 29:DG:51:ARG:CZ | 2.41 | 0.51 |
| 46:BX:11:ARG:CB | 46:BX:12:PRO:CD | 2.86 | 0.51 |
| 23:BA:1343:G:O2' | 23:BA:1344:G:H5' | 2.11 | 0.51 |
| 47:BY:9:GLN:CA | 47:BY:12:GLU:HB3 | 2.41 | 0.51 |
| 1:AA:353:A:H2' | 1:AA:354:G:OP2 | 2.11 | 0.51 |
| 1:CA:600:C:H2' | 1:CA:601:C:H6 | 1.74 | 0.51 |
| 1:AA:629:G:C2 | 1:AA:630:G:O6 | 2.64 | 0.51 |
| 23:DA:910:A:C4 | 35:DM:13:GLN:OE1 | 2.63 | 0.51 |
| 23:DA:1045:A:H4' | 23:DA:1046:A:H5'' | 1.93 | 0.51 |
| 2:AB:98:LEU:HB2 | 2:AB:101:MET:CG | 2.40 | 0.51 |
| 1:AA:171:A:H2' | 1:AA:172:A:C8 | 2.45 | 0.51 |
| 23:DA:947:G:N2 | 23:DA:971:C:C2 | 2.79 | 0.51 |
| 30:DH:8:PRO:HB3 | 30:DH:14:ASP:OD1 | 2.11 | 0.51 |
| 36:BN:99:LYS:N | 36:BN:99:LYS:HD2 | 2.26 | 0.51 |
| 23:BA:2638:G:P | 26:BD:82:ARG:HH22 | 2.34 | 0.51 |
| 44:DV:179:ASP:CG | 44:DV:180:VAL:H | 2.13 | 0.51 |
| 17:AQ:29:HIS:CE1 | 17:AQ:32:TYR:CD1 | 2.99 | 0.51 |
| 35:DM:20:ALA:HB2 | 35:DM:99:PRO:HB2 | 1.91 | 0.51 |
| 35:BM:22:LYS:C | 35:BM:22:LYS:HD3 | 2.32 | 0.51 |
| 8:CH:87:SER:HB2 | 8:CH:93:VAL:HB | 1.91 | 0.51 |
| 23:BA:1568:G:P | 25:BC:63:ARG:HH22 | 2.34 | 0.51 |
| 1:CA:765:G:H5'' | 1:CA:766:A:OP1 | 2.11 | 0.51 |
| 6:AF:33:TYR:HE1 | 6:AF:75:LEU:HA | 1.75 | 0.51 |
| 1:CA:1254:C:OP1 | 10:CJ:45:ARG:HD3 | 2.11 | 0.51 |
| 35:BM:111:GLU:O | 35:BM:115:MET:HB2 | 2.10 | 0.51 |
| 23:DA:825:C:O2 | 34:DL:55:ARG:NH2 | 2.41 | 0.51 |
| 23:DA:1705:G:O2' | 23:DA:1706:U:H5' | 2.10 | 0.51 |
| 7:CG:61:VAL:O | 7:CG:65:ALA:HB2 | 2.11 | 0.51 |
| 23:BA:226:G:H21 | 23:BA:228:A:H62 | 1.56 | 0.51 |
| 15:AO:7:GLU:HG3 | 15:AO:10:LYS:HD3 | 1.93 | 0.51 |
| 23:DA:2689:U:P | 23:DA:2719:G:H22 | 2.34 | 0.51 |
| 1:AA:539:A:C6 | 1:AA:540:G:C6 | 2.99 | 0.51 |
| 20:AT:39:LYS:O | 20:AT:43:LEU:HG | 2.11 | 0.51 |
| 23:DA:1526:G:O2' | 23:DA:1527:G:H5' | 2.10 | 0.51 |
| 23:BA:1471:A:C2 | 23:BA:1472:A:C8 | 2.99 | 0.51 |
| 23:BA:1717:G:C5 | 23:BA:1743:G:C2 | 2.99 | 0.51 |
| 37:BO:98:VAL:O | 37:BO:101:LEU:HB3 | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1038:C:H2' | 1:AA:1039:C:C6 | 2.46 | 0.51 |
| 28:BF:121:ASN:HD22 | 28:BF:122:PRO:HD2 | 1.75 | 0.51 |
| 16:CP:50:LYS:O | 16:CP:51:VAL:HG23 | 2.11 | 0.51 |
| 26:BD:146:THR:HA | 26:BD:147:PRO:C | 2.31 | 0.51 |
| 23:BA:374:A:H3' | 23:BA:375:C:H6 | 1.75 | 0.51 |
| 20:AT:84:LEU:HD13 | 20:AT:85:MET:N | 2.26 | 0.51 |
| 38:DP:78:LEU:HD13 | 38:DP:78:LEU:O | 2.10 | 0.51 |
| 1:CA:131:C:H2' | 1:CA:132:C:C6 | 2.46 | 0.51 |
| 23:BA:13:A:N3 | 23:BA:15:G:C6 | 2.79 | 0.51 |
| 23:BA:433:C:C4 | 23:BA:434:U:O4 | 2.64 | 0.51 |
| 23:DA:2250:G:OP2 | 23:DA:2275:C:H2' | 2.11 | 0.51 |
| 23:BA:860:U:O4' | 23:BA:860:U:O2 | 2.28 | 0.51 |
| 43:DU:8:LYS:N | 43:DU:8:LYS:NZ | 2.57 | 0.51 |
| 22:AV:6194:C:C2' | 22:AV:6195:G:H8 | 2.05 | 0.51 |
| 22:CV:6191:A:O2' | 22:CV:6192:G:H5' | 2.11 | 0.51 |
| 23:BA:2320:A:C8 | 23:BA:2333:A:N6 | 2.79 | 0.51 |
| 2:CB:70:PHE:O | 2:CB:71:VAL:HG13 | 2.10 | 0.51 |
| 23:BA:1657:C:H2' | 23:BA:1658:C:C6 | 2.46 | 0.51 |
| 27:DE:164:ARG:CG | 27:DE:164:ARG:HH11 | 2.08 | 0.51 |
| 47:DY:17:SER:O | 47:DY:21:LEU:N | 2.22 | 0.51 |
| 39:DQ:106:PHE:O | 39:DQ:110:VAL:HG23 | 2.11 | 0.51 |
| 41:DS:86:LEU:HD12 | 41:DS:87:PRO:HD2 | 1.92 | 0.51 |
| 30:BH:129:THR:HA | 30:BH:138:ILE:O | 2.10 | 0.51 |
| 39:BQ:92:ARG:HD2 | 39:BQ:95:LEU:N | 2.25 | 0.51 |
| 40:BR:47:VAL:O | 40:BR:48:GLY:C | 2.50 | 0.51 |
| 34:BL:47:ASP:CB | 34:BL:51:PHE:HB2 | 2.40 | 0.51 |
| 25:DC:127:VAL:HA | 25:DC:193:VAL:CG1 | 2.41 | 0.51 |
| 20:AT:72:LEU:HD21 | 20:AT:76:ALA:C | 2.31 | 0.51 |
| 23:DA:137(B):G:H2' | 23:DA:139:G:N7 | 2.26 | 0.51 |
| 2:CB:173:ALA:O | 2:CB:176:GLU:N | 2.44 | 0.51 |
| 23:BA:848:G:C4 | 23:BA:933:A:C8 | 2.99 | 0.51 |
| 30:BH:135:GLU:HG3 | 30:BH:135:GLU:O | 2.09 | 0.51 |
| 23:DA:2328:A:C2 | 23:DA:2329:G:C4 | 2.99 | 0.51 |
| 23:DA:1884:A:N3 | 23:DA:1885:A:C8 | 2.79 | 0.51 |
| 37:BO:58:LEU:N | 37:BO:58:LEU:HD12 | 2.26 | 0.51 |
| 1:CA:1150:U:H5'' | 1:CA:1151:A:OP2 | 2.12 | 0.51 |
| 1:AA:632:A:H8 | 1:AA:633:G:C8 | 2.29 | 0.51 |
| 1:CA:782:A:O3' | 1:CA:1515:C:H4' | 2.11 | 0.51 |
| 11:CK:84:VAL:HG23 | 11:CK:110:ASP:OD1 | 2.10 | 0.51 |
| 43:DU:44:ILE:HG22 | 43:DU:45:VAL:N | 2.24 | 0.51 |
| 38:BP:27:THR:O | 38:BP:89:VAL:HG13 | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 38:BP:27:THR:HG23 | 38:BP:90:GLN:HB3 | 1.93 | 0.51 |
| 23:BA:2101:G:H2' | 23:BA:2102:U:C5' | 2.39 | 0.51 |
| 1:CA:657:G:O2' | 1:CA:658:G:H5' | 2.10 | 0.51 |
| 29:DG:91:GLY:O | 29:DG:92:ILE:O | 2.29 | 0.51 |
| 35:BM:21:THR:O | 35:BM:22:LYS:C | 2.48 | 0.51 |
| 23:DA:1728:G:O5' | 23:DA:1728:G:C8 | 2.62 | 0.51 |
| 29:DG:102:ALA:CB | 29:DG:116:GLU:HA | 2.41 | 0.51 |
| 1:CA:1228:C:N4 | 1:CA:1229:A:N6 | 2.59 | 0.51 |
| 23:DA:2051:A:H4' | 26:DD:141:ILE:CG2 | 2.41 | 0.51 |
| 19:AS:31:ILE:CG2 | 19:AS:49:ILE:HA | 2.40 | 0.51 |
| 1:CA:639:G:H2' | 1:CA:640:A:H8 | 1.75 | 0.51 |
| 41:BS:36:LEU:HD12 | 41:BS:48:ALA:CA | 2.41 | 0.51 |
| 19:CS:5:LEU:HG | 19:CS:10:PHE:HB3 | 1.93 | 0.51 |
| 23:DA:1442:G:C2 | 23:DA:1550:C:O2 | 2.64 | 0.51 |
| 23:DA:2837:G:C6 | 23:DA:2838:G:C5 | 2.99 | 0.51 |
| 23:BA:1851:U:C4 | 23:BA:1852:C:C4 | 2.99 | 0.51 |
| 23:BA:1471:A:C2 | 23:BA:1472:A:N9 | 2.79 | 0.51 |
| 39:DQ:47:TYR:C | 39:DQ:47:TYR:CD2 | 2.84 | 0.51 |
| 1:CA:419:C:O2 | 1:CA:425:G:C2 | 2.63 | 0.51 |
| 28:DF:18:GLU:HG2 | 28:DF:175:LEU:HD22 | 1.93 | 0.51 |
| 23:BA:718:A:H8 | 23:BA:718:A:O5' | 1.93 | 0.51 |
| 23:BA:762:U:H4' | 23:BA:763:G:O5' | 2.10 | 0.51 |
| 51:B3:11:LEU:O | 51:B3:24:GLU:HB2 | 2.11 | 0.51 |
| 9:AI:27:THR:O | 9:AI:62:TYR:HA | 2.11 | 0.51 |
| 1:CA:966:G:H2' | 1:CA:967:C:C6 | 2.46 | 0.51 |
| 23:BA:245:G:H2' | 23:BA:246:C:H6 | 1.75 | 0.51 |
| 34:DL:61:ARG:CA | 34:DL:62:LEU:HD13 | 2.41 | 0.50 |
| 38:DP:50:ILE:HA | 38:DP:99:LEU:CD1 | 2.41 | 0.50 |
| 22:AV:6188:G:N2 | 22:AV:6216:U:N3 | 2.59 | 0.50 |
| 22:AV:6191:A:N1 | 22:AV:6213:A:C6 | 2.80 | 0.50 |
| 22:CV:6191:A:H2' | 22:CV:6192:G:H8 | 1.76 | 0.50 |
| 23:BA:2342:C:O2' | 23:BA:2374:C:H5'' | 2.11 | 0.50 |
| 23:DA:587:C:O2 | 34:DL:33:ARG:HD3 | 2.10 | 0.50 |
| 23:DA:1159:U:H2' | 23:DA:1160:G:C8 | 2.45 | 0.50 |
| 1:CA:376:G:P | 16:CP:67:THR:HG21 | 2.51 | 0.50 |
| 30:BH:82:ARG:HB3 | 30:BH:89:TYR:HB2 | 1.94 | 0.50 |
| 1:CA:671:G:H2' | 1:CA:672:U:C6 | 2.46 | 0.50 |
| 37:DO:27:SER:HA | 37:DO:88:ASP:HB3 | 1.93 | 0.50 |
| 30:DH:81:VAL:HG11 | 30:DH:90:GLY:HA3 | 1.94 | 0.50 |
| 2:CB:187:LEU:HD22 | 2:CB:188:ALA:N | 2.26 | 0.50 |
| 3:CC:151:VAL:O | 3:CC:152:ILE:HG13 | 2.10 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:CE:11:ILE:HG22 | 5:CE:12:LEU:N | 2.26 | 0.50 |
| 5:AE:33:VAL:HG13 | 5:AE:109:ILE:HD13 | 1.93 | 0.50 |
| 48:DZ:40:THR:OG1 | 48:DZ:41:PRO:HD2 | 2.10 | 0.50 |
| 1:AA:1149:C:O2' | 1:AA:1280:A:N1 | 2.43 | 0.50 |
| 35:DM:55:VAL:CG2 | 35:DM:56:ARG:N | 2.74 | 0.50 |
| 8:CH:28:ALA:HA | 8:CH:59:LEU:HD21 | 1.93 | 0.50 |
| 25:BC:24:ILE:HD11 | 25:BC:84:TYR:HB2 | 1.93 | 0.50 |
| 23:BA:1105:U:H2' | 23:BA:1106:G:H8 | 1.75 | 0.50 |
| 27:BE:68:LYS:C | 27:BE:70:THR:H | 2.14 | 0.50 |
| 1:AA:874:G:C5 | 1:AA:875:C:C5 | 3.00 | 0.50 |
| 1:AA:632:A:N7 | 1:AA:633:G:C4 | 2.79 | 0.50 |
| 1:CA:457:C:N4 | 1:CA:475:G:H1 | 2.09 | 0.50 |
| 32:DJ:69:VAL:O | 32:DJ:70:ALA:HB3 | 2.11 | 0.50 |
| 23:DA:2531:A:H4' | 29:DG:157:TYR:CE2 | 2.46 | 0.50 |
| 27:DE:199:TRP:CZ2 | 27:DE:203:GLN:NE2 | 2.79 | 0.50 |
| 36:BN:73:VAL:O | 36:BN:76:VAL:HG22 | 2.11 | 0.50 |
| 23:DA:966:G:C5 | 23:DA:967:C:H5 | 2.29 | 0.50 |
| 1:CA:278:G:OP2 | 17:CQ:41:LYS:NZ | 2.43 | 0.50 |
| 47:BY:46:GLN:HB2 | 47:BY:49:LYS:HZ1 | 1.73 | 0.50 |
| 23:BA:2287:A:C5 | 23:BA:2289:G:C5 | 2.99 | 0.50 |
| 35:BM:20:ALA:HA | 35:BM:98:LYS:HB3 | 1.92 | 0.50 |
| 35:BM:19:GLY:O | 35:BM:98:LYS:HD3 | 2.11 | 0.50 |
| 33:DK:19:ILE:HB | 33:DK:41:ALA:HB1 | 1.93 | 0.50 |
| 44:BV:23:LYS:HB3 | 44:BV:38:TYR:CD1 | 2.40 | 0.50 |
| 41:BS:59:VAL:HG12 | 41:BS:60:ASN:N | 2.25 | 0.50 |
| 23:BA:1909:C:N3 | 23:BA:1922:G:C2 | 2.79 | 0.50 |
| 13:CM:99:ARG:HB2 | 13:CM:101:GLN:HE21 | 1.76 | 0.50 |
| 24:BB:30:C:H1' | 24:BB:58:A:N1 | 2.27 | 0.50 |
| 12:AL:74:HIS:CD2 | 12:AL:76:LEU:H | 2.26 | 0.50 |
| 14:CN:43:CYS:SG | 14:CN:44:LEU:N | 2.84 | 0.50 |
| 12:CL:54:VAL:HG12 | 12:CL:55:ALA:N | 2.26 | 0.50 |
| 46:DX:67:ILE:N | 46:DX:68:PRO:HD2 | 2.25 | 0.50 |
| 47:BY:36:ARG:HA | 47:BY:39:ALA:HB3 | 1.93 | 0.50 |
| 48:DZ:23:LEU:N | 48:DZ:23:LEU:CD1 | 2.73 | 0.50 |
| 1:AA:1501:C:C5 | 1:AA:1504:G:C5 | 2.98 | 0.50 |
| 1:CA:1217:C:H5'' | 14:CN:9:LYS:NZ | 2.26 | 0.50 |
| 23:BA:1403:C:H5'' | 23:BA:1471:A:C1' | 2.41 | 0.50 |
| 23:DA:449:A:H2' | 23:DA:450:G:H5' | 1.92 | 0.50 |
| 1:CA:575:G:C5 | 1:CA:881:G:C2 | 3.00 | 0.50 |
| 25:DC:124:PRO:HG2 | 25:DC:129:ASN:ND2 | 2.26 | 0.50 |
| 23:BA:36:G:C5 | 23:BA:37:C:C5 | 2.99 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:BE:93:LYS:HB3 | 27:BE:94:PRO:HD2 | 1.92 | 0.50 |
| 49:B1:47:VAL:HG12 | 49:B1:49:GLU:OE1 | 2.11 | 0.50 |
| 1:CA:292:G:C5 | 1:CA:293:G:H1' | 2.46 | 0.50 |
| 15:AO:3:ILE:HA | 15:AO:38:ARG:NH2 | 2.27 | 0.50 |
| 1:AA:785:G:N2 | 1:AA:798:G:C4 | 2.79 | 0.50 |
| 10:AJ:65:LEU:HD13 | 14:AN:56:VAL:HG22 | 1.93 | 0.50 |
| 35:DM:83:MET:HG3 | 35:DM:83:MET:O | 2.11 | 0.50 |
| 18:CR:76:LEU:HD22 | 18:CR:76:LEU:N | 2.26 | 0.50 |
| 1:AA:156:G:C2 | 1:AA:166:G:C2 | 2.99 | 0.50 |
| 23:DA:57:C:H2' | 23:DA:58:G:O4' | 2.11 | 0.50 |
| 47:BY:1:MET:CE | 47:BY:4:SER:HB2 | 2.40 | 0.50 |
| 33:DK:71:ARG:NH2 | 33:DK:77:ILE:HG21 | 2.26 | 0.50 |
| 26:BD:11:MET:CE | 26:BD:186:GLY:HA2 | 2.41 | 0.50 |
| 40:DR:2:PHE:HE2 | 40:DR:13:ARG:CD | 2.23 | 0.50 |
| 47:BY:17:SER:HB3 | 47:BY:18:PRO:CD | 2.37 | 0.50 |
| 25:BC:72:LYS:HE2 | 25:BC:101:GLU:HG2 | 1.93 | 0.50 |
| 1:CA:76:G:O2' | 1:CA:77:C:H5' | 2.10 | 0.50 |
| 1:AA:878:G:H1' | 8:AH:3:THR:HG21 | 1.92 | 0.50 |
| 1:CA:402:G:C6 | 1:CA:403:C:C5 | 2.99 | 0.50 |
| 45:BW:31:VAL:HG11 | 45:BW:67:VAL:HG23 | 1.93 | 0.50 |
| 1:AA:488:C:H6 | 1:AA:488:C:O5' | 1.94 | 0.50 |
| 36:DN:57:ARG:CD | 36:DN:59:ASP:OD2 | 2.59 | 0.50 |
| 1:AA:1149:C:OP1 | 9:AI:14:VAL:HG21 | 2.12 | 0.50 |
| 36:DN:67:LEU:O | 36:DN:70:LEU:O | 2.28 | 0.50 |
| 41:BS:29:LEU:CG | 41:BS:33:ARG:HE | 2.24 | 0.50 |
| 46:BX:13:ILE:HA | 46:BX:66:HIS:ND1 | 2.26 | 0.50 |
| 5:CE:53:LEU:HD23 | 5:CE:53:LEU:N | 2.25 | 0.50 |
| 23:DA:1105:U:H2' | 23:DA:1106:G:H8 | 1.75 | 0.50 |
| 23:BA:1508:A:N6 | 23:BA:1509:A:C6 | 2.79 | 0.50 |
| 23:BA:1045:A:H4' | 23:BA:1046:A:H5'' | 1.93 | 0.50 |
| 41:DS:42:ARG:HG2 | 41:DS:42:ARG:HH11 | 1.76 | 0.50 |
| 1:CA:677:U:H2' | 1:CA:678:U:C6 | 2.46 | 0.50 |
| 23:BA:761:A:H8 | 23:BA:761:A:O5' | 1.94 | 0.50 |
| 53:B5:57:ARG:CZ | 53:B5:57:ARG:HB2 | 2.41 | 0.50 |
| 4:AD:79:PHE:O | 4:AD:82:ALA:HB3 | 2.12 | 0.50 |
| 1:AA:1009:G:O2' | 1:AA:1010:G:H5' | 2.11 | 0.50 |
| 23:BA:2687:U:H2' | 23:BA:2688:U:O4' | 2.12 | 0.50 |
| 1:CA:73:G:O5' | 1:CA:73:G:H8 | 1.94 | 0.50 |
| 26:DD:117:MET:HE3 | 26:DD:136:ARG:HA | 1.93 | 0.50 |
| 36:BN:99:LYS:N | 36:BN:99:LYS:CD | 2.74 | 0.50 |
| 2:CB:73:THR:HG22 | 2:CB:94:ASN:O | 2.10 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DA:301:G:HO2' | 23:DA:302:C:H6 | 1.58 | 0.50 |
| 23:DA:1680:U:C2' | 23:DA:1681:G:O5' | 2.59 | 0.50 |
| 1:AA:934:C:C2 | 1:AA:1344:C:C5 | 3.00 | 0.50 |
| 23:BA:1290:C:H2' | 23:BA:1291:C:C6 | 2.42 | 0.50 |
| 1:CA:1022:G:H2' | 1:CA:1023:G:C8 | 2.43 | 0.50 |
| 35:BM:54:MET:O | 35:BM:57:HIS:HB3 | 2.10 | 0.50 |
| 43:DU:90:LEU:HD12 | 43:DU:91:GLU:HG3 | 1.93 | 0.50 |
| 24:BB:45:A:H1' | 28:BF:95:ARG:CZ | 2.41 | 0.50 |
| 1:CA:1504:G:H4' | 1:CA:1505:G:C4 | 2.45 | 0.50 |
| 23:BA:2572:A:H62 | 26:BD:145:LYS:HG3 | 1.76 | 0.50 |
| 33:BK:49:ARG:HA | 33:BK:53:LYS:HZ2 | 1.76 | 0.50 |
| 2:CB:53:ARG:HA | 2:CB:56:ARG:HD2 | 1.93 | 0.50 |
| 33:DK:7:TYR:CE1 | 33:DK:20:MET:HB3 | 2.46 | 0.50 |
| 44:DV:63:ASP:HB3 | 44:DV:65:GLN:HG3 | 1.93 | 0.50 |
| 30:BH:57:ARG:HG2 | 30:BH:57:ARG:O | 2.11 | 0.50 |
| 28:DF:49:ASP:HB3 | 28:DF:52:ILE:HG12 | 1.92 | 0.50 |
| 23:BA:1641:A:H2' | 23:BA:1642:G:O4' | 2.11 | 0.50 |
| 30:BH:76:THR:HG22 | 30:BH:141:LYS:HB2 | 1.92 | 0.50 |
| 23:DA:30:G:H2' | 23:DA:31:C:C6 | 2.46 | 0.50 |
| 1:AA:1318:A:O2' | 19:AS:37:ARG:HB2 | 2.10 | 0.50 |
| 29:DG:78:GLY:O | 29:DG:136:ILE:HG22 | 2.11 | 0.50 |
| 36:DN:25:ALA:O | 36:DN:26:LYS:C | 2.47 | 0.50 |
| 1:CA:1508:G:H2' | 1:CA:1509:C:O4' | 2.11 | 0.50 |
| 43:BU:14:LEU:C | 43:BU:14:LEU:HD23 | 2.31 | 0.50 |
| 32:BJ:49:LEU:O | 32:BJ:49:LEU:HD12 | 2.11 | 0.50 |
| 23:DA:1173:G:H1' | 23:DA:1177:A:H61 | 1.75 | 0.50 |
| 32:DJ:119:GLU:H | 32:DJ:119:GLU:CD | 2.11 | 0.50 |
| 22:AV:6181:C:C2 | 22:AV:6182:A:C8 | 3.00 | 0.50 |
| 1:AA:363:A:C6 | 1:AA:364:A:C6 | 2.99 | 0.50 |
| 13:CM:96:LEU:HD22 | 13:CM:103:THR:HG21 | 1.92 | 0.50 |
| 38:BP:56:GLY:O | 38:BP:59:THR:CG2 | 2.55 | 0.50 |
| 23:DA:2017:U:O2 | 50:D2:10:LYS:HB2 | 2.11 | 0.50 |
| 39:DQ:72:HIS:CE1 | 39:DQ:107:ALA:HA | 2.47 | 0.50 |
| 28:DF:72:ARG:HB3 | 28:DF:87:PRO:HD2 | 1.92 | 0.50 |
| 23:DA:1019:U:H2' | 23:DA:1020:A:C8 | 2.40 | 0.50 |
| 34:BL:50:ARG:HB2 | 53:B5:60:LEU:HD21 | 1.93 | 0.50 |
| 34:BL:50:ARG:HB3 | 34:BL:50:ARG:HH11 | 1.76 | 0.50 |
| 1:AA:501:C:H2' | 1:AA:502:G:C8 | 2.47 | 0.50 |
| 35:BM:88:GLY:C | 35:BM:89:ASN:CG | 2.67 | 0.50 |
| 3:CC:31:HIS:O | 3:CC:35:GLU:HG2 | 2.11 | 0.50 |
| 4:CD:3:ARG:HG2 | 4:CD:5:ILE:HD13 | 1.92 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:1347:G:C6 | 9:AI:107:ARG:NH2 | 2.75 | 0.50 |
| 1:CA:353:A:C2' | 1:CA:354:G:OP2 | 2.59 | 0.50 |
| 6:CF:61:LEU:HB3 | 6:CF:63:TYR:HE2 | 1.76 | 0.50 |
| 23:DA:1344:G:H5' | 23:DA:1384:A:C6 | 2.46 | 0.50 |
| 1:CA:879:C:O2' | 1:CA:880:C:H5' | 2.11 | 0.50 |
| 33:BK:34:THR:HG23 | 33:BK:35:VAL:N | 2.27 | 0.50 |
| 23:DA:1502:C:H2' | 23:DA:1503:U:C6 | 2.47 | 0.50 |
| 23:DA:2324:C:H42 | 23:DA:2331:G:H1 | 1.59 | 0.50 |
| 8:AH:87:SER:HB2 | 8:AH:93:VAL:HB | 1.92 | 0.50 |
| 23:BA:1324:G:N2 | 23:BA:1331:A:C4 | 2.79 | 0.50 |
| 6:AF:90:VAL:O | 6:AF:91:VAL:HG23 | 2.10 | 0.50 |
| 23:DA:954:G:H5'' | 35:DM:13:GLN:HG2 | 1.93 | 0.50 |
| 23:DA:1109:C:N4 | 23:DA:1110:G:C2 | 2.78 | 0.50 |
| 18:CR:26:LEU:CD1 | 18:CR:42:ARG:HD2 | 2.39 | 0.50 |
| 23:DA:2563:U:O2 | 23:DA:2565:A:H8 | 1.94 | 0.50 |
| 24:DB:78:A:N3 | 24:DB:99:A:C5 | 2.80 | 0.50 |
| 1:CA:68:G:C6 | 1:CA:69:G:N7 | 2.79 | 0.50 |
| 23:BA:598:G:H5' | 34:BL:15:ARG:HG2 | 1.93 | 0.50 |
| 24:BB:60:C:C2 | 24:BB:61:G:C8 | 2.99 | 0.50 |
| 43:DU:46:LYS:O | 43:DU:48:ALA:N | 2.44 | 0.50 |
| 1:CA:853:G:C2' | 1:CA:854:G:H5' | 2.42 | 0.50 |
| 8:CH:86:ILE:HG22 | 8:CH:93:VAL:HG21 | 1.92 | 0.50 |
| 50:B2:35:GLU:HB2 | 50:B2:49:CYS:SG | 2.51 | 0.50 |
| 23:DA:2468:G:O2' | 23:DA:2476:A:N7 | 2.41 | 0.50 |
| 29:BG:86:GLU:N | 29:BG:86:GLU:OE2 | 2.42 | 0.50 |
| 43:BU:76:CYS:SG | 43:BU:77:PRO:CD | 2.99 | 0.50 |
| 33:DK:19:ILE:N | 33:DK:19:ILE:HD13 | 2.22 | 0.50 |
| 1:AA:1055:A:N7 | 1:AA:1200:C:N4 | 2.57 | 0.50 |
| 23:DA:2638:G:OP2 | 26:DD:82:ARG:NH2 | 2.44 | 0.50 |
| 23:BA:1856:G:C2 | 23:BA:1887:C:N3 | 2.79 | 0.50 |
| 1:CA:109:A:N6 | 1:CA:326:G:C6 | 2.79 | 0.50 |
| 4:AD:13:ARG:HD2 | 4:AD:38:TYR:O | 2.12 | 0.50 |
| 7:AG:61:VAL:O | 7:AG:65:ALA:HB2 | 2.11 | 0.50 |
| 23:DA:1709:U:H2' | 23:DA:1710:C:C6 | 2.45 | 0.50 |
| 53:D5:39:LYS:HA | 53:D5:42:ARG:NH1 | 2.27 | 0.50 |
| 40:BR:72:VAL:HG23 | 40:BR:85:LYS:HB3 | 1.92 | 0.50 |
| 1:CA:799:G:C2' | 1:CA:800:G:O5' | 2.59 | 0.50 |
| 3:AC:191:THR:HB | 3:AC:193:TYR:CD2 | 2.46 | 0.50 |
| 23:BA:1354:A:C8 | 23:BA:1355:G:C8 | 3.00 | 0.50 |
| 23:BA:1516:U:H2' | 23:BA:1517:G:H8 | 1.75 | 0.50 |
| 23:DA:1833:U:O2' | 23:DA:1834:U:H5' | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BA:414:C:H2' | 23:BA:415:A:H8 | 1.75 | 0.50 |
| 1:AA:1167:A:H62 | 1:AA:1169:A:N6 | 2.09 | 0.50 |
| 23:BA:1204:A:N6 | 23:BA:1240:U:O2' | 2.44 | 0.50 |
| 23:DA:2302:G:C2' | 23:DA:2303:G:H5' | 2.42 | 0.50 |
| 1:CA:191(F):U:H2' | 1:CA:191(G):G:H8 | 1.76 | 0.50 |
| 23:BA:1118:C:H5'' | 44:BV:80:ARG:NH2 | 2.26 | 0.50 |
| 1:AA:826:C:H2' | 8:AH:15:ASN:HD22 | 1.76 | 0.50 |
| 23:BA:1050:A:C2 | 23:BA:2751:G:C5 | 2.99 | 0.50 |
| 39:DQ:36:ARG:HD3 | 39:DQ:40:PHE:CZ | 2.46 | 0.50 |
| 23:BA:2703:C:O2' | 23:BA:2704:C:H5' | 2.11 | 0.50 |
| 30:BH:25:TYR:CD1 | 30:BH:30:LEU:HD11 | 2.47 | 0.50 |
| 23:DA:2420:C:OP1 | 53:D5:34:TRP:HA | 2.11 | 0.50 |
| 34:DL:140:ALA:O | 34:DL:141:ALA:CB | 2.59 | 0.50 |
| 52:B4:10:ARG:NE | 52:B4:14:LYS:HD2 | 2.26 | 0.50 |
| 1:AA:1226:C:O2' | 13:AM:111:LYS:NZ | 2.45 | 0.50 |
| 26:BD:11:MET:CE | 26:BD:186:GLY:CA | 2.90 | 0.50 |
| 23:DA:810:U:H6 | 23:DA:810:U:O5' | 1.94 | 0.50 |
| 32:BJ:37:VAL:HG12 | 32:BJ:38:LEU:N | 2.26 | 0.50 |
| 23:BA:1022:G:C6 | 23:BA:1140:C:C4 | 2.99 | 0.50 |
| 23:BA:2579:C:O2' | 26:BD:131:ALA:HB3 | 2.12 | 0.50 |
| 39:DQ:79:PHE:CE2 | 39:DQ:106:PHE:CE1 | 3.00 | 0.50 |
| 1:CA:376:G:C5 | 1:CA:389:A:N1 | 2.80 | 0.50 |
| 25:DC:265:PRO:C | 25:DC:267:SER:N | 2.65 | 0.50 |
| 25:DC:270:ILE:C | 25:DC:271:ILE:HG12 | 2.32 | 0.50 |
| 1:CA:391:G:C6 | 1:CA:392:G:N7 | 2.79 | 0.50 |
| 2:CB:211:ILE:HG22 | 2:CB:215:LEU:HD23 | 1.93 | 0.50 |
| 28:BF:88:ILE:HD12 | 28:BF:89:GLY:N | 2.26 | 0.50 |
| 44:BV:163:LEU:CD2 | 44:BV:163:LEU:H | 2.25 | 0.50 |
| 1:CA:1074:G:C2 | 1:CA:1075:C:C2 | 3.00 | 0.50 |
| 1:AA:1352:C:H2' | 1:AA:1353:G:C8 | 2.46 | 0.50 |
| 46:BX:10:LYS:O | 46:BX:11:ARG:HB2 | 2.10 | 0.50 |
| 8:CH:20:TYR:HD1 | 8:CH:65:TYR:CE2 | 2.30 | 0.50 |
| 1:AA:817:C:H4' | 1:AA:818:G:OP1 | 2.10 | 0.50 |
| 23:BA:2750:A:C2 | 23:BA:2753:A:H2 | 2.28 | 0.50 |
| 23:BA:1502:C:H2' | 23:BA:1503:U:C6 | 2.46 | 0.50 |
| 23:BA:1502:C:H3' | 23:BA:1502:C:H6 | 1.76 | 0.50 |
| 1:CA:456:C:H42 | 1:CA:476:G:H1 | 1.57 | 0.50 |
| 36:DN:101:ALA:HB2 | 50:D2:44:THR:HB | 1.94 | 0.50 |
| 24:BB:49:C:H6 | 24:BB:49:C:O5' | 1.95 | 0.50 |
| 23:BA:1476:C:C6 | 23:BA:1476:C:H3' | 2.45 | 0.50 |
| 4:AD:82:ALA:HB1 | 4:AD:89:THR:HG23 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:DG:88:LEU:O | 29:DG:162:ILE:HA | 2.11 | 0.50 |
| 23:DA:270(H):C:C4 | 23:DA:270(I):C:C5 | 3.00 | 0.50 |
| 29:DG:86:GLU:OE2 | 29:DG:86:GLU:N | 2.42 | 0.50 |
| 2:AB:73:THR:HG22 | 2:AB:94:ASN:O | 2.11 | 0.50 |
| 17:CQ:60:ILE:O | 17:CQ:71:PHE:HA | 2.12 | 0.50 |
| 17:CQ:85:VAL:O | 17:CQ:89:LEU:HG | 2.11 | 0.50 |
| 1:AA:1053:G:H3' | 1:AA:1054:C:C5' | 2.41 | 0.50 |
| 23:BA:786:C:C2' | 23:BA:787:U:H5' | 2.42 | 0.50 |
| 13:CM:79:LYS:HA | 13:CM:82:MET:HB3 | 1.93 | 0.50 |
| 3:AC:23:TYR:CG | 3:AC:24:ALA:N | 2.80 | 0.50 |
| 16:CP:43:LYS:HG2 | 16:CP:48:TRP:CG | 2.46 | 0.50 |
| 1:AA:1378:C:H3' | 1:AA:1379:G:H5'' | 1.93 | 0.50 |
| 25:DC:260:ARG:O | 25:DC:260:ARG:HG2 | 2.11 | 0.50 |
| 28:DF:55:LYS:HD2 | 28:DF:58:GLN:NE2 | 2.27 | 0.50 |
| 51:B3:38:LYS:HG2 | 51:B3:39:TYR:N | 2.27 | 0.50 |
| 26:DD:112:GLY:O | 26:DD:159:HIS:HA | 2.12 | 0.50 |
| 1:CA:779:C:H2' | 1:CA:780:A:O4' | 2.11 | 0.50 |
| 12:CL:77:GLN:O | 12:CL:79:HIS:N | 2.43 | 0.50 |
| 23:DA:644:A:C2 | 23:DA:646:A:C4 | 3.00 | 0.50 |
| 24:BB:55:U:O2' | 24:BB:56:G:H5' | 2.11 | 0.50 |
| 23:BA:189:G:H2' | 23:BA:205:G:N2 | 2.27 | 0.50 |
| 23:BA:2506:U:C5 | 23:BA:2507:C:C5 | 3.00 | 0.50 |
| 1:AA:562:C:H1' | 12:AL:14:ARG:HB3 | 1.93 | 0.50 |
| 23:DA:1126:A:H8 | 23:DA:1126:A:O5' | 1.95 | 0.50 |
| 23:BA:2078:C:C2' | 23:BA:2079:U:H5' | 2.41 | 0.50 |
| 42:DT:3:THR:HA | 42:DT:6:ASP:OD2 | 2.12 | 0.50 |
| 7:AG:79:ARG:HA | 7:AG:83:ALA:O | 2.12 | 0.50 |
| 23:BA:1678:G:H2' | 23:BA:1678:G:N3 | 2.27 | 0.50 |
| 16:CP:45:THR:HB | 16:CP:46:PRO:HD2 | 1.93 | 0.50 |
| 10:AJ:30:SER:HB2 | 10:AJ:80:LYS:CG | 2.42 | 0.50 |
| 23:BA:2726:U:O2 | 23:BA:2726:U:H5' | 2.11 | 0.50 |
| 1:AA:619:U:N3 | 4:AD:135:LEU:HD11 | 2.26 | 0.50 |
| 1:AA:1171:G:H2' | 1:AA:1172:C:C6 | 2.47 | 0.50 |
| 3:CC:72:LYS:HG2 | 3:CC:74:GLY:H | 1.75 | 0.50 |
| 53:D5:22:VAL:CB | 53:D5:54:GLU:HG3 | 2.41 | 0.50 |
| 35:BM:81:VAL:C | 35:BM:82:ARG:HG2 | 2.25 | 0.50 |
| 2:AB:91:PRO:HG3 | 2:AB:154:LEU:HD21 | 1.92 | 0.50 |
| 2:AB:68:ILE:CG2 | 2:AB:70:PHE:CE1 | 2.94 | 0.50 |
| 34:BL:97:PRO:HA | 34:BL:112:LEU:HD12 | 1.92 | 0.50 |
| 9:AI:114:TYR:N | 9:AI:114:TYR:CD2 | 2.80 | 0.50 |
| 22:AV:6189:G:H2' | 22:AV:6190:U:C6 | 2.46 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:CV:6191:A:N1 | 22:CV:6213:A:C6 | 2.79 | 0.50 |
| 1:CA:363:A:C6 | 1:CA:364:A:C6 | 3.00 | 0.50 |
| 23:BA:1899:G:N2 | 23:BA:1902:C:C4 | 2.80 | 0.50 |
| 32:DJ:39:ILE:O | 32:DJ:78:VAL:HG22 | 2.11 | 0.50 |
| 28:BF:82:LEU:HD22 | 28:BF:87:PRO:HG3 | 1.92 | 0.50 |
| 28:DF:73:ALA:HB3 | 28:DF:76:SER:OG | 2.12 | 0.50 |
| 16:AP:58:TYR:O | 16:AP:61:SER:HB3 | 2.12 | 0.50 |
| 1:AA:408:A:C4 | 1:AA:409:G:C8 | 3.00 | 0.50 |
| 23:DA:142:G:C1' | 42:DT:37:THR:HG21 | 2.41 | 0.50 |
| 25:DC:158:ALA:C | 25:DC:161:THR:HG23 | 2.31 | 0.50 |
| 23:DA:2713:A:H3' | 23:DA:2714:G:C5' | 2.40 | 0.50 |
| 20:CT:71:THR:CG2 | 20:CT:72:LEU:H | 2.19 | 0.50 |
| 23:DA:1771:C:O2' | 23:DA:1786:A:H8 | 1.79 | 0.50 |
| 26:DD:49:LEU:HD22 | 26:DD:49:LEU:N | 2.17 | 0.50 |
| 5:CE:34:VAL:O | 5:CE:41:VAL:HA | 2.11 | 0.50 |
| 23:DA:2886:G:H2' | 23:DA:2887:U:C6 | 2.46 | 0.50 |
| 1:AA:191(G):G:C4 | 1:AA:192:U:C5 | 2.99 | 0.50 |
| 1:AA:1366:C:H2' | 1:AA:1367:C:H6 | 1.75 | 0.50 |
| 1:CA:353:A:H2' | 1:CA:354:G:OP2 | 2.12 | 0.50 |
| 1:CA:9:G:H2' | 1:CA:10:A:C8 | 2.46 | 0.50 |
| 6:CF:8:ILE:HD12 | 6:CF:26:ILE:HD13 | 1.93 | 0.50 |
| 23:BA:1487:G:H2' | 23:BA:1488:G:C8 | 2.36 | 0.50 |
| 11:CK:40:ILE:HD13 | 11:CK:40:ILE:N | 2.26 | 0.50 |
| 37:BO:62:LYS:O | 37:BO:65:VAL:HB | 2.11 | 0.50 |
| 16:CP:39:TYR:CE1 | 16:CP:73:LEU:HD13 | 2.47 | 0.50 |
| 1:AA:799:G:C2' | 1:AA:800:G:O5' | 2.59 | 0.50 |
| 1:CA:600:C:OP1 | 8:CH:97:VAL:HG12 | 2.12 | 0.50 |
| 53:B5:14:VAL:HG13 | 53:B5:22:VAL:HG13 | 1.93 | 0.50 |
| 1:AA:173:U:C2 | 1:AA:197:A:C2 | 2.99 | 0.50 |
| 23:BA:1478:G:N2 | 23:BA:1479:G:C4 | 2.79 | 0.50 |
| 25:BC:25:THR:HG21 | 25:BC:82:ILE:H | 1.74 | 0.50 |
| 23:DA:2346:A:C2 | 23:DA:2383:G:C2 | 2.98 | 0.50 |
| 30:DH:5:LEU:HD23 | 30:DH:17:GLN:O | 2.11 | 0.50 |
| 23:DA:783:A:H3' | 23:DA:783:A:C8 | 2.47 | 0.50 |
| 25:BC:181:GLU:HA | 25:BC:272:ALA:HB3 | 1.92 | 0.50 |
| 38:BP:28:VAL:HA | 38:BP:89:VAL:CG1 | 2.41 | 0.50 |
| 43:DU:76:CYS:SG | 43:DU:77:PRO:CD | 2.99 | 0.50 |
| 44:BV:39:VAL:CG2 | 44:BV:44:PHE:HB2 | 2.39 | 0.50 |
| 11:AK:21:ILE:HG13 | 11:AK:30:VAL:HG12 | 1.94 | 0.50 |
| 23:BA:282:A:C4 | 23:BA:359:A:C2 | 2.99 | 0.50 |
| 23:BA:636:G:OP1 | 34:BL:132:LYS:HD3 | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:592:G:N1 | 1:CA:648:A:C6 | 2.79 | 0.50 |
| 23:DA:1290:C:H2' | 23:DA:1291:C:C6 | 2.41 | 0.50 |
| 1:AA:938:A:N6 | 1:AA:939:G:C6 | 2.79 | 0.50 |
| 23:DA:825:C:C2' | 23:DA:826:U:H5' | 2.41 | 0.50 |
| 1:CA:953:G:C6 | 1:CA:1229:A:C6 | 3.00 | 0.50 |
| 6:AF:18:GLN:O | 6:AF:21:LEU:HB2 | 2.11 | 0.50 |
| 23:DA:795:C:H6 | 23:DA:795:C:O5' | 1.95 | 0.50 |
| 32:BJ:80:ALA:O | 32:BJ:83:ILE:HG13 | 2.11 | 0.50 |
| 44:BV:5:LEU:CG | 44:BV:47:VAL:HG21 | 2.42 | 0.50 |
| 1:AA:44:G:C2 | 1:AA:399:G:C2 | 2.99 | 0.50 |
| 23:BA:2001:A:H2' | 23:BA:2002:G:O4' | 2.12 | 0.50 |
| 23:DA:1773:A:C5 | 23:DA:1829:A:H1' | 2.46 | 0.50 |
| 23:DA:1204:A:N6 | 23:DA:1240:U:O2' | 2.45 | 0.50 |
| 23:DA:2078:C:C2' | 23:DA:2079:U:H5' | 2.42 | 0.50 |
| 23:BA:2836:U:H2' | 23:BA:2837:G:C8 | 2.47 | 0.50 |
| 32:BJ:51:THR:O | 32:BJ:54:ALA:HB3 | 2.11 | 0.50 |
| 2:AB:53:ARG:HA | 2:AB:56:ARG:HD2 | 1.92 | 0.50 |
| 11:AK:120:ARG:NH1 | 11:AK:126:ARG:HE | 2.08 | 0.50 |
| 47:BY:7:ARG:NE | 47:BY:11:GLU:OE2 | 2.44 | 0.50 |
| 26:DD:3:GLY:C | 26:DD:81:ILE:HD13 | 2.32 | 0.50 |
| 23:DA:1232:G:H2' | 23:DA:1233:C:H6 | 1.76 | 0.50 |
| 23:BA:1382:G:O2' | 23:BA:1383:C:H5' | 2.12 | 0.50 |
| 32:DJ:32:VAL:HG12 | 32:DJ:33:GLU:N | 2.26 | 0.50 |
| 30:DH:76:THR:HG22 | 30:DH:141:LYS:HB2 | 1.93 | 0.50 |
| 1:CA:1290:G:N3 | 1:CA:1290:G:H2' | 2.26 | 0.50 |
| 1:CA:697:U:H2' | 1:CA:698:G:H5' | 1.93 | 0.50 |
| 23:DA:1317:A:C6 | 23:DA:1318:C:C4 | 2.99 | 0.50 |
| 53:D5:14:VAL:HG13 | 53:D5:22:VAL:HG13 | 1.93 | 0.50 |
| 2:AB:61:LEU:HG | 2:AB:68:ILE:HD11 | 1.94 | 0.50 |
| 9:CI:14:VAL:O | 9:CI:65:VAL:HG23 | 2.10 | 0.50 |
| 22:CV:6189:G:C5 | 22:CV:6190:U:C5 | 2.99 | 0.50 |
| 1:CA:362:G:O3' | 12:CL:32:ARG:NH2 | 2.44 | 0.50 |
| 2:CB:61:LEU:HG | 2:CB:68:ILE:HD11 | 1.94 | 0.50 |
| 32:BJ:156:GLN:O | 32:BJ:157:ARG:HB2 | 2.12 | 0.50 |
| 40:DR:2:PHE:O | 40:DR:41:GLY:HA2 | 2.12 | 0.50 |
| 30:BH:142:VAL:O | 30:BH:143:SER:HB2 | 2.12 | 0.50 |
| 23:BA:994:C:OP1 | 39:BQ:53:ARG:NH2 | 2.45 | 0.50 |
| 24:DB:7:G:H4' | 37:DO:29:PHE:CG | 2.46 | 0.50 |
| 1:AA:376:G:H1 | 1:AA:387:U:H3 | 1.59 | 0.50 |
| 3:CC:19:GLU:HG3 | 3:CC:54:ARG:HD2 | 1.93 | 0.50 |
| 3:AC:113:ALA:HB2 | 3:AC:202:ILE:HG13 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:DH:128:LEU:O | 30:DH:139:GLN:HA | 2.11 | 0.50 |
| 20:AT:26:ASN:ND2 | 20:AT:26:ASN:N | 2.49 | 0.50 |
| 1:AA:76:G:O2' | 1:AA:77:C:H5' | 2.11 | 0.50 |
| 1:AA:79:G:H2' | 1:AA:80:G:C8 | 2.46 | 0.50 |
| 23:DA:2687:U:H2' | 23:DA:2688:U:O4' | 2.12 | 0.50 |
| 5:AE:9:LYS:HB3 | 5:AE:112:LEU:HD11 | 1.94 | 0.50 |
| 5:AE:48:ALA:C | 5:AE:50:GLU:H | 2.14 | 0.50 |
| 49:B1:50:THR:HG22 | 49:B1:51:TYR:N | 2.26 | 0.50 |
| 1:AA:1071:C:H5'' | 5:AE:49:PRO:HG2 | 1.92 | 0.50 |
| 1:AA:1072:G:C6 | 1:AA:1104:G:C2 | 2.99 | 0.50 |
| 40:DR:28:GLU:O | 40:DR:61:VAL:HG21 | 2.12 | 0.50 |
| 18:CR:56:THR:HB | 18:CR:58:LEU:HD12 | 1.93 | 0.50 |
| 23:BA:2305:A:H3' | 23:BA:2306:C:H5'' | 1.93 | 0.50 |
| 6:AF:22:GLU:O | 6:AF:26:ILE:HG13 | 2.11 | 0.50 |
| 1:CA:488:C:O5' | 1:CA:488:C:H6 | 1.95 | 0.50 |
| 23:BA:2785:C:O2' | 26:BD:66:HIS:CD2 | 2.64 | 0.50 |
| 8:CH:19:VAL:HG23 | 8:CH:21:LYS:HG2 | 1.93 | 0.50 |
| 1:AA:735:C:H1' | 18:AR:75:ILE:HD11 | 1.93 | 0.50 |
| 1:AA:457:C:O2 | 1:AA:457:C:C2' | 2.58 | 0.50 |
| 23:BA:1511:A:H2' | 23:BA:1512:G:C8 | 2.45 | 0.50 |
| 1:CA:619:U:H2' | 4:CD:135:LEU:CD2 | 2.41 | 0.50 |
| 23:DA:1858:G:H1' | 23:DA:1884:A:H62 | 1.71 | 0.50 |
| 1:CA:599:C:H2' | 1:CA:600:C:H6 | 1.75 | 0.50 |
| 1:CA:642:A:O2' | 8:CH:31:PHE:HE1 | 1.95 | 0.50 |
| 23:DA:1952:A:C5 | 33:DK:22:ILE:CD1 | 2.91 | 0.50 |
| 53:B5:57:ARG:NE | 53:B5:57:ARG:CA | 2.71 | 0.50 |
| 15:AO:39:LEU:HD13 | 15:AO:56:LEU:HB2 | 1.92 | 0.50 |
| 15:AO:53:HIS:CE1 | 23:BA:715:G:O6 | 2.62 | 0.50 |
| 1:AA:173:U:N1 | 1:AA:197:A:C2 | 2.79 | 0.50 |
| 23:DA:2658:C:H4' | 29:DG:158:HIS:NE2 | 2.27 | 0.50 |
| 1:CA:105:G:C6 | 1:CA:106:C:C4 | 3.00 | 0.50 |
| 34:BL:13:ASN:O | 34:BL:14:LYS:C | 2.50 | 0.50 |
| 44:BV:4:ARG:HD3 | 44:BV:60:GLU:HG3 | 1.94 | 0.50 |
| 1:AA:1357:A:N7 | 1:AA:1358:U:C4 | 2.79 | 0.50 |
| 23:DA:864:G:O2' | 23:DA:865:C:H5' | 2.12 | 0.50 |
| 35:DM:20:ALA:HA | 35:DM:98:LYS:HB3 | 1.92 | 0.50 |
| 32:BJ:62:ARG:NH2 | 32:BJ:64:ASP:OD2 | 2.40 | 0.50 |
| 23:BA:2862:G:C4 | 23:BA:2863:C:C5 | 2.99 | 0.50 |
| 1:CA:1443:G:H22 | 38:DP:119:LYS:HB2 | 1.76 | 0.50 |
| 23:BA:1775:U:H2' | 23:BA:1776:G:O5' | 2.12 | 0.50 |
| 23:BA:794:G:H2' | 23:BA:795:C:C6 | 2.47 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:760:G:H2' | 1:CA:761:G:H5' | 1.93 | 0.50 |
| 23:DA:816:C:O2' | 23:DA:817:C:H5' | 2.12 | 0.50 |
| 1:CA:109:A:C6 | 1:CA:326:G:C6 | 2.99 | 0.50 |
| 1:AA:522:C:N4 | 1:AA:528:C:H42 | 2.09 | 0.50 |
| 28:BF:17:PRO:HA | 28:BF:20:ILE:HG12 | 1.92 | 0.50 |
| 17:AQ:45:HIS:O | 17:AQ:73:VAL:HG23 | 2.12 | 0.50 |
| 17:AQ:45:HIS:HB3 | 17:AQ:72:ARG:HG2 | 1.93 | 0.50 |
| 26:DD:16:ARG:O | 26:DD:17:ASP:C | 2.47 | 0.50 |
| 23:BA:1831:G:C5 | 23:BA:1832:C:C5 | 3.00 | 0.50 |
| 23:DA:990:A:H5'' | 23:DA:991:C:OP2 | 2.10 | 0.50 |
| 1:CA:137:C:O2' | 1:CA:138:G:H5' | 2.12 | 0.50 |
| 8:AH:50:ARG:CD | 8:AH:50:ARG:H | 2.24 | 0.50 |
| 35:DM:40:ALA:CB | 35:DM:127:ILE:HD12 | 2.40 | 0.50 |
| 13:CM:14:ARG:NH1 | 13:CM:42:ALA:HA | 2.26 | 0.50 |
| 25:DC:198:ASN:ND2 | 25:DC:198:ASN:C | 2.64 | 0.50 |
| 1:AA:765:G:H5'' | 1:AA:766:A:OP1 | 2.11 | 0.50 |
| 23:DA:2482:G:H2' | 23:DA:2483:C:O4' | 2.11 | 0.50 |
| 23:DA:455:C:N3 | 23:DA:472:A:H2' | 2.27 | 0.50 |
| 16:AP:25:ARG:O | 16:AP:26:ARG:C | 2.50 | 0.50 |
| 28:BF:28:VAL:O | 28:BF:31:VAL:HG12 | 2.11 | 0.50 |
| 34:DL:100:LEU:HD22 | 34:DL:100:LEU:H | 1.77 | 0.50 |
| 44:BV:63:ASP:HB3 | 44:BV:65:GLN:HG3 | 1.94 | 0.50 |
| 1:AA:933:G:N7 | 7:AG:3:ARG:NH2 | 2.60 | 0.50 |
| 34:DL:101:VAL:CB | 34:DL:106:LEU:HB3 | 2.42 | 0.50 |
| 23:BA:310:A:P | 43:BU:18:GLY:HA2 | 2.52 | 0.50 |
| 23:DA:2250:G:H5'' | 23:DA:2250:G:N3 | 2.27 | 0.50 |
| 23:DA:1542:G:OP2 | 23:DA:1543:A:OP1 | 2.29 | 0.50 |
| 1:CA:1368:G:OP2 | 9:CI:112:LYS:HD3 | 2.11 | 0.50 |
| 9:CI:10:ARG:CD | 9:CI:11:LYS:HG3 | 2.40 | 0.50 |
| 23:DA:806:C:OP1 | 34:DL:39:LYS:HB3 | 2.12 | 0.50 |
| 1:CA:1324:A:O4' | 1:CA:136(A):C:H4' | 2.11 | 0.50 |
| 1:CA:46:G:H8 | 1:CA:46:G:O5' | 1.94 | 0.50 |
| 1:CA:503:C:OP1 | 12:CL:118:LYS:HE3 | 2.11 | 0.50 |
| 23:BA:518:G:H4' | 41:BS:18:ARG:NH1 | 2.27 | 0.50 |
| 28:BF:72:ARG:HB3 | 28:BF:87:PRO:HD2 | 1.94 | 0.50 |
| 23:DA:252:G:O2' | 23:DA:253:C:H5' | 2.12 | 0.50 |
| 30:BH:77:LEU:HD21 | 30:BH:104:GLN:HB2 | 1.93 | 0.50 |
| 39:BQ:79:PHE:HE2 | 39:BQ:106:PHE:CZ | 2.30 | 0.50 |
| 1:AA:376:G:C5 | 1:AA:389:A:N1 | 2.79 | 0.50 |
| 4:AD:141:ARG:O | 4:AD:144:ASP:OD2 | 2.29 | 0.50 |
| 42:DT:27:THR:HB | 42:DT:80:ILE:HB | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BA:1408:C:C2 | 23:BA:1595:G:N2 | 2.80 | 0.50 |
| 28:BF:88:ILE:HD12 | 28:BF:89:GLY:H | 1.77 | 0.50 |
| 23:DA:1209:G:N2 | 23:DA:1210:A:N6 | 2.58 | 0.50 |
| 1:CA:670:G:N2 | 1:CA:736:C:O2 | 2.42 | 0.50 |
| 1:CA:738:C:C2 | 1:CA:739:C:C5 | 3.00 | 0.50 |
| 5:AE:41:VAL:HG12 | 5:AE:112:LEU:O | 2.11 | 0.50 |
| 2:CB:98:LEU:HB2 | 2:CB:101:MET:CG | 2.42 | 0.50 |
| 23:BA:1439:A:C2 | 23:BA:1553:A:C4 | 2.99 | 0.50 |
| 10:AJ:33:GLN:O | 10:AJ:75:ILE:HG12 | 2.11 | 0.50 |
| 1:AA:1371:G:OP1 | 9:AI:11:LYS:HB3 | 2.10 | 0.50 |
| 9:AI:14:VAL:O | 9:AI:65:VAL:HG23 | 2.11 | 0.50 |
| 42:DT:57:LEU:N | 42:DT:57:LEU:HD12 | 2.26 | 0.50 |
| 36:BN:4:LEU:C | 36:BN:6:SER:H | 2.15 | 0.50 |
| 2:CB:27:LYS:CG | 2:CB:194:PRO:HD2 | 2.41 | 0.50 |
| 23:DA:1567:A:C8 | 25:DC:84:TYR:CE2 | 3.00 | 0.50 |
| 23:BA:1104:C:C4 | 23:BA:1105:U:C5 | 3.00 | 0.50 |
| 18:AR:56:THR:HB | 18:AR:58:LEU:HD12 | 1.93 | 0.50 |
| 1:CA:1009:G:O2' | 1:CA:1010:G:H5' | 2.12 | 0.50 |
| 36:BN:99:LYS:H | 36:BN:99:LYS:HD2 | 1.75 | 0.50 |
| 30:BH:2:LYS:HB3 | 30:BH:20:ASP:OD1 | 2.12 | 0.50 |
| 1:CA:832:C:N4 | 1:CA:855:G:O6 | 2.45 | 0.50 |
| 23:DA:1476:C:C6 | 23:DA:1476:C:C3' | 2.94 | 0.50 |
| 17:CQ:83:ASP:O | 17:CQ:86:GLU:HB2 | 2.12 | 0.50 |
| 3:CC:23:TYR:HB2 | 10:CJ:93:GLY:O | 2.11 | 0.50 |
| 3:CC:73:PRO:HA | 3:CC:76:VAL:HG13 | 1.93 | 0.50 |
| 1:AA:1254:C:OP1 | 10:AJ:45:ARG:HD3 | 2.12 | 0.50 |
| 10:CJ:9:ARG:HG2 | 10:CJ:69:ASN:OD1 | 2.12 | 0.50 |
| 1:CA:973:G:P | 10:CJ:57:LYS:HZ3 | 2.34 | 0.50 |
| 12:CL:6:ILE:N | 12:CL:6:ILE:HD12 | 2.25 | 0.50 |
| 23:DA:184:C:C2 | 23:DA:185:U:C5 | 3.00 | 0.50 |
| 23:DA:1164:G:H5' | 23:DA:1165:U:OP2 | 2.12 | 0.50 |
| 2:AB:200:ILE:HG22 | 2:AB:202:PRO:HD3 | 1.92 | 0.50 |
| 39:BQ:17:ILE:HG23 | 39:BQ:39:LEU:HD12 | 1.93 | 0.50 |
| 23:DA:188:G:C2' | 23:DA:189:G:H5' | 2.42 | 0.50 |
| 23:DA:188:G:H1 | 23:DA:208:C:H42 | 1.60 | 0.50 |
| 1:CA:1501:C:C5 | 1:CA:1504:G:C4 | 2.99 | 0.50 |
| 1:CA:683:G:C6 | 1:CA:684:A:C5 | 3.00 | 0.50 |
| 1:CA:685:G:O2' | 1:CA:686:U:H5' | 2.11 | 0.50 |
| 24:BB:5:C:O2 | 24:BB:116:G:N2 | 2.44 | 0.50 |
| 1:CA:247:G:C5 | 1:CA:248:C:C5 | 3.00 | 0.50 |
| 46:DX:58:ILE:HD11 | 46:DX:60:PHE:CE1 | 2.47 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DA:25:U:H2' | 23:DA:26:G:C8 | 2.47 | 0.50 |
| 41:DS:45:TYR:CD2 | 41:DS:45:TYR:O | 2.65 | 0.50 |
| 1:AA:1386:G:C2 | 1:AA:1387:G:C8 | 2.99 | 0.50 |
| 23:BA:915:C:O2' | 24:BB:100:G:H5' | 2.12 | 0.50 |
| 23:DA:1850:G:C4 | 23:DA:1851:U:C5 | 3.00 | 0.50 |
| 23:BA:2302:G:O2' | 23:BA:2303:G:H5' | 2.11 | 0.50 |
| 23:BA:1241:A:N7 | 23:BA:1242:A:C4 | 2.80 | 0.50 |
| 8:CH:127:LEU:HD13 | 8:CH:127:LEU:O | 2.12 | 0.50 |
| 32:DJ:133:GLY:O | 32:DJ:137:ARG:HG2 | 2.11 | 0.50 |
| 1:CA:934:C:C2 | 1:CA:1344:C:C5 | 2.99 | 0.50 |
| 23:DA:618(B):C:O2 | 23:DA:618(B):C:H2' | 2.12 | 0.50 |
| 1:CA:33:A:H2' | 1:CA:34:C:C6 | 2.46 | 0.50 |
| 1:AA:1004:A:N3 | 1:AA:1004:A:H3' | 2.26 | 0.50 |
| 49:B1:45:GLY:O | 49:B1:46:ASN:HB2 | 2.11 | 0.50 |
| 46:DX:77:ALA:HA | 46:DX:80:LEU:HB2 | 1.92 | 0.50 |
| 23:DA:1398:C:O3' | 42:DT:25:LYS:NZ | 2.40 | 0.50 |
| 4:CD:72:GLU:O | 4:CD:72:GLU:OE1 | 2.30 | 0.50 |
| 41:BS:42:ARG:HG2 | 41:BS:42:ARG:HH11 | 1.76 | 0.50 |
| 23:BA:1897:G:H2' | 23:BA:1898:U:O4' | 2.11 | 0.50 |
| 23:BA:673:C:H5'' | 27:BE:81:PRO:HD2 | 1.94 | 0.50 |
| 23:BA:806:C:OP1 | 34:BL:39:LYS:HB3 | 2.11 | 0.50 |
| 1:CA:982:U:H5'' | 14:CN:6:LEU:HD13 | 1.93 | 0.50 |
| 24:BB:7:G:H1' | 37:BO:38:GLN:HE21 | 1.75 | 0.50 |
| 23:BA:1658:C:H2' | 23:BA:1659:U:C6 | 2.47 | 0.50 |
| 23:BA:1188:U:H2' | 23:BA:1189:A:C5' | 2.42 | 0.50 |
| 34:BL:49:ARG:O | 34:BL:50:ARG:C | 2.50 | 0.50 |
| 4:AD:110:PHE:N | 4:AD:110:PHE:CD2 | 2.75 | 0.50 |
| 23:DA:94:G:N3 | 47:DY:47:ASN:ND2 | 2.60 | 0.50 |
| 1:CA:36:C:H4' | 12:CL:121:THR:O | 2.11 | 0.50 |
| 1:AA:392:G:N3 | 1:AA:393:A:C8 | 2.80 | 0.50 |
| 26:DD:36:ARG:HH11 | 26:DD:85:ASN:ND2 | 2.09 | 0.50 |
| 1:AA:191(G):G:H2' | 1:AA:192:U:C6 | 2.46 | 0.50 |
| 26:DD:51:PHE:C | 26:DD:51:PHE:CD1 | 2.85 | 0.50 |
| 23:BA:849:A:O2' | 48:BZ:17:LYS:HE3 | 2.12 | 0.50 |
| 46:DX:11:ARG:HG3 | 46:DX:61:ARG:O | 2.12 | 0.50 |
| 12:CL:70:PRO:O | 12:CL:101:ARG:NH1 | 2.44 | 0.50 |
| 46:DX:27:GLU:HB3 | 46:DX:33:LYS:HG3 | 1.93 | 0.50 |
| 6:AF:8:ILE:HD12 | 6:AF:26:ILE:HD13 | 1.94 | 0.50 |
| 46:BX:11:ARG:HG3 | 46:BX:11:ARG:NH1 | 2.23 | 0.50 |
| 19:AS:21:GLU:HG3 | 19:AS:22:LEU:HD23 | 1.93 | 0.50 |
| 23:DA:932:G:H3' | 23:DA:932:G:OP1 | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 47:DY:9:GLN:CA | 47:DY:12:GLU:HB3 | 2.41 | 0.50 |
| 1:AA:457:C:N4 | 1:AA:475:G:H1 | 2.09 | 0.50 |
| 16:AP:39:TYR:CE1 | 16:AP:73:LEU:HD13 | 2.47 | 0.50 |
| 23:BA:8:A:H2' | 23:BA:9:U:C6 | 2.47 | 0.50 |
| 9:AI:104:ARG:O | 9:AI:105:ASP:HB3 | 2.11 | 0.50 |
| 23:DA:2208:U:O4' | 25:DC:151:LYS:HE3 | 2.12 | 0.50 |
| 23:DA:7:G:H2' | 23:DA:8:A:O4' | 2.12 | 0.50 |
| 36:DN:100:LEU:N | 36:DN:100:LEU:HD23 | 2.27 | 0.50 |
| 11:AK:34:ASP:HB2 | 11:AK:35:PRO:HD2 | 1.92 | 0.50 |
| 34:BL:10:PRO:HD2 | 34:BL:11:GLY:N | 2.26 | 0.50 |
| 23:BA:909:A:C4 | 23:BA:912:C:C5 | 2.99 | 0.50 |
| 2:CB:74:LYS:CB | 2:CB:74:LYS:HZ2 | 2.24 | 0.50 |
| 17:AQ:60:ILE:O | 17:AQ:71:PHE:HA | 2.12 | 0.50 |
| 13:AM:99:ARG:HB2 | 13:AM:101:GLN:HE21 | 1.77 | 0.50 |
| 23:DA:2352:A:C4 | 23:DA:2366:A:C2 | 3.00 | 0.50 |
| 1:CA:1233:G:OP2 | 9:CI:124:GLN:HB2 | 2.11 | 0.50 |
| 1:CA:629:G:C2 | 1:CA:630:G:O6 | 2.65 | 0.50 |
| 2:AB:31:TYR:O | 2:AB:42:ILE:HD12 | 2.12 | 0.50 |
| 42:BT:64:LYS:HG2 | 42:BT:65:ARG:HH21 | 1.77 | 0.50 |
| 1:AA:1424:C:H2' | 1:AA:1425:U:O4' | 2.12 | 0.50 |
| 23:DA:26:G:H1' | 23:DA:514:A:N6 | 2.27 | 0.50 |
| 23:BA:270(O):G:C6 | 23:BA:270(Q):C:N4 | 2.80 | 0.50 |
| 18:AR:53:ARG:HH21 | 18:AR:60:ALA:N | 2.09 | 0.50 |
| 1:AA:503:C:C2 | 1:AA:504:C:C5 | 3.00 | 0.50 |
| 47:DY:38:GLN:HB3 | 47:DY:44:LEU:HB3 | 1.93 | 0.50 |
| 1:CA:744:C:C3' | 1:CA:744:C:C6 | 2.95 | 0.50 |
| 23:DA:1015:G:O2' | 23:DA:1016:G:H5' | 2.12 | 0.50 |
| 35:BM:55:VAL:CG2 | 35:BM:56:ARG:N | 2.74 | 0.50 |
| 17:CQ:11:VAL:N | 17:CQ:20:THR:O | 2.45 | 0.50 |
| 28:DF:28:VAL:O | 28:DF:31:VAL:HG12 | 2.11 | 0.50 |
| 23:DA:1932:A:H2' | 23:DA:1933:G:O4' | 2.11 | 0.50 |
| 23:BA:1815:A:P | 25:BC:54:ARG:HH22 | 2.35 | 0.50 |
| 35:DM:110:THR:OG1 | 35:DM:113:GLN:HB2 | 2.12 | 0.50 |
| 23:BA:1040:C:H2' | 23:BA:1041:C:C6 | 2.46 | 0.50 |
| 10:CJ:31:GLY:HA3 | 10:CJ:81:THR:CG2 | 2.42 | 0.50 |
| 1:AA:767:A:H2' | 1:AA:768:A:O4' | 2.11 | 0.50 |
| 1:CA:1147:C:O5' | 1:CA:1147:C:H6 | 1.95 | 0.50 |
| 38:BP:78:LEU:O | 38:BP:78:LEU:HD13 | 2.11 | 0.50 |
| 25:BC:69:ARG:NH2 | 25:BC:128:GLY:O | 2.44 | 0.50 |
| 25:DC:52:ARG:HB3 | 25:DC:53:PHE:CD2 | 2.47 | 0.50 |
| 10:AJ:17:ASP:O | 10:AJ:21:GLN:HB2 | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BA:1345:C:O2' | 23:BA:1346:G:H5' | 2.11 | 0.50 |
| 23:DA:1040:C:H2' | 23:DA:1041:C:C6 | 2.47 | 0.50 |
| 53:D5:53:PRO:O | 53:D5:57:ARG:NH1 | 2.44 | 0.50 |
| 23:BA:2393:A:H5'' | 34:BL:62:LEU:HB3 | 1.93 | 0.50 |
| 47:DY:3:LEU:O | 47:DY:4:SER:C | 2.51 | 0.50 |
| 23:DA:960:A:H61 | 35:DM:82:ARG:HH21 | 1.59 | 0.50 |
| 23:BA:1540:G:H3' | 23:BA:1541:U:H6 | 1.75 | 0.50 |
| 43:DU:27:VAL:CG2 | 43:DU:27:VAL:O | 2.56 | 0.50 |
| 32:DJ:122:LEU:O | 32:DJ:126:VAL:HG22 | 2.11 | 0.50 |
| 10:AJ:58:ASP:O | 10:AJ:60:ARG:N | 2.45 | 0.50 |
| 22:CV:6189:G:H2' | 22:CV:6190:U:C6 | 2.45 | 0.50 |
| 22:CV:6192:G:C5 | 22:CV:6193:U:C4 | 3.00 | 0.50 |
| 27:DE:65:TRP:HZ3 | 27:DE:73:ALA:O | 1.94 | 0.50 |
| 24:BB:7:G:H2' | 24:BB:8:U:O4' | 2.12 | 0.50 |
| 32:BJ:39:ILE:O | 32:BJ:78:VAL:HG22 | 2.11 | 0.50 |
| 23:BA:1971:A:C4 | 25:BC:241:PRO:HG3 | 2.47 | 0.50 |
| 40:BR:13:ARG:HG3 | 40:BR:13:ARG:HH11 | 1.77 | 0.50 |
| 40:BR:38:LEU:HD12 | 40:BR:57:VAL:HG12 | 1.94 | 0.50 |
| 34:BL:52:GLU:CA | 34:BL:52:GLU:OE1 | 2.60 | 0.50 |
| 37:DO:28:VAL:O | 37:DO:92:TYR:HE1 | 1.94 | 0.50 |
| 16:AP:32:TYR:O | 16:AP:32:TYR:HD2 | 1.95 | 0.50 |
| 25:DC:105:ILE:HD13 | 25:DC:106:ILE:H | 1.77 | 0.50 |
| 4:CD:75:PHE:CZ | 4:CD:93:PHE:HZ | 2.29 | 0.50 |
| 1:AA:414:A:H2' | 1:AA:415:A:C8 | 2.47 | 0.50 |
| 26:BD:4:ILE:HD11 | 26:BD:28:ALA:O | 2.11 | 0.50 |
| 23:DA:1487:G:O2' | 23:DA:1488:G:H5' | 2.12 | 0.50 |
| 23:DA:1511:A:O2' | 23:DA:1512:G:H5' | 2.10 | 0.50 |
| 23:DA:848:G:C4 | 23:DA:933:A:C8 | 3.00 | 0.50 |
| 23:DA:929:G:H8 | 23:DA:929:G:O5' | 1.95 | 0.50 |
| 23:DA:848:G:N9 | 23:DA:933:A:H8 | 2.09 | 0.50 |
| 23:DA:2328:A:H2' | 23:DA:2329:G:O4' | 2.12 | 0.50 |
| 17:AQ:54:GLY:HA3 | 17:AQ:82:MET:HE1 | 1.94 | 0.50 |
| 23:BA:2276:G:O2' | 23:BA:2277:G:H5' | 2.11 | 0.50 |
| 41:DS:47:VAL:HA | 41:DS:50:VAL:HG12 | 1.94 | 0.50 |
| 45:DW:53:MET:HA | 45:DW:58:THR:O | 2.12 | 0.50 |
| 40:DR:100:ARG:O | 40:DR:100:ARG:CG | 2.57 | 0.50 |
| 32:DJ:65:TRP:HA | 32:DJ:71:MET:HE1 | 1.93 | 0.50 |
| 23:DA:9:U:N3 | 23:DA:2629:A:C6 | 2.79 | 0.50 |
| 23:DA:8:A:C5 | 23:DA:9:U:C4 | 3.00 | 0.50 |
| 23:BA:270(H):C:C2 | 23:BA:270(I):C:C5 | 3.00 | 0.50 |
| 23:BA:270(H):C:C4 | 23:BA:270(I):C:C5 | 3.00 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:AK:40:ILE:N | 11:AK:40:ILE:HD13 | 2.27 | 0.50 |
| 25:BC:182:LEU:O | 25:BC:271:ILE:HG13 | 2.12 | 0.50 |
| 23:BA:2480:C:H2' | 23:BA:2481:G:H5' | 1.92 | 0.50 |
| 23:BA:1396:U:O2 | 23:BA:1396:U:C2' | 2.52 | 0.50 |
| 25:DC:76:PRO:HA | 25:DC:118:VAL:HG23 | 1.93 | 0.50 |
| 23:DA:2477:C:HO2' | 23:DA:2478:A:P | 2.35 | 0.50 |
| 1:CA:922:G:H5'' | 1:CA:923:A:OP2 | 2.12 | 0.50 |
| 23:BA:681:G:H2' | 23:BA:682:G:O5' | 2.12 | 0.50 |
| 23:DA:1593:G:C6 | 23:DA:1594:G:C6 | 3.00 | 0.50 |
| 45:DW:51:VAL:N | 45:DW:62:LEU:HD12 | 2.26 | 0.50 |
| 36:BN:93:GLY:C | 36:BN:95:THR:H | 2.15 | 0.50 |
| 1:AA:498:A:H4' | 1:AA:500:G:H5' | 1.93 | 0.50 |
| 5:AE:96:PRO:HA | 5:AE:117:ASP:OD2 | 2.11 | 0.50 |
| 3:CC:175:LEU:CD1 | 3:CC:201:TYR:CE2 | 2.95 | 0.50 |
| 23:DA:828:U:H4' | 23:DA:831:G:N1 | 2.27 | 0.50 |
| 23:DA:1909:C:N3 | 23:DA:1922:G:C2 | 2.79 | 0.50 |
| 36:DN:84:ALA:O | 36:DN:85:PRO:C | 2.50 | 0.50 |
| 23:DA:2215:G:H8 | 23:DA:2215:G:OP2 | 1.94 | 0.50 |
| 25:DC:40:THR:CG2 | 25:DC:41:GLY:N | 2.75 | 0.50 |
| 1:AA:538:G:N2 | 1:AA:539:A:H1' | 2.27 | 0.50 |
| 23:DA:1444:G:N2 | 23:DA:1548:C:C2 | 2.80 | 0.50 |
| 23:DA:270(Q):C:O2' | 23:DA:270(R):C:C6 | 2.62 | 0.50 |
| 53:D5:26:LYS:HA | 53:D5:48:PHE:CE2 | 2.46 | 0.50 |
| 27:DE:150:GLY:HA2 | 27:DE:172:TRP:CE3 | 2.47 | 0.50 |
| 7:CG:86:GLN:HB2 | 7:CG:148:ASN:ND2 | 2.27 | 0.50 |
| 10:AJ:31:GLY:HA3 | 10:AJ:81:THR:CG2 | 2.42 | 0.50 |
| 1:CA:243:A:C2 | 1:CA:246:A:C8 | 3.00 | 0.50 |
| 1:AA:983:A:H5' | 1:AA:984:C:OP2 | 2.12 | 0.50 |
| 23:BA:351:G:H5'' | 23:BA:352:G:OP1 | 2.11 | 0.50 |
| 30:BH:45:LYS:HA | 30:BH:48:GLU:HG2 | 1.93 | 0.50 |
| 23:DA:1523:U:H2' | 23:DA:1524:G:H8 | 1.75 | 0.50 |
| 23:DA:1570:A:H2' | 23:DA:1571:A:C8 | 2.47 | 0.50 |
| 23:BA:962:G:H2' | 23:BA:963:U:O4' | 2.12 | 0.50 |
| 23:BA:1292:U:H2' | 23:BA:1293:C:C6 | 2.47 | 0.50 |
| 23:BA:409:C:O2' | 23:BA:410:G:H5' | 2.11 | 0.50 |
| 36:BN:25:ALA:O | 36:BN:26:LYS:C | 2.49 | 0.50 |
| 44:DV:155:LEU:O | 44:DV:157:LEU:HD12 | 2.12 | 0.50 |
| 3:AC:72:LYS:HG2 | 3:AC:74:GLY:H | 1.76 | 0.50 |
| 23:DA:2408:U:O5' | 23:DA:2408:U:H6 | 1.95 | 0.50 |
| 3:CC:111:LEU:HD23 | 3:CC:146:ALA:HB2 | 1.94 | 0.50 |
| 49:D1:45:GLY:O | 49:D1:46:ASN:HB2 | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:D5:57:ARG:CZ | 53:D5:57:ARG:HA | 2.42 | 0.49 |
| 34:DL:132:LYS:CD | 34:DL:132:LYS:N | 2.75 | 0.49 |
| 23:BA:2577:A:H5'' | 23:BA:2578:G:C5' | 2.36 | 0.49 |
| 26:DD:103:ASP:OD1 | 26:DD:201:THR:HG23 | 2.12 | 0.49 |
| 26:DD:104:VAL:HG22 | 26:DD:198:VAL:HG13 | 1.94 | 0.49 |
| 23:DA:674:G:C1' | 27:DE:74:ARG:HD3 | 2.36 | 0.49 |
| 28:DF:76:SER:HB2 | 28:DF:83:ARG:CA | 2.43 | 0.49 |
| 4:AD:49:ARG:CZ | 4:AD:50:ARG:H | 2.24 | 0.49 |
| 23:BA:1813:G:O2' | 25:BC:50:THR:CG2 | 2.60 | 0.49 |
| 30:DH:113:ARG:O | 30:DH:131:LYS:N | 2.45 | 0.49 |
| 35:DM:141:GLN:NE2 | 44:DV:89:PHE:HD1 | 2.10 | 0.49 |
| 26:DD:36:ARG:NH1 | 26:DD:86:PRO:HD2 | 2.27 | 0.49 |
| 1:CA:1260:C:H4' | 1:CA:1284:C:H5' | 1.93 | 0.49 |
| 26:DD:61:ARG:HB3 | 26:DD:62:PRO:HD2 | 1.94 | 0.49 |
| 23:DA:1324:G:C5 | 23:DA:1328:G:O6 | 2.66 | 0.49 |
| 42:BT:35:THR:HG22 | 42:BT:36:LYS:H | 1.77 | 0.49 |
| 1:AA:1083:U:C5 | 1:AA:1084:G:C6 | 3.00 | 0.49 |
| 1:CA:402:G:H8 | 1:CA:402:G:O5' | 1.94 | 0.49 |
| 23:BA:2366:A:H2' | 23:BA:2367:G:O4' | 2.11 | 0.49 |
| 12:CL:52:ARG:NH1 | 12:CL:52:ARG:CG | 2.59 | 0.49 |
| 35:DM:47:ILE:HD11 | 35:DM:68:ILE:HD12 | 1.93 | 0.49 |
| 20:CT:10:LEU:O | 20:CT:12:ALA:N | 2.38 | 0.49 |
| 23:DA:322:A:P | 27:DE:169:ASN:HB2 | 2.52 | 0.49 |
| 23:DA:2305:A:C4 | 28:DF:154:GLY:HA3 | 2.47 | 0.49 |
| 23:BA:85:G:N3 | 23:BA:103:A:C2 | 2.80 | 0.49 |
| 23:BA:2563:U:H4' | 33:BK:28:SER:HA | 1.94 | 0.49 |
| 23:BA:2893:G:H5'' | 23:BA:2894:G:O4' | 2.12 | 0.49 |
| 30:BH:133:HIS:NE2 | 30:BH:135:GLU:HG2 | 2.27 | 0.49 |
| 23:DA:1509:A:O2' | 23:DA:1510:A:OP1 | 2.24 | 0.49 |
| 23:DA:1567:A:H5'' | 25:DC:58:HIS:CD2 | 2.47 | 0.49 |
| 1:AA:657:G:C2 | 1:AA:658:G:C8 | 3.01 | 0.49 |
| 1:AA:750:G:C6 | 1:AA:751:U:C5 | 3.00 | 0.49 |
| 23:BA:1109:C:N4 | 23:BA:1110:G:N2 | 2.59 | 0.49 |
| 33:BK:43:VAL:HG23 | 33:BK:56:ASP:O | 2.12 | 0.49 |
| 8:AH:25:ASP:C | 8:AH:26:VAL:HG12 | 2.32 | 0.49 |
| 1:AA:1118:C:H5'' | 9:AI:104:ARG:CG | 2.42 | 0.49 |
| 18:CR:22:VAL:O | 18:CR:22:VAL:HG12 | 2.12 | 0.49 |
| 23:BA:2657:A:H5'' | 23:BA:2658:C:OP2 | 2.12 | 0.49 |
| 50:D2:52:TYR:O | 50:D2:52:TYR:HD1 | 1.96 | 0.49 |
| 6:CF:50:TYR:HE1 | 18:CR:74:ARG:O | 1.95 | 0.49 |
| 1:CA:522:C:N4 | 1:CA:528:C:N4 | 2.60 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 50:B2:52:TYR:O | 50:B2:52:TYR:HD1 | 1.95 | 0.49 |
| 28:DF:7:LEU:HD22 | 28:DF:176:LEU:HD22 | 1.94 | 0.49 |
| 1:AA:1446:A:O2' | 1:AA:1447:G:H8 | 1.95 | 0.49 |
| 23:BA:1152:C:H5'' | 39:BQ:80:ILE:CG2 | 2.41 | 0.49 |
| 35:BM:134:ARG:HE | 35:BM:134:ARG:HA | 1.77 | 0.49 |
| 1:CA:434:U:H2' | 1:CA:435:C:C6 | 2.47 | 0.49 |
| 1:AA:927:G:C2 | 1:AA:1391:U:C2 | 3.00 | 0.49 |
| 25:BC:94:LEU:HD22 | 25:BC:95:LEU:N | 2.27 | 0.49 |
| 36:DN:93:GLY:C | 36:DN:95:THR:H | 2.16 | 0.49 |
| 23:DA:1169:G:H1 | 23:DA:1180:C:N4 | 2.08 | 0.49 |
| 48:BZ:23:LEU:CD1 | 48:BZ:50:VAL:HG11 | 2.42 | 0.49 |
| 46:DX:49:VAL:HG11 | 46:DX:70:VAL:HG11 | 1.93 | 0.49 |
| 23:BA:1796:U:H4' | 25:BC:256:GLY:HA2 | 1.94 | 0.49 |
| 48:DZ:23:LEU:CD1 | 48:DZ:50:VAL:HG11 | 2.42 | 0.49 |
| 1:CA:1089:G:C6 | 1:CA:1090:U:C4 | 3.00 | 0.49 |
| 1:CA:380:G:C2 | 1:CA:384:G:N1 | 2.80 | 0.49 |
| 12:CL:92:LEU:HB2 | 12:CL:95:VAL:CG2 | 2.41 | 0.49 |
| 44:BV:68:PRO:HG2 | 44:BV:91:LEU:O | 2.12 | 0.49 |
| 28:BF:171:ALA:O | 28:BF:175:LEU:HG | 2.11 | 0.49 |
| 23:BA:27:G:C4 | 23:BA:512:G:N2 | 2.80 | 0.49 |
| 1:CA:1508:G:H2' | 1:CA:1509:C:C6 | 2.47 | 0.49 |
| 23:DA:1689:A:H62 | 23:DA:1698:A:H2 | 1.60 | 0.49 |
| 23:BA:2567:G:H2' | 23:BA:2568:C:C6 | 2.47 | 0.49 |
| 23:BA:46:C:H42 | 23:BA:179:G:H1 | 1.60 | 0.49 |
| 23:DA:265:A:H1' | 23:DA:266:G:O4' | 2.12 | 0.49 |
| 23:BA:1753:G:N1 | 23:BA:1756:G:C2 | 2.80 | 0.49 |
| 23:DA:2750:A:C2 | 23:DA:2753:A:H2 | 2.30 | 0.49 |
| 1:CA:1004:A:N3 | 1:CA:1004:A:H3' | 2.27 | 0.49 |
| 1:CA:958:A:C6 | 1:CA:959:A:C6 | 3.00 | 0.49 |
| 24:BB:63:G:H2' | 24:BB:64:C:C6 | 2.46 | 0.49 |
| 1:AA:1290:G:N3 | 1:AA:1290:G:H2' | 2.27 | 0.49 |
| 5:AE:103:GLY:O | 5:AE:104:ALA:C | 2.50 | 0.49 |
| 22:AV:6185:U:C5 | 22:AV:6186:U:C5 | 3.00 | 0.49 |
| 36:BN:65:LEU:O | 36:BN:68:ARG:HB2 | 2.12 | 0.49 |
| 1:AA:450:G:H4' | 16:AP:41:PRO:HB2 | 1.94 | 0.49 |
| 1:AA:946:A:H2' | 1:AA:947:G:C8 | 2.47 | 0.49 |
| 26:BD:171:GLU:HG2 | 26:BD:185:LYS:HG2 | 1.94 | 0.49 |
| 28:BF:60:LEU:O | 28:BF:64:THR:HG22 | 2.11 | 0.49 |
| 32:DJ:110:LEU:O | 32:DJ:113:MET:HB2 | 2.11 | 0.49 |
| 23:DA:2579:C:H2' | 23:DA:2580:U:O4' | 2.12 | 0.49 |
| 4:CD:144:ASP:O | 4:CD:146:ILE:HG13 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 42:DT:30:VAL:HG21 | 42:DT:79:ALA:HB3 | 1.94 | 0.49 |
| 26:BD:36:ARG:HH11 | 26:BD:85:ASN:ND2 | 2.10 | 0.49 |
| 3:CC:173:VAL:H | 3:CC:174:PRO:HD3 | 1.75 | 0.49 |
| 36:DN:107:ASP:OD2 | 36:DN:108:GLY:N | 2.45 | 0.49 |
| 23:DA:1828:G:OP2 | 25:DC:239:ARG:CZ | 2.60 | 0.49 |
| 3:AC:33:LEU:O | 3:AC:36:ASP:HB3 | 2.13 | 0.49 |
| 26:DD:1:MET:O | 26:DD:2:LYS:O | 2.30 | 0.49 |
| 3:AC:130:VAL:HA | 3:AC:133:ALA:HB3 | 1.94 | 0.49 |
| 23:DA:2517:C:C6 | 23:DA:2542:A:C2 | 3.00 | 0.49 |
| 1:CA:1104:G:C2 | 1:CA:1105:A:C5 | 3.01 | 0.49 |
| 41:BS:8:ARG:HA | 41:BS:102:HIS:HA | 1.94 | 0.49 |
| 23:BA:1771:C:O2' | 23:BA:1786:A:H8 | 1.76 | 0.49 |
| 2:AB:187:LEU:HD22 | 2:AB:188:ALA:N | 2.27 | 0.49 |
| 40:DR:28:GLU:HB2 | 40:DR:31:ALA:CB | 2.42 | 0.49 |
| 23:DA:2893:G:H3' | 23:DA:2894:G:H5' | 1.95 | 0.49 |
| 23:BA:955:C:H5'' | 35:BM:85:LYS:HE2 | 1.94 | 0.49 |
| 23:BA:7:G:H2' | 23:BA:8:A:O4' | 2.11 | 0.49 |
| 1:CA:712:A:C6 | 1:CA:713:G:C6 | 3.01 | 0.49 |
| 1:AA:556:C:O2 | 1:AA:556:C:C2' | 2.55 | 0.49 |
| 1:CA:557:G:H2' | 1:CA:558:G:O4' | 2.12 | 0.49 |
| 23:BA:2531:A:H4' | 29:BG:157:TYR:CE2 | 2.47 | 0.49 |
| 39:DQ:62:ILE:HD11 | 39:DQ:93:LYS:HG2 | 1.94 | 0.49 |
| 18:AR:56:THR:O | 18:AR:58:LEU:HD12 | 2.12 | 0.49 |
| 1:CA:801:U:H2' | 1:CA:802:A:C8 | 2.47 | 0.49 |
| 30:DH:15:VAL:C | 30:DH:17:GLN:H | 2.16 | 0.49 |
| 1:AA:216:G:H2' | 1:AA:217:C:H6 | 1.76 | 0.49 |
| 1:CA:593:G:C2 | 1:CA:594:G:C4 | 2.99 | 0.49 |
| 1:CA:761:G:H2' | 1:CA:762:C:H6 | 1.77 | 0.49 |
| 12:AL:10:VAL:HG11 | 17:AQ:36:ILE:HG21 | 1.94 | 0.49 |
| 3:AC:73:PRO:HA | 3:AC:76:VAL:HG13 | 1.94 | 0.49 |
| 1:CA:972:C:H4' | 10:CJ:57:LYS:CG | 2.42 | 0.49 |
| 23:DA:826:U:H2' | 23:DA:828:U:O4' | 2.12 | 0.49 |
| 19:CS:30:LEU:HD23 | 19:CS:31:ILE:N | 2.27 | 0.49 |
| 17:CQ:27:PHE:O | 17:CQ:36:ILE:N | 2.43 | 0.49 |
| 23:BA:1833:U:C2' | 23:BA:1834:U:H5' | 2.41 | 0.49 |
| 23:DA:2372:G:O2' | 51:D3:46:HIS:CE1 | 2.65 | 0.49 |
| 23:DA:245:G:N3 | 23:DA:246:C:C6 | 2.80 | 0.49 |
| 23:DA:2459:A:C2 | 23:DA:2460:U:H1' | 2.47 | 0.49 |
| 5:AE:36:ASP:O | 5:AE:37:ARG:CB | 2.60 | 0.49 |
| 1:AA:356:A:H2' | 1:AA:357:G:O5' | 2.12 | 0.49 |
| 23:BA:2584:U:O5' | 23:BA:2584:U:H6 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BA:2297:C:H2' | 23:BA:2298:A:H8 | 1.77 | 0.49 |
| 24:DB:86:G:H2' | 24:DB:87:G:C8 | 2.47 | 0.49 |
| 1:CA:450:G:H4' | 16:CP:41:PRO:HB2 | 1.94 | 0.49 |
| 45:BW:82:ARG:O | 45:BW:84:LEU:HD23 | 2.12 | 0.49 |
| 41:DS:5:ALA:HB2 | 41:DS:54:ALA:HA | 1.93 | 0.49 |
| 23:BA:2721:A:H1' | 23:BA:2873:A:O2' | 2.12 | 0.49 |
| 23:DA:2105:C:H2' | 23:DA:2106:G:C8 | 2.47 | 0.49 |
| 23:DA:1360:A:H5' | 23:DA:1361:G:OP2 | 2.12 | 0.49 |
| 1:AA:794:A:H4' | 1:AA:1521:G:O2' | 2.12 | 0.49 |
| 1:AA:1438:G:C5 | 1:AA:1439:C:C5 | 3.00 | 0.49 |
| 23:DA:1855:G:N1 | 23:DA:1888:G:C8 | 2.80 | 0.49 |
| 23:DA:2416:C:N3 | 23:DA:2417:C:C5 | 2.79 | 0.49 |
| 34:DL:107:LYS:O | 34:DL:109:GLY:N | 2.44 | 0.49 |
| 23:DA:747:U:N3 | 50:D2:2:ALA:N | 2.61 | 0.49 |
| 23:DA:1543:A:C8 | 23:DA:1545:A:H5'' | 2.46 | 0.49 |
| 23:DA:1542:G:P | 23:DA:1543:A:OP1 | 2.70 | 0.49 |
| 25:BC:145:VAL:HG12 | 25:BC:146:GLU:N | 2.28 | 0.49 |
| 43:DU:14:LEU:HD23 | 43:DU:15:VAL:CA | 2.42 | 0.49 |
| 2:AB:70:PHE:CD2 | 2:AB:163:PHE:HB3 | 2.48 | 0.49 |
| 22:AV:6189:G:C5 | 22:AV:6190:U:C5 | 3.00 | 0.49 |
| 25:BC:142:VAL:HG22 | 25:BC:143:HIS:N | 2.27 | 0.49 |
| 25:BC:67:PHE:HB3 | 25:BC:153:ALA:H | 1.77 | 0.49 |
| 23:DA:1122:G:H2' | 23:DA:1122:G:N3 | 2.26 | 0.49 |
| 4:AD:49:ARG:O | 4:AD:51:PRO:HD3 | 2.13 | 0.49 |
| 23:BA:2729:G:C5 | 23:BA:2730:C:C5 | 2.99 | 0.49 |
| 47:BY:6:VAL:C | 47:BY:10:LEU:HG | 2.33 | 0.49 |
| 25:DC:182:LEU:O | 25:DC:271:ILE:HG13 | 2.12 | 0.49 |
| 4:AD:28:SER:HB3 | 4:AD:29:PRO:CD | 2.41 | 0.49 |
| 3:CC:116:VAL:HG21 | 3:CC:202:ILE:HD11 | 1.92 | 0.49 |
| 23:DA:2711:A:OP1 | 23:DA:712(B):A:OP1 | 2.30 | 0.49 |
| 23:BA:1493:C:H4' | 23:BA:1494:A:OP1 | 2.11 | 0.49 |
| 23:BA:548:A:H2' | 23:BA:549:G:H5' | 1.94 | 0.49 |
| 28:BF:41:GLN:HB2 | 28:BF:90:LEU:HB2 | 1.94 | 0.49 |
| 23:DA:363(C):G:O2' | 23:DA:363(D):G:H5' | 2.12 | 0.49 |
| 23:DA:2543:G:O4' | 23:DA:2766:G:H5' | 2.13 | 0.49 |
| 2:CB:97:TRP:HZ2 | 2:CB:102:LEU:CD1 | 2.20 | 0.49 |
| 23:BA:2605:U:H2' | 23:BA:2606:C:C6 | 2.47 | 0.49 |
| 1:AA:16:A:O2' | 5:AE:16:THR:HB | 2.12 | 0.49 |
| 1:CA:408:A:H2' | 1:CA:409:G:C8 | 2.48 | 0.49 |
| 23:DA:2378:A:H4' | 37:DO:84:GLN:NE2 | 2.27 | 0.49 |
| 50:B2:25:LEU:N | 50:B2:25:LEU:HD12 | 2.18 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 10:CJ:33:GLN:O | 10:CJ:75:ILE:HG12 | 2.11 | 0.49 |
| 43:DU:81:LYS:HD2 | 43:DU:96:ILE:HD12 | 1.94 | 0.49 |
| 12:CL:44:PRO:HD2 | 12:CL:49:SER:HA | 1.94 | 0.49 |
| 6:CF:5:GLU:OE1 | 6:CF:62:TRP:HZ2 | 1.95 | 0.49 |
| 23:DA:2683:C:OP1 | 38:DP:53:ARG:NH2 | 2.45 | 0.49 |
| 23:DA:1502:C:H6 | 23:DA:1502:C:H3' | 1.77 | 0.49 |
| 19:CS:21:GLU:HG3 | 19:CS:22:LEU:HD23 | 1.94 | 0.49 |
| 31:BI:4:LYS:HG2 | 31:BI:4:LYS:O | 2.11 | 0.49 |
| 1:AA:782:A:O3' | 1:AA:1515:C:H4' | 2.12 | 0.49 |
| 8:AH:10:LEU:HB3 | 8:AH:83:ILE:HD13 | 1.93 | 0.49 |
| 1:AA:68:G:N1 | 1:AA:69:G:C5 | 2.80 | 0.49 |
| 30:BH:15:VAL:HG12 | 30:BH:16:GLY:N | 2.27 | 0.49 |
| 30:BH:5:LEU:HD22 | 30:BH:19:VAL:HG12 | 1.94 | 0.49 |
| 1:CA:1014:A:C2 | 1:CA:1219:U:H1' | 2.48 | 0.49 |
| 1:CA:1118:C:P | 9:CI:104:ARG:HG3 | 2.53 | 0.49 |
| 23:DA:243:U:H2' | 23:DA:244:A:H5' | 1.93 | 0.49 |
| 1:CA:171:A:H2' | 1:CA:172:A:C8 | 2.48 | 0.49 |
| 1:CA:197:A:N7 | 1:CA:221:C:H4' | 2.26 | 0.49 |
| 36:DN:99:LYS:CD | 36:DN:99:LYS:N | 2.74 | 0.49 |
| 25:BC:270:ILE:C | 25:BC:271:ILE:HG12 | 2.33 | 0.49 |
| 23:DA:335:C:C2 | 23:DA:336:C:C5 | 3.00 | 0.49 |
| 23:BA:334:C:O2' | 23:BA:335:C:P | 2.70 | 0.49 |
| 23:BA:334:C:HO2' | 23:BA:335:C:P | 2.34 | 0.49 |
| 23:DA:1728:G:H3' | 23:DA:1728:G:C8 | 2.47 | 0.49 |
| 29:DG:40:GLU:O | 29:DG:55:PRO:HG3 | 2.12 | 0.49 |
| 33:DK:49:ARG:HA | 33:DK:53:LYS:HZ2 | 1.76 | 0.49 |
| 1:CA:1232:U:H5'' | 9:CI:124:GLN:O | 2.12 | 0.49 |
| 33:BK:2:ILE:CD1 | 33:BK:82:ASN:HD22 | 2.26 | 0.49 |
| 23:BA:479:A:H4' | 23:BA:480:A:O5' | 2.11 | 0.49 |
| 8:CH:36:LEU:HA | 8:CH:39:LEU:HB2 | 1.94 | 0.49 |
| 12:AL:5:THR:O | 12:AL:8:GLN:HB2 | 2.12 | 0.49 |
| 34:BL:75:ILE:CD1 | 34:BL:75:ILE:H | 2.21 | 0.49 |
| 53:B5:26:LYS:HG2 | 53:B5:48:PHE:CD2 | 2.47 | 0.49 |
| 23:BA:1131:G:C2 | 23:BA:1132:A:C5 | 3.00 | 0.49 |
| 15:CO:7:GLU:HG3 | 15:CO:10:LYS:HD3 | 1.93 | 0.49 |
| 23:BA:2065:C:O2' | 23:BA:2066:C:H5' | 2.11 | 0.49 |
| 1:AA:1058:G:C6 | 1:AA:1059:C:N3 | 2.81 | 0.49 |
| 24:BB:28:C:H2' | 24:BB:29:A:O4' | 2.12 | 0.49 |
| 3:CC:191:THR:C | 3:CC:193:TYR:H | 2.15 | 0.49 |
| 23:DA:2836:U:C5 | 23:DA:2883:A:N6 | 2.81 | 0.49 |
| 1:AA:685:G:N2 | 1:AA:686:U:C4 | 2.81 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:836:G:OP1 | 18:AR:61:LYS:HE2 | 2.12 | 0.49 |
| 7:CG:70:LYS:HG3 | 7:CG:96:GLN:HB3 | 1.93 | 0.49 |
| 1:CA:1169:A:N6 | 1:CA:1170:A:N1 | 2.60 | 0.49 |
| 1:CA:1090:U:H2' | 1:CA:1091:U:C6 | 2.47 | 0.49 |
| 23:BA:553:U:C2' | 23:BA:554:U:H5' | 2.42 | 0.49 |
| 23:BA:466:A:H5'' | 23:BA:467:G:OP2 | 2.12 | 0.49 |
| 1:AA:595:G:H1' | 1:AA:596:C:H5 | 1.77 | 0.49 |
| 23:BA:772:C:H2' | 23:BA:772:C:O2 | 2.11 | 0.49 |
| 35:BM:137:TYR:HB3 | 44:BV:76:LEU:HD21 | 1.93 | 0.49 |
| 23:DA:1881:C:H2' | 23:DA:1882:C:H6 | 1.78 | 0.49 |
| 1:AA:830:G:C2 | 1:AA:831:U:C2 | 3.01 | 0.49 |
| 23:DA:2343:C:O2' | 23:DA:2373:G:O2' | 2.24 | 0.49 |
| 1:AA:958:A:C6 | 1:AA:959:A:C6 | 3.00 | 0.49 |
| 23:DA:2315:G:H2' | 23:DA:2316:C:C6 | 2.47 | 0.49 |
| 1:AA:243:A:C2 | 1:AA:246:A:C8 | 3.00 | 0.49 |
| 1:AA:1321:C:C5 | 1:AA:1322:C:C2 | 3.01 | 0.49 |
| 1:AA:1320:C:N3 | 19:AS:72:GLY:HA3 | 2.26 | 0.49 |
| 10:CJ:48:THR:CG2 | 10:CJ:62:HIS:ND1 | 2.73 | 0.49 |
| 1:AA:46:G:H8 | 1:AA:46:G:O5' | 1.95 | 0.49 |
| 38:BP:61:PHE:CE2 | 38:BP:76:PHE:HB2 | 2.47 | 0.49 |
| 23:BA:2295:C:N3 | 23:BA:2296:U:H5 | 2.10 | 0.49 |
| 23:DA:727:A:H2 | 25:DC:9:TYR:CD2 | 2.30 | 0.49 |
| 42:DT:44:GLU:HG2 | 42:DT:49:VAL:O | 2.13 | 0.49 |
| 39:BQ:53:ARG:O | 39:BQ:56:ASP:HB2 | 2.12 | 0.49 |
| 40:BR:4:ILE:HD13 | 40:BR:13:ARG:HA | 1.93 | 0.49 |
| 16:AP:21:VAL:O | 16:AP:21:VAL:HG23 | 2.12 | 0.49 |
| 1:AA:437:U:C4 | 1:AA:438:G:C6 | 3.00 | 0.49 |
| 4:AD:31:CYS:O | 4:AD:31:CYS:SG | 2.71 | 0.49 |
| 42:DT:30:VAL:HG21 | 42:DT:79:ALA:CB | 2.42 | 0.49 |
| 42:BT:30:VAL:HG11 | 42:BT:39:ILE:HD13 | 1.94 | 0.49 |
| 8:AH:88:LYS:HB3 | 8:AH:89:PRO:HD2 | 1.93 | 0.49 |
| 1:CA:1329:A:C2 | 1:CA:1330:U:C2 | 3.00 | 0.49 |
| 44:DV:54:HIS:CG | 44:DV:101:PRO:HG3 | 2.47 | 0.49 |
| 29:DG:138:LYS:O | 29:DG:139:GLN:C | 2.51 | 0.49 |
| 29:DG:46:GLU:HG3 | 29:DG:51:ARG:HE | 1.73 | 0.49 |
| 23:BA:1512:G:C2 | 23:BA:1513:C:C2 | 3.01 | 0.49 |
| 33:BK:97:ARG:H | 33:BK:117:LEU:CD2 | 2.25 | 0.49 |
| 16:AP:71:ARG:C | 16:AP:73:LEU:H | 2.15 | 0.49 |
| 8:AH:25:ASP:HA | 8:AH:59:LEU:O | 2.11 | 0.49 |
| 23:BA:1359:A:C8 | 23:BA:1372:U:O4 | 2.65 | 0.49 |
| 28:DF:131:TYR:CD2 | 28:DF:133:LEU:HD22 | 2.48 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:DA:998:C:C2' | 23:DA:999:U:O5' | 2.60 | 0.49 |
| 29:BG:95:ARG:NH1 | 29:BG:97:ARG:HE | 2.11 | 0.49 |
| 25:BC:25:THR:HG21 | 25:BC:81:ALA:CB | 2.43 | 0.49 |
| 23:DA:2287:A:C6 | 23:DA:2289:G:C4 | 3.01 | 0.49 |
| 1:AA:105:G:C6 | 1:AA:106:C:C4 | 3.00 | 0.49 |
| 23:BA:257:A:C2' | 23:BA:258:G:O5' | 2.60 | 0.49 |
| 39:DQ:98:LEU:O | 39:DQ:99:ALA:C | 2.51 | 0.49 |
| 25:BC:182:LEU:N | 25:BC:272:ALA:HB3 | 2.22 | 0.49 |
| 40:DR:19:LYS:HA | 40:DR:94:LEU:O | 2.12 | 0.49 |
| 23:BA:2479:G:H5'' | 23:BA:2537:U:O4' | 2.13 | 0.49 |
| 23:BA:1953:A:C2 | 23:BA:2549:G:N3 | 2.80 | 0.49 |
| 44:BV:179:ASP:CG | 44:BV:180:VAL:N | 2.65 | 0.49 |
| 39:DQ:111:GLU:HA | 39:DQ:114:LYS:HB2 | 1.95 | 0.49 |
| 33:DK:43:VAL:HG23 | 33:DK:56:ASP:O | 2.12 | 0.49 |
| 33:BK:121:VAL:O | 38:BP:43:GLN:NE2 | 2.44 | 0.49 |
| 34:BL:115:LEU:HA | 34:BL:134:ALA:CB | 2.42 | 0.49 |
| 23:DA:2865:U:C5 | 23:DA:2866:U:C4 | 3.01 | 0.49 |
| 8:AH:17:THR:HG21 | 8:AH:80:ILE:HD13 | 1.94 | 0.49 |
| 23:BA:1746:G:N3 | 23:BA:1747:G:C8 | 2.80 | 0.49 |
| 1:CA:775:G:O2' | 1:CA:776:G:H5' | 2.12 | 0.49 |
| 23:DA:2065:C:O2' | 23:DA:2066:C:H5' | 2.12 | 0.49 |
| 23:DA:298:G:P | 43:DU:85:VAL:HG22 | 2.52 | 0.49 |
| 39:BQ:46:ALA:O | 39:BQ:47:TYR:C | 2.50 | 0.49 |
| 1:AA:932:C:OP1 | 7:AG:4:ARG:HG2 | 2.12 | 0.49 |
| 1:CA:983:A:H5' | 1:CA:984:C:OP2 | 2.12 | 0.49 |
| 1:AA:1432:G:OP1 | 38:BP:107:ASP:HB2 | 2.12 | 0.49 |
| 2:CB:157:ARG:O | 2:CB:159:PRO:HD3 | 2.12 | 0.49 |
| 23:BA:1570:A:H2' | 23:BA:1571:A:C8 | 2.47 | 0.49 |
| 1:CA:1402:C:C5 | 1:CA:1403:C:C4 | 3.00 | 0.49 |
| 23:BA:337:C:H2' | 23:BA:338:G:O5' | 2.13 | 0.49 |
| 23:DA:1815:A:P | 25:DC:54:ARG:HH22 | 2.35 | 0.49 |
| 23:BA:2328:A:H2' | 23:BA:2329:G:O4' | 2.12 | 0.49 |
| 23:BA:1268:A:C2 | 23:BA:2013:A:C4 | 3.01 | 0.49 |
| 1:AA:1234:C:C2' | 1:AA:1235:U:H5' | 2.42 | 0.49 |
| 7:AG:113:GLU:O | 7:AG:119:ARG:HD3 | 2.12 | 0.49 |
| 23:BA:587:C:C4 | 34:BL:33:ARG:HB2 | 2.48 | 0.49 |
| 22:CV:6181:C:C2 | 22:CV:6182:A:C8 | 3.01 | 0.49 |
| 23:DA:805:G:H4' | 23:DA:806:C:OP2 | 2.13 | 0.49 |
| 23:BA:2338:G:C2 | 23:BA:2339:G:C8 | 3.00 | 0.49 |
| 25:DC:36:PRO:O | 25:DC:37:LEU:HB2 | 2.12 | 0.49 |
| 42:BT:50:LYS:N | 42:BT:87:GLN:HE22 | 1.91 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:408:A:H2' | 1:AA:409:G:C8 | 2.48 | 0.49 |
| 47:BY:57:ILE:HA | 47:BY:60:LEU:HB2 | 1.93 | 0.49 |
| 4:AD:21:LEU:HD12 | 4:AD:21:LEU:N | 2.26 | 0.49 |
| 4:AD:75:PHE:CZ | 4:AD:93:PHE:HZ | 2.29 | 0.49 |
| 35:BM:141:GLN:NE2 | 44:BV:89:PHE:HD1 | 2.10 | 0.49 |
| 41:DS:75:TYR:CE2 | 41:DS:104:THR:CB | 2.91 | 0.49 |
| 1:CA:404:U:C2 | 1:CA:405:U:C5 | 3.01 | 0.49 |
| 45:BW:64:ASP:OD1 | 45:BW:64:ASP:N | 2.46 | 0.49 |
| 8:CH:91:ARG:NH1 | 8:CH:91:ARG:HG3 | 2.22 | 0.49 |
| 1:AA:1148:U:C2 | 9:AI:16:ARG:NH2 | 2.81 | 0.49 |
| 30:BH:130:TYR:C | 30:BH:132:PRO:HD3 | 2.33 | 0.49 |
| 29:DG:12:PRO:HB2 | 29:DG:49:VAL:HA | 1.93 | 0.49 |
| 1:AA:1329:A:C2 | 1:AA:1330:U:C2 | 3.00 | 0.49 |
| 23:DA:1512:G:C6 | 23:DA:1513:C:N3 | 2.81 | 0.49 |
| 35:DM:8:LYS:HG3 | 35:DM:9:TYR:N | 2.25 | 0.49 |
| 28:BF:133:LEU:H | 28:BF:133:LEU:HD23 | 1.78 | 0.49 |
| 1:CA:1068:G:OP2 | 1:CA:1068:G:H8 | 1.96 | 0.49 |
| 25:BC:166:GLN:HB2 | 25:BC:174:ILE:HG22 | 1.94 | 0.49 |
| 29:DG:95:ARG:NH1 | 29:DG:97:ARG:HE | 2.10 | 0.49 |
| 38:DP:28:VAL:HA | 38:DP:89:VAL:HG12 | 1.94 | 0.49 |
| 24:DB:21:G:H2' | 24:DB:22:U:H6 | 1.77 | 0.49 |
| 23:DA:2478:A:H2' | 23:DA:2479:G:O4' | 2.12 | 0.49 |
| 12:CL:21:SER:C | 12:CL:23:VAL:H | 2.15 | 0.49 |
| 44:DV:85:HIS:C | 44:DV:85:HIS:HD1 | 2.16 | 0.49 |
| 23:DA:1717:G:C6 | 23:DA:1743:G:C6 | 3.00 | 0.49 |
| 3:CC:76:VAL:HG23 | 3:CC:77:ILE:HG13 | 1.94 | 0.49 |
| 3:CC:175:LEU:CD1 | 3:CC:201:TYR:HE2 | 2.25 | 0.49 |
| 23:DA:117:G:H5'' | 23:DA:118:A:OP2 | 2.12 | 0.49 |
| 23:DA:978:G:C2 | 23:DA:986:C:C2 | 3.01 | 0.49 |
| 25:BC:40:THR:CG2 | 25:BC:41:GLY:N | 2.75 | 0.49 |
| 23:BA:2738:A:C2 | 23:BA:2739:U:N1 | 2.80 | 0.49 |
| 23:DA:851:U:O2' | 48:DZ:45:GLY:HA3 | 2.12 | 0.49 |
| 23:BA:1442:G:C2 | 23:BA:1550:C:O2 | 2.65 | 0.49 |
| 38:BP:41:ARG:HB3 | 38:BP:41:ARG:HH11 | 1.78 | 0.49 |
| 12:AL:46:LYS:CB | 12:AL:47:PRO:HD3 | 2.43 | 0.49 |
| 1:CA:635:G:C5 | 1:CA:636:U:C5 | 3.01 | 0.49 |
| 23:BA:25:U:H2' | 23:BA:26:G:C8 | 2.47 | 0.49 |
| 23:BA:1818:U:H2' | 25:BC:157:ARG:HG3 | 1.94 | 0.49 |
| 48:BZ:3:ARG:NH1 | 48:BZ:59:VAL:HG11 | 2.27 | 0.49 |
| 29:BG:78:GLY:O | 29:BG:136:ILE:HG22 | 2.13 | 0.49 |
| 23:BA:107:C:C2' | 23:BA:108:U:H5' | 2.42 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DA:447:A:C4 | 23:DA:473:G:N7 | 2.80 | 0.49 |
| 40:DR:75:PHE:C | 40:DR:75:PHE:CD1 | 2.84 | 0.49 |
| 23:BA:601:C:H4' | 27:BE:104:LYS:HE2 | 1.95 | 0.49 |
| 24:DB:63:G:H2' | 24:DB:64:C:C6 | 2.47 | 0.49 |
| 23:DA:2703:C:O2' | 23:DA:2704:C:H5' | 2.12 | 0.49 |
| 53:D5:21:LYS:HA | 53:D5:54:GLU:OE2 | 2.12 | 0.49 |
| 53:D5:57:ARG:HB2 | 53:D5:57:ARG:CZ | 2.42 | 0.49 |
| 43:BU:71:LYS:NZ | 43:BU:71:LYS:HB2 | 2.27 | 0.49 |
| 23:DA:2439:A:H8 | 23:DA:2439:A:H5'' | 1.76 | 0.49 |
| 34:BL:80:TYR:CE1 | 34:BL:111:ARG:HG2 | 2.48 | 0.49 |
| 1:CA:1366:C:H2' | 1:CA:1367:C:H6 | 1.78 | 0.49 |
| 38:BP:54:ARG:NH1 | 38:BP:54:ARG:CG | 2.61 | 0.49 |
| 12:CL:26:LEU:HB3 | 12:CL:29:ALA:CB | 2.42 | 0.49 |
| 2:CB:91:PRO:HB3 | 2:CB:154:LEU:HD11 | 1.94 | 0.49 |
| 23:BA:1899:G:N2 | 23:BA:1902:C:H5 | 2.09 | 0.49 |
| 23:DA:114(B):A:O2' | 23:DA:1143:A:H3' | 2.13 | 0.49 |
| 30:BH:128:LEU:O | 30:BH:139:GLN:HA | 2.12 | 0.49 |
| 40:BR:44:LYS:HB3 | 40:BR:46:VAL:HG13 | 1.95 | 0.49 |
| 53:B5:7:HIS:HB2 | 53:B5:60:LEU:HB3 | 1.95 | 0.49 |
| 25:DC:267:SER:C | 25:DC:269:PHE:H | 2.14 | 0.49 |
| 3:CC:113:ALA:HB2 | 3:CC:202:ILE:HG13 | 1.94 | 0.49 |
| 20:AT:69:GLY:O | 20:AT:73:HIS:ND1 | 2.45 | 0.49 |
| 28:DF:88:ILE:HD12 | 28:DF:89:GLY:N | 2.27 | 0.49 |
| 20:CT:69:GLY:O | 20:CT:73:HIS:CE1 | 2.66 | 0.49 |
| 4:AD:105:VAL:O | 4:AD:105:VAL:CG1 | 2.59 | 0.49 |
| 3:AC:66:VAL:HB | 3:AC:101:LEU:CD2 | 2.39 | 0.49 |
| 5:CE:9:LYS:HB3 | 5:CE:112:LEU:HD11 | 1.94 | 0.49 |
| 5:CE:32:VAL:O | 5:CE:43:LEU:HA | 2.12 | 0.49 |
| 5:CE:76:ILE:HG12 | 5:CE:142:LEU:HD22 | 1.94 | 0.49 |
| 23:DA:2723:C:O5' | 23:DA:2723:C:H6 | 1.96 | 0.49 |
| 12:AL:70:PRO:O | 12:AL:101:ARG:NH1 | 2.44 | 0.49 |
| 44:BV:102:LEU:HD23 | 44:BV:137:ILE:HB | 1.95 | 0.49 |
| 13:CM:84:ILE:HG23 | 19:CS:74:PHE:HE1 | 1.77 | 0.49 |
| 23:BA:932:G:H3' | 23:BA:932:G:OP1 | 2.12 | 0.49 |
| 25:DC:185:VAL:HG12 | 25:DC:186:HIS:N | 2.28 | 0.49 |
| 13:AM:84:ILE:HG23 | 19:AS:74:PHE:HE1 | 1.77 | 0.49 |
| 23:DA:318:C:O2' | 23:DA:319:C:H5' | 2.13 | 0.49 |
| 18:CR:56:THR:O | 18:CR:58:LEU:N | 2.45 | 0.49 |
| 23:DA:1577:C:H5'' | 23:DA:1578:U:OP2 | 2.12 | 0.49 |
| 47:DY:49:LYS:HD2 | 47:DY:49:LYS:H | 1.77 | 0.49 |
| 23:BA:380:U:O2 | 23:BA:380:U:H2' | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 37:BO:56:LEU:HG | 37:BO:57:LYS:HB3 | 1.94 | 0.49 |
| 16:AP:39:TYR:CD2 | 16:AP:40:ASP:N | 2.81 | 0.49 |
| 1:AA:611:A:H61 | 1:AA:629:G:H1 | 1.61 | 0.49 |
| 1:AA:832:C:N4 | 1:AA:855:G:O6 | 2.46 | 0.49 |
| 39:DQ:61:TRP:O | 39:DQ:62:ILE:C | 2.51 | 0.49 |
| 1:AA:173:U:C2 | 1:AA:197:A:N1 | 2.81 | 0.49 |
| 1:AA:197:A:N6 | 1:AA:221:C:C5' | 2.76 | 0.49 |
| 23:BA:1434:A:H2' | 23:BA:1435:G:C8 | 2.48 | 0.49 |
| 1:AA:1128:C:O2' | 1:AA:1130:A:C4 | 2.65 | 0.49 |
| 23:BA:1682:G:H2' | 23:BA:1683:C:C6 | 2.47 | 0.49 |
| 23:DA:773:U:H4' | 25:DC:47:GLY:CA | 2.41 | 0.49 |
| 27:BE:153:SER:OG | 27:BE:190:GLU:HG3 | 2.13 | 0.49 |
| 18:CR:44:LEU:HD11 | 18:CR:70:ILE:HG21 | 1.95 | 0.49 |
| 23:DA:2102:U:C4 | 23:DA:2103:C:N4 | 2.81 | 0.49 |
| 35:BM:40:ALA:CB | 35:BM:127:ILE:HD12 | 2.41 | 0.49 |
| 4:CD:79:PHE:CD1 | 4:CD:207:TYR:HD1 | 2.31 | 0.49 |
| 1:CA:1446:A:O2' | 1:CA:1447:G:H8 | 1.95 | 0.49 |
| 1:AA:236:G:H5'' | 17:AQ:42:TYR:OH | 2.11 | 0.49 |
| 1:CA:1423:G:H2' | 1:CA:1424:C:C6 | 2.47 | 0.49 |
| 1:CA:373:A:C4 | 1:CA:482:A:N7 | 2.81 | 0.49 |
| 1:AA:754:C:C2' | 1:AA:755:G:OP1 | 2.61 | 0.49 |
| 32:BJ:68:ASN:HD22 | 32:BJ:68:ASN:H | 1.59 | 0.49 |
| 6:AF:44:GLY:HA2 | 6:AF:59:TYR:CE2 | 2.48 | 0.49 |
| 23:BA:571:A:C8 | 23:BA:2030:A:N6 | 2.80 | 0.49 |
| 51:D3:38:LYS:HG2 | 51:D3:39:TYR:N | 2.26 | 0.49 |
| 1:AA:1311:G:N2 | 1:AA:1327:C:C2 | 2.81 | 0.49 |
| 37:BO:20:ARG:HH12 | 45:BW:48:GLY:H | 1.60 | 0.49 |
| 1:CA:525:C:O2' | 1:CA:526:C:H5' | 2.12 | 0.49 |
| 26:BD:72:VAL:O | 26:BD:73:GLU:C | 2.50 | 0.49 |
| 23:DA:1798:U:H5'' | 25:DC:259:THR:O | 2.13 | 0.49 |
| 48:DZ:23:LEU:HD12 | 48:DZ:50:VAL:HG11 | 1.92 | 0.49 |
| 23:BA:2831:G:O4' | 23:BA:2883:A:C2 | 2.65 | 0.49 |
| 23:BA:57:C:H6 | 23:BA:57:C:O5' | 1.95 | 0.49 |
| 23:DA:1465:G:H21 | 23:DA:1466:G:H1' | 1.78 | 0.49 |
| 8:AH:42:GLU:HG3 | 8:AH:109:ILE:HD12 | 1.92 | 0.49 |
| 23:BA:963:U:H2' | 23:BA:964:C:C6 | 2.47 | 0.49 |
| 23:BA:963:U:H2' | 23:BA:964:C:H6 | 1.77 | 0.49 |
| 23:BA:2473:U:C4 | 23:BA:2474:C:C4 | 3.00 | 0.49 |
| 23:DA:1322:A:O3' | 41:DS:84:ARG:NH2 | 2.41 | 0.49 |
| 23:BA:2105:C:H2' | 23:BA:2106:G:C8 | 2.47 | 0.49 |
| 23:BA:1368:G:C2 | 23:BA:1369:G:C8 | 3.00 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 32:DJ:151:HIS:CD2 | 32:DJ:151:HIS:C | 2.86 | 0.49 |
| 23:DA:2734:A:H2' | 23:DA:2735:G:H5' | 1.95 | 0.49 |
| 19:CS:33:THR:HG23 | 19:CS:51:VAL:HA | 1.94 | 0.49 |
| 28:DF:106:LEU:HD12 | 28:DF:110:ALA:HB3 | 1.95 | 0.49 |
| 30:DH:45:LYS:HA | 30:DH:48:GLU:HG2 | 1.94 | 0.49 |
| 42:BT:3:THR:HA | 42:BT:6:ASP:OD2 | 2.13 | 0.49 |
| 23:BA:127:A:H5' | 23:BA:128:C:C6 | 2.47 | 0.49 |
| 16:AP:47:ASP:O | 16:AP:49:LEU:N | 2.45 | 0.49 |
| 3:AC:79:ARG:O | 3:AC:82:GLU:HG3 | 2.13 | 0.49 |
| 23:BA:2495:G:C2' | 23:BA:2496:C:O5' | 2.60 | 0.49 |
| 34:BL:57:THR:CG2 | 34:BL:59:LEU:CD2 | 2.75 | 0.49 |
| 1:AA:1123:A:H1' | 10:AJ:37:PRO:O | 2.12 | 0.49 |
| 2:AB:184:VAL:O | 2:AB:198:ASP:HB2 | 2.13 | 0.49 |
| 32:DJ:143:LEU:CD1 | 32:DJ:143:LEU:C | 2.81 | 0.49 |
| 1:AA:947:G:O3' | 13:AM:109:THR:OG1 | 2.28 | 0.49 |
| 22:AV:6192:G:C5 | 22:AV:6193:U:C4 | 3.00 | 0.49 |
| 33:BK:71:ARG:NH2 | 33:BK:77:ILE:HG21 | 2.27 | 0.49 |
| 38:BP:58:ASN:HD22 | 38:BP:58:ASN:C | 2.16 | 0.49 |
| 1:CA:551:U:HO2' | 12:CL:85:ARG:HD2 | 1.78 | 0.49 |
| 23:BA:1902:C:H2' | 23:BA:1903:G:O5' | 2.13 | 0.49 |
| 23:BA:1187:G:O5' | 23:BA:1187:G:H8 | 1.96 | 0.49 |
| 28:BF:83:ARG:HG3 | 28:BF:84:LYS:H | 1.77 | 0.49 |
| 16:CP:3:LYS:O | 16:CP:21:VAL:HA | 2.13 | 0.49 |
| 3:AC:182:ILE:HD11 | 3:AC:203:PHE:HD1 | 1.77 | 0.49 |
| 1:CA:76:G:C6 | 1:CA:77:C:N4 | 2.81 | 0.49 |
| 44:DV:163:LEU:H | 44:DV:163:LEU:CD2 | 2.25 | 0.49 |
| 23:BA:2681:C:O2 | 23:BA:2681:C:O5' | 2.31 | 0.49 |
| 1:AA:256:U:C2 | 1:AA:257:G:C8 | 3.00 | 0.49 |
| 43:DU:81:LYS:HD3 | 43:DU:96:ILE:HG13 | 1.93 | 0.49 |
| 23:DA:1343:G:O2' | 23:DA:1344:G:H5' | 2.13 | 0.49 |
| 20:CT:12:ALA:O | 20:CT:15:ARG:HB2 | 2.13 | 0.49 |
| 3:AC:195:VAL:CG1 | 3:AC:196:LEU:N | 2.65 | 0.49 |
| 1:CA:586:C:H1' | 1:CA:878:G:O2' | 2.12 | 0.49 |
| 4:CD:162:LEU:HD11 | 4:CD:181:MET:HG2 | 1.94 | 0.49 |
| 25:BC:120:GLY:HA2 | 25:BC:190:TYR:OH | 2.13 | 0.49 |
| 1:AA:321:A:O2' | 1:AA:322:C:H5' | 2.11 | 0.49 |
| 1:AA:987:G:H2' | 1:AA:988:G:H8 | 1.78 | 0.49 |
| 1:CA:1531:A:H8 | 1:CA:1531:A:O5' | 1.95 | 0.49 |
| 23:BA:661:C:O3' | 34:BL:18:ARG:HG2 | 2.13 | 0.49 |
| 23:DA:1952:A:C6 | 33:DK:22:ILE:HD11 | 2.48 | 0.49 |
| 30:BH:5:LEU:CD2 | 30:BH:5:LEU:N | 2.76 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:DA:2287:A:O2' | 23:DA:2288:A:P | 2.70 | 0.49 |
| 23:DA:226:G:N2 | 23:DA:227:A:C2 | 2.81 | 0.49 |
| 11:AK:32:ILE:O | 11:AK:40:ILE:HG12 | 2.13 | 0.49 |
| 43:BU:42:VAL:CG1 | 43:BU:65:ALA:HB3 | 2.41 | 0.49 |
| 28:DF:77:ILE:CG2 | 28:DF:80:PHE:H | 2.23 | 0.49 |
| 33:BK:88:ASN:ND2 | 33:BK:90:GLN:HB3 | 2.28 | 0.49 |
| 23:BA:105:C:C2 | 23:BA:106:C:C5 | 3.00 | 0.49 |
| 23:BA:2593:U:C2 | 23:BA:2594:C:C5 | 3.01 | 0.49 |
| 23:DA:1476:C:C5 | 23:DA:1477:A:N7 | 2.80 | 0.49 |
| 9:CI:114:TYR:N | 9:CI:114:TYR:CD2 | 2.77 | 0.49 |
| 1:CA:522:C:H2' | 1:CA:523:A:H5' | 1.94 | 0.49 |
| 1:CA:20:U:H2' | 1:CA:21:G:H5' | 1.94 | 0.49 |
| 25:BC:30:GLU:HG3 | 25:BC:63:ARG:NE | 2.27 | 0.49 |
| 25:BC:61:LEU:HB3 | 25:BC:63:ARG:NH1 | 2.28 | 0.49 |
| 12:CL:23:VAL:O | 12:CL:23:VAL:HG12 | 2.10 | 0.49 |
| 1:AA:127:G:C2 | 1:AA:128:G:C8 | 3.00 | 0.49 |
| 23:DA:2225:A:H1' | 23:DA:2226:C:OP2 | 2.13 | 0.49 |
| 23:DA:1746:G:N2 | 23:DA:1747:G:C4 | 2.80 | 0.49 |
| 3:CC:76:VAL:CG2 | 3:CC:77:ILE:HG13 | 2.43 | 0.49 |
| 3:CC:77:ILE:O | 3:CC:83:ARG:HB3 | 2.12 | 0.49 |
| 23:DA:304:G:N2 | 23:DA:314:A:C4 | 2.80 | 0.49 |
| 40:BR:12:TYR:CD2 | 40:BR:12:TYR:N | 2.81 | 0.49 |
| 1:AA:1089:G:C6 | 1:AA:1090:U:C4 | 3.01 | 0.49 |
| 39:BQ:50:ARG:HH12 | 40:BR:72:VAL:HG12 | 1.77 | 0.49 |
| 23:BA:1726:G:H2' | 23:BA:1727:U:H6 | 1.73 | 0.49 |
| 36:DN:79:LEU:HA | 36:DN:83:ILE:HG13 | 1.95 | 0.49 |
| 1:AA:639:G:H2' | 1:AA:640:A:H8 | 1.77 | 0.49 |
| 16:CP:13:HIS:C | 16:CP:15:PRO:HD3 | 2.33 | 0.49 |
| 7:AG:70:LYS:HG3 | 7:AG:96:GLN:HB3 | 1.94 | 0.49 |
| 1:CA:562:C:N4 | 1:CA:884:U:C6 | 2.80 | 0.49 |
| 33:DK:9:GLU:O | 33:DK:83:ALA:HA | 2.13 | 0.49 |
| 1:CA:380:G:N1 | 1:CA:384:G:C6 | 2.80 | 0.49 |
| 44:DV:91:LEU:CD2 | 44:DV:96:VAL:HG11 | 2.43 | 0.49 |
| 21:CU:12:LYS:HB3 | 21:CU:17:THR:O | 2.13 | 0.49 |
| 1:AA:801:U:H2' | 1:AA:802:A:H8 | 1.77 | 0.49 |
| 23:DA:57:C:O5' | 23:DA:57:C:H6 | 1.95 | 0.49 |
| 32:DJ:32:VAL:HG12 | 32:DJ:33:GLU:O | 2.12 | 0.49 |
| 1:CA:32:A:H2' | 1:CA:33:A:C8 | 2.47 | 0.49 |
| 38:BP:50:ILE:HA | 38:BP:99:LEU:CD1 | 2.43 | 0.49 |
| 6:AF:82:ARG:HB2 | 6:AF:85:VAL:CG2 | 2.43 | 0.49 |
| 20:AT:32:ALA:O | 20:AT:36:LEU:HD23 | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:DF:74:LYS:HA | 28:DF:74:LYS:HE3 | 1.94 | 0.49 |
| 23:DA:762:U:H4' | 23:DA:763:G:O5' | 2.12 | 0.49 |
| 23:DA:636:G:OP1 | 34:DL:132:LYS:HD3 | 2.13 | 0.49 |
| 9:CI:118:LYS:O | 9:CI:119:ALA:HB3 | 2.12 | 0.49 |
| 22:AV:6190:U:C4 | 22:AV:6191:A:N7 | 2.81 | 0.49 |
| 22:AV:6190:U:O4 | 22:AV:6191:A:N6 | 2.45 | 0.49 |
| 34:BL:50:ARG:HB2 | 53:B5:60:LEU:CD2 | 2.42 | 0.49 |
| 24:DB:7:G:H2' | 24:DB:8:U:O4' | 2.12 | 0.49 |
| 1:AA:1260:C:H4' | 1:AA:1284:C:H5' | 1.94 | 0.49 |
| 28:DF:41:GLN:HB2 | 28:DF:90:LEU:HB2 | 1.94 | 0.49 |
| 1:CA:79:G:H2' | 1:CA:80:G:C8 | 2.48 | 0.49 |
| 1:CA:95:G:H2' | 1:CA:96:G:O4' | 2.12 | 0.49 |
| 23:BA:137(B):G:C4 | 23:BA:139:G:N7 | 2.81 | 0.49 |
| 24:DB:71:C:C4 | 24:DB:72:G:N7 | 2.81 | 0.49 |
| 1:CA:397:A:N6 | 1:CA:548:G:N7 | 2.61 | 0.49 |
| 26:DD:84:PHE:CD2 | 26:DD:84:PHE:C | 2.86 | 0.49 |
| 23:DA:2886:G:N2 | 23:DA:2887:U:C2 | 2.81 | 0.49 |
| 1:AA:1064:G:C1' | 1:AA:1065:U:OP2 | 2.61 | 0.49 |
| 23:BA:929:G:H8 | 23:BA:929:G:O5' | 1.96 | 0.49 |
| 4:CD:3:ARG:HD2 | 4:CD:3:ARG:H | 1.76 | 0.49 |
| 37:DO:84:GLN:C | 37:DO:86:ALA:H | 2.16 | 0.49 |
| 46:DX:10:LYS:O | 46:DX:11:ARG:HB2 | 2.11 | 0.49 |
| 12:CL:44:PRO:CG | 12:CL:52:ARG:HE | 2.24 | 0.49 |
| 23:BA:2875:C:C4' | 38:BP:5:ALA:HB2 | 2.36 | 0.49 |
| 29:DG:20:ALA:HB1 | 29:DG:21:PRO:HD2 | 1.94 | 0.49 |
| 23:DA:319:C:N4 | 23:DA:320:A:C6 | 2.81 | 0.49 |
| 23:BA:2307:G:O5' | 23:BA:2307:G:C8 | 2.66 | 0.49 |
| 43:BU:27:VAL:O | 43:BU:27:VAL:CG2 | 2.58 | 0.49 |
| 23:BA:2784:C:H2' | 23:BA:2785:C:C6 | 2.47 | 0.49 |
| 23:DA:1401:G:C2' | 23:DA:1402:C:H6 | 2.22 | 0.49 |
| 23:BA:1496:A:C8 | 23:BA:1577:C:O2' | 2.65 | 0.49 |
| 23:BA:1511:A:O2' | 23:BA:1512:G:H5' | 2.12 | 0.49 |
| 1:CA:618:C:N4 | 1:CA:621:A:N7 | 2.60 | 0.49 |
| 1:AA:73:G:H8 | 1:AA:73:G:O5' | 1.95 | 0.49 |
| 23:DA:286:C:C2 | 23:DA:287:C:C5 | 3.01 | 0.49 |
| 33:BK:88:ASN:N | 33:BK:92:GLU:O | 2.39 | 0.49 |
| 38:DP:27:THR:O | 38:DP:89:VAL:HG13 | 2.12 | 0.49 |
| 18:AR:44:LEU:HD11 | 18:AR:70:ILE:HG21 | 1.95 | 0.49 |
| 4:AD:13:ARG:CD | 4:AD:38:TYR:O | 2.61 | 0.49 |
| 1:AA:1090:U:H2' | 1:AA:1091:U:C6 | 2.48 | 0.49 |
| 1:CA:1311:G:N2 | 1:CA:1327:C:C2 | 2.81 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:1327:C:O2' | 1:AA:1328:C:H5' | 2.12 | 0.49 |
| 23:DA:245:G:C4 | 23:DA:246:C:C5 | 3.00 | 0.49 |
| 23:BA:852:G:H2' | 23:BA:853:G:C8 | 2.48 | 0.49 |
| 6:AF:12:PRO:HD3 | 6:AF:58:GLY:HA2 | 1.95 | 0.49 |
| 3:CC:191:THR:HB | 3:CC:193:TYR:CD2 | 2.47 | 0.49 |
| 23:DA:270(O):G:C6 | 23:DA:270(Q):C:N4 | 2.81 | 0.49 |
| 1:AA:44:G:N2 | 1:AA:399:G:C4 | 2.80 | 0.49 |
| 23:DA:2435:A:H2' | 23:DA:2436:G:O5' | 2.11 | 0.49 |
| 2:CB:15:VAL:H | 2:CB:16:HIS:CE1 | 2.31 | 0.49 |
| 23:BA:1444:G:N2 | 23:BA:1548:C:C2 | 2.81 | 0.49 |
| 39:DQ:65:ILE:O | 39:DQ:66:ASN:C | 2.51 | 0.49 |
| 1:CA:294:U:H2' | 1:CA:295:C:C6 | 2.47 | 0.49 |
| 23:DA:1394:U:C5 | 23:DA:1395:A:C4 | 3.00 | 0.49 |
| 23:BA:1241:A:N6 | 23:BA:1242:A:N1 | 2.60 | 0.49 |
| 1:AA:1480:G:C4 | 1:AA:1481:U:C6 | 3.00 | 0.49 |
| 1:CA:743:U:O2' | 1:CA:744:C:H5' | 2.13 | 0.49 |
| 8:CH:120:THR:H | 8:CH:123:GLU:HB2 | 1.78 | 0.49 |
| 23:DA:2648:C:H2' | 23:DA:2649:U:C6 | 2.48 | 0.49 |
| 36:DN:30:THR:HG22 | 36:DN:31:HIS:CE1 | 2.48 | 0.49 |
| 23:BA:851:U:O2' | 48:BZ:45:GLY:HA3 | 2.13 | 0.49 |
| 23:BA:1678:G:N3 | 23:BA:1678:G:C2' | 2.74 | 0.49 |
| 17:CQ:11:VAL:O | 17:CQ:11:VAL:HG13 | 2.12 | 0.49 |
| 16:AP:49:LEU:HG | 16:AP:50:LYS:N | 2.28 | 0.49 |
| 6:AF:82:ARG:HB2 | 6:AF:85:VAL:HG23 | 1.94 | 0.49 |
| 23:DA:1930:G:N2 | 23:DA:1968:G:H2' | 2.28 | 0.49 |
| 1:CA:945:G:C6 | 1:CA:1337:G:C6 | 3.01 | 0.49 |
| 1:CA:1061:G:OP2 | 3:CC:3:ASN:ND2 | 2.42 | 0.49 |
| 9:CI:27:THR:O | 9:CI:62:TYR:HA | 2.12 | 0.49 |
| 30:DH:1:MET:HG3 | 30:DH:23:PRO:HG3 | 1.95 | 0.49 |
| 23:DA:702:G:C2 | 23:DA:731:C:C2 | 3.01 | 0.49 |
| 8:CH:54:ASP:O | 8:CH:56:LYS:HG3 | 2.12 | 0.49 |
| 23:DA:2024:G:H2' | 23:DA:2025:C:H6 | 1.77 | 0.49 |
| 24:BB:86:G:H2' | 24:BB:87:G:C8 | 2.48 | 0.49 |
| 23:BA:1665:A:H4' | 33:BK:67:LYS:HB2 | 1.95 | 0.49 |
| 7:CG:49:ILE:O | 7:CG:49:ILE:HG22 | 2.11 | 0.49 |
| 23:BA:2261:C:O2' | 23:BA:2262:U:H5' | 2.12 | 0.49 |
| 47:DY:1:MET:CE | 47:DY:4:SER:HB2 | 2.42 | 0.49 |
| 23:DA:1542:G:H3' | 23:DA:1542:G:P | 2.53 | 0.49 |
| 10:AJ:50:ILE:CG2 | 14:AN:41:ARG:HH21 | 2.26 | 0.49 |
| 7:AG:113:GLU:HB3 | 7:AG:118:VAL:CG2 | 2.42 | 0.49 |
| 23:BA:2846:G:P | 38:BP:54:ARG:HB2 | 2.52 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:DR:13:ARG:NH1 | 40:DR:13:ARG:HG3 | 2.28 | 0.49 |
| 25:DC:83:GLU:OE1 | 25:DC:104:TYR:OH | 2.19 | 0.49 |
| 23:DA:860:U:O2' | 23:DA:861:A:C5' | 2.52 | 0.49 |
| 28:DF:85:GLY:C | 28:DF:86:MET:HG3 | 2.32 | 0.49 |
| 17:CQ:45:HIS:O | 17:CQ:73:VAL:HG23 | 2.12 | 0.49 |
| 23:BA:556:G:H2' | 23:BA:557:U:H6 | 1.77 | 0.49 |
| 23:BA:2563:U:O2 | 23:BA:2565:A:H8 | 1.96 | 0.49 |
| 23:BA:379:G:C2 | 46:BX:20:ARG:NH2 | 2.81 | 0.49 |
| 23:BA:1567:A:C8 | 25:BC:84:TYR:CE2 | 3.01 | 0.49 |
| 37:BO:53:SER:O | 37:BO:56:LEU:HB3 | 2.13 | 0.49 |
| 9:CI:28:VAL:HG13 | 9:CI:63:ILE:HG22 | 1.95 | 0.49 |
| 25:DC:134:ARG:HD3 | 25:DC:135:PHE:HE1 | 1.74 | 0.49 |
| 1:CA:987:G:H2' | 1:CA:988:G:H8 | 1.78 | 0.49 |
| 11:CK:21:ILE:HG13 | 11:CK:30:VAL:HG12 | 1.95 | 0.49 |
| 1:CA:1053:G:H3' | 1:CA:1054:C:C5' | 2.41 | 0.49 |
| 50:B2:40:LYS:CD | 50:B2:46:CYS:HB3 | 2.43 | 0.49 |
| 23:DA:2636:U:H2' | 23:DA:2637:U:H6 | 1.77 | 0.49 |
| 1:CA:938:A:N6 | 1:CA:939:G:C6 | 2.81 | 0.49 |
| 1:AA:754:C:P | 15:AO:72:ARG:HH22 | 2.36 | 0.49 |
| 23:DA:2190:G:C4 | 23:DA:2191:G:C8 | 3.00 | 0.49 |
| 26:BD:112:GLY:O | 26:BD:159:HIS:HA | 2.13 | 0.49 |
| 43:DU:30:VAL:CG2 | 43:DU:37:VAL:HG12 | 2.42 | 0.49 |
| 23:DA:1749:A:H2' | 23:DA:1750:G:O4' | 2.12 | 0.49 |
| 23:DA:2828:C:C2' | 23:DA:2829:C:H5' | 2.41 | 0.49 |
| 1:CA:1511:G:C6 | 1:CA:1512:U:C4 | 3.01 | 0.49 |
| 36:BN:103:ARG:HH12 | 36:BN:110:PRO:HG3 | 1.78 | 0.49 |
| 23:DA:2836:U:H2' | 23:DA:2837:G:C8 | 2.47 | 0.49 |
| 1:AA:1465:C:H2' | 1:AA:1466:C:O4' | 2.13 | 0.49 |
| 1:CA:525:C:H5'' | 12:CL:90:LYS:CE | 2.43 | 0.49 |
| 1:AA:1315:U:H2' | 1:AA:1316:G:O4' | 2.12 | 0.49 |
| 1:AA:1047:G:O2' | 1:AA:1048:G:H5' | 2.13 | 0.49 |
| 20:CT:39:LYS:O | 20:CT:43:LEU:HG | 2.12 | 0.49 |
| 23:DA:1465:G:N2 | 23:DA:1466:G:H1' | 2.28 | 0.49 |
| 13:AM:14:ARG:NH1 | 13:AM:42:ALA:HA | 2.27 | 0.49 |
| 1:AA:420:U:O2 | 1:AA:424:G:N1 | 2.46 | 0.49 |
| 23:BA:2026:C:N3 | 23:BA:2027:G:C8 | 2.81 | 0.49 |
| 12:AL:92:LEU:HB2 | 12:AL:95:VAL:CG2 | 2.43 | 0.49 |
| 41:DS:54:ALA:HB1 | 41:DS:107:LEU:HD22 | 1.95 | 0.49 |
| 1:CA:149:A:H2' | 1:CA:150:C:C6 | 2.48 | 0.49 |
| 45:DW:47:PRO:HB2 | 45:DW:48:GLY:H | 1.47 | 0.49 |
| 30:BH:51:ILE:HG22 | 30:BH:52:ARG:N | 2.28 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BA:1465:G:C2 | 23:BA:1466:G:C8 | 3.01 | 0.49 |
| 23:DA:343:C:O2' | 23:DA:344:G:H5' | 2.12 | 0.49 |
| 23:DA:1168:G:C2 | 23:DA:1182:A:C2 | 3.01 | 0.49 |
| 45:DW:82:ARG:O | 45:DW:84:LEU:HD23 | 2.13 | 0.49 |
| 13:AM:49:THR:O | 13:AM:53:VAL:HG23 | 2.12 | 0.49 |
| 33:BK:9:GLU:O | 33:BK:83:ALA:HA | 2.13 | 0.49 |
| 23:DA:2679:A:H4' | 26:DD:165:VAL:HG11 | 1.94 | 0.49 |
| 41:BS:78:GLU:OE2 | 41:BS:99:ARG:HD3 | 2.13 | 0.49 |
| 23:BA:231:C:N4 | 23:BA:232:G:N1 | 2.61 | 0.49 |
| 52:B4:36:GLN:HG2 | 52:B4:36:GLN:O | 2.09 | 0.49 |
| 1:CA:385:C:H3' | 1:CA:385:C:H6 | 1.77 | 0.49 |
| 1:AA:525:C:OP1 | 12:AL:90:LYS:HG2 | 2.12 | 0.49 |
| 25:BC:212:SER:O | 25:BC:217:ARG:HG3 | 2.13 | 0.49 |
| 23:DA:1678:G:H22 | 23:DA:1989:G:H22 | 1.60 | 0.49 |
| 23:DA:1314:C:C2' | 23:DA:1315:C:H5' | 2.43 | 0.49 |
| 23:DA:2361:A:OP1 | 53:D5:27:THR:OG1 | 2.30 | 0.49 |
| 23:BA:1542:G:OP2 | 23:BA:1543:A:OP1 | 2.30 | 0.49 |
| 7:CG:113:GLU:HB3 | 7:CG:118:VAL:CG2 | 2.43 | 0.49 |
| 23:DA:103:A:O5' | 23:DA:103:A:H8 | 1.96 | 0.49 |
| 9:AI:114:TYR:N | 9:AI:114:TYR:HD2 | 2.10 | 0.49 |
| 13:AM:91:ARG:NH1 | 19:AS:81:ARG:NH2 | 2.61 | 0.49 |
| 28:BF:56:ALA:O | 28:BF:60:LEU:HB2 | 2.12 | 0.49 |
| 23:BA:727:A:H2 | 25:BC:9:TYR:CD2 | 2.30 | 0.49 |
| 24:BB:7:G:H5'' | 37:BO:29:PHE:CD2 | 2.47 | 0.49 |
| 1:AA:672:U:O2' | 1:AA:673:G:H5' | 2.13 | 0.49 |
| 37:DO:87:PHE:CD1 | 37:DO:102:ALA:HB2 | 2.48 | 0.49 |
| 25:DC:105:ILE:HD13 | 25:DC:106:ILE:N | 2.28 | 0.49 |
| 1:AA:413:G:H22 | 1:AA:429:U:P | 2.36 | 0.49 |
| 1:AA:689:C:H2' | 1:AA:690:G:O4' | 2.11 | 0.49 |
| 3:AC:172:ARG:HE | 3:AC:174:PRO:CG | 2.26 | 0.49 |
| 14:AN:37:PHE:CE1 | 14:AN:53:LEU:HD13 | 2.48 | 0.49 |
| 5:CE:78:HIS:HE1 | 5:CE:142:LEU:HA | 1.77 | 0.49 |
| 5:CE:79:GLU:HB3 | 5:CE:92:LYS:HA | 1.93 | 0.49 |
| 35:BM:141:GLN:OE1 | 44:BV:97:GLU:O | 2.31 | 0.49 |
| 3:AC:134:ILE:HG23 | 3:AC:151:VAL:CB | 2.35 | 0.49 |
| 23:DA:1608:A:HO2' | 23:DA:1610:A:P | 2.36 | 0.49 |
| 23:DA:2681:C:O2 | 23:DA:2681:C:O5' | 2.30 | 0.49 |
| 4:AD:162:LEU:HD11 | 4:AD:181:MET:HG2 | 1.95 | 0.49 |
| 1:AA:1369:C:OP1 | 9:AI:111:ARG:HG3 | 2.12 | 0.49 |
| 36:DN:72:ASP:O | 36:DN:76:VAL:HG13 | 2.12 | 0.49 |
| 4:CD:127:THR:OG1 | 4:CD:128:VAL:N | 2.46 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DA:2746:U:C2' | 23:DA:2747:G:O5' | 2.61 | 0.49 |
| 46:BX:45:ASN:ND2 | 46:BX:47:GLN:HE21 | 2.11 | 0.49 |
| 23:DA:1503:U:N3 | 23:DA:1504:C:N4 | 2.61 | 0.49 |
| 29:BG:43:VAL:HG12 | 29:BG:52:VAL:CG2 | 2.43 | 0.49 |
| 11:CK:32:ILE:HD11 | 11:CK:68:ALA:HB1 | 1.95 | 0.49 |
| 1:AA:632:A:C2' | 1:AA:633:G:H5' | 2.42 | 0.49 |
| 1:CA:327:A:C6 | 1:CA:329:A:C5 | 3.01 | 0.49 |
| 1:CA:102:G:C4 | 1:CA:103:C:C5 | 3.01 | 0.49 |
| 29:DG:86:GLU:O | 29:DG:86:GLU:CG | 2.61 | 0.49 |
| 28:BF:111:LEU:HA | 28:BF:114:ILE:HD11 | 1.95 | 0.49 |
| 38:DP:28:VAL:HA | 38:DP:89:VAL:CG1 | 2.42 | 0.49 |
| 38:DP:27:THR:HG23 | 38:DP:90:GLN:HB3 | 1.94 | 0.49 |
| 35:DM:21:THR:O | 35:DM:23:GLY:N | 2.45 | 0.49 |
| 39:DQ:117:GLN:HA | 39:DQ:117:GLN:OE1 | 2.13 | 0.49 |
| 23:DA:1389:G:N2 | 23:DA:1390:U:C2 | 2.80 | 0.49 |
| 20:AT:13:LEU:O | 20:AT:16:HIS:N | 2.46 | 0.49 |
| 23:DA:1289:C:H2' | 23:DA:1290:C:C6 | 2.47 | 0.49 |
| 16:CP:8:ARG:O | 16:CP:9:PHE:HD2 | 1.95 | 0.49 |
| 1:AA:941:G:C6 | 1:AA:1343:G:C6 | 3.00 | 0.49 |
| 13:AM:79:LYS:HA | 13:AM:82:MET:HB3 | 1.95 | 0.49 |
| 1:CA:1412:C:H2' | 1:CA:1413:A:C8 | 2.47 | 0.49 |
| 1:CA:632:A:C2' | 1:CA:633:G:H5' | 2.42 | 0.49 |
| 8:AH:38:ILE:HD11 | 8:AH:118:VAL:O | 2.13 | 0.49 |
| 23:BA:1842:G:H1' | 25:BC:255:LYS:HZ3 | 1.78 | 0.49 |
| 23:BA:569:U:C4 | 23:BA:570:G:C6 | 3.00 | 0.49 |
| 3:CC:179:ARG:O | 3:CC:179:ARG:HG3 | 2.13 | 0.49 |
| 1:AA:506:G:C4 | 1:AA:507:C:C5 | 3.00 | 0.49 |
| 36:DN:78:LYS:O | 36:DN:83:ILE:HG12 | 2.12 | 0.49 |
| 1:CA:1493:A:H4' | 1:CA:1494:G:OP2 | 2.13 | 0.49 |
| 46:BX:49:VAL:HG11 | 46:BX:70:VAL:HG11 | 1.94 | 0.49 |
| 23:DA:26:G:C6 | 23:DA:27:G:N1 | 2.80 | 0.49 |
| 23:DA:915:C:O2' | 24:DB:100:G:H5' | 2.13 | 0.49 |
| 35:DM:29:PHE:N | 35:DM:105:GLU:OE2 | 2.45 | 0.49 |
| 1:AA:926:G:C6 | 1:AA:1505:G:C6 | 3.01 | 0.49 |
| 1:CA:1525:G:OP1 | 11:CK:120:ARG:NH2 | 2.46 | 0.49 |
| 23:BA:2025:C:H2' | 23:BA:2026:C:C6 | 2.48 | 0.49 |
| 1:AA:958:A:N6 | 1:AA:959:A:N6 | 2.61 | 0.49 |
| 19:AS:33:THR:HG23 | 19:AS:51:VAL:HA | 1.94 | 0.49 |
| 1:AA:6:G:O2' | 1:AA:7:G:H5' | 2.13 | 0.49 |
| 23:DA:2849:U:H4' | 23:DA:2868:A:C2 | 2.47 | 0.49 |
| 19:CS:52:TYR:CE1 | 19:CS:56:GLN:HA | 2.48 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 52:B4:18:PHE:CE2 | 52:B4:22:MET:HG3 | 2.48 | 0.49 |
| 23:DA:1926:U:O2 | 23:DA:1929:G:C2 | 2.66 | 0.49 |
| 3:AC:179:ARG:HG3 | 3:AC:179:ARG:O | 2.13 | 0.49 |
| 28:DF:56:ALA:O | 28:DF:60:LEU:HB2 | 2.13 | 0.48 |
| 28:BF:64:THR:HG23 | 28:BF:66:GLN:N | 2.28 | 0.48 |
| 14:CN:2:ALA:HB1 | 14:CN:6:LEU:HD12 | 1.95 | 0.48 |
| 5:AE:101:ILE:HG12 | 5:AE:118:ILE:O | 2.13 | 0.48 |
| 23:DA:1971:A:C2 | 25:DC:241:PRO:HD3 | 2.47 | 0.48 |
| 23:BA:114(B):A:C4 | 23:BA:1144:G:N7 | 2.81 | 0.48 |
| 30:BH:98:ALA:O | 30:BH:109:ILE:HD11 | 2.13 | 0.48 |
| 39:BQ:69:CYS:SG | 39:BQ:79:PHE:CD2 | 3.06 | 0.48 |
| 37:DO:89:ARG:HG2 | 37:DO:89:ARG:O | 2.13 | 0.48 |
| 3:AC:114:PRO:HD3 | 3:AC:183:ASP:OD1 | 2.13 | 0.48 |
| 30:DH:82:ARG:HB3 | 30:DH:89:TYR:HB2 | 1.95 | 0.48 |
| 24:DB:44:G:N3 | 24:DB:47:C:N4 | 2.60 | 0.48 |
| 20:CT:26:ASN:HB2 | 20:CT:71:THR:CG2 | 2.33 | 0.48 |
| 1:AA:394:G:C4 | 1:AA:395:C:C5 | 3.01 | 0.48 |
| 4:CD:31:CYS:O | 4:CD:31:CYS:SG | 2.71 | 0.48 |
| 5:CE:139:LEU:O | 5:CE:141:GLN:N | 2.45 | 0.48 |
| 23:DA:2887:U:C2 | 23:DA:2888:C:C5 | 3.00 | 0.48 |
| 1:AA:1190:G:OP1 | 3:AC:4:LYS:HA | 2.13 | 0.48 |
| 23:DA:1788:C:OP1 | 25:DC:222:ARG:NH2 | 2.46 | 0.48 |
| 2:AB:211:ILE:HG22 | 2:AB:215:LEU:HD23 | 1.94 | 0.48 |
| 1:AA:187:C:H2' | 1:AA:188:U:O4' | 2.13 | 0.48 |
| 1:CA:1292:U:N3 | 1:CA:1293:G:N7 | 2.61 | 0.48 |
| 41:DS:69:LEU:HA | 41:DS:108:GLY:O | 2.13 | 0.48 |
| 36:BN:38:VAL:CB | 36:BN:39:PRO:HD3 | 2.36 | 0.48 |
| 12:AL:44:PRO:HG3 | 12:AL:52:ARG:HD3 | 1.95 | 0.48 |
| 12:AL:52:ARG:NH1 | 12:AL:52:ARG:HG3 | 2.24 | 0.48 |
| 6:AF:46:ARG:HH12 | 18:AR:37:VAL:HG21 | 1.78 | 0.48 |
| 2:AB:141:GLU:O | 2:AB:145:LEU:HD23 | 2.13 | 0.48 |
| 29:BG:67:LEU:HG | 29:BG:71:LEU:HD23 | 1.95 | 0.48 |
| 23:BA:966:G:C4 | 23:BA:967:C:H5 | 2.30 | 0.48 |
| 16:AP:45:THR:HB | 16:AP:46:PRO:HD2 | 1.94 | 0.48 |
| 33:DK:12:ASP:HA | 33:DK:98:VAL:HA | 1.94 | 0.48 |
| 23:BA:1401:G:C5 | 23:BA:1402:C:C5 | 3.01 | 0.48 |
| 23:BA:2100:G:H21 | 23:BA:2101:G:H1' | 1.76 | 0.48 |
| 23:DA:301:G:C6 | 23:DA:302:C:N4 | 2.81 | 0.48 |
| 23:BA:2863:C:O2' | 23:BA:2864:G:H5' | 2.12 | 0.48 |
| 24:DB:75:G:HO2' | 44:DV:85:HIS:CD2 | 2.31 | 0.48 |
| 45:DW:64:ASP:OD1 | 45:DW:64:ASP:N | 2.45 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:862:C:O2' | 1:AA:863:U:H5' | 2.12 | 0.48 |
| 33:BK:2:ILE:CD1 | 33:BK:82:ASN:ND2 | 2.76 | 0.48 |
| 23:BA:493:G:H2' | 23:BA:494:G:O4' | 2.13 | 0.48 |
| 34:DL:55:ARG:HG3 | 34:DL:56:SER:N | 2.28 | 0.48 |
| 23:BA:444:C:OP2 | 39:BQ:2:PRO:HD3 | 2.12 | 0.48 |
| 43:BU:68:HIS:C | 43:BU:70:SER:H | 2.16 | 0.48 |
| 8:CH:39:LEU:C | 8:CH:45:ILE:HG12 | 2.34 | 0.48 |
| 27:DE:127:GLU:OE2 | 27:DE:127:GLU:O | 2.31 | 0.48 |
| 38:BP:84:GLN:HG3 | 38:BP:85:LYS:HG3 | 1.95 | 0.48 |
| 23:DA:2862:G:C4 | 23:DA:2863:C:C5 | 3.01 | 0.48 |
| 45:BW:11:LYS:O | 45:BW:14:ARG:NH2 | 2.40 | 0.48 |
| 23:DA:2738:A:C2 | 23:DA:2739:U:N1 | 2.81 | 0.48 |
| 33:DK:14:THR:HG22 | 33:DK:14:THR:O | 2.11 | 0.48 |
| 15:CO:5:LYS:HD3 | 15:CO:5:LYS:N | 2.27 | 0.48 |
| 1:CA:827:U:H2' | 1:CA:870:U:O4 | 2.13 | 0.48 |
| 23:DA:46:C:N4 | 23:DA:179:G:H1 | 2.11 | 0.48 |
| 23:DA:1241:A:N6 | 23:DA:1242:A:N1 | 2.61 | 0.48 |
| 34:BL:135:LEU:O | 34:BL:139:LYS:HB2 | 2.13 | 0.48 |
| 1:AA:928:G:C2 | 1:AA:1390:U:O2 | 2.66 | 0.48 |
| 30:DH:28:ASN:C | 30:DH:32:PRO:HG2 | 2.34 | 0.48 |
| 23:DA:443:A:N7 | 27:DE:45:ARG:HG2 | 2.28 | 0.48 |
| 38:BP:50:ILE:HA | 38:BP:99:LEU:HD11 | 1.94 | 0.48 |
| 1:AA:780:A:C2 | 1:AA:803:G:N1 | 2.81 | 0.48 |
| 23:DA:2620:C:C4' | 26:DD:156:MET:HG3 | 2.43 | 0.48 |
| 26:BD:102:VAL:HA | 26:BD:199:ARG:O | 2.13 | 0.48 |
| 23:DA:811:U:OP2 | 34:DL:24:GLY:HA2 | 2.13 | 0.48 |
| 23:DA:569:U:O2' | 23:DA:983:A:N1 | 2.45 | 0.48 |
| 4:CD:190:ASP:O | 4:CD:194:LEU:HD23 | 2.13 | 0.48 |
| 1:CA:1400:C:H6 | 1:CA:1400:C:O5' | 1.96 | 0.48 |
| 36:DN:104:ARG:CB | 36:DN:104:ARG:HH11 | 2.25 | 0.48 |
| 27:DE:122:LYS:N | 27:DE:122:LYS:HD2 | 2.28 | 0.48 |
| 4:AD:143:GLY:H | 4:AD:185:PHE:HB3 | 1.78 | 0.48 |
| 1:AA:149:A:H2' | 1:AA:150:C:C6 | 2.47 | 0.48 |
| 23:DA:2416:C:H6 | 23:DA:2416:C:O5' | 1.96 | 0.48 |
| 23:BA:2250:G:H5'' | 23:BA:2250:G:N3 | 2.28 | 0.48 |
| 23:DA:306:U:H2' | 23:DA:307:G:O4' | 2.13 | 0.48 |
| 1:CA:1368:G:OP1 | 9:CI:111:ARG:NH2 | 2.44 | 0.48 |
| 26:BD:170:LEU:HB3 | 26:BD:185:LYS:HB2 | 1.95 | 0.48 |
| 22:AV:6189:G:N2 | 22:AV:6215:C:C2 | 2.81 | 0.48 |
| 24:BB:7:G:H4' | 37:BO:29:PHE:CG | 2.48 | 0.48 |
| 23:BA:2334:G:C4 | 37:BO:12:PHE:HZ | 2.32 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:DJ:157:ARG:O | 32:DJ:158:PRO:C | 2.49 | 0.48 |
| 34:DL:40:SER:C | 34:DL:41:ARG:HD3 | 2.32 | 0.48 |
| 16:CP:28:ARG:CG | 16:CP:28:ARG:NH1 | 2.74 | 0.48 |
| 3:AC:19:GLU:HG3 | 3:AC:54:ARG:HD2 | 1.93 | 0.48 |
| 39:BQ:92:ARG:O | 39:BQ:94:ASN:N | 2.46 | 0.48 |
| 23:DA:2320:A:C8 | 23:DA:2333:A:N6 | 2.80 | 0.48 |
| 1:AA:32:A:H2' | 1:AA:33:A:C8 | 2.48 | 0.48 |
| 12:AL:116:ARG:HH21 | 12:AL:123:LYS:HB2 | 1.77 | 0.48 |
| 1:AA:552:U:H4' | 12:AL:85:ARG:HG2 | 1.95 | 0.48 |
| 20:AT:69:GLY:O | 20:AT:73:HIS:CE1 | 2.67 | 0.48 |
| 23:DA:1827:C:O2' | 23:DA:1828:G:H5' | 2.13 | 0.48 |
| 41:BS:75:TYR:CD2 | 41:BS:104:THR:HB | 2.46 | 0.48 |
| 23:BA:2712:U:O2' | 23:BA:2713:A:H5' | 2.13 | 0.48 |
| 23:DA:1331:A:O2' | 23:DA:1332:G:C8 | 2.63 | 0.48 |
| 1:CA:1072:G:C6 | 1:CA:1104:G:C2 | 3.01 | 0.48 |
| 1:CA:1106:G:C2 | 1:CA:1107:C:C5 | 3.01 | 0.48 |
| 1:AA:1074:G:C2 | 1:AA:1075:C:C2 | 3.01 | 0.48 |
| 23:DA:1788:C:H2' | 23:DA:1789:A:O4' | 2.12 | 0.48 |
| 25:DC:222:ARG:NH1 | 25:DC:224:ALA:HB3 | 2.27 | 0.48 |
| 48:DZ:26:LEU:HD13 | 48:DZ:47:VAL:HG22 | 1.94 | 0.48 |
| 6:CF:46:ARG:HH12 | 18:CR:37:VAL:HG21 | 1.78 | 0.48 |
| 12:AL:51:LEU:HD12 | 12:AL:51:LEU:N | 2.28 | 0.48 |
| 1:CA:1321:C:C5 | 1:CA:1322:C:C2 | 3.01 | 0.48 |
| 25:DC:235:GLY:O | 25:DC:237:GLU:N | 2.46 | 0.48 |
| 1:AA:1014:A:C2 | 1:AA:1219:U:H1' | 2.48 | 0.48 |
| 23:BA:2746:U:H4' | 29:BG:138:LYS:HD3 | 1.95 | 0.48 |
| 23:BA:1323:U:H2' | 23:BA:1324:G:H5' | 1.95 | 0.48 |
| 27:DE:89:VAL:O | 27:DE:91:GLY:N | 2.44 | 0.48 |
| 24:DB:12:C:O2' | 45:DW:74:ARG:HG2 | 2.13 | 0.48 |
| 28:BF:131:TYR:CD2 | 28:BF:133:LEU:HD22 | 2.48 | 0.48 |
| 44:BV:150:LEU:HD23 | 44:BV:171:ILE:HB | 1.94 | 0.48 |
| 29:BG:44:VAL:O | 29:BG:50:VAL:HG13 | 2.12 | 0.48 |
| 23:DA:1152:C:HO2' | 39:DQ:76:TYR:HE2 | 1.58 | 0.48 |
| 1:CA:627:G:O2' | 1:CA:628:G:H5' | 2.13 | 0.48 |
| 1:CA:1083:U:C5 | 1:CA:1084:G:C6 | 3.01 | 0.48 |
| 23:BA:2477:C:O2' | 23:BA:2478:A:P | 2.70 | 0.48 |
| 35:DM:60:ARG:HA | 44:DV:179:ASP:HB2 | 1.95 | 0.48 |
| 23:BA:2102:U:C4 | 23:BA:2103:C:N4 | 2.81 | 0.48 |
| 1:CA:657:G:C2 | 1:CA:658:G:C8 | 3.01 | 0.48 |
| 23:DA:2100:G:N2 | 23:DA:2101:G:N3 | 2.61 | 0.48 |
| 2:CB:76:GLN:NE2 | 2:CB:76:GLN:H | 2.11 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BA:588:U:C2 | 23:BA:589:C:C5 | 3.01 | 0.48 |
| 34:BL:132:LYS:CD | 34:BL:132:LYS:N | 2.76 | 0.48 |
| 23:BA:814:C:C5 | 34:BL:27:HIS:NE2 | 2.81 | 0.48 |
| 23:BA:1164:G:H5' | 23:BA:1165:U:OP2 | 2.12 | 0.48 |
| 1:CA:941:G:C6 | 1:CA:1343:G:C6 | 3.01 | 0.48 |
| 1:CA:560:U:O5' | 1:CA:566:G:N2 | 2.46 | 0.48 |
| 34:DL:105:LEU:N | 34:DL:105:LEU:HD12 | 2.27 | 0.48 |
| 23:DA:2228:G:P | 25:DC:263:ARG:HH21 | 2.36 | 0.48 |
| 1:CA:356:A:H2' | 1:CA:357:G:O5' | 2.13 | 0.48 |
| 23:DA:2862:G:C5 | 23:DA:2863:C:C5 | 3.00 | 0.48 |
| 23:DA:2738:A:C6 | 23:DA:2739:U:C5 | 3.01 | 0.48 |
| 23:BA:2718:G:H2' | 23:BA:2719:G:C8 | 2.48 | 0.48 |
| 13:AM:32:GLU:CD | 13:AM:64:TRP:CH2 | 2.86 | 0.48 |
| 8:CH:13:ILE:O | 8:CH:17:THR:HG23 | 2.13 | 0.48 |
| 27:BE:78:ILE:H | 27:BE:78:ILE:HG13 | 1.27 | 0.48 |
| 9:AI:26:VAL:O | 9:AI:26:VAL:HG12 | 2.12 | 0.48 |
| 1:AA:1296:C:C6 | 1:AA:1297:C:H5 | 2.30 | 0.48 |
| 1:AA:1038:C:C2 | 1:AA:1039:C:C5 | 3.01 | 0.48 |
| 23:BA:2032:G:H21 | 26:BD:146:THR:HG23 | 1.77 | 0.48 |
| 1:AA:134:A:N6 | 16:AP:25:ARG:HH12 | 2.09 | 0.48 |
| 39:BQ:36:ARG:HD3 | 39:BQ:40:PHE:CZ | 2.49 | 0.48 |
| 23:DA:2813:A:H2' | 23:DA:2814:C:O4' | 2.13 | 0.48 |
| 23:BA:270(Z):G:C2 | 23:BA:271(A):U:O4 | 2.66 | 0.48 |
| 23:DA:1118:C:H5'' | 44:DV:80:ARG:NH2 | 2.27 | 0.48 |
| 23:BA:1937:A:N7 | 23:BA:1939:U:H2' | 2.28 | 0.48 |
| 23:DA:516:C:P | 50:D2:13:LYS:HZ1 | 2.35 | 0.48 |
| 12:CL:51:LEU:N | 12:CL:51:LEU:HD12 | 2.28 | 0.48 |
| 32:BJ:133:GLY:O | 32:BJ:137:ARG:HG2 | 2.12 | 0.48 |
| 23:BA:611:C:C2 | 23:BA:612:G:C8 | 3.02 | 0.48 |
| 34:DL:80:TYR:CE1 | 34:DL:111:ARG:CG | 2.96 | 0.48 |
| 23:BA:2388:A:C8 | 23:BA:2389:G:C5 | 3.02 | 0.48 |
| 43:BU:8:LYS:NZ | 43:BU:8:LYS:CA | 2.76 | 0.48 |
| 52:B4:8:ASN:ND2 | 52:B4:9:ARG:N | 2.56 | 0.48 |
| 25:BC:155:LEU:HD12 | 25:BC:155:LEU:N | 2.28 | 0.48 |
| 23:BA:2272:U:C5' | 23:BA:2272:U:C6 | 2.88 | 0.48 |
| 1:CA:1315:U:H2' | 1:CA:1316:G:O4' | 2.13 | 0.48 |
| 2:CB:91:PRO:CB | 2:CB:154:LEU:HD11 | 2.44 | 0.48 |
| 23:BA:1188:U:C2' | 23:BA:1189:A:C5' | 2.91 | 0.48 |
| 40:BR:77:ALA:O | 40:BR:79:VAL:N | 2.46 | 0.48 |
| 42:DT:49:VAL:HG21 | 42:DT:83:VAL:CG1 | 2.42 | 0.48 |
| 48:DZ:52:HIS:HD2 | 48:DZ:52:HIS:H | 1.58 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:DB:7:G:H1' | 37:DO:38:GLN:HE21 | 1.78 | 0.48 |
| 1:AA:406:G:H2' | 1:AA:407:G:H8 | 1.78 | 0.48 |
| 23:DA:973:A:O4' | 23:DA:1188:U:C6 | 2.66 | 0.48 |
| 28:BF:128:ARG:HH21 | 28:BF:129:GLY:C | 2.16 | 0.48 |
| 26:BD:61:ARG:HB3 | 26:BD:62:PRO:HD2 | 1.95 | 0.48 |
| 3:CC:91:LEU:CD1 | 3:CC:101:LEU:HD21 | 2.43 | 0.48 |
| 14:CN:37:PHE:CE1 | 14:CN:53:LEU:HD13 | 2.49 | 0.48 |
| 36:DN:10:LEU:HB3 | 36:DN:17:ARG:CZ | 2.42 | 0.48 |
| 23:DA:1327:C:H2' | 23:DA:1328:G:O4' | 2.14 | 0.48 |
| 6:CF:90:VAL:O | 6:CF:91:VAL:HG23 | 2.12 | 0.48 |
| 48:BZ:26:LEU:HB2 | 48:BZ:28:LEU:CD1 | 2.43 | 0.48 |
| 36:DN:55:ALA:O | 36:DN:57:ARG:O | 2.32 | 0.48 |
| 30:BH:132:PRO:O | 30:BH:134:PRO:HD3 | 2.12 | 0.48 |
| 26:BD:111:ARG:CD | 26:BD:160:TYR:CE1 | 2.92 | 0.48 |
| 23:BA:2893:G:H3' | 23:BA:2894:G:H5' | 1.95 | 0.48 |
| 23:BA:2396:G:N3 | 23:BA:2421:G:C2 | 2.81 | 0.48 |
| 23:DA:1505:C:H2' | 23:DA:1506:C:C6 | 2.49 | 0.48 |
| 11:CK:34:ASP:HB2 | 11:CK:35:PRO:HD2 | 1.95 | 0.48 |
| 44:BV:151:HIS:O | 44:BV:171:ILE:HG12 | 2.14 | 0.48 |
| 18:AR:56:THR:O | 18:AR:58:LEU:N | 2.46 | 0.48 |
| 23:DA:105:C:C2 | 23:DA:106:C:C5 | 3.02 | 0.48 |
| 10:AJ:34:VAL:CG1 | 10:AJ:74:ILE:HG22 | 2.43 | 0.48 |
| 25:BC:267:SER:C | 25:BC:269:PHE:H | 2.17 | 0.48 |
| 17:CQ:69:LYS:C | 17:CQ:70:ARG:HD2 | 2.32 | 0.48 |
| 24:BB:78:A:N3 | 24:BB:99:A:C5 | 2.81 | 0.48 |
| 1:AA:976:G:H5'' | 1:AA:1358:U:O2' | 2.14 | 0.48 |
| 23:BA:1386:C:H2' | 23:BA:1387:C:C6 | 2.43 | 0.48 |
| 44:DV:4:ARG:HD3 | 44:DV:60:GLU:HG3 | 1.94 | 0.48 |
| 23:BA:814:C:O2' | 23:BA:815:C:H5' | 2.13 | 0.48 |
| 23:DA:2638:G:P | 26:DD:82:ARG:HH22 | 2.36 | 0.48 |
| 23:BA:637:A:OP1 | 34:BL:133:SER:HB3 | 2.13 | 0.48 |
| 23:DA:2663:G:C5 | 23:DA:2664:G:C5 | 3.01 | 0.48 |
| 26:DD:4:ILE:HD11 | 26:DD:28:ALA:O | 2.13 | 0.48 |
| 53:B5:39:LYS:HA | 53:B5:42:ARG:NH1 | 2.27 | 0.48 |
| 39:BQ:62:ILE:O | 39:BQ:63:VAL:C | 2.49 | 0.48 |
| 23:DA:814:C:H2' | 23:DA:815:C:H6 | 1.78 | 0.48 |
| 3:AC:175:LEU:CD1 | 3:AC:201:TYR:CE2 | 2.96 | 0.48 |
| 23:BA:2853:C:O2' | 23:BA:2854:G:H5' | 2.13 | 0.48 |
| 23:BA:2190:G:H2' | 23:BA:2191:G:C8 | 2.45 | 0.48 |
| 23:BA:2465:C:O2 | 23:BA:2486:G:C2 | 2.66 | 0.48 |
| 1:AA:152:A:H62 | 1:AA:169:C:H42 | 1.61 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:DO:93:LYS:O | 37:DO:93:LYS:HG3 | 2.13 | 0.48 |
| 24:BB:56:G:H4' | 24:BB:57:A:H8 | 1.79 | 0.48 |
| 1:CA:112:G:C2 | 1:CA:113:G:C8 | 3.01 | 0.48 |
| 8:CH:50:ARG:H | 8:CH:50:ARG:CD | 2.27 | 0.48 |
| 23:BA:1015:G:O2' | 23:BA:1016:G:H5' | 2.13 | 0.48 |
| 1:AA:1502:A:C8 | 1:AA:1505:G:N2 | 2.82 | 0.48 |
| 1:CA:1048:G:OP1 | 14:CN:4:LYS:HB2 | 2.13 | 0.48 |
| 23:BA:2557:G:H2' | 23:BA:2558:C:H6 | 1.78 | 0.48 |
| 35:BM:130:LYS:HZ2 | 44:BV:80:ARG:HE | 1.60 | 0.48 |
| 23:DA:2734:A:C8 | 23:DA:2735:G:C8 | 3.01 | 0.48 |
| 35:BM:131:ILE:HG22 | 35:BM:132:VAL:N | 2.28 | 0.48 |
| 1:CA:1244:C:H2' | 1:CA:1245:A:C8 | 2.49 | 0.48 |
| 43:DU:75:ILE:HG13 | 43:DU:79:CYS:HA | 1.94 | 0.48 |
| 23:BA:725:G:C6 | 23:BA:726:G:N1 | 2.82 | 0.48 |
| 23:BA:1929:G:H5'' | 23:BA:1929:G:N3 | 2.28 | 0.48 |
| 23:BA:649:G:H2' | 23:BA:650:C:C6 | 2.48 | 0.48 |
| 23:BA:1881:C:H2' | 23:BA:1882:C:H6 | 1.78 | 0.48 |
| 32:DJ:58:ARG:O | 32:DJ:60:LYS:N | 2.46 | 0.48 |
| 23:BA:2062:A:O2' | 23:BA:2063:C:H5' | 2.13 | 0.48 |
| 27:BE:118:ALA:HB2 | 27:BE:123:LEU:HD23 | 1.96 | 0.48 |
| 23:BA:1309:G:H3' | 52:B4:9:ARG:HH12 | 1.78 | 0.48 |
| 2:AB:68:ILE:HG22 | 2:AB:70:PHE:CE1 | 2.48 | 0.48 |
| 13:AM:108:ARG:HA | 13:AM:111:LYS:HB2 | 1.93 | 0.48 |
| 23:DA:2261:C:H1' | 23:DA:2388:A:N3 | 2.28 | 0.48 |
| 1:CA:1234:C:C2' | 1:CA:1235:U:H5' | 2.43 | 0.48 |
| 38:BP:54:ARG:HA | 38:BP:59:THR:OG1 | 2.14 | 0.48 |
| 12:CL:82:VAL:CG1 | 12:CL:83:LEU:N | 2.76 | 0.48 |
| 23:DA:1900:A:C2 | 23:DA:1970:A:C5 | 3.00 | 0.48 |
| 23:BA:1122:G:N3 | 23:BA:1122:G:H2' | 2.29 | 0.48 |
| 23:BA:1141:U:OP2 | 32:BJ:86:THR:HG21 | 2.14 | 0.48 |
| 32:DJ:156:GLN:O | 32:DJ:157:ARG:HB2 | 2.13 | 0.48 |
| 23:DA:1264:G:H5' | 50:D2:11:THR:HG23 | 1.94 | 0.48 |
| 41:BS:18:ARG:HG2 | 41:BS:18:ARG:HH11 | 1.78 | 0.48 |
| 40:BR:3:ALA:HB1 | 40:BR:38:LEU:HD21 | 1.95 | 0.48 |
| 25:BC:33:LEU:H | 25:BC:33:LEU:HD23 | 1.78 | 0.48 |
| 1:AA:691:G:H2' | 1:AA:692:U:C6 | 2.49 | 0.48 |
| 25:DC:141:VAL:O | 25:DC:141:VAL:HG22 | 2.14 | 0.48 |
| 44:BV:102:LEU:HD21 | 44:BV:124:ILE:HD11 | 1.96 | 0.48 |
| 44:BV:128:VAL:CG2 | 44:BV:132:ASN:HB2 | 2.43 | 0.48 |
| 1:CA:687:A:H1' | 1:CA:688:G:OP2 | 2.13 | 0.48 |
| 23:DA:2305:A:O2' | 28:DF:136:ARG:NE | 2.46 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:BU:9:LYS:O | 43:BU:27:VAL:CG2 | 2.61 | 0.48 |
| 20:AT:12:ALA:O | 20:AT:15:ARG:HB2 | 2.13 | 0.48 |
| 1:CA:556:C:C2' | 1:CA:556:C:O2 | 2.55 | 0.48 |
| 32:DJ:59:GLY:O | 32:DJ:65:TRP:CE3 | 2.65 | 0.48 |
| 25:DC:17:THR:H | 25:DC:205:VAL:HG12 | 1.77 | 0.48 |
| 23:DA:2784:C:H2' | 23:DA:2785:C:C6 | 2.49 | 0.48 |
| 17:AQ:69:LYS:C | 17:AQ:70:ARG:HD2 | 2.34 | 0.48 |
| 24:DB:75:G:O2' | 44:DV:85:HIS:CD2 | 2.66 | 0.48 |
| 1:AA:1051:C:C4 | 1:AA:1052:U:C4 | 3.02 | 0.48 |
| 1:CA:564:C:C4 | 17:CQ:31:LEU:HD11 | 2.49 | 0.48 |
| 23:BA:442:G:C4' | 27:BE:46:ARG:HD3 | 2.44 | 0.48 |
| 1:CA:256:U:H2' | 1:CA:257:G:C8 | 2.48 | 0.48 |
| 29:BG:102:ALA:CB | 29:BG:116:GLU:HA | 2.41 | 0.48 |
| 1:CA:373:A:C2 | 1:CA:374:A:C8 | 3.01 | 0.48 |
| 12:AL:6:ILE:O | 12:AL:10:VAL:CG2 | 2.59 | 0.48 |
| 43:DU:63:LYS:HG3 | 43:DU:64:GLU:N | 2.28 | 0.48 |
| 23:BA:226:G:N2 | 23:BA:227:A:C2 | 2.82 | 0.48 |
| 1:CA:1328:C:H5'' | 13:CM:28:ALA:CB | 2.42 | 0.48 |
| 23:DA:904:C:H2' | 23:DA:905:U:C6 | 2.48 | 0.48 |
| 23:BA:2461:C:O2 | 23:BA:2461:C:C2' | 2.52 | 0.48 |
| 1:CA:464:G:O6 | 1:CA:466:G:H5' | 2.12 | 0.48 |
| 35:DM:38:GLU:HB2 | 35:DM:127:ILE:CG1 | 2.43 | 0.48 |
| 23:DA:2079:U:H2' | 23:DA:2080:G:O4' | 2.14 | 0.48 |
| 1:AA:1504:G:H4' | 1:AA:1505:G:C4 | 2.48 | 0.48 |
| 1:CA:1296:C:C5 | 1:CA:1297:C:C5 | 3.02 | 0.48 |
| 28:DF:18:GLU:HG2 | 28:DF:175:LEU:CD2 | 2.43 | 0.48 |
| 1:CA:575:G:H4' | 1:CA:575:G:OP1 | 2.13 | 0.48 |
| 23:BA:1301:A:N3 | 23:BA:1301:A:H2' | 2.28 | 0.48 |
| 48:BZ:8:LEU:HD13 | 48:BZ:31:LEU:HD12 | 1.94 | 0.48 |
| 23:BA:30:G:H2' | 23:BA:31:C:C6 | 2.49 | 0.48 |
| 23:BA:447:A:C4 | 23:BA:473:G:N7 | 2.82 | 0.48 |
| 44:BV:155:LEU:O | 44:BV:157:LEU:HD12 | 2.13 | 0.48 |
| 1:AA:772:U:C2' | 1:AA:773:G:H5' | 2.44 | 0.48 |
| 41:DS:95:ILE:O | 41:DS:95:ILE:HG13 | 2.13 | 0.48 |
| 1:CA:238:G:P | 17:CQ:25:ARG:HH22 | 2.36 | 0.48 |
| 24:DB:76:G:OP1 | 44:DV:15:PRO:HG3 | 2.13 | 0.48 |
| 23:DA:122(A):C:H2' | 23:DA:1222:C:H6 | 1.78 | 0.48 |
| 23:DA:2392:A:OP2 | 53:D5:31:HIS:HE1 | 1.95 | 0.48 |
| 47:BY:1:MET:SD | 47:BY:1:MET:O | 2.71 | 0.48 |
| 23:BA:857:C:C2 | 23:BA:858:U:C5 | 3.02 | 0.48 |
| 23:DA:328:U:H4' | 43:DU:68:HIS:CE1 | 2.48 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:BD:24:THR:HG21 | 26:BD:188:VAL:HG12 | 1.95 | 0.48 |
| 22:AV:6192:G:C6 | 22:AV:6193:U:C4 | 3.01 | 0.48 |
| 1:CA:971:G:H1' | 1:CA:1365:G:HO2' | 1.78 | 0.48 |
| 1:CA:501:C:H2' | 1:CA:502:G:C8 | 2.49 | 0.48 |
| 41:BS:14:PRO:O | 41:BS:16:LYS:N | 2.46 | 0.48 |
| 30:BH:86:THR:O | 30:BH:86:THR:HG22 | 2.14 | 0.48 |
| 4:AD:109:GLY:O | 4:AD:111:ALA:N | 2.46 | 0.48 |
| 1:CA:394:G:C2 | 1:CA:395:C:C6 | 3.01 | 0.48 |
| 3:CC:148:GLY:HA3 | 3:CC:203:PHE:HB3 | 1.94 | 0.48 |
| 30:DH:101:LEU:O | 30:DH:107:ILE:HG22 | 2.13 | 0.48 |
| 23:BA:2210:G:C3' | 23:BA:2210:G:N3 | 2.75 | 0.48 |
| 23:DA:1826:G:P | 25:DC:233:HIS:HD2 | 2.36 | 0.48 |
| 5:AE:139:LEU:C | 5:AE:141:GLN:H | 2.17 | 0.48 |
| 42:BT:35:THR:HG22 | 42:BT:36:LYS:N | 2.28 | 0.48 |
| 1:AA:878:G:C1' | 8:AH:3:THR:HG21 | 2.43 | 0.48 |
| 1:CA:42:G:N2 | 1:CA:401:C:O2 | 2.47 | 0.48 |
| 1:CA:408:A:C2 | 1:CA:409:G:C4 | 3.02 | 0.48 |
| 1:CA:409:G:C2' | 1:CA:410:G:O5' | 2.61 | 0.48 |
| 29:DG:23:ARG:H | 29:DG:23:ARG:HD3 | 1.78 | 0.48 |
| 23:DA:2307:G:O5' | 23:DA:2307:G:C8 | 2.67 | 0.48 |
| 1:CA:487:A:H2' | 1:CA:488:C:O4' | 2.13 | 0.48 |
| 1:CA:706:A:O4' | 11:CK:29:ILE:HD11 | 2.14 | 0.48 |
| 15:CO:29:VAL:HG12 | 15:CO:85:LEU:CD1 | 2.42 | 0.48 |
| 1:AA:66:G:H5' | 1:AA:173:U:O4 | 2.13 | 0.48 |
| 25:DC:15:PHE:O | 25:DC:205:VAL:CG1 | 2.62 | 0.48 |
| 34:DL:13:ASN:O | 34:DL:14:LYS:C | 2.51 | 0.48 |
| 23:DA:260:G:C6 | 23:DA:261:G:C8 | 3.02 | 0.48 |
| 29:DG:87:LEU:CD2 | 29:DG:164:TYR:HD1 | 2.25 | 0.48 |
| 1:CA:832:C:N4 | 1:CA:854:G:H1 | 2.05 | 0.48 |
| 44:BV:58:VAL:HG11 | 44:BV:66:SER:HB2 | 1.95 | 0.48 |
| 1:AA:401:C:C6 | 1:AA:401:C:H3' | 2.48 | 0.48 |
| 44:DV:179:ASP:CG | 44:DV:180:VAL:N | 2.66 | 0.48 |
| 25:DC:79:VAL:HG11 | 25:DC:111:LEU:CD1 | 2.43 | 0.48 |
| 50:B2:35:GLU:OE2 | 50:B2:51:TYR:HA | 2.12 | 0.48 |
| 1:AA:236:G:H1' | 17:AQ:4:LYS:HE3 | 1.95 | 0.48 |
| 23:DA:2636:U:H4' | 26:DD:80:GLU:OE1 | 2.14 | 0.48 |
| 1:CA:1423:G:H5'' | 33:DK:49:ARG:NH2 | 2.27 | 0.48 |
| 23:DA:2094:G:C2 | 23:DA:2196:C:C2 | 3.02 | 0.48 |
| 1:AA:1298:C:C5 | 7:AG:114:ARG:NH1 | 2.80 | 0.48 |
| 1:AA:1088:G:C5 | 1:AA:1089:G:N7 | 2.82 | 0.48 |
| 44:DV:5:LEU:CG | 44:DV:47:VAL:HG21 | 2.42 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BA:566:U:H2' | 23:BA:567:A:O4' | 2.14 | 0.48 |
| 1:AA:444:C:H2' | 1:AA:445:G:C8 | 2.49 | 0.48 |
| 23:DA:693:C:H2' | 23:DA:694:U:H6 | 1.77 | 0.48 |
| 7:AG:30:ILE:HD13 | 7:AG:105:VAL:HG13 | 1.94 | 0.48 |
| 16:AP:12:LYS:O | 16:AP:13:HIS:HB2 | 2.11 | 0.48 |
| 23:DA:1773:A:N7 | 23:DA:1829:A:H1' | 2.28 | 0.48 |
| 23:DA:914:C:C5 | 23:DA:915:C:C6 | 3.02 | 0.48 |
| 38:BP:80:SER:C | 38:BP:82:LEU:N | 2.67 | 0.48 |
| 1:AA:356:A:H2' | 1:AA:357:G:C8 | 2.48 | 0.48 |
| 23:BA:176:G:O2' | 23:BA:177:G:H5' | 2.14 | 0.48 |
| 11:CK:120:ARG:NH1 | 11:CK:126:ARG:HE | 2.11 | 0.48 |
| 1:AA:515:G:N2 | 1:AA:537:G:C4 | 2.82 | 0.48 |
| 1:AA:760:G:H2' | 1:AA:761:G:H5' | 1.96 | 0.48 |
| 26:DD:3:GLY:HA3 | 26:DD:81:ILE:HD13 | 1.95 | 0.48 |
| 1:CA:698:G:C6 | 1:CA:699:C:C4 | 3.02 | 0.48 |
| 23:DA:2025:C:H2' | 23:DA:2026:C:C6 | 2.48 | 0.48 |
| 23:DA:1929:G:H5'' | 23:DA:1929:G:N3 | 2.29 | 0.48 |
| 1:AA:779:C:H2' | 1:AA:780:A:O4' | 2.13 | 0.48 |
| 7:CG:77:SER:HA | 7:CG:85:TYR:O | 2.14 | 0.48 |
| 3:AC:6:HIS:HD2 | 3:AC:7:PRO:HD2 | 1.78 | 0.48 |
| 1:AA:597:G:C8 | 1:AA:598:U:C5 | 3.02 | 0.48 |
| 39:DQ:53:ARG:O | 39:DQ:56:ASP:HB2 | 2.14 | 0.48 |
| 36:DN:96:ARG:HD3 | 36:DN:98:LEU:HD21 | 1.95 | 0.48 |
| 28:BF:74:LYS:HA | 28:BF:74:LYS:HE3 | 1.95 | 0.48 |
| 23:BA:1582:C:O5' | 23:BA:1582:C:H6 | 1.97 | 0.48 |
| 23:BA:247:G:H4' | 23:BA:386:G:C5 | 2.49 | 0.48 |
| 23:BA:343:C:O2' | 23:BA:344:G:H5' | 2.14 | 0.48 |
| 1:CA:1351:U:H4' | 7:CG:33:ASP:OD2 | 2.13 | 0.48 |
| 12:CL:31:PHE:CB | 12:CL:83:LEU:HD11 | 2.43 | 0.48 |
| 23:BA:1188:U:H2' | 23:BA:1189:A:O5' | 2.13 | 0.48 |
| 32:DJ:38:LEU:C | 32:DJ:39:ILE:HG12 | 2.33 | 0.48 |
| 32:DJ:116:THR:OG1 | 32:DJ:117:HIS:N | 2.46 | 0.48 |
| 1:CA:386:C:H2' | 1:CA:387:U:O4' | 2.14 | 0.48 |
| 1:CA:672:U:O2' | 1:CA:673:G:H5' | 2.14 | 0.48 |
| 34:BL:50:ARG:HD2 | 34:BL:51:PHE:CA | 2.44 | 0.48 |
| 23:DA:2334:G:C4 | 37:DO:12:PHE:HZ | 2.32 | 0.48 |
| 8:AH:120:THR:H | 8:AH:123:GLU:HB2 | 1.78 | 0.48 |
| 1:AA:76:G:C6 | 1:AA:95:G:N1 | 2.82 | 0.48 |
| 44:BV:30:ASN:HA | 44:BV:89:PHE:HE2 | 1.78 | 0.48 |
| 5:AE:91:LEU:HD22 | 5:AE:110:LEU:HD11 | 1.95 | 0.48 |
| 23:DA:1313:U:H4' | 23:DA:1332:G:H4' | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:BA:71:A:OP2 | 23:BA:113:G:H5' | 2.14 | 0.48 |
| 23:BA:2516:G:C6 | 23:BA:2517:C:N4 | 2.81 | 0.48 |
| 1:CA:403:C:O2' | 1:CA:404:U:H5' | 2.13 | 0.48 |
| 1:CA:438:G:H4' | 4:CD:123:HIS:ND1 | 2.28 | 0.48 |
| 46:BX:10:LYS:O | 46:BX:11:ARG:CG | 2.61 | 0.48 |
| 29:BG:46:GLU:HG3 | 29:BG:51:ARG:CZ | 2.43 | 0.48 |
| 23:BA:1503:U:H2' | 23:BA:1504:C:C6 | 2.49 | 0.48 |
| 23:BA:2277:G:C5' | 35:BM:85:LYS:HB2 | 2.43 | 0.48 |
| 1:AA:175:C:H4' | 20:AT:25:ARG:NH1 | 2.29 | 0.48 |
| 3:CC:68:VAL:HG12 | 3:CC:70:VAL:HG23 | 1.95 | 0.48 |
| 36:BN:72:ASP:O | 36:BN:76:VAL:HG13 | 2.13 | 0.48 |
| 25:BC:30:GLU:CG | 25:BC:63:ARG:NH2 | 2.77 | 0.48 |
| 23:BA:2631:G:N3 | 23:BA:2810:A:C2 | 2.77 | 0.48 |
| 23:BA:795:C:H6 | 23:BA:795:C:O5' | 1.97 | 0.48 |
| 23:DA:1412:A:H2' | 23:DA:1413:G:O4' | 2.14 | 0.48 |
| 8:AH:97:VAL:CG1 | 8:AH:98:LYS:H | 2.24 | 0.48 |
| 33:DK:32:TYR:N | 33:DK:32:TYR:CD1 | 2.80 | 0.48 |
| 43:DU:6:HIS:CD2 | 43:DU:35:TYR:CE1 | 2.97 | 0.48 |
| 23:BA:1152:C:O2' | 23:BA:1153:C:H5' | 2.14 | 0.48 |
| 18:AR:45:SER:H | 18:AR:51:LEU:CD1 | 2.26 | 0.48 |
| 18:AR:66:LEU:CG | 18:AR:70:ILE:HD11 | 2.44 | 0.48 |
| 35:DM:134:ARG:HA | 35:DM:134:ARG:HE | 1.78 | 0.48 |
| 23:BA:739:G:H4' | 23:BA:740:U:OP1 | 2.14 | 0.48 |
| 23:BA:2190:G:C4 | 23:BA:2191:G:C8 | 3.02 | 0.48 |
| 23:BA:2739:U:C2' | 23:BA:2739:U:O2 | 2.54 | 0.48 |
| 1:CA:1160:G:C6 | 1:CA:1181:G:O6 | 2.66 | 0.48 |
| 25:BC:122:ASP:CG | 25:BC:123:ALA:N | 2.67 | 0.48 |
| 17:CQ:99:SER:O | 17:CQ:100:LYS:HD3 | 2.14 | 0.48 |
| 1:AA:294:U:H2' | 1:AA:295:C:C6 | 2.49 | 0.48 |
| 23:DA:618(A):G:H2' | 23:DA:618(B):C:H6 | 1.77 | 0.48 |
| 1:CA:451:A:N7 | 1:CA:481:G:C6 | 2.82 | 0.48 |
| 38:DP:34:VAL:HG21 | 38:DP:43:GLN:HB2 | 1.96 | 0.48 |
| 1:CA:1452:C:H1' | 1:CA:1453:G:N2 | 2.29 | 0.48 |
| 1:AA:142:G:N2 | 1:AA:143:A:C4 | 2.81 | 0.48 |
| 23:DA:312:G:H2' | 23:DA:312:G:N3 | 2.29 | 0.48 |
| 23:BA:861:A:C2 | 23:BA:917:A:C4 | 3.01 | 0.48 |
| 21:AU:14:TRP:HE3 | 21:AU:15:ARG:HG2 | 1.78 | 0.48 |
| 22:AV:6182:A:C2 | 22:AV:6195:G:N2 | 2.82 | 0.48 |
| 22:CV:6189:G:N2 | 22:CV:6215:C:C2 | 2.81 | 0.48 |
| 22:CV:6213:A:C4 | 22:CV:6214:C:C5 | 3.01 | 0.48 |
| 13:CM:105:THR:O | 13:CM:106:ASN:O | 2.30 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 42:BT:12:VAL:HG12 | 42:BT:28:PHE:HA | 1.95 | 0.48 |
| 23:BA:2728:U:H2' | 23:BA:2728:U:O2 | 2.13 | 0.48 |
| 23:BA:2729:G:H1' | 26:BD:187:ALA:CB | 2.31 | 0.48 |
| 23:BA:194:G:H2' | 23:BA:195:A:O4' | 2.13 | 0.48 |
| 26:BD:36:ARG:NH1 | 26:BD:86:PRO:HD2 | 2.28 | 0.48 |
| 23:DA:1188:U:H2' | 23:DA:1189:A:C5' | 2.44 | 0.48 |
| 49:D1:50:THR:HG22 | 49:D1:51:TYR:N | 2.26 | 0.48 |
| 23:BA:1407:C:H2' | 23:BA:1408:C:H6 | 1.77 | 0.48 |
| 23:BA:141(A):A:N6 | 23:BA:1596:A:H5' | 2.29 | 0.48 |
| 23:DA:1826:G:OP1 | 25:DC:233:HIS:CD2 | 2.59 | 0.48 |
| 23:DA:1827:C:C2' | 23:DA:1828:G:H5' | 2.44 | 0.48 |
| 1:AA:76:G:C6 | 1:AA:77:C:N4 | 2.82 | 0.48 |
| 26:BD:51:PHE:CD1 | 26:BD:51:PHE:C | 2.86 | 0.48 |
| 28:BF:8:LYS:HD3 | 28:BF:9:ARG:CG | 2.44 | 0.48 |
| 36:BN:17:ARG:O | 36:BN:20:LEU:HB3 | 2.14 | 0.48 |
| 1:AA:9:G:H5'' | 5:AE:122:GLU:OE1 | 2.13 | 0.48 |
| 12:CL:44:PRO:HG3 | 12:CL:52:ARG:HD3 | 1.93 | 0.48 |
| 1:AA:1294:G:H2' | 1:AA:1295:G:H8 | 1.74 | 0.48 |
| 41:BS:29:LEU:HD22 | 41:BS:69:LEU:HD11 | 1.96 | 0.48 |
| 46:BX:46:LEU:HD23 | 46:BX:46:LEU:C | 2.34 | 0.48 |
| 23:DA:1104:C:C4 | 23:DA:1105:U:C5 | 3.01 | 0.48 |
| 53:B5:21:LYS:HA | 53:B5:54:GLU:OE2 | 2.14 | 0.48 |
| 6:CF:78:GLU:HA | 6:CF:81:ILE:CD1 | 2.44 | 0.48 |
| 30:DH:4:ILE:HA | 30:DH:17:GLN:O | 2.13 | 0.48 |
| 29:BG:29:PRO:HD2 | 29:BG:79:VAL:O | 2.13 | 0.48 |
| 25:BC:182:LEU:HA | 25:BC:182:LEU:HD23 | 1.55 | 0.48 |
| 15:CO:39:LEU:CD1 | 15:CO:56:LEU:HB2 | 2.44 | 0.48 |
| 50:D2:40:LYS:HD3 | 50:D2:46:CYS:HB3 | 1.95 | 0.48 |
| 1:CA:1058:G:C6 | 1:CA:1059:C:N3 | 2.81 | 0.48 |
| 35:DM:21:THR:C | 35:DM:23:GLY:N | 2.67 | 0.48 |
| 1:CA:1056:U:O2 | 1:CA:1056:U:H2' | 2.13 | 0.48 |
| 1:CA:1443:G:N2 | 38:DP:119:LYS:CA | 2.74 | 0.48 |
| 45:BW:37:LEU:HG | 45:BW:60:PHE:HA | 1.96 | 0.48 |
| 23:DA:118:A:C8 | 23:DA:119:A:C8 | 3.02 | 0.48 |
| 8:AH:36:LEU:HA | 8:AH:39:LEU:HD23 | 1.95 | 0.48 |
| 36:BN:85:PRO:HA | 36:BN:88:ARG:HH11 | 1.78 | 0.48 |
| 24:DB:30:C:H1' | 24:DB:58:A:N1 | 2.28 | 0.48 |
| 1:CA:754:C:C2' | 1:CA:755:G:OP1 | 2.62 | 0.48 |
| 25:DC:94:LEU:HD22 | 25:DC:94:LEU:C | 2.34 | 0.48 |
| 23:DA:641:C:O2' | 23:DA:2350:C:OP1 | 2.28 | 0.48 |
| 1:CA:1327:C:O2' | 1:CA:1328:C:H5' | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:1379:G:O2' | 1:AA:1380:U:H5' | 2.13 | 0.48 |
| 7:CG:69:VAL:HG22 | 7:CG:135:VAL:HG22 | 1.95 | 0.48 |
| 35:BM:70:PRO:HA | 35:BM:94:VAL:O | 2.14 | 0.48 |
| 26:BD:176:ILE:N | 26:BD:176:ILE:CD1 | 2.76 | 0.48 |
| 1:CA:806:C:O2 | 1:CA:807:A:C8 | 2.67 | 0.48 |
| 23:BA:1917:U:O2' | 23:BA:1918:A:H5' | 2.13 | 0.48 |
| 1:AA:178:C:C2' | 1:AA:179:A:H5' | 2.44 | 0.48 |
| 1:CA:114:U:H2' | 1:CA:115:G:H8 | 1.79 | 0.48 |
| 23:DA:1336:A:H2' | 23:DA:1337:G:C8 | 2.49 | 0.48 |
| 1:CA:1047:G:O2' | 1:CA:1048:G:H5' | 2.14 | 0.48 |
| 23:DA:531:C:H4' | 23:DA:532:A:H5'' | 1.94 | 0.48 |
| 37:DO:20:ARG:HH12 | 45:DW:48:GLY:H | 1.61 | 0.48 |
| 1:CA:1415:G:O2' | 1:CA:1416:G:H5' | 2.14 | 0.48 |
| 23:DA:220:G:N1 | 23:DA:428:A:OP2 | 2.32 | 0.48 |
| 31:BI:57:THR:HG23 | 31:BI:60:ARG:HH12 | 1.77 | 0.48 |
| 3:CC:6:HIS:HD2 | 3:CC:7:PRO:HD2 | 1.79 | 0.48 |
| 23:DA:1839:G:C8 | 23:DA:1927:A:H1' | 2.48 | 0.48 |
| 23:BA:1523:U:H2' | 23:BA:1524:G:H8 | 1.77 | 0.48 |
| 34:BL:61:ARG:HD3 | 53:B5:13:ARG:HD2 | 1.96 | 0.48 |
| 23:DA:1174:A:H3' | 23:DA:1175:U:C5' | 2.17 | 0.48 |
| 1:AA:977:A:HO2' | 1:AA:978:A:H5'' | 1.78 | 0.48 |
| 1:AA:972:C:H4' | 10:AJ:57:LYS:HG3 | 1.96 | 0.48 |
| 34:BL:32:THR:HG21 | 34:BL:37:GLY:HA2 | 1.94 | 0.48 |
| 22:CV:6182:A:C6 | 22:CV:6195:G:N1 | 2.82 | 0.48 |
| 38:DP:58:ASN:C | 38:DP:58:ASN:HD22 | 2.17 | 0.48 |
| 1:AA:954:G:H2' | 1:AA:955:U:C6 | 2.48 | 0.48 |
| 32:BJ:157:ARG:O | 32:BJ:158:PRO:C | 2.51 | 0.48 |
| 39:DQ:72:HIS:HE1 | 39:DQ:107:ALA:HA | 1.77 | 0.48 |
| 39:DQ:106:PHE:O | 39:DQ:109:LEU:N | 2.47 | 0.48 |
| 34:DL:41:ARG:HA | 34:DL:41:ARG:HD2 | 1.56 | 0.48 |
| 42:BT:44:GLU:HG2 | 42:BT:49:VAL:O | 2.14 | 0.48 |
| 41:DS:14:PRO:C | 41:DS:16:LYS:H | 2.16 | 0.48 |
| 39:BQ:106:PHE:O | 39:BQ:109:LEU:N | 2.46 | 0.48 |
| 28:DF:161:THR:C | 28:DF:163:ALA:N | 2.67 | 0.48 |
| 23:DA:1812:A:H2' | 23:DA:1813:G:H5' | 1.95 | 0.48 |
| 47:BY:24:LEU:HD22 | 47:BY:60:LEU:CD1 | 2.43 | 0.48 |
| 25:BC:45:ASN:OD1 | 25:BC:45:ASN:C | 2.50 | 0.48 |
| 30:DH:130:TYR:C | 30:DH:132:PRO:HD3 | 2.34 | 0.48 |
| 1:AA:391:G:C6 | 1:AA:392:G:N7 | 2.81 | 0.48 |
| 23:BA:1639:U:H4' | 23:BA:2699:C:H4' | 1.94 | 0.48 |
| 44:BV:126:VAL:HG12 | 44:BV:163:LEU:HA | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:DD:5:LEU:C | 26:DD:51:PHE:HE2 | 2.17 | 0.48 |
| 2:AB:167:PRO:HG3 | 2:AB:188:ALA:HB2 | 1.94 | 0.48 |
| 23:BA:2352:A:C4 | 23:BA:2366:A:C2 | 3.02 | 0.48 |
| 1:AA:1152:A:C4 | 1:AA:1153:C:C5 | 3.02 | 0.48 |
| 25:DC:172:TYR:CE1 | 25:DC:186:HIS:HA | 2.49 | 0.48 |
| 6:AF:35:ALA:O | 6:AF:37:VAL:N | 2.47 | 0.48 |
| 18:AR:38:GLU:HA | 18:AR:38:GLU:OE2 | 2.13 | 0.48 |
| 23:DA:1486:A:C6 | 23:DA:1504:C:N4 | 2.80 | 0.48 |
| 23:DA:528:A:N1 | 23:DA:2043:C:O5' | 2.47 | 0.48 |
| 34:BL:18:ARG:C | 34:BL:19:VAL:HG22 | 2.33 | 0.48 |
| 1:CA:324:G:OP1 | 20:CT:70:SER:CB | 2.61 | 0.48 |
| 1:AA:29:G:C2 | 1:AA:555:C:N3 | 2.82 | 0.48 |
| 39:DQ:62:ILE:HD12 | 39:DQ:76:TYR:CE1 | 2.49 | 0.48 |
| 1:CA:173:U:N1 | 1:CA:197:A:C2 | 2.82 | 0.48 |
| 23:BA:1799:G:H8 | 25:BC:181:GLU:CD | 2.16 | 0.48 |
| 1:CA:235:C:H2' | 1:CA:236:G:H8 | 1.77 | 0.48 |
| 24:BB:78:A:H61 | 24:BB:98:G:H1' | 1.79 | 0.48 |
| 24:BB:75:G:HO2' | 44:BV:85:HIS:CD2 | 2.31 | 0.48 |
| 44:BV:82:ARG:HG2 | 44:BV:83:PRO:HD2 | 1.96 | 0.48 |
| 23:BA:2470:G:C6 | 23:BA:2471:C:C5 | 3.02 | 0.48 |
| 39:DQ:25:TRP:C | 39:DQ:25:TRP:CD1 | 2.87 | 0.48 |
| 18:CR:66:LEU:CG | 18:CR:70:ILE:HD11 | 2.43 | 0.48 |
| 23:BA:2549:G:C2' | 23:BA:2550:G:H5' | 2.43 | 0.48 |
| 23:BA:1467:C:C2' | 23:BA:1468:C:H5' | 2.43 | 0.48 |
| 1:AA:1195:C:H5'' | 1:AA:1196:U:OP2 | 2.14 | 0.48 |
| 23:BA:1909:C:C2 | 23:BA:1922:G:C2 | 3.01 | 0.48 |
| 34:DL:27:HIS:CD2 | 34:DL:27:HIS:C | 2.86 | 0.48 |
| 23:DA:1862:G:C2 | 23:DA:1863:G:C5 | 3.01 | 0.48 |
| 1:AA:109:A:C6 | 1:AA:326:G:C6 | 3.02 | 0.48 |
| 1:CA:300:A:H2' | 1:CA:301:G:H5' | 1.96 | 0.48 |
| 7:CG:46:ALA:O | 7:CG:50:ILE:HG12 | 2.14 | 0.48 |
| 36:BN:84:ALA:HB3 | 36:BN:85:PRO:HD3 | 1.94 | 0.48 |
| 8:CH:36:LEU:HA | 8:CH:39:LEU:HD23 | 1.96 | 0.48 |
| 20:CT:84:LEU:HD13 | 20:CT:85:MET:N | 2.28 | 0.48 |
| 23:DA:151:C:C2 | 23:DA:176:G:N2 | 2.81 | 0.48 |
| 1:CA:1182:G:H4' | 1:CA:1183:A:C5' | 2.44 | 0.48 |
| 23:BA:2717:G:C6 | 23:BA:2718:G:C5 | 3.02 | 0.48 |
| 10:CJ:98:ILE:O | 10:CJ:99:LYS:HD3 | 2.13 | 0.48 |
| 23:DA:2297:C:H2' | 23:DA:2298:A:H8 | 1.78 | 0.48 |
| 28:DF:62:LEU:HB3 | 28:DF:143:GLU:HG3 | 1.96 | 0.48 |
| 1:CA:826:C:C2' | 8:CH:15:ASN:HD22 | 2.25 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BA:415:A:H2' | 23:BA:416:C:C6 | 2.48 | 0.48 |
| 25:BC:52:ARG:CB | 25:BC:53:PHE:CD2 | 2.97 | 0.48 |
| 23:DA:533:G:N3 | 39:DQ:45:TYR:HE1 | 2.11 | 0.48 |
| 2:AB:76:GLN:H | 2:AB:76:GLN:NE2 | 2.12 | 0.48 |
| 17:AQ:11:VAL:N | 17:AQ:20:THR:O | 2.45 | 0.48 |
| 44:DV:63:ASP:C | 44:DV:65:GLN:H | 2.16 | 0.48 |
| 23:BA:516:C:P | 50:B2:13:LYS:HZ1 | 2.37 | 0.48 |
| 5:AE:20:GLN:O | 5:AE:23:GLY:O | 2.31 | 0.48 |
| 1:CA:35:G:C2 | 1:CA:550:G:C2 | 3.01 | 0.48 |
| 23:BA:2410:G:H2' | 23:BA:2411:A:O4' | 2.14 | 0.48 |
| 4:AD:199:ASN:ND2 | 4:AD:202:LEU:HG | 2.28 | 0.48 |
| 23:DA:1583:A:O5' | 23:DA:1583:A:H8 | 1.97 | 0.48 |
| 34:DL:59:LEU:N | 34:DL:61:ARG:HE | 2.11 | 0.48 |
| 34:DL:64:LYS:HB2 | 53:D5:25:MET:HG3 | 1.95 | 0.48 |
| 26:BD:104:VAL:HG11 | 26:BD:188:VAL:HG21 | 1.96 | 0.48 |
| 23:BA:2292:C:N4 | 23:BA:2293:C:N4 | 2.62 | 0.48 |
| 34:DL:32:THR:CG2 | 34:DL:37:GLY:H | 2.27 | 0.48 |
| 35:DM:75:THR:C | 35:DM:88:GLY:HA2 | 2.34 | 0.48 |
| 32:DJ:95:TYR:CD2 | 32:DJ:113:MET:HG3 | 2.48 | 0.48 |
| 3:AC:19:GLU:HG2 | 3:AC:40:ARG:NH2 | 2.28 | 0.48 |
| 23:DA:2730:C:C2' | 23:DA:2731:G:H5' | 2.43 | 0.48 |
| 25:DC:108:PRO:CB | 25:DC:143:HIS:HE1 | 2.26 | 0.48 |
| 23:BA:1593:G:C6 | 23:BA:1594:G:C6 | 3.02 | 0.48 |
| 23:DA:1786:A:H2 | 23:DA:2606:C:H1' | 1.78 | 0.48 |
| 5:CE:61:TYR:HA | 5:CE:64:ARG:HB3 | 1.95 | 0.48 |
| 23:DA:2687:U:N3 | 23:DA:2688:U:C6 | 2.82 | 0.48 |
| 1:CA:669:U:C2 | 1:CA:670:G:C8 | 3.02 | 0.48 |
| 23:DA:2516:G:C6 | 23:DA:2517:C:N4 | 2.82 | 0.48 |
| 1:AA:15:G:H4' | 5:AE:24:ARG:NH1 | 2.27 | 0.48 |
| 23:BA:849:A:H5'' | 23:BA:850:C:OP2 | 2.13 | 0.48 |
| 1:AA:1366:C:C4 | 1:AA:1367:C:N4 | 2.82 | 0.48 |
| 36:DN:48:VAL:HA | 36:DN:51:LEU:HD12 | 1.94 | 0.48 |
| 23:BA:528:A:O2' | 23:BA:529:A:H5' | 2.13 | 0.48 |
| 18:AR:37:VAL:HG12 | 18:AR:78:LEU:HB3 | 1.95 | 0.48 |
| 23:DA:1496:A:C8 | 23:DA:1577:C:O2' | 2.67 | 0.48 |
| 1:AA:1529:G:H4' | 1:AA:1530:G:OP2 | 2.12 | 0.48 |
| 23:DA:2893:G:H5'' | 23:DA:2894:G:O4' | 2.13 | 0.48 |
| 8:CH:119:LEU:HD12 | 8:CH:124:ALA:HA | 1.94 | 0.48 |
| 30:BH:15:VAL:C | 30:BH:17:GLN:H | 2.17 | 0.48 |
| 4:AD:79:PHE:CE1 | 4:AD:204:ILE:HA | 2.48 | 0.48 |
| 1:CA:1128:C:O2' | 1:CA:1130:A:C4 | 2.65 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:1064:G:C1' | 1:CA:1065:U:OP2 | 2.59 | 0.48 |
| 11:AK:34:ASP:CB | 11:AK:35:PRO:CD | 2.92 | 0.48 |
| 34:BL:27:HIS:C | 34:BL:27:HIS:CD2 | 2.87 | 0.48 |
| 21:CU:14:TRP:HE3 | 21:CU:15:ARG:HG2 | 1.78 | 0.48 |
| 1:AA:1056:U:H2' | 1:AA:1056:U:O2 | 2.14 | 0.48 |
| 1:AA:934:C:C5 | 1:AA:1345:U:C6 | 3.02 | 0.48 |
| 1:AA:939:G:N1 | 1:AA:940:C:N4 | 2.62 | 0.48 |
| 23:DA:1871:A:O2' | 23:DA:1872:A:H5' | 2.14 | 0.48 |
| 36:BN:52:ILE:CG2 | 36:BN:94:TYR:CG | 2.97 | 0.48 |
| 1:AA:730:G:C5 | 1:AA:731:G:H1' | 2.49 | 0.48 |
| 13:AM:24:GLY:O | 13:AM:25:ILE:HD13 | 2.13 | 0.48 |
| 6:CF:12:PRO:HD3 | 6:CF:58:GLY:HA2 | 1.95 | 0.48 |
| 23:DA:1909:C:C2 | 23:DA:1922:G:C2 | 3.02 | 0.48 |
| 1:CA:300:A:C3' | 1:CA:300:A:C8 | 2.96 | 0.48 |
| 23:DA:442:G:C4' | 27:DE:46:ARG:HD3 | 2.43 | 0.48 |
| 7:AG:17:VAL:HG21 | 7:AG:44:TYR:CE2 | 2.48 | 0.48 |
| 23:BA:2394:C:P | 34:BL:63:PRO:HD2 | 2.54 | 0.48 |
| 44:BV:9:TYR:CG | 44:BV:35:ARG:NH1 | 2.82 | 0.48 |
| 7:AG:69:VAL:HG22 | 7:AG:135:VAL:HG22 | 1.96 | 0.48 |
| 23:DA:2853:C:O2' | 23:DA:2854:G:H5' | 2.14 | 0.48 |
| 1:CA:464:G:C6 | 1:CA:466:G:H5' | 2.49 | 0.48 |
| 38:DP:80:SER:C | 38:DP:82:LEU:N | 2.66 | 0.48 |
| 42:DT:40:LYS:C | 42:DT:42:ALA:N | 2.67 | 0.48 |
| 1:AA:357:G:C2 | 1:AA:358:U:C5 | 3.02 | 0.48 |
| 19:CS:40:ILE:HG13 | 19:CS:69:HIS:O | 2.14 | 0.48 |
| 23:DA:2506:U:OP2 | 23:DA:2576:G:N1 | 2.31 | 0.48 |
| 1:AA:380:G:N1 | 1:AA:384:G:C6 | 2.82 | 0.48 |
| 6:CF:97:PHE:HD2 | 18:CR:31:LEU:HD21 | 1.79 | 0.48 |
| 8:AH:54:ASP:C | 8:AH:56:LYS:H | 2.17 | 0.48 |
| 39:DQ:27:LEU:HD23 | 39:DQ:27:LEU:O | 2.14 | 0.48 |
| 23:DA:30:G:C5 | 23:DA:31:C:C4 | 3.00 | 0.48 |
| 1:CA:958:A:N6 | 1:CA:959:A:N6 | 2.62 | 0.48 |
| 38:BP:105:LEU:O | 38:BP:107:ASP:CG | 2.52 | 0.48 |
| 1:AA:525:C:O2' | 1:AA:526:C:H5' | 2.14 | 0.48 |
| 23:DA:1678:G:N3 | 23:DA:1678:G:H2' | 2.29 | 0.48 |
| 27:BE:126:VAL:O | 27:BE:196:LEU:HG | 2.13 | 0.48 |
| 14:AN:45:ARG:O | 14:AN:49:HIS:CD2 | 2.67 | 0.48 |
| 44:BV:165:VAL:HG23 | 44:BV:166:SER:O | 2.13 | 0.48 |
| 1:AA:1401:G:C2 | 1:AA:1402:C:H1' | 2.49 | 0.48 |
| 23:BA:685:A:H1' | 23:BA:688:U:O4 | 2.14 | 0.48 |
| 36:BN:28:LEU:HA | 36:BN:28:LEU:HD23 | 1.69 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:BD:3:GLY:HA3 | 26:BD:81:ILE:HD13 | 1.96 | 0.48 |
| 15:CO:3:ILE:HA | 15:CO:38:ARG:NH2 | 2.29 | 0.48 |
| 1:AA:1244:C:H2' | 1:AA:1245:A:C8 | 2.49 | 0.48 |
| 23:DA:2416:C:C4 | 23:DA:2417:C:C5 | 3.02 | 0.48 |
| 23:BA:631:A:OP1 | 34:BL:64:LYS:HE3 | 2.13 | 0.48 |
| 38:DP:75:ILE:HG22 | 38:DP:75:ILE:O | 2.13 | 0.48 |
| 32:DJ:51:THR:HG22 | 32:DJ:52:LYS:N | 2.29 | 0.48 |
| 1:AA:986:A:C6 | 1:AA:1220:G:N1 | 2.82 | 0.48 |
| 1:CA:969:A:C2' | 1:CA:970:C:H5' | 2.44 | 0.48 |
| 23:BA:2846:G:C5 | 23:BA:2847:U:C4 | 3.02 | 0.48 |
| 23:BA:1022:G:N2 | 23:BA:114(B):A:H2 | 2.12 | 0.48 |
| 32:BJ:95:TYR:CD2 | 32:BJ:113:MET:HG3 | 2.49 | 0.48 |
| 32:BJ:116:THR:OG1 | 32:BJ:117:HIS:N | 2.46 | 0.48 |
| 23:BA:1012:U:O4 | 32:BJ:48:ARG:HA | 2.13 | 0.48 |
| 40:DR:45:THR:O | 40:DR:46:VAL:HG22 | 2.13 | 0.48 |
| 25:BC:143:HIS:HD2 | 25:BC:144:ALA:HB2 | 1.79 | 0.48 |
| 34:DL:50:ARG:HB2 | 53:D5:60:LEU:HD21 | 1.95 | 0.48 |
| 23:DA:114(B):A:C4 | 23:DA:1144:G:N7 | 2.82 | 0.48 |
| 25:DC:155:LEU:HG | 25:DC:177:LEU:HD22 | 1.95 | 0.48 |
| 4:AD:106:TYR:O | 4:AD:109:GLY:N | 2.44 | 0.48 |
| 1:AA:33:A:H2' | 1:AA:34:C:C6 | 2.49 | 0.48 |
| 47:BY:60:LEU:O | 47:BY:62:THR:N | 2.47 | 0.48 |
| 1:CA:76:G:C6 | 1:CA:95:G:N1 | 2.81 | 0.48 |
| 36:DN:4:LEU:C | 36:DN:6:SER:N | 2.66 | 0.48 |
| 44:BV:53:ILE:CG2 | 44:BV:71:VAL:O | 2.62 | 0.48 |
| 1:CA:198:G:O2' | 1:CA:199:G:H5' | 2.14 | 0.48 |
| 23:BA:96:G:O5' | 47:BY:48:HIS:HE1 | 1.96 | 0.48 |
| 1:CA:57:G:N2 | 1:CA:388:G:C6 | 2.82 | 0.48 |
| 23:BA:1264:G:H5' | 50:B2:11:THR:HG23 | 1.92 | 0.48 |
| 18:CR:38:GLU:OE2 | 18:CR:38:GLU:HA | 2.12 | 0.48 |
| 18:CR:37:VAL:HG23 | 18:CR:38:GLU:N | 2.29 | 0.48 |
| 23:DA:2746:U:O3' | 29:DG:138:LYS:HD3 | 2.14 | 0.48 |
| 1:CA:878:G:C1' | 8:CH:3:THR:HG21 | 2.44 | 0.48 |
| 23:DA:1487:G:H2' | 23:DA:1488:G:C8 | 2.35 | 0.48 |
| 1:AA:669:U:C2 | 1:AA:670:G:C8 | 3.02 | 0.48 |
| 1:CA:624:C:H4' | 16:CP:10:GLY:HA2 | 1.95 | 0.48 |
| 33:BK:97:ARG:H | 33:BK:117:LEU:HD22 | 1.79 | 0.48 |
| 1:CA:1280:A:C8 | 10:CJ:41:PRO:HD3 | 2.49 | 0.48 |
| 41:DS:42:ARG:HG2 | 41:DS:42:ARG:NH1 | 2.29 | 0.48 |
| 8:CH:97:VAL:CG1 | 8:CH:98:LYS:H | 2.26 | 0.48 |
| 23:BA:732:C:H2' | 23:BA:733:G:H5' | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:104:G:C2 | 1:CA:105:G:N7 | 2.82 | 0.48 |
| 43:BU:36:ALA:HA | 43:BU:67:LEU:O | 2.13 | 0.48 |
| 24:BB:21:G:N2 | 24:BB:62:C:N3 | 2.58 | 0.48 |
| 24:BB:75:G:N1 | 24:BB:102:G:N2 | 2.62 | 0.48 |
| 23:DA:333:G:C4 | 23:DA:334:C:C5 | 3.01 | 0.48 |
| 4:AD:121:VAL:O | 4:AD:134:ASP:HA | 2.14 | 0.48 |
| 23:BA:1387:C:C2 | 23:BA:1388:G:C8 | 3.02 | 0.48 |
| 35:BM:60:ARG:HA | 44:BV:179:ASP:HB2 | 1.96 | 0.48 |
| 44:BV:13:GLU:CD | 44:BV:13:GLU:H | 2.18 | 0.48 |
| 34:BL:85:LEU:HD23 | 34:BL:117:GLU:O | 2.14 | 0.48 |
| 1:CA:862:C:O2' | 1:CA:863:U:H5' | 2.14 | 0.48 |
| 1:AA:545:C:OP2 | 4:AD:62:GLN:NE2 | 2.47 | 0.48 |
| 5:CE:96:PRO:HA | 5:CE:117:ASP:OD2 | 2.13 | 0.48 |
| 23:DA:304:G:H2' | 23:DA:305:U:O4' | 2.14 | 0.48 |
| 1:AA:1412:C:H2' | 1:AA:1413:A:H8 | 1.79 | 0.48 |
| 12:CL:6:ILE:O | 12:CL:10:VAL:CG2 | 2.62 | 0.48 |
| 1:CA:428:G:C8 | 1:CA:430:A:C4 | 3.01 | 0.48 |
| 19:AS:30:LEU:HD23 | 19:AS:31:ILE:N | 2.28 | 0.48 |
| 1:CA:754:C:H3' | 1:CA:754:C:O2 | 2.14 | 0.48 |
| 1:AA:382:A:C2 | 1:AA:383:A:C4 | 3.02 | 0.48 |
| 23:DA:903:C:O2' | 23:DA:904:C:H5' | 2.14 | 0.48 |
| 26:BD:117:MET:CE | 26:BD:136:ARG:HA | 2.44 | 0.48 |
| 27:DE:12:LEU:HD11 | 27:DE:17:ARG:HG2 | 1.96 | 0.48 |
| 1:CA:1409:C:OP1 | 23:DA:1916:A:H2 | 1.97 | 0.48 |
| 23:BA:2039:C:C2 | 23:BA:2040:C:C5 | 3.02 | 0.48 |
| 1:AA:1360:A:C6 | 1:AA:1361:G:C2 | 3.01 | 0.48 |
| 5:AE:53:LEU:HD23 | 5:AE:53:LEU:N | 2.28 | 0.48 |
| 2:CB:17:PHE:CG | 2:CB:44:LEU:HD21 | 2.49 | 0.48 |
| 35:DM:26:TYR:HD1 | 35:DM:26:TYR:O | 1.94 | 0.48 |
| 1:CA:1167:A:H62 | 1:CA:1169:A:N6 | 2.12 | 0.48 |
| 34:BL:135:LEU:HD22 | 34:BL:135:LEU:HA | 1.53 | 0.48 |
| 26:DD:173:VAL:O | 26:DD:174:ASP:C | 2.51 | 0.48 |
| 23:BA:2744:G:C2 | 23:BA:2761:G:C6 | 3.01 | 0.48 |
| 16:CP:47:ASP:O | 16:CP:49:LEU:N | 2.47 | 0.48 |
| 3:CC:111:LEU:HD11 | 3:CC:144:SER:OG | 2.13 | 0.48 |
| 42:BT:4:ALA:C | 42:BT:6:ASP:H | 2.16 | 0.48 |
| 33:BK:9:GLU:OE1 | 33:BK:18:LYS:HE2 | 2.14 | 0.48 |
| 1:CA:608:A:C4 | 1:CA:609:A:C8 | 3.01 | 0.48 |
| 23:DA:476:G:O4' | 23:DA:505:A:C2 | 2.66 | 0.48 |
| 44:DV:144:LEU:HB3 | 44:DV:174:VAL:HG21 | 1.96 | 0.48 |
| 37:DO:64:GLU:O | 37:DO:68:GLN:HG3 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:AL:54:VAL:HG12 | 12:AL:55:ALA:H | 1.77 | 0.48 |
| 36:BN:14:SER:O | 36:BN:15:SER:C | 2.52 | 0.48 |
| 33:BK:3:GLN:HG3 | 33:BK:4:PRO:HD2 | 1.96 | 0.48 |
| 1:CA:118:U:O4 | 1:CA:288:A:H2' | 2.14 | 0.48 |
| 23:DA:1292:U:H2' | 23:DA:1293:C:C6 | 2.49 | 0.48 |
| 1:AA:850:U:H6 | 1:AA:850:U:O5' | 1.97 | 0.48 |
| 39:BQ:34:LYS:HE3 | 39:BQ:34:LYS:HA | 1.96 | 0.48 |
| 23:BA:2393:A:C5' | 34:BL:62:LEU:HD12 | 2.42 | 0.47 |
| 23:BA:1175:U:H2' | 23:BA:1176:G:C8 | 2.49 | 0.47 |
| 25:BC:15:PHE:O | 25:BC:205:VAL:CG1 | 2.61 | 0.47 |
| 23:DA:2846:G:H2' | 23:DA:2847:U:O4' | 2.14 | 0.47 |
| 23:BA:2683:C:OP1 | 38:BP:55:ASN:ND2 | 2.41 | 0.47 |
| 40:DR:44:LYS:HB3 | 40:DR:46:VAL:HG13 | 1.95 | 0.47 |
| 40:DR:47:VAL:O | 40:DR:48:GLY:C | 2.51 | 0.47 |
| 39:BQ:113:ALA:HA | 39:BQ:116:ALA:HB3 | 1.96 | 0.47 |
| 34:BL:41:ARG:HD2 | 34:BL:41:ARG:HA | 1.50 | 0.47 |
| 1:CA:393:A:N3 | 1:CA:394:G:C8 | 2.82 | 0.47 |
| 1:CA:394:G:C4 | 1:CA:395:C:C5 | 3.01 | 0.47 |
| 30:DH:69:LYS:HD3 | 30:DH:138:ILE:HG12 | 1.95 | 0.47 |
| 28:DF:88:ILE:HD12 | 28:DF:89:GLY:H | 1.79 | 0.47 |
| 28:BF:161:THR:C | 28:BF:163:ALA:N | 2.68 | 0.47 |
| 8:AH:127:LEU:O | 8:AH:127:LEU:HD13 | 2.14 | 0.47 |
| 3:AC:173:VAL:H | 3:AC:174:PRO:HD3 | 1.77 | 0.47 |
| 3:CC:15:THR:HG21 | 3:CC:181:ASN:CA | 2.44 | 0.47 |
| 23:BA:2886:G:H2' | 23:BA:2887:U:C6 | 2.48 | 0.47 |
| 5:CE:129:ILE:O | 5:CE:132:ALA:HB3 | 2.13 | 0.47 |
| 23:DA:1999:C:OP1 | 23:DA:2723:C:O2' | 2.32 | 0.47 |
| 1:CA:737:A:C4 | 1:CA:738:C:C5 | 3.01 | 0.47 |
| 1:AA:16:A:C2 | 1:AA:17:U:C6 | 3.02 | 0.47 |
| 5:CE:126:ARG:NH1 | 5:CE:126:ARG:CG | 2.59 | 0.47 |
| 1:AA:1346:A:C2 | 1:AA:1348:U:O4 | 2.67 | 0.47 |
| 23:DA:2621:A:OP1 | 26:DD:119:ARG:NH2 | 2.46 | 0.47 |
| 1:AA:9:G:O2' | 1:AA:10:A:H5' | 2.13 | 0.47 |
| 1:AA:9:G:H2' | 1:AA:10:A:C8 | 2.49 | 0.47 |
| 12:AL:44:PRO:HD2 | 12:AL:49:SER:HA | 1.96 | 0.47 |
| 27:DE:173:VAL:HG12 | 27:DE:174:VAL:N | 2.28 | 0.47 |
| 23:BA:1578:U:H2' | 23:BA:1578:U:O2 | 2.14 | 0.47 |
| 23:DA:1508:A:N6 | 23:DA:1509:A:C6 | 2.82 | 0.47 |
| 1:CA:619:U:N3 | 4:CD:135:LEU:HD11 | 2.28 | 0.47 |
| 40:DR:24:LYS:HA | 40:DR:92:THR:CG2 | 2.39 | 0.47 |
| 23:BA:954:G:C6 | 23:BA:955:C:C5 | 3.02 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:1152:A:C4 | 1:CA:1153:C:C5 | 3.02 | 0.47 |
| 23:DA:588:U:C2 | 27:DE:90:PHE:CE1 | 3.02 | 0.47 |
| 1:AA:1180:A:OP1 | 9:AI:103:THR:OG1 | 2.27 | 0.47 |
| 9:CI:104:ARG:O | 9:CI:105:ASP:HB3 | 2.13 | 0.47 |
| 36:BN:67:LEU:O | 36:BN:70:LEU:O | 2.31 | 0.47 |
| 28:DF:112:PRO:HB3 | 49:D1:62:CYS:O | 2.14 | 0.47 |
| 43:DU:76:CYS:O | 43:DU:77:PRO:C | 2.52 | 0.47 |
| 24:BB:21:G:H2' | 24:BB:22:U:C6 | 2.48 | 0.47 |
| 23:BA:2550:G:C6 | 23:BA:2551:C:C4 | 3.01 | 0.47 |
| 1:CA:841:U:H4' | 1:CA:842:C:C5 | 2.49 | 0.47 |
| 50:B2:33:CYS:HB2 | 50:B2:34:PRO:HD2 | 1.95 | 0.47 |
| 23:BA:828:U:H2' | 23:BA:828:U:O2 | 2.14 | 0.47 |
| 23:DA:1591:G:H2' | 23:DA:1592:C:C6 | 2.49 | 0.47 |
| 23:DA:1592:C:H2' | 23:DA:1593:G:C8 | 2.46 | 0.47 |
| 28:BF:11:TYR:HB2 | 28:BF:176:LEU:HD21 | 1.96 | 0.47 |
| 8:AH:36:LEU:HA | 8:AH:39:LEU:HB2 | 1.95 | 0.47 |
| 1:AA:559:A:H4' | 1:AA:560:U:H3' | 1.96 | 0.47 |
| 12:AL:37:THR:OG1 | 12:AL:38:VAL:N | 2.47 | 0.47 |
| 1:CA:381:C:H2' | 1:CA:382:A:C8 | 2.49 | 0.47 |
| 36:DN:88:ARG:C | 36:DN:90:ARG:H | 2.17 | 0.47 |
| 6:AF:47:ARG:HH12 | 6:AF:56:PRO:HB2 | 1.79 | 0.47 |
| 1:CA:1183:A:H5'' | 1:CA:1184:G:OP2 | 2.14 | 0.47 |
| 41:DS:59:VAL:HG12 | 41:DS:60:ASN:N | 2.29 | 0.47 |
| 34:BL:140:ALA:O | 34:BL:141:ALA:CB | 2.62 | 0.47 |
| 1:AA:1182:G:H4' | 1:AA:1183:A:H5'' | 1.96 | 0.47 |
| 1:AA:380:G:C2 | 1:AA:384:G:N1 | 2.82 | 0.47 |
| 49:D1:41:ILE:HD13 | 49:D1:47:VAL:HG13 | 1.96 | 0.47 |
| 23:BA:1424:G:H2' | 23:BA:1425:G:O4' | 2.14 | 0.47 |
| 30:DH:73:GLU:C | 30:DH:75:LEU:H | 2.18 | 0.47 |
| 23:DA:1677:A:H2' | 23:DA:1678:G:O4' | 2.14 | 0.47 |
| 21:AU:12:LYS:HB3 | 21:AU:17:THR:O | 2.14 | 0.47 |
| 1:CA:614:A:OP1 | 4:CD:85:LYS:HE2 | 2.14 | 0.47 |
| 30:BH:12:LEU:N | 30:BH:12:LEU:HD22 | 2.28 | 0.47 |
| 23:DA:337:C:H2' | 23:DA:338:G:O5' | 2.14 | 0.47 |
| 23:DA:616:A:C4 | 27:DE:180:GLY:HA2 | 2.49 | 0.47 |
| 1:AA:892:A:C2 | 1:AA:907:A:C4 | 3.02 | 0.47 |
| 1:CA:1407:C:O5' | 1:CA:1407:C:H6 | 1.97 | 0.47 |
| 1:AA:1339:A:H2' | 1:AA:1340:A:O4' | 2.13 | 0.47 |
| 23:DA:653:C:H6 | 23:DA:653:C:O5' | 1.97 | 0.47 |
| 34:DL:115:LEU:HB3 | 34:DL:131:SER:HB2 | 1.96 | 0.47 |
| 23:BA:630:G:N2 | 23:BA:633:A:OP2 | 2.33 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:BL:57:THR:OG1 | 34:BL:58:THR:N | 2.46 | 0.47 |
| 23:BA:1542:G:P | 23:BA:1543:A:OP1 | 2.72 | 0.47 |
| 23:BA:1545:A:O2' | 23:BA:1546:A:H5' | 2.13 | 0.47 |
| 23:DA:1175:U:H2' | 23:DA:1176:G:C8 | 2.48 | 0.47 |
| 34:BL:111:ARG:HD2 | 34:BL:128:HIS:CD2 | 2.49 | 0.47 |
| 1:AA:1060:C:H5'' | 10:AJ:51:ARG:HG2 | 1.97 | 0.47 |
| 5:CE:81:GLU:HG2 | 5:CE:90:VAL:HG22 | 1.97 | 0.47 |
| 13:CM:91:ARG:NH1 | 19:CS:81:ARG:NH2 | 2.61 | 0.47 |
| 12:CL:116:ARG:NH2 | 12:CL:123:LYS:HB2 | 2.29 | 0.47 |
| 27:DE:65:TRP:HB3 | 27:DE:66:PRO:HD2 | 1.96 | 0.47 |
| 37:BO:12:PHE:O | 37:BO:12:PHE:HD1 | 1.97 | 0.47 |
| 30:BH:88:ILE:CG2 | 30:BH:89:TYR:N | 2.77 | 0.47 |
| 53:B5:60:LEU:N | 53:B5:60:LEU:HD23 | 2.29 | 0.47 |
| 34:BL:51:PHE:HB3 | 34:BL:52:GLU:H | 1.37 | 0.47 |
| 47:BY:13:ALA:O | 47:BY:17:SER:OG | 2.22 | 0.47 |
| 1:AA:386:C:H2' | 1:AA:387:U:O4' | 2.13 | 0.47 |
| 42:DT:38:GLU:O | 42:DT:39:ILE:C | 2.48 | 0.47 |
| 30:DH:69:LYS:HD2 | 30:DH:138:ILE:HG23 | 1.95 | 0.47 |
| 4:AD:68:TYR:CE2 | 4:AD:97:LEU:HB3 | 2.49 | 0.47 |
| 26:BD:52:LEU:CB | 26:BD:76:ARG:HB2 | 2.44 | 0.47 |
| 27:DE:124:LEU:CD1 | 27:DE:125:LEU:O | 2.62 | 0.47 |
| 4:AD:64:LEU:HB2 | 4:AD:198:VAL:HG11 | 1.95 | 0.47 |
| 4:AD:61:LYS:HA | 4:AD:203:VAL:HG22 | 1.96 | 0.47 |
| 23:DA:1328:G:H2' | 23:DA:1330:C:C5 | 2.49 | 0.47 |
| 1:CA:1103:C:C2 | 1:CA:1104:G:C8 | 3.03 | 0.47 |
| 6:CF:90:VAL:CG1 | 6:CF:91:VAL:H | 2.26 | 0.47 |
| 48:BZ:43:ILE:HD13 | 48:BZ:43:ILE:H | 1.76 | 0.47 |
| 45:BW:51:VAL:N | 45:BW:62:LEU:HD12 | 2.29 | 0.47 |
| 1:AA:1372:U:C5 | 1:AA:1373:G:C4 | 3.02 | 0.47 |
| 9:AI:111:ARG:HG3 | 14:AN:61:TRP:HE1 | 1.79 | 0.47 |
| 20:CT:10:LEU:C | 20:CT:10:LEU:HD12 | 2.34 | 0.47 |
| 27:DE:174:VAL:HG21 | 27:DE:189:THR:HG21 | 1.97 | 0.47 |
| 1:CA:595:G:H1' | 1:CA:596:C:H5 | 1.79 | 0.47 |
| 23:DA:2308:G:HO2' | 23:DA:2310:A:P | 2.37 | 0.47 |
| 46:BX:10:LYS:O | 46:BX:13:ILE:CG2 | 2.62 | 0.47 |
| 1:AA:818:G:N3 | 1:AA:820:U:C6 | 2.82 | 0.47 |
| 23:DA:557:U:C2 | 23:DA:558:G:C8 | 3.02 | 0.47 |
| 23:BA:1512:G:C2 | 23:BA:1513:C:O2 | 2.67 | 0.47 |
| 24:DB:10:C:N3 | 24:DB:11:C:C5 | 2.82 | 0.47 |
| 28:BF:131:TYR:CE2 | 28:BF:133:LEU:HB3 | 2.48 | 0.47 |
| 23:DA:270(H):C:C2 | 23:DA:270(I):C:C5 | 3.03 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:CC:59:ARG:HH21 | 3:CC:97:LYS:HE2 | 1.80 | 0.47 |
| 23:DA:967:C:O2' | 23:DA:968:G:H5' | 2.14 | 0.47 |
| 23:DA:2591:C:H2' | 23:DA:2592:G:C8 | 2.49 | 0.47 |
| 26:DD:117:MET:CE | 26:DD:136:ARG:HA | 2.44 | 0.47 |
| 23:DA:1478:G:O2' | 23:DA:1558:A:C2 | 2.67 | 0.47 |
| 1:AA:564:C:C4 | 17:AQ:31:LEU:HD11 | 2.48 | 0.47 |
| 1:CA:1051:C:C4 | 1:CA:1052:U:C4 | 3.02 | 0.47 |
| 23:BA:2862:G:H2' | 23:BA:2863:C:H6 | 1.78 | 0.47 |
| 17:AQ:59:ILE:CG2 | 17:AQ:71:PHE:CD1 | 2.97 | 0.47 |
| 1:CA:539:A:C6 | 1:CA:540:G:C6 | 3.02 | 0.47 |
| 1:CA:540:G:C6 | 1:CA:541:G:C5 | 3.02 | 0.47 |
| 1:CA:921:U:H5'' | 1:CA:922:G:OP2 | 2.14 | 0.47 |
| 1:CA:728:A:C6 | 15:CO:54:ARG:HD2 | 2.48 | 0.47 |
| 36:BN:101:ALA:HB2 | 50:B2:44:THR:HB | 1.96 | 0.47 |
| 23:BA:1923:U:H2' | 23:BA:1924:C:C6 | 2.49 | 0.47 |
| 23:DA:1923:U:H2' | 23:DA:1924:C:C6 | 2.49 | 0.47 |
| 1:CA:444:C:H2' | 1:CA:445:G:C8 | 2.48 | 0.47 |
| 8:CH:36:LEU:O | 8:CH:39:LEU:N | 2.47 | 0.47 |
| 7:AG:46:ALA:O | 7:AG:50:ILE:HG12 | 2.14 | 0.47 |
| 1:AA:445:G:H2' | 1:AA:446:G:H8 | 1.79 | 0.47 |
| 36:DN:84:ALA:N | 36:DN:85:PRO:HD2 | 2.29 | 0.47 |
| 23:BA:1832:C:H2' | 23:BA:1833:U:O4' | 2.14 | 0.47 |
| 15:CO:67:LEU:HD23 | 15:CO:78:TYR:HE1 | 1.78 | 0.47 |
| 2:CB:106:LYS:HE2 | 2:CB:110:GLN:HE21 | 1.77 | 0.47 |
| 26:BD:16:ARG:O | 26:BD:17:ASP:C | 2.52 | 0.47 |
| 7:AG:70:LYS:HE2 | 7:AG:96:GLN:CD | 2.34 | 0.47 |
| 16:CP:25:ARG:O | 16:CP:26:ARG:C | 2.50 | 0.47 |
| 23:BA:414:C:H2' | 23:BA:415:A:C8 | 2.48 | 0.47 |
| 1:AA:635:G:C5 | 1:AA:636:U:C5 | 3.02 | 0.47 |
| 1:AA:1399:C:C4 | 1:AA:1502:A:C2 | 3.03 | 0.47 |
| 1:AA:288:A:O2' | 1:AA:289:G:H5' | 2.14 | 0.47 |
| 23:DA:1465:G:C2 | 23:DA:1466:G:N9 | 2.82 | 0.47 |
| 23:BA:2770:G:H5'' | 23:BA:2771:C:OP2 | 2.14 | 0.47 |
| 11:CK:111:ASP:O | 11:CK:112:THR:C | 2.52 | 0.47 |
| 1:CA:1465:C:H2' | 1:CA:1466:C:O4' | 2.13 | 0.47 |
| 23:BA:2744:G:H1' | 23:BA:2761:G:H22 | 1.79 | 0.47 |
| 32:BJ:33:GLU:HA | 32:BJ:34:PRO:HD3 | 1.75 | 0.47 |
| 23:BA:374:A:C2 | 23:BA:401:A:C4 | 3.02 | 0.47 |
| 23:BA:1381:G:H2' | 23:BA:1382:G:H5' | 1.95 | 0.47 |
| 23:BA:1368:G:O2' | 23:BA:1369:G:H5' | 2.15 | 0.47 |
| 23:BA:2019:A:O4' | 39:BQ:34:LYS:HD2 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:DC:210:GLY:HA2 | 25:DC:213:ARG:HG3 | 1.95 | 0.47 |
| 23:DA:2694:G:C6 | 23:DA:2695:C:C4 | 3.02 | 0.47 |
| 23:BA:1281:G:C5 | 23:BA:1282:U:C5 | 3.01 | 0.47 |
| 27:BE:11:VAL:O | 27:BE:12:LEU:HD12 | 2.14 | 0.47 |
| 23:DA:1456:G:C2' | 23:DA:1457:A:H5' | 2.45 | 0.47 |
| 23:DA:1641:A:H2' | 23:DA:1642:G:O4' | 2.14 | 0.47 |
| 23:BA:2359:C:H2' | 23:BA:2360:A:C8 | 2.49 | 0.47 |
| 15:AO:48:LYS:HA | 15:AO:48:LYS:HE2 | 1.96 | 0.47 |
| 1:AA:531:U:O3' | 1:AA:532:A:H4' | 2.14 | 0.47 |
| 23:DA:2523:G:H2' | 23:DA:2524:G:H5' | 1.96 | 0.47 |
| 23:BA:2495:G:H2' | 23:BA:2496:C:O5' | 2.14 | 0.47 |
| 34:BL:59:LEU:C | 34:BL:59:LEU:HD23 | 2.35 | 0.47 |
| 38:DP:63:VAL:O | 38:DP:73:GLU:HA | 2.13 | 0.47 |
| 23:BA:674:G:C1' | 27:BE:74:ARG:HD3 | 2.35 | 0.47 |
| 1:AA:960:U:C6 | 1:AA:1225:A:C8 | 3.01 | 0.47 |
| 22:AV:6213:A:C4 | 22:AV:6214:C:C5 | 3.02 | 0.47 |
| 23:BA:664:C:H4' | 23:BA:941:A:OP1 | 2.14 | 0.47 |
| 1:CA:977:A:H2' | 1:CA:978:A:C5' | 2.44 | 0.47 |
| 38:BP:61:PHE:CD2 | 38:BP:61:PHE:N | 2.81 | 0.47 |
| 1:CA:552:U:C2' | 1:CA:553:A:H5' | 2.45 | 0.47 |
| 23:BA:2419:U:OP2 | 53:B5:41:ILE:CD1 | 2.62 | 0.47 |
| 23:DA:1899:G:HO2' | 23:DA:1900:A:P | 2.37 | 0.47 |
| 30:BH:69:LYS:HD2 | 30:BH:138:ILE:HG23 | 1.95 | 0.47 |
| 23:DA:2334:G:H4' | 23:DA:2335:A:OP2 | 2.15 | 0.47 |
| 1:AA:402:G:C6 | 1:AA:403:C:C5 | 3.02 | 0.47 |
| 1:AA:687:A:N3 | 1:AA:688:G:H1' | 2.30 | 0.47 |
| 30:DH:101:LEU:HD23 | 30:DH:109:ILE:HG13 | 1.96 | 0.47 |
| 26:DD:6:GLY:CA | 26:DD:51:PHE:HE2 | 2.27 | 0.47 |
| 52:B4:19:ARG:CB | 52:B4:19:ARG:HH11 | 2.27 | 0.47 |
| 1:AA:1105:A:C2 | 1:AA:1106:G:C8 | 3.01 | 0.47 |
| 2:AB:80:ILE:HD11 | 2:AB:208:ILE:HG22 | 1.95 | 0.47 |
| 29:DG:19:VAL:HG13 | 29:DG:43:VAL:CG2 | 2.44 | 0.47 |
| 4:CD:155:LEU:HD23 | 4:CD:156:GLU:OE2 | 2.14 | 0.47 |
| 25:BC:131:LEU:HD11 | 25:BC:136:ILE:HG13 | 1.97 | 0.47 |
| 8:AH:112:LEU:HA | 8:AH:134:ILE:H | 1.79 | 0.47 |
| 23:BA:1486:A:C6 | 23:BA:1504:C:N4 | 2.75 | 0.47 |
| 16:CP:10:GLY:O | 16:CP:11:SER:O | 2.33 | 0.47 |
| 37:BO:49:VAL:HG11 | 37:BO:76:LYS:HB2 | 1.95 | 0.47 |
| 23:BA:910:A:C4 | 35:BM:13:GLN:OE1 | 2.66 | 0.47 |
| 1:CA:328:C:H4' | 1:CA:329:A:C5' | 2.43 | 0.47 |
| 11:CK:29:ILE:HB | 11:CK:44:SER:HB3 | 1.95 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 23:DA:1359:A:C8 | 23:DA:1372:U:O4 | 2.67 | 0.47 |
| 23:DA:2785:C:O2' | 26:DD:66:HIS:CD2 | 2.67 | 0.47 |
| 2:AB:72:GLY:HA3 | 2:AB:165:VAL:HG11 | 1.95 | 0.47 |
| 23:BA:582:G:OP1 | 39:BQ:14:HIS:CD2 | 2.67 | 0.47 |
| 10:CJ:55:LYS:O | 10:CJ:56:HIS:CG | 2.67 | 0.47 |
| 23:BA:1820:U:O2 | 25:BC:201:HIS:HB3 | 2.14 | 0.47 |
| 8:AH:49:GLU:HG3 | 8:AH:51:VAL:HG23 | 1.96 | 0.47 |
| 40:BR:19:LYS:HA | 40:BR:94:LEU:O | 2.13 | 0.47 |
| 1:CA:922:G:C6 | 1:CA:923:A:N6 | 2.82 | 0.47 |
| 10:AJ:9:ARG:HG2 | 10:AJ:69:ASN:OD1 | 2.14 | 0.47 |
| 32:DJ:80:ALA:C | 32:DJ:82:LYS:H | 2.17 | 0.47 |
| 36:BN:88:ARG:C | 36:BN:90:ARG:H | 2.17 | 0.47 |
| 5:AE:140:ARG:CG | 5:AE:140:ARG:O | 2.62 | 0.47 |
| 1:AA:381:C:H2' | 1:AA:382:A:C8 | 2.49 | 0.47 |
| 23:DA:2001:A:H2' | 23:DA:2002:G:O4' | 2.14 | 0.47 |
| 23:DA:1550:C:H2' | 23:DA:1551:C:H6 | 1.79 | 0.47 |
| 1:CA:1505:G:H4' | 1:CA:1506:U:H5'' | 1.94 | 0.47 |
| 23:DA:1526:G:H2' | 23:DA:1527:G:C8 | 2.49 | 0.47 |
| 1:CA:55:A:C5 | 1:CA:56:U:C5 | 3.02 | 0.47 |
| 23:BA:1997:G:O2' | 23:BA:1998:G:H5' | 2.14 | 0.47 |
| 35:DM:38:GLU:C | 35:DM:127:ILE:HD11 | 2.34 | 0.47 |
| 35:BM:24:GLY:HA2 | 35:BM:101:ARG:HA | 1.96 | 0.47 |
| 1:AA:577:G:H1' | 1:AA:816:A:C4 | 2.49 | 0.47 |
| 1:CA:112:G:OP1 | 16:CP:27:LYS:HE2 | 2.14 | 0.47 |
| 1:AA:574:A:H1' | 1:AA:883:C:O4' | 2.15 | 0.47 |
| 23:BA:1796:U:H2' | 23:BA:1797:C:C6 | 2.49 | 0.47 |
| 2:AB:17:PHE:HB2 | 2:AB:44:LEU:HD21 | 1.96 | 0.47 |
| 1:AA:575:G:C5 | 1:AA:881:G:C2 | 3.02 | 0.47 |
| 23:BA:1127:A:C2' | 23:BA:1128:A:H5'' | 2.43 | 0.47 |
| 30:BH:26:ALA:HA | 30:BH:30:LEU:HB2 | 1.95 | 0.47 |
| 1:AA:451:A:N7 | 1:AA:481:G:C6 | 2.82 | 0.47 |
| 23:BA:1265:A:H5' | 23:BA:1267:U:H1' | 1.95 | 0.47 |
| 7:AG:77:SER:HA | 7:AG:85:TYR:O | 2.14 | 0.47 |
| 1:CA:1438:G:O2' | 1:CA:1439:C:H5' | 2.14 | 0.47 |
| 23:DA:1345:C:O2' | 23:DA:1346:G:H5' | 2.15 | 0.47 |
| 1:AA:879:C:O2' | 1:AA:880:C:H5' | 2.15 | 0.47 |
| 1:CA:572:A:H5'' | 1:CA:917:G:H4' | 1.95 | 0.47 |
| 44:DV:140:ASP:N | 44:DV:140:ASP:OD2 | 2.47 | 0.47 |
| 27:BE:28:ILE:O | 27:BE:28:ILE:HG13 | 2.14 | 0.47 |
| 26:DD:14:ILE:C | 26:DD:14:ILE:HD12 | 2.34 | 0.47 |
| 15:CO:32:LEU:O | 15:CO:35:ARG:N | 2.46 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:BL:62:LEU:HD21 | 53:B5:25:MET:HB2 | 1.96 | 0.47 |
| 34:BL:62:LEU:CD1 | 53:B5:27:THR:HG22 | 2.45 | 0.47 |
| 43:BU:14:LEU:HD23 | 43:BU:15:VAL:CA | 2.43 | 0.47 |
| 43:BU:17:SER:CB | 43:BU:71:LYS:HD2 | 2.43 | 0.47 |
| 32:BJ:123:GLU:C | 32:BJ:125:ALA:H | 2.16 | 0.47 |
| 34:BL:97:PRO:O | 34:BL:101:VAL:HG12 | 2.15 | 0.47 |
| 1:CA:1368:G:H5'' | 14:CN:61:TRP:HZ2 | 1.78 | 0.47 |
| 26:BD:11:MET:HE3 | 26:BD:186:GLY:CA | 2.41 | 0.47 |
| 23:DA:673:C:C2' | 23:DA:674:G:H5' | 2.45 | 0.47 |
| 1:CA:981:U:OP1 | 14:CN:6:LEU:HD21 | 2.15 | 0.47 |
| 23:DA:1971:A:C5 | 25:DC:241:PRO:HG3 | 2.50 | 0.47 |
| 23:BA:1970:A:H4' | 23:BA:1971:A:OP1 | 2.14 | 0.47 |
| 25:DC:9:TYR:C | 25:DC:10:THR:HG22 | 2.34 | 0.47 |
| 40:DR:3:ALA:HB1 | 40:DR:38:LEU:HD21 | 1.97 | 0.47 |
| 30:BH:143:SER:O | 30:BH:145:VAL:N | 2.46 | 0.47 |
| 40:BR:6:LYS:CG | 40:BR:11:GLN:HG2 | 2.43 | 0.47 |
| 28:DF:25:TYR:CZ | 28:DF:32:PRO:HD3 | 2.49 | 0.47 |
| 25:DC:143:HIS:C | 25:DC:143:HIS:CD2 | 2.87 | 0.47 |
| 1:AA:407:G:C2 | 1:AA:436:C:C2 | 3.02 | 0.47 |
| 11:AK:27:ASN:HA | 11:AK:55:LYS:O | 2.15 | 0.47 |
| 28:BF:129:GLY:HA3 | 28:BF:163:ALA:CB | 2.44 | 0.47 |
| 1:AA:88:C:H2' | 1:AA:89:U:O4' | 2.15 | 0.47 |
| 27:BE:174:VAL:HG21 | 27:BE:189:THR:HG21 | 1.95 | 0.47 |
| 36:DN:2:ARG:O | 36:DN:3:HIS:CG | 2.68 | 0.47 |
| 5:AE:76:ILE:HG12 | 5:AE:142:LEU:HD22 | 1.96 | 0.47 |
| 26:DD:52:LEU:CB | 26:DD:76:ARG:HB2 | 2.45 | 0.47 |
| 24:BB:106:G:C6 | 24:BB:107:U:C4 | 3.03 | 0.47 |
| 9:AI:28:VAL:HG13 | 9:AI:63:ILE:HG22 | 1.96 | 0.47 |
| 1:AA:1291:G:C6 | 1:AA:1292:U:C4 | 3.02 | 0.47 |
| 23:DA:2746:U:H4' | 29:DG:138:LYS:HD3 | 1.96 | 0.47 |
| 23:BA:2305:A:O2' | 28:BF:136:ARG:NE | 2.48 | 0.47 |
| 4:CD:110:PHE:CD2 | 4:CD:110:PHE:N | 2.82 | 0.47 |
| 2:CB:83:MET:CE | 2:CB:234:PRO:HG2 | 2.44 | 0.47 |
| 29:BG:151:ILE:HD13 | 29:BG:151:ILE:H | 1.79 | 0.47 |
| 1:AA:783:C:H2' | 1:AA:784:C:H6 | 1.80 | 0.47 |
| 1:AA:54:C:N4 | 1:AA:353:A:OP2 | 2.45 | 0.47 |
| 1:AA:627:G:O2' | 1:AA:628:G:H5' | 2.15 | 0.47 |
| 23:DA:588:U:H2' | 23:DA:589:C:H6 | 1.79 | 0.47 |
| 23:DA:1109:C:H42 | 23:DA:1110:G:N2 | 2.12 | 0.47 |
| 23:DA:1952:A:C6 | 23:DA:1953:A:C6 | 3.03 | 0.47 |
| 23:DA:1516:U:H2' | 23:DA:1517:G:H8 | 1.77 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:AR:22:VAL:HG12 | 18:AR:22:VAL:O | 2.14 | 0.47 |
| 25:DC:176:ARG:HG2 | 25:DC:176:ARG:NH1 | 2.27 | 0.47 |
| 4:CD:13:ARG:HD2 | 4:CD:38:TYR:O | 2.14 | 0.47 |
| 4:CD:13:ARG:O | 4:CD:39:PRO:HA | 2.14 | 0.47 |
| 10:CJ:34:VAL:HG22 | 10:CJ:74:ILE:HG22 | 1.97 | 0.47 |
| 23:DA:1030:G:OP2 | 35:DM:128:LYS:HG2 | 2.15 | 0.47 |
| 32:BJ:135:LEU:O | 32:BJ:139:LEU:HG | 2.14 | 0.47 |
| 1:CA:652:U:O4 | 1:CA:752:G:O2' | 2.20 | 0.47 |
| 23:BA:627:A:H4' | 23:BA:628:G:OP1 | 2.14 | 0.47 |
| 45:DW:50:ASN:HD22 | 45:DW:83:PRO:HD3 | 1.78 | 0.47 |
| 8:AH:97:VAL:CG1 | 8:AH:98:LYS:N | 2.76 | 0.47 |
| 23:DA:2850:A:C4 | 23:DA:2851:A:C8 | 3.03 | 0.47 |
| 28:DF:178:PHE:O | 28:DF:180:PHE:CD1 | 2.67 | 0.47 |
| 10:AJ:40:LEU:HB2 | 10:AJ:69:ASN:CB | 2.42 | 0.47 |
| 23:DA:815:C:C2 | 23:DA:816:C:C5 | 3.03 | 0.47 |
| 35:BM:32:PHE:CZ | 35:BM:111:GLU:HG2 | 2.45 | 0.47 |
| 28:BF:7:LEU:HD22 | 28:BF:176:LEU:HD22 | 1.96 | 0.47 |
| 23:BA:2094:G:C2 | 23:BA:2196:C:C2 | 3.02 | 0.47 |
| 23:DA:1184:G:C6 | 23:DA:1185:C:C4 | 3.03 | 0.47 |
| 23:BA:904:C:H2' | 23:BA:905:U:C6 | 2.49 | 0.47 |
| 23:DA:189:G:H2' | 23:DA:205:G:N2 | 2.29 | 0.47 |
| 23:DA:1443:G:H1 | 23:DA:1548:C:H42 | 1.63 | 0.47 |
| 28:BF:62:LEU:HB3 | 28:BF:143:GLU:HG3 | 1.97 | 0.47 |
| 23:BA:1919:A:H5'' | 23:BA:1920:C:OP2 | 2.14 | 0.47 |
| 1:AA:814:A:C8 | 1:AA:816:A:C8 | 3.03 | 0.47 |
| 5:AE:53:LEU:CD2 | 5:AE:53:LEU:H | 2.27 | 0.47 |
| 35:BM:26:TYR:HD1 | 35:BM:26:TYR:O | 1.97 | 0.47 |
| 27:BE:150:GLY:HA2 | 27:BE:172:TRP:CE3 | 2.49 | 0.47 |
| 1:CA:932:C:OP1 | 7:CG:4:ARG:HG2 | 2.14 | 0.47 |
| 23:BA:270(G):U:H3 | 23:BA:270(U):G:H1 | 1.63 | 0.47 |
| 35:DM:125:LEU:HB3 | 35:DM:126:PRO:HD2 | 1.97 | 0.47 |
| 23:DA:2193:G:O2' | 23:DA:2194:G:H5' | 2.14 | 0.47 |
| 25:DC:89:SER:HB2 | 25:DC:159:ALA:HB2 | 1.97 | 0.47 |
| 42:BT:27:THR:HB | 42:BT:80:ILE:HB | 1.94 | 0.47 |
| 36:BN:104:ARG:HH11 | 36:BN:104:ARG:CB | 2.28 | 0.47 |
| 48:DZ:38:GLU:OE1 | 48:DZ:38:GLU:N | 2.45 | 0.47 |
| 39:BQ:97:ASP:CG | 39:BQ:97:ASP:O | 2.52 | 0.47 |
| 5:AE:72:GLN:O | 5:AE:73:ASN:CB | 2.61 | 0.47 |
| 28:DF:17:PRO:HA | 28:DF:20:ILE:HG12 | 1.96 | 0.47 |
| 23:DA:1665:A:H4' | 33:DK:67:LYS:HB2 | 1.95 | 0.47 |
| 10:CJ:65:LEU:HD13 | 14:CN:56:VAL:HG22 | 1.95 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DA:2251:G:C6 | 23:DA:2252:G:C6 | 3.03 | 0.47 |
| 4:CD:201:GLN:O | 4:CD:205:GLU:HG3 | 2.13 | 0.47 |
| 23:DA:627:A:C2 | 23:DA:636:G:N3 | 2.83 | 0.47 |
| 1:CA:1347:G:H22 | 1:CA:1373:G:C2' | 2.28 | 0.47 |
| 23:BA:2439:A:O2' | 23:BA:2440:C:OP2 | 2.25 | 0.47 |
| 22:CV:6192:G:C6 | 22:CV:6193:U:C4 | 3.02 | 0.47 |
| 1:CA:950:U:H4' | 1:CA:971:G:H22 | 1.78 | 0.47 |
| 38:BP:64:ARG:HD2 | 38:BP:73:GLU:OE2 | 2.14 | 0.47 |
| 28:BF:73:ALA:HB3 | 28:BF:76:SER:OG | 2.14 | 0.47 |
| 39:DQ:92:ARG:HD2 | 39:DQ:95:LEU:CG | 2.44 | 0.47 |
| 30:BH:101:LEU:HD23 | 30:BH:109:ILE:HG13 | 1.97 | 0.47 |
| 41:DS:17:VAL:O | 41:DS:18:ARG:C | 2.50 | 0.47 |
| 23:BA:1159:U:H2' | 23:BA:1160:G:C8 | 2.47 | 0.47 |
| 39:BQ:98:LEU:O | 39:BQ:101:ARG:N | 2.47 | 0.47 |
| 1:AA:376:G:C2' | 1:AA:377:G:O5' | 2.62 | 0.47 |
| 4:CD:51:PRO:HB3 | 4:CD:55:ALA:CB | 2.43 | 0.47 |
| 4:AD:109:GLY:C | 4:AD:111:ALA:N | 2.67 | 0.47 |
| 23:BA:1412:A:H2' | 23:BA:1413:G:O4' | 2.14 | 0.47 |
| 2:CB:80:ILE:HD11 | 2:CB:208:ILE:HG22 | 1.95 | 0.47 |
| 1:AA:90:C:N3 | 1:AA:91:C:C4 | 2.82 | 0.47 |
| 23:DA:137(B):G:O6 | 23:DA:139:G:O2' | 2.29 | 0.47 |
| 23:BA:2887:U:C2 | 23:BA:2888:C:C5 | 3.02 | 0.47 |
| 5:CE:139:LEU:C | 5:CE:141:GLN:H | 2.16 | 0.47 |
| 37:DO:53:SER:O | 37:DO:56:LEU:HB3 | 2.14 | 0.47 |
| 1:AA:878:G:C5' | 8:AH:89:PRO:HG2 | 2.44 | 0.47 |
| 23:BA:850:C:O2' | 48:BZ:46:ASN:ND2 | 2.47 | 0.47 |
| 45:BW:62:LEU:O | 45:BW:63:VAL:HG13 | 2.15 | 0.47 |
| 12:CL:49:SER:O | 12:CL:50:ALA:HB2 | 2.15 | 0.47 |
| 18:CR:37:VAL:HG12 | 18:CR:78:LEU:HB3 | 1.97 | 0.47 |
| 4:CD:126:ILE:CG2 | 4:CD:127:THR:N | 2.78 | 0.47 |
| 6:AF:26:ILE:C | 6:AF:30:LEU:HD12 | 2.35 | 0.47 |
| 6:AF:5:GLU:OE1 | 6:AF:62:TRP:HZ2 | 1.96 | 0.47 |
| 23:DA:528:A:OP2 | 32:DJ:134:PRO:HB3 | 2.14 | 0.47 |
| 9:CI:28:VAL:HG22 | 9:CI:63:ILE:H | 1.78 | 0.47 |
| 23:DA:2791:C:H4' | 23:DA:2792:G:OP1 | 2.14 | 0.47 |
| 23:DA:2406:U:O4 | 34:DL:70:GLN:HB3 | 2.13 | 0.47 |
| 23:DA:2287:A:C5 | 23:DA:2289:G:N7 | 2.83 | 0.47 |
| 1:CA:1084:G:C6 | 1:CA:1085:U:O4 | 2.68 | 0.47 |
| 23:DA:2629:A:N3 | 23:DA:2629:A:H2' | 2.29 | 0.47 |
| 30:DH:15:VAL:HG12 | 30:DH:16:GLY:N | 2.29 | 0.47 |
| 28:DF:111:LEU:HA | 28:DF:114:ILE:HD11 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DA:1131:G:N2 | 23:DA:1132:A:C4 | 2.83 | 0.47 |
| 1:CA:832:C:O2' | 1:CA:833:U:P | 2.72 | 0.47 |
| 25:BC:176:ARG:HH11 | 25:BC:176:ARG:CG | 2.26 | 0.47 |
| 12:CL:46:LYS:CB | 12:CL:47:PRO:HD3 | 2.45 | 0.47 |
| 12:CL:45:LYS:HB3 | 12:CL:46:LYS:H | 1.39 | 0.47 |
| 35:BM:60:ARG:H | 44:BV:179:ASP:CB | 2.26 | 0.47 |
| 1:CA:1054:C:O2 | 1:CA:1054:C:H3' | 2.14 | 0.47 |
| 23:BA:118:A:C8 | 23:BA:119:A:C8 | 3.02 | 0.47 |
| 33:DK:1:MET:HE2 | 33:DK:32:TYR:CG | 2.50 | 0.47 |
| 3:AC:23:TYR:CD1 | 10:AJ:10:GLY:HA2 | 2.49 | 0.47 |
| 23:BA:540:G:C5 | 23:BA:541:C:C5 | 3.02 | 0.47 |
| 23:BA:540:G:C4 | 23:BA:541:C:C6 | 3.02 | 0.47 |
| 40:BR:12:TYR:CZ | 40:BR:22:VAL:HG22 | 2.49 | 0.47 |
| 29:BG:40:GLU:O | 29:BG:55:PRO:HG3 | 2.13 | 0.47 |
| 1:AA:565:U:C6 | 1:AA:566:G:C8 | 3.03 | 0.47 |
| 23:BA:1832:C:N4 | 23:BA:1833:U:C4 | 2.82 | 0.47 |
| 23:BA:1833:U:N3 | 23:BA:1834:U:C5 | 2.83 | 0.47 |
| 26:DD:179:GLU:HB3 | 26:DD:181:LEU:HD22 | 1.97 | 0.47 |
| 23:DA:2299:G:C6 | 23:DA:2318:G:N2 | 2.83 | 0.47 |
| 23:BA:1850:G:C5 | 23:BA:1851:U:C5 | 3.02 | 0.47 |
| 19:CS:11:VAL:HG23 | 19:CS:38:SER:HB2 | 1.96 | 0.47 |
| 1:CA:1289:A:OP1 | 21:CU:10:ARG:HD3 | 2.14 | 0.47 |
| 7:CG:70:LYS:HE2 | 7:CG:96:GLN:CD | 2.35 | 0.47 |
| 25:BC:141:VAL:O | 25:BC:141:VAL:HG22 | 2.14 | 0.47 |
| 2:CB:17:PHE:HB2 | 2:CB:44:LEU:HD21 | 1.96 | 0.47 |
| 23:DA:2428:G:H5'' | 23:DA:2429:G:O5' | 2.14 | 0.47 |
| 1:CA:993:G:H2' | 1:CA:993:G:N3 | 2.29 | 0.47 |
| 23:DA:1851:U:C4 | 23:DA:1852:C:C4 | 3.02 | 0.47 |
| 33:DK:60:ALA:CB | 33:DK:86:ILE:HA | 2.43 | 0.47 |
| 23:DA:2302:G:O2' | 23:DA:2303:G:H5' | 2.15 | 0.47 |
| 14:CN:4:LYS:O | 14:CN:7:ILE:HG13 | 2.15 | 0.47 |
| 18:AR:36:ASN:HB2 | 18:AR:39:VAL:CG2 | 2.45 | 0.47 |
| 1:AA:240:C:H2' | 1:AA:241:C:C6 | 2.49 | 0.47 |
| 23:BA:2025:C:C2 | 23:BA:2026:C:C5 | 3.02 | 0.47 |
| 4:AD:23:GLY:HA3 | 4:AD:112:VAL:CG2 | 2.45 | 0.47 |
| 30:BH:28:ASN:C | 30:BH:32:PRO:HG2 | 2.34 | 0.47 |
| 23:BA:433:C:H2' | 23:BA:434:U:C6 | 2.49 | 0.47 |
| 44:BV:63:ASP:C | 44:BV:65:GLN:H | 2.17 | 0.47 |
| 23:DA:2104:G:H2' | 23:DA:2105:C:C6 | 2.49 | 0.47 |
| 23:DA:136:G:C5 | 23:DA:137(A):C:C5 | 3.02 | 0.47 |
| 1:AA:743:U:O2' | 1:AA:744:C:H5' | 2.13 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DA:13:A:N1 | 23:DA:525:U:C2 | 2.83 | 0.47 |
| 1:CA:1272:G:H2' | 1:CA:1273:G:C8 | 2.49 | 0.47 |
| 23:DA:273(B):G:C2 | 23:DA:364:C:N3 | 2.82 | 0.47 |
| 1:CA:1461:G:O5' | 1:CA:1461:G:H8 | 1.98 | 0.47 |
| 4:CD:8:VAL:HG11 | 4:CD:115:ARG:NH1 | 2.29 | 0.47 |
| 43:DU:68:HIS:ND1 | 43:DU:70:SER:HB3 | 2.29 | 0.47 |
| 1:CA:1372:U:C5 | 1:CA:1373:G:C4 | 3.03 | 0.47 |
| 1:AA:977:A:H2' | 1:AA:978:A:C5' | 2.45 | 0.47 |
| 1:AA:1223:C:P | 19:AS:78:ARG:HH21 | 2.37 | 0.47 |
| 25:BC:6:PHE:HD1 | 25:BC:16:MET:O | 1.97 | 0.47 |
| 23:DA:2846:G:C5 | 23:DA:2847:U:C4 | 3.02 | 0.47 |
| 1:CA:1224:G:H4' | 13:CM:102:ARG:NH2 | 2.30 | 0.47 |
| 41:BS:17:VAL:O | 41:BS:18:ARG:C | 2.51 | 0.47 |
| 53:D5:7:HIS:CB | 53:D5:60:LEU:HB3 | 2.45 | 0.47 |
| 28:DF:72:ARG:HG2 | 28:DF:86:MET:O | 2.14 | 0.47 |
| 1:CA:673:G:H5'' | 6:CF:87:ARG:NH1 | 2.29 | 0.47 |
| 23:DA:2293:C:H5'' | 37:DO:89:ARG:NH1 | 2.30 | 0.47 |
| 37:DO:14:VAL:O | 37:DO:18:ILE:HG12 | 2.15 | 0.47 |
| 47:BY:20:GLU:O | 47:BY:21:LEU:C | 2.52 | 0.47 |
| 26:BD:92:THR:O | 26:BD:95:ILE:HG12 | 2.14 | 0.47 |
| 23:BA:197:A:C8 | 23:BA:197:A:C4' | 2.98 | 0.47 |
| 20:CT:69:GLY:O | 20:CT:73:HIS:ND1 | 2.47 | 0.47 |
| 2:AB:193:ASP:O | 2:AB:196:LEU:HG | 2.15 | 0.47 |
| 44:DV:126:VAL:HG12 | 44:DV:163:LEU:HA | 1.96 | 0.47 |
| 44:DV:56:VAL:HG12 | 44:DV:57:ILE:N | 2.30 | 0.47 |
| 23:BA:2697:G:C2 | 23:BA:2711:A:C2 | 3.03 | 0.47 |
| 4:CD:9:CYS:SG | 4:CD:31:CYS:O | 2.72 | 0.47 |
| 43:DU:29:GLU:O | 43:DU:38:ILE:N | 2.44 | 0.47 |
| 1:AA:130:A:C8 | 17:AQ:63:ARG:HG3 | 2.50 | 0.47 |
| 1:AA:448:A:H2' | 1:AA:449:C:H6 | 1.78 | 0.47 |
| 36:DN:59:ASP:OD1 | 36:DN:61:HIS:HB3 | 2.14 | 0.47 |
| 43:DU:96:ILE:HD11 | 43:DU:99:CYS:SG | 2.54 | 0.47 |
| 5:CE:126:ARG:HH11 | 5:CE:126:ARG:HG3 | 1.75 | 0.47 |
| 36:BN:10:LEU:HB3 | 36:BN:17:ARG:CZ | 2.44 | 0.47 |
| 25:BC:185:VAL:HG12 | 25:BC:186:HIS:H | 1.80 | 0.47 |
| 30:BH:113:ARG:O | 30:BH:131:LYS:N | 2.47 | 0.47 |
| 23:BA:2790:A:H2' | 23:BA:2791:C:C5' | 2.39 | 0.47 |
| 1:AA:1531:A:H8 | 1:AA:1531:A:O5' | 1.96 | 0.47 |
| 37:BO:39:ILE:O | 37:BO:39:ILE:HG22 | 2.14 | 0.47 |
| 23:BA:967:C:O2' | 23:BA:968:G:H5' | 2.14 | 0.47 |
| 4:AD:166:LYS:HD2 | 4:AD:166:LYS:O | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:DK:90:GLN:O | 33:DK:90:GLN:HG3 | 2.15 | 0.47 |
| 1:AA:618:C:N4 | 1:AA:621:A:N7 | 2.63 | 0.47 |
| 23:DA:783:A:C3' | 23:DA:783:A:C8 | 2.98 | 0.47 |
| 15:AO:29:VAL:O | 15:AO:30:ALA:C | 2.51 | 0.47 |
| 44:BV:24:LEU:HD12 | 44:BV:85:HIS:HA | 1.94 | 0.47 |
| 24:DB:49:C:O5' | 24:DB:49:C:H6 | 1.98 | 0.47 |
| 23:BA:2189:U:O2 | 23:BA:2189:U:H2' | 2.15 | 0.47 |
| 38:DP:105:LEU:O | 38:DP:106:SER:C | 2.52 | 0.47 |
| 23:DA:1467:C:C2' | 23:DA:1468:C:H5' | 2.44 | 0.47 |
| 12:AL:21:SER:C | 12:AL:23:VAL:H | 2.16 | 0.47 |
| 1:CA:515:G:N2 | 1:CA:537:G:C4 | 2.83 | 0.47 |
| 23:BA:319:C:H2' | 23:BA:320:A:C8 | 2.49 | 0.47 |
| 23:BA:826:U:H2' | 23:BA:828:U:O4' | 2.14 | 0.47 |
| 23:DA:1248:G:C8 | 39:DQ:3:ARG:HB2 | 2.49 | 0.47 |
| 38:BP:1:MET:O | 38:BP:3:ARG:N | 2.48 | 0.47 |
| 25:DC:257:LEU:C | 25:DC:257:LEU:CD2 | 2.83 | 0.47 |
| 23:DA:2433:A:H5'' | 23:DA:2434:A:OP1 | 2.15 | 0.47 |
| 23:BA:1945:G:H2' | 23:BA:1946:U:C6 | 2.50 | 0.47 |
| 8:AH:118:VAL:HG12 | 8:AH:118:VAL:O | 2.14 | 0.47 |
| 1:CA:1126:U:H2' | 1:CA:1127:G:H8 | 1.76 | 0.47 |
| 35:BM:10:ARG:HD3 | 35:BM:10:ARG:HA | 1.71 | 0.47 |
| 4:CD:4:TYR:CE1 | 4:CD:11:LEU:HD11 | 2.49 | 0.47 |
| 23:DA:2460:U:C4 | 23:DA:2461:C:C5 | 3.02 | 0.47 |
| 24:DB:56:G:H4' | 24:DB:57:A:H8 | 1.80 | 0.47 |
| 12:CL:38:VAL:HG12 | 12:CL:39:VAL:N | 2.29 | 0.47 |
| 8:AH:50:ARG:CD | 8:AH:50:ARG:N | 2.77 | 0.47 |
| 23:DA:779:U:OP1 | 25:DC:49:ILE:HD12 | 2.15 | 0.47 |
| 23:BA:1992:G:OP1 | 23:BA:1992:G:H8 | 1.96 | 0.47 |
| 1:AA:464:G:O6 | 1:AA:466:G:H5' | 2.14 | 0.47 |
| 1:AA:1169:A:N6 | 1:AA:1170:A:N1 | 2.62 | 0.47 |
| 23:BA:2837:G:C6 | 23:BA:2838:G:C5 | 3.03 | 0.47 |
| 1:CA:127:G:HO2' | 17:CQ:2:PRO:N | 2.13 | 0.47 |
| 7:AG:31:MET:CG | 7:AG:35:LYS:H | 2.27 | 0.47 |
| 23:BA:2734:A:C8 | 23:BA:2735:G:C8 | 3.02 | 0.47 |
| 12:AL:54:VAL:HG12 | 12:AL:55:ALA:N | 2.29 | 0.47 |
| 23:DA:338:G:N2 | 23:DA:339:U:H1' | 2.29 | 0.47 |
| 1:AA:757:U:O2' | 1:AA:879:C:H1' | 2.15 | 0.47 |
| 23:DA:13:A:N3 | 23:DA:15:G:C6 | 2.83 | 0.47 |
| 23:DA:1017:G:C2 | 23:DA:1146:C:O2 | 2.68 | 0.47 |
| 28:BF:33:ARG:HD3 | 28:BF:162:THR:HG21 | 1.96 | 0.47 |
| 7:CG:106:GLN:O | 7:CG:110:GLN:HG3 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BA:1196:C:H1' | 23:BA:1226:A:N3 | 2.29 | 0.47 |
| 23:DA:1050:A:C2 | 23:DA:2751:G:C5 | 3.02 | 0.47 |
| 37:DO:79:ALA:O | 37:DO:80:LEU:HD23 | 2.15 | 0.47 |
| 48:DZ:5:LYS:HE2 | 48:DZ:34:GLU:OE1 | 2.14 | 0.47 |
| 40:BR:87:HIS:CD2 | 40:BR:87:HIS:O | 2.67 | 0.47 |
| 23:BA:2813:A:H2' | 23:BA:2814:C:O4' | 2.14 | 0.47 |
| 4:AD:88:VAL:HG13 | 5:AE:97:GLY:CA | 2.44 | 0.47 |
| 23:DA:671:C:H2' | 23:DA:672:C:H6 | 1.79 | 0.47 |
| 23:DA:2393:A:H5'' | 34:DL:62:LEU:HB3 | 1.96 | 0.47 |
| 34:BL:61:ARG:HD2 | 53:B5:13:ARG:HD2 | 1.96 | 0.47 |
| 23:BA:306:U:H2' | 23:BA:307:G:O4' | 2.14 | 0.47 |
| 47:DY:2:LYS:O | 47:DY:5:GLU:HG3 | 2.15 | 0.47 |
| 48:BZ:19:GLN:HE22 | 48:BZ:52:HIS:CE1 | 2.32 | 0.47 |
| 23:DA:85:G:N3 | 23:DA:103:A:C2 | 2.83 | 0.47 |
| 32:DJ:119:GLU:O | 32:DJ:123:GLU:HG3 | 2.14 | 0.47 |
| 1:CA:1346:A:C2 | 1:CA:1348:U:C4 | 3.03 | 0.47 |
| 26:BD:167:VAL:CG1 | 26:BD:189:PRO:HD3 | 2.44 | 0.47 |
| 23:BA:1190:G:H2' | 23:BA:1191:G:H8 | 1.79 | 0.47 |
| 1:AA:365:U:O4' | 1:AA:365:U:O2 | 2.30 | 0.47 |
| 38:DP:57:PHE:CD2 | 38:DP:58:ASN:N | 2.82 | 0.47 |
| 1:AA:953:G:C6 | 1:AA:1229:A:C6 | 3.02 | 0.47 |
| 23:DA:1902:C:H2' | 23:DA:1903:G:O4' | 2.14 | 0.47 |
| 32:DJ:37:VAL:HG12 | 32:DJ:38:LEU:H | 1.80 | 0.47 |
| 36:DN:39:PRO:O | 36:DN:40:LYS:C | 2.53 | 0.47 |
| 27:DE:164:ARG:CG | 27:DE:164:ARG:NH1 | 2.71 | 0.47 |
| 26:BD:137:HIS:CB | 26:BD:138:PRO:HD2 | 2.44 | 0.47 |
| 39:DQ:92:ARG:HG2 | 40:DR:11:GLN:HE21 | 1.74 | 0.47 |
| 35:DM:75:THR:CA | 35:DM:88:GLY:CA | 2.78 | 0.47 |
| 23:DA:1021:A:H8 | 23:DA:1022:G:H5'' | 1.79 | 0.47 |
| 16:CP:20:VAL:CG2 | 16:CP:21:VAL:N | 2.78 | 0.47 |
| 16:CP:32:TYR:HD2 | 16:CP:32:TYR:O | 1.97 | 0.47 |
| 39:BQ:54:LYS:O | 39:BQ:55:ARG:C | 2.51 | 0.47 |
| 34:BL:40:SER:C | 34:BL:41:ARG:HD3 | 2.32 | 0.47 |
| 47:BY:17:SER:O | 47:BY:21:LEU:N | 2.23 | 0.47 |
| 1:AA:376:G:C2 | 1:AA:377:G:C8 | 3.03 | 0.47 |
| 1:AA:376:G:P | 16:AP:67:THR:HG21 | 2.54 | 0.47 |
| 25:DC:143:HIS:CD2 | 25:DC:144:ALA:N | 2.83 | 0.47 |
| 3:CC:19:GLU:HG2 | 3:CC:40:ARG:NH2 | 2.30 | 0.47 |
| 3:AC:148:GLY:HA3 | 3:AC:203:PHE:HB3 | 1.97 | 0.47 |
| 1:AA:409:G:C2' | 1:AA:410:G:O5' | 2.62 | 0.47 |
| 4:CD:61:LYS:HA | 4:CD:203:VAL:CG2 | 2.45 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:428:G:C8 | 1:AA:430:A:C4 | 3.02 | 0.47 |
| 3:CC:182:ILE:HD11 | 3:CC:203:PHE:CD1 | 2.50 | 0.47 |
| 23:DA:72:U:C4 | 23:DA:112:U:H4' | 2.49 | 0.47 |
| 30:DH:123:LEU:HD11 | 30:DH:145:VAL:OXT | 2.14 | 0.47 |
| 30:DH:88:ILE:CG2 | 30:DH:89:TYR:N | 2.78 | 0.47 |
| 23:DA:1639:U:O2' | 23:DA:1640:C:H5'' | 2.15 | 0.47 |
| 24:BB:44:G:N3 | 24:BB:47:C:N4 | 2.62 | 0.47 |
| 44:DV:30:ASN:O | 44:DV:33:LEU:N | 2.48 | 0.47 |
| 1:AA:78:G:N1 | 1:AA:92:G:C6 | 2.83 | 0.47 |
| 25:BC:158:ALA:C | 25:BC:161:THR:HG23 | 2.35 | 0.47 |
| 44:BV:30:ASN:HB3 | 44:BV:90:VAL:HB | 1.97 | 0.47 |
| 37:DO:49:VAL:HG11 | 37:DO:76:LYS:HB2 | 1.97 | 0.47 |
| 37:DO:56:LEU:HG | 37:DO:57:LYS:HB3 | 1.95 | 0.47 |
| 41:BS:8:ARG:O | 41:BS:9:TYR:HB2 | 2.15 | 0.47 |
| 1:AA:1107:C:N3 | 1:AA:1108:G:C8 | 2.83 | 0.47 |
| 3:AC:15:THR:HG21 | 3:AC:181:ASN:CA | 2.44 | 0.47 |
| 14:AN:27:CYS:SG | 14:AN:29:ARG:HB2 | 2.54 | 0.47 |
| 12:CL:53:LYS:N | 12:CL:53:LYS:HD2 | 2.30 | 0.47 |
| 26:BD:120:TRP:NE1 | 26:BD:155:LYS:HB3 | 2.28 | 0.47 |
| 44:DV:128:VAL:CG2 | 44:DV:132:ASN:HB2 | 2.44 | 0.47 |
| 12:CL:44:PRO:CD | 12:CL:50:ALA:H | 2.28 | 0.47 |
| 41:DS:35:ILE:O | 41:DS:36:LEU:C | 2.52 | 0.47 |
| 1:CA:54:C:N4 | 1:CA:353:A:OP2 | 2.48 | 0.47 |
| 43:BU:81:LYS:HD2 | 43:BU:96:ILE:CD1 | 2.43 | 0.47 |
| 36:BN:4:LEU:C | 36:BN:6:SER:N | 2.68 | 0.47 |
| 1:CA:448:A:H2' | 1:CA:449:C:H6 | 1.80 | 0.47 |
| 23:BA:2791:C:H4' | 23:BA:2792:G:OP1 | 2.14 | 0.47 |
| 23:DA:1503:U:H2' | 23:DA:1504:C:C6 | 2.50 | 0.47 |
| 6:CF:44:GLY:HA2 | 6:CF:59:TYR:CE2 | 2.50 | 0.47 |
| 23:DA:1056:G:N2 | 23:DA:1104:C:N3 | 2.63 | 0.47 |
| 23:BA:1109:C:H42 | 23:BA:1110:G:N2 | 2.12 | 0.47 |
| 27:BE:65:TRP:HB3 | 27:BE:66:PRO:HD2 | 1.96 | 0.47 |
| 1:AA:722:A:H2' | 1:AA:724:G:C8 | 2.49 | 0.47 |
| 33:DK:34:THR:HG23 | 33:DK:35:VAL:N | 2.29 | 0.47 |
| 37:BO:34:HIS:ND1 | 37:BO:54:LEU:HB3 | 2.28 | 0.47 |
| 23:BA:1327:C:H2' | 23:BA:1328:G:O4' | 2.15 | 0.47 |
| 1:CA:1149:C:O2' | 1:CA:1280:A:N1 | 2.44 | 0.47 |
| 23:DA:1000:A:H62 | 23:DA:1154:G:H2' | 1.80 | 0.47 |
| 23:BA:1476:C:C2' | 23:BA:1477:A:H5' | 2.45 | 0.47 |
| 1:CA:1116:C:N3 | 1:CA:1117:G:C8 | 2.83 | 0.47 |
| 1:CA:1190:G:OP1 | 3:CC:4:LYS:HA | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:DH:5:LEU:CD2 | 30:DH:5:LEU:N | 2.77 | 0.47 |
| 30:DH:6:LEU:N | 30:DH:6:LEU:HD23 | 2.29 | 0.47 |
| 45:BW:36:ILE:HG23 | 45:BW:58:THR:CG2 | 2.44 | 0.47 |
| 28:BF:106:LEU:HD12 | 28:BF:110:ALA:HB3 | 1.95 | 0.47 |
| 29:BG:92:ILE:HD12 | 29:BG:92:ILE:N | 2.29 | 0.47 |
| 36:BN:113:LEU:HA | 36:BN:113:LEU:HD12 | 1.49 | 0.47 |
| 35:DM:60:ARG:H | 44:DV:179:ASP:CB | 2.27 | 0.47 |
| 33:BK:12:ASP:HA | 33:BK:98:VAL:HA | 1.95 | 0.47 |
| 1:AA:841:U:H4' | 1:AA:842:C:C5 | 2.49 | 0.47 |
| 1:CA:1053:G:C3' | 1:CA:1054:C:C5' | 2.92 | 0.47 |
| 43:BU:76:CYS:O | 43:BU:77:PRO:C | 2.51 | 0.47 |
| 1:AA:1194:U:H4' | 5:AE:22:GLY:O | 2.13 | 0.47 |
| 1:AA:236:G:OP1 | 17:AQ:40:LYS:NZ | 2.48 | 0.47 |
| 1:CA:513:C:C2 | 1:CA:539:A:C2 | 3.02 | 0.47 |
| 23:BA:333:G:C4 | 23:BA:334:C:C5 | 3.02 | 0.47 |
| 23:BA:115:C:O2' | 23:BA:116:C:H5' | 2.15 | 0.47 |
| 32:DJ:160:LYS:HD2 | 32:DJ:160:LYS:HA | 1.53 | 0.47 |
| 23:BA:198:C:H6 | 23:BA:198:C:O5' | 1.98 | 0.47 |
| 23:BA:1788:C:H2' | 23:BA:1789:A:O4' | 2.14 | 0.47 |
| 25:DC:257:LEU:HD23 | 25:DC:258:LYS:N | 2.29 | 0.47 |
| 4:AD:38:TYR:CZ | 4:AD:45:GLN:NE2 | 2.80 | 0.47 |
| 13:CM:24:GLY:O | 13:CM:25:ILE:HD13 | 2.15 | 0.47 |
| 1:AA:560:U:C5' | 1:AA:566:G:N2 | 2.77 | 0.47 |
| 1:AA:1126:U:H2' | 1:AA:1127:G:H8 | 1.74 | 0.47 |
| 7:AG:50:ILE:HB | 7:AG:58:PRO:HG3 | 1.96 | 0.47 |
| 8:AH:119:LEU:HD12 | 8:AH:124:ALA:HA | 1.96 | 0.47 |
| 23:DA:635:C:O2' | 23:DA:639:U:OP1 | 2.33 | 0.47 |
| 1:CA:640:A:N3 | 8:CH:115:SER:HB2 | 2.30 | 0.47 |
| 23:BA:2372:G:O2' | 51:B3:46:HIS:CE1 | 2.67 | 0.47 |
| 1:CA:1261:A:N7 | 1:CA:1262:C:C5 | 2.83 | 0.47 |
| 23:DA:956:G:OP1 | 35:DM:86:GLY:N | 2.47 | 0.47 |
| 36:DN:94:TYR:C | 36:DN:117:VAL:HG12 | 2.35 | 0.47 |
| 30:DH:86:THR:O | 30:DH:86:THR:HG22 | 2.14 | 0.47 |
| 23:DA:49:A:H5'' | 23:DA:51:G:O4' | 2.14 | 0.47 |
| 23:DA:1901:A:N3 | 23:DA:1901:A:C2' | 2.78 | 0.47 |
| 23:DA:1832:C:H2' | 23:DA:1833:U:O4' | 2.15 | 0.47 |
| 1:CA:247:G:C4 | 1:CA:248:C:C5 | 3.03 | 0.47 |
| 1:AA:993:G:N3 | 1:AA:993:G:H2' | 2.30 | 0.47 |
| 11:CK:101:SER:OG | 11:CK:102:GLY:N | 2.48 | 0.47 |
| 8:CH:17:THR:HG21 | 8:CH:80:ILE:HD13 | 1.97 | 0.47 |
| 9:CI:48:GLU:N | 9:CI:49:PRO:CD | 2.77 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:CH:50:ARG:CD | 8:CH:50:ARG:N | 2.77 | 0.47 |
| 1:CA:562:C:C4 | 1:CA:884:U:C5 | 3.03 | 0.47 |
| 23:DA:2039:C:H2' | 23:DA:2040:C:H6 | 1.78 | 0.47 |
| 36:BN:96:ARG:HD2 | 36:BN:115:GLU:OE1 | 2.15 | 0.47 |
| 23:DA:1356:G:C6 | 23:DA:1357:U:C4 | 3.03 | 0.47 |
| 23:DA:2506:U:C5 | 23:DA:2507:C:C5 | 3.03 | 0.47 |
| 1:AA:575:G:C5 | 1:AA:881:G:N2 | 2.83 | 0.47 |
| 1:AA:165:C:H2' | 1:AA:166:G:O4' | 2.14 | 0.47 |
| 30:BH:75:LEU:HG | 30:BH:76:THR:O | 2.15 | 0.47 |
| 23:DA:1231:G:O2' | 23:DA:1232:G:H5' | 2.15 | 0.47 |
| 1:CA:934:C:C5 | 1:CA:1345:U:C6 | 3.03 | 0.47 |
| 41:DS:107:LEU:N | 41:DS:107:LEU:HD13 | 2.29 | 0.47 |
| 1:AA:1438:G:O2' | 1:AA:1439:C:H5' | 2.14 | 0.47 |
| 23:BA:1905:C:O2' | 23:BA:1929:G:H1' | 2.15 | 0.47 |
| 1:AA:1403:C:H6 | 1:AA:1403:C:O5' | 1.98 | 0.47 |
| 36:BN:13:HIS:CE1 | 36:BN:15:SER:HB3 | 2.50 | 0.47 |
| 23:DA:1685:C:O2' | 23:DA:1686:C:H5' | 2.14 | 0.47 |
| 9:AI:8:GLY:HA3 | 9:AI:76:ALA:O | 2.13 | 0.47 |
| 4:AD:176:LEU:HG | 4:AD:178:VAL:HG22 | 1.96 | 0.47 |
| 23:BA:1769:G:C5 | 23:BA:1984:G:C6 | 3.03 | 0.47 |
| 41:BS:79:GLY:C | 41:BS:100:THR:HG22 | 2.35 | 0.47 |
| 1:AA:385:C:H6 | 1:AA:385:C:H3' | 1.78 | 0.47 |
| 29:BG:34:GLU:O | 29:BG:36:PRO:HD3 | 2.15 | 0.47 |
| 1:AA:1272:G:H2' | 1:AA:1273:G:C8 | 2.50 | 0.47 |
| 1:CA:1241:G:C2 | 1:CA:1242:C:C4 | 3.03 | 0.47 |
| 3:CC:79:ARG:O | 3:CC:82:GLU:HG3 | 2.15 | 0.47 |
| 4:CD:76:ARG:NH2 | 4:CD:80:GLU:OE1 | 2.48 | 0.47 |
| 13:CM:81:LEU:HD22 | 13:CM:86:CYS:SG | 2.54 | 0.47 |
| 23:DA:1364:G:OP2 | 46:DX:8:SER:HB2 | 2.14 | 0.47 |
| 1:AA:945:G:C6 | 1:AA:1337:G:C6 | 3.03 | 0.47 |
| 23:BA:500:G:N2 | 23:BA:502:A:H3' | 2.29 | 0.47 |
| 32:BJ:58:ARG:O | 32:BJ:60:LYS:N | 2.48 | 0.47 |
| 49:B1:39:ARG:O | 49:B1:57:ILE:HB | 2.15 | 0.47 |
| 5:CE:60:TYR:C | 5:CE:60:TYR:CD1 | 2.87 | 0.47 |
| 23:DA:2760:C:H2' | 23:DA:2760:C:O2 | 2.13 | 0.47 |
| 23:DA:409:C:O2' | 23:DA:410:G:H5' | 2.15 | 0.47 |
| 23:BA:2330:G:C2' | 23:BA:2331:G:H5' | 2.44 | 0.47 |
| 26:DD:104:VAL:HG11 | 26:DD:188:VAL:HG21 | 1.95 | 0.47 |
| 23:BA:861:A:H2' | 23:BA:862:G:O4' | 2.14 | 0.47 |
| 24:BB:83:G:C6 | 24:BB:84:C:C5 | 3.03 | 0.47 |
| 1:AA:1308:U:OP1 | 13:AM:97:PRO:HA | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:979:C:C5 | 1:AA:980:C:C6 | 3.03 | 0.47 |
| 27:DE:65:TRP:CH2 | 27:DE:75:HIS:HD2 | 2.33 | 0.47 |
| 32:DJ:37:VAL:HG12 | 32:DJ:38:LEU:N | 2.29 | 0.47 |
| 39:DQ:92:ARG:O | 39:DQ:94:ASN:N | 2.48 | 0.47 |
| 40:DR:47:VAL:CG1 | 40:DR:50:PRO:O | 2.63 | 0.47 |
| 30:BH:69:LYS:HD3 | 30:BH:138:ILE:HG12 | 1.96 | 0.47 |
| 23:DA:1799:G:C8 | 25:DC:181:GLU:CD | 2.88 | 0.47 |
| 1:AA:403:C:O2' | 1:AA:404:U:H5' | 2.14 | 0.47 |
| 1:AA:408:A:C2 | 1:AA:409:G:C4 | 3.03 | 0.47 |
| 1:AA:35:G:O2' | 12:AL:117:SER:O | 2.28 | 0.47 |
| 30:DH:110:ASP:HB3 | 30:DH:111:PRO:HD2 | 1.95 | 0.47 |
| 23:DA:2697:G:C2 | 23:DA:2711:A:C2 | 3.02 | 0.47 |
| 23:BA:94:G:N3 | 47:BY:47:ASN:ND2 | 2.62 | 0.47 |
| 1:CA:187:C:H2' | 1:CA:188:U:O4' | 2.14 | 0.47 |
| 39:DQ:60:LEU:HD22 | 39:DQ:60:LEU:O | 2.15 | 0.47 |
| 49:B1:40:ILE:HG23 | 49:B1:59:VAL:CG2 | 2.45 | 0.47 |
| 23:DA:2723:C:H4' | 36:DN:2:ARG:HH21 | 1.78 | 0.47 |
| 4:AD:63:LYS:HD2 | 4:AD:198:VAL:CG2 | 2.44 | 0.47 |
| 25:BC:248:SER:HB2 | 25:BC:250:TRP:CE3 | 2.49 | 0.47 |
| 37:DO:58:LEU:HD12 | 37:DO:58:LEU:N | 2.30 | 0.47 |
| 26:DD:57:LYS:CG | 26:DD:58:ARG:N | 2.78 | 0.47 |
| 29:DG:72:ILE:O | 29:DG:75:ALA:N | 2.47 | 0.47 |
| 48:BZ:28:LEU:CD1 | 48:BZ:28:LEU:N | 2.76 | 0.47 |
| 1:CA:437:U:C4 | 1:CA:438:G:C6 | 3.03 | 0.47 |
| 25:DC:223:GLY:HA3 | 25:DC:231:HIS:ND1 | 2.30 | 0.47 |
| 46:DX:11:ARG:HB3 | 46:DX:12:PRO:HD3 | 1.91 | 0.47 |
| 7:AG:9:VAL:HG12 | 7:AG:10:ARG:H | 1.79 | 0.47 |
| 36:DN:47:PHE:O | 36:DN:51:LEU:HD12 | 2.14 | 0.47 |
| 41:DS:36:LEU:HD12 | 41:DS:48:ALA:CA | 2.45 | 0.47 |
| 30:BH:110:ASP:OD2 | 30:BH:113:ARG:HG3 | 2.14 | 0.47 |
| 4:CD:128:VAL:HA | 4:CD:145:GLU:O | 2.15 | 0.47 |
| 46:BX:46:LEU:HD21 | 46:BX:61:ARG:HG3 | 1.96 | 0.47 |
| 1:AA:749:C:O2 | 1:AA:749:C:H2' | 2.14 | 0.47 |
| 23:BA:1056:G:N2 | 23:BA:1104:C:N3 | 2.63 | 0.47 |
| 1:CA:1530:G:H2' | 1:CA:1531:A:C8 | 2.50 | 0.47 |
| 23:BA:1314:C:OP1 | 23:BA:1332:G:H5'' | 2.15 | 0.47 |
| 23:BA:2629:A:N3 | 23:BA:2629:A:H2' | 2.29 | 0.47 |
| 23:DA:955:C:OP1 | 35:DM:85:LYS:HE2 | 2.14 | 0.47 |
| 28:DF:131:TYR:CE2 | 28:DF:133:LEU:HB3 | 2.49 | 0.47 |
| 1:AA:101:A:C6 | 1:AA:102:G:C5 | 3.02 | 0.47 |
| 23:DA:282:A:C4 | 23:DA:359:A:C2 | 3.03 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:BK:90:GLN:HG3 | 33:BK:90:GLN:O | 2.14 | 0.47 |
| 38:BP:88:ILE:CD1 | 38:BP:89:VAL:H | 2.27 | 0.47 |
| 17:CQ:59:ILE:HG23 | 17:CQ:71:PHE:HD1 | 1.79 | 0.47 |
| 29:BG:92:ILE:O | 29:BG:93:GLY:C | 2.53 | 0.47 |
| 44:BV:85:HIS:ND1 | 44:BV:85:HIS:C | 2.68 | 0.47 |
| 24:DB:19:G:N2 | 24:DB:65:C:C2 | 2.83 | 0.47 |
| 6:CF:50:TYR:CE1 | 18:CR:77:GLY:HA2 | 2.50 | 0.47 |
| 24:DB:59:A:H2' | 24:DB:60:C:O4' | 2.15 | 0.47 |
| 23:DA:2189:U:H2' | 23:DA:2189:U:O2 | 2.14 | 0.47 |
| 27:DE:36:VAL:HG11 | 27:DE:183:VAL:CG1 | 2.45 | 0.47 |
| 8:AH:51:VAL:HG21 | 8:AH:60:ARG:HG2 | 1.94 | 0.47 |
| 44:DV:13:GLU:CD | 44:DV:13:GLU:H | 2.18 | 0.47 |
| 1:CA:1443:G:H22 | 38:DP:119:LYS:CB | 2.28 | 0.47 |
| 44:DV:82:ARG:HG2 | 44:DV:83:PRO:HD2 | 1.97 | 0.47 |
| 1:CA:650:G:C2 | 1:CA:651:C:C6 | 3.03 | 0.47 |
| 1:AA:1056:U:H5 | 1:AA:1200:C:N4 | 2.13 | 0.47 |
| 23:DA:2401:U:O2' | 23:DA:2402:C:H5'' | 2.14 | 0.47 |
| 1:CA:730:G:C5 | 1:CA:731:G:H1' | 2.50 | 0.47 |
| 1:CA:976:G:H5'' | 1:CA:1358:U:O2' | 2.14 | 0.47 |
| 32:DJ:101:TYR:N | 32:DJ:101:TYR:CD1 | 2.83 | 0.47 |
| 3:AC:175:LEU:CD1 | 3:AC:201:TYR:HE2 | 2.27 | 0.47 |
| 1:CA:1429:C:H2' | 1:CA:1430:C:C6 | 2.50 | 0.47 |
| 1:CA:1298:C:H4' | 1:CA:1299:A:C4 | 2.49 | 0.47 |
| 23:BA:2663:G:C5 | 23:BA:2664:G:C5 | 3.02 | 0.47 |
| 23:BA:1894:C:H2' | 23:BA:1895:C:H6 | 1.80 | 0.47 |
| 25:BC:260:ARG:HG2 | 25:BC:260:ARG:O | 2.15 | 0.47 |
| 23:BA:1920:C:H2' | 23:BA:1920:C:O2 | 2.14 | 0.47 |
| 23:DA:27:G:C4 | 23:DA:512:G:N2 | 2.82 | 0.47 |
| 1:AA:562:C:N3 | 1:AA:884:U:C5 | 2.83 | 0.47 |
| 1:AA:479:C:C2 | 1:AA:480:U:C6 | 3.03 | 0.47 |
| 23:DA:165:U:H2' | 23:DA:171:G:O4' | 2.14 | 0.47 |
| 48:DZ:50:VAL:O | 48:DZ:50:VAL:HG23 | 2.14 | 0.47 |
| 12:AL:19:LYS:HD3 | 12:AL:19:LYS:N | 2.30 | 0.47 |
| 23:DA:948:G:N2 | 23:DA:970:C:O2 | 2.48 | 0.47 |
| 1:CA:191(G):G:C4 | 1:CA:192:U:C5 | 3.02 | 0.47 |
| 1:CA:191(G):G:H2' | 1:CA:192:U:C6 | 2.50 | 0.47 |
| 1:CA:1038:C:C2 | 1:CA:1039:C:C5 | 3.03 | 0.47 |
| 1:CA:897:C:H42 | 1:CA:902:G:H1 | 1.63 | 0.47 |
| 23:BA:1678:G:H22 | 23:BA:1989:G:H22 | 1.63 | 0.47 |
| 23:BA:2298:A:H2' | 23:BA:2299:G:O4' | 2.15 | 0.47 |
| 1:CA:1438:G:C5 | 1:CA:1439:C:C5 | 3.02 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:744:C:C6 | 1:AA:744:C:H3' | 2.49 | 0.47 |
| 23:DA:896:A:H1' | 44:DV:176:PRO:HG3 | 1.96 | 0.47 |
| 41:DS:10:VAL:HG23 | 41:DS:101:SER:O | 2.15 | 0.47 |
| 23:BA:1668:A:N7 | 23:BA:1674:G:C6 | 2.83 | 0.47 |
| 42:DT:18:TYR:CD1 | 42:DT:18:TYR:N | 2.79 | 0.47 |
| 8:CH:74:PRO:O | 8:CH:76:PRO:HD3 | 2.13 | 0.47 |
| 29:BG:105:LEU:HD23 | 29:BG:105:LEU:N | 2.30 | 0.47 |
| 23:BA:1790:C:H2' | 23:BA:1791:A:C5 | 2.49 | 0.47 |
| 1:AA:1400:C:H6 | 1:AA:1400:C:O5' | 1.98 | 0.47 |
| 32:BJ:151:HIS:CD2 | 32:BJ:151:HIS:C | 2.87 | 0.47 |
| 27:BE:156:LEU:HD12 | 27:BE:193:VAL:HG12 | 1.97 | 0.47 |
| 23:BA:2193:G:O2' | 23:BA:2194:G:H5' | 2.14 | 0.47 |
| 34:DL:66:GLY:O | 34:DL:67:MET:HB2 | 2.15 | 0.47 |
| 23:DA:2439:A:O2' | 23:DA:2440:C:OP2 | 2.25 | 0.47 |
| 23:BA:747:U:N3 | 50:B2:2:ALA:N | 2.63 | 0.47 |
| 26:DD:101:ARG:HB3 | 26:DD:169:ASN:HD22 | 1.80 | 0.47 |
| 26:DD:167:VAL:CG1 | 26:DD:189:PRO:HD3 | 2.44 | 0.47 |
| 43:DU:17:SER:CB | 43:DU:71:LYS:HD2 | 2.45 | 0.47 |
| 38:DP:51:ARG:CD | 38:DP:62:THR:HG23 | 2.43 | 0.47 |
| 1:CA:1367:C:C2 | 1:CA:1368:G:C8 | 3.03 | 0.47 |
| 1:CA:954:G:H2' | 1:CA:955:U:C6 | 2.50 | 0.47 |
| 23:BA:1021:A:H8 | 23:BA:1022:G:H5'' | 1.80 | 0.47 |
| 34:DL:51:PHE:HB3 | 34:DL:52:GLU:H | 1.39 | 0.47 |
| 40:BR:47:VAL:HG11 | 40:BR:50:PRO:O | 2.15 | 0.47 |
| 1:AA:373:A:C2 | 1:AA:482:A:N6 | 2.82 | 0.47 |
| 1:CA:392:G:C4 | 1:CA:393:A:N7 | 2.83 | 0.47 |
| 30:DH:68:LEU:O | 30:DH:72:LEU:HB2 | 2.15 | 0.47 |
| 26:BD:57:LYS:CG | 26:BD:58:ARG:N | 2.78 | 0.47 |
| 1:CA:37:U:H2' | 1:CA:38:G:C8 | 2.50 | 0.47 |
| 27:BE:173:VAL:HG12 | 27:BE:174:VAL:N | 2.29 | 0.47 |
| 37:DO:62:LYS:O | 37:DO:65:VAL:HB | 2.14 | 0.47 |
| 1:CA:1075:C:OP1 | 2:CB:103:THR:HG21 | 2.15 | 0.47 |
| 2:AB:100:GLY:O | 2:AB:104:ASN:N | 2.47 | 0.47 |
| 1:CA:404:U:H2' | 1:CA:405:U:C6 | 2.46 | 0.47 |
| 46:DX:9:GLY:O | 46:DX:13:ILE:CG2 | 2.63 | 0.47 |
| 10:AJ:33:GLN:HB2 | 10:AJ:75:ILE:CD1 | 2.45 | 0.47 |
| 1:CA:1301:U:H3' | 1:CA:1302:U:C5' | 2.45 | 0.47 |
| 1:CA:692:U:H2' | 1:CA:694:A:OP2 | 2.15 | 0.47 |
| 1:AA:1292:U:N3 | 1:AA:1293:G:N7 | 2.63 | 0.47 |
| 41:DS:48:ALA:O | 41:DS:51:LEU:N | 2.48 | 0.47 |
| 1:CA:59:A:H5'' | 1:CA:60:A:C5' | 2.44 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 36:BN:60:LEU:HA | 36:BN:63:ARG:HB3 | 1.95 | 0.47 |
| 2:AB:27:LYS:CG | 2:AB:194:PRO:HD2 | 2.41 | 0.47 |
| 23:DA:2744:G:N3 | 23:DA:2761:G:C2 | 2.83 | 0.47 |
| 23:BA:84:A:H4' | 23:BA:85:G:O5' | 2.15 | 0.47 |
| 1:AA:1530:G:H2' | 1:AA:1531:A:C8 | 2.50 | 0.47 |
| 15:AO:18:PHE:O | 15:AO:19:PRO:O | 2.32 | 0.47 |
| 27:BE:66:PRO:HB3 | 27:BE:68:LYS:NZ | 2.30 | 0.47 |
| 29:DG:29:PRO:HD2 | 29:DG:79:VAL:O | 2.15 | 0.47 |
| 23:DA:2562:U:C2' | 23:DA:2563:U:H5' | 2.45 | 0.47 |
| 28:DF:111:LEU:HA | 28:DF:114:ILE:CD1 | 2.45 | 0.47 |
| 6:CF:98:LEU:CD1 | 6:CF:101:ALA:HB2 | 2.41 | 0.47 |
| 9:CI:58:ARG:HG2 | 9:CI:58:ARG:O | 2.14 | 0.47 |
| 23:BA:2476:A:N3 | 23:BA:2476:A:C2' | 2.77 | 0.47 |
| 4:CD:38:TYR:CZ | 4:CD:45:GLN:NE2 | 2.81 | 0.47 |
| 1:CA:592:G:H2' | 1:CA:593:G:H8 | 1.79 | 0.47 |
| 17:CQ:29:HIS:CE1 | 17:CQ:32:TYR:HD1 | 2.32 | 0.47 |
| 30:DH:2:LYS:HB3 | 30:DH:20:ASP:OD1 | 2.15 | 0.47 |
| 23:BA:302:C:H2' | 23:BA:303:U:H6 | 1.76 | 0.47 |
| 1:CA:576:G:N2 | 1:CA:759:A:OP1 | 2.48 | 0.47 |
| 1:CA:17:U:H2' | 1:CA:18:C:C6 | 2.49 | 0.47 |
| 6:AF:50:TYR:CE1 | 18:AR:74:ARG:O | 2.68 | 0.47 |
| 6:CF:47:ARG:HH12 | 6:CF:56:PRO:HB2 | 1.80 | 0.47 |
| 35:DM:32:PHE:CZ | 35:DM:111:GLU:HG2 | 2.46 | 0.47 |
| 38:DP:41:ARG:CB | 38:DP:41:ARG:NH1 | 2.78 | 0.47 |
| 36:BN:84:ALA:N | 36:BN:85:PRO:HD2 | 2.30 | 0.47 |
| 23:DA:1218:C:OP2 | 39:DQ:15:LYS:NZ | 2.39 | 0.47 |
| 1:AA:1261:A:N7 | 1:AA:1262:C:C5 | 2.83 | 0.47 |
| 7:CG:30:ILE:HD13 | 7:CG:105:VAL:HG13 | 1.97 | 0.47 |
| 23:DA:2298:A:H2' | 23:DA:2299:G:O4' | 2.15 | 0.47 |
| 1:CA:1386:G:N3 | 1:CA:1387:G:C8 | 2.83 | 0.47 |
| 23:BA:1027:A:C6 | 23:BA:1126:A:C5 | 3.03 | 0.47 |
| 23:DA:2617:C:O2' | 23:DA:2618:G:H5' | 2.14 | 0.47 |
| 1:AA:247:G:C5 | 1:AA:248:C:C5 | 3.03 | 0.47 |
| 3:AC:125:GLU:OE2 | 3:AC:189:ALA:HA | 2.14 | 0.47 |
| 1:CA:1480:G:C4 | 1:CA:1481:U:C6 | 3.03 | 0.47 |
| 23:BA:2079:U:H2' | 23:BA:2080:G:O4' | 2.15 | 0.47 |
| 23:DA:1015:G:H2' | 23:DA:1016:G:H5' | 1.96 | 0.47 |
| 11:CK:86:GLY:C | 11:CK:88:GLY:H | 2.18 | 0.47 |
| 1:CA:165:C:H2' | 1:CA:166:G:O4' | 2.14 | 0.47 |
| 23:BA:26:G:C6 | 23:BA:27:G:N1 | 2.83 | 0.47 |
| 23:BA:1570:A:H4' | 25:BC:38:LYS:HE2 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:837:G:H1 | 1:AA:849:C:H42 | 1.63 | 0.47 |
| 24:BB:87:G:N2 | 24:BB:89(A):G:C8 | 2.83 | 0.47 |
| 23:BA:270(F):G:H2' | 23:BA:270(G):U:O4' | 2.14 | 0.47 |
| 23:DA:1897:G:H2' | 23:DA:1898:U:O4' | 2.15 | 0.47 |
| 23:BA:1751:C:H2' | 23:BA:1752:C:C6 | 2.50 | 0.47 |
| 23:DA:2011:U:H2' | 23:DA:2012:G:O4' | 2.14 | 0.47 |
| 23:DA:487:C:H1' | 41:DS:53:SER:HB2 | 1.97 | 0.47 |
| 11:CK:115:PRO:C | 11:CK:117:ASN:H | 2.17 | 0.47 |
| 23:DA:2405:G:O2' | 23:DA:2411:A:N6 | 2.46 | 0.47 |
| 23:DA:2409:G:C6 | 23:DA:2410:G:C5 | 3.03 | 0.47 |
| 16:AP:1:MET:HG2 | 16:AP:2:VAL:O | 2.14 | 0.47 |
| 43:BU:17:SER:HB2 | 43:BU:71:LYS:HD2 | 1.98 | 0.47 |
| 32:BJ:143:LEU:CD1 | 32:BJ:143:LEU:C | 2.82 | 0.47 |
| 24:BB:81:G:C6 | 24:BB:82:G:N7 | 2.83 | 0.47 |
| 28:DF:64:THR:HG23 | 28:DF:66:GLN:N | 2.29 | 0.47 |
| 1:AA:84:U:H5'' | 1:AA:85:U:OP2 | 2.15 | 0.47 |
| 10:AJ:55:LYS:O | 10:AJ:56:HIS:CG | 2.68 | 0.47 |
| 1:CA:1226:C:H2' | 13:CM:103:THR:CB | 2.42 | 0.47 |
| 23:BA:2291:U:O2' | 23:BA:2374:C:O2 | 2.32 | 0.47 |
| 23:BA:1826:G:OP1 | 25:BC:233:HIS:CD2 | 2.63 | 0.47 |
| 23:DA:2731:G:H2' | 23:DA:2732:G:C8 | 2.50 | 0.47 |
| 53:B5:11:LYS:N | 53:B5:61:LEU:HD21 | 2.30 | 0.47 |
| 1:AA:376:G:C4 | 1:AA:389:A:N1 | 2.83 | 0.47 |
| 1:CA:391:G:C5 | 1:CA:392:G:C8 | 3.03 | 0.47 |
| 3:CC:114:PRO:HD3 | 3:CC:183:ASP:OD1 | 2.15 | 0.47 |
| 4:CD:21:LEU:HD12 | 4:CD:21:LEU:N | 2.28 | 0.47 |
| 23:BA:1812:A:C2 | 23:BA:1813:G:C4 | 3.03 | 0.47 |
| 30:DH:79:ILE:HG22 | 30:DH:81:VAL:CG2 | 2.43 | 0.47 |
| 40:DR:76:LYS:O | 40:DR:79:VAL:HG12 | 2.14 | 0.47 |
| 44:DV:92:SER:O | 44:DV:93:ASP:HB3 | 2.14 | 0.47 |
| 1:AA:1076:C:C2' | 1:AA:1077:G:H5' | 2.45 | 0.47 |
| 1:AA:1080:A:C5' | 1:AA:1081:G:OP2 | 2.63 | 0.47 |
| 1:AA:1192:C:OP2 | 3:AC:4:LYS:NZ | 2.36 | 0.47 |
| 23:DA:1586:A:H2' | 23:DA:1587:A:H5' | 1.97 | 0.47 |
| 6:AF:30:LEU:HD11 | 6:AF:63:TYR:CE1 | 2.50 | 0.47 |
| 25:BC:134:ARG:HG3 | 25:BC:135:PHE:HD1 | 1.79 | 0.47 |
| 23:BA:2745:C:C4 | 23:BA:2746:U:C5 | 3.03 | 0.47 |
| 15:CO:81:LEU:HD12 | 15:CO:81:LEU:O | 2.15 | 0.47 |
| 53:B5:22:VAL:CB | 53:B5:54:GLU:HG3 | 2.41 | 0.47 |
| 1:CA:101:A:C6 | 1:CA:102:G:C5 | 3.03 | 0.47 |
| 34:BL:10:PRO:CD | 34:BL:11:GLY:H | 2.26 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:BN:48:VAL:O | 36:BN:51:LEU:N | 2.48 | 0.47 |
| 8:CH:49:GLU:HG3 | 8:CH:51:VAL:HG23 | 1.96 | 0.47 |
| 23:DA:2477:C:O2' | 23:DA:2478:A:OP2 | 2.30 | 0.47 |
| 23:BA:781:A:H2' | 23:BA:1777:U:O2' | 2.15 | 0.47 |
| 23:BA:627:A:C5 | 23:BA:637:A:N7 | 2.83 | 0.47 |
| 34:BL:85:LEU:HD22 | 34:BL:85:LEU:H | 1.79 | 0.47 |
| 23:DA:1024:G:OP2 | 23:DA:1025:G:H3' | 2.16 | 0.47 |
| 23:BA:987:G:H2' | 23:BA:988:A:C5' | 2.45 | 0.47 |
| 6:AF:50:TYR:HE1 | 18:AR:74:ARG:O | 1.97 | 0.47 |
| 23:DA:1894:C:C2 | 23:DA:1895:C:C5 | 3.02 | 0.47 |
| 23:BA:60:G:C6 | 23:BA:74:A:N6 | 2.83 | 0.47 |
| 53:D5:29:LYS:O | 53:D5:29:LYS:HG2 | 2.15 | 0.47 |
| 23:BA:164:U:C4 | 23:BA:165:U:C4 | 3.03 | 0.47 |
| 18:CR:45:SER:H | 18:CR:51:LEU:CD1 | 2.28 | 0.47 |
| 48:DZ:19:GLN:O | 48:DZ:23:LEU:HD13 | 2.14 | 0.47 |
| 9:AI:48:GLU:N | 9:AI:49:PRO:CD | 2.78 | 0.47 |
| 1:CA:1305:G:H5'' | 21:CU:4:GLY:C | 2.35 | 0.47 |
| 23:DA:2584:U:O5' | 23:DA:2584:U:C6 | 2.68 | 0.47 |
| 11:AK:111:ASP:O | 11:AK:112:THR:C | 2.53 | 0.47 |
| 37:DO:20:ARG:HH12 | 45:DW:47:PRO:HB2 | 1.79 | 0.47 |
| 23:BA:1301:A:H2 | 23:BA:1626:G:N3 | 2.12 | 0.47 |
| 50:D2:6:VAL:HG13 | 50:D2:7:PRO:HD2 | 1.97 | 0.47 |
| 23:BA:735:A:C8 | 23:BA:736:C:C5 | 3.03 | 0.47 |
| 1:AA:1493:A:H4' | 1:AA:1494:G:OP2 | 2.15 | 0.47 |
| 23:BA:769:G:C2' | 23:BA:770:G:H5' | 2.45 | 0.47 |
| 23:DA:153:C:OP1 | 46:DX:92:LYS:HE2 | 2.15 | 0.47 |
| 23:BA:1421:G:C2 | 23:BA:1422:G:C8 | 3.02 | 0.47 |
| 44:DV:46:LYS:O | 44:DV:50:GLN:OE1 | 2.33 | 0.47 |
| 34:DL:62:LEU:HD21 | 53:D5:25:MET:HB2 | 1.97 | 0.46 |
| 23:BA:2416:C:H6 | 23:BA:2416:C:O5' | 1.97 | 0.46 |
| 23:BA:2416:C:C4 | 23:BA:2417:C:C5 | 3.03 | 0.46 |
| 10:AJ:48:THR:CG2 | 10:AJ:62:HIS:ND1 | 2.75 | 0.46 |
| 43:DU:68:HIS:C | 43:DU:70:SER:H | 2.19 | 0.46 |
| 38:DP:64:ARG:HD2 | 38:DP:73:GLU:CG | 2.45 | 0.46 |
| 1:CA:1353:G:H1 | 1:CA:1369:C:N4 | 2.12 | 0.46 |
| 1:CA:84:U:H5'' | 1:CA:85:U:OP2 | 2.14 | 0.46 |
| 34:DL:38:GLN:CG | 34:DL:39:LYS:N | 2.71 | 0.46 |
| 23:DA:1657:C:O2' | 23:DA:1658:C:H5' | 2.16 | 0.46 |
| 39:DQ:83:LEU:HD12 | 39:DQ:83:LEU:N | 2.30 | 0.46 |
| 41:DS:86:LEU:C | 41:DS:86:LEU:HD12 | 2.35 | 0.46 |
| 1:CA:376:G:O2' | 1:CA:377:G:C5' | 2.63 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:CP:28:ARG:NH1 | 16:CP:28:ARG:HG2 | 2.14 | 0.46 |
| 30:BH:82:ARG:HB3 | 30:BH:89:TYR:CB | 2.45 | 0.46 |
| 26:DD:137:HIS:CB | 26:DD:138:PRO:HD2 | 2.44 | 0.46 |
| 13:CM:56:LEU:O | 13:CM:59:TYR:HB3 | 2.14 | 0.46 |
| 26:BD:86:PRO:HB2 | 26:BD:87:GLU:H | 1.38 | 0.46 |
| 1:CA:78:G:N1 | 1:CA:92:G:C6 | 2.84 | 0.46 |
| 2:CB:167:PRO:HG3 | 2:CB:188:ALA:HB2 | 1.96 | 0.46 |
| 26:DD:35:GLN:HG2 | 26:DD:36:ARG:N | 2.30 | 0.46 |
| 1:CA:1104:G:N1 | 1:CA:1105:A:C5 | 2.82 | 0.46 |
| 1:AA:1072:G:O6 | 1:AA:1104:G:C6 | 2.68 | 0.46 |
| 46:DX:9:GLY:O | 46:DX:13:ILE:HG21 | 2.15 | 0.46 |
| 10:CJ:33:GLN:HB2 | 10:CJ:75:ILE:CD1 | 2.46 | 0.46 |
| 12:CL:52:ARG:HG2 | 12:CL:52:ARG:HH11 | 1.73 | 0.46 |
| 4:CD:129:ASN:OD1 | 4:CD:129:ASN:N | 2.48 | 0.46 |
| 18:AR:37:VAL:HG23 | 18:AR:38:GLU:N | 2.30 | 0.46 |
| 1:CA:11:G:C5 | 1:CA:12:U:C5 | 3.03 | 0.46 |
| 43:BU:81:LYS:CD | 43:BU:96:ILE:HG13 | 2.45 | 0.46 |
| 23:BA:1884:A:C2 | 23:BA:1885:A:C8 | 3.03 | 0.46 |
| 25:BC:79:VAL:HG11 | 25:BC:111:LEU:CD1 | 2.45 | 0.46 |
| 23:BA:1486:A:N1 | 23:BA:1504:C:C4 | 2.83 | 0.46 |
| 29:BG:20:ALA:HB1 | 29:BG:21:PRO:HD2 | 1.95 | 0.46 |
| 23:BA:1313:U:H4' | 23:BA:1332:G:H4' | 1.98 | 0.46 |
| 23:DA:1418:G:O5' | 23:DA:1418:G:C8 | 2.54 | 0.46 |
| 25:DC:134:ARG:HG3 | 25:DC:135:PHE:HD1 | 1.75 | 0.46 |
| 8:AH:11:THR:O | 8:AH:12:ARG:C | 2.52 | 0.46 |
| 1:AA:1116:C:N3 | 1:AA:1117:G:C8 | 2.83 | 0.46 |
| 23:DA:2274:A:C5 | 23:DA:2276:G:C8 | 3.03 | 0.46 |
| 23:DA:2550:G:C6 | 23:DA:2551:C:C4 | 3.03 | 0.46 |
| 1:AA:855:G:C6 | 1:AA:856:C:C4 | 3.03 | 0.46 |
| 27:BE:52:LYS:HB3 | 27:BE:56:GLU:HB2 | 1.96 | 0.46 |
| 34:DL:70:GLN:O | 34:DL:73:GLY:N | 2.48 | 0.46 |
| 23:DA:8:A:C5 | 23:DA:9:U:O4 | 2.68 | 0.46 |
| 1:CA:173:U:C2 | 1:CA:197:A:C2 | 3.04 | 0.46 |
| 23:BA:2590:A:O2' | 23:BA:2591:C:H5' | 2.14 | 0.46 |
| 4:AD:102:ASP:OD2 | 4:AD:136:PRO:HB3 | 2.15 | 0.46 |
| 10:CJ:58:ASP:C | 10:CJ:60:ARG:N | 2.69 | 0.46 |
| 24:DB:21:G:H2' | 24:DB:22:U:O4' | 2.15 | 0.46 |
| 29:DG:92:ILE:HD12 | 29:DG:92:ILE:N | 2.30 | 0.46 |
| 17:CQ:54:GLY:HA3 | 17:CQ:82:MET:CE | 2.45 | 0.46 |
| 32:BJ:69:VAL:CG1 | 32:BJ:71:MET:HG3 | 2.42 | 0.46 |
| 1:AA:236:G:C6 | 1:AA:237:C:C4 | 3.03 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:CD:52:SER:C | 4:CD:54:TYR:N | 2.67 | 0.46 |
| 23:BA:1728:G:H3' | 23:BA:1728:G:C8 | 2.50 | 0.46 |
| 1:CA:762:C:C2 | 1:CA:763:G:C8 | 3.03 | 0.46 |
| 27:BE:46:ARG:CZ | 27:BE:46:ARG:HB3 | 2.45 | 0.46 |
| 1:CA:976:G:C8 | 1:CA:1358:U:C2' | 2.96 | 0.46 |
| 23:DA:229:A:H5' | 23:DA:230:U:O5' | 2.15 | 0.46 |
| 13:CM:70:LEU:C | 13:CM:70:LEU:HD23 | 2.35 | 0.46 |
| 1:CA:560:U:C5' | 1:CA:566:G:N2 | 2.78 | 0.46 |
| 7:CG:17:VAL:HG21 | 7:CG:44:TYR:CE2 | 2.50 | 0.46 |
| 8:CH:118:VAL:O | 8:CH:118:VAL:HG12 | 2.15 | 0.46 |
| 43:BU:6:HIS:CD2 | 43:BU:35:TYR:CE1 | 3.00 | 0.46 |
| 1:AA:1090:U:H2' | 1:AA:1091:U:H6 | 1.80 | 0.46 |
| 23:DA:442:G:H4' | 27:DE:46:ARG:HD3 | 1.96 | 0.46 |
| 14:AN:26:ARG:HD2 | 14:AN:47:LEU:HD11 | 1.96 | 0.46 |
| 23:BA:2228:G:P | 25:BC:263:ARG:HH21 | 2.38 | 0.46 |
| 1:AA:114:U:H2' | 1:AA:115:G:H8 | 1.76 | 0.46 |
| 1:AA:1059:C:O2 | 10:AJ:53:PRO:HG2 | 2.15 | 0.46 |
| 35:BM:116:GLU:O | 35:BM:117:ALA:C | 2.54 | 0.46 |
| 1:CA:152:A:H62 | 1:CA:169:C:H42 | 1.63 | 0.46 |
| 1:AA:464:G:C6 | 1:AA:466:G:H5' | 2.50 | 0.46 |
| 41:DS:45:TYR:CD2 | 41:DS:46:PHE:CD1 | 3.01 | 0.46 |
| 23:DA:164:U:C4 | 23:DA:165:U:C4 | 3.03 | 0.46 |
| 23:BA:2837:G:C5 | 23:BA:2838:G:N7 | 2.84 | 0.46 |
| 23:BA:1471:A:N7 | 23:BA:1522:G:C6 | 2.83 | 0.46 |
| 23:DA:2823:A:C5 | 23:DA:2824:C:C5 | 3.04 | 0.46 |
| 7:CG:80:VAL:C | 7:CG:82:GLY:H | 2.19 | 0.46 |
| 35:BM:77:LYS:NZ | 35:BM:84:GLY:O | 2.42 | 0.46 |
| 25:BC:198:ASN:C | 25:BC:198:ASN:ND2 | 2.69 | 0.46 |
| 23:BA:298:G:P | 43:BU:85:VAL:HG22 | 2.55 | 0.46 |
| 48:BZ:3:ARG:HH11 | 48:BZ:59:VAL:HG11 | 1.79 | 0.46 |
| 23:DA:2027:G:H2' | 23:DA:2028:U:O4' | 2.15 | 0.46 |
| 1:CA:1244:C:H2' | 1:CA:1245:A:H8 | 1.79 | 0.46 |
| 23:DA:2410:G:H2' | 23:DA:2411:A:O4' | 2.15 | 0.46 |
| 23:BA:769:G:O2' | 23:BA:770:G:H5' | 2.15 | 0.46 |
| 1:AA:654:G:H1' | 1:AA:753:A:N1 | 2.31 | 0.46 |
| 42:BT:40:LYS:O | 42:BT:42:ALA:N | 2.47 | 0.46 |
| 16:CP:75:ARG:C | 16:CP:77:ALA:H | 2.18 | 0.46 |
| 43:BU:31:LEU:HA | 43:BU:32:PRO:HD3 | 1.74 | 0.46 |
| 1:CA:6:G:O2' | 1:CA:7:G:H5' | 2.14 | 0.46 |
| 8:AH:107:LEU:HD23 | 8:AH:107:LEU:N | 2.30 | 0.46 |
| 20:AT:24:LEU:H | 20:AT:24:LEU:HD22 | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:398:C:H6 | 1:AA:398:C:O5' | 1.98 | 0.46 |
| 1:CA:850:U:O5' | 1:CA:850:U:H6 | 1.98 | 0.46 |
| 35:BM:125:LEU:N | 35:BM:125:LEU:HD23 | 2.30 | 0.46 |
| 26:BD:103:ASP:OD2 | 26:BD:201:THR:HA | 2.15 | 0.46 |
| 23:BA:2014:A:H2' | 23:BA:2015:A:C8 | 2.50 | 0.46 |
| 23:BA:1169:G:H1 | 23:BA:1180:C:N4 | 2.12 | 0.46 |
| 43:DU:9:LYS:O | 43:DU:27:VAL:CG2 | 2.63 | 0.46 |
| 1:CA:1366:C:C4 | 1:CA:1367:C:N4 | 2.83 | 0.46 |
| 22:CV:6190:U:C4 | 22:CV:6191:A:N7 | 2.83 | 0.46 |
| 12:CL:26:LEU:O | 12:CL:28:GLY:N | 2.49 | 0.46 |
| 2:CB:183:PRO:HA | 2:CB:198:ASP:OD1 | 2.14 | 0.46 |
| 41:BS:14:PRO:C | 41:BS:16:LYS:N | 2.66 | 0.46 |
| 24:DB:83:G:C6 | 24:DB:84:C:C5 | 3.03 | 0.46 |
| 23:DA:593:G:H4' | 53:D5:62:LEU:HD11 | 1.96 | 0.46 |
| 32:DJ:110:LEU:HD22 | 32:DJ:110:LEU:O | 2.15 | 0.46 |
| 39:BQ:83:LEU:CG | 39:BQ:88:ILE:HD11 | 2.34 | 0.46 |
| 23:DA:2295:C:N3 | 23:DA:2296:U:H5 | 2.12 | 0.46 |
| 25:DC:182:LEU:N | 25:DC:272:ALA:HB3 | 2.28 | 0.46 |
| 3:AC:182:ILE:CG1 | 3:AC:203:PHE:HD1 | 2.27 | 0.46 |
| 25:BC:31:LYS:HE2 | 25:BC:102:LYS:NZ | 2.29 | 0.46 |
| 28:DF:70:VAL:HG12 | 28:DF:90:LEU:CD2 | 2.44 | 0.46 |
| 24:DB:73:A:N6 | 24:DB:104:A:H1' | 2.29 | 0.46 |
| 44:DV:30:ASN:HA | 44:DV:89:PHE:HE2 | 1.81 | 0.46 |
| 23:DA:661:C:O3' | 34:DL:18:ARG:HD2 | 2.15 | 0.46 |
| 1:AA:394:G:C2 | 1:AA:395:C:C5 | 3.03 | 0.46 |
| 1:CA:130:A:C8 | 17:CQ:63:ARG:HG3 | 2.49 | 0.46 |
| 1:AA:1070:U:O2 | 1:AA:1106:G:C2 | 2.68 | 0.46 |
| 44:DV:134:PRO:C | 44:DV:136:PHE:N | 2.68 | 0.46 |
| 23:DA:2327:A:H2' | 23:DA:2328:A:H8 | 1.75 | 0.46 |
| 23:BA:1503:U:C2 | 23:BA:1504:C:H5 | 2.33 | 0.46 |
| 44:DV:151:HIS:O | 44:DV:171:ILE:HG12 | 2.15 | 0.46 |
| 23:BA:9:U:N3 | 23:BA:2629:A:C6 | 2.83 | 0.46 |
| 40:BR:66:ARG:HD2 | 40:BR:88:ARG:NE | 2.29 | 0.46 |
| 24:DB:10:C:C4 | 24:DB:11:C:C5 | 3.04 | 0.46 |
| 1:AA:556:C:H2' | 1:AA:557:G:C5' | 2.44 | 0.46 |
| 1:AA:102:G:C4 | 1:AA:103:C:C5 | 3.02 | 0.46 |
| 23:BA:1476:C:C6 | 23:BA:1476:C:C3' | 2.98 | 0.46 |
| 1:AA:1143:G:O5' | 1:AA:1143:G:H8 | 1.99 | 0.46 |
| 1:CA:1143:G:O5' | 1:CA:1143:G:H8 | 1.98 | 0.46 |
| 43:BU:50:ARG:CD | 43:BU:51:VAL:H | 2.25 | 0.46 |
| 25:BC:235:GLY:C | 25:BC:237:GLU:H | 2.17 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:DH:14:ASP:H | 30:DH:17:GLN:NE2 | 2.13 | 0.46 |
| 30:DH:5:LEU:HD22 | 30:DH:19:VAL:HG12 | 1.96 | 0.46 |
| 1:AA:624:C:H4' | 16:AP:10:GLY:HA2 | 1.97 | 0.46 |
| 23:DA:359:A:C8 | 23:DA:360:G:C8 | 3.03 | 0.46 |
| 24:BB:21:G:H2' | 24:BB:22:U:O4' | 2.14 | 0.46 |
| 23:BA:2477:C:O2' | 23:BA:2478:A:OP2 | 2.33 | 0.46 |
| 50:D2:32:PRO:HA | 50:D2:38:ALA:O | 2.16 | 0.46 |
| 33:BK:21:CYS:SG | 33:BK:22:ILE:N | 2.88 | 0.46 |
| 9:AI:58:ARG:HG2 | 9:AI:58:ARG:O | 2.15 | 0.46 |
| 23:BA:2287:A:H62 | 23:BA:2344:U:H3 | 1.63 | 0.46 |
| 44:DV:58:VAL:CG1 | 44:DV:66:SER:HB2 | 2.45 | 0.46 |
| 1:AA:1288:A:C6 | 1:AA:1289:A:C5 | 3.03 | 0.46 |
| 25:BC:176:ARG:NH1 | 25:BC:176:ARG:HG2 | 2.27 | 0.46 |
| 23:BA:1349:A:N6 | 23:BA:1598:C:N4 | 2.62 | 0.46 |
| 23:BA:2850:A:H2' | 23:BA:2851:A:O4' | 2.16 | 0.46 |
| 1:CA:1441:G:H8 | 1:CA:1441:G:O5' | 1.97 | 0.46 |
| 23:BA:2226:C:O5' | 23:BA:2226:C:H6 | 1.98 | 0.46 |
| 1:CA:511:C:C5 | 1:CA:541:G:N2 | 2.83 | 0.46 |
| 1:CA:1424:C:H2' | 1:CA:1425:U:O4' | 2.15 | 0.46 |
| 23:DA:987:G:H2' | 23:DA:988:A:C5' | 2.45 | 0.46 |
| 20:CT:93:GLU:O | 20:CT:93:GLU:HG2 | 2.15 | 0.46 |
| 1:CA:565:U:C5 | 1:CA:566:G:C5 | 3.03 | 0.46 |
| 23:DA:1682:G:H2' | 23:DA:1683:C:C6 | 2.50 | 0.46 |
| 39:DQ:29:SER:OG | 39:DQ:30:LYS:HE3 | 2.16 | 0.46 |
| 23:DA:1734:C:H2' | 23:DA:1735:U:O4' | 2.16 | 0.46 |
| 36:DN:84:ALA:HB3 | 36:DN:85:PRO:HD3 | 1.98 | 0.46 |
| 1:CA:1511:G:H2' | 1:CA:1512:U:O4' | 2.15 | 0.46 |
| 23:BA:1734:C:H2' | 23:BA:1735:U:O4' | 2.16 | 0.46 |
| 2:AB:106:LYS:HE2 | 2:AB:110:GLN:HE21 | 1.76 | 0.46 |
| 23:DA:189:G:H1 | 23:DA:205:G:HO2' | 1.62 | 0.46 |
| 3:AC:30:ARG:O | 3:AC:34:LEU:HB2 | 2.15 | 0.46 |
| 1:CA:1182:G:H4' | 1:CA:1183:A:H5'' | 1.96 | 0.46 |
| 10:AJ:98:ILE:O | 10:AJ:99:LYS:HD3 | 2.15 | 0.46 |
| 23:DA:2837:G:C6 | 23:DA:2838:G:N7 | 2.83 | 0.46 |
| 1:AA:1160:G:C6 | 1:AA:1181:G:O6 | 2.68 | 0.46 |
| 23:BA:2038:G:C5 | 23:BA:2039:C:C5 | 3.03 | 0.46 |
| 41:DS:45:TYR:CZ | 41:DS:49:LYS:HE3 | 2.49 | 0.46 |
| 2:AB:15:VAL:H | 2:AB:16:HIS:CE1 | 2.33 | 0.46 |
| 53:B5:29:LYS:O | 53:B5:29:LYS:HG2 | 2.15 | 0.46 |
| 1:CA:636:U:O2' | 1:CA:637:G:H5' | 2.15 | 0.46 |
| 3:AC:108:ASN:HB3 | 3:AC:111:LEU:HD12 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:419:C:C2' | 1:AA:420:U:H5' | 2.45 | 0.46 |
| 23:DA:532:A:C8 | 23:DA:2021:C:C4 | 3.03 | 0.46 |
| 23:BA:2435:A:H2' | 23:BA:2436:G:O5' | 2.15 | 0.46 |
| 27:BE:139:PHE:CB | 27:BE:166:ALA:HB1 | 2.44 | 0.46 |
| 23:BA:771:G:C4 | 23:BA:772:C:C5 | 3.03 | 0.46 |
| 23:BA:1678:G:H22 | 23:BA:1989:G:N2 | 2.13 | 0.46 |
| 23:BA:1381:G:C2' | 23:BA:1382:G:H5' | 2.46 | 0.46 |
| 38:BP:105:LEU:HA | 38:BP:105:LEU:HD23 | 1.70 | 0.46 |
| 23:DA:1678:G:H22 | 23:DA:1989:G:N2 | 2.12 | 0.46 |
| 23:DA:476:G:H4' | 23:DA:502:A:N1 | 2.31 | 0.46 |
| 1:AA:645:C:H2' | 1:AA:646:U:O4' | 2.14 | 0.46 |
| 16:CP:1:MET:HG2 | 16:CP:2:VAL:O | 2.15 | 0.46 |
| 28:DF:121:ASN:ND2 | 28:DF:122:PRO:HD2 | 2.30 | 0.46 |
| 6:AF:28:ARG:O | 6:AF:32:ASN:N | 2.48 | 0.46 |
| 4:CD:176:LEU:HG | 4:CD:178:VAL:HG22 | 1.97 | 0.46 |
| 1:CA:857:C:H2' | 1:CA:858:G:O4' | 2.15 | 0.46 |
| 48:BZ:38:GLU:OE1 | 48:BZ:38:GLU:N | 2.49 | 0.46 |
| 6:CF:42:GLU:HG2 | 6:CF:42:GLU:O | 2.15 | 0.46 |
| 44:DV:131:ARG:HD2 | 44:DV:131:ARG:H | 1.79 | 0.46 |
| 29:DG:103:LEU:HG | 29:DG:103:LEU:O | 2.15 | 0.46 |
| 23:DA:637:A:OP1 | 34:DL:133:SER:HB3 | 2.15 | 0.46 |
| 34:DL:122:PRO:HB3 | 34:DL:141:ALA:O | 2.15 | 0.46 |
| 23:BA:2331:G:H8 | 23:BA:2331:G:O5' | 1.98 | 0.46 |
| 26:BD:103:ASP:OD1 | 26:BD:201:THR:HG23 | 2.16 | 0.46 |
| 23:BA:1542:G:H3' | 23:BA:1542:G:P | 2.55 | 0.46 |
| 25:BC:155:LEU:HD13 | 25:BC:155:LEU:H | 1.80 | 0.46 |
| 1:CA:1367:C:N3 | 1:CA:1368:G:N7 | 2.63 | 0.46 |
| 22:AV:6182:A:C6 | 22:AV:6195:G:N1 | 2.84 | 0.46 |
| 1:CA:960:U:C6 | 1:CA:1225:A:C8 | 3.04 | 0.46 |
| 23:BA:2846:G:H2' | 23:BA:2847:U:O4' | 2.14 | 0.46 |
| 23:DA:861:A:O2' | 35:DM:18:LYS:NZ | 2.46 | 0.46 |
| 1:CA:390:C:O3' | 16:CP:28:ARG:NH2 | 2.46 | 0.46 |
| 16:CP:68:ASP:C | 16:CP:70:ALA:H | 2.19 | 0.46 |
| 1:AA:37:U:H2' | 1:AA:38:G:C8 | 2.49 | 0.46 |
| 1:AA:692:U:O4 | 11:AK:52:GLY:C | 2.54 | 0.46 |
| 1:AA:1252:A:H61 | 1:AA:1285:A:N6 | 2.11 | 0.46 |
| 1:CA:90:C:N3 | 1:CA:91:C:C4 | 2.83 | 0.46 |
| 28:BF:25:TYR:CZ | 28:BF:32:PRO:HD3 | 2.51 | 0.46 |
| 35:DM:141:GLN:OE1 | 44:DV:97:GLU:O | 2.32 | 0.46 |
| 1:CA:1105:A:C2 | 1:CA:1106:G:C8 | 3.03 | 0.46 |
| 23:BA:2543:G:O4' | 23:BA:2766:G:H5' | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:DZ:43:ILE:O | 48:DZ:47:VAL:HG23 | 2.15 | 0.46 |
| 23:BA:1438:U:O2' | 23:BA:1439:A:H5' | 2.15 | 0.46 |
| 1:AA:1353:G:H1 | 1:AA:1369:C:N4 | 2.13 | 0.46 |
| 36:BN:9:LYS:C | 36:BN:10:LEU:CG | 2.82 | 0.46 |
| 25:DC:172:TYR:CD1 | 25:DC:186:HIS:CA | 2.92 | 0.46 |
| 23:DA:2745:C:C4 | 23:DA:2746:U:C4 | 3.02 | 0.46 |
| 23:DA:1495:A:C4 | 23:DA:1496:A:C2 | 3.04 | 0.46 |
| 43:BU:96:ILE:HD11 | 43:BU:99:CYS:HB2 | 1.97 | 0.46 |
| 2:AB:83:MET:CE | 2:AB:234:PRO:HG2 | 2.45 | 0.46 |
| 1:CA:1221:G:OP1 | 1:CA:1321:C:N3 | 2.47 | 0.46 |
| 23:BA:1496:A:C8 | 23:BA:1498:C:N3 | 2.84 | 0.46 |
| 4:CD:110:PHE:HE1 | 4:CD:148:VAL:HG23 | 1.80 | 0.46 |
| 1:AA:557:G:H2' | 1:AA:558:G:O4' | 2.14 | 0.46 |
| 53:B5:51:ALA:H | 53:B5:54:GLU:CB | 2.24 | 0.46 |
| 30:BH:8:PRO:HA | 30:BH:14:ASP:HA | 1.98 | 0.46 |
| 44:BV:74:VAL:CG2 | 44:BV:86:VAL:HG13 | 2.45 | 0.46 |
| 50:D2:52:TYR:C | 50:D2:52:TYR:HD1 | 2.18 | 0.46 |
| 23:DA:534:U:C2' | 39:DQ:49:HIS:HD2 | 2.28 | 0.46 |
| 50:B2:52:TYR:C | 50:B2:52:TYR:HD1 | 2.18 | 0.46 |
| 29:DG:62:LYS:O | 29:DG:63:SER:C | 2.54 | 0.46 |
| 28:DF:11:TYR:HB2 | 28:DF:176:LEU:HD21 | 1.96 | 0.46 |
| 25:DC:257:LEU:HD23 | 25:DC:258:LYS:O | 2.16 | 0.46 |
| 1:CA:631:G:N2 | 1:CA:632:A:C2 | 2.83 | 0.46 |
| 23:DA:775:G:C4 | 23:DA:794:G:C8 | 3.04 | 0.46 |
| 7:AG:15:ASP:OD1 | 7:AG:18:TYR:HD1 | 1.98 | 0.46 |
| 23:BA:575:A:OP2 | 23:BA:2499:C:O2' | 2.31 | 0.46 |
| 2:AB:158:LEU:N | 2:AB:158:LEU:HD12 | 2.30 | 0.46 |
| 40:DR:22:VAL:O | 40:DR:23:GLU:C | 2.54 | 0.46 |
| 26:BD:117:MET:HE1 | 26:BD:136:ARG:HA | 1.97 | 0.46 |
| 23:DA:189:G:C8 | 23:DA:189:G:H3' | 2.51 | 0.46 |
| 23:BA:2738:A:C2 | 23:BA:2739:U:H1' | 2.50 | 0.46 |
| 23:BA:1894:C:C2 | 23:BA:1895:C:C5 | 3.04 | 0.46 |
| 23:DA:414:C:H2' | 23:DA:415:A:C8 | 2.51 | 0.46 |
| 23:DA:1471:A:C2 | 23:DA:1472:A:C8 | 3.03 | 0.46 |
| 35:BM:36:ALA:O | 35:BM:100:GLY:N | 2.40 | 0.46 |
| 24:DB:5:C:O2' | 24:DB:27:C:H1' | 2.15 | 0.46 |
| 23:DA:1027:A:N6 | 23:DA:1126:A:C4 | 2.84 | 0.46 |
| 5:CE:38:GLN:HG2 | 5:CE:38:GLN:O | 2.15 | 0.46 |
| 1:CA:574:A:H1' | 1:CA:883:C:O4' | 2.15 | 0.46 |
| 23:BA:1761:C:H5'' | 23:BA:1762:A:OP2 | 2.16 | 0.46 |
| 23:BA:1717:G:O6 | 23:BA:1743:G:C6 | 2.69 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:BO:35:ILE:CG1 | 37:BO:101:LEU:HD23 | 2.46 | 0.46 |
| 23:DA:1232:G:C5 | 23:DA:1233:C:C5 | 3.04 | 0.46 |
| 23:BA:723:G:H2' | 23:BA:724:U:O4' | 2.15 | 0.46 |
| 23:BA:476:G:O4' | 23:BA:505:A:C2 | 2.68 | 0.46 |
| 35:BM:125:LEU:HB3 | 35:BM:126:PRO:HD2 | 1.97 | 0.46 |
| 5:CE:69:VAL:HG12 | 5:CE:71:LEU:HG | 1.98 | 0.46 |
| 8:AH:68:ARG:HG2 | 8:AH:69:ARG:H | 1.81 | 0.46 |
| 4:CD:88:VAL:HG13 | 5:CE:97:GLY:CA | 2.45 | 0.46 |
| 23:BA:270(W):G:C4 | 23:BA:270(X):G:C8 | 3.03 | 0.46 |
| 23:BA:38:A:H2' | 23:BA:39:C:C6 | 2.50 | 0.46 |
| 23:BA:896:A:H1' | 44:BV:176:PRO:HG3 | 1.98 | 0.46 |
| 41:DS:31:GLU:O | 41:DS:34:ASN:HB2 | 2.16 | 0.46 |
| 1:CA:654:G:H1' | 1:CA:753:A:N1 | 2.29 | 0.46 |
| 44:BV:131:ARG:HD2 | 44:BV:131:ARG:H | 1.80 | 0.46 |
| 4:CD:166:LYS:O | 4:CD:166:LYS:HD2 | 2.15 | 0.46 |
| 1:AA:789:U:H6 | 1:AA:789:U:O5' | 1.97 | 0.46 |
| 23:DA:1206:G:C6 | 23:DA:1207:C:C4 | 3.03 | 0.46 |
| 23:DA:60:G:C6 | 23:DA:74:A:N6 | 2.82 | 0.46 |
| 12:CL:125:LYS:HE2 | 12:CL:127:ALA:H | 1.79 | 0.46 |
| 23:DA:627:A:C5 | 23:DA:637:A:N7 | 2.83 | 0.46 |
| 23:BA:2330:G:H1' | 45:BW:41:ARG:HB3 | 1.96 | 0.46 |
| 45:DW:26:TYR:HB2 | 45:DW:29:GLN:NE2 | 2.30 | 0.46 |
| 27:DE:68:LYS:C | 27:DE:70:THR:H | 2.19 | 0.46 |
| 39:DQ:79:PHE:CE2 | 39:DQ:106:PHE:CZ | 3.04 | 0.46 |
| 40:DR:2:PHE:CE2 | 40:DR:13:ARG:CD | 2.88 | 0.46 |
| 23:DA:1022:G:H8 | 32:DJ:92:GLN:NE2 | 2.12 | 0.46 |
| 28:DF:33:ARG:HD3 | 28:DF:162:THR:HG21 | 1.98 | 0.46 |
| 1:AA:373:A:C8 | 1:AA:482:A:C8 | 3.03 | 0.46 |
| 12:AL:25:ALA:O | 12:AL:26:LEU:HB2 | 2.15 | 0.46 |
| 4:CD:64:LEU:HB2 | 4:CD:198:VAL:HG11 | 1.98 | 0.46 |
| 42:DT:43:VAL:HG11 | 42:DT:81:VAL:HG11 | 1.97 | 0.46 |
| 13:AM:56:LEU:O | 13:AM:59:TYR:HB3 | 2.16 | 0.46 |
| 23:BA:1590:U:O2 | 23:BA:1591:G:C8 | 2.68 | 0.46 |
| 44:DV:125:LEU:HD23 | 44:DV:126:VAL:N | 2.31 | 0.46 |
| 35:BM:47:ILE:HG22 | 35:BM:48:GLU:H | 1.73 | 0.46 |
| 27:DE:118:ALA:HB2 | 27:DE:123:LEU:HD23 | 1.97 | 0.46 |
| 23:DA:1404:C:C2' | 23:DA:1405:U:H5' | 2.46 | 0.46 |
| 5:CE:76:ILE:CG1 | 5:CE:77:PRO:HD2 | 2.40 | 0.46 |
| 35:BM:141:GLN:OE1 | 44:BV:72:ARG:CZ | 2.63 | 0.46 |
| 23:DA:1324:G:C4 | 23:DA:1328:G:O6 | 2.69 | 0.46 |
| 1:CA:1104:G:N3 | 1:CA:1105:A:C8 | 2.84 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 19:CS:60:VAL:HG21 | 19:CS:74:PHE:HB3 | 1.97 | 0.46 |
| 12:CL:52:ARG:NH1 | 12:CL:52:ARG:HG3 | 2.20 | 0.46 |
| 6:CF:5:GLU:OE1 | 6:CF:62:TRP:CZ2 | 2.68 | 0.46 |
| 13:AM:10:PRO:CG | 13:AM:22:ILE:HD11 | 2.45 | 0.46 |
| 29:DG:151:ILE:H | 29:DG:151:ILE:HD13 | 1.78 | 0.46 |
| 46:BX:13:ILE:O | 46:BX:14:VAL:HB | 2.16 | 0.46 |
| 35:DM:6:ARG:HE | 35:DM:6:ARG:HB2 | 1.56 | 0.46 |
| 1:AA:819:A:N6 | 1:AA:1529:G:C5 | 2.83 | 0.46 |
| 8:CH:25:ASP:C | 8:CH:26:VAL:HG12 | 2.34 | 0.46 |
| 23:DA:2809:A:C2 | 23:DA:2892:A:C4 | 3.03 | 0.46 |
| 1:CA:1279:A:O2' | 1:CA:1282:C:N4 | 2.48 | 0.46 |
| 8:CH:113:SER:O | 8:CH:114:THR:HG23 | 2.15 | 0.46 |
| 53:B5:57:ARG:HA | 53:B5:57:ARG:CZ | 2.45 | 0.46 |
| 23:DA:380:U:O2 | 23:DA:380:U:H2' | 2.13 | 0.46 |
| 13:AM:71:ARG:O | 13:AM:74:VAL:HB | 2.15 | 0.46 |
| 11:AK:13:GLN:HG3 | 11:AK:75:TYR:O | 2.16 | 0.46 |
| 47:BY:49:LYS:H | 47:BY:49:LYS:HD2 | 1.80 | 0.46 |
| 44:BV:24:LEU:HD11 | 44:BV:85:HIS:HA | 1.96 | 0.46 |
| 23:DA:1557:C:OP2 | 23:DA:1558:A:O2' | 2.25 | 0.46 |
| 33:DK:2:ILE:CD1 | 33:DK:82:ASN:HD22 | 2.28 | 0.46 |
| 23:BA:816:C:O2' | 23:BA:817:C:H5' | 2.16 | 0.46 |
| 36:BN:52:ILE:HG21 | 36:BN:94:TYR:CB | 2.44 | 0.46 |
| 38:DP:96:ARG:CZ | 38:DP:96:ARG:HB2 | 2.45 | 0.46 |
| 26:DD:9:VAL:HG22 | 26:DD:25:VAL:HB | 1.98 | 0.46 |
| 1:CA:1379:G:C6 | 1:CA:1380:U:O4 | 2.69 | 0.46 |
| 1:AA:1412:C:H2' | 1:AA:1413:A:C8 | 2.51 | 0.46 |
| 23:BA:444:C:H4' | 27:BE:49:ALA:HB2 | 1.96 | 0.46 |
| 23:DA:794:G:H2' | 23:DA:795:C:C6 | 2.49 | 0.46 |
| 44:DV:108:PRO:HG3 | 44:DV:141:VAL:HG22 | 1.96 | 0.46 |
| 23:DA:2436:G:C4 | 23:DA:2437:U:C6 | 3.03 | 0.46 |
| 1:CA:1504:G:OP1 | 1:CA:1507:A:H4' | 2.15 | 0.46 |
| 28:BF:55:LYS:HD2 | 28:BF:58:GLN:NE2 | 2.29 | 0.46 |
| 35:DM:38:GLU:HB2 | 35:DM:127:ILE:HG12 | 1.97 | 0.46 |
| 1:CA:1286:A:C8 | 1:CA:1288:A:OP1 | 2.69 | 0.46 |
| 23:DA:2572:A:C8 | 26:DD:144:ARG:HB3 | 2.50 | 0.46 |
| 47:BY:36:ARG:HA | 47:BY:39:ALA:HB2 | 1.98 | 0.46 |
| 23:BA:533:G:N3 | 39:BQ:45:TYR:HE1 | 2.11 | 0.46 |
| 23:BA:2078:C:H2' | 23:BA:2079:U:C6 | 2.51 | 0.46 |
| 1:CA:634:C:H2' | 1:CA:635:G:H8 | 1.78 | 0.46 |
| 6:AF:97:PHE:HD2 | 18:AR:31:LEU:HD21 | 1.80 | 0.46 |
| 23:BA:948:G:C2 | 23:BA:970:C:O2 | 2.68 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BA:245:G:C5 | 23:BA:246:C:C5 | 3.04 | 0.46 |
| 23:DA:1523:U:H2' | 23:DA:1524:G:C8 | 2.51 | 0.46 |
| 1:AA:142:G:C2 | 1:AA:143:A:C5 | 3.03 | 0.46 |
| 23:BA:353:G:H2' | 23:BA:354:G:H8 | 1.80 | 0.46 |
| 23:DA:238:C:O2' | 23:DA:608:A:H1' | 2.15 | 0.46 |
| 23:DA:2557:G:H2' | 23:DA:2558:C:C6 | 2.50 | 0.46 |
| 11:CK:18:ARG:HD2 | 11:CK:83:ILE:HD11 | 1.96 | 0.46 |
| 23:BA:653:C:H6 | 23:BA:653:C:O5' | 1.96 | 0.46 |
| 1:CA:1114:C:O5' | 1:CA:1114:C:H6 | 1.98 | 0.46 |
| 53:D5:32:LEU:N | 53:D5:32:LEU:HD23 | 2.30 | 0.46 |
| 23:DA:2361:A:H5' | 53:D5:27:THR:OG1 | 2.15 | 0.46 |
| 23:DA:1309:G:P | 52:D4:9:ARG:HD2 | 2.56 | 0.46 |
| 1:AA:946:A:H61 | 1:AA:1235:U:H3 | 1.63 | 0.46 |
| 22:CV:6190:U:O4 | 22:CV:6191:A:N6 | 2.48 | 0.46 |
| 1:CA:946:A:H2' | 1:CA:947:G:C8 | 2.50 | 0.46 |
| 23:DA:809:G:O2' | 23:DA:810:U:H5' | 2.15 | 0.46 |
| 40:BR:45:THR:O | 40:BR:46:VAL:HG22 | 2.16 | 0.46 |
| 53:B5:7:HIS:CB | 53:B5:60:LEU:HB3 | 2.46 | 0.46 |
| 16:AP:5:ARG:CB | 16:AP:67:THR:OG1 | 2.63 | 0.46 |
| 4:CD:75:PHE:CZ | 4:CD:93:PHE:CZ | 3.04 | 0.46 |
| 3:CC:112:SER:O | 3:CC:116:VAL:HG23 | 2.15 | 0.46 |
| 44:DV:3:TYR:O | 44:DV:57:ILE:HA | 2.16 | 0.46 |
| 23:BA:363(B):A:C2 | 23:BA:363(C):G:C5 | 3.04 | 0.46 |
| 36:DN:9:LYS:HG2 | 36:DN:43:GLU:OE2 | 2.15 | 0.46 |
| 1:CA:1107:C:N3 | 1:CA:1108:G:C8 | 2.84 | 0.46 |
| 25:BC:175:LEU:HD23 | 25:BC:175:LEU:HA | 1.76 | 0.46 |
| 18:CR:56:THR:O | 18:CR:58:LEU:HD12 | 2.16 | 0.46 |
| 43:BU:81:LYS:HD3 | 43:BU:97:ARG:CB | 2.42 | 0.46 |
| 33:BK:28:SER:O | 33:BK:29:ASN:HB3 | 2.15 | 0.46 |
| 23:BA:2807:G:N1 | 23:BA:2893:G:O6 | 2.48 | 0.46 |
| 5:CE:48:ALA:C | 5:CE:50:GLU:H | 2.19 | 0.46 |
| 1:AA:1238:A:N3 | 1:AA:1238:A:H2' | 2.30 | 0.46 |
| 9:CI:28:VAL:CG2 | 9:CI:63:ILE:HB | 2.44 | 0.46 |
| 1:CA:599:C:H4' | 8:CH:130:GLY:C | 2.35 | 0.46 |
| 1:CA:642:A:C2' | 8:CH:113:SER:OG | 2.64 | 0.46 |
| 28:DF:131:TYR:HD2 | 28:DF:133:LEU:HD22 | 1.81 | 0.46 |
| 53:B5:22:VAL:HB | 53:B5:54:GLU:CG | 2.43 | 0.46 |
| 1:CA:1117:G:N2 | 1:CA:1180:A:H1' | 2.23 | 0.46 |
| 1:CA:1145:C:H4' | 1:CA:1146:A:C8 | 2.49 | 0.46 |
| 45:BW:36:ILE:HD12 | 45:BW:58:THR:CG2 | 2.42 | 0.46 |
| 34:BL:10:PRO:HD2 | 34:BL:11:GLY:H | 1.81 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BN:54:LEU:CD2 | 36:BN:62:ALA:HB1 | 2.45 | 0.46 |
| 23:DA:2784:C:H2' | 23:DA:2785:C:H6 | 1.81 | 0.46 |
| 23:DA:2591:C:H2' | 23:DA:2592:G:H8 | 1.79 | 0.46 |
| 1:CA:278:G:OP2 | 17:CQ:41:LYS:CE | 2.64 | 0.46 |
| 17:CQ:59:ILE:CG2 | 17:CQ:71:PHE:CD1 | 2.99 | 0.46 |
| 23:BA:580:C:O2' | 23:BA:581:C:H5' | 2.15 | 0.46 |
| 23:DA:737:C:H2' | 23:DA:738:G:C5' | 2.42 | 0.46 |
| 9:AI:58:ARG:NH2 | 9:AI:59:PHE:HE1 | 2.14 | 0.46 |
| 23:BA:2287:A:C2 | 23:BA:2289:G:C8 | 3.04 | 0.46 |
| 8:CH:51:VAL:HG21 | 8:CH:60:ARG:HG2 | 1.98 | 0.46 |
| 38:DP:3:ARG:HD2 | 38:DP:6:LEU:HD23 | 1.97 | 0.46 |
| 1:CA:515:G:C2 | 1:CA:537:G:N3 | 2.83 | 0.46 |
| 29:DG:16:SER:HB2 | 29:DG:27:LYS:HB2 | 1.98 | 0.46 |
| 23:DA:1414:G:N2 | 23:DA:1589:C:C2 | 2.84 | 0.46 |
| 23:DA:2226:C:H6 | 23:DA:2226:C:O5' | 1.99 | 0.46 |
| 23:BA:997:G:H2' | 23:BA:998:C:H5' | 1.97 | 0.46 |
| 29:DG:98:LEU:HB2 | 29:DG:125:VAL:CG2 | 2.46 | 0.46 |
| 19:CS:29:ARG:HD2 | 19:CS:30:LEU:N | 2.30 | 0.46 |
| 7:CG:50:ILE:HB | 7:CG:58:PRO:HG3 | 1.98 | 0.46 |
| 34:BL:75:ILE:N | 34:BL:75:ILE:HD12 | 2.30 | 0.46 |
| 1:CA:382:A:C2 | 1:CA:383:A:C4 | 3.04 | 0.46 |
| 1:AA:186(D):G:N1 | 1:AA:186(E):C:C4 | 2.84 | 0.46 |
| 23:DA:991:C:C5 | 23:DA:1185:C:N3 | 2.84 | 0.46 |
| 23:BA:1024:G:OP2 | 23:BA:1025:G:H3' | 2.15 | 0.46 |
| 37:BO:14:VAL:O | 37:BO:18:ILE:HG12 | 2.16 | 0.46 |
| 23:DA:1127:A:H2' | 23:DA:1128:A:H5'' | 1.97 | 0.46 |
| 26:BD:181:LEU:HA | 26:BD:181:LEU:HD12 | 1.73 | 0.46 |
| 23:BA:188:G:C2' | 23:BA:189:G:H5' | 2.45 | 0.46 |
| 23:DA:491:G:O6 | 41:DS:49:LYS:HD3 | 2.15 | 0.46 |
| 23:BA:1203:G:H3' | 23:BA:1204:A:C5' | 2.45 | 0.46 |
| 23:DA:2038:G:C5 | 23:DA:2039:C:C4 | 3.03 | 0.46 |
| 1:AA:117:G:H2' | 1:AA:118:U:O4' | 2.16 | 0.46 |
| 25:BC:159:ALA:HB1 | 25:BC:198:ASN:O | 2.16 | 0.46 |
| 4:AD:135:LEU:HD13 | 4:AD:135:LEU:N | 2.30 | 0.46 |
| 1:CA:1401:G:C2 | 1:CA:1402:C:H1' | 2.50 | 0.46 |
| 8:CH:54:ASP:C | 8:CH:56:LYS:H | 2.19 | 0.46 |
| 1:AA:1244:C:H2' | 1:AA:1245:A:H8 | 1.80 | 0.46 |
| 1:AA:757:U:H2' | 1:AA:758:G:O4' | 2.15 | 0.46 |
| 5:AE:72:GLN:O | 5:AE:73:ASN:HB3 | 2.16 | 0.46 |
| 1:AA:645:C:C2' | 1:AA:646:U:H5' | 2.45 | 0.46 |
| 28:DF:121:ASN:HD22 | 28:DF:122:PRO:HD2 | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 11:CK:87:THR:HA | 11:CK:91:ARG:HH21 | 1.79 | 0.46 |
| 48:BZ:5:LYS:HE2 | 48:BZ:34:GLU:OE1 | 2.16 | 0.46 |
| 2:CB:47:THR:HA | 2:CB:202:PRO:HG2 | 1.97 | 0.46 |
| 6:AF:41:GLU:O | 6:AF:43:LEU:N | 2.49 | 0.46 |
| 1:CA:789:U:H6 | 1:CA:789:U:O5' | 1.99 | 0.46 |
| 35:BM:73:PRO:HB3 | 35:BM:93:TYR:CE2 | 2.50 | 0.46 |
| 34:DL:115:LEU:HA | 34:DL:134:ALA:HB2 | 1.96 | 0.46 |
| 23:BA:2416:C:C2 | 23:BA:2417:C:C5 | 3.03 | 0.46 |
| 47:BY:1:MET:SD | 47:BY:5:GLU:OE2 | 2.73 | 0.46 |
| 2:AB:91:PRO:CB | 2:AB:154:LEU:HD11 | 2.46 | 0.46 |
| 2:AB:91:PRO:HB3 | 2:AB:154:LEU:HD11 | 1.98 | 0.46 |
| 1:CA:1371:G:O3' | 9:CI:69:GLY:HA3 | 2.15 | 0.46 |
| 26:BD:169:ASN:HD22 | 26:BD:169:ASN:C | 2.19 | 0.46 |
| 28:BF:60:LEU:HA | 28:BF:63:ILE:HD11 | 1.97 | 0.46 |
| 1:CA:551:U:H5' | 12:CL:118:LYS:HZ3 | 1.80 | 0.46 |
| 2:CB:71:VAL:CG2 | 2:CB:164:VAL:HG13 | 2.38 | 0.46 |
| 32:BJ:36:TRP:N | 32:BJ:36:TRP:CD1 | 2.81 | 0.46 |
| 40:DR:38:LEU:HD12 | 40:DR:57:VAL:HG12 | 1.98 | 0.46 |
| 25:BC:105:ILE:HD13 | 25:BC:106:ILE:N | 2.30 | 0.46 |
| 23:BA:1828:G:OP2 | 25:BC:239:ARG:CZ | 2.64 | 0.46 |
| 40:BR:5:VAL:HG11 | 40:BR:14:VAL:HG21 | 1.98 | 0.46 |
| 23:DA:1639:U:H4' | 23:DA:2699:C:H4' | 1.98 | 0.46 |
| 1:CA:262:A:H5' | 20:CT:74:LYS:HG3 | 1.98 | 0.46 |
| 20:CT:73:HIS:CD2 | 20:CT:74:LYS:H | 2.33 | 0.46 |
| 28:BF:126:ASP:O | 28:BF:128:ARG:N | 2.42 | 0.46 |
| 1:AA:198:G:O2' | 1:AA:199:G:H5' | 2.16 | 0.46 |
| 23:DA:1323:U:H2' | 23:DA:1324:G:H5' | 1.97 | 0.46 |
| 1:CA:1074:G:N3 | 1:CA:1102:A:C2 | 2.84 | 0.46 |
| 25:DC:231:HIS:HD2 | 25:DC:249:PRO:CA | 2.18 | 0.46 |
| 1:AA:1279:A:O2' | 1:AA:1282:C:N4 | 2.48 | 0.46 |
| 19:AS:60:VAL:HG21 | 19:AS:74:PHE:HB3 | 1.97 | 0.46 |
| 1:CA:321:A:O2' | 1:CA:322:C:H5' | 2.16 | 0.46 |
| 1:CA:722:A:H2' | 1:CA:724:G:C8 | 2.50 | 0.46 |
| 23:DA:1401:G:C5 | 23:DA:1402:C:C5 | 3.03 | 0.46 |
| 23:BA:380:U:H4' | 46:BX:21:ARG:O | 2.15 | 0.46 |
| 1:AA:670:G:N2 | 1:AA:736:C:O2 | 2.47 | 0.46 |
| 40:BR:24:LYS:HA | 40:BR:92:THR:CG2 | 2.41 | 0.46 |
| 33:DK:96:THR:O | 33:DK:97:ARG:C | 2.54 | 0.46 |
| 23:BA:2276:G:C2' | 23:BA:2277:G:H5' | 2.45 | 0.46 |
| 8:AH:137:VAL:HG12 | 8:AH:138:TRP:N | 2.31 | 0.46 |
| 40:BR:100:ARG:O | 40:BR:100:ARG:CG | 2.56 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BA:732:C:C2' | 23:BA:733:G:H5' | 2.45 | 0.46 |
| 33:DK:88:ASN:HB3 | 33:DK:92:GLU:H | 1.80 | 0.46 |
| 15:AO:53:HIS:HE1 | 23:BA:715:G:C6 | 2.34 | 0.46 |
| 28:BF:77:ILE:CG2 | 28:BF:80:PHE:H | 2.23 | 0.46 |
| 23:BA:2406:U:O4 | 34:BL:70:GLN:HB3 | 2.16 | 0.46 |
| 10:AJ:34:VAL:HG22 | 10:AJ:74:ILE:HG22 | 1.97 | 0.46 |
| 23:BA:497:A:C6 | 23:BA:498:G:C5 | 3.04 | 0.46 |
| 28:BF:111:LEU:HA | 28:BF:114:ILE:CD1 | 2.45 | 0.46 |
| 1:AA:41:G:O6 | 1:AA:401:C:N3 | 2.49 | 0.46 |
| 30:DH:66:GLU:HB3 | 30:DH:67:ARG:NH1 | 2.31 | 0.46 |
| 23:BA:2100:G:N2 | 23:BA:2101:G:N3 | 2.63 | 0.46 |
| 1:AA:976:G:C8 | 1:AA:1358:U:C2' | 2.97 | 0.46 |
| 1:AA:1286:A:C8 | 1:AA:1288:A:OP1 | 2.69 | 0.46 |
| 1:CA:527:G:H2' | 1:CA:528:C:H5' | 1.97 | 0.46 |
| 25:DC:61:LEU:HB3 | 25:DC:63:ARG:NH1 | 2.30 | 0.46 |
| 27:BE:89:VAL:O | 27:BE:91:GLY:N | 2.44 | 0.46 |
| 23:DA:1349:A:N6 | 23:DA:1598:C:N4 | 2.64 | 0.46 |
| 23:BA:1289:C:H2' | 23:BA:1290:C:C6 | 2.51 | 0.46 |
| 1:AA:300:A:C8 | 1:AA:300:A:C3' | 2.98 | 0.46 |
| 36:BN:85:PRO:HA | 36:BN:88:ARG:NH1 | 2.30 | 0.46 |
| 23:BA:1844:C:O3' | 25:BC:258:LYS:NZ | 2.45 | 0.46 |
| 20:CT:84:LEU:HD13 | 20:CT:84:LEU:C | 2.36 | 0.46 |
| 23:DA:493:G:H2' | 23:DA:494:G:O4' | 2.16 | 0.46 |
| 40:DR:12:TYR:CZ | 40:DR:22:VAL:HG22 | 2.50 | 0.46 |
| 1:AA:160:A:N7 | 1:AA:161:A:C5 | 2.84 | 0.46 |
| 23:DA:2718:G:C2' | 23:DA:2719:G:O5' | 2.64 | 0.46 |
| 23:BA:923:C:O2' | 23:BA:924:C:H5' | 2.16 | 0.46 |
| 3:CC:30:ARG:O | 3:CC:34:LEU:HB2 | 2.15 | 0.46 |
| 12:CL:38:VAL:HG12 | 12:CL:39:VAL:H | 1.81 | 0.46 |
| 1:CA:1399:C:C4 | 1:CA:1502:A:N1 | 2.83 | 0.46 |
| 28:BF:58:GLN:O | 28:BF:61:ALA:HB3 | 2.15 | 0.46 |
| 1:CA:1386:G:C2 | 1:CA:1387:G:N7 | 2.83 | 0.46 |
| 38:BP:41:ARG:CB | 38:BP:41:ARG:HH11 | 2.29 | 0.46 |
| 19:CS:61:TYR:CG | 19:CS:62:ILE:N | 2.84 | 0.46 |
| 23:DA:1904:G:C2' | 23:DA:1905:C:H5' | 2.46 | 0.46 |
| 1:AA:1508:G:H2' | 1:AA:1509:C:C6 | 2.51 | 0.46 |
| 7:CG:31:MET:CG | 7:CG:35:LYS:H | 2.28 | 0.46 |
| 1:CA:575:G:C8 | 1:CA:881:G:N2 | 2.83 | 0.46 |
| 39:DQ:36:ARG:HD3 | 39:DQ:40:PHE:CE1 | 2.50 | 0.46 |
| 1:CA:451:A:C8 | 1:CA:481:G:C6 | 3.04 | 0.46 |
| 12:AL:88:ARG:NH1 | 12:AL:90:LYS:HD3 | 2.31 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DM:34:LEU:HD11 | 35:DM:129:THR:HB | 1.98 | 0.46 |
| 35:DM:34:LEU:HD12 | 35:DM:130:LYS:O | 2.16 | 0.46 |
| 25:DC:69:ARG:NH2 | 25:DC:128:GLY:O | 2.49 | 0.46 |
| 42:BT:18:TYR:CD1 | 42:BT:18:TYR:N | 2.83 | 0.46 |
| 44:BV:144:LEU:HB3 | 44:BV:174:VAL:HG21 | 1.97 | 0.46 |
| 19:AS:52:TYR:CE1 | 19:AS:56:GLN:HA | 2.51 | 0.46 |
| 23:DA:1354:A:C8 | 23:DA:1355:G:C8 | 3.03 | 0.46 |
| 1:CA:645:C:H2' | 1:CA:646:U:O4' | 2.16 | 0.46 |
| 23:DA:448:U:H1' | 27:DE:84:VAL:HG21 | 1.96 | 0.46 |
| 23:DA:2495:G:H2' | 23:DA:2496:C:O5' | 2.15 | 0.46 |
| 27:DE:144:LYS:O | 27:DE:146:ALA:N | 2.43 | 0.46 |
| 23:DA:1001:A:H2' | 23:DA:1002:G:O4' | 2.16 | 0.46 |
| 23:DA:1582:C:O5' | 23:DA:1582:C:H6 | 1.98 | 0.46 |
| 14:CN:42:ILE:H | 14:CN:42:ILE:HG12 | 1.60 | 0.46 |
| 43:BU:71:LYS:HB2 | 43:BU:71:LYS:HZ3 | 1.81 | 0.46 |
| 23:DA:1540:G:C4 | 23:DA:1541:U:C6 | 3.03 | 0.46 |
| 34:BL:101:VAL:CB | 34:BL:106:LEU:HB3 | 2.43 | 0.46 |
| 1:CA:1366:C:OP1 | 9:CI:117:HIS:CE1 | 2.69 | 0.46 |
| 1:AA:974:A:OP2 | 14:AN:41:ARG:NH1 | 2.49 | 0.46 |
| 10:AJ:56:HIS:O | 10:AJ:58:ASP:N | 2.46 | 0.46 |
| 10:AJ:58:ASP:C | 10:AJ:60:ARG:N | 2.68 | 0.46 |
| 1:CA:950:U:O2' | 1:CA:951:G:H5' | 2.15 | 0.46 |
| 42:DT:63:LYS:CE | 42:DT:72:LYS:HB3 | 2.45 | 0.46 |
| 23:BA:2335:A:N7 | 23:BA:2337:G:C5 | 2.84 | 0.46 |
| 37:BO:87:PHE:CD1 | 37:BO:102:ALA:HB2 | 2.50 | 0.46 |
| 23:DA:1903:G:OP2 | 25:DC:241:PRO:HB3 | 2.16 | 0.46 |
| 25:BC:105:ILE:HD11 | 25:BC:192:THR:HG21 | 1.98 | 0.46 |
| 23:BA:1826:G:C4' | 25:BC:242:ARG:HE | 2.13 | 0.46 |
| 1:AA:671:G:C4 | 1:AA:672:U:C6 | 3.03 | 0.46 |
| 1:CA:375:U:C2' | 1:CA:376:G:H5' | 2.46 | 0.46 |
| 25:DC:143:HIS:HD2 | 25:DC:144:ALA:HB2 | 1.78 | 0.46 |
| 25:DC:182:LEU:HA | 25:DC:182:LEU:HD23 | 1.50 | 0.46 |
| 25:BC:44:ASN:CG | 25:BC:45:ASN:H | 2.17 | 0.46 |
| 30:DH:82:ARG:HB3 | 30:DH:89:TYR:CB | 2.46 | 0.46 |
| 20:AT:73:HIS:CD2 | 20:AT:74:LYS:H | 2.34 | 0.46 |
| 24:DB:73:A:C4 | 24:DB:104:A:C2 | 3.04 | 0.46 |
| 35:DM:141:GLN:OE1 | 44:DV:72:ARG:CZ | 2.64 | 0.46 |
| 26:BD:5:LEU:C | 26:BD:51:PHE:HE2 | 2.18 | 0.46 |
| 26:BD:59:VAL:C | 26:BD:61:ARG:H | 2.19 | 0.46 |
| 47:DY:57:ILE:O | 47:DY:61:LEU:HB2 | 2.15 | 0.46 |
| 24:BB:10:C:N3 | 24:BB:11:C:C5 | 2.83 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:AL:53:LYS:N | 12:AL:53:LYS:HD2 | 2.31 | 0.46 |
| 44:BV:134:PRO:C | 44:BV:136:PHE:N | 2.69 | 0.46 |
| 11:AK:59:TYR:O | 11:AK:62:GLN:HB3 | 2.16 | 0.46 |
| 1:AA:1372:U:C5 | 1:AA:1373:G:C5 | 3.03 | 0.46 |
| 19:AS:40:ILE:CD1 | 19:AS:62:ILE:HD11 | 2.46 | 0.46 |
| 1:CA:321:A:C2 | 1:CA:333:G:N2 | 2.84 | 0.46 |
| 18:CR:88:LYS:OXT | 18:CR:88:LYS:HG3 | 2.15 | 0.46 |
| 23:BA:2784:C:H2' | 23:BA:2785:C:H6 | 1.81 | 0.46 |
| 1:AA:1330:U:O4 | 1:AA:1331:G:C2 | 2.69 | 0.46 |
| 1:CA:825:G:N2 | 8:CH:11:THR:HG21 | 2.30 | 0.46 |
| 42:BT:23:GLU:HG3 | 42:BT:24:GLY:H | 1.80 | 0.46 |
| 23:DA:2276:G:C2' | 23:DA:2277:G:H5' | 2.45 | 0.46 |
| 24:DB:13:A:O4' | 45:DW:74:ARG:NH2 | 2.49 | 0.46 |
| 23:DA:1670:C:OP2 | 23:DA:2550:G:OP1 | 2.34 | 0.46 |
| 23:DA:8:A:C6 | 23:DA:9:U:O4 | 2.69 | 0.46 |
| 1:AA:104:G:C2 | 1:AA:105:G:N7 | 2.84 | 0.46 |
| 29:BG:28:GLY:HA3 | 29:BG:79:VAL:HB | 1.96 | 0.46 |
| 33:BK:31:LYS:HB3 | 33:BK:32:TYR:CD1 | 2.50 | 0.46 |
| 50:D2:33:CYS:HB2 | 50:D2:34:PRO:HD2 | 1.97 | 0.46 |
| 23:DA:908:C:O2' | 23:DA:909:A:H5' | 2.16 | 0.46 |
| 25:DC:77:ALA:HB2 | 25:DC:97:TYR:CG | 2.51 | 0.46 |
| 27:BE:205:ARG:C | 27:BE:206:ILE:HG13 | 2.36 | 0.46 |
| 21:CU:14:TRP:CE3 | 21:CU:15:ARG:HG2 | 2.51 | 0.46 |
| 1:AA:1054:C:O2' | 1:AA:1055:A:H5'' | 2.15 | 0.46 |
| 1:AA:1054:C:H6 | 1:AA:1196:U:O2 | 1.99 | 0.46 |
| 33:BK:63:VAL:HG23 | 33:BK:64:ARG:HG3 | 1.97 | 0.46 |
| 4:AD:8:VAL:O | 4:AD:10:ARG:N | 2.48 | 0.46 |
| 10:CJ:49:VAL:HG23 | 14:CN:34:TYR:OH | 2.15 | 0.46 |
| 7:CG:44:TYR:O | 7:CG:47:CYS:HB2 | 2.16 | 0.46 |
| 25:BC:257:LEU:HD23 | 25:BC:258:LYS:O | 2.15 | 0.46 |
| 1:AA:1298:C:H4' | 1:AA:1299:A:C4 | 2.50 | 0.46 |
| 1:CA:413:G:H22 | 1:CA:429:U:P | 2.39 | 0.46 |
| 1:AA:643:C:H5' | 8:AH:31:PHE:CD1 | 2.51 | 0.46 |
| 41:BS:24:ILE:CG2 | 41:BS:36:LEU:HD21 | 2.46 | 0.46 |
| 1:CA:1161:C:H2' | 1:CA:1162:C:C6 | 2.50 | 0.46 |
| 33:BK:86:ILE:HD12 | 33:BK:86:ILE:N | 2.30 | 0.46 |
| 1:AA:1501:C:C5 | 1:AA:1504:G:C4 | 3.04 | 0.46 |
| 1:AA:697:U:H2' | 1:AA:698:G:H5' | 1.98 | 0.46 |
| 23:DA:2584:U:H5'' | 23:DA:2585:U:OP2 | 2.15 | 0.46 |
| 23:DA:270(S):G:H2' | 23:DA:270(T):G:H8 | 1.81 | 0.46 |
| 23:DA:1301:A:H2 | 23:DA:1626:G:N3 | 2.14 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BA:26:G:H1' | 23:BA:514:A:N6 | 2.31 | 0.46 |
| 23:DA:844:C:O2' | 23:DA:845:G:H5' | 2.16 | 0.46 |
| 1:AA:450:G:C8 | 1:AA:481:G:C6 | 3.04 | 0.46 |
| 23:BA:79:G:H1 | 23:BA:107:C:H42 | 1.62 | 0.46 |
| 1:CA:794:A:H4' | 1:CA:1521:G:O2' | 2.15 | 0.46 |
| 28:DF:44:GLY:O | 28:DF:47:LYS:HB2 | 2.16 | 0.46 |
| 23:DA:2462:U:H2' | 23:DA:2463:C:O4' | 2.16 | 0.46 |
| 23:BA:844:C:C2' | 23:BA:845:G:H5' | 2.46 | 0.46 |
| 23:DA:723:G:H2' | 23:DA:724:U:O4' | 2.16 | 0.46 |
| 23:DA:374:A:C2 | 23:DA:401:A:C4 | 3.04 | 0.46 |
| 35:BM:97:VAL:O | 35:BM:97:VAL:HG12 | 2.14 | 0.46 |
| 27:BE:33:LEU:HD12 | 27:BE:33:LEU:HA | 1.68 | 0.46 |
| 23:DA:2075:U:H2' | 23:DA:2238:G:N2 | 2.31 | 0.46 |
| 43:DU:11:ASP:H | 43:DU:27:VAL:HG22 | 1.81 | 0.46 |
| 27:BE:74:ARG:O | 27:BE:74:ARG:HG2 | 2.14 | 0.46 |
| 1:CA:1226:C:C2' | 13:CM:103:THR:HB | 2.43 | 0.46 |
| 1:CA:47:C:O2 | 1:CA:49:U:C5 | 2.69 | 0.46 |
| 23:DA:1902:C:H2' | 23:DA:1903:G:O5' | 2.15 | 0.46 |
| 23:BA:1657:C:O2' | 23:BA:1658:C:H5' | 2.16 | 0.46 |
| 23:BA:1144:G:C4 | 23:BA:1145:C:C5 | 3.03 | 0.46 |
| 1:CA:376:G:N3 | 1:CA:377:G:C8 | 2.83 | 0.46 |
| 16:CP:6:LEU:HB3 | 16:CP:17:TYR:HB3 | 1.97 | 0.46 |
| 23:BA:1614:A:C6 | 41:BS:87:PRO:HB3 | 2.50 | 0.46 |
| 16:AP:5:ARG:HB2 | 16:AP:67:THR:HG1 | 1.80 | 0.46 |
| 4:AD:3:ARG:O | 4:AD:5:ILE:N | 2.49 | 0.46 |
| 25:BC:36:PRO:HA | 25:BC:62:TYR:O | 2.16 | 0.46 |
| 25:BC:74:GLY:O | 25:BC:76:PRO:HD3 | 2.16 | 0.46 |
| 30:DH:110:ASP:OD2 | 30:DH:113:ARG:HG3 | 2.16 | 0.46 |
| 30:DH:98:ALA:HB1 | 30:DH:109:ILE:HG12 | 1.98 | 0.46 |
| 24:DB:104:A:O4' | 44:DV:29:TYR:CE1 | 2.66 | 0.46 |
| 23:DA:363(B):A:C2 | 23:DA:363(C):G:C5 | 3.03 | 0.46 |
| 1:AA:392:G:C4 | 1:AA:393:A:N7 | 2.84 | 0.46 |
| 1:CA:130:A:OP2 | 1:CA:189:U:C2 | 2.69 | 0.46 |
| 5:CE:110:LEU:O | 5:CE:115:VAL:HG23 | 2.16 | 0.46 |
| 4:CD:119:GLN:O | 4:CD:123:HIS:CD2 | 2.68 | 0.46 |
| 36:BN:9:LYS:HG2 | 36:BN:43:GLU:OE2 | 2.16 | 0.46 |
| 44:DV:102:LEU:HD23 | 44:DV:137:ILE:HB | 1.96 | 0.46 |
| 23:DA:1577:C:H2' | 23:DA:1578:U:C1' | 2.46 | 0.46 |
| 23:BA:2562:U:C2' | 23:BA:2563:U:H5' | 2.45 | 0.46 |
| 23:DA:2892:A:C2' | 23:DA:2893:G:H5' | 2.45 | 0.46 |
| 18:CR:54:ARG:CD | 18:CR:54:ARG:H | 2.24 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:BF:133:LEU:HD21 | 28:BF:157:ILE:HG13 | 1.98 | 0.46 |
| 23:DA:2550:G:C5 | 23:DA:2551:C:C5 | 3.04 | 0.46 |
| 33:DK:22:ILE:HA | 33:DK:22:ILE:HD13 | 1.42 | 0.46 |
| 15:AO:60:VAL:HG11 | 23:BA:715:G:O4' | 2.16 | 0.46 |
| 23:BA:1519:G:O2' | 23:BA:1520:U:H5' | 2.16 | 0.46 |
| 36:BN:47:PHE:O | 36:BN:51:LEU:HD12 | 2.16 | 0.46 |
| 33:BK:88:ASN:HB3 | 33:BK:92:GLU:H | 1.80 | 0.46 |
| 29:BG:92:ILE:CG2 | 29:BG:93:GLY:N | 2.74 | 0.46 |
| 1:CA:1060:C:O2 | 1:CA:1198:G:C2 | 2.68 | 0.46 |
| 9:AI:58:ARG:NH2 | 9:AI:59:PHE:CE1 | 2.83 | 0.46 |
| 23:BA:912:C:C2' | 23:BA:912:C:O2 | 2.63 | 0.46 |
| 4:CD:79:PHE:O | 4:CD:82:ALA:HB3 | 2.16 | 0.46 |
| 1:CA:1446:A:N1 | 38:DP:118:ARG:CZ | 2.78 | 0.46 |
| 23:BA:2092:U:C4 | 23:BA:2226:C:OP2 | 2.68 | 0.46 |
| 1:CA:590:C:OP1 | 8:CH:29:SER:HA | 2.16 | 0.46 |
| 1:AA:593:G:C2 | 1:AA:594:G:C4 | 3.03 | 0.46 |
| 13:AM:70:LEU:HD23 | 13:AM:70:LEU:C | 2.36 | 0.46 |
| 1:AA:109:A:N6 | 1:AA:326:G:C6 | 2.83 | 0.46 |
| 20:AT:86:ARG:O | 20:AT:90:GLN:HG3 | 2.16 | 0.46 |
| 23:DA:2050:C:C2' | 23:DA:2051:A:O5' | 2.64 | 0.46 |
| 27:DE:53:THR:C | 27:DE:55:GLY:H | 2.18 | 0.46 |
| 51:B3:44:ARG:O | 51:B3:45:LYS:HG2 | 2.15 | 0.46 |
| 38:DP:84:GLN:HG3 | 38:DP:85:LYS:HG3 | 1.98 | 0.46 |
| 23:DA:1127:A:C2' | 23:DA:1128:A:H5'' | 2.46 | 0.46 |
| 12:CL:78:GLU:CD | 12:CL:78:GLU:O | 2.54 | 0.46 |
| 23:DA:646:A:H2' | 23:DA:647:G:O5' | 2.16 | 0.46 |
| 19:AS:11:VAL:HG23 | 19:AS:38:SER:HB2 | 1.97 | 0.46 |
| 35:BM:24:GLY:HA2 | 35:BM:100:GLY:O | 2.16 | 0.46 |
| 7:CG:148:ASN:C | 7:CG:150:ALA:H | 2.19 | 0.46 |
| 23:DA:1775:U:H2' | 23:DA:1776:G:O5' | 2.15 | 0.46 |
| 1:CA:927:G:N1 | 1:CA:1391:U:C2 | 2.84 | 0.46 |
| 13:CM:32:GLU:CD | 13:CM:64:TRP:CH2 | 2.89 | 0.46 |
| 14:AN:4:LYS:O | 14:AN:7:ILE:HG13 | 2.16 | 0.46 |
| 23:BA:2836:U:C5 | 23:BA:2883:A:N6 | 2.84 | 0.46 |
| 4:CD:23:GLY:HA3 | 4:CD:112:VAL:CG2 | 2.46 | 0.46 |
| 23:DA:2026:C:C4 | 23:DA:2027:G:N7 | 2.84 | 0.46 |
| 4:AD:88:VAL:HG13 | 5:AE:97:GLY:HA3 | 1.96 | 0.46 |
| 23:BA:1687:G:H2' | 23:BA:1688:U:H6 | 1.81 | 0.46 |
| 1:AA:195:A:C5 | 1:AA:196:A:N1 | 2.84 | 0.46 |
| 4:AD:190:ASP:O | 4:AD:194:LEU:HD23 | 2.15 | 0.46 |
| 50:B2:32:PRO:HA | 50:B2:38:ALA:O | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:BP:13:ARG:C | 38:BP:15:VAL:H | 2.19 | 0.46 |
| 23:BA:2084:C:O2' | 23:BA:2085:C:H5' | 2.16 | 0.46 |
| 24:BB:76:G:OP1 | 44:BV:15:PRO:HG3 | 2.15 | 0.46 |
| 52:B4:31:LEU:HA | 52:B4:31:LEU:HD12 | 1.68 | 0.46 |
| 5:AE:60:TYR:CD1 | 5:AE:60:TYR:C | 2.88 | 0.46 |
| 1:AA:1461:G:O5' | 1:AA:1461:G:H8 | 1.98 | 0.46 |
| 23:BA:2408:U:O5' | 23:BA:2408:U:H6 | 1.99 | 0.46 |
| 13:CM:94:ARG:NH2 | 19:CS:80:TYR:HE2 | 2.14 | 0.46 |
| 15:AO:17:ARG:NH1 | 15:AO:77:ARG:HH12 | 2.13 | 0.46 |
| 23:DA:629:G:H2' | 23:DA:630:G:C8 | 2.51 | 0.46 |
| 28:DF:60:LEU:HA | 28:DF:63:ILE:HG12 | 1.97 | 0.46 |
| 1:CA:1369:C:H2' | 1:CA:1370:G:C8 | 2.51 | 0.46 |
| 22:CV:6193:U:C5 | 22:CV:6194:C:C5 | 3.04 | 0.46 |
| 27:DE:68:LYS:H | 27:DE:70:THR:HG22 | 1.80 | 0.46 |
| 2:CB:70:PHE:CD2 | 2:CB:163:PHE:HB3 | 2.51 | 0.46 |
| 32:BJ:38:LEU:C | 32:BJ:39:ILE:HG12 | 2.36 | 0.46 |
| 32:BJ:109:PRO:HG2 | 32:BJ:112:LYS:HB2 | 1.98 | 0.46 |
| 32:BJ:110:LEU:O | 32:BJ:113:MET:HB2 | 2.15 | 0.46 |
| 36:DN:40:LYS:HE3 | 36:DN:40:LYS:HB2 | 1.77 | 0.46 |
| 24:DB:82:G:C2' | 24:DB:83:G:H5' | 2.45 | 0.46 |
| 53:D5:7:HIS:CD2 | 53:D5:60:LEU:HD13 | 2.51 | 0.46 |
| 30:BH:88:ILE:CG1 | 30:BH:123:LEU:HA | 2.45 | 0.46 |
| 39:BQ:79:PHE:O | 39:BQ:79:PHE:CD1 | 2.69 | 0.46 |
| 42:BT:14:SER:OG | 42:BT:17:ALA:HB2 | 2.16 | 0.46 |
| 23:DA:2729:G:C5 | 23:DA:2730:C:C5 | 3.04 | 0.46 |
| 16:AP:3:LYS:O | 16:AP:21:VAL:HA | 2.16 | 0.46 |
| 42:DT:35:THR:HB | 42:DT:38:GLU:H | 1.81 | 0.46 |
| 20:AT:22:ARG:O | 20:AT:26:ASN:ND2 | 2.49 | 0.46 |
| 1:CA:88:C:H2' | 1:CA:89:U:O4' | 2.16 | 0.46 |
| 20:CT:30:LYS:O | 20:CT:33:ILE:HB | 2.16 | 0.46 |
| 35:DM:141:GLN:OXT | 44:DV:53:ILE:O | 2.34 | 0.46 |
| 36:DN:4:LEU:C | 36:DN:6:SER:H | 2.19 | 0.46 |
| 5:AE:13:ILE:HA | 5:AE:29:GLY:O | 2.15 | 0.46 |
| 1:AA:194:C:O2' | 20:AT:68:LYS:HD3 | 2.15 | 0.46 |
| 1:CA:1102:A:C5 | 1:CA:1103:C:C5 | 3.04 | 0.46 |
| 23:BA:95:G:HO2' | 47:BY:48:HIS:CE1 | 2.28 | 0.46 |
| 1:AA:1150:U:H5'' | 1:AA:1151:A:OP2 | 2.15 | 0.46 |
| 1:AA:1347:G:C2 | 1:AA:1373:G:C5 | 3.04 | 0.46 |
| 19:AS:61:TYR:CG | 19:AS:62:ILE:N | 2.82 | 0.46 |
| 19:AS:66:MET:HB3 | 19:AS:74:PHE:CZ | 2.51 | 0.46 |
| 36:BN:39:PRO:O | 36:BN:40:LYS:C | 2.54 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:757:U:H2' | 1:CA:758:G:O4' | 2.16 | 0.46 |
| 23:BA:1577:C:H5'' | 23:BA:1578:U:OP2 | 2.16 | 0.46 |
| 4:CD:152:SER:O | 4:CD:153:ARG:C | 2.54 | 0.46 |
| 23:DA:2630:G:H1' | 23:DA:2894:G:H1' | 1.97 | 0.46 |
| 29:BG:138:LYS:O | 29:BG:139:GLN:C | 2.54 | 0.46 |
| 23:BA:1503:U:N3 | 23:BA:1504:C:N4 | 2.64 | 0.46 |
| 23:BA:8:A:C5 | 23:BA:9:U:C4 | 3.04 | 0.46 |
| 8:CH:97:VAL:CG1 | 8:CH:98:LYS:N | 2.79 | 0.46 |
| 15:AO:39:LEU:HA | 15:AO:39:LEU:HD23 | 1.80 | 0.46 |
| 1:CA:556:C:O2 | 1:CA:557:G:O4' | 2.34 | 0.46 |
| 1:CA:1118:C:O4' | 1:CA:1179:A:C4 | 2.69 | 0.46 |
| 1:CA:783:C:H2' | 1:CA:784:C:H6 | 1.79 | 0.46 |
| 1:CA:66:G:H5' | 1:CA:173:U:O4 | 2.15 | 0.46 |
| 38:BP:88:ILE:CG1 | 38:BP:89:VAL:N | 2.78 | 0.46 |
| 20:CT:13:LEU:O | 20:CT:16:HIS:N | 2.48 | 0.46 |
| 13:AM:3:ARG:HA | 13:AM:9:ILE:HG12 | 1.97 | 0.46 |
| 10:CJ:34:VAL:CG1 | 10:CJ:74:ILE:HG22 | 2.45 | 0.46 |
| 1:CA:522:C:O2' | 1:CA:523:A:H5' | 2.16 | 0.46 |
| 24:BB:19:G:N2 | 24:BB:65:C:C2 | 2.83 | 0.46 |
| 1:CA:1054:C:H6 | 1:CA:1196:U:O2 | 1.99 | 0.46 |
| 33:DK:2:ILE:CD1 | 33:DK:82:ASN:ND2 | 2.79 | 0.46 |
| 17:CQ:31:LEU:O | 17:CQ:31:LEU:HG | 2.16 | 0.46 |
| 29:BG:98:LEU:HB2 | 29:BG:125:VAL:CG2 | 2.46 | 0.46 |
| 1:AA:1441:G:O5' | 1:AA:1441:G:H8 | 1.99 | 0.46 |
| 3:CC:73:PRO:O | 3:CC:76:VAL:HG22 | 2.16 | 0.46 |
| 39:BQ:62:ILE:HD13 | 39:BQ:62:ILE:N | 2.30 | 0.46 |
| 4:AD:4:TYR:OH | 4:AD:66:ARG:HG2 | 2.15 | 0.46 |
| 1:CA:611:A:H61 | 1:CA:629:G:H1 | 1.64 | 0.46 |
| 1:CA:937:A:C2 | 1:CA:1379:G:C6 | 3.04 | 0.46 |
| 1:AA:434:U:H2' | 1:AA:435:C:C6 | 2.50 | 0.46 |
| 19:AS:29:ARG:HD2 | 19:AS:30:LEU:N | 2.30 | 0.46 |
| 39:BQ:111:GLU:HA | 39:BQ:114:LYS:HB2 | 1.98 | 0.46 |
| 1:AA:1311:G:H1 | 1:AA:1326:C:N4 | 2.13 | 0.46 |
| 1:AA:638:G:C6 | 1:AA:639:G:N7 | 2.83 | 0.46 |
| 16:CP:12:LYS:O | 16:CP:13:HIS:HB2 | 2.16 | 0.46 |
| 44:DV:178:GLU:HG3 | 44:DV:178:GLU:O | 2.16 | 0.46 |
| 40:DR:1:MET:N | 40:DR:16:PRO:HD3 | 2.30 | 0.46 |
| 20:CT:82:SER:O | 20:CT:86:ARG:CB | 2.64 | 0.46 |
| 23:BA:1239:G:C6 | 23:BA:1240:U:C4 | 3.04 | 0.46 |
| 18:AR:53:ARG:O | 18:AR:55:ARG:N | 2.49 | 0.46 |
| 23:DA:948:G:OP1 | 23:DA:962:G:OP1 | 2.34 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BA:1465:G:N2 | 23:BA:1466:G:H1' | 2.30 | 0.46 |
| 13:CM:86:CYS:HA | 19:CS:73:GLU:O | 2.16 | 0.46 |
| 23:DA:2495:G:C2' | 23:DA:2496:C:O5' | 2.63 | 0.46 |
| 37:DO:98:VAL:O | 37:DO:101:LEU:HB3 | 2.15 | 0.46 |
| 23:BA:1360:A:C5' | 23:BA:1361:G:OP2 | 2.64 | 0.46 |
| 4:AD:76:ARG:NH2 | 4:AD:80:GLU:OE1 | 2.49 | 0.46 |
| 30:DH:51:ILE:HG22 | 30:DH:52:ARG:N | 2.30 | 0.46 |
| 23:DA:270(Z):G:C2 | 23:DA:271(A):U:O4 | 2.69 | 0.46 |
| 15:AO:25:THR:OG1 | 15:AO:26:GLU:N | 2.49 | 0.46 |
| 23:BA:2257:U:O2' | 23:BA:2258:C:H5' | 2.15 | 0.46 |
| 45:BW:55:ARG:NH1 | 45:BW:55:ARG:HB3 | 2.31 | 0.46 |
| 36:DN:116:LEU:HA | 36:DN:116:LEU:HD23 | 1.61 | 0.46 |
| 33:DK:3:GLN:HG3 | 33:DK:4:PRO:HD2 | 1.97 | 0.46 |
| 7:AG:106:GLN:O | 7:AG:110:GLN:HG3 | 2.16 | 0.46 |
| 23:DA:2393:A:H4' | 34:DL:61:ARG:O | 2.16 | 0.46 |
| 32:BJ:119:GLU:O | 32:BJ:123:GLU:HG3 | 2.16 | 0.46 |
| 23:BA:806:C:O5' | 23:BA:806:C:H6 | 1.99 | 0.46 |
| 1:CA:1347:G:C2 | 1:CA:1373:G:C5 | 3.03 | 0.46 |
| 9:CI:111:ARG:HG3 | 14:CN:61:TRP:HE1 | 1.81 | 0.46 |
| 1:AA:950:U:O2' | 1:AA:951:G:H5' | 2.15 | 0.46 |
| 21:AU:14:TRP:CE3 | 21:AU:15:ARG:HG2 | 2.50 | 0.46 |
| 22:AV:6191:A:C2 | 22:AV:6192:G:C4 | 3.04 | 0.46 |
| 7:AG:115:ARG:O | 7:AG:119:ARG:HG3 | 2.16 | 0.46 |
| 22:CV:6182:A:C2 | 22:CV:6195:G:N2 | 2.83 | 0.46 |
| 23:DA:2846:G:P | 38:DP:54:ARG:HB2 | 2.56 | 0.46 |
| 42:DT:62:LYS:H | 42:DT:62:LYS:HG2 | 1.58 | 0.46 |
| 25:DC:32:SER:O | 25:DC:33:LEU:O | 2.34 | 0.46 |
| 23:DA:242:G:N7 | 53:D5:5:LYS:HG2 | 2.31 | 0.46 |
| 34:DL:50:ARG:HB2 | 53:D5:60:LEU:CD2 | 2.46 | 0.46 |
| 30:BH:88:ILE:HG13 | 30:BH:144:VAL:CG1 | 2.46 | 0.46 |
| 39:BQ:72:HIS:CE1 | 39:BQ:107:ALA:HA | 2.51 | 0.46 |
| 40:BR:2:PHE:HE2 | 40:BR:13:ARG:CG | 2.29 | 0.46 |
| 23:DA:2728:U:O2 | 23:DA:2729:G:C8 | 2.68 | 0.46 |
| 37:DO:12:PHE:O | 37:DO:12:PHE:HD1 | 1.98 | 0.46 |
| 4:AD:119:GLN:O | 4:AD:123:HIS:CD2 | 2.69 | 0.46 |
| 4:AD:108:LEU:HB3 | 4:AD:110:PHE:CD2 | 2.49 | 0.46 |
| 23:BA:323:G:H5' | 27:BE:169:ASN:ND2 | 2.21 | 0.46 |
| 46:DX:10:LYS:O | 46:DX:13:ILE:CG2 | 2.64 | 0.46 |
| 1:CA:1291:G:C6 | 1:CA:1292:U:C4 | 3.04 | 0.46 |
| 44:DV:101:PRO:O | 44:DV:102:LEU:HD23 | 2.16 | 0.46 |
| 19:AS:40:ILE:HG13 | 19:AS:69:HIS:O | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 18:AR:35:ARG:O | 18:AR:37:VAL:N | 2.45 | 0.46 |
| 1:AA:1309:G:N2 | 1:AA:1329:A:H1' | 2.30 | 0.46 |
| 1:CA:624:C:H4' | 16:CP:11:SER:N | 2.20 | 0.46 |
| 27:BE:68:LYS:H | 27:BE:70:THR:HG22 | 1.81 | 0.46 |
| 34:BL:16:ARG:C | 34:BL:16:ARG:NE | 2.61 | 0.46 |
| 23:BA:733:G:H8 | 23:BA:733:G:O5' | 1.99 | 0.46 |
| 1:CA:1219:U:OP1 | 14:CN:19:ARG:NH2 | 2.35 | 0.46 |
| 23:DA:2287:A:C5 | 23:DA:2289:G:C5 | 3.04 | 0.46 |
| 2:AB:63:MET:C | 2:AB:65:GLY:H | 2.19 | 0.46 |
| 11:AK:32:ILE:HD11 | 11:AK:68:ALA:HB1 | 1.97 | 0.46 |
| 23:BA:2636:U:C2 | 23:BA:2637:U:C5 | 3.04 | 0.46 |
| 23:BA:2467:C:H4' | 35:BM:123:HIS:ND1 | 2.31 | 0.46 |
| 50:D2:35:GLU:OE2 | 50:D2:51:TYR:HA | 2.16 | 0.46 |
| 24:DB:21:G:N2 | 24:DB:62:C:N3 | 2.59 | 0.46 |
| 35:DM:21:THR:O | 35:DM:22:LYS:C | 2.54 | 0.46 |
| 23:DA:2661:G:C6 | 23:DA:2662:A:C2 | 3.03 | 0.46 |
| 23:BA:1728:G:C8 | 23:BA:1728:G:O5' | 2.63 | 0.46 |
| 1:AA:649:G:N3 | 1:AA:650:G:C8 | 2.83 | 0.46 |
| 23:DA:1820:U:H4' | 23:DA:1821:A:OP2 | 2.16 | 0.46 |
| 1:AA:1511:G:H2' | 1:AA:1512:U:O4' | 2.16 | 0.46 |
| 20:AT:93:GLU:O | 20:AT:93:GLU:HG2 | 2.15 | 0.46 |
| 28:BF:16:ARG:O | 28:BF:20:ILE:HG12 | 2.16 | 0.46 |
| 23:BA:979:G:H3' | 23:BA:980:A:C5' | 2.46 | 0.46 |
| 23:BA:2661:G:H2' | 23:BA:2662:A:O4' | 2.16 | 0.46 |
| 1:AA:433:C:C6 | 1:AA:434:U:H5 | 2.34 | 0.46 |
| 23:DA:775:G:O5' | 23:DA:777:A:H1' | 2.15 | 0.46 |
| 19:AS:18:LYS:HG2 | 19:AS:31:ILE:HD13 | 1.98 | 0.46 |
| 1:CA:638:G:C6 | 1:CA:639:G:N7 | 2.84 | 0.46 |
| 41:BS:47:VAL:HA | 41:BS:50:VAL:HG12 | 1.98 | 0.46 |
| 5:AE:38:GLN:HG2 | 5:AE:38:GLN:O | 2.15 | 0.46 |
| 1:CA:178:C:C2' | 1:CA:179:A:H5' | 2.46 | 0.46 |
| 11:CK:103:LEU:HA | 11:CK:103:LEU:HD12 | 1.83 | 0.46 |
| 1:CA:1288:A:C6 | 1:CA:1289:A:C5 | 3.03 | 0.46 |
| 1:CA:141:A:C5 | 1:CA:142:G:N7 | 2.84 | 0.46 |
| 40:BR:1:MET:N | 40:BR:16:PRO:HD3 | 2.31 | 0.46 |
| 23:BA:1717:G:C5 | 23:BA:1743:G:N1 | 2.84 | 0.46 |
| 11:CK:86:GLY:N | 11:CK:112:THR:OG1 | 2.43 | 0.46 |
| 23:BA:2582:G:C2 | 23:BA:2583:G:C8 | 3.04 | 0.46 |
| 3:CC:108:ASN:HB3 | 3:CC:111:LEU:HD12 | 1.98 | 0.46 |
| 12:AL:89:VAL:O | 12:AL:90:LYS:C | 2.52 | 0.46 |
| 1:CA:892:A:C6 | 1:CA:893:C:C4 | 3.04 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BA:1984:G:H2' | 23:BA:1985:G:O5' | 2.15 | 0.46 |
| 23:BA:696:G:H2' | 23:BA:697:C:H6 | 1.81 | 0.46 |
| 23:BA:1455:G:C2 | 23:BA:1456:G:C8 | 3.03 | 0.46 |
| 5:CE:72:GLN:O | 5:CE:73:ASN:CB | 2.63 | 0.46 |
| 23:BA:2620:C:C4' | 26:BD:156:MET:HG3 | 2.46 | 0.46 |
| 35:DM:131:ILE:HG22 | 35:DM:132:VAL:N | 2.31 | 0.46 |
| 48:DZ:56:VAL:O | 48:DZ:57:GLU:HG2 | 2.16 | 0.46 |
| 15:AO:42:HIS:CD2 | 15:AO:43:LEU:HD23 | 2.51 | 0.46 |
| 23:DA:2726:U:H5' | 23:DA:2726:U:O2 | 2.15 | 0.46 |
| 23:BA:1603:A:OP1 | 23:BA:1604:C:OP2 | 2.34 | 0.46 |
| 1:AA:360:A:H2' | 1:AA:361:G:C8 | 2.51 | 0.46 |
| 34:BL:62:LEU:O | 34:BL:62:LEU:CD2 | 2.62 | 0.45 |
| 23:BA:857:C:N3 | 23:BA:858:U:C4 | 2.84 | 0.45 |
| 23:BA:860:U:C5 | 23:BA:2268:A:C8 | 3.05 | 0.45 |
| 23:BA:918:A:H5'' | 23:BA:919:G:OP2 | 2.16 | 0.45 |
| 48:BZ:15:TYR:HB3 | 48:BZ:19:GLN:NE2 | 2.31 | 0.45 |
| 7:CG:115:ARG:O | 7:CG:119:ARG:HG3 | 2.15 | 0.45 |
| 1:CA:1369:C:P | 9:CI:111:ARG:HG3 | 2.56 | 0.45 |
| 1:AA:1221:G:OP1 | 1:AA:1321:C:N3 | 2.49 | 0.45 |
| 25:BC:208:LYS:HG3 | 25:BC:211:ARG:H | 1.80 | 0.45 |
| 22:CV:6194:C:C2 | 22:CV:6195:G:C8 | 3.04 | 0.45 |
| 13:CM:108:ARG:HA | 13:CM:111:LYS:HB2 | 1.99 | 0.45 |
| 23:BA:2392:A:H2 | 23:BA:2424:C:N4 | 2.08 | 0.45 |
| 23:DA:664:C:H4' | 23:DA:941:A:OP1 | 2.16 | 0.45 |
| 23:DA:1899:G:N2 | 23:DA:1902:C:H5 | 2.10 | 0.45 |
| 23:BA:1971:A:H5'' | 23:BA:1971:A:H8 | 1.80 | 0.45 |
| 41:DS:86:LEU:HD12 | 41:DS:87:PRO:CD | 2.46 | 0.45 |
| 53:D5:2:PRO:O | 53:D5:3:LYS:HB2 | 2.16 | 0.45 |
| 34:DL:46:LYS:HB3 | 34:DL:52:GLU:HG2 | 1.98 | 0.45 |
| 39:BQ:83:LEU:N | 39:BQ:83:LEU:HD12 | 2.31 | 0.45 |
| 25:BC:97:TYR:HB2 | 25:BC:101:GLU:O | 2.16 | 0.45 |
| 30:DH:98:ALA:O | 30:DH:109:ILE:HD11 | 2.15 | 0.45 |
| 1:AA:390:C:O3' | 16:AP:28:ARG:NH2 | 2.47 | 0.45 |
| 25:DC:233:HIS:HE1 | 25:DC:247:ALA:N | 2.11 | 0.45 |
| 4:AD:110:PHE:HE1 | 4:AD:148:VAL:HG23 | 1.81 | 0.45 |
| 3:AC:91:LEU:HD12 | 3:AC:101:LEU:HD21 | 1.99 | 0.45 |
| 36:DN:9:LYS:O | 36:DN:10:LEU:HD23 | 2.17 | 0.45 |
| 44:BV:92:SER:O | 44:BV:93:ASP:HB3 | 2.16 | 0.45 |
| 37:DO:57:LYS:HB3 | 37:DO:58:LEU:HD12 | 1.98 | 0.45 |
| 12:AL:68:TYR:HB3 | 12:AL:98:HIS:CD2 | 2.52 | 0.45 |
| 13:CM:10:PRO:CG | 13:CM:22:ILE:HD11 | 2.43 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:CD:100:ARG:NH2 | 4:CD:118:ARG:NH1 | 2.60 | 0.45 |
| 1:AA:130:A:OP2 | 1:AA:189:U:C2 | 2.69 | 0.45 |
| 46:DX:11:ARG:NH1 | 46:DX:61:ARG:N | 2.63 | 0.45 |
| 12:CL:68:TYR:HB3 | 12:CL:98:HIS:CD2 | 2.51 | 0.45 |
| 1:CA:1292:U:C2 | 1:CA:1293:G:N7 | 2.84 | 0.45 |
| 36:BN:40:LYS:HB2 | 36:BN:40:LYS:HE3 | 1.73 | 0.45 |
| 1:CA:319:G:H2' | 1:CA:320:C:O4' | 2.17 | 0.45 |
| 1:CA:758:G:H4' | 1:CA:880:C:H4' | 1.98 | 0.45 |
| 46:BX:11:ARG:C | 46:BX:13:ILE:N | 2.64 | 0.45 |
| 26:BD:25:VAL:C | 26:BD:26:ILE:HD13 | 2.37 | 0.45 |
| 23:BA:2809:A:C2 | 23:BA:2892:A:C4 | 3.04 | 0.45 |
| 1:AA:319:G:H2' | 1:AA:320:C:O4' | 2.16 | 0.45 |
| 37:DO:104:GLY:HA2 | 37:DO:107:GLU:CG | 2.41 | 0.45 |
| 24:BB:50:G:OP1 | 37:BO:63:THR:OG1 | 2.34 | 0.45 |
| 27:BE:65:TRP:HZ3 | 27:BE:73:ALA:O | 1.99 | 0.45 |
| 23:BA:662:G:OP1 | 34:BL:18:ARG:NH1 | 2.49 | 0.45 |
| 1:AA:175:C:H4' | 20:AT:25:ARG:HH11 | 1.81 | 0.45 |
| 1:CA:642:A:H1' | 8:CH:113:SER:OG | 2.16 | 0.45 |
| 45:DW:73:GLY:O | 45:DW:74:ARG:C | 2.54 | 0.45 |
| 30:BH:5:LEU:HD23 | 30:BH:17:GLN:O | 2.16 | 0.45 |
| 25:BC:26:LYS:HE3 | 25:BC:26:LYS:HB2 | 1.69 | 0.45 |
| 1:CA:236:G:H5'' | 17:CQ:42:TYR:OH | 2.15 | 0.45 |
| 13:CM:3:ARG:HA | 13:CM:9:ILE:HG12 | 1.98 | 0.45 |
| 9:CI:58:ARG:NH2 | 9:CI:59:PHE:CE1 | 2.84 | 0.45 |
| 23:DA:1477:A:C4 | 23:DA:1478:G:C8 | 3.04 | 0.45 |
| 10:CJ:56:HIS:O | 10:CJ:58:ASP:N | 2.41 | 0.45 |
| 23:BA:359:A:C8 | 23:BA:360:G:C8 | 3.05 | 0.45 |
| 12:CL:46:LYS:HD3 | 12:CL:47:PRO:HG3 | 1.97 | 0.45 |
| 1:AA:707:C:O2' | 1:AA:708:C:H5' | 2.16 | 0.45 |
| 23:BA:534:U:C2' | 39:BQ:49:HIS:HD2 | 2.29 | 0.45 |
| 1:CA:531:U:O3' | 1:CA:532:A:H4' | 2.16 | 0.45 |
| 32:BJ:160:LYS:HD2 | 32:BJ:160:LYS:HA | 1.58 | 0.45 |
| 4:CD:79:PHE:CD1 | 4:CD:207:TYR:CD1 | 3.04 | 0.45 |
| 10:CJ:16:LEU:O | 10:CJ:70:ARG:HD2 | 2.15 | 0.45 |
| 45:DW:31:VAL:HG13 | 45:DW:65:GLY:O | 2.16 | 0.45 |
| 33:BK:38:VAL:O | 33:BK:38:VAL:HG23 | 2.15 | 0.45 |
| 18:AR:44:LEU:HA | 18:AR:49:LYS:O | 2.15 | 0.45 |
| 15:CO:27:VAL:O | 15:CO:28:GLN:C | 2.54 | 0.45 |
| 23:BA:1749:A:H2' | 23:BA:1750:G:O4' | 2.15 | 0.45 |
| 24:DB:31:C:C2' | 24:DB:31:C:O2 | 2.64 | 0.45 |
| 23:DA:189:G:C3' | 23:DA:189:G:C8 | 2.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 23:DA:643:A:C2 | 23:DA:644:A:N9 | 2.84 | 0.45 |
| 23:BA:2738:A:C6 | 23:BA:2739:U:C5 | 3.04 | 0.45 |
| 23:DA:887:A:N3 | 23:DA:889:C:C5 | 2.84 | 0.45 |
| 23:BA:886:C:C2' | 23:BA:887:A:H4' | 2.46 | 0.45 |
| 23:DA:414:C:H2' | 23:DA:415:A:H8 | 1.80 | 0.45 |
| 1:AA:1183:A:H5'' | 1:AA:1184:G:OP2 | 2.15 | 0.45 |
| 23:DA:1471:A:C2 | 23:DA:1472:A:N9 | 2.84 | 0.45 |
| 23:BA:164:U:C4 | 23:BA:165:U:O4 | 2.69 | 0.45 |
| 27:BE:29:ASN:N | 27:BE:112:MET:HE1 | 2.32 | 0.45 |
| 9:AI:45:ALA:O | 9:AI:48:GLU:HB2 | 2.16 | 0.45 |
| 23:BA:1204:A:C2 | 23:BA:1241:A:N1 | 2.84 | 0.45 |
| 1:CA:1090:U:H2' | 1:CA:1091:U:H6 | 1.80 | 0.45 |
| 1:CA:744:C:H3' | 1:CA:744:C:H6 | 1.81 | 0.45 |
| 1:AA:1296:C:C5 | 1:AA:1297:C:C5 | 3.04 | 0.45 |
| 23:DA:770:G:H2' | 23:DA:771:G:O5' | 2.16 | 0.45 |
| 23:BA:1993:U:H4' | 26:BD:128:SER:HB3 | 1.97 | 0.45 |
| 23:BA:2584:U:C6 | 23:BA:2584:U:O5' | 2.68 | 0.45 |
| 40:BR:75:PHE:O | 40:BR:75:PHE:HD1 | 1.98 | 0.45 |
| 1:AA:826:C:C5' | 1:AA:827:U:OP2 | 2.65 | 0.45 |
| 1:AA:932:C:H2' | 1:AA:933:G:H8 | 1.81 | 0.45 |
| 1:CA:1004:A:H2 | 1:CA:1024:G:N3 | 2.14 | 0.45 |
| 1:AA:451:A:C8 | 1:AA:481:G:C6 | 3.04 | 0.45 |
| 23:BA:2104:G:H2' | 23:BA:2105:C:C6 | 2.52 | 0.45 |
| 23:BA:31:C:C4 | 23:BA:32:C:C5 | 3.05 | 0.45 |
| 23:DA:2359:C:H2' | 23:DA:2360:A:C8 | 2.51 | 0.45 |
| 27:BE:135:LYS:O | 27:BE:136:THR:C | 2.54 | 0.45 |
| 23:BA:2490:G:H4' | 23:BA:2491:U:OP1 | 2.15 | 0.45 |
| 1:AA:1489:G:C6 | 1:AA:1490:C:N4 | 2.85 | 0.45 |
| 1:AA:1031:G:H2' | 1:AA:103(A):A:O4' | 2.16 | 0.45 |
| 2:CB:100:GLY:O | 2:CB:104:ASN:N | 2.49 | 0.45 |
| 23:BA:1975:G:H2' | 23:BA:1976:U:H6 | 1.81 | 0.45 |
| 24:BB:95:U:H2' | 24:BB:96:G:C8 | 2.51 | 0.45 |
| 1:CA:582:U:OP1 | 15:CO:68:ARG:NH2 | 2.49 | 0.45 |
| 23:BA:2330:G:H1' | 45:BW:41:ARG:CB | 2.46 | 0.45 |
| 43:DU:8:LYS:HD2 | 43:DU:13:VAL:CG2 | 2.42 | 0.45 |
| 32:DJ:126:VAL:O | 32:DJ:127:LYS:C | 2.55 | 0.45 |
| 1:AA:81:G:C5 | 1:AA:82:U:C4 | 3.05 | 0.45 |
| 26:BD:188:VAL:HA | 26:BD:189:PRO:HD3 | 1.67 | 0.45 |
| 13:AM:94:ARG:NH2 | 19:AS:80:TYR:HE2 | 2.15 | 0.45 |
| 12:CL:25:ALA:O | 12:CL:26:LEU:HB2 | 2.15 | 0.45 |
| 37:BO:29:PHE:CD2 | 37:BO:92:TYR:OH | 2.69 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 32:BJ:157:ARG:O | 32:BJ:159:GLU:N | 2.49 | 0.45 |
| 1:CA:389:A:C5 | 1:CA:390:C:H1' | 2.51 | 0.45 |
| 16:CP:58:TYR:O | 16:CP:61:SER:HB3 | 2.16 | 0.45 |
| 23:BA:2730:C:C2' | 23:BA:2731:G:H5' | 2.46 | 0.45 |
| 23:DA:2727:G:C4 | 23:DA:2728:U:H5 | 2.30 | 0.45 |
| 23:DA:2291:U:H2' | 23:DA:2292:C:C6 | 2.51 | 0.45 |
| 1:AA:492:G:C4 | 1:AA:493:G:C8 | 3.05 | 0.45 |
| 42:DT:31:HIS:HA | 42:DT:32:PRO:HD3 | 1.85 | 0.45 |
| 23:DA:2712:U:HO2' | 23:DA:712(B):A:H5'' | 1.80 | 0.45 |
| 49:D1:40:ILE:HG23 | 49:D1:59:VAL:CG2 | 2.46 | 0.45 |
| 26:BD:55:ASN:O | 26:BD:59:VAL:HG23 | 2.16 | 0.45 |
| 3:AC:172:ARG:HE | 3:AC:174:PRO:HG2 | 1.81 | 0.45 |
| 23:DA:1329:U:H5'' | 23:DA:1330:C:C5 | 2.43 | 0.45 |
| 42:BT:39:ILE:HG12 | 42:BT:39:ILE:H | 1.55 | 0.45 |
| 41:DS:75:TYR:CD2 | 41:DS:75:TYR:C | 2.90 | 0.45 |
| 3:AC:181:ASN:HB3 | 3:AC:205:GLY:HA3 | 1.98 | 0.45 |
| 41:BS:20:VAL:O | 41:BS:23:LEU:HB2 | 2.15 | 0.45 |
| 43:DU:95:LYS:HE2 | 43:DU:100:ALA:HB2 | 1.98 | 0.45 |
| 4:AD:152:SER:O | 4:AD:153:ARG:C | 2.54 | 0.45 |
| 29:DG:67:LEU:O | 29:DG:71:LEU:HB2 | 2.16 | 0.45 |
| 23:BA:85:G:N3 | 23:BA:103:A:H2 | 2.14 | 0.45 |
| 23:BA:2892:A:C2' | 23:BA:2893:G:H5' | 2.46 | 0.45 |
| 11:CK:13:GLN:HG3 | 11:CK:75:TYR:O | 2.16 | 0.45 |
| 11:CK:32:ILE:O | 11:CK:40:ILE:HG12 | 2.16 | 0.45 |
| 1:CA:1148:U:H2' | 1:CA:1149:C:O4' | 2.16 | 0.45 |
| 1:AA:783:C:N4 | 1:AA:799:G:H1 | 2.14 | 0.45 |
| 1:AA:875:C:O2' | 8:AH:14:ARG:NH1 | 2.45 | 0.45 |
| 33:DK:63:VAL:HG23 | 33:DK:64:ARG:HG3 | 1.98 | 0.45 |
| 1:AA:302:G:N3 | 1:AA:556:C:H4' | 2.32 | 0.45 |
| 25:DC:148:GLU:HB2 | 25:DC:151:LYS:HD3 | 1.97 | 0.45 |
| 34:DL:70:GLN:O | 34:DL:71:VAL:C | 2.53 | 0.45 |
| 43:BU:50:ARG:HD3 | 43:BU:51:VAL:N | 2.25 | 0.45 |
| 43:BU:42:VAL:CG2 | 43:BU:67:LEU:HD11 | 2.46 | 0.45 |
| 16:AP:10:GLY:O | 16:AP:11:SER:O | 2.35 | 0.45 |
| 36:BN:99:LYS:HA | 36:BN:112:ALA:HB2 | 1.98 | 0.45 |
| 43:DU:46:LYS:O | 43:DU:47:LYS:C | 2.55 | 0.45 |
| 23:DA:1388:G:N3 | 23:DA:1389:G:C8 | 2.84 | 0.45 |
| 23:DA:1389:G:H2' | 23:DA:1390:U:H6 | 1.80 | 0.45 |
| 29:BG:87:LEU:CD2 | 29:BG:164:TYR:HD1 | 2.30 | 0.45 |
| 3:CC:23:TYR:CD1 | 10:CJ:10:GLY:HA2 | 2.50 | 0.45 |
| 45:DW:81:VAL:O | 45:DW:83:PRO:HD3 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 45:DW:31:VAL:HG21 | 45:DW:61:ALA:HB2 | 1.98 | 0.45 |
| 1:CA:1410:G:H2' | 1:CA:1411:C:H6 | 1.81 | 0.45 |
| 23:BA:635:C:O2' | 23:BA:639:U:OP1 | 2.32 | 0.45 |
| 1:AA:543:C:C2 | 1:AA:544:G:C8 | 3.05 | 0.45 |
| 4:AD:4:TYR:CE1 | 4:AD:11:LEU:HD11 | 2.50 | 0.45 |
| 1:CA:560:U:H5' | 1:CA:566:G:N2 | 2.31 | 0.45 |
| 23:BA:978:G:C2 | 23:BA:986:C:C2 | 3.05 | 0.45 |
| 17:AQ:51:TYR:CD1 | 17:AQ:73:VAL:HG11 | 2.51 | 0.45 |
| 1:CA:638:G:C2 | 1:CA:639:G:C8 | 3.04 | 0.45 |
| 44:DV:121:HIS:CE1 | 44:DV:169:GLU:OE2 | 2.69 | 0.45 |
| 23:BA:1230:C:H2' | 23:BA:1231:G:H8 | 1.81 | 0.45 |
| 1:CA:357:G:C2 | 1:CA:358:U:C5 | 3.04 | 0.45 |
| 27:BE:84:VAL:C | 27:BE:86:GLY:H | 2.20 | 0.45 |
| 23:DA:644:A:N1 | 23:DA:646:A:C4 | 2.84 | 0.45 |
| 10:AJ:6:ILE:HG22 | 10:AJ:98:ILE:HG12 | 1.98 | 0.45 |
| 1:AA:1182:G:H4' | 1:AA:1183:A:C5' | 2.45 | 0.45 |
| 23:DA:1833:U:H2' | 23:DA:1834:U:H6 | 1.80 | 0.45 |
| 23:BA:969:U:H2' | 23:BA:970:C:C6 | 2.51 | 0.45 |
| 4:CD:23:GLY:HA3 | 4:CD:112:VAL:HG22 | 1.98 | 0.45 |
| 16:CP:50:LYS:HD3 | 16:CP:51:VAL:N | 2.31 | 0.45 |
| 23:BA:374:A:H3' | 23:BA:375:C:C6 | 2.51 | 0.45 |
| 20:AT:84:LEU:HD13 | 20:AT:84:LEU:C | 2.36 | 0.45 |
| 23:BA:13:A:N1 | 23:BA:525:U:C2 | 2.84 | 0.45 |
| 35:BM:34:LEU:HD12 | 35:BM:130:LYS:O | 2.16 | 0.45 |
| 19:CS:33:THR:CG2 | 19:CS:51:VAL:HA | 2.46 | 0.45 |
| 16:AP:47:ASP:C | 16:AP:49:LEU:H | 2.19 | 0.45 |
| 16:AP:50:LYS:HD3 | 16:AP:51:VAL:N | 2.32 | 0.45 |
| 1:AA:646:U:C4 | 1:AA:647:C:N4 | 2.84 | 0.45 |
| 23:BA:1360:A:H5' | 23:BA:1361:G:OP2 | 2.16 | 0.45 |
| 1:AA:292:G:C5 | 1:AA:293:G:H1' | 2.52 | 0.45 |
| 22:CV:6185:U:C5 | 22:CV:6186:U:C5 | 3.04 | 0.45 |
| 23:BA:153:C:OP1 | 46:BX:92:LYS:HE2 | 2.16 | 0.45 |
| 1:CA:245:C:O2 | 1:CA:283:C:N3 | 2.50 | 0.45 |
| 23:BA:1417:C:H42 | 23:BA:1581:G:H1 | 1.64 | 0.45 |
| 38:DP:14:TYR:H | 38:DP:14:TYR:HD1 | 1.62 | 0.45 |
| 38:BP:101:PHE:CD2 | 38:BP:101:PHE:C | 2.89 | 0.45 |
| 48:DZ:18:ASP:N | 48:DZ:18:ASP:OD1 | 2.48 | 0.45 |
| 26:BD:14:ILE:C | 26:BD:14:ILE:HD12 | 2.36 | 0.45 |
| 8:CH:107:LEU:HD23 | 8:CH:107:LEU:N | 2.31 | 0.45 |
| 40:DR:95:LEU:HD23 | 40:DR:96:ILE:N | 2.31 | 0.45 |
| 53:B5:23:VAL:HG12 | 53:B5:47:LYS:HB3 | 1.97 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 34:BL:62:LEU:CD1 | 34:BL:62:LEU:N | 2.79 | 0.45 |
| 26:DD:169:ASN:HD22 | 26:DD:169:ASN:C | 2.19 | 0.45 |
| 1:AA:961:U:OP2 | 1:AA:1223:C:C1' | 2.64 | 0.45 |
| 13:CM:87:TYR:O | 13:CM:91:ARG:HG2 | 2.16 | 0.45 |
| 32:BJ:112:LYS:O | 32:BJ:116:THR:CG2 | 2.65 | 0.45 |
| 47:DY:18:PRO:O | 47:DY:22:GLU:HG3 | 2.17 | 0.45 |
| 28:DF:32:PRO:HA | 28:DF:162:THR:OG1 | 2.17 | 0.45 |
| 1:AA:376:G:C2 | 1:AA:389:A:C2 | 3.03 | 0.45 |
| 1:AA:35:G:C6 | 1:AA:36:C:N4 | 2.84 | 0.45 |
| 25:DC:45:ASN:C | 25:DC:45:ASN:OD1 | 2.54 | 0.45 |
| 3:CC:66:VAL:HB | 3:CC:101:LEU:CD2 | 2.40 | 0.45 |
| 5:CE:91:LEU:HD22 | 5:CE:110:LEU:HD11 | 1.98 | 0.45 |
| 5:CE:79:GLU:OE2 | 8:CH:104:ARG:HA | 2.16 | 0.45 |
| 15:CO:45:VAL:HG22 | 15:CO:46:HIS:ND1 | 2.32 | 0.45 |
| 5:AE:80:ILE:HD12 | 5:AE:138:ALA:HB1 | 1.99 | 0.45 |
| 4:AD:61:LYS:HA | 4:AD:203:VAL:CG2 | 2.46 | 0.45 |
| 8:AH:92:ARG:CB | 8:AH:94:TYR:HE2 | 2.21 | 0.45 |
| 23:DA:1439:A:H2' | 23:DA:1440:G:H5' | 1.99 | 0.45 |
| 52:B4:19:ARG:HG3 | 52:B4:19:ARG:NH1 | 2.16 | 0.45 |
| 1:AA:15:G:H2' | 1:AA:16:A:C8 | 2.51 | 0.45 |
| 1:CA:57:G:C6 | 1:CA:58:C:C4 | 3.04 | 0.45 |
| 1:CA:57:G:H2' | 1:CA:58:C:O4' | 2.16 | 0.45 |
| 46:BX:91:LYS:HA | 46:BX:94:LEU:HD23 | 1.99 | 0.45 |
| 1:AA:1347:G:H22 | 1:AA:1373:G:C2' | 2.27 | 0.45 |
| 1:AA:1376:U:O2' | 1:AA:1377:A:H5' | 2.16 | 0.45 |
| 2:CB:141:GLU:O | 2:CB:145:LEU:HD23 | 2.16 | 0.45 |
| 23:BA:2308:G:HO2' | 23:BA:2310:A:P | 2.39 | 0.45 |
| 1:CA:725:G:H2' | 1:CA:726:C:H6 | 1.81 | 0.45 |
| 25:BC:132:PRO:CG | 25:BC:190:TYR:CE1 | 2.97 | 0.45 |
| 23:BA:2009:G:O2' | 23:BA:2010:G:H5' | 2.16 | 0.45 |
| 23:BA:2753:A:H2' | 23:BA:2754:U:H5' | 1.98 | 0.45 |
| 29:BG:19:VAL:HG13 | 29:BG:43:VAL:CG2 | 2.47 | 0.45 |
| 1:CA:818:G:HO2' | 1:CA:820:U:H6 | 1.61 | 0.45 |
| 23:BA:1332:G:H22 | 23:BA:1610:A:H8 | 1.63 | 0.45 |
| 8:AH:25:ASP:OD1 | 8:AH:25:ASP:N | 2.49 | 0.45 |
| 27:BE:53:THR:C | 27:BE:55:GLY:H | 2.19 | 0.45 |
| 39:DQ:61:TRP:O | 39:DQ:64:ARG:HB2 | 2.16 | 0.45 |
| 9:CI:58:ARG:NH2 | 9:CI:59:PHE:HE1 | 2.14 | 0.45 |
| 44:DV:180:VAL:C | 44:DV:182:LYS:N | 2.69 | 0.45 |
| 24:DB:21:G:H2' | 24:DB:22:U:C6 | 2.50 | 0.45 |
| 23:BA:908:C:O2' | 23:BA:909:A:H5' | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DA:540:G:H2' | 23:DA:541:C:C6 | 2.43 | 0.45 |
| 23:DA:247:G:H4' | 23:DA:386:G:C5 | 2.52 | 0.45 |
| 45:DW:62:LEU:O | 45:DW:63:VAL:HG13 | 2.16 | 0.45 |
| 1:AA:922:G:H5'' | 1:AA:923:A:OP2 | 2.16 | 0.45 |
| 23:DA:300:A:P | 43:DU:84:ARG:NH2 | 2.89 | 0.45 |
| 1:CA:952:U:O2' | 1:CA:953:G:H5' | 2.17 | 0.45 |
| 1:CA:433:C:C6 | 1:CA:434:U:H5 | 2.34 | 0.45 |
| 23:BA:2661:G:C6 | 23:BA:2662:A:C2 | 3.04 | 0.45 |
| 27:DE:46:ARG:HB3 | 27:DE:46:ARG:NH1 | 2.32 | 0.45 |
| 7:AG:50:ILE:O | 7:AG:54:THR:O | 2.34 | 0.45 |
| 23:DA:634:C:H2' | 23:DA:635:C:H6 | 1.81 | 0.45 |
| 1:AA:1378:C:H5 | 1:AA:1379:G:C8 | 2.35 | 0.45 |
| 23:DA:1164:G:C5 | 23:DA:1165:U:C4 | 3.03 | 0.45 |
| 15:CO:67:LEU:HD23 | 15:CO:78:TYR:CE1 | 2.51 | 0.45 |
| 1:CA:804:U:H5'' | 1:CA:805:C:OP2 | 2.16 | 0.45 |
| 14:CN:43:CYS:O | 14:CN:46:GLU:N | 2.49 | 0.45 |
| 34:BL:122:PRO:HB3 | 34:BL:141:ALA:O | 2.16 | 0.45 |
| 1:CA:1360:A:C6 | 1:CA:1361:G:C2 | 3.04 | 0.45 |
| 27:BE:160:ASN:OD1 | 27:BE:163:VAL:HG23 | 2.15 | 0.45 |
| 18:CR:84:LYS:H | 18:CR:84:LYS:HG2 | 1.35 | 0.45 |
| 1:AA:123:C:H5'' | 1:AA:311:C:O2' | 2.16 | 0.45 |
| 23:DA:1239:G:C6 | 23:DA:1240:U:C4 | 3.04 | 0.45 |
| 23:DA:164:U:C4 | 23:DA:165:U:O4 | 2.69 | 0.45 |
| 1:AA:247:G:C4 | 1:AA:248:C:C5 | 3.04 | 0.45 |
| 26:DD:146:THR:HA | 26:DD:147:PRO:C | 2.37 | 0.45 |
| 23:DA:1382:G:H4' | 23:DA:1573:G:C2 | 2.52 | 0.45 |
| 3:AC:111:LEU:HD11 | 3:AC:144:SER:OG | 2.15 | 0.45 |
| 23:DA:768:G:C4 | 23:DA:769:G:C8 | 3.04 | 0.45 |
| 1:AA:662:G:C2 | 1:AA:744:C:O2 | 2.70 | 0.45 |
| 23:BA:476:G:H4' | 23:BA:502:A:N1 | 2.32 | 0.45 |
| 23:BA:537:C:H2' | 23:BA:539:G:O4' | 2.17 | 0.45 |
| 27:BE:144:LYS:C | 27:BE:146:ALA:H | 2.20 | 0.45 |
| 4:CD:143:GLY:H | 4:CD:185:PHE:HB3 | 1.82 | 0.45 |
| 23:DA:1274:A:N3 | 23:DA:1297:C:H1' | 2.31 | 0.45 |
| 1:AA:608:A:C4 | 1:AA:609:A:C8 | 3.03 | 0.45 |
| 28:BF:44:GLY:O | 28:BF:47:LYS:HB2 | 2.17 | 0.45 |
| 23:BA:220:G:N1 | 23:BA:428:A:OP2 | 2.35 | 0.45 |
| 53:D5:23:VAL:HG12 | 53:D5:47:LYS:HB3 | 1.99 | 0.45 |
| 23:BA:309:G:O3' | 43:BU:18:GLY:HA2 | 2.16 | 0.45 |
| 43:BU:8:LYS:HE2 | 43:BU:8:LYS:HB2 | 1.55 | 0.45 |
| 23:DA:2014:A:H2' | 23:DA:2015:A:C8 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:AB:157:ARG:O | 2:AB:159:PRO:HD3 | 2.15 | 0.45 |
| 23:BA:804:A:C5' | 23:BA:805:G:OP1 | 2.54 | 0.45 |
| 1:AA:969:A:C2' | 1:AA:970:C:H5' | 2.46 | 0.45 |
| 37:BO:11:LYS:O | 37:BO:12:PHE:CB | 2.64 | 0.45 |
| 23:DA:2502:G:C5' | 23:DA:2503:A:C5' | 2.89 | 0.45 |
| 39:DQ:88:ILE:HB | 39:DQ:90:VAL:CG1 | 2.29 | 0.45 |
| 39:DQ:91:ASP:OD2 | 39:DQ:96:ALA:CB | 2.61 | 0.45 |
| 25:BC:105:ILE:HD13 | 25:BC:106:ILE:H | 1.80 | 0.45 |
| 28:DF:86:MET:O | 28:DF:87:PRO:O | 2.34 | 0.45 |
| 32:DJ:110:LEU:CD2 | 32:DJ:110:LEU:O | 2.65 | 0.45 |
| 1:CA:376:G:C2' | 1:CA:377:G:O5' | 2.65 | 0.45 |
| 1:CA:376:G:C4 | 1:CA:389:A:N1 | 2.85 | 0.45 |
| 30:BH:88:ILE:HG13 | 30:BH:144:VAL:HG11 | 1.99 | 0.45 |
| 16:AP:4:ILE:HA | 16:AP:20:VAL:O | 2.17 | 0.45 |
| 1:AA:404:U:C2 | 1:AA:405:U:C5 | 3.05 | 0.45 |
| 4:AD:111:ALA:HB1 | 4:AD:116:GLN:CG | 2.47 | 0.45 |
| 42:DT:12:VAL:HG22 | 42:DT:17:ALA:HB2 | 1.99 | 0.45 |
| 30:DH:88:ILE:CG1 | 30:DH:123:LEU:HA | 2.44 | 0.45 |
| 1:CA:233:C:C2' | 1:CA:234:C:H5' | 2.47 | 0.45 |
| 23:DA:139:G:N3 | 23:DA:141(A):A:N1 | 2.64 | 0.45 |
| 4:CD:29:PRO:O | 4:CD:30:LYS:CB | 2.65 | 0.45 |
| 44:BV:56:VAL:HG12 | 44:BV:57:ILE:N | 2.31 | 0.45 |
| 24:BB:13:A:O4' | 45:BW:74:ARG:NH2 | 2.49 | 0.45 |
| 37:DO:69:VAL:HA | 37:DO:72:ALA:HB2 | 1.98 | 0.45 |
| 26:DD:52:LEU:O | 26:DD:75:VAL:HA | 2.16 | 0.45 |
| 1:AA:1067:A:N3 | 1:AA:1068:G:H1' | 2.31 | 0.45 |
| 1:CA:407:G:C2 | 1:CA:436:C:C2 | 3.04 | 0.45 |
| 36:DN:57:ARG:HG2 | 36:DN:58:GLY:N | 2.28 | 0.45 |
| 4:AD:158:ILE:HG22 | 4:AD:159:ARG:N | 2.29 | 0.45 |
| 1:AA:1367:C:C2 | 1:AA:1368:G:C8 | 3.04 | 0.45 |
| 1:AA:1374:A:C4 | 1:AA:1375:A:C8 | 3.05 | 0.45 |
| 23:DA:2745:C:C4 | 23:DA:2746:U:C5 | 3.04 | 0.45 |
| 23:BA:2308:G:O2' | 23:BA:2310:A:P | 2.74 | 0.45 |
| 6:AF:5:GLU:OE1 | 6:AF:62:TRP:CZ2 | 2.70 | 0.45 |
| 41:DS:8:ARG:O | 41:DS:9:TYR:HB2 | 2.16 | 0.45 |
| 23:DA:1503:U:C2 | 23:DA:1504:C:H5 | 2.34 | 0.45 |
| 23:DA:1104:C:C2' | 23:DA:1105:U:H5' | 2.46 | 0.45 |
| 1:AA:1237:C:C5 | 1:AA:1336:C:N3 | 2.85 | 0.45 |
| 1:CA:1529:G:H4' | 1:CA:1530:G:OP2 | 2.16 | 0.45 |
| 23:BA:910:A:H2' | 23:BA:2264:C:O2' | 2.15 | 0.45 |
| 18:AR:88:LYS:OXT | 18:AR:88:LYS:HG3 | 2.15 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BE:157:VAL:HG21 | 27:BE:194:MET:HE3 | 1.97 | 0.45 |
| 16:AP:8:ARG:O | 16:AP:9:PHE:HD2 | 1.95 | 0.45 |
| 1:AA:1118:C:O4' | 1:AA:1179:A:C4 | 2.69 | 0.45 |
| 23:DA:601:C:H4' | 27:DE:104:LYS:HE2 | 1.98 | 0.45 |
| 1:CA:556:C:H2' | 1:CA:557:G:C5' | 2.44 | 0.45 |
| 39:DQ:76:TYR:CZ | 39:DQ:80:ILE:HG12 | 2.52 | 0.45 |
| 1:CA:170:U:HO2' | 1:CA:171:A:H5' | 1.81 | 0.45 |
| 43:BU:20:TYR:N | 43:BU:20:TYR:CD1 | 2.84 | 0.45 |
| 39:DQ:98:LEU:O | 39:DQ:101:ARG:N | 2.50 | 0.45 |
| 23:BA:2476:A:C2 | 23:BA:2477:C:C5 | 3.04 | 0.45 |
| 17:AQ:29:HIS:HA | 17:AQ:30:PRO:HD2 | 1.64 | 0.45 |
| 23:DA:2100:G:C2 | 23:DA:2101:G:C4 | 3.04 | 0.45 |
| 23:BA:1030:G:OP2 | 35:BM:128:LYS:HG2 | 2.16 | 0.45 |
| 35:BM:38:GLU:C | 35:BM:127:ILE:HD11 | 2.37 | 0.45 |
| 23:DA:540:G:C4 | 23:DA:541:C:C6 | 3.04 | 0.45 |
| 44:BV:180:VAL:C | 44:BV:182:LYS:N | 2.65 | 0.45 |
| 1:CA:1056:U:C5 | 1:CA:1200:C:C4 | 3.05 | 0.45 |
| 1:CA:216:G:H2' | 1:CA:217:C:H6 | 1.77 | 0.45 |
| 1:CA:913:A:O2' | 1:CA:914:A:OP2 | 2.32 | 0.45 |
| 23:BA:814:C:H2' | 23:BA:815:C:H6 | 1.81 | 0.45 |
| 46:DX:23:LYS:HB3 | 46:DX:37:ILE:CG1 | 2.47 | 0.45 |
| 1:CA:543:C:C2 | 1:CA:544:G:C8 | 3.04 | 0.45 |
| 1:AA:939:G:C2 | 1:AA:940:C:C4 | 3.04 | 0.45 |
| 23:DA:2366:A:H2' | 23:DA:2367:G:O4' | 2.16 | 0.45 |
| 1:CA:255:G:C5 | 1:CA:256:U:C5 | 3.05 | 0.45 |
| 1:CA:17:U:O4' | 1:CA:1080:A:H1' | 2.16 | 0.45 |
| 33:BK:2:ILE:HD11 | 33:BK:82:ASN:ND2 | 2.32 | 0.45 |
| 23:DA:1006:C:C2 | 23:DA:1138:G:N2 | 2.85 | 0.45 |
| 19:CS:18:LYS:HG2 | 19:CS:31:ILE:HD13 | 1.99 | 0.45 |
| 23:BA:327:G:O2' | 23:BA:328:U:H5' | 2.17 | 0.45 |
| 8:CH:36:LEU:C | 8:CH:38:ILE:N | 2.69 | 0.45 |
| 7:CG:95:ARG:CZ | 7:CG:99:LEU:HD11 | 2.47 | 0.45 |
| 23:BA:1930:G:O2' | 23:BA:1931:U:P | 2.75 | 0.45 |
| 23:BA:2347:C:H4' | 51:B3:39:TYR:CE1 | 2.52 | 0.45 |
| 23:DA:245:G:C4 | 23:DA:246:C:C6 | 3.04 | 0.45 |
| 1:CA:716:A:N3 | 11:CK:118:GLY:HA2 | 2.31 | 0.45 |
| 33:BK:26:LYS:HB3 | 33:BK:27:GLY:H | 1.68 | 0.45 |
| 11:AK:101:SER:OG | 11:AK:102:GLY:N | 2.48 | 0.45 |
| 1:AA:1038:C:H2' | 1:AA:1039:C:H6 | 1.81 | 0.45 |
| 23:BA:245:G:C4 | 23:BA:246:C:C5 | 3.04 | 0.45 |
| 48:BZ:3:ARG:NH1 | 48:BZ:59:VAL:CG1 | 2.79 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:DA:569:U:C4 | 23:DA:570:G:C6 | 3.03 | 0.45 |
| 48:BZ:8:LEU:HA | 48:BZ:8:LEU:HD23 | 1.74 | 0.45 |
| 23:BA:735:A:H3' | 23:BA:736:C:H6 | 1.81 | 0.45 |
| 20:CT:94:ALA:O | 20:CT:95:ALA:HB3 | 2.16 | 0.45 |
| 52:D4:35:ARG:HG3 | 52:D4:42:LEU:HD11 | 1.98 | 0.45 |
| 1:CA:1340:A:C5 | 1:CA:1341:U:C6 | 3.04 | 0.45 |
| 30:DH:26:ALA:HA | 30:DH:30:LEU:HB2 | 1.98 | 0.45 |
| 33:BK:7:TYR:HE1 | 33:BK:20:MET:HE3 | 1.81 | 0.45 |
| 10:AJ:26:ALA:HB1 | 10:AJ:84:GLN:HG2 | 1.99 | 0.45 |
| 51:D3:36:LEU:N | 51:D3:36:LEU:HD23 | 2.31 | 0.45 |
| 44:BV:140:ASP:N | 44:BV:140:ASP:OD2 | 2.50 | 0.45 |
| 1:AA:1407:C:H6 | 1:AA:1407:C:O5' | 1.99 | 0.45 |
| 2:AB:221:LEU:HA | 2:AB:221:LEU:HD22 | 1.86 | 0.45 |
| 6:AF:42:GLU:HG2 | 6:AF:42:GLU:O | 2.16 | 0.45 |
| 1:AA:1455:G:H2' | 1:AA:1459:C:C6 | 2.50 | 0.45 |
| 23:DA:627:A:H4' | 23:DA:628:G:OP1 | 2.17 | 0.45 |
| 26:DD:170:LEU:N | 26:DD:170:LEU:CD2 | 2.79 | 0.45 |
| 23:DA:1530:G:C6 | 23:DA:1531:C:C4 | 3.04 | 0.45 |
| 23:DA:99:U:C6 | 23:DA:102:G:N1 | 2.84 | 0.45 |
| 1:CA:1346:A:H5'' | 9:CI:120:ARG:HH12 | 1.81 | 0.45 |
| 14:AN:32:SER:HB3 | 14:AN:41:ARG:HG2 | 1.99 | 0.45 |
| 10:AJ:49:VAL:HG23 | 14:AN:34:TYR:OH | 2.16 | 0.45 |
| 1:CA:946:A:H61 | 1:CA:1235:U:H3 | 1.63 | 0.45 |
| 2:CB:68:ILE:CG2 | 2:CB:70:PHE:CE1 | 2.99 | 0.45 |
| 23:BA:1021:A:N6 | 23:BA:1141:U:N3 | 2.54 | 0.45 |
| 23:BA:1827:C:O2' | 23:BA:1828:G:H5' | 2.17 | 0.45 |
| 34:DL:52:GLU:CA | 34:DL:52:GLU:OE1 | 2.63 | 0.45 |
| 53:B5:11:LYS:HD2 | 53:B5:64:TYR:CE2 | 2.50 | 0.45 |
| 23:BA:243:U:H2' | 23:BA:244:A:H5' | 1.97 | 0.45 |
| 1:AA:376:G:O3' | 16:AP:5:ARG:HD2 | 2.16 | 0.45 |
| 1:AA:404:U:H2' | 1:AA:405:U:C6 | 2.48 | 0.45 |
| 4:AD:106:TYR:C | 4:AD:109:GLY:H | 2.20 | 0.45 |
| 1:AA:36:C:N4 | 1:AA:37:U:C4 | 2.85 | 0.45 |
| 1:AA:327:A:C6 | 1:AA:329:A:C5 | 3.04 | 0.45 |
| 1:AA:328:C:H4' | 1:AA:329:A:C5' | 2.46 | 0.45 |
| 28:DF:69:ALA:O | 28:DF:90:LEU:HD13 | 2.15 | 0.45 |
| 24:BB:46:A:C5 | 24:BB:47:C:C4 | 3.05 | 0.45 |
| 26:BD:59:VAL:O | 26:BD:61:ARG:N | 2.50 | 0.45 |
| 23:DA:2210:G:C3' | 23:DA:2210:G:N3 | 2.77 | 0.45 |
| 17:CQ:51:TYR:CD1 | 17:CQ:73:VAL:HG11 | 2.51 | 0.45 |
| 1:CA:1435:G:H2' | 1:CA:1436:U:H6 | 1.70 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:AE:65:ASN:O | 5:AE:66:MET:HG3 | 2.17 | 0.45 |
| 1:AA:191(G):G:C5 | 1:AA:192:U:C5 | 3.04 | 0.45 |
| 1:AA:15:G:N3 | 1:AA:16:A:C8 | 2.85 | 0.45 |
| 4:CD:119:GLN:O | 4:CD:123:HIS:HD2 | 1.99 | 0.45 |
| 1:CA:1330:U:O4 | 1:CA:1331:G:C2 | 2.69 | 0.45 |
| 9:AI:16:ARG:HB2 | 9:AI:64:THR:HB | 1.99 | 0.45 |
| 38:BP:24:PRO:O | 38:BP:94:ALA:HB2 | 2.16 | 0.45 |
| 41:DS:24:ILE:CG2 | 41:DS:36:LEU:HD21 | 2.46 | 0.45 |
| 29:DG:143:GLN:O | 29:DG:144:VAL:C | 2.54 | 0.45 |
| 1:CA:583:A:N6 | 1:CA:758:G:H1' | 2.32 | 0.45 |
| 8:CH:88:LYS:HB3 | 8:CH:89:PRO:HD2 | 1.97 | 0.45 |
| 23:DA:2311:A:O2' | 23:DA:2312:U:O4' | 2.34 | 0.45 |
| 46:BX:9:GLY:O | 46:BX:10:LYS:O | 2.35 | 0.45 |
| 1:AA:321:A:C2 | 1:AA:333:G:C2 | 3.05 | 0.45 |
| 8:AH:86:ILE:HG22 | 8:AH:93:VAL:HG21 | 1.98 | 0.45 |
| 1:AA:657:G:O2' | 1:AA:658:G:H5' | 2.16 | 0.45 |
| 37:BO:57:LYS:HB3 | 37:BO:58:LEU:HD12 | 1.98 | 0.45 |
| 25:DC:25:THR:CG2 | 25:DC:81:ALA:HB1 | 2.45 | 0.45 |
| 44:DV:150:LEU:HD23 | 44:DV:171:ILE:HB | 1.97 | 0.45 |
| 1:CA:711:G:N2 | 1:CA:712:A:N3 | 2.64 | 0.45 |
| 1:CA:1014:A:H5' | 19:CS:14:HIS:CG | 2.50 | 0.45 |
| 34:DL:10:PRO:CD | 34:DL:11:GLY:N | 2.80 | 0.45 |
| 10:CJ:27:ALA:HB1 | 10:CJ:34:VAL:HG21 | 1.98 | 0.45 |
| 25:DC:61:LEU:HB2 | 25:DC:63:ARG:HH12 | 1.82 | 0.45 |
| 32:BJ:66:THR:HB | 32:BJ:71:MET:HE3 | 1.98 | 0.45 |
| 23:BA:1871:A:O2' | 23:BA:1872:A:H5' | 2.16 | 0.45 |
| 1:CA:913:A:C2' | 1:CA:914:A:OP2 | 2.64 | 0.45 |
| 23:DA:2476:A:C2' | 23:DA:2476:A:N3 | 2.80 | 0.45 |
| 34:BL:55:ARG:HG3 | 34:BL:56:SER:N | 2.31 | 0.45 |
| 36:BN:94:TYR:C | 36:BN:117:VAL:HG12 | 2.37 | 0.45 |
| 23:DA:1717:G:C5 | 23:DA:1743:G:C2 | 3.04 | 0.45 |
| 23:DA:2850:A:H2' | 23:DA:2851:A:O4' | 2.16 | 0.45 |
| 1:AA:527:G:H2' | 1:AA:528:C:H5' | 1.99 | 0.45 |
| 8:AH:64:LYS:CG | 8:AH:79:VAL:HG21 | 2.45 | 0.45 |
| 35:DM:115:MET:HE2 | 35:DM:115:MET:HA | 1.98 | 0.45 |
| 35:DM:135:ASP:N | 35:DM:135:ASP:OD1 | 2.49 | 0.45 |
| 35:DM:43:THR:HG1 | 35:DM:46:GLN:HG3 | 1.82 | 0.45 |
| 1:AA:1413:A:C6 | 1:AA:1414:U:C4 | 3.04 | 0.45 |
| 1:CA:492:G:C4 | 1:CA:493:G:C8 | 3.05 | 0.45 |
| 7:AG:16:LEU:O | 7:AG:17:VAL:HG23 | 2.17 | 0.45 |
| 7:AG:54:THR:C | 7:AG:56:GLN:H | 2.20 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:639:G:O2' | 1:CA:640:A:H5' | 2.17 | 0.45 |
| 23:DA:1870:C:C2' | 23:DA:1870:C:O2 | 2.65 | 0.45 |
| 7:CG:103:TRP:O | 7:CG:104:LEU:C | 2.55 | 0.45 |
| 41:BS:36:LEU:HD11 | 41:BS:47:VAL:HB | 1.97 | 0.45 |
| 23:DA:205:G:O2' | 23:DA:206:U:P | 2.75 | 0.45 |
| 23:DA:2863:C:O2' | 23:DA:2864:G:H5' | 2.16 | 0.45 |
| 16:AP:13:HIS:C | 16:AP:15:PRO:HD3 | 2.37 | 0.45 |
| 26:DD:96:PHE:HA | 26:DD:100:GLU:OE1 | 2.16 | 0.45 |
| 46:BX:68:PRO:O | 46:BX:70:VAL:N | 2.50 | 0.45 |
| 23:DA:1204:A:C2 | 23:DA:1241:A:N1 | 2.85 | 0.45 |
| 44:BV:14:LYS:HB2 | 44:BV:17:ALA:HB3 | 1.98 | 0.45 |
| 23:DA:2037:G:C6 | 23:DA:2038:G:C6 | 3.05 | 0.45 |
| 1:CA:1088:G:C5 | 1:CA:1089:G:N7 | 2.85 | 0.45 |
| 23:BA:503:A:C4 | 23:BA:506:G:N7 | 2.85 | 0.45 |
| 7:AG:35:LYS:O | 7:AG:38:LEU:N | 2.49 | 0.45 |
| 7:AG:80:VAL:C | 7:AG:82:GLY:H | 2.19 | 0.45 |
| 23:DA:537:C:H2' | 23:DA:539:G:C8 | 2.51 | 0.45 |
| 49:B1:41:ILE:HD13 | 49:B1:47:VAL:HG13 | 1.97 | 0.45 |
| 23:BA:1345:C:C2' | 23:BA:1346:G:H5' | 2.46 | 0.45 |
| 36:DN:96:ARG:HD2 | 36:DN:115:GLU:OE1 | 2.17 | 0.45 |
| 23:BA:2410:G:C2 | 23:BA:2411:A:H1' | 2.52 | 0.45 |
| 4:CD:8:VAL:O | 4:CD:10:ARG:N | 2.49 | 0.45 |
| 32:BJ:151:HIS:NE2 | 32:BJ:153:HIS:HA | 2.32 | 0.45 |
| 28:DF:45:GLU:C | 28:DF:47:LYS:H | 2.19 | 0.45 |
| 30:DH:3:VAL:HG12 | 30:DH:37:VAL:O | 2.17 | 0.45 |
| 5:CE:80:ILE:HD12 | 5:CE:138:ALA:HB1 | 1.98 | 0.45 |
| 6:CF:82:ARG:HB2 | 6:CF:85:VAL:CG2 | 2.46 | 0.45 |
| 13:AM:81:LEU:HD22 | 13:AM:86:CYS:SG | 2.56 | 0.45 |
| 23:DA:1484:G:H2' | 23:DA:1485:G:H8 | 1.81 | 0.45 |
| 4:AD:201:GLN:O | 4:AD:205:GLU:HG3 | 2.16 | 0.45 |
| 34:DL:126:VAL:HG23 | 34:DL:145:PRO:HG2 | 1.99 | 0.45 |
| 34:BL:57:THR:HG21 | 34:BL:59:LEU:HD22 | 1.89 | 0.45 |
| 1:AA:946:A:OP2 | 13:AM:114:ARG:NH2 | 2.49 | 0.45 |
| 1:AA:978:A:H5'' | 1:AA:979:C:OP2 | 2.17 | 0.45 |
| 13:AM:105:THR:O | 13:AM:106:ASN:O | 2.35 | 0.45 |
| 13:AM:91:ARG:NH1 | 19:AS:81:ARG:HH22 | 2.06 | 0.45 |
| 23:DA:1971:A:H5'' | 23:DA:1971:A:H8 | 1.82 | 0.45 |
| 32:DJ:157:ARG:O | 32:DJ:159:GLU:N | 2.50 | 0.45 |
| 41:BS:14:PRO:O | 41:BS:15:ARG:C | 2.54 | 0.45 |
| 39:DQ:107:ALA:O | 39:DQ:110:VAL:HB | 2.17 | 0.45 |
| 35:DM:74:TYR:O | 35:DM:89:ASN:N | 2.44 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:BC:127:VAL:HA | 25:BC:193:VAL:HG12 | 1.96 | 0.45 |
| 16:CP:18:ARG:O | 16:CP:19:ILE:O | 2.34 | 0.45 |
| 30:BH:107:ILE:HD12 | 30:BH:108:THR:H | 1.82 | 0.45 |
| 42:BT:12:VAL:HG22 | 42:BT:17:ALA:HB2 | 1.99 | 0.45 |
| 23:BA:1614:A:C6 | 41:BS:87:PRO:HA | 2.50 | 0.45 |
| 23:DA:2338:G:C2 | 23:DA:2339:G:C8 | 3.04 | 0.45 |
| 1:AA:373:A:C2 | 1:AA:374:A:C8 | 3.04 | 0.45 |
| 1:AA:687:A:H1' | 1:AA:688:G:OP2 | 2.15 | 0.45 |
| 30:DH:126:TYR:HB2 | 30:DH:142:VAL:HG21 | 1.98 | 0.45 |
| 30:DH:143:SER:O | 30:DH:145:VAL:N | 2.47 | 0.45 |
| 23:BA:1404:C:C2' | 23:BA:1405:U:H5' | 2.46 | 0.45 |
| 49:D1:40:ILE:N | 49:D1:40:ILE:HD12 | 2.31 | 0.45 |
| 24:DB:16:G:O6 | 24:DB:69:G:C2 | 2.69 | 0.45 |
| 3:CC:35:GLU:O | 3:CC:39:ILE:HG13 | 2.17 | 0.45 |
| 27:BE:155:LEU:HD12 | 27:BE:174:VAL:O | 2.17 | 0.45 |
| 23:BA:2712:U:O2 | 23:BA:2712:U:H5'' | 2.15 | 0.45 |
| 26:DD:84:PHE:CE2 | 26:DD:86:PRO:HG3 | 2.52 | 0.45 |
| 24:BB:12:C:O2' | 45:BW:74:ARG:HG2 | 2.16 | 0.45 |
| 5:AE:78:HIS:HE1 | 5:AE:142:LEU:HA | 1.80 | 0.45 |
| 1:AA:1074:G:N3 | 1:AA:1102:A:C2 | 2.84 | 0.45 |
| 26:DD:119:ARG:HD3 | 26:DD:120:TRP:NE1 | 2.31 | 0.45 |
| 24:DB:106:G:C6 | 24:DB:107:U:C4 | 3.04 | 0.45 |
| 46:BX:11:ARG:NH1 | 46:BX:11:ARG:CG | 2.79 | 0.45 |
| 46:BX:13:ILE:HG23 | 46:BX:14:VAL:N | 2.29 | 0.45 |
| 23:BA:2630:G:H1' | 23:BA:2894:G:H1' | 1.99 | 0.45 |
| 23:DA:96:G:O5' | 47:DY:48:HIS:HE1 | 1.99 | 0.45 |
| 23:DA:2807:G:N1 | 23:DA:2893:G:O6 | 2.49 | 0.45 |
| 4:CD:135:LEU:HD13 | 4:CD:135:LEU:N | 2.32 | 0.45 |
| 16:AP:72:ARG:HD3 | 16:AP:73:LEU:HD21 | 1.99 | 0.45 |
| 1:CA:1237:C:C5 | 1:CA:1336:C:N3 | 2.85 | 0.45 |
| 3:CC:70:VAL:CG1 | 3:CC:71:ALA:N | 2.80 | 0.45 |
| 24:BB:48:A:H2' | 24:BB:49:C:C6 | 2.51 | 0.45 |
| 29:DG:73:ALA:O | 29:DG:76:VAL:HB | 2.17 | 0.45 |
| 1:CA:1064:G:O4' | 1:CA:1066:C:C6 | 2.70 | 0.45 |
| 23:DA:1478:G:C2 | 23:DA:1479:G:C5 | 3.05 | 0.45 |
| 8:CH:51:VAL:CG1 | 8:CH:52:ASP:N | 2.79 | 0.45 |
| 32:BJ:70:ALA:HB2 | 32:BJ:135:LEU:HD11 | 1.99 | 0.45 |
| 8:CH:86:ILE:HG22 | 8:CH:87:SER:N | 2.31 | 0.45 |
| 27:BE:46:ARG:NH1 | 27:BE:46:ARG:CG | 2.79 | 0.45 |
| 28:DF:178:PHE:HA | 28:DF:179:PRO:HD3 | 1.69 | 0.45 |
| 23:BA:1010:A:H5' | 39:BQ:62:ILE:HG21 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:AD:72:GLU:O | 4:AD:72:GLU:OE1 | 2.34 | 0.45 |
| 1:AA:719:C:O2' | 18:AR:49:LYS:HB3 | 2.17 | 0.45 |
| 32:DJ:80:ALA:C | 32:DJ:82:LYS:N | 2.70 | 0.45 |
| 7:AG:27:ILE:HD12 | 7:AG:40:ALA:HA | 1.99 | 0.45 |
| 1:AA:1379:G:C6 | 1:AA:1380:U:O4 | 2.69 | 0.45 |
| 2:AB:47:THR:HA | 2:AB:202:PRO:HG2 | 1.99 | 0.45 |
| 1:AA:505:G:O2' | 1:AA:506:G:H5' | 2.17 | 0.45 |
| 23:BA:1230:C:O2' | 23:BA:1231:G:H5' | 2.17 | 0.45 |
| 23:DA:2862:G:H2' | 23:DA:2863:C:H6 | 1.82 | 0.45 |
| 27:BE:179:GLU:CD | 27:BE:179:GLU:N | 2.69 | 0.45 |
| 26:BD:67:PHE:CD1 | 26:BD:74:PRO:HB3 | 2.50 | 0.45 |
| 23:DA:2572:A:OP2 | 26:DD:144:ARG:HB2 | 2.17 | 0.45 |
| 33:DK:86:ILE:N | 33:DK:86:ILE:HD12 | 2.30 | 0.45 |
| 1:CA:883:C:C2' | 1:CA:884:U:H5' | 2.47 | 0.45 |
| 1:CA:744:C:O5' | 1:CA:744:C:H6 | 2.00 | 0.45 |
| 23:DA:1465:G:C2 | 23:DA:1466:G:C4 | 3.05 | 0.45 |
| 1:CA:425:G:C6 | 1:CA:426:G:C5 | 3.05 | 0.45 |
| 23:BA:511:U:C5 | 23:BA:512:G:C5 | 3.05 | 0.45 |
| 23:BA:2744:G:N3 | 23:BA:2761:G:C2 | 2.85 | 0.45 |
| 28:DF:16:ARG:O | 28:DF:20:ILE:HG12 | 2.16 | 0.45 |
| 23:BA:1685:C:O2' | 23:BA:1686:C:H5' | 2.16 | 0.45 |
| 34:BL:21:ARG:H | 34:BL:21:ARG:HG2 | 1.57 | 0.45 |
| 23:DA:270(F):G:H2' | 23:DA:270(G):U:O4' | 2.16 | 0.45 |
| 23:BA:586:A:N1 | 23:BA:809:G:O2' | 2.37 | 0.45 |
| 11:AK:81:ASP:OD1 | 11:AK:106:LYS:HB3 | 2.16 | 0.45 |
| 23:BA:2380:C:H6 | 23:BA:2380:C:O5' | 1.99 | 0.45 |
| 1:CA:891:U:O2 | 1:CA:891:U:H2' | 2.17 | 0.45 |
| 2:AB:9:GLU:CD | 2:AB:9:GLU:C | 2.75 | 0.45 |
| 39:BQ:84:LYS:HA | 39:BQ:84:LYS:HD3 | 1.89 | 0.45 |
| 34:DL:114:ILE:H | 34:DL:114:ILE:CD1 | 1.98 | 0.45 |
| 23:BA:2415:G:O2' | 23:BA:2416:C:H5' | 2.16 | 0.45 |
| 23:BA:1309:G:H3' | 52:B4:9:ARG:HH11 | 1.80 | 0.45 |
| 23:BA:1180:C:O2' | 23:BA:1181:C:H5' | 2.17 | 0.45 |
| 1:CA:1350:A:C6 | 1:CA:1351:U:N3 | 2.85 | 0.45 |
| 1:AA:946:A:C6 | 1:AA:1236:A:C2 | 3.04 | 0.45 |
| 10:AJ:49:VAL:CG2 | 14:AN:41:ARG:HB3 | 2.46 | 0.45 |
| 25:BC:17:THR:H | 25:BC:205:VAL:HG12 | 1.80 | 0.45 |
| 2:CB:154:LEU:C | 2:CB:154:LEU:HD22 | 2.37 | 0.45 |
| 23:DA:1900:A:N1 | 23:DA:1970:A:C5 | 2.85 | 0.45 |
| 25:DC:35:LYS:HA | 25:DC:35:LYS:HD3 | 1.70 | 0.45 |
| 23:DA:1022:G:N2 | 23:DA:114(B):A:H2 | 2.13 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DA:1021:A:N6 | 23:DA:1141:U:N3 | 2.53 | 0.45 |
| 34:BL:40:SER:O | 34:BL:41:ARG:CD | 2.52 | 0.45 |
| 1:AA:375:U:C2' | 1:AA:376:G:H5' | 2.47 | 0.45 |
| 12:AL:100:VAL:CG1 | 12:AL:103:VAL:HG23 | 2.46 | 0.45 |
| 1:AA:37:U:P | 12:AL:122:LYS:HG3 | 2.57 | 0.45 |
| 28:BF:70:VAL:HG12 | 28:BF:90:LEU:CD2 | 2.44 | 0.45 |
| 35:DM:140:ALA:HB3 | 44:DV:53:ILE:CG1 | 2.47 | 0.45 |
| 41:BS:75:TYR:C | 41:BS:75:TYR:CD2 | 2.89 | 0.45 |
| 1:CA:36:C:N4 | 1:CA:37:U:C4 | 2.85 | 0.45 |
| 1:AA:393:A:N3 | 1:AA:394:G:C8 | 2.85 | 0.45 |
| 41:BS:4:LYS:CD | 41:BS:6:ILE:HD11 | 2.47 | 0.45 |
| 36:DN:2:ARG:O | 36:DN:3:HIS:CD2 | 2.69 | 0.45 |
| 24:BB:10:C:C2 | 24:BB:11:C:C5 | 3.05 | 0.45 |
| 26:DD:55:ASN:O | 26:DD:59:VAL:HG23 | 2.17 | 0.45 |
| 25:DC:86:PRO:HD2 | 25:DC:87:ASN:HD21 | 1.81 | 0.45 |
| 1:AA:586:C:O2' | 1:AA:878:G:H4' | 2.17 | 0.45 |
| 19:CS:66:MET:HB3 | 19:CS:74:PHE:CZ | 2.52 | 0.45 |
| 3:AC:205:GLY:O | 3:AC:206:GLU:HB2 | 2.17 | 0.45 |
| 37:BO:84:GLN:C | 37:BO:86:ALA:H | 2.20 | 0.45 |
| 1:AA:1148:U:H2' | 1:AA:1149:C:O4' | 2.17 | 0.45 |
| 9:AI:118:LYS:C | 9:AI:120:ARG:H | 2.20 | 0.45 |
| 36:DN:50:HIS:CD2 | 36:DN:50:HIS:C | 2.89 | 0.45 |
| 23:DA:2744:G:N2 | 23:DA:2761:G:C4 | 2.85 | 0.45 |
| 1:CA:644:G:H5' | 8:CH:92:ARG:HH21 | 1.81 | 0.45 |
| 23:BA:2311:A:O2' | 23:BA:2312:U:O4' | 2.34 | 0.45 |
| 1:CA:986:A:C6 | 1:CA:1220:G:N1 | 2.84 | 0.45 |
| 1:AA:737:A:C4 | 1:AA:738:C:C5 | 3.05 | 0.45 |
| 23:BA:2747:G:C6 | 23:BA:2754:U:C6 | 3.05 | 0.45 |
| 29:BG:74:ASN:ND2 | 29:BG:138:LYS:HD2 | 2.31 | 0.45 |
| 11:CK:34:ASP:CB | 11:CK:35:PRO:CD | 2.94 | 0.45 |
| 1:AA:631:G:N2 | 1:AA:632:A:C2 | 2.84 | 0.45 |
| 45:DW:73:GLY:O | 45:DW:75:LEU:N | 2.50 | 0.45 |
| 23:DA:379:G:N2 | 46:DX:20:ARG:NH2 | 2.64 | 0.45 |
| 30:BH:4:ILE:HA | 30:BH:17:GLN:O | 2.16 | 0.45 |
| 23:BA:1478:G:C2 | 23:BA:1479:G:C5 | 3.05 | 0.45 |
| 4:AD:52:SER:C | 4:AD:54:TYR:N | 2.70 | 0.45 |
| 43:BU:44:ILE:HG22 | 43:BU:45:VAL:N | 2.25 | 0.45 |
| 4:CD:102:ASP:OD2 | 4:CD:136:PRO:HB3 | 2.17 | 0.45 |
| 1:CA:277:C:OP1 | 17:CQ:41:LYS:HE3 | 2.16 | 0.45 |
| 23:DA:483:A:H1' | 43:DU:47:LYS:O | 2.17 | 0.45 |
| 23:BA:2468:G:C2 | 23:BA:2481:G:N3 | 2.85 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:DG:92:ILE:O | 29:DG:93:GLY:C | 2.55 | 0.45 |
| 8:AH:51:VAL:CG1 | 8:AH:52:ASP:N | 2.79 | 0.45 |
| 1:AA:706:A:H2' | 1:AA:707:C:H5' | 1.99 | 0.45 |
| 2:CB:72:GLY:HA2 | 2:CB:165:VAL:HG22 | 1.98 | 0.45 |
| 25:DC:97:TYR:HB2 | 25:DC:101:GLU:O | 2.16 | 0.45 |
| 17:CQ:32:TYR:O | 17:CQ:34:LYS:N | 2.49 | 0.45 |
| 23:DA:1411:C:O2' | 23:DA:1412:A:H5' | 2.17 | 0.45 |
| 38:BP:3:ARG:HD2 | 38:BP:6:LEU:HD23 | 1.97 | 0.45 |
| 39:BQ:61:TRP:O | 39:BQ:62:ILE:C | 2.55 | 0.45 |
| 18:AR:43:PHE:C | 18:AR:44:LEU:HD12 | 2.37 | 0.45 |
| 2:CB:122:PHE:HD1 | 2:CB:139:LYS:HZ2 | 1.65 | 0.45 |
| 23:BA:2869:G:C6 | 23:BA:2870:C:C4 | 3.04 | 0.45 |
| 15:AO:27:VAL:O | 15:AO:28:GLN:C | 2.53 | 0.45 |
| 7:CG:54:THR:C | 7:CG:56:GLN:H | 2.20 | 0.45 |
| 23:DA:651:G:OP1 | 53:D5:19:SER:CB | 2.63 | 0.45 |
| 23:BA:738:G:H2' | 23:BA:739:G:C8 | 2.52 | 0.45 |
| 25:BC:244:ARG:HB2 | 25:BC:245:PRO:HD3 | 1.99 | 0.45 |
| 1:CA:381:C:C2 | 1:CA:382:A:C8 | 3.05 | 0.45 |
| 41:DS:57:ASN:O | 41:DS:58:ALA:C | 2.54 | 0.45 |
| 27:DE:53:THR:C | 27:DE:55:GLY:N | 2.69 | 0.45 |
| 7:CG:68:ASN:O | 7:CG:135:VAL:HG13 | 2.17 | 0.45 |
| 15:AO:5:LYS:N | 15:AO:5:LYS:HD3 | 2.30 | 0.45 |
| 51:B3:18:ARG:HB3 | 51:B3:19:ARG:H | 1.52 | 0.45 |
| 1:AA:927:G:N1 | 1:AA:1391:U:C2 | 2.85 | 0.45 |
| 39:BQ:17:ILE:HA | 39:BQ:20:LEU:HD23 | 1.98 | 0.45 |
| 7:AG:68:ASN:O | 7:AG:135:VAL:HG13 | 2.17 | 0.45 |
| 1:AA:639:G:O2' | 1:AA:640:A:H5' | 2.16 | 0.45 |
| 36:BN:31:HIS:C | 36:BN:33:ARG:H | 2.19 | 0.45 |
| 23:BA:136:G:C4 | 23:BA:137(A):C:C5 | 3.05 | 0.45 |
| 1:AA:1161:C:H2' | 1:AA:1162:C:C6 | 2.52 | 0.45 |
| 1:CA:525:C:OP1 | 12:CL:90:LYS:HE2 | 2.16 | 0.45 |
| 46:DX:51:VAL:HG12 | 46:DX:58:ILE:HG12 | 1.99 | 0.45 |
| 46:DX:68:PRO:O | 46:DX:70:VAL:N | 2.49 | 0.45 |
| 9:CI:45:ALA:O | 9:CI:48:GLU:HB2 | 2.17 | 0.45 |
| 23:BA:1612:C:H4' | 52:B4:5:TRP:O | 2.17 | 0.45 |
| 23:BA:234:C:H2' | 23:BA:235:U:C6 | 2.52 | 0.45 |
| 23:DA:2511:U:O4 | 23:DA:2575:C:N3 | 2.49 | 0.45 |
| 39:DQ:24:TYR:HE1 | 39:DQ:39:LEU:HD23 | 1.81 | 0.45 |
| 1:CA:897:C:N4 | 1:CA:902:G:H1 | 2.15 | 0.45 |
| 23:BA:644:A:C2 | 23:BA:646:A:C4 | 3.04 | 0.45 |
| 33:BK:3:GLN:CB | 33:BK:4:PRO:HD2 | 2.47 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:BA:260:G:N2 | 23:BA:261:G:H1' | 2.32 | 0.45 |
| 1:AA:857:C:H2' | 1:AA:858:G:O4' | 2.17 | 0.45 |
| 8:AH:29:SER:OG | 8:AH:32:LYS:HG3 | 2.17 | 0.45 |
| 10:AJ:22:LYS:NZ | 10:AJ:88:LEU:HG | 2.32 | 0.45 |
| 1:AA:1452:C:H1' | 1:AA:1453:G:N2 | 2.31 | 0.45 |
| 23:DA:629:G:H2' | 23:DA:630:G:H8 | 1.81 | 0.45 |
| 34:DL:85:LEU:HD23 | 34:DL:117:GLU:O | 2.16 | 0.45 |
| 34:DL:62:LEU:CD2 | 34:DL:62:LEU:O | 2.62 | 0.45 |
| 26:DD:11:MET:CE | 26:DD:186:GLY:CA | 2.94 | 0.45 |
| 23:DA:83:G:N2 | 23:DA:84:A:N6 | 2.65 | 0.45 |
| 43:DU:15:VAL:O | 43:DU:15:VAL:HG12 | 2.17 | 0.45 |
| 43:DU:8:LYS:HB2 | 43:DU:8:LYS:HE2 | 1.51 | 0.45 |
| 32:DJ:123:GLU:C | 32:DJ:125:ALA:H | 2.19 | 0.45 |
| 1:AA:948:C:OP1 | 13:AM:107:ALA:HA | 2.17 | 0.45 |
| 22:CV:6195:G:N2 | 22:CV:6196:A:N3 | 2.65 | 0.45 |
| 23:DA:2388:A:C8 | 23:DA:2389:G:C5 | 3.05 | 0.45 |
| 5:AE:81:GLU:HG2 | 5:AE:90:VAL:HG22 | 1.98 | 0.45 |
| 27:DE:67:GLN:O | 27:DE:68:LYS:HB3 | 2.17 | 0.45 |
| 23:DA:587:C:C4 | 34:DL:33:ARG:HB2 | 2.52 | 0.45 |
| 32:BJ:36:TRP:CZ2 | 32:BJ:74:PHE:CD2 | 3.05 | 0.45 |
| 23:BA:819:A:OP2 | 23:BA:1187:G:N2 | 2.30 | 0.45 |
| 23:BA:2579:C:O2' | 26:BD:131:ALA:CB | 2.64 | 0.45 |
| 23:DA:993:G:C6 | 23:DA:994:C:C5 | 3.05 | 0.45 |
| 25:DC:36:PRO:HA | 25:DC:62:TYR:O | 2.17 | 0.45 |
| 23:BA:1826:G:H2' | 23:BA:1827:C:H6 | 1.82 | 0.45 |
| 28:DF:128:ARG:HH21 | 28:DF:129:GLY:C | 2.20 | 0.45 |
| 4:AD:119:GLN:O | 4:AD:123:HIS:HD2 | 2.00 | 0.45 |
| 4:AD:29:PRO:O | 4:AD:30:LYS:CB | 2.64 | 0.45 |
| 3:CC:182:ILE:HD11 | 3:CC:203:PHE:HD1 | 1.81 | 0.45 |
| 25:DC:50:THR:HG23 | 25:DC:51:VAL:N | 2.32 | 0.45 |
| 1:CA:186(G):C:H2' | 1:CA:187:C:O4' | 2.17 | 0.45 |
| 14:CN:24:CYS:SG | 14:CN:27:CYS:SG | 3.08 | 0.45 |
| 23:DA:1786:A:C2 | 23:DA:2606:C:H1' | 2.52 | 0.45 |
| 47:DY:60:LEU:HD23 | 47:DY:60:LEU:HA | 1.38 | 0.45 |
| 49:B1:40:ILE:HD12 | 49:B1:40:ILE:N | 2.32 | 0.45 |
| 1:CA:1072:G:C5 | 1:CA:1073:U:C4 | 3.04 | 0.45 |
| 41:BS:23:LEU:HD22 | 50:B2:25:LEU:HD13 | 1.99 | 0.45 |
| 23:BA:1439:A:C2' | 23:BA:1440:G:H5' | 2.47 | 0.45 |
| 1:CA:687:A:N3 | 1:CA:688:G:H1' | 2.32 | 0.45 |
| 1:CA:688:G:C4 | 1:CA:689:C:C5 | 3.04 | 0.45 |
| 1:AA:1149:C:H2' | 1:AA:1150:U:C6 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:AI:9:ARG:O | 9:AI:10:ARG:HB2 | 2.17 | 0.45 |
| 35:DM:55:VAL:O | 35:DM:56:ARG:C | 2.54 | 0.45 |
| 1:AA:9:G:OP2 | 5:AE:121:LYS:HG3 | 2.17 | 0.45 |
| 41:DS:32:ALA:O | 41:DS:33:ARG:C | 2.55 | 0.45 |
| 32:DJ:142:ARG:CG | 32:DJ:142:ARG:HH11 | 2.20 | 0.45 |
| 46:DX:86:SER:HB3 | 46:DX:89:GLU:HB2 | 1.99 | 0.45 |
| 33:BK:35:VAL:HG11 | 33:BK:103:ALA:CB | 2.46 | 0.45 |
| 41:DS:8:ARG:HA | 41:DS:102:HIS:HA | 1.98 | 0.45 |
| 1:AA:750:G:O2' | 15:AO:21:ASP:HA | 2.16 | 0.45 |
| 23:BA:1104:C:C2' | 23:BA:1105:U:H5' | 2.47 | 0.45 |
| 23:BA:1314:C:C2' | 23:BA:1315:C:H5' | 2.47 | 0.45 |
| 25:DC:25:THR:O | 25:DC:27:THR:CB | 2.64 | 0.45 |
| 23:BA:733:G:C5 | 23:BA:761:A:C6 | 3.05 | 0.45 |
| 27:DE:203:GLN:OE1 | 27:DE:207:GLY:CA | 2.64 | 0.45 |
| 43:BU:19:LYS:HB3 | 43:BU:20:TYR:CE1 | 2.52 | 0.45 |
| 23:BA:295:G:H4' | 43:BU:2:ARG:NH1 | 2.32 | 0.45 |
| 1:CA:236:G:H2' | 1:CA:237:C:O4' | 2.17 | 0.45 |
| 44:DV:60:GLU:OE1 | 44:DV:66:SER:HB3 | 2.17 | 0.45 |
| 23:DA:2470:G:C6 | 23:DA:2471:C:C5 | 3.05 | 0.45 |
| 1:AA:1135:U:H4' | 1:AA:1136:U:C5 | 2.52 | 0.45 |
| 33:BK:104:ARG:HG2 | 33:BK:121:VAL:HG12 | 1.99 | 0.45 |
| 1:AA:236:G:C5 | 1:AA:237:C:C5 | 3.04 | 0.45 |
| 23:BA:318:C:O2' | 23:BA:319:C:H5' | 2.16 | 0.45 |
| 23:DA:988:A:C8 | 48:DZ:13:ILE:HD12 | 2.52 | 0.45 |
| 1:CA:1076:C:C2' | 1:CA:1077:G:H5' | 2.47 | 0.45 |
| 1:CA:1327:C:H2' | 1:CA:1328:C:C6 | 2.52 | 0.45 |
| 38:BP:84:GLN:HG3 | 38:BP:85:LYS:CG | 2.47 | 0.45 |
| 23:DA:1051:G:C5 | 23:DA:1052:C:N3 | 2.84 | 0.45 |
| 23:DA:2852:G:H2' | 23:DA:2853:C:C6 | 2.51 | 0.45 |
| 23:BA:887:A:N3 | 23:BA:889:C:C5 | 2.84 | 0.45 |
| 12:CL:88:ARG:NH1 | 12:CL:90:LYS:HD3 | 2.32 | 0.45 |
| 48:BZ:23:LEU:HD12 | 48:BZ:50:VAL:HG11 | 1.99 | 0.45 |
| 1:AA:1316:G:H2' | 1:AA:1317:C:H5" | 1.99 | 0.45 |
| 23:BA:165:U:H2' | 23:BA:171:G:O4' | 2.16 | 0.45 |
| 38:BP:41:ARG:NH1 | 38:BP:41:ARG:CB | 2.80 | 0.45 |
| 23:DA:231:C:C5 | 23:DA:232:G:C6 | 3.05 | 0.45 |
| 4:AD:23:GLY:HA3 | 4:AD:112:VAL:HG22 | 1.98 | 0.45 |
| 1:AA:932:C:H2' | 1:AA:933:G:C8 | 2.52 | 0.45 |
| 24:DB:87:G:N2 | 24:DB:89(A):G:C8 | 2.85 | 0.45 |
| 23:DA:1759:A:C8 | 23:DA:2696:U:H1' | 2.52 | 0.45 |
| 23:BA:1751:C:H2' | 23:BA:1752:C:H6 | 1.82 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DA:2410:G:C2 | 23:DA:2411:A:H1' | 2.52 | 0.45 |
| 27:DE:144:LYS:C | 27:DE:146:ALA:H | 2.19 | 0.45 |
| 23:DA:270(G):U:H3 | 23:DA:270(U):G:H1 | 1.64 | 0.45 |
| 18:CR:23:LYS:C | 18:CR:25:THR:H | 2.19 | 0.45 |
| 23:BA:2679:A:H4' | 26:BD:165:VAL:HG11 | 1.99 | 0.45 |
| 1:AA:1186:G:H4' | 9:AI:110:GLU:OE2 | 2.16 | 0.45 |
| 1:CA:474:G:H5' | 16:CP:81:ARG:HG3 | 1.98 | 0.45 |
| 23:DA:735:A:H3' | 23:DA:736:C:H6 | 1.81 | 0.45 |
| 15:AO:32:LEU:O | 15:AO:35:ARG:N | 2.50 | 0.45 |
| 39:BQ:59:ARG:HE | 39:BQ:59:ARG:HB2 | 1.53 | 0.45 |
| 48:DZ:49:LYS:HD3 | 48:DZ:49:LYS:HA | 1.44 | 0.45 |
| 26:BD:125:GLY:HA2 | 26:BD:126:PRO:HD3 | 1.74 | 0.45 |
| 26:DD:12:THR:O | 26:DD:23:VAL:O | 2.35 | 0.45 |
| 36:DN:12:ARG:CG | 36:DN:16:HIS:CD2 | 2.78 | 0.45 |
| 22:AV:6214:C:H2' | 22:AV:6215:C:C6 | 2.52 | 0.45 |
| 28:BF:60:LEU:HA | 28:BF:63:ILE:HG12 | 1.99 | 0.45 |
| 23:BA:1275:A:C5 | 36:BN:16:HIS:ND1 | 2.85 | 0.45 |
| 1:AA:8:A:H5' | 5:AE:120:THR:O | 2.17 | 0.45 |
| 25:BC:142:VAL:CG2 | 25:BC:192:THR:O | 2.65 | 0.45 |
| 30:BH:143:SER:O | 30:BH:145:VAL:HG23 | 2.17 | 0.45 |
| 1:AA:436:C:H2' | 1:AA:437:U:H6 | 1.81 | 0.45 |
| 1:AA:413:G:H4' | 1:AA:414:A:H5'' | 1.98 | 0.45 |
| 25:DC:158:ALA:HB3 | 25:DC:161:THR:CG2 | 2.33 | 0.45 |
| 4:AD:75:PHE:CZ | 4:AD:93:PHE:CZ | 3.05 | 0.45 |
| 49:D1:60:GLU:N | 49:D1:60:GLU:CD | 2.70 | 0.45 |
| 1:CA:36:C:O3' | 12:CL:122:LYS:HA | 2.17 | 0.45 |
| 1:AA:391:G:C5 | 1:AA:392:G:C8 | 3.05 | 0.45 |
| 47:DY:28:LYS:HG3 | 47:DY:60:LEU:HD12 | 1.99 | 0.45 |
| 36:DN:2:ARG:HA | 36:DN:2:ARG:HD2 | 1.42 | 0.45 |
| 44:BV:125:LEU:HD23 | 44:BV:126:VAL:N | 2.32 | 0.45 |
| 1:CA:1252:A:H61 | 1:CA:1285:A:N6 | 2.12 | 0.45 |
| 44:BV:101:PRO:O | 44:BV:102:LEU:HD23 | 2.16 | 0.45 |
| 44:BV:137:ILE:HG22 | 44:BV:138:GLU:N | 2.31 | 0.45 |
| 42:BT:51:VAL:HG11 | 42:BT:81:VAL:CG1 | 2.45 | 0.45 |
| 29:DG:35:VAL:HG21 | 29:DG:75:ALA:HB2 | 1.98 | 0.45 |
| 1:AA:1074:G:H1' | 2:AB:104:ASN:HD22 | 1.82 | 0.45 |
| 1:CA:401:C:C3' | 1:CA:401:C:C6 | 3.00 | 0.45 |
| 43:DU:81:LYS:HD3 | 43:DU:97:ARG:CB | 2.43 | 0.45 |
| 9:AI:28:VAL:HG22 | 9:AI:63:ILE:H | 1.82 | 0.45 |
| 4:AD:126:ILE:CG2 | 4:AD:127:THR:H | 2.22 | 0.45 |
| 23:DA:1586:A:C2' | 23:DA:1587:A:H5' | 2.46 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:AE:126:ARG:NH1 | 5:AE:126:ARG:HG2 | 2.24 | 0.45 |
| 6:AF:63:TYR:H | 6:AF:63:TYR:HD2 | 1.59 | 0.45 |
| 36:BN:2:ARG:HA | 36:BN:2:ARG:HD2 | 1.44 | 0.45 |
| 1:CA:724:G:N3 | 1:CA:725:G:C8 | 2.85 | 0.45 |
| 40:BR:30:GLY:HA2 | 40:BR:61:VAL:O | 2.16 | 0.45 |
| 23:DA:528:A:O2' | 23:DA:529:A:H5' | 2.17 | 0.45 |
| 23:BA:1502:C:C6 | 23:BA:1502:C:H3' | 2.52 | 0.45 |
| 1:CA:601:C:H2' | 1:CA:602:A:H8 | 1.73 | 0.45 |
| 30:DH:133:HIS:NE2 | 30:DH:135:GLU:HG2 | 2.32 | 0.45 |
| 1:AA:625:G:O2' | 1:AA:626:U:H5' | 2.17 | 0.45 |
| 3:AC:59:ARG:HG2 | 3:AC:63:ASN:O | 2.17 | 0.45 |
| 1:CA:236:G:H1' | 17:CQ:4:LYS:NZ | 2.32 | 0.45 |
| 24:BB:61:G:C6 | 24:BB:62:C:C4 | 3.05 | 0.45 |
| 10:CJ:58:ASP:O | 10:CJ:60:ARG:N | 2.50 | 0.45 |
| 1:AA:976:G:H8 | 1:AA:1358:U:C2' | 2.30 | 0.45 |
| 23:DA:2468:G:C2 | 23:DA:2481:G:N3 | 2.84 | 0.45 |
| 2:CB:63:MET:C | 2:CB:65:GLY:H | 2.19 | 0.45 |
| 44:BV:18:LEU:O | 44:BV:21:ALA:HB3 | 2.17 | 0.45 |
| 38:BP:34:VAL:O | 38:BP:40:THR:HA | 2.17 | 0.45 |
| 41:BS:60:ASN:N | 41:BS:60:ASN:OD1 | 2.50 | 0.45 |
| 1:CA:1080:A:C5' | 1:CA:1081:G:OP2 | 2.65 | 0.45 |
| 1:CA:1418:A:N3 | 23:DA:1959:G:H1' | 2.32 | 0.45 |
| 10:CJ:45:ARG:HB3 | 10:CJ:47:PHE:CE1 | 2.52 | 0.45 |
| 40:BR:7:THR:CG2 | 40:BR:22:VAL:HG11 | 2.44 | 0.45 |
| 8:AH:114:THR:OG1 | 8:AH:119:LEU:HG | 2.17 | 0.45 |
| 40:DR:7:THR:CG2 | 40:DR:22:VAL:HG11 | 2.47 | 0.45 |
| 1:AA:806:C:O2 | 1:AA:807:A:C8 | 2.69 | 0.45 |
| 1:AA:1327:C:H2' | 1:AA:1328:C:C6 | 2.51 | 0.45 |
| 46:BX:70:VAL:O | 46:BX:74:VAL:HG23 | 2.17 | 0.45 |
| 1:AA:356:A:H1' | 1:AA:368:U:O2' | 2.17 | 0.45 |
| 23:BA:2300:G:C6 | 23:BA:2301:C:C4 | 3.05 | 0.45 |
| 1:CA:191(G):G:C5 | 1:CA:192:U:C5 | 3.05 | 0.45 |
| 1:AA:166:G:O2' | 1:AA:167:G:H5' | 2.17 | 0.45 |
| 23:DA:30:G:C6 | 23:DA:31:C:C4 | 3.05 | 0.45 |
| 41:BS:42:ARG:HG2 | 41:BS:42:ARG:NH1 | 2.32 | 0.45 |
| 25:DC:52:ARG:CZ | 25:DC:53:PHE:CE2 | 3.00 | 0.45 |
| 25:DC:52:ARG:NH1 | 25:DC:53:PHE:HE2 | 2.15 | 0.45 |
| 19:AS:33:THR:CG2 | 19:AS:51:VAL:HA | 2.47 | 0.45 |
| 1:CA:614:A:P | 4:CD:85:LYS:HE2 | 2.57 | 0.45 |
| 23:DA:2360:A:O5' | 23:DA:2360:A:H8 | 1.99 | 0.45 |
| 23:BA:1260:G:H2' | 23:BA:1261:C:O4' | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:642:A:N3 | 8:AH:113:SER:OG | 2.32 | 0.45 |
| 9:AI:5:TYR:CG | 9:AI:6:GLY:N | 2.85 | 0.45 |
| 24:DB:95:U:H2' | 24:DB:96:G:C8 | 2.51 | 0.45 |
| 23:DA:1983:C:O2' | 23:DA:1984:G:H5' | 2.16 | 0.45 |
| 36:DN:65:LEU:O | 36:DN:68:ARG:HB2 | 2.17 | 0.45 |
| 1:CA:452:A:C4 | 1:CA:453:A:C8 | 3.05 | 0.45 |
| 23:BA:1394:U:C5 | 23:BA:1395:A:C5 | 3.04 | 0.45 |
| 23:DA:2672:G:H2' | 23:DA:2673:G:O5' | 2.17 | 0.45 |
| 23:BA:1214:A:H2' | 23:BA:1215:G:O4' | 2.17 | 0.45 |
| 7:AG:41:ARG:O | 7:AG:45:ASP:N | 2.40 | 0.45 |
| 23:BA:2082:A:H2' | 23:BA:2083:G:O4' | 2.15 | 0.45 |
| 5:CE:28:PHE:CD1 | 5:CE:28:PHE:N | 2.85 | 0.45 |
| 7:CG:36:LYS:HB2 | 7:CG:36:LYS:NZ | 2.31 | 0.45 |
| 5:AE:26:PHE:CD1 | 5:AE:26:PHE:N | 2.84 | 0.45 |
| 23:DA:2587:A:O5' | 23:DA:2587:A:H8 | 1.99 | 0.45 |
| 23:DA:2795:G:H3' | 23:DA:2797:U:C5' | 2.47 | 0.45 |
| 23:DA:1417:C:H42 | 23:DA:1581:G:H1 | 1.64 | 0.45 |
| 1:AA:1241:G:C2 | 1:AA:1242:C:C4 | 3.04 | 0.45 |
| 34:DL:61:ARG:HD2 | 53:D5:13:ARG:HD2 | 1.99 | 0.45 |
| 34:DL:97:PRO:O | 34:DL:101:VAL:HG12 | 2.17 | 0.45 |
| 34:DL:57:THR:OG1 | 34:DL:58:THR:N | 2.49 | 0.45 |
| 23:BA:2416:C:N3 | 23:BA:2417:C:C5 | 2.85 | 0.45 |
| 1:CA:1372:U:C5 | 1:CA:1373:G:C5 | 3.04 | 0.45 |
| 1:AA:973:G:OP1 | 10:AJ:57:LYS:NZ | 2.50 | 0.45 |
| 34:BL:33:ARG:NE | 34:BL:36:LYS:HD3 | 2.10 | 0.45 |
| 23:BA:2846:G:C6 | 23:BA:2847:U:C4 | 3.04 | 0.45 |
| 1:CA:362:G:O2' | 12:CL:32:ARG:NH2 | 2.49 | 0.45 |
| 53:B5:32:LEU:HD23 | 53:B5:32:LEU:N | 2.32 | 0.45 |
| 25:BC:233:HIS:HE1 | 25:BC:247:ALA:N | 2.06 | 0.45 |
| 34:DL:49:ARG:O | 34:DL:51:PHE:N | 2.50 | 0.45 |
| 28:DF:73:ALA:H | 28:DF:87:PRO:HD2 | 1.82 | 0.45 |
| 50:D2:17:ASP:O | 50:D2:20:ARG:HB2 | 2.16 | 0.45 |
| 1:CA:671:G:C4 | 1:CA:672:U:C6 | 3.05 | 0.45 |
| 37:DO:88:ASP:O | 37:DO:90:GLY:N | 2.45 | 0.45 |
| 4:AD:31:CYS:O | 4:AD:32:ALA:HB3 | 2.17 | 0.45 |
| 42:DT:28:PHE:HE1 | 42:DT:81:VAL:CG2 | 2.30 | 0.45 |
| 13:AM:37:THR:OG1 | 13:AM:56:LEU:HD23 | 2.17 | 0.45 |
| 24:DB:68:C:H2' | 24:DB:69:G:O4' | 2.17 | 0.45 |
| 44:DV:97:GLU:O | 44:DV:98:MET:HB3 | 2.17 | 0.45 |
| 23:DA:661:C:O3' | 34:DL:18:ARG:CG | 2.65 | 0.45 |
| 47:DY:60:LEU:C | 47:DY:62:THR:N | 2.70 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:CE:13:ILE:HA | 5:CE:29:GLY:O | 2.17 | 0.45 |
| 5:AE:136:MET:O | 5:AE:139:LEU:N | 2.50 | 0.45 |
| 23:BA:2766:G:H5'' | 23:BA:2767:C:OP2 | 2.16 | 0.45 |
| 23:DA:1438:U:O2' | 23:DA:1439:A:H5' | 2.16 | 0.45 |
| 14:AN:24:CYS:SG | 14:AN:27:CYS:SG | 3.15 | 0.45 |
| 25:BC:175:LEU:HD12 | 25:BC:185:VAL:HG21 | 1.99 | 0.45 |
| 1:AA:1301:U:H3' | 1:AA:1302:U:C5' | 2.46 | 0.45 |
| 42:DT:29:TRP:CZ3 | 42:DT:78:LYS:CG | 3.00 | 0.45 |
| 23:DA:1578:U:O2 | 23:DA:1578:U:H2' | 2.17 | 0.45 |
| 4:AD:92:VAL:O | 4:AD:96:LEU:HB2 | 2.17 | 0.45 |
| 17:AQ:85:VAL:O | 17:AQ:89:LEU:HG | 2.17 | 0.45 |
| 1:CA:1149:C:H2' | 1:CA:1150:U:C6 | 2.52 | 0.45 |
| 8:CH:112:LEU:HD12 | 8:CH:114:THR:HG23 | 1.98 | 0.45 |
| 27:DE:89:VAL:CG1 | 27:DE:90:PHE:H | 2.19 | 0.45 |
| 1:CA:324:G:C2 | 1:CA:327:A:C8 | 3.05 | 0.45 |
| 1:CA:710:G:C4 | 1:CA:711:G:C8 | 3.05 | 0.45 |
| 23:DA:2286:A:C8 | 23:DA:2287:A:C6 | 3.05 | 0.45 |
| 23:BA:497:A:C5 | 23:BA:498:G:C8 | 3.05 | 0.45 |
| 23:BA:581:C:H2' | 23:BA:582:G:H8 | 1.81 | 0.45 |
| 44:BV:25:PRO:O | 44:BV:85:HIS:HB2 | 2.17 | 0.45 |
| 1:AA:913:A:C2' | 1:AA:914:A:OP2 | 2.64 | 0.45 |
| 18:CR:44:LEU:HG | 18:CR:50:ILE:HD13 | 1.99 | 0.45 |
| 38:BP:34:VAL:HG21 | 38:BP:43:GLN:HB2 | 1.99 | 0.45 |
| 23:DA:247:G:N7 | 23:DA:249:C:C2 | 2.85 | 0.45 |
| 23:DA:1413:G:C2' | 23:DA:1414:G:H5' | 2.47 | 0.45 |
| 1:CA:949:A:C2 | 1:CA:1233:G:N3 | 2.85 | 0.45 |
| 1:CA:256:U:OP1 | 17:CQ:17:LYS:NZ | 2.39 | 0.45 |
| 23:BA:1789:A:OP1 | 25:BC:222:ARG:HG3 | 2.16 | 0.45 |
| 35:BM:111:GLU:OE2 | 35:BM:133:ARG:CZ | 2.65 | 0.45 |
| 35:DM:116:GLU:O | 35:DM:117:ALA:C | 2.55 | 0.45 |
| 38:DP:41:ARG:HH11 | 38:DP:41:ARG:CB | 2.28 | 0.45 |
| 12:CL:7:ASN:HA | 12:CL:10:VAL:HG23 | 1.99 | 0.45 |
| 23:BA:17:G:H2' | 23:BA:18:C:C6 | 2.52 | 0.45 |
| 23:DA:2347:C:H4' | 51:D3:39:TYR:CE1 | 2.52 | 0.45 |
| 1:CA:1269:A:H5'' | 21:CU:24:ARG:NH1 | 2.32 | 0.45 |
| 25:DC:221:VAL:HG22 | 25:DC:226:MET:CE | 2.47 | 0.45 |
| 1:CA:1181:G:N2 | 1:CA:1182:G:N2 | 2.65 | 0.45 |
| 23:DA:496:G:C1' | 41:DS:61:ASN:HD21 | 2.30 | 0.45 |
| 33:BK:59:LYS:O | 33:BK:86:ILE:HG23 | 2.16 | 0.45 |
| 1:AA:224:C:H2' | 1:AA:225:C:H6 | 1.81 | 0.45 |
| 12:AL:58:ARG:HA | 12:AL:64:GLU:HG2 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:577:G:H1' | 1:AA:816:A:N3 | 2.32 | 0.45 |
| 1:CA:123:C:H5'' | 1:CA:311:C:O2' | 2.17 | 0.45 |
| 24:DB:27:C:N4 | 24:DB:28:C:N4 | 2.65 | 0.45 |
| 23:BA:1126:A:H8 | 23:BA:1126:A:O5' | 2.00 | 0.45 |
| 23:DA:1241:A:N7 | 23:DA:1242:A:C4 | 2.85 | 0.45 |
| 1:AA:497:U:C2' | 1:AA:497:U:O2 | 2.65 | 0.45 |
| 23:DA:1425:G:N2 | 23:DA:1573:G:N7 | 2.64 | 0.45 |
| 23:BA:2079:U:C2' | 23:BA:2080:G:O5' | 2.64 | 0.45 |
| 23:DA:771:G:C4 | 23:DA:772:C:C5 | 3.05 | 0.45 |
| 30:DH:75:LEU:HG | 30:DH:76:THR:O | 2.16 | 0.45 |
| 8:AH:68:ARG:HG2 | 8:AH:69:ARG:N | 2.32 | 0.45 |
| 1:CA:645:C:C2' | 1:CA:646:U:H5' | 2.46 | 0.45 |
| 5:CE:72:GLN:O | 5:CE:73:ASN:HB3 | 2.17 | 0.45 |
| 1:CA:1339:A:H2' | 1:CA:1340:A:O4' | 2.17 | 0.45 |
| 6:CF:82:ARG:HD2 | 6:CF:82:ARG:HA | 1.79 | 0.45 |
| 6:CF:82:ARG:HB2 | 6:CF:85:VAL:HG23 | 1.98 | 0.45 |
| 24:DB:95:U:C2 | 24:DB:96:G:N7 | 2.85 | 0.45 |
| 23:DA:1790:C:H2' | 23:DA:1791:A:C5 | 2.51 | 0.45 |
| 23:DA:2046:G:O5' | 50:D2:19:ARG:HA | 2.16 | 0.45 |
| 23:BA:1632:A:C6 | 23:BA:1633:G:C6 | 3.05 | 0.45 |
| 23:BA:1632:A:H8 | 23:BA:1632:A:O5' | 2.00 | 0.45 |
| 38:BP:114:LEU:HD23 | 38:BP:114:LEU:HA | 1.56 | 0.45 |
| 23:BA:838:C:C4 | 23:BA:839:U:C5 | 3.05 | 0.45 |
| 23:BA:1564:C:O2' | 23:BA:1565:C:H5' | 2.17 | 0.45 |
| 23:BA:606:U:H4' | 23:BA:658:C:H4' | 1.99 | 0.45 |
| 38:DP:108:ARG:O | 38:DP:111:ARG:HB2 | 2.17 | 0.45 |
| 23:DA:575:A:H2' | 23:DA:575:A:N3 | 2.32 | 0.45 |
| 9:CI:8:GLY:HA3 | 9:CI:76:ALA:O | 2.17 | 0.45 |
| 23:DA:1835:G:C4 | 23:DA:1836:C:C5 | 3.05 | 0.45 |
| 23:BA:1889:A:H2' | 23:BA:1890:A:O4' | 2.17 | 0.45 |
| 10:CJ:89:ASP:C | 10:CJ:91:PRO:HD3 | 2.37 | 0.45 |
| 40:DR:82:ARG:C | 40:DR:83:ARG:HG2 | 2.37 | 0.45 |
| 41:DS:78:GLU:OE2 | 41:DS:99:ARG:HD3 | 2.17 | 0.45 |
| 23:DA:1540:G:C2 | 23:DA:1541:U:C2 | 3.05 | 0.44 |
| 23:DA:1541:U:O3' | 23:DA:1542:G:H3' | 2.16 | 0.44 |
| 27:DE:64:ILE:HG23 | 27:DE:65:TRP:CD1 | 2.52 | 0.44 |
| 42:BT:63:LYS:HE3 | 42:BT:72:LYS:HG2 | 1.98 | 0.44 |
| 23:BA:603:A:C2 | 23:BA:655:A:C2 | 3.06 | 0.44 |
| 25:BC:142:VAL:HG23 | 25:BC:192:THR:O | 2.17 | 0.44 |
| 34:DL:47:ASP:HB2 | 34:DL:51:PHE:HB2 | 1.98 | 0.44 |
| 23:DA:1022:G:C6 | 23:DA:1140:C:C4 | 3.05 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:BQ:79:PHE:O | 39:BQ:79:PHE:HD1 | 1.98 | 0.44 |
| 39:BQ:92:ARG:HD2 | 39:BQ:95:LEU:CG | 2.46 | 0.44 |
| 1:AA:378:G:C6 | 1:AA:379:C:N4 | 2.84 | 0.44 |
| 1:AA:501:C:H3' | 1:AA:501:C:H6 | 1.82 | 0.44 |
| 12:AL:82:VAL:CG1 | 12:AL:83:LEU:N | 2.80 | 0.44 |
| 25:BC:77:ALA:HB2 | 25:BC:97:TYR:CG | 2.53 | 0.44 |
| 4:CD:106:TYR:C | 4:CD:109:GLY:H | 2.19 | 0.44 |
| 16:AP:28:ARG:NH1 | 16:AP:28:ARG:CG | 2.71 | 0.44 |
| 3:CC:172:ARG:O | 3:CC:173:VAL:CG2 | 2.52 | 0.44 |
| 2:CB:204:ASN:CG | 2:CB:205:ASP:H | 2.20 | 0.44 |
| 25:DC:242:ARG:H | 25:DC:242:ARG:HH11 | 1.64 | 0.44 |
| 23:DA:662:G:H5' | 34:DL:18:ARG:HA | 1.97 | 0.44 |
| 26:DD:2:LYS:HD3 | 26:DD:95:ILE:O | 2.16 | 0.44 |
| 47:DY:25:VAL:HG21 | 47:DY:61:LEU:HD13 | 1.98 | 0.44 |
| 23:DA:2722:G:C5 | 23:DA:2723:C:C4 | 3.05 | 0.44 |
| 36:DN:17:ARG:O | 36:DN:20:LEU:HB3 | 2.17 | 0.44 |
| 42:BT:43:VAL:HG11 | 42:BT:81:VAL:HG11 | 1.99 | 0.44 |
| 28:BF:5:LEU:HD22 | 28:BF:6:ALA:H | 1.81 | 0.44 |
| 1:AA:1104:G:C2 | 1:AA:1105:A:C5 | 3.05 | 0.44 |
| 45:BW:49:LYS:HB2 | 45:BW:80:HIS:CB | 2.46 | 0.44 |
| 1:AA:1369:C:C2' | 1:AA:1370:G:O4' | 2.66 | 0.44 |
| 36:DN:54:LEU:CD2 | 36:DN:62:ALA:HB1 | 2.45 | 0.44 |
| 1:CA:506:G:C6 | 1:CA:507:C:N4 | 2.84 | 0.44 |
| 19:AS:39:THR:HG22 | 19:AS:40:ILE:N | 2.32 | 0.44 |
| 36:BN:57:ARG:CD | 36:BN:59:ASP:OD2 | 2.64 | 0.44 |
| 23:DA:2305:A:C5' | 28:DF:134:GLY:HA3 | 2.46 | 0.44 |
| 43:BU:81:LYS:HZ3 | 43:BU:97:ARG:HD3 | 1.80 | 0.44 |
| 46:BX:13:ILE:O | 46:BX:13:ILE:HD12 | 2.17 | 0.44 |
| 25:BC:131:LEU:HG | 25:BC:136:ILE:HD11 | 1.99 | 0.44 |
| 25:DC:25:THR:O | 25:DC:26:LYS:C | 2.55 | 0.44 |
| 1:AA:556:C:O2' | 1:AA:557:G:H5' | 2.17 | 0.44 |
| 28:DF:133:LEU:H | 28:DF:133:LEU:HD23 | 1.81 | 0.44 |
| 3:AC:59:ARG:HH21 | 3:AC:97:LYS:HE2 | 1.81 | 0.44 |
| 1:AA:66:G:C4' | 1:AA:173:U:C5 | 2.99 | 0.44 |
| 23:BA:1475:G:C2 | 23:BA:1476:C:O2 | 2.70 | 0.44 |
| 27:BE:117:ARG:HH21 | 27:BE:187:VAL:HA | 1.82 | 0.44 |
| 1:CA:833:U:C2 | 1:CA:834:C:C5 | 3.05 | 0.44 |
| 43:BU:63:LYS:CG | 43:BU:64:GLU:N | 2.80 | 0.44 |
| 23:BA:2550:G:C5 | 23:BA:2551:C:C5 | 3.05 | 0.44 |
| 17:CQ:89:LEU:O | 17:CQ:93:GLN:HG3 | 2.16 | 0.44 |
| 23:DA:540:G:C5 | 23:DA:541:C:C5 | 3.05 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:DE:50:SER:OG | 27:DE:51:THR:N | 2.46 | 0.44 |
| 29:BG:90:LYS:O | 29:BG:94:TYR:HB2 | 2.17 | 0.44 |
| 23:DA:2009:G:O2' | 23:DA:2010:G:H5' | 2.17 | 0.44 |
| 4:CD:82:ALA:CB | 4:CD:89:THR:HG23 | 2.47 | 0.44 |
| 1:AA:236:G:H2' | 1:AA:237:C:O4' | 2.17 | 0.44 |
| 1:CA:1135:U:H4' | 1:CA:1136:U:C5 | 2.53 | 0.44 |
| 1:CA:511:C:H1' | 4:CD:43:HIS:HE2 | 1.81 | 0.44 |
| 23:DA:2664:G:H2' | 23:DA:2665:A:OP2 | 2.17 | 0.44 |
| 23:BA:795:C:H2' | 23:BA:796:C:C6 | 2.47 | 0.44 |
| 23:BA:1184:G:C6 | 23:BA:1185:C:C4 | 3.04 | 0.44 |
| 23:BA:1922:G:C6 | 23:BA:1923:U:N3 | 2.84 | 0.44 |
| 1:CA:976:G:H8 | 1:CA:1358:U:C2' | 2.29 | 0.44 |
| 7:CG:15:ASP:OD1 | 7:CG:18:TYR:HD1 | 1.99 | 0.44 |
| 8:AH:36:LEU:C | 8:AH:38:ILE:N | 2.69 | 0.44 |
| 1:CA:492:G:C6 | 1:CA:493:G:C5 | 3.05 | 0.44 |
| 38:BP:96:ARG:CZ | 38:BP:96:ARG:HB2 | 2.47 | 0.44 |
| 1:CA:413:G:H4' | 1:CA:414:A:H5'' | 1.98 | 0.44 |
| 12:AL:5:THR:O | 12:AL:9:LEU:HD12 | 2.18 | 0.44 |
| 23:DA:494:G:N2 | 41:DS:57:ASN:HD21 | 2.15 | 0.44 |
| 45:BW:14:ARG:O | 45:BW:15:ASP:HB2 | 2.17 | 0.44 |
| 1:CA:334:C:O2' | 1:CA:335:C:H5' | 2.17 | 0.44 |
| 36:BN:27:SER:O | 36:BN:31:HIS:N | 2.50 | 0.44 |
| 3:AC:191:THR:C | 3:AC:193:TYR:H | 2.21 | 0.44 |
| 46:BX:68:PRO:O | 46:BX:71:TYR:N | 2.49 | 0.44 |
| 1:AA:994:A:O5' | 1:AA:994:A:H8 | 2.00 | 0.44 |
| 1:AA:563:A:C8 | 1:AA:567:G:H1' | 2.51 | 0.44 |
| 1:CA:119:A:C4 | 1:CA:240:C:C4 | 3.05 | 0.44 |
| 26:DD:72:VAL:O | 26:DD:73:GLU:C | 2.54 | 0.44 |
| 19:CS:39:THR:HG22 | 19:CS:40:ILE:N | 2.32 | 0.44 |
| 23:DA:1647:G:H3' | 23:DA:1647:G:P | 2.57 | 0.44 |
| 20:CT:78:ALA:O | 20:CT:79:ARG:C | 2.55 | 0.44 |
| 23:BA:900:A:H2' | 23:BA:901:A:O4' | 2.17 | 0.44 |
| 38:BP:107:ASP:H | 38:BP:110:ILE:HG13 | 1.82 | 0.44 |
| 23:DA:2026:C:C2 | 23:DA:2027:G:C8 | 3.05 | 0.44 |
| 30:BH:12:LEU:H | 30:BH:12:LEU:HD22 | 1.81 | 0.44 |
| 37:BO:64:GLU:O | 37:BO:68:GLN:HG3 | 2.17 | 0.44 |
| 15:CO:17:ARG:NH1 | 15:CO:77:ARG:HH12 | 2.16 | 0.44 |
| 26:BD:8:LYS:HG2 | 26:BD:192:ASN:HD22 | 1.81 | 0.44 |
| 2:AB:228:GLY:O | 2:AB:230:VAL:N | 2.50 | 0.44 |
| 7:AG:36:LYS:HB2 | 7:AG:36:LYS:NZ | 2.32 | 0.44 |
| 52:B4:3:ARG:HA | 52:B4:3:ARG:HD3 | 1.74 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:AB:189:ASP:N | 2:AB:189:ASP:OD1 | 2.50 | 0.44 |
| 23:DA:2231:C:H2' | 23:DA:2232:U:O4' | 2.17 | 0.44 |
| 15:CO:25:THR:OG1 | 15:CO:26:GLU:N | 2.49 | 0.44 |
| 34:DL:85:LEU:CA | 34:DL:88:LEU:HB2 | 2.46 | 0.44 |
| 34:BL:66:GLY:O | 34:BL:67:MET:HB2 | 2.17 | 0.44 |
| 47:BY:3:LEU:O | 47:BY:5:GLU:N | 2.50 | 0.44 |
| 23:BA:312:G:H2' | 23:BA:312:G:N3 | 2.32 | 0.44 |
| 43:DU:14:LEU:CD2 | 43:DU:15:VAL:N | 2.69 | 0.44 |
| 2:AB:164:VAL:O | 2:AB:186:ALA:HB1 | 2.17 | 0.44 |
| 1:AA:1226:C:H42 | 13:AM:104:ARG:HD2 | 1.82 | 0.44 |
| 1:CA:81:G:C5 | 1:CA:82:U:C4 | 3.05 | 0.44 |
| 34:BL:33:ARG:O | 34:BL:34:GLY:C | 2.55 | 0.44 |
| 1:CA:1225:A:C5' | 1:CA:1226:C:OP2 | 2.66 | 0.44 |
| 1:CA:1316:G:H2' | 1:CA:1317:C:H5'' | 1.99 | 0.44 |
| 27:DE:64:ILE:O | 27:DE:65:TRP:CD1 | 2.70 | 0.44 |
| 23:BA:1902:C:H2' | 23:BA:1903:G:O4' | 2.17 | 0.44 |
| 28:BF:73:ALA:H | 28:BF:87:PRO:HD2 | 1.82 | 0.44 |
| 23:DA:748:G:OP2 | 41:DS:88:ARG:HG3 | 2.17 | 0.44 |
| 23:DA:194:G:H2' | 23:DA:195:A:O4' | 2.17 | 0.44 |
| 23:DA:197:A:C5' | 23:DA:197:A:C8 | 2.95 | 0.44 |
| 25:DC:70:TRP:O | 25:DC:70:TRP:HD1 | 2.01 | 0.44 |
| 24:DB:16:G:C6 | 24:DB:69:G:N2 | 2.85 | 0.44 |
| 44:DV:57:ILE:HG22 | 44:DV:59:LEU:HG | 1.99 | 0.44 |
| 26:DD:87:GLU:O | 26:DD:88:GLY:C | 2.53 | 0.44 |
| 5:CE:75:THR:HG23 | 5:CE:76:ILE:H | 1.81 | 0.44 |
| 1:CA:668:G:H2' | 1:CA:669:U:H6 | 1.81 | 0.44 |
| 1:AA:1067:A:N3 | 1:AA:1068:G:C1' | 2.80 | 0.44 |
| 1:AA:1076:C:H2' | 1:AA:1077:G:H5' | 1.99 | 0.44 |
| 1:AA:1064:G:N2 | 1:AA:1190:G:H2' | 2.22 | 0.44 |
| 41:DS:4:LYS:CD | 41:DS:6:ILE:HD11 | 2.45 | 0.44 |
| 1:AA:186(G):C:H2' | 1:AA:187:C:O4' | 2.16 | 0.44 |
| 23:DA:1454:U:C5 | 23:DA:2702:U:O4 | 2.71 | 0.44 |
| 23:DA:1454:U:O4' | 36:DN:63:ARG:HD3 | 2.17 | 0.44 |
| 25:BC:164:GLN:O | 25:BC:175:LEU:HD23 | 2.17 | 0.44 |
| 23:DA:2747:G:O2' | 23:DA:2748:A:O4' | 2.27 | 0.44 |
| 8:CH:25:ASP:N | 8:CH:25:ASP:OD1 | 2.50 | 0.44 |
| 8:AH:10:LEU:N | 8:AH:10:LEU:HD23 | 2.32 | 0.44 |
| 24:DB:10:C:C2 | 24:DB:11:C:C5 | 3.06 | 0.44 |
| 1:AA:832:C:O2' | 1:AA:833:U:P | 2.74 | 0.44 |
| 3:AC:59:ARG:CG | 3:AC:64:VAL:HG22 | 2.43 | 0.44 |
| 44:BV:74:VAL:HG22 | 44:BV:86:VAL:CG1 | 2.47 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DA:498:G:O2' | 43:DU:47:LYS:HD3 | 2.17 | 0.44 |
| 23:BA:2476:A:N1 | 23:BA:2477:C:C5 | 2.85 | 0.44 |
| 23:BA:1389:G:C2 | 23:BA:1390:U:C2 | 3.05 | 0.44 |
| 17:CQ:53:LEU:HD12 | 17:CQ:54:GLY:H | 1.82 | 0.44 |
| 7:CG:131:LYS:HE3 | 7:CG:136:LYS:HZ1 | 1.81 | 0.44 |
| 38:DP:3:ARG:HB3 | 38:DP:6:LEU:HB3 | 1.98 | 0.44 |
| 23:DA:1649:G:C6 | 23:DA:2009:G:C6 | 3.05 | 0.44 |
| 23:DA:2467:C:C2' | 23:DA:2468:G:H5' | 2.47 | 0.44 |
| 1:AA:128:G:O2' | 17:AQ:3:LYS:HE2 | 2.18 | 0.44 |
| 23:BA:56:A:C2 | 23:BA:115:C:O2 | 2.70 | 0.44 |
| 1:AA:649:G:C4 | 1:AA:650:G:C8 | 3.05 | 0.44 |
| 33:DK:31:LYS:HB3 | 33:DK:32:TYR:CD1 | 2.53 | 0.44 |
| 38:BP:3:ARG:HB3 | 38:BP:6:LEU:HB3 | 1.99 | 0.44 |
| 23:DA:814:C:C5 | 34:DL:27:HIS:NE2 | 2.85 | 0.44 |
| 23:DA:1945:G:H2' | 23:DA:1946:U:C6 | 2.52 | 0.44 |
| 23:DA:1684:C:C2 | 23:DA:1705:G:N2 | 2.86 | 0.44 |
| 7:CG:27:ILE:HD12 | 7:CG:40:ALA:HA | 1.99 | 0.44 |
| 23:BA:571:A:H4' | 23:BA:572:A:OP1 | 2.17 | 0.44 |
| 26:DD:176:ILE:CD1 | 26:DD:176:ILE:N | 2.80 | 0.44 |
| 44:BV:108:PRO:HG3 | 44:BV:141:VAL:HG22 | 1.99 | 0.44 |
| 36:DN:79:LEU:HD23 | 36:DN:83:ILE:CB | 2.47 | 0.44 |
| 1:CA:356:A:C2' | 1:CA:357:G:O5' | 2.65 | 0.44 |
| 1:AA:512:U:H3 | 1:AA:539:A:H61 | 1.65 | 0.44 |
| 25:DC:221:VAL:HG22 | 25:DC:226:MET:HE3 | 1.99 | 0.44 |
| 8:AH:50:ARG:H | 8:AH:50:ARG:HD3 | 1.81 | 0.44 |
| 1:AA:1160:G:O2' | 1:AA:1161:C:H5' | 2.16 | 0.44 |
| 38:DP:80:SER:O | 38:DP:82:LEU:N | 2.50 | 0.44 |
| 11:CK:109:VAL:HG11 | 18:CR:84:LYS:HB2 | 1.99 | 0.44 |
| 51:D3:18:ARG:HH22 | 51:D3:44:ARG:HB2 | 1.82 | 0.44 |
| 23:DA:1203:G:H3' | 23:DA:1204:A:C5' | 2.47 | 0.44 |
| 23:DA:1027:A:C6 | 23:DA:1126:A:C4 | 3.04 | 0.44 |
| 15:AO:67:LEU:HD23 | 15:AO:78:TYR:HE1 | 1.83 | 0.44 |
| 5:CE:36:ASP:O | 5:CE:37:ARG:CB | 2.65 | 0.44 |
| 23:BA:1203:G:H3' | 23:BA:1204:A:H5'' | 1.99 | 0.44 |
| 23:BA:262:A:O2' | 23:BA:263:C:H5' | 2.17 | 0.44 |
| 1:CA:662:G:C2 | 1:CA:744:C:O2 | 2.71 | 0.44 |
| 23:DA:1464:C:C2 | 23:DA:1465:G:C8 | 3.05 | 0.44 |
| 16:CP:49:LEU:HG | 16:CP:50:LYS:N | 2.32 | 0.44 |
| 15:AO:3:ILE:HG21 | 15:AO:34:LEU:HD23 | 1.99 | 0.44 |
| 27:DE:135:LYS:O | 27:DE:136:THR:C | 2.56 | 0.44 |
| 23:BA:2795:G:H3' | 23:BA:2797:U:C5' | 2.47 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:B3:13:CYS:O | 51:B3:21:TYR:HA | 2.17 | 0.44 |
| 1:CA:930:C:C4 | 1:CA:931:C:C5 | 3.05 | 0.44 |
| 53:B5:15:LYS:CG | 53:B5:16:ILE:N | 2.80 | 0.44 |
| 48:BZ:18:ASP:N | 48:BZ:18:ASP:OD1 | 2.49 | 0.44 |
| 20:AT:94:ALA:O | 20:AT:95:ALA:HB3 | 2.17 | 0.44 |
| 34:DL:126:VAL:CA | 34:DL:145:PRO:HG2 | 2.46 | 0.44 |
| 34:DL:62:LEU:CD1 | 53:D5:27:THR:HG22 | 2.48 | 0.44 |
| 23:BA:1540:G:C2 | 23:BA:1541:U:C2 | 3.05 | 0.44 |
| 23:BA:1540:G:C4 | 23:BA:1541:U:C6 | 3.04 | 0.44 |
| 1:CA:948:C:OP1 | 13:CM:107:ALA:HA | 2.17 | 0.44 |
| 23:BA:2295:C:C4 | 23:BA:2296:U:H5 | 2.36 | 0.44 |
| 25:DC:10:THR:CG2 | 25:DC:13:ARG:CB | 2.92 | 0.44 |
| 32:BJ:110:LEU:O | 32:BJ:110:LEU:HD22 | 2.17 | 0.44 |
| 34:DL:50:ARG:HD2 | 34:DL:51:PHE:CB | 2.47 | 0.44 |
| 16:CP:6:LEU:HB3 | 16:CP:17:TYR:HD2 | 1.82 | 0.44 |
| 39:BQ:72:HIS:HE1 | 39:BQ:107:ALA:HA | 1.82 | 0.44 |
| 39:BQ:79:PHE:HE1 | 39:BQ:83:LEU:CD2 | 2.29 | 0.44 |
| 43:BU:29:GLU:O | 43:BU:38:ILE:N | 2.40 | 0.44 |
| 1:AA:407:G:N2 | 1:AA:436:C:C2 | 2.86 | 0.44 |
| 1:CA:393:A:C4 | 1:CA:394:G:C8 | 3.05 | 0.44 |
| 2:CB:205:ASP:O | 2:CB:207:ALA:N | 2.49 | 0.44 |
| 35:BM:140:ALA:HB3 | 44:BV:53:ILE:CG1 | 2.46 | 0.44 |
| 23:BA:142:G:H2' | 23:BA:143:C:H6 | 1.81 | 0.44 |
| 1:AA:1072:G:C6 | 1:AA:1104:G:N1 | 2.85 | 0.44 |
| 1:AA:1251:A:H1' | 1:AA:1369:C:O2' | 2.17 | 0.44 |
| 4:AD:128:VAL:HA | 4:AD:145:GLU:O | 2.17 | 0.44 |
| 25:DC:164:GLN:O | 25:DC:175:LEU:HD23 | 2.18 | 0.44 |
| 44:DV:137:ILE:HG22 | 44:DV:138:GLU:N | 2.31 | 0.44 |
| 35:DM:47:ILE:HG22 | 35:DM:48:GLU:H | 1.78 | 0.44 |
| 23:DA:1576:U:N3 | 23:DA:1577:C:C5 | 2.85 | 0.44 |
| 1:AA:1238:A:C5 | 1:AA:1303:C:H1' | 2.53 | 0.44 |
| 23:DA:2330:G:H1' | 45:DW:41:ARG:HB3 | 1.98 | 0.44 |
| 23:BA:1284:A:H2' | 23:BA:1285:G:O4' | 2.17 | 0.44 |
| 41:DS:41:LYS:C | 41:DS:43:GLY:N | 2.69 | 0.44 |
| 23:DA:953:A:O2' | 23:DA:954:G:H5' | 2.17 | 0.44 |
| 4:CD:92:VAL:O | 4:CD:96:LEU:HB2 | 2.17 | 0.44 |
| 11:CK:21:ILE:HG13 | 11:CK:30:VAL:CG1 | 2.47 | 0.44 |
| 1:CA:173:U:C2 | 1:CA:197:A:N1 | 2.85 | 0.44 |
| 1:CA:69:G:H1 | 1:CA:99:C:H42 | 1.65 | 0.44 |
| 27:BE:37:VAL:HG23 | 27:BE:183:VAL:HG22 | 1.99 | 0.44 |
| 4:CD:79:PHE:HZ | 4:CD:204:ILE:HA | 1.81 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DA:2471:C:H2' | 23:DA:2472:G:O4' | 2.17 | 0.44 |
| 44:DV:39:VAL:HG21 | 44:DV:44:PHE:CD2 | 2.52 | 0.44 |
| 23:BA:1777:U:O2' | 23:BA:1778:U:H5' | 2.17 | 0.44 |
| 23:BA:2427:C:H5'' | 23:BA:2428:G:OP1 | 2.17 | 0.44 |
| 1:AA:949:A:C2 | 1:AA:1233:G:N3 | 2.85 | 0.44 |
| 23:BA:2401:U:O2' | 23:BA:2402:C:H5'' | 2.16 | 0.44 |
| 25:BC:221:VAL:HG22 | 25:BC:226:MET:HE3 | 1.98 | 0.44 |
| 1:CA:445:G:H2' | 1:CA:446:G:C8 | 2.52 | 0.44 |
| 43:BU:91:GLU:HB3 | 43:BU:92:ASN:H | 1.65 | 0.44 |
| 5:CE:137:GLU:HG2 | 5:CE:140:ARG:NH1 | 2.31 | 0.44 |
| 23:BA:1217:C:OP1 | 39:BQ:15:LYS:HE2 | 2.17 | 0.44 |
| 23:DA:693:C:C2' | 23:DA:694:U:O5' | 2.66 | 0.44 |
| 41:BS:45:TYR:HD2 | 41:BS:46:PHE:CE1 | 2.34 | 0.44 |
| 23:DA:2280:G:C2' | 23:DA:2281:C:H5' | 2.47 | 0.44 |
| 23:DA:958:U:C2' | 23:DA:959:A:OP2 | 2.65 | 0.44 |
| 24:BB:26:A:N7 | 24:BB:27:C:C4 | 2.85 | 0.44 |
| 23:BA:2572:A:C8 | 26:BD:144:ARG:HB3 | 2.52 | 0.44 |
| 48:BZ:50:VAL:O | 48:BZ:54:VAL:HG22 | 2.17 | 0.44 |
| 12:AL:46:LYS:HD3 | 12:AL:47:PRO:HG3 | 1.99 | 0.44 |
| 23:DA:1381:G:H2' | 23:DA:1382:G:H5' | 1.97 | 0.44 |
| 23:BA:1471:A:C2 | 23:BA:1472:A:C4 | 3.05 | 0.44 |
| 1:CA:932:C:H2' | 1:CA:933:G:C8 | 2.52 | 0.44 |
| 1:AA:575:G:C8 | 1:AA:881:G:N2 | 2.86 | 0.44 |
| 23:BA:273(B):G:C2 | 23:BA:364:C:C2 | 3.05 | 0.44 |
| 28:DF:52:ILE:HG23 | 28:DF:153:ARG:HH22 | 1.83 | 0.44 |
| 23:DA:447:A:C4 | 23:DA:473:G:C8 | 3.05 | 0.44 |
| 23:BA:724:U:H2' | 23:BA:725:G:O4' | 2.18 | 0.44 |
| 42:BT:18:TYR:O | 42:BT:19:ALA:C | 2.56 | 0.44 |
| 13:AM:86:CYS:HA | 19:AS:73:GLU:O | 2.17 | 0.44 |
| 9:AI:5:TYR:O | 9:AI:84:ALA:HA | 2.18 | 0.44 |
| 23:BA:443:A:H1' | 23:BA:1201:C:O4' | 2.18 | 0.44 |
| 23:BA:2794:C:N4 | 23:BA:2802:G:H1 | 2.15 | 0.44 |
| 23:BA:1655:A:C8 | 23:BA:1656:C:C5 | 3.05 | 0.44 |
| 23:BA:487:C:H1' | 41:BS:53:SER:HB2 | 1.98 | 0.44 |
| 39:BQ:78:THR:O | 39:BQ:81:HIS:HB3 | 2.17 | 0.44 |
| 23:DA:2666:C:C6 | 23:DA:2667:C:C6 | 3.05 | 0.44 |
| 1:CA:1417:G:N2 | 1:CA:1482:G:H2' | 2.33 | 0.44 |
| 50:D2:14:ALA:O | 50:D2:15:ARG:C | 2.55 | 0.44 |
| 23:DA:836:G:C5 | 23:DA:837:C:C4 | 3.05 | 0.44 |
| 48:BZ:11:SER:OG | 48:BZ:13:ILE:HG13 | 2.17 | 0.44 |
| 6:AF:64:GLN:HE21 | 6:AF:64:GLN:HB2 | 1.60 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:BZ:32:GLN:OE1 | 48:BZ:32:GLN:HA | 2.17 | 0.44 |
| 4:CD:14:ARG:HA | 4:CD:14:ARG:HD3 | 1.84 | 0.44 |
| 2:CB:9:GLU:C | 2:CB:9:GLU:CD | 2.75 | 0.44 |
| 23:BA:1987:G:H2' | 23:BA:1988:C:H6 | 1.83 | 0.44 |
| 34:DL:107:LYS:C | 34:DL:109:GLY:H | 2.20 | 0.44 |
| 25:BC:155:LEU:CD1 | 25:BC:155:LEU:H | 2.29 | 0.44 |
| 1:CA:1369:C:O2' | 1:CA:1370:G:O4' | 2.34 | 0.44 |
| 1:CA:1374:A:C4 | 1:CA:1375:A:C8 | 3.05 | 0.44 |
| 1:AA:978:A:O2' | 1:AA:1322:C:N3 | 2.48 | 0.44 |
| 26:BD:24:THR:HG22 | 26:BD:186:GLY:H | 1.82 | 0.44 |
| 27:DE:67:GLN:O | 27:DE:68:LYS:CB | 2.65 | 0.44 |
| 23:DA:577:G:OP1 | 23:DA:2502:G:H2' | 2.16 | 0.44 |
| 32:BJ:95:TYR:N | 32:BJ:108:ILE:O | 2.40 | 0.44 |
| 41:DS:14:PRO:O | 41:DS:15:ARG:C | 2.55 | 0.44 |
| 4:AD:104:VAL:C | 4:AD:106:TYR:N | 2.70 | 0.44 |
| 1:AA:430:A:OP1 | 4:AD:9:CYS:N | 2.44 | 0.44 |
| 4:AD:19:LEU:O | 4:AD:31:CYS:SG | 2.75 | 0.44 |
| 23:DA:2712:U:O2' | 23:DA:712(B):A:C5' | 2.64 | 0.44 |
| 23:BA:2210:G:N2 | 23:BA:2211:G:C5' | 2.60 | 0.44 |
| 44:DV:163:LEU:HD23 | 44:DV:163:LEU:H | 1.83 | 0.44 |
| 23:BA:1299:G:H3' | 23:BA:1639:U:O4 | 2.16 | 0.44 |
| 24:BB:10:C:C4 | 24:BB:11:C:C5 | 3.06 | 0.44 |
| 24:BB:68:C:H2' | 24:BB:69:G:O4' | 2.16 | 0.44 |
| 10:CJ:76:ASN:HA | 10:CJ:77:PRO:HD3 | 1.87 | 0.44 |
| 1:AA:1346:A:C2 | 1:AA:1348:U:C4 | 3.06 | 0.44 |
| 41:DS:19:LEU:HB3 | 50:D2:25:LEU:HD11 | 1.99 | 0.44 |
| 1:AA:1292:U:C2 | 1:AA:1293:G:N7 | 2.86 | 0.44 |
| 29:DG:44:VAL:O | 29:DG:50:VAL:HG13 | 2.18 | 0.44 |
| 23:BA:2723:C:H6 | 23:BA:2723:C:O5' | 2.00 | 0.44 |
| 1:AA:1331:G:OP1 | 1:AA:1331:G:H4' | 2.17 | 0.44 |
| 40:BR:28:GLU:HB2 | 40:BR:31:ALA:HB2 | 1.99 | 0.44 |
| 25:DC:166:GLN:NE2 | 25:DC:166:GLN:CA | 2.62 | 0.44 |
| 25:DC:166:GLN:HB2 | 25:DC:174:ILE:HG22 | 1.99 | 0.44 |
| 1:CA:349:A:C2' | 1:CA:350:G:H5' | 2.47 | 0.44 |
| 17:AQ:85:VAL:O | 17:AQ:86:GLU:C | 2.54 | 0.44 |
| 33:BK:96:THR:O | 33:BK:97:ARG:C | 2.56 | 0.44 |
| 33:DK:35:VAL:HG11 | 33:DK:103:ALA:CB | 2.47 | 0.44 |
| 23:BA:956:G:OP1 | 35:BM:86:GLY:N | 2.49 | 0.44 |
| 9:CI:16:ARG:HB2 | 9:CI:64:THR:HB | 1.99 | 0.44 |
| 1:CA:828:A:C5' | 1:CA:859:A:C2 | 2.96 | 0.44 |
| 37:DO:34:HIS:HB3 | 37:DO:36:TYR:CE1 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DA:1010:A:H5' | 39:DQ:62:ILE:HG21 | 1.99 | 0.44 |
| 23:DA:295:G:H4' | 43:DU:2:ARG:NH1 | 2.32 | 0.44 |
| 23:DA:1518:C:H2' | 23:DA:1519:G:H8 | 1.82 | 0.44 |
| 45:BW:53:MET:HA | 45:BW:58:THR:O | 2.17 | 0.44 |
| 1:CA:67:C:O2' | 1:CA:171:A:H1' | 2.17 | 0.44 |
| 23:BA:483:A:H2' | 23:BA:483:A:N3 | 2.33 | 0.44 |
| 29:BG:91:GLY:O | 29:BG:92:ILE:O | 2.35 | 0.44 |
| 23:BA:1401:G:C5 | 23:BA:1402:C:C4 | 3.06 | 0.44 |
| 1:AA:401:C:C6 | 1:AA:401:C:C3' | 3.00 | 0.44 |
| 23:BA:2467:C:C2' | 23:BA:2468:G:H5' | 2.47 | 0.44 |
| 23:BA:2467:C:C5' | 35:BM:123:HIS:CE1 | 3.00 | 0.44 |
| 23:BA:909:A:H2' | 23:BA:912:C:H5 | 1.83 | 0.44 |
| 1:CA:521:G:C2 | 1:CA:522:C:C6 | 3.05 | 0.44 |
| 2:CB:165:VAL:HG23 | 2:CB:166:ASP:N | 2.33 | 0.44 |
| 33:DK:2:ILE:HD12 | 33:DK:2:ILE:HA | 1.76 | 0.44 |
| 44:DV:74:VAL:CG2 | 44:DV:86:VAL:HG13 | 2.47 | 0.44 |
| 1:AA:1053:G:C3' | 1:AA:1054:C:C5' | 2.92 | 0.44 |
| 36:BN:79:LEU:CD2 | 36:BN:83:ILE:HB | 2.46 | 0.44 |
| 8:AH:13:ILE:O | 8:AH:17:THR:HG23 | 2.17 | 0.44 |
| 23:BA:997:G:OP1 | 39:BQ:93:LYS:HD2 | 2.17 | 0.44 |
| 1:CA:559:A:H4' | 1:CA:560:U:H3' | 2.00 | 0.44 |
| 8:AH:36:LEU:O | 8:AH:39:LEU:N | 2.50 | 0.44 |
| 1:CA:411:A:N6 | 1:CA:413:G:N3 | 2.66 | 0.44 |
| 32:BJ:80:ALA:C | 32:BJ:82:LYS:H | 2.21 | 0.44 |
| 44:BV:121:HIS:CE1 | 44:BV:169:GLU:OE2 | 2.71 | 0.44 |
| 2:CB:28:PHE:CD1 | 2:CB:190:THR:HG22 | 2.53 | 0.44 |
| 23:DA:2705:A:H3' | 23:DA:2706:G:H8 | 1.83 | 0.44 |
| 26:DD:172:VAL:HG13 | 26:DD:182:LEU:HD11 | 1.98 | 0.44 |
| 1:AA:1181:G:N2 | 1:AA:1182:G:N2 | 2.65 | 0.44 |
| 23:DA:2604:U:O2 | 23:DA:2604:U:C2' | 2.65 | 0.44 |
| 1:AA:577:G:C5 | 1:AA:578:C:C5 | 3.05 | 0.44 |
| 23:BA:1773:A:C5 | 23:BA:1829:A:H1' | 2.52 | 0.44 |
| 3:AC:186:PHE:CD1 | 3:AC:187:ALA:N | 2.85 | 0.44 |
| 3:CC:186:PHE:CD1 | 3:CC:187:ALA:N | 2.86 | 0.44 |
| 33:DK:7:TYR:HE1 | 33:DK:20:MET:CE | 2.29 | 0.44 |
| 1:AA:515:G:C2 | 1:AA:537:G:N3 | 2.86 | 0.44 |
| 23:DA:772:C:C2' | 23:DA:772:C:O2 | 2.64 | 0.44 |
| 1:AA:762:C:C2 | 1:AA:763:G:C8 | 3.06 | 0.44 |
| 1:CA:1038:C:H2' | 1:CA:1039:C:H6 | 1.82 | 0.44 |
| 28:DF:153:ARG:HB3 | 28:DF:153:ARG:NH1 | 2.32 | 0.44 |
| 26:DD:3:GLY:HA3 | 26:DD:81:ILE:HG21 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BA:1425:G:N2 | 23:BA:1573:G:N7 | 2.65 | 0.44 |
| 36:BN:13:HIS:HE1 | 36:BN:15:SER:HB3 | 1.82 | 0.44 |
| 23:DA:608:A:C4 | 23:DA:621:A:C6 | 3.06 | 0.44 |
| 28:BF:45:GLU:C | 28:BF:47:LYS:H | 2.20 | 0.44 |
| 5:CE:84:PHE:O | 5:CE:86:ALA:N | 2.45 | 0.44 |
| 38:DP:114:LEU:HA | 38:DP:114:LEU:HD23 | 1.54 | 0.44 |
| 10:AJ:89:ASP:C | 10:AJ:91:PRO:HD3 | 2.38 | 0.44 |
| 1:AA:131:C:H2' | 1:AA:132:C:C6 | 2.53 | 0.44 |
| 23:DA:2490:G:H4' | 23:DA:2491:U:OP1 | 2.17 | 0.44 |
| 23:BA:2248:C:C2' | 23:BA:2249:U:H5' | 2.47 | 0.44 |
| 40:BR:95:LEU:HD23 | 40:BR:96:ILE:N | 2.33 | 0.44 |
| 5:AE:137:GLU:OE2 | 5:AE:137:GLU:O | 2.35 | 0.44 |
| 10:CJ:22:LYS:NZ | 10:CJ:88:LEU:HG | 2.33 | 0.44 |
| 23:BA:2230:G:C6 | 23:BA:2231:C:C4 | 3.05 | 0.44 |
| 23:DA:679:C:H2' | 23:DA:680:G:H8 | 1.83 | 0.44 |
| 42:BT:89:ILE:HG22 | 42:BT:91:ALA:HB3 | 1.99 | 0.44 |
| 52:B4:10:ARG:HE | 52:B4:14:LYS:HD2 | 1.82 | 0.44 |
| 32:DJ:121:VAL:HG23 | 32:DJ:122:LEU:N | 2.33 | 0.44 |
| 1:CA:1349:A:P | 9:CI:118:LYS:NZ | 2.91 | 0.44 |
| 1:CA:1369:C:C2' | 1:CA:1370:G:O4' | 2.65 | 0.44 |
| 1:CA:977:A:C2' | 1:CA:978:A:H5'' | 2.47 | 0.44 |
| 38:BP:63:VAL:O | 38:BP:73:GLU:HA | 2.17 | 0.44 |
| 1:AA:952:U:O2' | 1:AA:953:G:H5' | 2.18 | 0.44 |
| 1:CA:501:C:OP2 | 12:CL:123:LYS:HD2 | 2.18 | 0.44 |
| 27:BE:63:LYS:CE | 27:BE:67:GLN:HB3 | 2.48 | 0.44 |
| 23:BA:1902:C:C2' | 23:BA:1903:G:O5' | 2.65 | 0.44 |
| 39:DQ:79:PHE:HE1 | 39:DQ:83:LEU:CD2 | 2.31 | 0.44 |
| 40:DR:2:PHE:HE2 | 40:DR:13:ARG:CG | 2.31 | 0.44 |
| 34:BL:46:LYS:HG2 | 34:BL:52:GLU:CD | 2.38 | 0.44 |
| 30:DH:143:SER:O | 30:DH:145:VAL:HG23 | 2.18 | 0.44 |
| 35:BM:141:GLN:N | 44:BV:53:ILE:HB | 2.29 | 0.44 |
| 26:DD:59:VAL:O | 26:DD:61:ARG:N | 2.51 | 0.44 |
| 52:B4:19:ARG:CG | 52:B4:19:ARG:NH1 | 2.65 | 0.44 |
| 1:CA:436:C:H2' | 1:CA:437:U:H6 | 1.81 | 0.44 |
| 4:CD:137:SER:O | 4:CD:138:TYR:C | 2.55 | 0.44 |
| 23:BA:2376:A:H2' | 23:BA:2377:A:O4' | 2.18 | 0.44 |
| 11:CK:52:GLY:H | 11:CK:55:LYS:HE2 | 1.83 | 0.44 |
| 1:AA:1367:C:N3 | 1:AA:1368:G:N7 | 2.66 | 0.44 |
| 25:DC:175:LEU:HD23 | 25:DC:175:LEU:HA | 1.84 | 0.44 |
| 1:CA:505:G:N3 | 1:CA:506:G:C8 | 2.85 | 0.44 |
| 6:CF:62:TRP:CG | 18:CR:35:ARG:NH1 | 2.86 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:CF:60:PHE:CE2 | 18:CR:78:LEU:HD21 | 2.53 | 0.44 |
| 40:DR:28:GLU:HB2 | 40:DR:31:ALA:HB2 | 1.99 | 0.44 |
| 41:DS:9:TYR:N | 41:DS:102:HIS:CD2 | 2.83 | 0.44 |
| 23:BA:2757:A:H2' | 23:BA:2758:A:H5' | 2.00 | 0.44 |
| 29:BG:23:ARG:H | 29:BG:23:ARG:HD3 | 1.83 | 0.44 |
| 1:AA:340:U:H2' | 1:AA:341:C:C6 | 2.52 | 0.44 |
| 23:BA:8:A:C5 | 23:BA:9:U:O4 | 2.71 | 0.44 |
| 33:DK:115:VAL:O | 33:DK:118:ALA:HB3 | 2.17 | 0.44 |
| 4:CD:92:VAL:HG12 | 4:CD:96:LEU:CD2 | 2.41 | 0.44 |
| 28:DF:133:LEU:HD21 | 28:DF:157:ILE:HG13 | 1.99 | 0.44 |
| 3:AC:58:GLU:O | 3:AC:64:VAL:HA | 2.17 | 0.44 |
| 30:BH:6:LEU:HD23 | 30:BH:6:LEU:N | 2.32 | 0.44 |
| 20:AT:91:LEU:HD23 | 20:AT:91:LEU:HA | 1.67 | 0.44 |
| 23:BA:1434:A:C2 | 23:BA:1435:G:C4 | 3.05 | 0.44 |
| 1:CA:1180:A:H5' | 9:CI:103:THR:HG23 | 2.00 | 0.44 |
| 29:DG:28:GLY:HA3 | 29:DG:79:VAL:HB | 1.99 | 0.44 |
| 1:CA:616:G:N3 | 1:CA:625:G:C2 | 2.85 | 0.44 |
| 23:BA:2596:U:C2' | 23:BA:2597:G:H5' | 2.47 | 0.44 |
| 25:BC:182:LEU:N | 25:BC:272:ALA:CB | 2.80 | 0.44 |
| 1:CA:236:G:H1' | 17:CQ:4:LYS:CE | 2.47 | 0.44 |
| 44:BV:24:LEU:HB2 | 44:BV:41:LEU:HG | 1.97 | 0.44 |
| 30:BH:2:LYS:HG3 | 30:BH:39:ALA:CB | 2.44 | 0.44 |
| 23:DA:333:G:C6 | 23:DA:334:C:C4 | 3.06 | 0.44 |
| 23:BA:2469:A:C2 | 23:BA:2470:G:C5 | 3.05 | 0.44 |
| 25:DC:176:ARG:HH11 | 25:DC:176:ARG:CG | 2.25 | 0.44 |
| 1:AA:939:G:H1 | 1:AA:1344:C:H42 | 1.66 | 0.44 |
| 1:CA:760:G:H2' | 1:CA:761:G:C5' | 2.48 | 0.44 |
| 27:BE:46:ARG:NH1 | 27:BE:46:ARG:HB3 | 2.32 | 0.44 |
| 1:CA:909:A:H3' | 1:CA:910:C:H6 | 1.82 | 0.44 |
| 1:AA:921:U:H5'' | 1:AA:922:G:OP2 | 2.18 | 0.44 |
| 1:CA:1483:A:H1' | 23:DA:1948:G:H1' | 2.00 | 0.44 |
| 1:CA:1483:A:C2 | 23:DA:1959:G:N3 | 2.84 | 0.44 |
| 7:CG:17:VAL:HG12 | 7:CG:18:TYR:CD1 | 2.52 | 0.44 |
| 23:BA:1746:G:N2 | 23:BA:1747:G:C4 | 2.85 | 0.44 |
| 43:BU:46:LYS:O | 43:BU:48:ALA:N | 2.50 | 0.44 |
| 8:CH:36:LEU:C | 8:CH:38:ILE:H | 2.21 | 0.44 |
| 1:AA:381:C:C2 | 1:AA:382:A:C8 | 3.05 | 0.44 |
| 35:BM:43:THR:HG1 | 35:BM:46:GLN:HG3 | 1.81 | 0.44 |
| 1:AA:538:G:OP2 | 12:AL:114:LYS:HB2 | 2.17 | 0.44 |
| 23:DA:2738:A:C2 | 23:DA:2739:U:C6 | 3.06 | 0.44 |
| 23:DA:646:A:H2' | 23:DA:647:G:O4' | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:BA:2001:A:H4' | 23:BA:2689:U:O2' | 2.16 | 0.44 |
| 23:BA:2051:A:H4' | 26:BD:141:ILE:CG2 | 2.48 | 0.44 |
| 33:DK:26:LYS:HB3 | 33:DK:27:GLY:H | 1.65 | 0.44 |
| 23:BA:2572:A:P | 26:BD:144:ARG:HB2 | 2.57 | 0.44 |
| 1:CA:313:A:H2' | 1:CA:314:C:C6 | 2.52 | 0.44 |
| 48:DZ:8:LEU:HD23 | 48:DZ:8:LEU:HA | 1.75 | 0.44 |
| 42:DT:75:ASP:C | 42:DT:76:ARG:HG3 | 2.38 | 0.44 |
| 2:CB:96:ARG:N | 2:CB:96:ARG:HD2 | 2.32 | 0.44 |
| 1:AA:380:G:N2 | 1:AA:384:G:C5 | 2.86 | 0.44 |
| 23:BA:77:C:OP1 | 47:BY:59:ARG:HD3 | 2.16 | 0.44 |
| 23:DA:466:A:O3' | 52:D4:33:ARG:NH1 | 2.50 | 0.44 |
| 23:BA:646:A:H2' | 23:BA:647:G:O5' | 2.17 | 0.44 |
| 23:BA:2823:A:C5 | 23:BA:2824:C:C5 | 3.05 | 0.44 |
| 32:BJ:32:VAL:HG12 | 32:BJ:33:GLU:O | 2.17 | 0.44 |
| 1:AA:1004:A:H2 | 1:AA:1024:G:N3 | 2.15 | 0.44 |
| 1:CA:837:G:H1 | 1:CA:849:C:H42 | 1.65 | 0.44 |
| 1:AA:744:C:C6 | 1:AA:744:C:C3' | 3.01 | 0.44 |
| 1:CA:1272:G:H2' | 1:CA:1273:G:H8 | 1.82 | 0.44 |
| 23:BA:1422:G:C6 | 23:BA:1423:G:C5 | 3.06 | 0.44 |
| 8:AH:69:ARG:HA | 8:AH:69:ARG:HD3 | 1.79 | 0.44 |
| 30:DH:25:TYR:CD1 | 30:DH:30:LEU:HD11 | 2.52 | 0.44 |
| 13:AM:116:THR:O | 13:AM:117:VAL:O | 2.36 | 0.44 |
| 23:DA:2082:A:H2' | 23:DA:2083:G:O4' | 2.17 | 0.44 |
| 26:BD:153:GLY:O | 26:BD:154:LYS:C | 2.55 | 0.44 |
| 23:BA:1001:A:H2' | 23:BA:1002:G:O4' | 2.16 | 0.44 |
| 23:DA:270(W):G:C4 | 23:DA:270(X):G:C8 | 3.06 | 0.44 |
| 23:DA:38:A:H2' | 23:DA:39:C:C6 | 2.52 | 0.44 |
| 3:AC:61:ALA:O | 3:AC:62:ASP:HB2 | 2.18 | 0.44 |
| 32:DJ:41:ALA:HB3 | 32:DJ:79:ASN:O | 2.18 | 0.44 |
| 27:DE:140:LEU:HD12 | 27:DE:140:LEU:HA | 1.80 | 0.44 |
| 34:BL:100:LEU:HD22 | 34:BL:100:LEU:H | 1.82 | 0.44 |
| 38:BP:14:TYR:H | 38:BP:14:TYR:HD1 | 1.64 | 0.44 |
| 11:CK:81:ASP:OD1 | 11:CK:106:LYS:HB3 | 2.18 | 0.44 |
| 23:BA:307:G:N1 | 23:BA:310:A:OP2 | 2.50 | 0.44 |
| 43:DU:71:LYS:NZ | 43:DU:71:LYS:HB2 | 2.32 | 0.44 |
| 1:CA:961:U:OP2 | 1:CA:1223:C:C1' | 2.66 | 0.44 |
| 1:CA:977:A:H2' | 1:CA:978:A:H5'' | 2.00 | 0.44 |
| 1:CA:979:C:C5 | 1:CA:980:C:C6 | 3.05 | 0.44 |
| 5:AE:101:ILE:HD11 | 5:AE:119:LEU:CD2 | 2.23 | 0.44 |
| 27:DE:164:ARG:HA | 27:DE:175:THR:OG1 | 2.17 | 0.44 |
| 53:D5:11:LYS:HD2 | 53:D5:64:TYR:CE2 | 2.52 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DA:195:A:N7 | 23:DA:197:A:OP1 | 2.51 | 0.44 |
| 30:BH:68:LEU:O | 30:BH:72:LEU:HB2 | 2.17 | 0.44 |
| 34:BL:50:ARG:CD | 34:BL:51:PHE:N | 2.79 | 0.44 |
| 25:DC:155:LEU:CD1 | 25:DC:155:LEU:N | 2.80 | 0.44 |
| 1:AA:411:A:N6 | 1:AA:413:G:N3 | 2.66 | 0.44 |
| 4:CD:141:ARG:O | 4:CD:144:ASP:OD2 | 2.36 | 0.44 |
| 1:AA:689:C:H2' | 1:AA:689:C:O2 | 2.16 | 0.44 |
| 30:DH:100:ALA:O | 30:DH:104:GLN:HG3 | 2.17 | 0.44 |
| 1:CA:91:C:C2 | 1:CA:92:G:N7 | 2.86 | 0.44 |
| 1:CA:93:U:C2' | 1:CA:95:G:C8 | 2.98 | 0.44 |
| 26:DD:77:ILE:HD13 | 26:DD:195:LEU:CD1 | 2.42 | 0.44 |
| 42:BT:35:THR:HB | 42:BT:38:GLU:H | 1.83 | 0.44 |
| 1:CA:41:G:O6 | 1:CA:401:C:N3 | 2.51 | 0.44 |
| 1:AA:266:G:C5' | 1:AA:267:C:C5 | 2.94 | 0.44 |
| 36:BN:2:ARG:O | 36:BN:3:HIS:CG | 2.71 | 0.44 |
| 46:BX:27:GLU:HB3 | 46:BX:33:LYS:HG3 | 1.97 | 0.44 |
| 38:DP:53:ARG:CG | 38:DP:53:ARG:HH11 | 2.16 | 0.44 |
| 23:BA:379:G:C5 | 23:BA:380:U:C5 | 3.05 | 0.44 |
| 23:BA:1587:A:C5 | 23:BA:1588:C:C4 | 3.06 | 0.44 |
| 27:BE:68:LYS:O | 27:BE:70:THR:N | 2.49 | 0.44 |
| 42:DT:21:PHE:O | 42:DT:23:GLU:O | 2.36 | 0.44 |
| 10:CJ:13:HIS:CB | 10:CJ:68:HIS:NE2 | 2.80 | 0.44 |
| 23:BA:661:C:H5'' | 34:BL:18:ARG:HD3 | 2.00 | 0.44 |
| 28:BF:131:TYR:HD2 | 28:BF:133:LEU:HD22 | 1.82 | 0.44 |
| 1:CA:370:C:C2' | 1:CA:371:G:H5' | 2.48 | 0.44 |
| 1:AA:68:G:C6 | 1:AA:69:G:C5 | 3.06 | 0.44 |
| 23:BA:1477:A:C4 | 23:BA:1478:G:C8 | 3.06 | 0.44 |
| 25:BC:25:THR:HG21 | 25:BC:81:ALA:HB1 | 2.00 | 0.44 |
| 26:DD:37:ARG:NH1 | 26:DD:42:ASP:OD1 | 2.51 | 0.44 |
| 11:AK:21:ILE:HG13 | 11:AK:30:VAL:CG1 | 2.46 | 0.44 |
| 44:DV:179:ASP:O | 44:DV:182:LYS:HB2 | 2.18 | 0.44 |
| 1:CA:658:G:N1 | 1:CA:749:C:C4 | 2.85 | 0.44 |
| 23:BA:947:G:N3 | 23:BA:984:A:H2 | 2.16 | 0.44 |
| 25:DC:30:GLU:HG3 | 25:DC:63:ARG:NE | 2.32 | 0.44 |
| 23:DA:2467:C:H4' | 35:DM:123:HIS:ND1 | 2.32 | 0.44 |
| 1:CA:512:U:H3 | 1:CA:539:A:H61 | 1.65 | 0.44 |
| 34:BL:84:ASN:HB3 | 34:BL:86:LYS:HG2 | 2.00 | 0.44 |
| 10:CJ:49:VAL:CG2 | 14:CN:41:ARG:HB3 | 2.47 | 0.44 |
| 23:BA:2705:A:H2' | 23:BA:2706:G:O4' | 2.18 | 0.44 |
| 7:CG:16:LEU:O | 7:CG:17:VAL:HG23 | 2.17 | 0.44 |
| 8:CH:40:ALA:HB2 | 8:CH:45:ILE:HD11 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BA:2889:C:H2' | 23:BA:2891:G:H8 | 1.83 | 0.44 |
| 23:BA:2853:C:H2' | 23:BA:2854:G:C8 | 2.51 | 0.44 |
| 29:BG:62:LYS:O | 29:BG:63:SER:C | 2.56 | 0.44 |
| 47:BY:50:ILE:O | 47:BY:51:ARG:C | 2.55 | 0.44 |
| 40:DR:12:TYR:N | 40:DR:12:TYR:CD2 | 2.85 | 0.44 |
| 1:CA:186(D):G:N1 | 1:CA:186(E):C:C4 | 2.86 | 0.44 |
| 2:AB:20:GLU:OE1 | 2:AB:20:GLU:HA | 2.17 | 0.44 |
| 2:AB:35:GLU:HG3 | 2:AB:40:HIS:HA | 2.00 | 0.44 |
| 23:BA:903:C:O2' | 23:BA:904:C:H5' | 2.17 | 0.44 |
| 1:CA:358:U:H2' | 1:CA:358:U:O2 | 2.16 | 0.44 |
| 23:DA:886:C:C2' | 23:DA:887:A:H4' | 2.47 | 0.44 |
| 1:CA:926:G:C6 | 1:CA:1505:G:C6 | 3.05 | 0.44 |
| 23:BA:2039:C:H2' | 23:BA:2040:C:C6 | 2.50 | 0.44 |
| 23:DA:926:A:H2' | 23:DA:928:G:H8 | 1.83 | 0.44 |
| 1:CA:479:C:C2 | 1:CA:480:U:C6 | 3.05 | 0.44 |
| 51:D3:44:ARG:O | 51:D3:45:LYS:HG2 | 2.18 | 0.44 |
| 23:BA:1027:A:N6 | 23:BA:1126:A:N9 | 2.66 | 0.44 |
| 23:DA:463:G:H5'' | 23:DA:464:U:OP2 | 2.17 | 0.44 |
| 27:BE:112:MET:HA | 27:BE:115:ALA:HB3 | 1.99 | 0.44 |
| 23:BA:192:C:H5'' | 23:BA:193:U:OP2 | 2.17 | 0.44 |
| 23:DA:1368:G:N3 | 23:DA:1369:G:C8 | 2.85 | 0.44 |
| 1:AA:740:U:O2' | 1:AA:741:G:H5' | 2.18 | 0.44 |
| 23:DA:2506:U:C5 | 23:DA:2507:C:H5 | 2.35 | 0.44 |
| 23:BA:621:A:H5' | 23:BA:622:G:OP2 | 2.17 | 0.44 |
| 10:CJ:30:SER:HB2 | 10:CJ:80:LYS:HG3 | 1.99 | 0.44 |
| 1:CA:1037:C:H2' | 1:CA:1038:C:C6 | 2.53 | 0.44 |
| 23:BA:298:G:H5'' | 23:BA:299:A:OP1 | 2.18 | 0.44 |
| 1:AA:744:C:H6 | 1:AA:744:C:O5' | 2.01 | 0.44 |
| 44:BV:146:ILE:HG23 | 44:BV:174:VAL:HG12 | 1.99 | 0.44 |
| 15:AO:35:ARG:C | 15:AO:59:MET:HE1 | 2.38 | 0.44 |
| 10:CJ:78:ASN:O | 10:CJ:82:ILE:HG12 | 2.18 | 0.44 |
| 23:DA:1803:A:H2 | 23:DA:1822:G:N3 | 2.15 | 0.44 |
| 23:DA:649:G:H2' | 23:DA:650:C:C6 | 2.52 | 0.44 |
| 41:BS:63:ASP:C | 41:BS:63:ASP:OD2 | 2.56 | 0.44 |
| 23:DA:2248:C:H2' | 23:DA:2249:U:O4' | 2.16 | 0.44 |
| 23:DA:1956:U:H1' | 23:DA:2552:U:OP1 | 2.17 | 0.44 |
| 53:D5:15:LYS:HG3 | 53:D5:16:ILE:N | 2.32 | 0.44 |
| 38:DP:13:ARG:C | 38:DP:15:VAL:H | 2.20 | 0.44 |
| 34:DL:114:ILE:CD1 | 34:DL:130:PHE:CE1 | 2.97 | 0.44 |
| 52:B4:9:ARG:O | 52:B4:10:ARG:C | 2.52 | 0.44 |
| 24:BB:82:G:C4 | 24:BB:83:G:C8 | 3.06 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:BC:145:VAL:HB | 25:BC:155:LEU:HB2 | 1.99 | 0.44 |
| 23:DA:1177:A:H5'' | 23:DA:1178:C:OP2 | 2.18 | 0.44 |
| 28:DF:60:LEU:HA | 28:DF:63:ILE:HD11 | 1.99 | 0.44 |
| 1:CA:1347:G:C8 | 9:CI:107:ARG:O | 2.71 | 0.44 |
| 1:AA:961:U:OP2 | 1:AA:1223:C:H1' | 2.17 | 0.44 |
| 26:BD:24:THR:HG23 | 26:BD:184:VAL:HG23 | 1.99 | 0.44 |
| 1:CA:961:U:OP2 | 1:CA:1223:C:H1' | 2.18 | 0.44 |
| 23:BA:2293:C:H5'' | 37:BO:89:ARG:NH1 | 2.33 | 0.44 |
| 23:DA:861:A:C2 | 23:DA:917:A:C4 | 3.05 | 0.44 |
| 25:BC:238:GLY:C | 25:BC:239:ARG:O | 2.53 | 0.44 |
| 28:DF:72:ARG:HD3 | 28:DF:86:MET:HA | 2.00 | 0.44 |
| 1:CA:673:G:C4 | 1:CA:734:G:C2 | 3.06 | 0.44 |
| 25:DC:105:ILE:HD11 | 25:DC:192:THR:HG21 | 1.99 | 0.44 |
| 1:AA:397:A:N6 | 1:AA:548:G:N7 | 2.66 | 0.44 |
| 1:AA:429:U:OP1 | 4:AD:9:CYS:O | 2.35 | 0.44 |
| 1:CA:76:G:C6 | 1:CA:77:C:C4 | 3.05 | 0.44 |
| 24:BB:41:U:OP1 | 24:BB:42:C:H5 | 1.99 | 0.44 |
| 3:CC:29:TYR:HE1 | 3:CC:33:LEU:HD22 | 1.83 | 0.44 |
| 1:AA:367:U:C6 | 1:AA:394:G:C2 | 3.06 | 0.44 |
| 47:DY:57:ILE:HA | 47:DY:60:LEU:HB2 | 2.00 | 0.44 |
| 49:B1:60:GLU:CD | 49:B1:60:GLU:N | 2.71 | 0.44 |
| 24:BB:71:C:N3 | 24:BB:72:G:C8 | 2.86 | 0.44 |
| 24:BB:9:G:C6 | 24:BB:10:C:C4 | 3.06 | 0.44 |
| 19:CS:63:THR:HG23 | 19:CS:65:ASN:N | 2.33 | 0.44 |
| 45:BW:31:VAL:HG13 | 45:BW:65:GLY:O | 2.17 | 0.44 |
| 20:CT:57:ARG:C | 20:CT:59:ALA:N | 2.70 | 0.44 |
| 24:DB:106:G:C2' | 24:DB:107:U:H5' | 2.48 | 0.44 |
| 23:DA:2746:U:H2' | 23:DA:2747:G:C5' | 2.47 | 0.44 |
| 12:AL:44:PRO:CD | 12:AL:50:ALA:H | 2.31 | 0.44 |
| 23:BA:99:U:C6 | 23:BA:102:G:N1 | 2.85 | 0.44 |
| 40:BR:88:ARG:H | 40:BR:88:ARG:HG3 | 1.59 | 0.44 |
| 23:DA:998:C:H2' | 23:DA:999:U:O4' | 2.18 | 0.44 |
| 23:DA:2287:A:N1 | 23:DA:2346:A:H2 | 2.15 | 0.44 |
| 23:DA:1132:A:C2' | 23:DA:1133:U:H5' | 2.48 | 0.44 |
| 23:DA:479:A:H4' | 23:DA:480:A:O5' | 2.17 | 0.44 |
| 9:CI:114:TYR:HE1 | 10:CJ:60:ARG:O | 2.00 | 0.44 |
| 1:CA:659:U:C2' | 1:CA:660:G:H5' | 2.48 | 0.44 |
| 46:BX:23:LYS:CG | 46:BX:23:LYS:O | 2.65 | 0.44 |
| 1:AA:708:C:O2' | 1:AA:709:G:H5' | 2.17 | 0.44 |
| 1:AA:235:C:H2' | 1:AA:236:G:H8 | 1.83 | 0.44 |
| 29:DG:54:ARG:HA | 29:DG:55:PRO:HD2 | 1.70 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:942:G:H21 | 9:AI:124:GLN:NE2 | 2.16 | 0.44 |
| 1:AA:650:G:C2 | 1:AA:651:C:C6 | 3.06 | 0.44 |
| 36:BN:79:LEU:HD23 | 36:BN:79:LEU:HA | 1.71 | 0.44 |
| 23:DA:1746:G:C2 | 23:DA:1747:G:C5 | 3.06 | 0.44 |
| 1:CA:255:G:H5' | 17:CQ:16:GLN:O | 2.17 | 0.44 |
| 1:CA:1077:G:C2 | 1:CA:1081:G:C5 | 3.05 | 0.44 |
| 18:AR:74:ARG:H | 18:AR:74:ARG:HG3 | 1.49 | 0.44 |
| 8:CH:64:LYS:CG | 8:CH:79:VAL:HG21 | 2.45 | 0.44 |
| 43:BU:68:HIS:C | 43:BU:70:SER:N | 2.71 | 0.44 |
| 1:CA:1428:A:H2' | 1:CA:1429:C:C6 | 2.53 | 0.44 |
| 7:AG:17:VAL:HG12 | 7:AG:18:TYR:CD1 | 2.52 | 0.44 |
| 1:AA:186(E):C:H2' | 1:AA:186(F):C:C6 | 2.53 | 0.44 |
| 1:AA:936:C:H2' | 1:AA:937:A:O4' | 2.18 | 0.44 |
| 1:CA:1112:C:C5 | 3:CC:178:LEU:HD23 | 2.53 | 0.44 |
| 28:DF:58:GLN:O | 28:DF:61:ALA:HB3 | 2.18 | 0.44 |
| 23:BA:853:G:H1 | 23:BA:924:C:H42 | 1.65 | 0.44 |
| 2:CB:158:LEU:HD12 | 2:CB:158:LEU:N | 2.32 | 0.44 |
| 1:CA:1408:A:O2' | 1:CA:1409:C:H5' | 2.17 | 0.44 |
| 23:DA:2867:G:O6 | 38:DP:23:ARG:HD3 | 2.17 | 0.44 |
| 23:BA:189:G:H3' | 23:BA:189:G:C8 | 2.53 | 0.44 |
| 23:BA:2572:A:H2' | 26:BD:144:ARG:HG3 | 2.00 | 0.44 |
| 44:DV:14:LYS:HB2 | 44:DV:17:ALA:HB3 | 1.99 | 0.44 |
| 1:AA:634:C:H2' | 1:AA:635:G:H8 | 1.82 | 0.44 |
| 23:BA:914:C:C5 | 23:BA:915:C:C6 | 3.05 | 0.44 |
| 33:DK:59:LYS:O | 33:DK:86:ILE:HG23 | 2.17 | 0.44 |
| 1:CA:439:A:C8 | 1:CA:440:A:C8 | 3.06 | 0.44 |
| 7:AG:78:ARG:HG2 | 7:AG:79:ARG:N | 2.33 | 0.44 |
| 2:AB:17:PHE:CG | 2:AB:44:LEU:HD21 | 2.52 | 0.44 |
| 23:DA:841:A:C2 | 23:DA:938:G:N3 | 2.86 | 0.44 |
| 23:DA:2342:C:O2 | 23:DA:2374:C:H4' | 2.18 | 0.44 |
| 23:BA:36:G:H4' | 23:BA:451:C:C2 | 2.53 | 0.44 |
| 1:AA:451:A:C5 | 1:AA:481:G:C5 | 3.05 | 0.44 |
| 23:BA:1523:U:H2' | 23:BA:1524:G:C8 | 2.53 | 0.44 |
| 4:CD:88:VAL:HG13 | 5:CE:97:GLY:HA3 | 1.99 | 0.44 |
| 30:DH:31:LEU:HA | 30:DH:31:LEU:HD13 | 1.73 | 0.44 |
| 7:AG:111:ARG:CZ | 7:AG:122:HIS:HB3 | 2.48 | 0.44 |
| 23:DA:2692:C:H2' | 23:DA:2693:A:O4' | 2.18 | 0.44 |
| 26:DD:116:VAL:HG13 | 26:DD:122:PHE:CD2 | 2.53 | 0.44 |
| 32:BJ:41:ALA:O | 32:BJ:44:LYS:HG2 | 2.17 | 0.44 |
| 20:CT:41:VAL:O | 20:CT:44:ALA:HB3 | 2.18 | 0.44 |
| 12:CL:36:CYS:SG | 12:CL:80:SER:HB2 | 2.58 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1141:C:H2' | 1:AA:1142:G:H8 | 1.83 | 0.44 |
| 34:DL:21:ARG:H | 34:DL:21:ARG:HG2 | 1.60 | 0.44 |
| 39:DQ:84:LYS:HA | 39:DQ:84:LYS:HD3 | 1.89 | 0.44 |
| 22:AV:6212:U:H2' | 22:AV:6212:U:O2 | 2.17 | 0.44 |
| 18:AR:23:LYS:C | 18:AR:25:THR:H | 2.20 | 0.44 |
| 23:BA:2462:U:H2' | 23:BA:2463:C:O4' | 2.18 | 0.44 |
| 23:BA:960:A:H61 | 35:BM:82:ARG:NH2 | 2.15 | 0.44 |
| 23:BA:1530:G:C6 | 23:BA:1531:C:C4 | 3.06 | 0.44 |
| 32:DJ:114:LEU:HA | 32:DJ:118:PRO:CB | 2.46 | 0.44 |
| 1:AA:960:U:C5 | 1:AA:1225:A:C8 | 3.06 | 0.44 |
| 1:AA:977:A:C2' | 1:AA:978:A:H5'' | 2.48 | 0.44 |
| 13:AM:91:ARG:NH2 | 13:AM:96:LEU:HB3 | 2.33 | 0.44 |
| 22:AV:6193:U:C5 | 22:AV:6194:C:C5 | 3.06 | 0.44 |
| 36:BN:11:ASN:O | 36:BN:12:ARG:CB | 2.64 | 0.44 |
| 25:BC:10:THR:CG2 | 25:BC:13:ARG:CB | 2.90 | 0.44 |
| 23:DA:2846:G:C6 | 23:DA:2847:U:C4 | 3.05 | 0.44 |
| 1:CA:47:C:H5'' | 1:CA:365:U:C6 | 2.53 | 0.44 |
| 32:DJ:36:TRP:HB2 | 32:DJ:156:GLN:CB | 2.48 | 0.44 |
| 23:DA:242:G:H5' | 53:D5:63:PRO:CB | 2.48 | 0.44 |
| 39:BQ:105:VAL:CG1 | 40:BR:40:LEU:HD13 | 2.47 | 0.44 |
| 39:BQ:104:GLN:HB3 | 40:BR:44:LYS:CE | 2.48 | 0.44 |
| 23:BA:242:G:C8 | 53:B5:5:LYS:HG2 | 2.53 | 0.44 |
| 34:BL:49:ARG:O | 34:BL:51:PHE:N | 2.50 | 0.44 |
| 28:DF:161:THR:CG2 | 28:DF:172:LEU:HD23 | 2.47 | 0.44 |
| 16:AP:34:GLU:OE1 | 16:AP:55:ARG:NH1 | 2.51 | 0.44 |
| 1:AA:406:G:OP1 | 4:AD:5:ILE:HG21 | 2.18 | 0.44 |
| 3:CC:182:ILE:CG1 | 3:CC:203:PHE:HD1 | 2.30 | 0.44 |
| 4:CD:106:TYR:O | 4:CD:109:GLY:N | 2.46 | 0.44 |
| 26:BD:84:PHE:C | 26:BD:84:PHE:CD2 | 2.91 | 0.44 |
| 23:DA:1188:U:H2' | 23:DA:1189:A:H5' | 2.00 | 0.44 |
| 24:DB:43:C:H2' | 24:DB:44:G:H5'' | 1.99 | 0.44 |
| 5:CE:33:VAL:HG12 | 5:CE:34:VAL:N | 2.32 | 0.44 |
| 44:BV:92:SER:HB2 | 44:BV:94:GLU:CD | 2.38 | 0.44 |
| 5:AE:129:ILE:O | 5:AE:132:ALA:HB3 | 2.18 | 0.44 |
| 12:AL:69:ILE:HA | 12:AL:70:PRO:HD3 | 1.69 | 0.44 |
| 1:AA:1064:G:O4' | 1:AA:1066:C:C6 | 2.70 | 0.44 |
| 1:AA:130:A:H5'' | 1:AA:190:G:O2' | 2.18 | 0.44 |
| 46:DX:45:ASN:HD22 | 46:DX:46:LEU:H | 1.63 | 0.44 |
| 1:AA:1201:A:C2' | 1:AA:1202:G:OP2 | 2.66 | 0.44 |
| 10:CJ:32:ALA:HB3 | 10:CJ:76:ASN:CB | 2.37 | 0.44 |
| 1:CA:53:A:C2 | 1:CA:54:C:C1' | 3.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:BH:110:ASP:HB3 | 30:BH:111:PRO:HD2 | 1.99 | 0.44 |
| 29:DG:74:ASN:ND2 | 29:DG:138:LYS:HD2 | 2.32 | 0.44 |
| 12:AL:43:THR:HA | 12:AL:44:PRO:HD3 | 1.72 | 0.44 |
| 23:DA:2304:G:H5' | 23:DA:2305:A:OP2 | 2.18 | 0.44 |
| 23:BA:1497:U:H5' | 23:BA:1498:C:H5 | 1.83 | 0.44 |
| 23:BA:1884:A:C4 | 23:BA:1885:A:C8 | 3.06 | 0.44 |
| 4:CD:158:ILE:HG22 | 4:CD:159:ARG:N | 2.32 | 0.44 |
| 23:DA:589:C:O3' | 27:DE:95:ARG:NH1 | 2.51 | 0.44 |
| 45:DW:36:ILE:HD12 | 45:DW:58:THR:CG2 | 2.41 | 0.44 |
| 1:AA:67:C:O2' | 1:AA:171:A:H1' | 2.18 | 0.44 |
| 23:BA:385:C:HO2' | 23:BA:390:A:H2 | 1.65 | 0.44 |
| 23:BA:256:A:H2' | 23:BA:257:A:H5' | 1.97 | 0.44 |
| 10:AJ:27:ALA:HB1 | 10:AJ:34:VAL:HG21 | 2.00 | 0.44 |
| 23:DA:259:G:C2 | 23:DA:260:G:C8 | 3.06 | 0.44 |
| 1:CA:236:G:C6 | 1:CA:237:C:C4 | 3.06 | 0.44 |
| 23:BA:2469:A:C8 | 23:BA:2482:G:C4 | 3.06 | 0.44 |
| 44:DV:182:LYS:O | 44:DV:186:GLU:HB2 | 2.18 | 0.44 |
| 13:CM:71:ARG:O | 13:CM:74:VAL:HB | 2.17 | 0.44 |
| 23:BA:1389:G:C2 | 23:BA:1399:C:O2 | 2.71 | 0.44 |
| 23:DA:2479:G:H5'' | 23:DA:2537:U:O4' | 2.17 | 0.44 |
| 28:BF:178:PHE:O | 28:BF:180:PHE:CD1 | 2.71 | 0.44 |
| 33:BK:25:LEU:HD23 | 33:BK:25:LEU:HA | 1.69 | 0.44 |
| 36:BN:78:LYS:O | 36:BN:83:ILE:HG12 | 2.18 | 0.44 |
| 23:DA:1138:G:O2' | 32:DJ:128:GLY:HA3 | 2.17 | 0.44 |
| 23:BA:2275:C:C5' | 23:BA:2275:C:H6 | 2.29 | 0.44 |
| 1:CA:193:C:O4' | 20:CT:60:GLU:OE2 | 2.36 | 0.44 |
| 23:DA:150:C:H2' | 23:DA:151:C:C6 | 2.53 | 0.44 |
| 23:BA:1930:G:O2' | 23:BA:1931:U:OP2 | 2.31 | 0.44 |
| 23:BA:136:G:H2' | 23:BA:137(A):C:H6 | 1.83 | 0.44 |
| 10:CJ:6:ILE:HG12 | 10:CJ:72:VAL:O | 2.17 | 0.44 |
| 15:CO:61:GLY:O | 15:CO:64:ARG:N | 2.51 | 0.44 |
| 7:CG:148:ASN:C | 7:CG:150:ALA:N | 2.70 | 0.44 |
| 1:AA:356:A:C2' | 1:AA:357:G:O5' | 2.65 | 0.44 |
| 2:CB:17:PHE:CE1 | 2:CB:44:LEU:HD11 | 2.53 | 0.44 |
| 23:DA:718:A:H2' | 23:DA:719:C:H5' | 1.99 | 0.44 |
| 23:DA:2065:C:H2' | 23:DA:2066:C:C6 | 2.52 | 0.44 |
| 35:DM:24:GLY:HA2 | 35:DM:101:ARG:HA | 1.99 | 0.44 |
| 41:DS:62:HIS:O | 41:DS:64:MET:N | 2.47 | 0.44 |
| 23:BA:532:A:C8 | 23:BA:2021:C:C5 | 3.06 | 0.44 |
| 2:AB:17:PHE:CE1 | 2:AB:44:LEU:HD11 | 2.52 | 0.44 |
| 11:CK:38:ASN:HA | 11:CK:39:PRO:HD2 | 1.74 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:DA:900:A:H2' | 23:DA:901:A:O4' | 2.17 | 0.44 |
| 23:BA:772:C:C2' | 23:BA:772:C:O2 | 2.65 | 0.44 |
| 23:BA:1382:G:H4' | 23:BA:1573:G:C2 | 2.53 | 0.44 |
| 1:AA:452:A:C4 | 1:AA:453:A:C8 | 3.05 | 0.44 |
| 23:BA:1665:A:H2' | 23:BA:1666:G:O4' | 2.18 | 0.44 |
| 23:DA:2849:U:OP2 | 38:DP:95:ARG:NH1 | 2.44 | 0.44 |
| 1:AA:803:G:H2' | 1:AA:804:U:O4' | 2.17 | 0.44 |
| 23:BA:270(F):G:C6 | 23:BA:270(G):U:C4 | 3.05 | 0.44 |
| 1:CA:581:G:O2' | 1:CA:582:U:H5' | 2.16 | 0.44 |
| 25:DC:214:TRP:C | 25:DC:216:GLY:H | 2.21 | 0.44 |
| 25:DC:122:ASP:CG | 25:DC:123:ALA:N | 2.71 | 0.44 |
| 23:BA:2672:G:H2' | 23:BA:2673:G:O5' | 2.17 | 0.44 |
| 23:BA:2676:C:C2' | 23:BA:2677:G:H5' | 2.47 | 0.44 |
| 10:CJ:26:ALA:HB1 | 10:CJ:84:GLN:HG2 | 2.00 | 0.44 |
| 46:BX:35:THR:HB | 46:BX:36:GLY:H | 1.49 | 0.44 |
| 1:CA:1001:G:H2' | 1:CA:1002:G:O4' | 2.18 | 0.44 |
| 23:DA:606:U:H4' | 23:DA:658:C:H4' | 2.00 | 0.44 |
| 27:DE:33:LEU:HD12 | 27:DE:33:LEU:HA | 1.66 | 0.44 |
| 51:B3:36:LEU:N | 51:B3:36:LEU:HD23 | 2.32 | 0.44 |
| 23:BA:1693:U:H4' | 23:BA:1694:C:OP2 | 2.18 | 0.44 |
| 49:D1:53:THR:C | 49:D1:54:LYS:HD2 | 2.38 | 0.44 |
| 44:BV:75:ASN:O | 44:BV:84:GLU:HB2 | 2.18 | 0.44 |
| 48:BZ:1:MET:HB3 | 48:BZ:39:ASP:HB3 | 2.00 | 0.44 |
| 23:DA:630:G:H22 | 23:DA:632:A:H3' | 1.81 | 0.44 |
| 23:DA:1173:G:O5' | 23:DA:1173:G:H8 | 2.01 | 0.44 |
| 2:AB:61:LEU:HG | 2:AB:68:ILE:CG1 | 2.47 | 0.44 |
| 22:CV:6188:G:O2' | 22:CV:6189:G:H5' | 2.17 | 0.44 |
| 23:DA:2282:G:H4' | 23:DA:2389:G:O2' | 2.18 | 0.44 |
| 1:CA:946:A:C6 | 1:CA:1236:A:C2 | 3.06 | 0.44 |
| 1:CA:503:C:OP1 | 12:CL:118:LYS:CE | 2.65 | 0.44 |
| 12:CL:30:PRO:HD2 | 12:CL:31:PHE:H | 1.83 | 0.44 |
| 23:DA:587:C:C2 | 34:DL:33:ARG:HD3 | 2.53 | 0.44 |
| 47:DY:17:SER:HB3 | 47:DY:18:PRO:CD | 2.37 | 0.44 |
| 28:BF:72:ARG:HD3 | 28:BF:86:MET:HA | 2.00 | 0.44 |
| 50:D2:16:ARG:HG2 | 50:D2:17:ASP:N | 2.31 | 0.44 |
| 30:BH:81:VAL:HG12 | 30:BH:90:GLY:N | 2.33 | 0.44 |
| 34:BL:47:ASP:HB3 | 34:BL:51:PHE:CB | 2.47 | 0.44 |
| 13:CM:37:THR:OG1 | 13:CM:56:LEU:HD23 | 2.18 | 0.44 |
| 23:BA:1414:G:H2' | 23:BA:1415:U:C6 | 2.51 | 0.44 |
| 26:BD:50:GLY:HA3 | 26:BD:75:VAL:HG11 | 2.00 | 0.44 |
| 26:DD:92:THR:O | 26:DD:95:ILE:HG12 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DA:2687:U:C4 | 23:DA:2688:U:H5 | 2.31 | 0.44 |
| 45:BW:73:GLY:O | 45:BW:74:ARG:C | 2.56 | 0.44 |
| 24:DB:50:G:OP1 | 37:DO:63:THR:OG1 | 2.36 | 0.44 |
| 23:DA:2767:C:C2' | 23:DA:2768:C:H5' | 2.48 | 0.44 |
| 23:DA:850:C:O2' | 48:DZ:46:ASN:ND2 | 2.51 | 0.44 |
| 41:BS:23:LEU:HD12 | 41:BS:23:LEU:HA | 1.79 | 0.44 |
| 1:CA:1293:G:O2' | 1:CA:1294:G:H5' | 2.18 | 0.44 |
| 1:CA:693:G:H2' | 1:CA:694:A:C8 | 2.53 | 0.44 |
| 12:AL:44:PRO:CG | 12:AL:52:ARG:HE | 2.29 | 0.44 |
| 23:DA:2305:A:H1' | 28:DF:135:LEU:O | 2.18 | 0.44 |
| 23:BA:2722:G:C5 | 23:BA:2723:C:C4 | 3.06 | 0.44 |
| 23:BA:2563:U:O2 | 23:BA:2565:A:C8 | 2.71 | 0.44 |
| 5:CE:53:LEU:CD2 | 5:CE:53:LEU:H | 2.24 | 0.44 |
| 23:DA:849:A:O2' | 48:DZ:17:LYS:HE3 | 2.17 | 0.44 |
| 8:CH:25:ASP:HA | 8:CH:59:LEU:O | 2.18 | 0.44 |
| 37:BO:104:GLY:HA2 | 37:BO:107:GLU:CG | 2.40 | 0.44 |
| 23:BA:966:G:C5 | 23:BA:967:C:H5 | 2.35 | 0.44 |
| 18:AR:54:ARG:H | 18:AR:54:ARG:CD | 2.24 | 0.44 |
| 23:DA:997:G:OP1 | 39:DQ:93:LYS:HD2 | 2.18 | 0.44 |
| 32:DJ:64:ASP:O | 32:DJ:71:MET:HE1 | 2.17 | 0.44 |
| 4:AD:79:PHE:C | 4:AD:79:PHE:CD2 | 2.91 | 0.44 |
| 23:DA:2287:A:HO2' | 23:DA:2288:A:C5' | 2.30 | 0.44 |
| 23:BA:2074:U:O2' | 23:BA:2597:G:H1' | 2.18 | 0.44 |
| 1:AA:104:G:N3 | 1:AA:105:G:C8 | 2.86 | 0.44 |
| 44:BV:58:VAL:CG1 | 44:BV:66:SER:HB2 | 2.48 | 0.44 |
| 23:BA:1820:U:H4' | 23:BA:1821:A:OP2 | 2.18 | 0.44 |
| 27:DE:117:ARG:HH21 | 27:DE:187:VAL:HA | 1.82 | 0.44 |
| 32:BJ:66:THR:HB | 32:BJ:69:VAL:HG11 | 2.00 | 0.44 |
| 1:CA:1441:G:H5' | 1:CA:1442:G:O5' | 2.17 | 0.44 |
| 23:DA:1800:C:OP2 | 25:DC:183:ARG:NH2 | 2.47 | 0.44 |
| 1:CA:865:A:H2 | 1:CA:918:A:H4' | 1.82 | 0.44 |
| 23:DA:1592:C:O2' | 23:DA:1593:G:H5' | 2.18 | 0.44 |
| 23:BA:118:A:N3 | 23:BA:178:G:H1' | 2.33 | 0.44 |
| 1:AA:592:G:H2' | 1:AA:593:G:H8 | 1.82 | 0.44 |
| 1:CA:565:U:C4 | 1:CA:566:G:C5 | 3.06 | 0.44 |
| 23:DA:245:G:C5 | 23:DA:246:C:C5 | 3.06 | 0.44 |
| 44:DV:121:HIS:C | 44:DV:123:ASP:H | 2.22 | 0.44 |
| 23:DA:2861:G:C2 | 23:DA:2862:G:C8 | 3.05 | 0.44 |
| 27:DE:110:LEU:HD12 | 27:DE:110:LEU:HA | 1.70 | 0.44 |
| 1:CA:1160:G:O2' | 1:CA:1161:C:H5' | 2.17 | 0.44 |
| 23:DA:2837:G:C4 | 23:DA:2838:G:C8 | 3.06 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 10:CJ:6:ILE:HG22 | 10:CJ:98:ILE:HG12 | 1.99 | 0.44 |
| 1:CA:826:C:H5'' | 1:CA:827:U:OP2 | 2.18 | 0.44 |
| 51:D3:18:ARG:HB3 | 51:D3:19:ARG:H | 1.51 | 0.44 |
| 24:DB:5:C:O2 | 24:DB:116:G:N2 | 2.50 | 0.44 |
| 24:DB:26:A:N7 | 24:DB:27:C:C4 | 2.86 | 0.44 |
| 23:BA:2464:C:C2 | 23:BA:2487:G:C2 | 3.06 | 0.44 |
| 1:CA:1089:G:C6 | 1:CA:1090:U:C5 | 3.06 | 0.44 |
| 7:CG:35:LYS:O | 7:CG:38:LEU:N | 2.49 | 0.44 |
| 32:DJ:137:ARG:HG2 | 32:DJ:137:ARG:H | 1.55 | 0.44 |
| 1:AA:450:G:H2' | 1:AA:451:A:OP1 | 2.17 | 0.44 |
| 1:CA:451:A:C5 | 1:CA:481:G:C5 | 3.05 | 0.44 |
| 1:CA:450:G:C8 | 1:CA:481:G:C6 | 3.06 | 0.44 |
| 35:DM:130:LYS:HZ2 | 44:DV:80:ARG:HE | 1.65 | 0.44 |
| 28:DF:20:ILE:O | 28:DF:24:GLY:HA2 | 2.18 | 0.44 |
| 35:BM:73:PRO:HA | 35:BM:93:TYR:CD2 | 2.53 | 0.44 |
| 23:DA:725:G:C6 | 23:DA:726:G:N1 | 2.86 | 0.44 |
| 33:BK:20:MET:HG3 | 33:BK:20:MET:O | 2.16 | 0.44 |
| 38:DP:113:LYS:O | 38:DP:114:LEU:HD23 | 2.18 | 0.44 |
| 32:BJ:41:ALA:HB3 | 32:BJ:79:ASN:O | 2.17 | 0.44 |
| 1:CA:1062:U:H2' | 1:CA:1063:C:C6 | 2.53 | 0.44 |
| 34:DL:77:ARG:HA | 34:DL:78:PRO:HD3 | 1.87 | 0.44 |
| 23:BA:1855:G:N1 | 23:BA:1888:G:C8 | 2.86 | 0.44 |
| 1:CA:296:U:H2' | 1:CA:297:G:C8 | 2.52 | 0.44 |
| 9:CI:125:TYR:CD1 | 9:CI:126:SER:N | 2.86 | 0.44 |
| 35:BM:135:ASP:OD1 | 35:BM:135:ASP:N | 2.50 | 0.44 |
| 34:BL:94:GLU:O | 34:BL:96:THR:HG23 | 2.18 | 0.44 |
| 34:DL:107:LYS:C | 34:DL:108:LYS:HG2 | 2.38 | 0.43 |
| 52:D4:9:ARG:O | 52:D4:10:ARG:C | 2.53 | 0.43 |
| 23:DA:1309:G:O5' | 23:DA:1309:G:H8 | 2.00 | 0.43 |
| 36:DN:11:ASN:O | 36:DN:12:ARG:CB | 2.64 | 0.43 |
| 32:BJ:122:LEU:O | 32:BJ:126:VAL:HG22 | 2.18 | 0.43 |
| 38:DP:50:ILE:HD11 | 38:DP:102:ILE:HG12 | 2.00 | 0.43 |
| 1:AA:1060:C:O2 | 1:AA:1198:G:C2 | 2.71 | 0.43 |
| 13:AM:87:TYR:O | 13:AM:91:ARG:HG2 | 2.18 | 0.43 |
| 14:AN:31:ARG:O | 14:AN:32:SER:HB2 | 2.18 | 0.43 |
| 25:BC:9:TYR:CZ | 25:BC:13:ARG:HD3 | 2.52 | 0.43 |
| 33:BK:77:ILE:HD12 | 38:BP:73:GLU:O | 2.18 | 0.43 |
| 1:CA:502:G:H2' | 1:CA:503:C:O4' | 2.18 | 0.43 |
| 12:CL:118:LYS:C | 12:CL:119:TYR:CD1 | 2.91 | 0.43 |
| 1:CA:363:A:H8 | 12:CL:32:ARG:HH21 | 1.66 | 0.43 |
| 34:BL:83:VAL:O | 34:BL:114:ILE:HA | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BA:2335:A:C8 | 23:BA:2337:G:N7 | 2.86 | 0.43 |
| 23:BA:1266:G:O6 | 41:BS:16:LYS:HD2 | 2.18 | 0.43 |
| 24:DB:80:U:C2 | 24:DB:81:G:N2 | 2.86 | 0.43 |
| 24:DB:84:C:O2 | 24:DB:84:C:C2' | 2.67 | 0.43 |
| 16:CP:21:VAL:HG23 | 16:CP:33:ILE:HB | 2.00 | 0.43 |
| 30:BH:114:LEU:HD21 | 30:BH:128:LEU:HD13 | 1.99 | 0.43 |
| 1:CA:674:G:H2' | 1:CA:675:A:C8 | 2.47 | 0.43 |
| 37:DO:11:LYS:O | 37:DO:12:PHE:CB | 2.64 | 0.43 |
| 16:AP:20:VAL:CG2 | 16:AP:21:VAL:N | 2.81 | 0.43 |
| 3:CC:18:TRP:O | 3:CC:19:GLU:C | 2.57 | 0.43 |
| 3:CC:182:ILE:HA | 3:CC:202:ILE:O | 2.18 | 0.43 |
| 49:D1:42:CYS:HB3 | 49:D1:59:VAL:HB | 1.99 | 0.43 |
| 3:CC:181:ASN:HB3 | 3:CC:205:GLY:HA3 | 2.00 | 0.43 |
| 26:DD:59:VAL:C | 26:DD:61:ARG:H | 2.21 | 0.43 |
| 23:DA:2768:C:C5 | 23:DA:2769:C:C5 | 3.05 | 0.43 |
| 29:DG:35:VAL:HG21 | 29:DG:75:ALA:CB | 2.48 | 0.43 |
| 11:CK:59:TYR:O | 11:CK:62:GLN:HB3 | 2.18 | 0.43 |
| 1:CA:691:G:H2' | 1:CA:692:U:C6 | 2.53 | 0.43 |
| 46:DX:26:ARG:O | 46:DX:27:GLU:HB3 | 2.18 | 0.43 |
| 23:BA:2396:G:H4' | 46:BX:31:GLY:HA2 | 2.00 | 0.43 |
| 4:CD:156:GLU:O | 4:CD:160:GLN:HG3 | 2.17 | 0.43 |
| 23:DA:1502:C:C6 | 23:DA:1502:C:H3' | 2.52 | 0.43 |
| 42:BT:9:LEU:O | 42:BT:10:ALA:HB2 | 2.18 | 0.43 |
| 25:DC:174:ILE:N | 25:DC:174:ILE:CD1 | 2.81 | 0.43 |
| 1:AA:1145:C:H4' | 1:AA:1146:A:C8 | 2.51 | 0.43 |
| 1:CA:104:G:N1 | 1:CA:105:G:C5 | 2.86 | 0.43 |
| 1:CA:104:G:N3 | 1:CA:105:G:C8 | 2.86 | 0.43 |
| 2:AB:72:GLY:HA2 | 2:AB:165:VAL:HG22 | 2.00 | 0.43 |
| 9:CI:58:ARG:HH21 | 9:CI:59:PHE:HE1 | 1.62 | 0.43 |
| 23:DA:480:A:H5' | 43:DU:46:LYS:HG3 | 2.00 | 0.43 |
| 23:DA:737:C:O2' | 23:DA:738:G:H5' | 2.18 | 0.43 |
| 23:DA:1478:G:H2' | 23:DA:1479:G:H8 | 1.83 | 0.43 |
| 23:BA:2209:C:C2 | 23:BA:2216:G:N1 | 2.86 | 0.43 |
| 23:BA:2100:G:C2 | 23:BA:2101:G:C4 | 3.05 | 0.43 |
| 23:BA:1387:C:N4 | 23:BA:1400:G:H1 | 2.16 | 0.43 |
| 23:DA:2476:A:C2 | 23:DA:2477:C:C5 | 3.06 | 0.43 |
| 1:CA:336:C:H2' | 1:CA:337:C:C6 | 2.52 | 0.43 |
| 1:CA:1233:G:P | 9:CI:124:GLN:H | 2.41 | 0.43 |
| 1:CA:939:G:H2' | 1:CA:940:C:H6 | 1.83 | 0.43 |
| 3:CC:86:VAL:O | 3:CC:89:GLU:HB3 | 2.18 | 0.43 |
| 1:CA:17:U:N3 | 1:CA:18:C:C4 | 2.86 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 39:BQ:62:ILE:CD1 | 39:BQ:93:LYS:HG2 | 2.48 | 0.43 |
| 28:BF:16:ARG:HB3 | 28:BF:17:PRO:HD3 | 1.99 | 0.43 |
| 27:DE:46:ARG:HB3 | 27:DE:46:ARG:CZ | 2.48 | 0.43 |
| 43:BU:90:LEU:HD12 | 43:BU:91:GLU:HG3 | 2.00 | 0.43 |
| 39:BQ:29:SER:C | 39:BQ:30:LYS:HG2 | 2.37 | 0.43 |
| 6:CF:77:ARG:HB3 | 6:CF:77:ARG:CZ | 2.48 | 0.43 |
| 1:AA:925:G:C2 | 1:AA:1392:G:C2 | 3.06 | 0.43 |
| 1:CA:774:G:N2 | 1:CA:806:C:C6 | 2.86 | 0.43 |
| 20:AT:42:GLN:HG3 | 20:AT:43:LEU:N | 2.33 | 0.43 |
| 1:CA:577:G:C6 | 1:CA:578:C:C5 | 3.06 | 0.43 |
| 23:BA:2511:U:O4 | 23:BA:2575:C:N3 | 2.50 | 0.43 |
| 1:AA:1386:G:C2 | 1:AA:1387:G:N7 | 2.86 | 0.43 |
| 23:DA:1991:U:H2' | 23:DA:1992:G:C5' | 2.48 | 0.43 |
| 24:DB:116:G:H8 | 24:DB:116:G:O5' | 2.01 | 0.43 |
| 1:AA:636:U:O2' | 1:AA:637:G:H5' | 2.18 | 0.43 |
| 35:DM:30:GLY:CA | 35:DM:107:ALA:HB2 | 2.48 | 0.43 |
| 1:CA:1391:U:H2' | 1:CA:1392:G:C8 | 2.53 | 0.43 |
| 20:CT:42:GLN:HG3 | 20:CT:43:LEU:N | 2.33 | 0.43 |
| 1:CA:932:C:H2' | 1:CA:933:G:H8 | 1.81 | 0.43 |
| 26:BD:173:VAL:O | 26:BD:174:ASP:C | 2.56 | 0.43 |
| 23:BA:646:A:H2' | 23:BA:647:G:O4' | 2.17 | 0.43 |
| 5:AE:104:ALA:O | 5:AE:107:ARG:HB3 | 2.17 | 0.43 |
| 23:DA:1678:G:N3 | 23:DA:1678:G:C2' | 2.75 | 0.43 |
| 32:BJ:137:ARG:HG2 | 32:BJ:137:ARG:H | 1.50 | 0.43 |
| 1:AA:1340:A:C5 | 1:AA:1341:U:C6 | 3.06 | 0.43 |
| 23:BA:270(F):G:C5 | 23:BA:270(G):U:C5 | 3.06 | 0.43 |
| 1:CA:5:U:O2' | 1:CA:6:G:C4 | 2.71 | 0.43 |
| 23:BA:2313:C:H4' | 28:BF:91:ARG:HG3 | 2.00 | 0.43 |
| 9:CI:41:VAL:O | 9:CI:44:VAL:HG22 | 2.17 | 0.43 |
| 1:CA:195:A:C5 | 1:CA:196:A:N1 | 2.86 | 0.43 |
| 23:DA:2515:C:O2 | 23:DA:2570:G:C2 | 2.71 | 0.43 |
| 23:DA:32:C:O2' | 23:DA:33:U:H5' | 2.18 | 0.43 |
| 23:BA:671:C:H2' | 23:BA:672:C:H6 | 1.83 | 0.43 |
| 7:CG:60:LYS:HD2 | 7:CG:60:LYS:HA | 1.76 | 0.43 |
| 34:DL:138:LEU:O | 34:DL:141:ALA:N | 2.51 | 0.43 |
| 34:DL:85:LEU:CD2 | 34:DL:85:LEU:N | 2.79 | 0.43 |
| 23:DA:1309:G:H3' | 52:D4:9:ARG:HH12 | 1.79 | 0.43 |
| 43:DU:68:HIS:C | 43:DU:70:SER:N | 2.72 | 0.43 |
| 12:CL:100:VAL:O | 12:CL:100:VAL:HG12 | 2.17 | 0.43 |
| 2:CB:61:LEU:HG | 2:CB:68:ILE:CG1 | 2.48 | 0.43 |
| 32:BJ:107:LYS:O | 32:BJ:108:ILE:HD13 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BA:603:A:H2 | 23:BA:655:A:N3 | 2.14 | 0.43 |
| 39:BQ:79:PHE:CE1 | 39:BQ:83:LEU:CD1 | 3.02 | 0.43 |
| 40:BR:49:THR:O | 40:BR:50:PRO:C | 2.56 | 0.43 |
| 23:BA:242:G:H5' | 53:B5:63:PRO:CB | 2.48 | 0.43 |
| 1:AA:551:U:O2' | 12:AL:85:ARG:HD2 | 2.17 | 0.43 |
| 30:DH:88:ILE:HG13 | 30:DH:144:VAL:CG1 | 2.48 | 0.43 |
| 1:AA:324:G:C2 | 1:AA:327:A:C8 | 3.07 | 0.43 |
| 1:CA:78:G:H2' | 1:CA:79:G:C8 | 2.54 | 0.43 |
| 1:CA:323:U:H4' | 20:CT:22:ARG:HB3 | 1.99 | 0.43 |
| 23:DA:1842:G:H1' | 25:DC:255:LYS:HZ3 | 1.83 | 0.43 |
| 1:CA:397:A:C6 | 1:CA:548:G:N7 | 2.86 | 0.43 |
| 49:B1:42:CYS:HB3 | 49:B1:59:VAL:HB | 2.00 | 0.43 |
| 44:BV:3:TYR:O | 44:BV:57:ILE:HA | 2.18 | 0.43 |
| 44:BV:94:GLU:CD | 44:BV:94:GLU:N | 2.66 | 0.43 |
| 1:AA:1064:G:H21 | 1:AA:1190:G:C2' | 2.24 | 0.43 |
| 1:AA:448:A:H2' | 1:AA:449:C:C6 | 2.53 | 0.43 |
| 10:AJ:3:LYS:N | 10:AJ:75:ILE:HA | 2.33 | 0.43 |
| 1:CA:1294:G:H2' | 1:CA:1295:G:H8 | 1.74 | 0.43 |
| 1:AA:1369:C:H2' | 1:AA:1370:G:C8 | 2.53 | 0.43 |
| 1:AA:1347:G:N7 | 9:AI:107:ARG:HB3 | 2.31 | 0.43 |
| 25:BC:172:TYR:CE1 | 25:BC:186:HIS:HA | 2.50 | 0.43 |
| 23:DA:1496:A:C8 | 23:DA:1498:C:N3 | 2.86 | 0.43 |
| 4:CD:108:LEU:O | 4:CD:110:PHE:CD2 | 2.71 | 0.43 |
| 23:DA:1502:C:C6 | 23:DA:1502:C:C3' | 3.01 | 0.43 |
| 25:BC:134:ARG:HD3 | 25:BC:135:PHE:HE1 | 1.82 | 0.43 |
| 25:DC:24:ILE:HD13 | 25:DC:84:TYR:HB2 | 2.00 | 0.43 |
| 1:CA:1238:A:N3 | 1:CA:1238:A:H2' | 2.33 | 0.43 |
| 1:AA:625:G:C6 | 1:AA:626:U:C4 | 3.06 | 0.43 |
| 1:CA:708:C:O2' | 1:CA:709:G:H5' | 2.18 | 0.43 |
| 44:BV:151:HIS:HA | 44:BV:170:THR:HA | 2.00 | 0.43 |
| 25:DC:148:GLU:HB2 | 25:DC:151:LYS:HD2 | 1.99 | 0.43 |
| 3:AC:70:VAL:CG1 | 3:AC:71:ALA:N | 2.81 | 0.43 |
| 23:DA:1358:G:H1' | 23:DA:1373:A:H61 | 1.83 | 0.43 |
| 1:CA:29:G:C2 | 1:CA:555:C:N3 | 2.86 | 0.43 |
| 27:BE:53:THR:C | 27:BE:55:GLY:N | 2.70 | 0.43 |
| 1:AA:69:G:H1 | 1:AA:99:C:H42 | 1.66 | 0.43 |
| 25:BC:25:THR:O | 25:BC:26:LYS:C | 2.57 | 0.43 |
| 1:AA:233:C:C2' | 1:AA:234:C:H5' | 2.48 | 0.43 |
| 23:DA:2590:A:O2' | 23:DA:2591:C:H5' | 2.17 | 0.43 |
| 1:AA:39:G:N1 | 1:AA:40:C:C5 | 2.86 | 0.43 |
| 23:BA:2549:G:H2' | 23:BA:2550:G:H5' | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:CO:12:ILE:HG21 | 15:CO:22:THR:HG22 | 1.99 | 0.43 |
| 35:DM:54:MET:O | 35:DM:57:HIS:HB3 | 2.17 | 0.43 |
| 23:BA:285:C:H2' | 23:BA:286:C:C6 | 2.54 | 0.43 |
| 6:AF:78:GLU:HA | 6:AF:81:ILE:HD11 | 2.00 | 0.43 |
| 25:BC:61:LEU:HD13 | 25:BC:61:LEU:HA | 1.51 | 0.43 |
| 1:CA:510:A:H5'' | 1:CA:511:C:OP2 | 2.17 | 0.43 |
| 23:BA:825:C:H4' | 23:BA:2428:G:N7 | 2.33 | 0.43 |
| 23:DA:2663:G:C6 | 23:DA:2664:G:C5 | 3.06 | 0.43 |
| 23:BA:442:G:H4' | 27:BE:46:ARG:HD3 | 1.99 | 0.43 |
| 1:CA:256:U:P | 17:CQ:17:LYS:HZ3 | 2.40 | 0.43 |
| 23:DA:1248:G:OP1 | 39:DQ:2:PRO:CD | 2.64 | 0.43 |
| 23:BA:1789:A:OP1 | 25:BC:221:VAL:HA | 2.18 | 0.43 |
| 25:BC:222:ARG:NH1 | 25:BC:224:ALA:HB3 | 2.33 | 0.43 |
| 3:AC:73:PRO:O | 3:AC:76:VAL:HG22 | 2.18 | 0.43 |
| 14:CN:32:SER:HB3 | 14:CN:41:ARG:HG2 | 2.00 | 0.43 |
| 43:DU:43:ASN:OD1 | 43:DU:64:GLU:HA | 2.18 | 0.43 |
| 12:AL:78:GLU:O | 12:AL:78:GLU:CD | 2.57 | 0.43 |
| 23:BA:566:U:H3 | 23:BA:575:A:H61 | 1.66 | 0.43 |
| 36:DN:85:PRO:HA | 36:DN:88:ARG:HH11 | 1.82 | 0.43 |
| 44:BV:120:ILE:HG12 | 44:BV:172:ALA:HA | 1.99 | 0.43 |
| 1:AA:160:A:H4' | 1:AA:344:A:N1 | 2.33 | 0.43 |
| 29:DG:169:VAL:O | 29:DG:170:ARG:HB2 | 2.18 | 0.43 |
| 23:BA:853:G:H1 | 23:BA:924:C:N4 | 2.17 | 0.43 |
| 1:AA:639:G:H2' | 1:AA:640:A:C8 | 2.53 | 0.43 |
| 23:DA:1443:G:O2' | 23:DA:1444:G:H5' | 2.17 | 0.43 |
| 23:DA:1980:G:H4' | 23:DA:1981:A:OP2 | 2.17 | 0.43 |
| 23:DA:2435:A:C2' | 23:DA:2436:G:O5' | 2.66 | 0.43 |
| 27:DE:160:ASN:OD1 | 27:DE:163:VAL:HG23 | 2.18 | 0.43 |
| 23:DA:1833:U:H2' | 23:DA:1834:U:H5' | 1.98 | 0.43 |
| 24:BB:5:C:O2' | 24:BB:27:C:H1' | 2.18 | 0.43 |
| 12:AL:64:GLU:OE1 | 12:AL:64:GLU:C | 2.57 | 0.43 |
| 23:BA:2828:C:C2' | 23:BA:2829:C:H5' | 2.48 | 0.43 |
| 1:AA:1386:G:N3 | 1:AA:1387:G:C8 | 2.86 | 0.43 |
| 23:DA:914:C:C6 | 23:DA:914:C:H3' | 2.52 | 0.43 |
| 24:DB:27:C:C4 | 24:DB:28:C:C4 | 3.06 | 0.43 |
| 3:AC:137:ALA:O | 3:AC:141:VAL:HG23 | 2.18 | 0.43 |
| 1:CA:993:G:H4' | 1:CA:994:A:OP2 | 2.19 | 0.43 |
| 23:BA:150:C:H2' | 23:BA:151:C:C6 | 2.53 | 0.43 |
| 23:DA:1424:G:H2' | 23:DA:1425:G:O4' | 2.18 | 0.43 |
| 18:CR:53:ARG:O | 18:CR:55:ARG:N | 2.51 | 0.43 |
| 1:CA:1210:C:H4' | 1:CA:1214:C:C5 | 2.52 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:DM:24:GLY:HA2 | 35:DM:100:GLY:O | 2.18 | 0.43 |
| 26:DD:68:ALA:C | 26:DD:70:ALA:H | 2.22 | 0.43 |
| 42:BT:75:ASP:C | 42:BT:76:ARG:HG3 | 2.39 | 0.43 |
| 23:DA:2564:A:C2 | 23:DA:2647:U:H4' | 2.53 | 0.43 |
| 23:DA:1629:U:H2' | 23:DA:1630:G:O4' | 2.18 | 0.43 |
| 23:BA:2734:A:C2' | 23:BA:2735:G:H5' | 2.48 | 0.43 |
| 20:CT:78:ALA:O | 20:CT:81:LYS:N | 2.51 | 0.43 |
| 1:AA:983:A:H3' | 1:AA:983:A:N3 | 2.34 | 0.43 |
| 23:DA:2734:A:C2' | 23:DA:2735:G:H5' | 2.48 | 0.43 |
| 23:DA:1930:G:O2' | 23:DA:1931:U:P | 2.76 | 0.43 |
| 2:CB:200:ILE:HG22 | 2:CB:202:PRO:HD3 | 2.00 | 0.43 |
| 33:DK:3:GLN:CB | 33:DK:4:PRO:HD2 | 2.48 | 0.43 |
| 5:CE:135:THR:O | 5:CE:138:ALA:HB3 | 2.18 | 0.43 |
| 1:CA:1463:C:OP1 | 38:DP:111:ARG:HD2 | 2.19 | 0.43 |
| 38:BP:14:TYR:N | 38:BP:14:TYR:CD1 | 2.85 | 0.43 |
| 16:AP:75:ARG:C | 16:AP:77:ALA:H | 2.21 | 0.43 |
| 6:AF:99:ALA:HB3 | 18:AR:29:PHE:CE1 | 2.53 | 0.43 |
| 23:DA:660:G:O3' | 27:DE:38:ARG:NH2 | 2.51 | 0.43 |
| 40:DR:62:LEU:HA | 40:DR:62:LEU:HD12 | 1.77 | 0.43 |
| 44:BV:70:LEU:HD23 | 44:BV:70:LEU:H | 1.83 | 0.43 |
| 25:DC:220:HIS:C | 25:DC:220:HIS:CD2 | 2.92 | 0.43 |
| 38:DP:101:PHE:C | 38:DP:101:PHE:CD2 | 2.91 | 0.43 |
| 34:DL:84:ASN:HB3 | 34:DL:86:LYS:HG2 | 1.99 | 0.43 |
| 34:DL:91:PHE:CE2 | 34:DL:95:VAL:HG12 | 2.53 | 0.43 |
| 23:BA:1177:A:H5'' | 23:BA:1178:C:OP2 | 2.17 | 0.43 |
| 23:DA:1541:U:H5'' | 23:DA:1543:A:OP2 | 2.17 | 0.43 |
| 1:AA:964:A:N3 | 1:AA:969:A:O2' | 2.48 | 0.43 |
| 1:AA:1060:C:O2' | 10:AJ:56:HIS:CD2 | 2.71 | 0.43 |
| 22:AV:6194:C:C2 | 22:AV:6195:G:C8 | 3.07 | 0.43 |
| 5:CE:101:ILE:HD11 | 5:CE:119:LEU:CD2 | 2.23 | 0.43 |
| 38:DP:54:ARG:HA | 38:DP:59:THR:OG1 | 2.19 | 0.43 |
| 23:DA:2259:G:C2 | 23:DA:2282:G:N1 | 2.87 | 0.43 |
| 12:CL:29:ALA:HA | 12:CL:30:PRO:HD3 | 1.76 | 0.43 |
| 23:BA:1188:U:C2' | 23:BA:1189:A:O5' | 2.66 | 0.43 |
| 28:BF:86:MET:O | 28:BF:87:PRO:O | 2.36 | 0.43 |
| 39:DQ:79:PHE:CE1 | 39:DQ:83:LEU:CD1 | 3.02 | 0.43 |
| 40:DR:49:THR:O | 40:DR:50:PRO:C | 2.56 | 0.43 |
| 25:DC:32:SER:O | 25:DC:36:PRO:HD2 | 2.19 | 0.43 |
| 34:DL:46:LYS:HG2 | 34:DL:52:GLU:CD | 2.38 | 0.43 |
| 23:DA:1021:A:N6 | 23:DA:1141:U:C2 | 2.87 | 0.43 |
| 23:DA:2292:C:N4 | 23:DA:2293:C:N4 | 2.66 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:DC:147:LEU:HD13 | 25:DC:155:LEU:CD1 | 2.48 | 0.43 |
| 30:DH:88:ILE:HG13 | 30:DH:144:VAL:HG11 | 2.00 | 0.43 |
| 26:BD:35:GLN:HG2 | 26:BD:36:ARG:N | 2.33 | 0.43 |
| 47:DY:24:LEU:HD22 | 47:DY:60:LEU:CD1 | 2.47 | 0.43 |
| 39:DQ:57:PHE:O | 39:DQ:60:LEU:N | 2.52 | 0.43 |
| 1:CA:1104:G:C2 | 1:CA:1105:A:C4 | 3.07 | 0.43 |
| 1:CA:1106:G:C2 | 1:CA:1107:C:C6 | 3.06 | 0.43 |
| 23:BA:1786:A:H2 | 23:BA:2606:C:H1' | 1.82 | 0.43 |
| 25:BC:172:TYR:CD1 | 25:BC:186:HIS:CA | 2.93 | 0.43 |
| 1:CA:505:G:H5' | 1:CA:534:U:C2 | 2.53 | 0.43 |
| 23:DA:2744:G:H1' | 23:DA:2761:G:N2 | 2.33 | 0.43 |
| 23:BA:83:G:N2 | 23:BA:84:A:N6 | 2.66 | 0.43 |
| 6:CF:28:ARG:O | 6:CF:32:ASN:N | 2.47 | 0.43 |
| 15:AO:45:VAL:HG22 | 15:AO:46:HIS:ND1 | 2.33 | 0.43 |
| 1:AA:349:A:C2' | 1:AA:350:G:H5' | 2.47 | 0.43 |
| 1:CA:818:G:N3 | 1:CA:820:U:C6 | 2.86 | 0.43 |
| 23:BA:2274:A:C5 | 23:BA:2276:G:C8 | 3.06 | 0.43 |
| 8:AH:26:VAL:O | 8:AH:27:PRO:C | 2.55 | 0.43 |
| 23:DA:952:G:C6 | 23:DA:953:A:N7 | 2.87 | 0.43 |
| 23:DA:1953:A:C2 | 23:DA:2549:G:N3 | 2.84 | 0.43 |
| 23:DA:2658:C:H2' | 23:DA:2658:C:O2 | 2.18 | 0.43 |
| 17:CQ:15:MET:CB | 17:CQ:18:THR:HB | 2.45 | 0.43 |
| 23:DA:1131:G:C2 | 23:DA:1132:A:C5 | 3.06 | 0.43 |
| 1:CA:855:G:C6 | 1:CA:856:C:C4 | 3.06 | 0.43 |
| 23:BA:588:U:H2' | 23:BA:589:C:H6 | 1.81 | 0.43 |
| 32:BJ:160:LYS:O | 32:BJ:161:LEU:HD23 | 2.18 | 0.43 |
| 23:BA:332:A:C4 | 23:BA:335:C:C4 | 3.06 | 0.43 |
| 1:AA:939:G:H2' | 1:AA:940:C:H6 | 1.83 | 0.43 |
| 1:CA:731:G:C6 | 1:CA:732:C:C4 | 3.06 | 0.43 |
| 23:DA:273(G):C:H2' | 23:DA:274:G:C5' | 2.46 | 0.43 |
| 2:AB:22:LYS:HZ3 | 2:AB:22:LYS:N | 2.14 | 0.43 |
| 1:AA:754:C:H3' | 1:AA:754:C:O2 | 2.17 | 0.43 |
| 23:BA:978:G:O2' | 23:BA:979:G:H5' | 2.18 | 0.43 |
| 8:AH:40:ALA:O | 8:AH:41:ARG:C | 2.56 | 0.43 |
| 23:BA:737:C:H2' | 23:BA:738:G:C5' | 2.47 | 0.43 |
| 7:AG:44:TYR:O | 7:AG:47:CYS:HB2 | 2.19 | 0.43 |
| 1:AA:506:G:C6 | 1:AA:507:C:N4 | 2.86 | 0.43 |
| 23:BA:1526:G:O2' | 23:BA:1527:G:H5' | 2.18 | 0.43 |
| 26:BD:172:VAL:HG13 | 26:BD:182:LEU:HD11 | 2.00 | 0.43 |
| 23:DA:880:G:N2 | 23:DA:898:C:C4 | 2.86 | 0.43 |
| 1:AA:294:U:N3 | 1:AA:295:C:C5 | 2.86 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:BP:23:ARG:CG | 38:BP:23:ARG:NH1 | 2.82 | 0.43 |
| 25:BC:52:ARG:CZ | 25:BC:53:PHE:CE2 | 3.02 | 0.43 |
| 23:BA:2096:U:H2' | 23:BA:2097:C:C6 | 2.53 | 0.43 |
| 23:DA:948:G:C2 | 23:DA:970:C:O2 | 2.72 | 0.43 |
| 11:AK:124:LYS:HB2 | 11:AK:124:LYS:HE3 | 1.75 | 0.43 |
| 23:BA:1338:G:H2' | 23:BA:1339:G:H5' | 2.00 | 0.43 |
| 2:AB:96:ARG:N | 2:AB:96:ARG:HD2 | 2.33 | 0.43 |
| 1:AA:1037:C:H2' | 1:AA:1038:C:C6 | 2.51 | 0.43 |
| 23:DA:107:C:H2' | 23:DA:108:U:H5' | 2.01 | 0.43 |
| 1:AA:167:G:C2' | 1:AA:168:G:H5' | 2.48 | 0.43 |
| 28:DF:106:LEU:HA | 28:DF:110:ALA:HB3 | 2.00 | 0.43 |
| 23:DA:1221:C:H2' | 23:DA:122(A):C:H6 | 1.83 | 0.43 |
| 1:CA:892:A:C2 | 1:CA:907:A:C4 | 3.07 | 0.43 |
| 10:AJ:61:GLU:OE2 | 14:AN:45:ARG:NH1 | 2.51 | 0.43 |
| 23:BA:2231:C:H2' | 23:BA:2232:U:O4' | 2.18 | 0.43 |
| 1:CA:1433:A:N1 | 1:CA:1434:A:C2 | 2.86 | 0.43 |
| 17:CQ:77:VAL:O | 17:CQ:78:GLU:HB3 | 2.18 | 0.43 |
| 33:DK:47:ILE:HD12 | 33:DK:47:ILE:HA | 1.66 | 0.43 |
| 2:AB:21:ARG:HG3 | 2:AB:21:ARG:O | 2.18 | 0.43 |
| 52:D4:3:ARG:HA | 52:D4:3:ARG:HD3 | 1.72 | 0.43 |
| 20:AT:55:ILE:HA | 20:AT:55:ILE:HD12 | 1.84 | 0.43 |
| 53:B5:37:SER:OG | 53:B5:40:GLU:HG2 | 2.18 | 0.43 |
| 23:DA:1779:U:C6 | 23:DA:1783:A:N7 | 2.86 | 0.43 |
| 9:CI:5:TYR:CG | 9:CI:6:GLY:N | 2.85 | 0.43 |
| 9:AI:41:VAL:O | 9:AI:44:VAL:HG22 | 2.18 | 0.43 |
| 53:D5:23:VAL:HG11 | 53:D5:47:LYS:HD3 | 2.01 | 0.43 |
| 34:DL:97:PRO:CD | 34:DL:126:VAL:HG12 | 2.44 | 0.43 |
| 34:DL:79:ARG:O | 34:DL:111:ARG:HB2 | 2.19 | 0.43 |
| 23:BA:747:U:O2 | 23:BA:2014:A:H1' | 2.18 | 0.43 |
| 43:DU:11:ASP:O | 43:DU:26:LYS:HA | 2.18 | 0.43 |
| 43:DU:8:LYS:CA | 43:DU:8:LYS:HZ3 | 2.30 | 0.43 |
| 28:DF:60:LEU:HA | 28:DF:63:ILE:CG1 | 2.48 | 0.43 |
| 32:DJ:143:LEU:HD13 | 32:DJ:144:LYS:N | 2.34 | 0.43 |
| 26:BD:101:ARG:HB3 | 26:BD:169:ASN:HD22 | 1.82 | 0.43 |
| 7:AG:108:ALA:O | 7:AG:119:ARG:HD2 | 2.18 | 0.43 |
| 5:CE:101:ILE:HG12 | 5:CE:118:ILE:O | 2.17 | 0.43 |
| 23:BA:1019:U:C2 | 23:BA:1020:A:N7 | 2.86 | 0.43 |
| 23:DA:918:A:H5'' | 23:DA:919:G:OP2 | 2.17 | 0.43 |
| 23:DA:593:G:C6 | 23:DA:594:U:C4 | 3.07 | 0.43 |
| 1:AA:673:G:C4 | 1:AA:734:G:C2 | 3.07 | 0.43 |
| 28:DF:86:MET:H | 28:DF:87:PRO:HD2 | 1.83 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:B5:59:LYS:O | 53:B5:62:LEU:HG | 2.19 | 0.43 |
| 3:CC:19:GLU:HA | 3:CC:54:ARG:NH2 | 2.33 | 0.43 |
| 1:AA:409:G:OP1 | 4:AD:24:GLU:N | 2.51 | 0.43 |
| 1:AA:692:U:H2' | 1:AA:694:A:OP2 | 2.17 | 0.43 |
| 23:DA:1825:A:O3' | 25:DC:233:HIS:CD2 | 2.71 | 0.43 |
| 24:BB:46:A:H2' | 24:BB:47:C:H6 | 1.81 | 0.43 |
| 44:BV:31:ARG:CZ | 44:BV:94:GLU:HG3 | 2.49 | 0.43 |
| 23:DA:1285:G:C5 | 23:DA:1329:U:C4 | 3.06 | 0.43 |
| 23:DA:1313:U:O2 | 23:DA:1313:U:C2' | 2.64 | 0.43 |
| 23:DA:1332:G:N2 | 23:DA:1610:A:H8 | 2.13 | 0.43 |
| 1:CA:1071:C:O2 | 1:CA:1072:G:C8 | 2.71 | 0.43 |
| 23:BA:2768:C:C5 | 23:BA:2769:C:C5 | 3.06 | 0.43 |
| 1:AA:1368:G:C2 | 1:AA:1369:C:C6 | 3.06 | 0.43 |
| 9:AI:118:LYS:O | 9:AI:119:ALA:HB3 | 2.17 | 0.43 |
| 9:AI:29:ASN:ND2 | 9:AI:65:VAL:O | 2.51 | 0.43 |
| 10:AJ:13:HIS:CB | 10:AJ:68:HIS:NE2 | 2.81 | 0.43 |
| 1:CA:59:A:H1' | 1:CA:354:G:C2 | 2.53 | 0.43 |
| 23:BA:1454:U:O4' | 36:BN:63:ARG:HD3 | 2.19 | 0.43 |
| 23:DA:1401:G:C4 | 23:DA:1402:C:C5 | 3.06 | 0.43 |
| 23:BA:2790:A:C2 | 23:BA:2791:C:H2' | 2.54 | 0.43 |
| 4:CD:108:LEU:HB3 | 4:CD:110:PHE:CD2 | 2.51 | 0.43 |
| 23:DA:2809:A:N1 | 23:DA:2892:A:C4 | 2.86 | 0.43 |
| 23:BA:951:C:C2' | 23:BA:952:G:H5' | 2.49 | 0.43 |
| 23:BA:954:G:C4 | 23:BA:955:C:C6 | 3.06 | 0.43 |
| 8:CH:114:THR:OG1 | 8:CH:119:LEU:HG | 2.18 | 0.43 |
| 23:BA:874:G:H2' | 23:BA:875:G:O4' | 2.19 | 0.43 |
| 53:B5:53:PRO:O | 53:B5:57:ARG:NH1 | 2.51 | 0.43 |
| 32:DJ:135:LEU:O | 32:DJ:136:GLY:C | 2.56 | 0.43 |
| 29:BG:95:ARG:HH12 | 29:BG:97:ARG:HE | 1.67 | 0.43 |
| 23:BA:1478:G:H2' | 23:BA:1479:G:H8 | 1.83 | 0.43 |
| 1:AA:232:G:H2' | 1:AA:233:C:O4' | 2.18 | 0.43 |
| 1:CA:102:G:C5 | 1:CA:103:C:C5 | 3.07 | 0.43 |
| 23:BA:498:G:O2' | 43:BU:47:LYS:HD3 | 2.18 | 0.43 |
| 13:CM:3:ARG:HG2 | 13:CM:9:ILE:HD13 | 1.99 | 0.43 |
| 28:BF:112:PRO:HB3 | 49:B1:62:CYS:O | 2.17 | 0.43 |
| 11:AK:21:ILE:HD13 | 11:AK:84:VAL:HG12 | 2.00 | 0.43 |
| 36:BN:100:LEU:H | 36:BN:112:ALA:HA | 1.83 | 0.43 |
| 23:BA:2636:U:H2' | 23:BA:2637:U:C6 | 2.53 | 0.43 |
| 9:CI:114:TYR:H | 9:CI:114:TYR:HD2 | 1.62 | 0.43 |
| 1:CA:749:C:O2 | 1:CA:749:C:H2' | 2.18 | 0.43 |
| 1:CA:1054:C:O2' | 1:CA:1055:A:H5'' | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1056:U:OP1 | 3:CC:163:ALA:N | 2.49 | 0.43 |
| 1:CA:1442:G:C8 | 1:CA:1446:A:C2 | 3.07 | 0.43 |
| 29:BG:86:GLU:O | 29:BG:87:LEU:HD23 | 2.17 | 0.43 |
| 8:CH:29:SER:OG | 8:CH:32:LYS:HG3 | 2.19 | 0.43 |
| 1:CA:864:A:N1 | 1:CA:865:A:C2 | 2.86 | 0.43 |
| 23:BA:775:G:C4 | 23:BA:794:G:C8 | 3.05 | 0.43 |
| 23:BA:117:G:H5'' | 23:BA:118:A:OP2 | 2.18 | 0.43 |
| 1:CA:1232:U:H2' | 1:CA:1232:U:O2 | 2.17 | 0.43 |
| 23:BA:1607:C:N4 | 23:BA:1622:G:OP2 | 2.46 | 0.43 |
| 23:DA:1716:U:O2' | 23:DA:1717:G:H5' | 2.18 | 0.43 |
| 1:AA:570:G:H2' | 1:AA:571:U:C6 | 2.54 | 0.43 |
| 23:BA:997:G:OP1 | 39:BQ:93:LYS:CD | 2.66 | 0.43 |
| 23:DA:814:C:H2' | 23:DA:815:C:C6 | 2.53 | 0.43 |
| 23:BA:2275:C:H5' | 23:BA:2275:C:C6 | 2.48 | 0.43 |
| 1:CA:565:U:OP2 | 1:CA:566:G:O2' | 2.28 | 0.43 |
| 23:BA:753:C:H2' | 23:BA:754:C:H6 | 1.83 | 0.43 |
| 41:DS:65:LEU:HB2 | 41:DS:68:ARG:NE | 2.31 | 0.43 |
| 27:BE:127:GLU:O | 27:BE:127:GLU:OE2 | 2.37 | 0.43 |
| 44:BV:7:ALA:HB3 | 44:BV:61:LEU:HD23 | 2.01 | 0.43 |
| 1:AA:382:A:O2' | 1:AA:383:A:H5' | 2.19 | 0.43 |
| 23:BA:229:A:H5' | 23:BA:230:U:O5' | 2.16 | 0.43 |
| 1:CA:160:A:H4' | 1:CA:344:A:N1 | 2.33 | 0.43 |
| 12:CL:77:GLN:C | 12:CL:79:HIS:H | 2.22 | 0.43 |
| 16:AP:52:ASP:OD1 | 16:AP:54:GLU:HB2 | 2.17 | 0.43 |
| 46:DX:53:VAL:O | 46:DX:55:GLY:O | 2.37 | 0.43 |
| 1:CA:294:U:N3 | 1:CA:295:C:C5 | 2.86 | 0.43 |
| 1:AA:1504:G:H4' | 1:AA:1505:G:O4' | 2.18 | 0.43 |
| 23:DA:298:G:P | 43:DU:85:VAL:CG2 | 3.06 | 0.43 |
| 1:CA:1489:G:C6 | 1:CA:1490:C:C4 | 3.06 | 0.43 |
| 28:BF:153:ARG:HB3 | 28:BF:153:ARG:NH1 | 2.32 | 0.43 |
| 1:AA:826:C:H5'' | 1:AA:827:U:OP2 | 2.18 | 0.43 |
| 1:AA:1384:C:H2' | 1:AA:1385:G:H8 | 1.83 | 0.43 |
| 38:BP:105:LEU:O | 38:BP:106:SER:C | 2.56 | 0.43 |
| 6:AF:82:ARG:HD2 | 6:AF:82:ARG:HA | 1.80 | 0.43 |
| 23:BA:2409:G:C6 | 23:BA:2410:G:C5 | 3.06 | 0.43 |
| 1:AA:1415:G:C6 | 1:AA:1486:G:C6 | 3.06 | 0.43 |
| 23:DA:374:A:H3' | 23:DA:375:C:H6 | 1.82 | 0.43 |
| 23:BA:537:C:H6 | 23:BA:537:C:O5' | 2.02 | 0.43 |
| 23:DA:1297:C:H2' | 23:DA:1298:C:H6 | 1.82 | 0.43 |
| 23:DA:270(F):G:C6 | 23:DA:270(G):U:C4 | 3.06 | 0.43 |
| 23:BA:1854:A:H62 | 23:BA:1888:G:H8 | 1.65 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 23:BA:2666:C:C6 | 23:BA:2667:C:C6 | 3.07 | 0.43 |
| 23:BA:1462:C:C4 | 23:BA:1463:C:C4 | 3.06 | 0.43 |
| 24:BB:38:C:H2' | 24:BB:39:A:H8 | 1.83 | 0.43 |
| 23:BA:836:G:C5 | 23:BA:837:C:C4 | 3.05 | 0.43 |
| 23:BA:2075:U:H2' | 23:BA:2238:G:N2 | 2.34 | 0.43 |
| 19:CS:50:ALA:HB1 | 19:CS:57:HIS:HB3 | 2.00 | 0.43 |
| 23:DA:2493:U:C4 | 23:DA:2494:G:C8 | 3.07 | 0.43 |
| 1:AA:792:A:H4' | 1:AA:793:U:O5' | 2.17 | 0.43 |
| 1:CA:872:A:N3 | 1:CA:872:A:H2' | 2.33 | 0.43 |
| 25:BC:78:LYS:HG2 | 25:BC:114:GLY:O | 2.18 | 0.43 |
| 23:BA:2650:U:H6 | 23:BA:2650:U:O5' | 2.01 | 0.43 |
| 38:BP:87:ASP:N | 38:BP:87:ASP:OD1 | 2.51 | 0.43 |
| 17:AQ:14:LYS:HD2 | 17:AQ:14:LYS:H | 1.84 | 0.43 |
| 23:DA:1668:A:N7 | 23:DA:1674:G:C6 | 2.87 | 0.43 |
| 52:D4:18:PHE:CE2 | 52:D4:22:MET:HG3 | 2.53 | 0.43 |
| 1:AA:582:U:OP1 | 15:AO:68:ARG:NH2 | 2.51 | 0.43 |
| 49:D1:39:ARG:O | 49:D1:57:ILE:HB | 2.17 | 0.43 |
| 23:BA:690:G:H2' | 23:BA:691:C:O4' | 2.19 | 0.43 |
| 23:BA:1173:G:O5' | 23:BA:1173:G:H8 | 2.01 | 0.43 |
| 1:AA:1225:A:C5' | 1:AA:1226:C:OP2 | 2.66 | 0.43 |
| 9:AI:114:TYR:HE1 | 10:AJ:60:ARG:O | 2.00 | 0.43 |
| 22:CV:6191:A:C2 | 22:CV:6192:G:C4 | 3.06 | 0.43 |
| 22:CV:6213:A:C2 | 22:CV:6214:C:C4 | 3.07 | 0.43 |
| 37:BO:89:ARG:HG2 | 37:BO:89:ARG:O | 2.18 | 0.43 |
| 9:CI:13:ALA:HB2 | 9:CI:68:GLY:CA | 2.32 | 0.43 |
| 23:DA:1614:A:C6 | 41:DS:87:PRO:HA | 2.54 | 0.43 |
| 48:DZ:52:HIS:CD2 | 48:DZ:52:HIS:N | 2.85 | 0.43 |
| 53:D5:11:LYS:N | 53:D5:61:LEU:HD21 | 2.34 | 0.43 |
| 1:CA:375:U:H2' | 1:CA:376:G:H5' | 1.99 | 0.43 |
| 23:BA:2727:G:C2 | 23:BA:2728:U:C5 | 3.07 | 0.43 |
| 23:BA:2731:G:H2' | 23:BA:2732:G:C8 | 2.54 | 0.43 |
| 23:BA:252:G:O2' | 23:BA:253:C:H5' | 2.18 | 0.43 |
| 1:AA:375:U:H4' | 16:AP:17:TYR:CE2 | 2.53 | 0.43 |
| 4:AD:30:LYS:C | 4:AD:32:ALA:N | 2.70 | 0.43 |
| 4:CD:104:VAL:CG1 | 4:CD:146:ILE:HD13 | 2.33 | 0.43 |
| 47:BY:53:LEU:O | 47:BY:56:GLN:HB2 | 2.19 | 0.43 |
| 23:DA:1188:U:C2' | 23:DA:1189:A:C5' | 2.96 | 0.43 |
| 24:DB:69:G:C6 | 24:DB:70:C:C4 | 3.07 | 0.43 |
| 23:DA:94:G:C2 | 47:DY:47:ASN:ND2 | 2.86 | 0.43 |
| 1:AA:76:G:C6 | 1:AA:77:C:C4 | 3.07 | 0.43 |
| 3:CC:57:ILE:HD11 | 3:CC:66:VAL:HG22 | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:394:G:C2 | 1:AA:395:C:C6 | 3.07 | 0.43 |
| 23:BA:2713:A:H3' | 23:BA:2714:G:H5' | 1.99 | 0.43 |
| 4:CD:19:LEU:O | 4:CD:31:CYS:SG | 2.76 | 0.43 |
| 44:BV:30:ASN:O | 44:BV:31:ARG:C | 2.56 | 0.43 |
| 1:CA:668:G:H1' | 15:CO:46:HIS:CD2 | 2.43 | 0.43 |
| 5:AE:33:VAL:HG12 | 5:AE:34:VAL:N | 2.33 | 0.43 |
| 23:DA:2766:G:H5'' | 23:DA:2767:C:OP2 | 2.18 | 0.43 |
| 44:BV:54:HIS:CG | 44:BV:101:PRO:HG3 | 2.53 | 0.43 |
| 1:AA:1084:G:C6 | 1:AA:1085:U:O4 | 2.71 | 0.43 |
| 41:DS:74:ALA:HA | 41:DS:104:THR:O | 2.18 | 0.43 |
| 24:BB:106:G:C2' | 24:BB:107:U:H5' | 2.49 | 0.43 |
| 19:AS:46:GLY:HA2 | 19:AS:61:TYR:OH | 2.18 | 0.43 |
| 27:DE:167:ALA:O | 27:DE:170:LEU:HB2 | 2.18 | 0.43 |
| 1:CA:597:G:C8 | 1:CA:598:U:C5 | 3.07 | 0.43 |
| 1:CA:10:A:O2' | 1:CA:11:G:H5' | 2.18 | 0.43 |
| 25:BC:132:PRO:HD3 | 25:BC:190:TYR:CE1 | 2.52 | 0.43 |
| 23:DA:686:G:O6 | 52:D4:12:ARG:NH1 | 2.51 | 0.43 |
| 8:CH:10:LEU:HD23 | 8:CH:10:LEU:N | 2.33 | 0.43 |
| 23:BA:1509:A:O2' | 23:BA:1510:A:OP1 | 2.27 | 0.43 |
| 23:BA:1324:G:C4 | 23:BA:1328:G:O6 | 2.71 | 0.43 |
| 16:AP:71:ARG:O | 16:AP:73:LEU:N | 2.52 | 0.43 |
| 23:BA:661:C:O3' | 34:BL:18:ARG:HD2 | 2.18 | 0.43 |
| 1:CA:829:G:H2' | 1:CA:830:G:H8 | 1.83 | 0.43 |
| 23:DA:2285:C:C4 | 23:DA:2346:A:N6 | 2.87 | 0.43 |
| 1:CA:1067:A:N3 | 1:CA:1068:G:N9 | 2.66 | 0.43 |
| 27:DE:203:GLN:O | 27:DE:206:ILE:C | 2.57 | 0.43 |
| 1:AA:624:C:H4' | 16:AP:11:SER:N | 2.28 | 0.43 |
| 29:DG:124:GLU:N | 29:DG:132:ARG:O | 2.49 | 0.43 |
| 24:BB:59:A:H2' | 24:BB:60:C:O4' | 2.17 | 0.43 |
| 43:DU:46:LYS:C | 43:DU:48:ALA:N | 2.71 | 0.43 |
| 50:B2:28:PRO:O | 50:B2:29:ILE:HD13 | 2.19 | 0.43 |
| 1:CA:658:G:O2' | 1:CA:659:U:H5' | 2.18 | 0.43 |
| 43:DU:19:LYS:HB3 | 43:DU:20:TYR:CE1 | 2.53 | 0.43 |
| 23:BA:589:C:H2' | 23:BA:590:A:C8 | 2.52 | 0.43 |
| 23:DA:2467:C:H5' | 35:DM:123:HIS:CE1 | 2.53 | 0.43 |
| 29:BG:86:GLU:CG | 29:BG:86:GLU:O | 2.65 | 0.43 |
| 23:DA:1728:G:C3' | 23:DA:1728:G:C8 | 3.02 | 0.43 |
| 1:AA:939:G:C6 | 1:AA:940:C:N4 | 2.86 | 0.43 |
| 23:DA:1591:G:H2' | 23:DA:1592:C:H6 | 1.82 | 0.43 |
| 23:DA:923:C:O2' | 23:DA:924:C:H5' | 2.18 | 0.43 |
| 1:AA:1442:G:C8 | 1:AA:1446:A:C2 | 3.07 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:922:G:H3' | 1:AA:923:A:H8 | 1.84 | 0.43 |
| 23:DA:198:C:H6 | 23:DA:198:C:O5' | 2.01 | 0.43 |
| 23:BA:494:G:N2 | 41:BS:57:ASN:HD21 | 2.16 | 0.43 |
| 14:CN:31:ARG:O | 14:CN:32:SER:HB2 | 2.18 | 0.43 |
| 1:AA:1088:G:C4 | 1:AA:1089:G:C8 | 3.06 | 0.43 |
| 23:BA:570:G:O6 | 23:BA:2499:C:OP1 | 2.37 | 0.43 |
| 26:DD:181:LEU:HD12 | 26:DD:181:LEU:HA | 1.69 | 0.43 |
| 23:DA:1051:G:C2 | 23:DA:1052:C:O2 | 2.71 | 0.43 |
| 27:DE:112:MET:HE3 | 27:DE:112:MET:HB3 | 1.76 | 0.43 |
| 4:CD:4:TYR:OH | 4:CD:66:ARG:HG2 | 2.18 | 0.43 |
| 44:BV:178:GLU:O | 44:BV:178:GLU:HG3 | 2.18 | 0.43 |
| 23:DA:1180:C:O2' | 23:DA:1181:C:H5' | 2.18 | 0.43 |
| 23:BA:1356:G:C4 | 23:BA:1357:U:C6 | 3.06 | 0.43 |
| 16:CP:52:ASP:OD1 | 16:CP:54:GLU:HB2 | 2.18 | 0.43 |
| 35:DM:38:GLU:O | 35:DM:127:ILE:HD11 | 2.19 | 0.43 |
| 12:CL:63:TYR:HB3 | 12:CL:64:GLU:H | 1.63 | 0.43 |
| 12:CL:58:ARG:HA | 12:CL:64:GLU:HG2 | 1.99 | 0.43 |
| 1:CA:224:C:H2' | 1:CA:225:C:H6 | 1.82 | 0.43 |
| 1:AA:883:C:C2' | 1:AA:884:U:H5' | 2.48 | 0.43 |
| 23:BA:880:G:H1 | 23:BA:897:C:H42 | 1.66 | 0.43 |
| 1:CA:994:A:O5' | 1:CA:994:A:H8 | 2.01 | 0.43 |
| 23:DA:1227:G:OP2 | 39:DQ:16:LYS:NZ | 2.48 | 0.43 |
| 1:AA:269:C:H2' | 1:AA:270:A:C8 | 2.53 | 0.43 |
| 1:CA:240:C:H2' | 1:CA:241:C:C6 | 2.54 | 0.43 |
| 1:CA:1480:G:H2' | 1:CA:1481:U:H6 | 1.83 | 0.43 |
| 33:DK:6:THR:O | 33:DK:20:MET:HA | 2.18 | 0.43 |
| 23:BA:270(S):G:H2' | 23:BA:270(T):G:H8 | 1.82 | 0.43 |
| 1:CA:617:G:H5' | 16:CP:45:THR:HG22 | 1.99 | 0.43 |
| 4:AD:53:ASP:OD2 | 5:AE:107:ARG:HD2 | 2.18 | 0.43 |
| 16:AP:50:LYS:O | 16:AP:51:VAL:HG23 | 2.18 | 0.43 |
| 44:DV:146:ILE:HG23 | 44:DV:174:VAL:HG12 | 2.00 | 0.43 |
| 1:CA:117:G:H2' | 1:CA:118:U:O4' | 2.18 | 0.43 |
| 53:B5:15:LYS:HG3 | 53:B5:16:ILE:N | 2.33 | 0.43 |
| 34:DL:77:ARG:HG3 | 34:DL:77:ARG:O | 2.18 | 0.43 |
| 20:AT:37:SER:O | 20:AT:40:ALA:HB3 | 2.18 | 0.43 |
| 51:D3:13:CYS:O | 51:D3:21:TYR:HA | 2.18 | 0.43 |
| 44:DV:75:ASN:O | 44:DV:84:GLU:HB2 | 2.17 | 0.43 |
| 23:DA:458:G:O2' | 52:D4:39:ARG:HD3 | 2.18 | 0.43 |
| 23:DA:394:A:O2' | 23:DA:395:U:H5' | 2.19 | 0.43 |
| 49:B1:53:THR:C | 49:B1:54:LYS:HD2 | 2.39 | 0.43 |
| 16:AP:82:GLN:HE21 | 16:AP:82:GLN:HB3 | 1.57 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 17:CQ:43:LEU:HD12 | 17:CQ:43:LEU:HA | 1.57 | 0.43 |
| 44:DV:70:LEU:HD23 | 44:DV:70:LEU:H | 1.82 | 0.43 |
| 2:CB:21:ARG:HG3 | 2:CB:21:ARG:O | 2.18 | 0.43 |
| 51:D3:25:LYS:HD3 | 53:D5:34:TRP:HZ3 | 1.83 | 0.43 |
| 23:BA:2261:C:H1' | 23:BA:2388:A:N3 | 2.33 | 0.43 |
| 23:BA:673:C:C2' | 23:BA:674:G:H5' | 2.49 | 0.43 |
| 1:CA:1376:U:O2' | 1:CA:1377:A:H5' | 2.18 | 0.43 |
| 22:AV:6195:G:N2 | 22:AV:6196:A:N3 | 2.66 | 0.43 |
| 23:DA:2261:C:C2' | 23:DA:2262:U:H5' | 2.49 | 0.43 |
| 23:BA:2319:G:O6 | 23:BA:2334:G:OP2 | 2.37 | 0.43 |
| 2:CB:68:ILE:HG22 | 2:CB:70:PHE:CE1 | 2.54 | 0.43 |
| 32:BJ:89:LYS:O | 32:BJ:91:GLU:N | 2.51 | 0.43 |
| 41:BS:14:PRO:C | 41:BS:16:LYS:H | 2.22 | 0.43 |
| 40:DR:5:VAL:HG11 | 40:DR:14:VAL:HG21 | 1.98 | 0.43 |
| 23:DA:1019:U:O2' | 23:DA:1021:A:H2 | 2.01 | 0.43 |
| 16:CP:32:TYR:C | 16:CP:32:TYR:CD2 | 2.92 | 0.43 |
| 3:AC:19:GLU:HA | 3:AC:54:ARG:NH2 | 2.32 | 0.43 |
| 30:BH:82:ARG:CA | 30:BH:89:TYR:HB2 | 2.48 | 0.43 |
| 47:BY:10:LEU:O | 47:BY:13:ALA:HB3 | 2.18 | 0.43 |
| 1:AA:373:A:C4 | 1:AA:482:A:N7 | 2.86 | 0.43 |
| 25:DC:126:GLN:HB3 | 25:DC:126:GLN:HE21 | 1.53 | 0.43 |
| 25:DC:145:VAL:O | 25:DC:153:ALA:HA | 2.18 | 0.43 |
| 4:CD:49:ARG:O | 4:CD:51:PRO:HD3 | 2.19 | 0.43 |
| 1:AA:32:A:C2 | 1:AA:33:A:C4 | 3.06 | 0.43 |
| 42:DT:14:SER:OG | 42:DT:17:ALA:HB2 | 2.18 | 0.43 |
| 23:DA:2697:G:H2' | 23:DA:2698:U:O4' | 2.19 | 0.43 |
| 24:DB:71:C:N3 | 24:DB:72:G:C8 | 2.87 | 0.43 |
| 27:DE:9:ILE:HD11 | 27:DE:125:LEU:CD1 | 2.49 | 0.43 |
| 3:CC:35:GLU:OE1 | 3:CC:38:ARG:HD2 | 2.19 | 0.43 |
| 1:AA:1102:A:C5 | 1:AA:1103:C:C5 | 3.07 | 0.43 |
| 1:AA:1105:A:N3 | 1:AA:1106:G:C8 | 2.87 | 0.43 |
| 23:DA:1587:A:C5 | 23:DA:1588:C:C4 | 3.06 | 0.43 |
| 1:AA:1293:G:O2' | 1:AA:1294:G:H5' | 2.18 | 0.43 |
| 36:BN:57:ARG:HG2 | 36:BN:58:GLY:N | 2.29 | 0.43 |
| 23:DA:2744:G:N7 | 23:DA:2755:C:C2 | 2.87 | 0.43 |
| 1:CA:757:U:O2' | 1:CA:879:C:H1' | 2.18 | 0.43 |
| 26:BD:111:ARG:CA | 36:BN:2:ARG:HH11 | 2.26 | 0.43 |
| 16:AP:39:TYR:HE1 | 16:AP:73:LEU:HD22 | 1.83 | 0.43 |
| 41:DS:40:ASN:O | 41:DS:41:LYS:CG | 2.61 | 0.43 |
| 8:CH:119:LEU:CD1 | 8:CH:124:ALA:HA | 2.49 | 0.43 |
| 1:CA:711:G:N2 | 1:CA:712:A:C4 | 2.86 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:DA:601:C:O2' | 23:DA:605:C:H5'' | 2.18 | 0.43 |
| 3:CC:59:ARG:HG2 | 3:CC:63:ASN:O | 2.18 | 0.43 |
| 18:AR:26:LEU:CD1 | 18:AR:42:ARG:HD2 | 2.44 | 0.43 |
| 43:DU:50:ARG:HD3 | 43:DU:51:VAL:N | 2.28 | 0.43 |
| 23:DA:1476:C:H2' | 23:DA:1477:A:H5' | 2.00 | 0.43 |
| 13:CM:23:TYR:CE1 | 13:CM:71:ARG:HD3 | 2.53 | 0.43 |
| 13:AM:3:ARG:HG2 | 13:AM:9:ILE:HD13 | 2.00 | 0.43 |
| 23:BA:2286:A:C8 | 23:BA:2287:A:C6 | 3.06 | 0.43 |
| 2:CB:74:LYS:HD3 | 2:CB:76:GLN:OE1 | 2.19 | 0.43 |
| 50:B2:40:LYS:HD3 | 50:B2:46:CYS:HB3 | 1.99 | 0.43 |
| 23:BA:814:C:H2' | 23:BA:815:C:C6 | 2.53 | 0.43 |
| 1:CA:515:G:H2' | 1:CA:516:U:O4' | 2.18 | 0.43 |
| 23:DA:2402:C:C3' | 23:DA:2403:C:H5' | 2.48 | 0.43 |
| 23:BA:301:G:C6 | 23:BA:302:C:N4 | 2.86 | 0.43 |
| 1:CA:763:G:H2' | 1:CA:764:C:H6 | 1.83 | 0.43 |
| 23:DA:2092:U:C4 | 23:DA:2226:C:OP2 | 2.71 | 0.43 |
| 50:B2:41:PRO:O | 50:B2:44:THR:OG1 | 2.19 | 0.43 |
| 23:BA:198:C:H5' | 23:BA:2244:U:OP1 | 2.18 | 0.43 |
| 10:AJ:45:ARG:HB3 | 10:AJ:47:PHE:CE1 | 2.53 | 0.43 |
| 33:BK:2:ILE:HA | 33:BK:2:ILE:HD12 | 1.75 | 0.43 |
| 23:DA:2870:C:C5 | 23:DA:2871:C:C5 | 3.07 | 0.43 |
| 1:AA:522:C:N4 | 1:AA:528:C:N4 | 2.65 | 0.43 |
| 17:AQ:27:PHE:O | 17:AQ:36:ILE:N | 2.48 | 0.43 |
| 3:AC:83:ARG:O | 3:AC:86:VAL:HG22 | 2.19 | 0.43 |
| 6:CF:47:ARG:HH11 | 6:CF:47:ARG:CG | 2.31 | 0.43 |
| 10:CJ:52:GLY:O | 14:CN:41:ARG:NH2 | 2.51 | 0.43 |
| 10:CJ:50:ILE:HG22 | 14:CN:41:ARG:HH21 | 1.84 | 0.43 |
| 20:AT:82:SER:O | 20:AT:86:ARG:CB | 2.65 | 0.43 |
| 7:CG:50:ILE:O | 7:CG:54:THR:O | 2.36 | 0.43 |
| 8:AH:40:ALA:HB2 | 8:AH:45:ILE:HD11 | 1.99 | 0.43 |
| 8:CH:39:LEU:HB3 | 8:CH:45:ILE:CG2 | 2.46 | 0.43 |
| 23:BA:1748:G:C2 | 23:BA:1749:A:C4 | 3.07 | 0.43 |
| 12:AL:77:GLN:O | 12:AL:79:HIS:N | 2.47 | 0.43 |
| 12:AL:5:THR:CG2 | 12:AL:8:GLN:HG3 | 2.46 | 0.43 |
| 39:BQ:117:GLN:HA | 39:BQ:117:GLN:OE1 | 2.17 | 0.43 |
| 1:CA:775:G:H2' | 1:CA:776:G:H5' | 2.00 | 0.43 |
| 23:BA:2458:G:H21 | 23:BA:2459:A:N6 | 2.16 | 0.43 |
| 6:AF:77:ARG:CZ | 6:AF:77:ARG:HB3 | 2.48 | 0.43 |
| 7:AG:103:TRP:O | 7:AG:104:LEU:C | 2.57 | 0.43 |
| 41:DS:60:ASN:OD1 | 41:DS:60:ASN:N | 2.52 | 0.43 |
| 11:AK:48:ILE:N | 11:AK:48:ILE:HD13 | 2.33 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:179:A:C6 | 1:CA:180:U:C4 | 3.07 | 0.43 |
| 39:DQ:24:TYR:CE1 | 39:DQ:39:LEU:HD23 | 2.53 | 0.43 |
| 23:DA:173:G:H2' | 23:DA:174:C:H6 | 1.84 | 0.43 |
| 1:AA:1479:C:H2' | 1:AA:1480:G:H8 | 1.83 | 0.43 |
| 26:DD:67:PHE:CD1 | 26:DD:74:PRO:HB3 | 2.53 | 0.43 |
| 23:BA:1471:A:C5 | 23:BA:1522:G:N1 | 2.86 | 0.43 |
| 7:CG:78:ARG:HG2 | 7:CG:79:ARG:N | 2.33 | 0.43 |
| 23:BA:644:A:N1 | 23:BA:646:A:C4 | 2.86 | 0.43 |
| 16:CP:47:ASP:C | 16:CP:49:LEU:H | 2.21 | 0.43 |
| 1:AA:1403:C:H1' | 1:AA:1500:A:N1 | 2.34 | 0.43 |
| 27:BE:12:LEU:HD11 | 27:BE:17:ARG:HG2 | 2.01 | 0.43 |
| 1:AA:758:G:H4' | 1:AA:880:C:H4' | 2.00 | 0.43 |
| 23:DA:709:U:C2 | 23:DA:723:G:N2 | 2.87 | 0.43 |
| 15:AO:17:ARG:NH1 | 15:AO:77:ARG:NH1 | 2.67 | 0.43 |
| 37:DO:35:ILE:CG1 | 37:DO:101:LEU:HD23 | 2.49 | 0.43 |
| 23:BA:697:C:C2 | 23:BA:698:C:C5 | 3.07 | 0.43 |
| 48:DZ:12:PRO:O | 48:DZ:14:GLY:N | 2.51 | 0.43 |
| 23:BA:1262:A:N3 | 50:B2:10:LYS:HE3 | 2.34 | 0.43 |
| 1:AA:604:G:C2' | 1:AA:605:U:H5' | 2.48 | 0.43 |
| 23:BA:200:U:O4 | 23:BA:250:G:N2 | 2.52 | 0.43 |
| 36:BN:18:LEU:HD11 | 36:BN:22:ARG:NE | 2.33 | 0.43 |
| 34:DL:29:LYS:N | 34:DL:29:LYS:HD2 | 2.34 | 0.43 |
| 1:AA:1217:C:H5'' | 14:AN:9:LYS:HZ1 | 1.84 | 0.43 |
| 50:B2:6:VAL:HG13 | 50:B2:7:PRO:HD2 | 2.00 | 0.43 |
| 7:CG:21:VAL:HG23 | 7:CG:22:LEU:N | 2.34 | 0.43 |
| 23:DA:631:A:OP2 | 53:D5:47:LYS:NZ | 2.34 | 0.43 |
| 34:DL:143:GLY:O | 34:DL:145:PRO:HD3 | 2.19 | 0.43 |
| 23:BA:2250:G:C5 | 35:BM:82:ARG:HD2 | 2.53 | 0.43 |
| 32:BJ:143:LEU:C | 32:BJ:144:LYS:HD2 | 2.39 | 0.43 |
| 10:AJ:48:THR:HG22 | 10:AJ:62:HIS:CG | 2.54 | 0.43 |
| 23:BA:1528:A:N1 | 23:BA:1529:A:C2 | 2.87 | 0.43 |
| 38:DP:74:ARG:CD | 38:DP:76:PHE:CZ | 3.01 | 0.43 |
| 10:AJ:50:ILE:HA | 10:AJ:60:ARG:HB3 | 2.01 | 0.43 |
| 1:CA:1226:C:N4 | 13:CM:104:ARG:HB2 | 2.33 | 0.43 |
| 5:AE:102:ALA:HB2 | 5:AE:120:THR:HG21 | 1.98 | 0.43 |
| 23:DA:675:A:OP1 | 27:DE:63:LYS:NZ | 2.49 | 0.43 |
| 40:BR:77:ALA:C | 40:BR:79:VAL:N | 2.72 | 0.43 |
| 28:BF:86:MET:H | 28:BF:87:PRO:HD2 | 1.79 | 0.43 |
| 39:DQ:104:GLN:HB3 | 40:DR:44:LYS:CE | 2.49 | 0.43 |
| 40:DR:47:VAL:HG12 | 40:DR:49:THR:O | 2.18 | 0.43 |
| 16:CP:20:VAL:HG21 | 16:CP:32:TYR:CB | 2.49 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 30:BH:126:TYR:HB2 | 30:BH:142:VAL:HG21 | 1.99 | 0.43 |
| 23:DA:2295:C:H2' | 23:DA:2296:U:O5' | 2.19 | 0.43 |
| 1:AA:35:G:C2 | 1:AA:550:G:C2 | 3.05 | 0.43 |
| 12:AL:30:PRO:HD2 | 12:AL:31:PHE:H | 1.83 | 0.43 |
| 2:CB:193:ASP:O | 2:CB:196:LEU:HG | 2.19 | 0.43 |
| 23:DA:549:G:H2' | 23:DA:550:G:O4' | 2.18 | 0.43 |
| 25:DC:245:PRO:HA | 25:DC:246:PRO:HD3 | 1.84 | 0.43 |
| 24:DB:70:C:C2 | 24:DB:71:C:C5 | 3.07 | 0.43 |
| 1:AA:91:C:C2 | 1:AA:92:G:N7 | 2.86 | 0.43 |
| 23:DA:1209:G:N2 | 23:DA:1210:A:H62 | 2.02 | 0.43 |
| 3:CC:205:GLY:O | 3:CC:206:GLU:HB2 | 2.18 | 0.43 |
| 5:CE:110:LEU:HD23 | 5:CE:110:LEU:N | 2.34 | 0.43 |
| 23:DA:1651:G:H2' | 23:DA:1652:A:O4' | 2.19 | 0.43 |
| 44:BV:163:LEU:N | 44:BV:163:LEU:HD23 | 2.34 | 0.43 |
| 1:CA:1104:G:C2 | 1:CA:1105:A:C8 | 3.07 | 0.43 |
| 1:AA:1106:G:C2 | 1:AA:1107:C:C5 | 3.06 | 0.43 |
| 1:CA:41:G:C6 | 1:CA:42:G:C6 | 3.06 | 0.43 |
| 45:BW:31:VAL:HG21 | 45:BW:61:ALA:HB2 | 2.00 | 0.43 |
| 45:BW:49:LYS:N | 45:BW:80:HIS:ND1 | 2.55 | 0.43 |
| 46:DX:11:ARG:CB | 46:DX:12:PRO:CD | 2.88 | 0.43 |
| 36:DN:55:ALA:CA | 36:DN:80:PHE:CE1 | 2.93 | 0.43 |
| 4:AD:159:ARG:HA | 4:AD:162:LEU:HB2 | 2.00 | 0.43 |
| 1:AA:1349:A:OP1 | 9:AI:120:ARG:HB2 | 2.19 | 0.43 |
| 50:D2:25:LEU:HD12 | 50:D2:25:LEU:N | 2.19 | 0.43 |
| 41:DS:32:ALA:O | 41:DS:35:ILE:N | 2.52 | 0.43 |
| 23:BA:557:U:C2 | 23:BA:558:G:C8 | 3.07 | 0.43 |
| 23:DA:2757:A:H2' | 23:DA:2758:A:H5' | 2.00 | 0.43 |
| 23:DA:2744:G:C2 | 23:DA:2761:G:C6 | 3.07 | 0.43 |
| 26:BD:110:GLY:O | 36:BN:5:LYS:NZ | 2.48 | 0.43 |
| 43:BU:100:ALA:O | 43:BU:101:LYS:HB3 | 2.18 | 0.43 |
| 1:CA:1119:C:H2' | 1:CA:1120:G:C8 | 2.54 | 0.43 |
| 23:BA:1502:C:C6 | 23:BA:1502:C:C3' | 3.01 | 0.43 |
| 1:AA:659:U:C2' | 1:AA:660:G:H5' | 2.49 | 0.43 |
| 23:BA:1313:U:C2' | 23:BA:1313:U:O2 | 2.65 | 0.43 |
| 16:CP:72:ARG:HD3 | 16:CP:73:LEU:HD21 | 2.00 | 0.43 |
| 1:AA:59:A:H5'' | 1:AA:60:A:C5' | 2.48 | 0.43 |
| 1:CA:457:C:C2' | 1:CA:457:C:O2 | 2.60 | 0.43 |
| 23:DA:2549:G:C2' | 23:DA:2550:G:H5' | 2.49 | 0.43 |
| 1:AA:28:G:C6 | 1:AA:29:G:C5 | 3.07 | 0.43 |
| 3:AC:68:VAL:HG12 | 3:AC:70:VAL:CG2 | 2.49 | 0.43 |
| 1:CA:556:C:O2' | 1:CA:557:G:H5' | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1066:C:C2' | 1:CA:1066:C:O2 | 2.65 | 0.43 |
| 50:D2:42:PRO:HB2 | 50:D2:43:HIS:CD2 | 2.54 | 0.43 |
| 23:DA:258:G:C4 | 23:DA:259:G:C8 | 3.07 | 0.43 |
| 25:BC:181:GLU:HA | 25:BC:272:ALA:CB | 2.48 | 0.43 |
| 15:CO:39:LEU:HD23 | 15:CO:39:LEU:HA | 1.79 | 0.43 |
| 1:CA:1206:G:C6 | 1:CA:1207:G:C5 | 3.07 | 0.43 |
| 23:DA:302:C:H2' | 23:DA:303:U:H6 | 1.82 | 0.43 |
| 33:BK:102:VAL:HB | 33:BK:106:LEU:CD1 | 2.48 | 0.43 |
| 34:BL:88:LEU:HA | 34:BL:88:LEU:HD12 | 1.39 | 0.43 |
| 23:DA:2663:G:C5 | 23:DA:2664:G:N7 | 2.86 | 0.43 |
| 1:AA:570:G:C6 | 1:AA:873:A:C2 | 3.07 | 0.43 |
| 1:AA:918:A:H2' | 1:AA:919:A:C8 | 2.53 | 0.43 |
| 23:BA:988:A:H8 | 23:BA:988:A:O5' | 2.00 | 0.43 |
| 17:AQ:27:PHE:HB2 | 17:AQ:28:PRO:CD | 2.49 | 0.43 |
| 3:AC:35:GLU:O | 3:AC:39:ILE:HG13 | 2.18 | 0.43 |
| 25:BC:257:LEU:CD2 | 25:BC:257:LEU:C | 2.86 | 0.43 |
| 23:DA:186:G:H2' | 23:DA:187:G:H8 | 1.83 | 0.43 |
| 23:DA:2213:U:H6 | 23:DA:2213:U:O5' | 2.02 | 0.43 |
| 1:CA:186(E):C:H2' | 1:CA:186(F):C:C6 | 2.53 | 0.43 |
| 1:AA:638:G:C2 | 1:AA:639:G:C8 | 3.07 | 0.43 |
| 1:CA:803:G:H2' | 1:CA:804:U:O4' | 2.18 | 0.43 |
| 41:BS:45:TYR:CD2 | 41:BS:46:PHE:CE1 | 3.06 | 0.43 |
| 6:AF:16:GLN:HA | 6:AF:19:LEU:HB3 | 2.01 | 0.43 |
| 46:BX:67:ILE:HB | 46:BX:68:PRO:CD | 2.49 | 0.43 |
| 23:BA:1850:G:C4 | 23:BA:1851:U:C5 | 3.07 | 0.43 |
| 46:DX:59:THR:OG1 | 46:DX:60:PHE:N | 2.51 | 0.43 |
| 23:DA:511:U:H5 | 23:DA:512:G:C5 | 2.35 | 0.43 |
| 23:BA:880:G:N2 | 23:BA:898:C:C4 | 2.86 | 0.43 |
| 33:DK:7:TYR:CD1 | 33:DK:20:MET:HB3 | 2.54 | 0.43 |
| 29:DG:105:LEU:N | 29:DG:105:LEU:CD2 | 2.82 | 0.43 |
| 18:CR:36:ASN:HB2 | 18:CR:39:VAL:CG2 | 2.48 | 0.43 |
| 1:CA:419:C:C2' | 1:CA:420:U:H5' | 2.49 | 0.43 |
| 1:AA:764:C:H2' | 1:AA:765:G:O4' | 2.18 | 0.43 |
| 23:BA:298:G:P | 43:BU:85:VAL:CG2 | 3.06 | 0.43 |
| 28:DF:16:ARG:HB3 | 28:DF:17:PRO:HD3 | 1.99 | 0.43 |
| 6:AF:29:ALA:HA | 6:AF:32:ASN:OD1 | 2.18 | 0.43 |
| 1:CA:283:C:C2 | 1:CA:284:G:C8 | 3.06 | 0.43 |
| 23:DA:1416:G:HO2' | 23:DA:1417:C:H6 | 1.67 | 0.43 |
| 53:D5:15:LYS:CG | 53:D5:16:ILE:N | 2.82 | 0.43 |
| 23:DA:2794:C:N4 | 23:DA:2802:G:H1 | 2.17 | 0.43 |
| 36:BN:36:THR:HG23 | 36:BN:41:ALA:HB2 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:CB:60:ASP:O | 2:CB:64:ARG:CG | 2.66 | 0.43 |
| 10:AJ:78:ASN:O | 10:AJ:82:ILE:HG12 | 2.18 | 0.43 |
| 23:BA:1206:G:C6 | 23:BA:1207:C:C4 | 3.06 | 0.43 |
| 23:DA:2313:C:H4' | 28:DF:91:ARG:HG3 | 1.99 | 0.43 |
| 15:CO:66:LEU:N | 15:CO:66:LEU:CD1 | 2.82 | 0.43 |
| 23:BA:1955:U:O4 | 23:BA:2554:U:H5 | 2.01 | 0.43 |
| 34:BL:59:LEU:N | 34:BL:61:ARG:HE | 2.16 | 0.43 |
| 47:DY:3:LEU:O | 47:DY:5:GLU:N | 2.52 | 0.43 |
| 23:BA:858:U:O2 | 23:BA:2268:A:N3 | 2.51 | 0.43 |
| 34:BL:126:VAL:HG23 | 34:BL:145:PRO:HG2 | 2.00 | 0.43 |
| 7:CG:9:VAL:HG12 | 7:CG:10:ARG:H | 1.83 | 0.43 |
| 1:AA:986:A:C4 | 1:AA:1220:G:N2 | 2.87 | 0.43 |
| 22:CV:6193:U:C4 | 22:CV:6194:C:C4 | 3.07 | 0.43 |
| 23:DA:2845:G:C2 | 23:DA:2846:G:C5 | 3.06 | 0.43 |
| 1:CA:946:A:N3 | 1:CA:1333:A:H2 | 2.16 | 0.43 |
| 23:BA:1253:A:C3' | 23:BA:1254:A:H5' | 2.48 | 0.43 |
| 34:DL:32:THR:HB | 34:DL:36:LYS:HB2 | 2.00 | 0.43 |
| 11:AK:114:VAL:HA | 11:AK:115:PRO:HD2 | 1.73 | 0.43 |
| 16:CP:58:TYR:HE2 | 16:CP:59:TRP:CZ3 | 2.37 | 0.43 |
| 16:CP:5:ARG:CB | 16:CP:67:THR:OG1 | 2.67 | 0.43 |
| 23:BA:593:G:H4' | 53:B5:62:LEU:CD1 | 2.48 | 0.43 |
| 25:DC:177:LEU:HD23 | 25:DC:177:LEU:HA | 1.85 | 0.43 |
| 25:BC:36:PRO:O | 25:BC:37:LEU:HB2 | 2.18 | 0.43 |
| 4:CD:106:TYR:HE1 | 4:CD:113:SER:HA | 1.84 | 0.43 |
| 25:BC:50:THR:HG23 | 25:BC:51:VAL:N | 2.32 | 0.43 |
| 30:DH:77:LEU:HD23 | 30:DH:105:HIS:HE1 | 1.83 | 0.43 |
| 28:DF:41:GLN:HG2 | 28:DF:155:MET:CB | 2.47 | 0.43 |
| 23:BA:2634:G:H5' | 26:BD:61:ARG:NH1 | 2.33 | 0.43 |
| 1:AA:395:C:O2 | 1:AA:395:C:H2' | 2.18 | 0.43 |
| 23:BA:2713:A:C3' | 23:BA:2714:G:C5' | 2.96 | 0.43 |
| 23:DA:2634:G:O2' | 23:DA:2635:C:H5' | 2.19 | 0.43 |
| 26:DD:50:GLY:HA3 | 26:DD:75:VAL:HG21 | 2.01 | 0.43 |
| 1:CA:1331:G:H4' | 1:CA:1331:G:OP1 | 2.18 | 0.43 |
| 1:AA:57:G:C6 | 1:AA:58:C:C4 | 3.06 | 0.43 |
| 6:AF:45:LEU:O | 6:AF:46:ARG:HG2 | 2.19 | 0.43 |
| 1:CA:11:G:C6 | 1:CA:12:U:C4 | 3.06 | 0.43 |
| 46:BX:45:ASN:HD22 | 46:BX:46:LEU:H | 1.64 | 0.43 |
| 1:CA:725:G:C4 | 1:CA:726:C:C5 | 3.06 | 0.43 |
| 1:AA:1014:A:H5' | 19:AS:14:HIS:CG | 2.52 | 0.43 |
| 1:AA:987:G:H2' | 1:AA:988:G:C8 | 2.54 | 0.43 |
| 40:DR:34:GLU:O | 40:DR:36:PRO:CD | 2.59 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:819:A:N7 | 1:CA:1529:G:C2 | 2.87 | 0.43 |
| 1:AA:59:A:H3' | 1:AA:331:G:H22 | 1.83 | 0.43 |
| 1:AA:626:U:O2 | 1:AA:627:G:C8 | 2.71 | 0.43 |
| 45:DW:72:ARG:O | 45:DW:73:GLY:C | 2.56 | 0.43 |
| 28:BF:120:LEU:HD13 | 28:BF:133:LEU:HD13 | 2.01 | 0.43 |
| 15:CO:29:VAL:O | 15:CO:30:ALA:C | 2.56 | 0.43 |
| 32:DJ:66:THR:HB | 32:DJ:71:MET:HE3 | 2.00 | 0.43 |
| 23:DA:384:U:H2' | 23:DA:385:C:H6 | 1.83 | 0.43 |
| 1:CA:66:G:C6 | 1:CA:67:C:C5 | 3.07 | 0.43 |
| 3:CC:58:GLU:O | 3:CC:64:VAL:HA | 2.19 | 0.43 |
| 25:DC:136:ILE:HA | 25:DC:137:PRO:HD3 | 1.81 | 0.43 |
| 23:BA:1401:G:C4 | 23:BA:1402:C:C5 | 3.07 | 0.43 |
| 1:AA:913:A:O2' | 1:AA:914:A:OP2 | 2.36 | 0.43 |
| 23:BA:2207:C:H2' | 23:BA:2208:U:O4' | 2.19 | 0.43 |
| 23:BA:2101:G:C6 | 23:BA:2102:U:C4 | 3.06 | 0.43 |
| 23:BA:2864:G:C6 | 23:BA:2865:U:N3 | 2.87 | 0.43 |
| 1:CA:21:G:C2 | 1:CA:22:G:C6 | 3.06 | 0.43 |
| 3:CC:22:TRP:HZ3 | 3:CC:24:ALA:HB2 | 1.83 | 0.43 |
| 1:AA:128:G:H4' | 17:AQ:3:LYS:HG2 | 2.00 | 0.43 |
| 23:BA:319:C:C2 | 23:BA:333:G:N2 | 2.87 | 0.43 |
| 1:CA:570:G:C6 | 1:CA:873:A:C2 | 3.06 | 0.43 |
| 1:CA:918:A:C2 | 1:CA:919:A:C4 | 3.06 | 0.43 |
| 1:CA:918:A:H2' | 1:CA:919:A:C8 | 2.54 | 0.43 |
| 30:DH:2:LYS:HG3 | 30:DH:39:ALA:CB | 2.46 | 0.43 |
| 1:CA:1079:G:C2 | 1:CA:1080:A:C2 | 3.07 | 0.43 |
| 10:AJ:10:GLY:HA3 | 10:AJ:16:LEU:HD21 | 2.00 | 0.43 |
| 23:DA:2870:C:H2' | 23:DA:2871:C:O4' | 2.19 | 0.43 |
| 17:AQ:27:PHE:CE2 | 17:AQ:36:ILE:HG13 | 2.54 | 0.43 |
| 23:DA:1006:C:C2' | 23:DA:1007:C:H5' | 2.48 | 0.43 |
| 51:B3:30:THR:CG2 | 51:B3:31:PRO:HD2 | 2.48 | 0.43 |
| 35:DM:45:GLN:O | 35:DM:49:ALA:HB2 | 2.17 | 0.43 |
| 23:BA:2460:U:C2 | 23:BA:2461:C:C6 | 3.07 | 0.43 |
| 39:BQ:18:LEU:HD12 | 39:BQ:18:LEU:HA | 1.77 | 0.43 |
| 1:AA:638:G:H2' | 1:AA:639:G:H5' | 2.01 | 0.43 |
| 23:DA:1917:U:O2' | 23:DA:1918:A:H5' | 2.18 | 0.43 |
| 7:AG:30:ILE:HD12 | 7:AG:120:ILE:HD11 | 2.01 | 0.43 |
| 1:CA:928:G:N2 | 1:CA:1390:U:O2 | 2.52 | 0.43 |
| 23:BA:914:C:H3' | 23:BA:914:C:C6 | 2.53 | 0.43 |
| 44:DV:76:LEU:H | 44:DV:76:LEU:HD12 | 1.83 | 0.43 |
| 35:BM:30:GLY:CA | 35:BM:107:ALA:HB2 | 2.48 | 0.43 |
| 23:BA:2744:G:H1' | 23:BA:2761:G:N2 | 2.33 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BA:2703:C:C2' | 23:BA:2704:C:H5' | 2.49 | 0.43 |
| 1:CA:983:A:H3' | 1:CA:983:A:N3 | 2.34 | 0.43 |
| 23:DA:500:G:N2 | 23:DA:502:A:H3' | 2.33 | 0.43 |
| 23:DA:2695:C:H2' | 23:DA:2696:U:C6 | 2.54 | 0.43 |
| 23:DA:2194:G:C6 | 23:DA:2195:C:C4 | 3.07 | 0.43 |
| 23:BA:2194:G:C6 | 23:BA:2195:C:C4 | 3.06 | 0.43 |
| 1:CA:646:U:C4 | 1:CA:647:C:N4 | 2.87 | 0.43 |
| 23:BA:697:C:N3 | 23:BA:698:C:C5 | 2.87 | 0.43 |
| 33:BK:7:TYR:CE1 | 33:BK:20:MET:HB3 | 2.54 | 0.43 |
| 23:DA:1835:G:H2' | 23:DA:1835:G:N3 | 2.34 | 0.43 |
| 17:CQ:76:LEU:HD12 | 17:CQ:77:VAL:H | 1.83 | 0.43 |
| 9:CI:5:TYR:O | 9:CI:84:ALA:HA | 2.19 | 0.43 |
| 1:AA:791:G:C6 | 1:AA:792:A:N7 | 2.87 | 0.43 |
| 23:BA:1629:U:H2' | 23:BA:1630:G:O4' | 2.19 | 0.43 |
| 19:AS:50:ALA:HB1 | 19:AS:57:HIS:HB3 | 2.00 | 0.43 |
| 23:BA:702:G:C2 | 23:BA:731:C:C2 | 3.07 | 0.43 |
| 48:DZ:1:MET:HB3 | 48:DZ:39:ASP:HB3 | 2.00 | 0.43 |
| 23:BA:2612:C:H2' | 23:BA:2613:U:O5' | 2.19 | 0.43 |
| 17:CQ:14:LYS:HD2 | 17:CQ:14:LYS:H | 1.84 | 0.43 |
| 23:DA:2392:A:H2' | 23:DA:2393:A:H5' | 2.00 | 0.43 |
| 23:BA:2415:G:H4' | 34:BL:67:MET:N | 2.34 | 0.43 |
| 23:BA:310:A:N1 | 23:BA:312:G:H1' | 2.34 | 0.43 |
| 33:DK:77:ILE:HD11 | 38:DP:72:VAL:CG1 | 2.49 | 0.43 |
| 32:DJ:51:THR:O | 32:DJ:54:ALA:HB3 | 2.19 | 0.43 |
| 1:CA:1368:G:C2 | 1:CA:1369:C:C6 | 3.07 | 0.43 |
| 9:CI:9:ARG:O | 9:CI:10:ARG:HB2 | 2.19 | 0.43 |
| 25:BC:205:VAL:O | 25:BC:206:LEU:C | 2.55 | 0.43 |
| 25:BC:16:MET:HE2 | 25:BC:211:ARG:HD3 | 2.01 | 0.43 |
| 22:CV:6191:A:C6 | 22:CV:6192:G:C5 | 3.07 | 0.43 |
| 23:DA:2846:G:C8 | 23:DA:2847:U:C5 | 3.06 | 0.43 |
| 1:CA:977:A:HO2' | 1:CA:978:A:H5'' | 1.84 | 0.43 |
| 1:CA:551:U:H5' | 12:CL:118:LYS:HZ2 | 1.83 | 0.43 |
| 23:BA:2295:C:N3 | 23:BA:2296:U:C5 | 2.87 | 0.43 |
| 24:BB:7:G:H5'' | 37:BO:29:PHE:CZ | 2.53 | 0.43 |
| 2:CB:180:LEU:C | 2:CB:181:PHE:CD2 | 2.92 | 0.43 |
| 23:DA:1902:C:C2' | 23:DA:1903:G:O5' | 2.67 | 0.43 |
| 39:DQ:69:CYS:HB3 | 39:DQ:79:PHE:HD2 | 1.83 | 0.43 |
| 34:DL:50:ARG:CD | 34:DL:51:PHE:N | 2.78 | 0.43 |
| 16:AP:18:ARG:O | 16:AP:19:ILE:O | 2.37 | 0.43 |
| 1:AA:492:G:C6 | 1:AA:493:G:C5 | 3.06 | 0.43 |
| 1:CA:392:G:C2 | 1:CA:393:A:C4 | 3.07 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:BY:24:LEU:CD2 | 47:BY:28:LYS:HG2 | 2.49 | 0.43 |
| 47:BY:60:LEU:HD23 | 47:BY:60:LEU:HA | 1.49 | 0.43 |
| 42:DT:80:ILE:HG12 | 42:DT:80:ILE:O | 2.16 | 0.43 |
| 23:BA:1210:A:H4' | 23:BA:1211:U:O5' | 2.18 | 0.43 |
| 41:BS:75:TYR:HD2 | 41:BS:75:TYR:C | 2.22 | 0.43 |
| 1:AA:393:A:C4 | 1:AA:394:G:C8 | 3.07 | 0.43 |
| 23:BA:1640:C:H6 | 23:BA:1640:C:H5' | 1.84 | 0.43 |
| 20:AT:57:ARG:C | 20:AT:59:ALA:N | 2.72 | 0.43 |
| 42:BT:30:VAL:HG21 | 42:BT:79:ALA:HB3 | 2.00 | 0.43 |
| 46:BX:90:ILE:O | 46:BX:94:LEU:HD22 | 2.18 | 0.43 |
| 43:DU:100:ALA:O | 43:DU:101:LYS:HB3 | 2.19 | 0.43 |
| 43:DU:81:LYS:HG2 | 43:DU:97:ARG:HB3 | 2.01 | 0.43 |
| 25:DC:175:LEU:HD12 | 25:DC:185:VAL:HG21 | 2.00 | 0.43 |
| 26:DD:120:TRP:NE1 | 26:DD:155:LYS:HB3 | 2.34 | 0.43 |
| 23:BA:1263:U:O2' | 50:B2:11:THR:HG23 | 2.19 | 0.43 |
| 23:BA:528:A:C2' | 23:BA:529:A:O5' | 2.66 | 0.43 |
| 1:CA:598:U:H4' | 8:CH:94:TYR:CD1 | 2.54 | 0.43 |
| 6:AF:60:PHE:CE2 | 18:AR:78:LEU:HD21 | 2.54 | 0.43 |
| 46:BX:45:ASN:C | 46:BX:45:ASN:HD22 | 2.22 | 0.43 |
| 26:BD:37:ARG:HA | 26:BD:42:ASP:OD2 | 2.19 | 0.43 |
| 16:AP:71:ARG:C | 16:AP:73:LEU:N | 2.71 | 0.43 |
| 25:DC:25:THR:O | 25:DC:27:THR:HG22 | 2.18 | 0.43 |
| 33:DK:88:ASN:O | 33:DK:91:LEU:HA | 2.19 | 0.43 |
| 23:DA:380:U:H4' | 46:DX:21:ARG:O | 2.18 | 0.43 |
| 23:DA:2563:U:O2 | 23:DA:2565:A:C8 | 2.71 | 0.43 |
| 34:BL:70:GLN:O | 34:BL:71:VAL:C | 2.56 | 0.43 |
| 23:DA:475:U:C4 | 23:DA:481:G:O6 | 2.72 | 0.43 |
| 23:DA:1476:C:O2' | 23:DA:1477:A:H5' | 2.18 | 0.43 |
| 24:DB:61:G:C6 | 24:DB:62:C:C4 | 3.07 | 0.43 |
| 23:DA:2636:U:C2 | 23:DA:2637:U:C5 | 3.07 | 0.43 |
| 1:CA:865:A:H5' | 1:CA:1078:U:O4 | 2.19 | 0.43 |
| 23:BA:1166:C:H42 | 23:BA:1183:G:H1 | 1.67 | 0.43 |
| 25:BC:221:VAL:HG22 | 25:BC:226:MET:CE | 2.49 | 0.43 |
| 41:BS:57:ASN:O | 41:BS:58:ALA:C | 2.56 | 0.43 |
| 1:CA:427:U:O4 | 1:CA:428:G:N1 | 2.51 | 0.43 |
| 1:CA:1311:G:H1 | 1:CA:1326:C:N4 | 2.11 | 0.43 |
| 36:DN:85:PRO:HA | 36:DN:88:ARG:NH1 | 2.33 | 0.43 |
| 23:BA:1449:G:C4 | 23:BA:1450:C:C5 | 3.07 | 0.43 |
| 1:CA:160:A:N7 | 1:CA:161:A:C5 | 2.87 | 0.43 |
| 1:AA:1430:C:C2 | 1:AA:1471:G:C2 | 3.06 | 0.43 |
| 6:AF:55:ASP:OD1 | 6:AF:56:PRO:HD2 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:CG:26:PHE:O | 7:CG:30:ILE:HG12 | 2.19 | 0.43 |
| 1:CA:806:C:O2' | 1:CA:807:A:H5' | 2.18 | 0.43 |
| 23:BA:958:U:H5' | 35:BM:14:ARG:HH11 | 1.83 | 0.43 |
| 46:BX:51:VAL:HG12 | 46:BX:58:ILE:HG12 | 2.00 | 0.43 |
| 23:DA:1515:C:H2' | 23:DA:1515:C:O2 | 2.19 | 0.43 |
| 23:BA:189:G:C8 | 23:BA:189:G:C3' | 3.02 | 0.43 |
| 1:AA:991:U:O2' | 1:AA:993:G:H8 | 2.01 | 0.43 |
| 2:CB:144:ARG:O | 2:CB:147:LYS:HB3 | 2.18 | 0.43 |
| 23:DA:963:U:H2' | 23:DA:964:C:H6 | 1.84 | 0.43 |
| 33:DK:20:MET:HG3 | 33:DK:20:MET:O | 2.17 | 0.43 |
| 12:CL:19:LYS:N | 12:CL:19:LYS:HD3 | 2.33 | 0.43 |
| 23:BA:2564:A:C2 | 23:BA:2647:U:H4' | 2.54 | 0.43 |
| 7:AG:78:ARG:HH11 | 7:AG:154:TYR:HB3 | 1.84 | 0.43 |
| 1:CA:380:G:N2 | 1:CA:384:G:C5 | 2.87 | 0.43 |
| 1:CA:164:U:H2' | 1:CA:165:C:C6 | 2.54 | 0.43 |
| 1:CA:167:G:C2' | 1:CA:168:G:H5' | 2.48 | 0.43 |
| 36:DN:18:LEU:HD13 | 36:DN:19:ALA:N | 2.34 | 0.43 |
| 1:AA:164:U:H2' | 1:AA:165:C:C6 | 2.54 | 0.43 |
| 1:CA:242:C:H2' | 1:CA:243:A:H5'' | 2.01 | 0.43 |
| 1:CA:385:C:H3' | 1:CA:385:C:C6 | 2.54 | 0.43 |
| 23:BA:32:C:O2' | 23:BA:33:U:H5' | 2.19 | 0.43 |
| 1:CA:288:A:O2' | 1:CA:289:G:H5' | 2.19 | 0.43 |
| 1:AA:892:A:C6 | 1:AA:893:C:C4 | 3.06 | 0.43 |
| 1:AA:583:A:N6 | 1:AA:758:G:H1' | 2.34 | 0.43 |
| 23:BA:844:C:O2' | 23:BA:845:G:H5' | 2.19 | 0.43 |
| 30:DH:38:LEU:HA | 30:DH:38:LEU:HD13 | 1.87 | 0.43 |
| 23:DA:270(F):G:C5 | 23:DA:270(G):U:C5 | 3.06 | 0.43 |
| 23:DA:1603:A:OP1 | 23:DA:1604:C:OP2 | 2.37 | 0.43 |
| 27:BE:138:GLU:O | 27:BE:141:ALA:HB3 | 2.18 | 0.43 |
| 23:BA:1370:C:H2' | 23:BA:1371:G:C5' | 2.49 | 0.43 |
| 23:BA:1964:G:H4' | 23:BA:1965:C:OP2 | 2.19 | 0.43 |
| 27:DE:139:PHE:HB2 | 27:DE:166:ALA:HB1 | 2.00 | 0.43 |
| 26:DD:153:GLY:O | 26:DD:154:LYS:C | 2.55 | 0.43 |
| 29:DG:126:PRO:HG2 | 29:DG:130:ARG:HB3 | 2.01 | 0.43 |
| 23:BA:869:G:C4 | 23:BA:870:A:C8 | 3.07 | 0.43 |
| 33:BK:72:PRO:C | 33:BK:74:GLY:H | 2.21 | 0.43 |
| 23:DA:852:G:H2' | 23:DA:853:G:C8 | 2.54 | 0.43 |
| 23:DA:77:C:OP1 | 47:DY:59:ARG:HD3 | 2.19 | 0.43 |
| 34:DL:96:THR:HB | 34:DL:97:PRO:HD2 | 2.01 | 0.43 |
| 23:BA:310:A:OP1 | 43:BU:17:SER:O | 2.37 | 0.43 |
| 23:DA:1275:A:C5 | 36:DN:16:HIS:ND1 | 2.87 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 33:DK:75:SER:HB2 | 38:DP:75:ILE:O | 2.19 | 0.43 |
| 34:BL:107:LYS:C | 34:BL:109:GLY:H | 2.22 | 0.43 |
| 34:BL:80:TYR:CE1 | 34:BL:111:ARG:CG | 3.02 | 0.43 |
| 32:DJ:143:LEU:C | 32:DJ:144:LYS:HD2 | 2.39 | 0.43 |
| 1:CA:1348:U:H4' | 9:CI:120:ARG:HH11 | 1.84 | 0.43 |
| 1:AA:1364:U:H5' | 21:AU:14:TRP:CZ2 | 2.54 | 0.43 |
| 23:DA:2258:C:H4' | 23:DA:2259:G:OP2 | 2.19 | 0.43 |
| 23:BA:1899:G:H21 | 23:BA:1902:C:H5 | 1.67 | 0.43 |
| 23:BA:2579:C:H2' | 23:BA:2580:U:O4' | 2.19 | 0.43 |
| 39:DQ:82:GLY:CA | 39:DQ:113:ALA:HB1 | 2.42 | 0.43 |
| 6:AF:52:ILE:CD1 | 6:AF:87:ARG:HH21 | 2.31 | 0.43 |
| 23:DA:1144:G:C6 | 23:DA:1145:C:N4 | 2.87 | 0.43 |
| 1:AA:438:G:O2' | 1:AA:493:G:C2 | 2.65 | 0.43 |
| 1:AA:409:G:H5' | 4:AD:24:GLU:HB3 | 2.00 | 0.43 |
| 1:AA:36:C:H4' | 12:AL:121:THR:O | 2.19 | 0.43 |
| 25:BC:32:SER:O | 25:BC:36:PRO:HD2 | 2.18 | 0.43 |
| 1:CA:395:C:H2' | 1:CA:395:C:O2 | 2.17 | 0.43 |
| 23:DA:142:G:H2' | 23:DA:143:C:O4' | 2.19 | 0.43 |
| 30:DH:107:ILE:HD12 | 30:DH:108:THR:H | 1.84 | 0.43 |
| 13:AM:37:THR:OG1 | 13:AM:39:ILE:HG12 | 2.19 | 0.43 |
| 24:DB:45:A:C2 | 24:DB:46:A:O4' | 2.72 | 0.43 |
| 23:DA:1826:G:H2' | 23:DA:1827:C:H6 | 1.83 | 0.43 |
| 1:CA:397:A:N7 | 1:CA:548:G:H8 | 2.14 | 0.43 |
| 3:AC:57:ILE:HD11 | 3:AC:66:VAL:HG22 | 2.00 | 0.43 |
| 23:DA:1785:A:O2' | 23:DA:1786:A:H2' | 2.19 | 0.43 |
| 44:BV:48:PHE:CE2 | 44:BV:71:VAL:HG21 | 2.54 | 0.43 |
| 44:BV:57:ILE:HG22 | 44:BV:59:LEU:HG | 2.01 | 0.43 |
| 25:BC:231:HIS:CG | 25:BC:232:PRO:HD2 | 2.52 | 0.43 |
| 1:AA:194:C:H5'' | 20:AT:65:LYS:HG2 | 2.01 | 0.43 |
| 23:DA:1607:C:N4 | 23:DA:1621:U:C3' | 2.82 | 0.43 |
| 2:CB:97:TRP:CE3 | 2:CB:98:LEU:O | 2.72 | 0.43 |
| 23:BA:2767:C:C2' | 23:BA:2768:C:H5' | 2.49 | 0.43 |
| 1:AA:448:A:OP2 | 1:AA:485:G:N2 | 2.49 | 0.43 |
| 25:BC:172:TYR:CD1 | 25:BC:185:VAL:O | 2.66 | 0.43 |
| 1:CA:506:G:C5 | 1:CA:507:C:C4 | 3.07 | 0.43 |
| 1:AA:57:G:N7 | 1:AA:58:C:C5 | 2.87 | 0.43 |
| 27:DE:173:VAL:CG1 | 27:DE:174:VAL:N | 2.81 | 0.43 |
| 1:CA:586:C:O2' | 1:CA:878:G:H4' | 2.18 | 0.43 |
| 43:BU:81:LYS:HD2 | 43:BU:96:ILE:HD12 | 2.00 | 0.43 |
| 23:BA:1344:G:H5' | 23:BA:1384:A:N1 | 2.34 | 0.43 |
| 1:CA:448:A:H2' | 1:CA:449:C:C6 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:CD:159:ARG:O | 4:CD:162:LEU:N | 2.52 | 0.43 |
| 23:DA:1105:U:H2' | 23:DA:1106:G:C8 | 2.54 | 0.43 |
| 17:AQ:10:VAL:CG1 | 17:AQ:53:LEU:HA | 2.48 | 0.43 |
| 23:BA:1046:A:C3' | 23:BA:1047:G:C5' | 2.96 | 0.43 |
| 23:BA:1111:A:N3 | 23:BA:1112:G:H1' | 2.34 | 0.43 |
| 23:BA:954:G:H5'' | 35:BM:13:GLN:HG2 | 1.99 | 0.43 |
| 35:DM:16:ARG:CG | 35:DM:17:LEU:H | 2.32 | 0.43 |
| 23:DA:1046:A:C3' | 23:DA:1047:G:C5' | 2.96 | 0.43 |
| 1:AA:1119:C:H2' | 1:AA:1120:G:C8 | 2.54 | 0.43 |
| 3:CC:50:ALA:HB1 | 3:CC:70:VAL:HG11 | 2.01 | 0.43 |
| 23:DA:241:A:H5' | 23:DA:243:U:C1' | 2.47 | 0.43 |
| 1:AA:509:A:C6 | 1:AA:510:A:N1 | 2.86 | 0.43 |
| 1:CA:99:C:O2' | 1:CA:101:A:H8 | 2.01 | 0.43 |
| 26:DD:37:ARG:HA | 26:DD:42:ASP:OD2 | 2.19 | 0.43 |
| 36:BN:100:LEU:HG | 36:BN:112:ALA:HA | 2.01 | 0.43 |
| 23:DA:479:A:N3 | 23:DA:481:G:H5'' | 2.34 | 0.43 |
| 1:CA:664:G:N2 | 1:CA:742:G:C2 | 2.87 | 0.43 |
| 23:BA:1952:A:C6 | 33:BK:22:ILE:HD11 | 2.53 | 0.43 |
| 1:AA:1357:A:N6 | 1:AA:1358:U:H3 | 2.17 | 0.43 |
| 29:DG:92:ILE:HG22 | 29:DG:93:GLY:H | 1.80 | 0.43 |
| 23:DA:912:C:C2' | 23:DA:912:C:O2 | 2.64 | 0.43 |
| 8:AH:49:GLU:O | 8:AH:51:VAL:N | 2.45 | 0.43 |
| 23:DA:1399:C:H2' | 23:DA:1400:G:H8 | 1.82 | 0.43 |
| 17:AQ:70:ARG:N | 17:AQ:70:ARG:HD2 | 2.34 | 0.43 |
| 1:CA:651:C:O2' | 1:CA:652:U:H5' | 2.18 | 0.43 |
| 1:CA:510:A:H1' | 1:CA:543:C:O4' | 2.19 | 0.43 |
| 23:DA:1414:G:H2' | 23:DA:1415:U:C6 | 2.51 | 0.43 |
| 1:CA:15:G:H2' | 1:CA:16:A:C8 | 2.53 | 0.43 |
| 1:AA:909:A:H3' | 1:AA:910:C:H6 | 1.83 | 0.43 |
| 1:AA:1511:G:C6 | 1:AA:1512:U:C4 | 3.07 | 0.43 |
| 23:BA:1748:G:O2' | 23:BA:1749:A:H5' | 2.19 | 0.43 |
| 1:AA:1089:G:H1 | 1:AA:1096:C:H42 | 1.67 | 0.43 |
| 27:DE:46:ARG:CG | 27:DE:46:ARG:NH1 | 2.80 | 0.43 |
| 23:DA:1856:G:C2 | 23:DA:1887:C:C2 | 3.06 | 0.43 |
| 23:BA:1832:C:C4 | 23:BA:1833:U:C5 | 3.07 | 0.43 |
| 1:CA:639:G:H2' | 1:CA:640:A:C8 | 2.53 | 0.43 |
| 2:AB:144:ARG:O | 2:AB:147:LYS:HB3 | 2.19 | 0.43 |
| 23:DA:2001:A:H4' | 23:DA:2689:U:O2' | 2.19 | 0.43 |
| 3:AC:17:ASP:HB3 | 3:AC:21:ARG:HH22 | 1.84 | 0.43 |
| 23:BA:1232:G:C4 | 23:BA:1233:C:C5 | 3.07 | 0.43 |
| 23:DA:2738:A:H2' | 23:DA:2739:U:O5' | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:BN:32:GLY:C | 36:BN:33:ARG:HD2 | 2.38 | 0.43 |
| 33:DK:25:LEU:HA | 33:DK:25:LEU:HD23 | 1.56 | 0.43 |
| 1:AA:20:U:H2' | 1:AA:21:G:H5' | 2.00 | 0.43 |
| 1:AA:1162:C:O2' | 1:AA:1163:C:H5' | 2.19 | 0.43 |
| 5:AE:79:GLU:CG | 5:AE:92:LYS:HG3 | 2.49 | 0.43 |
| 23:DA:1471:A:C2 | 23:DA:1472:A:C4 | 3.07 | 0.43 |
| 23:BA:2604:U:C2' | 23:BA:2604:U:O2 | 2.67 | 0.43 |
| 23:BA:173:G:H2' | 23:BA:174:C:H6 | 1.83 | 0.43 |
| 1:AA:440:A:C8 | 1:AA:442:C:C5 | 3.07 | 0.43 |
| 1:CA:1165:C:C2' | 1:CA:1166:G:H5' | 2.49 | 0.43 |
| 5:CE:107:ARG:HG2 | 5:CE:108:ALA:N | 2.34 | 0.43 |
| 7:AG:49:ILE:CG2 | 7:AG:49:ILE:O | 2.66 | 0.43 |
| 15:AO:3:ILE:HG21 | 15:AO:34:LEU:CD2 | 2.49 | 0.43 |
| 30:BH:25:TYR:CE1 | 30:BH:30:LEU:HD11 | 2.53 | 0.43 |
| 23:BA:1905:C:O4' | 23:BA:1928:A:H2 | 2.02 | 0.43 |
| 38:DP:14:TYR:N | 38:DP:14:TYR:CD1 | 2.83 | 0.43 |
| 51:D3:13:CYS:HB2 | 51:D3:22:ALA:HB3 | 2.01 | 0.43 |
| 23:BA:1718:G:N2 | 23:BA:1742:C:C2 | 2.86 | 0.43 |
| 18:AR:65:ILE:O | 18:AR:69:THR:HG23 | 2.19 | 0.43 |
| 11:CK:17:GLY:HA3 | 11:CK:77:MET:SD | 2.59 | 0.43 |
| 23:DA:69:C:O2' | 23:DA:70:G:H5' | 2.19 | 0.43 |
| 46:BX:59:THR:OG1 | 46:BX:60:PHE:N | 2.51 | 0.43 |
| 13:CM:116:THR:O | 13:CM:117:VAL:O | 2.37 | 0.43 |
| 49:D1:36:VAL:HB | 49:D1:37:PRO:HD2 | 2.01 | 0.43 |
| 53:D5:30:ARG:HA | 53:D5:30:ARG:HD3 | 1.72 | 0.42 |
| 34:DL:115:LEU:CB | 34:DL:131:SER:HB2 | 2.48 | 0.42 |
| 24:BB:79:C:O5' | 24:BB:79:C:H6 | 2.02 | 0.42 |
| 25:BC:70:TRP:O | 25:BC:70:TRP:HD1 | 2.01 | 0.42 |
| 43:DU:17:SER:HB2 | 43:DU:71:LYS:HD2 | 2.00 | 0.42 |
| 38:DP:50:ILE:HG22 | 38:DP:51:ARG:HB3 | 2.01 | 0.42 |
| 1:AA:1320:C:N4 | 19:AS:36:ARG:HG3 | 2.12 | 0.42 |
| 1:CA:501:C:H3' | 1:CA:501:C:H6 | 1.84 | 0.42 |
| 37:BO:88:ASP:O | 37:BO:90:GLY:N | 2.50 | 0.42 |
| 23:BA:1903:G:OP2 | 25:BC:241:PRO:HB3 | 2.19 | 0.42 |
| 23:DA:705:A:C2 | 23:DA:727:A:H1' | 2.53 | 0.42 |
| 23:DA:195:A:OP1 | 34:DL:46:LYS:HE2 | 2.19 | 0.42 |
| 32:BJ:154:GLN:O | 32:BJ:155:ALA:HB2 | 2.19 | 0.42 |
| 32:DJ:109:PRO:HG2 | 32:DJ:112:LYS:HB2 | 2.00 | 0.42 |
| 1:CA:386:C:H2' | 1:CA:387:U:C4' | 2.49 | 0.42 |
| 39:BQ:72:HIS:ND1 | 39:BQ:110:VAL:HG21 | 2.34 | 0.42 |
| 37:DO:14:VAL:HG21 | 37:DO:89:ARG:HH21 | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:394:G:N3 | 1:CA:395:C:C6 | 2.87 | 0.42 |
| 30:DH:79:ILE:HB | 30:DH:143:SER:O | 2.19 | 0.42 |
| 24:DB:46:A:C5 | 24:DB:47:C:C4 | 3.07 | 0.42 |
| 25:DC:233:HIS:HE1 | 25:DC:246:PRO:HA | 1.83 | 0.42 |
| 25:DC:246:PRO:HD2 | 25:DC:255:LYS:HD2 | 2.01 | 0.42 |
| 44:DV:53:ILE:C | 44:DV:53:ILE:HD12 | 2.40 | 0.42 |
| 1:AA:78:G:H2' | 1:AA:79:G:C8 | 2.54 | 0.42 |
| 23:DA:1210:A:H4' | 23:DA:1211:U:O5' | 2.19 | 0.42 |
| 23:BA:322:A:P | 27:BE:169:ASN:HB2 | 2.58 | 0.42 |
| 1:CA:1202:G:O2' | 14:CN:27:CYS:HB2 | 2.19 | 0.42 |
| 36:DN:6:SER:OG | 36:DN:7:GLY:N | 2.51 | 0.42 |
| 24:BB:104:A:O4' | 44:BV:29:TYR:CE1 | 2.68 | 0.42 |
| 1:AA:191(F):U:H2' | 1:AA:191(G):G:C8 | 2.54 | 0.42 |
| 5:CE:126:ARG:NH1 | 5:CE:126:ARG:HG2 | 2.22 | 0.42 |
| 23:DA:2748:A:C4 | 23:DA:2757:A:C6 | 3.07 | 0.42 |
| 23:BA:1859:A:N6 | 23:BA:1884:A:C8 | 2.87 | 0.42 |
| 27:DE:102:PRO:O | 27:DE:106:ARG:HG2 | 2.19 | 0.42 |
| 15:AO:12:ILE:HG21 | 15:AO:22:THR:HG22 | 2.00 | 0.42 |
| 23:DA:589:C:H2' | 23:DA:590:A:C8 | 2.54 | 0.42 |
| 23:DA:2790:A:C2 | 23:DA:2791:C:H2' | 2.54 | 0.42 |
| 23:DA:947:G:N3 | 23:DA:984:A:H2 | 2.17 | 0.42 |
| 1:AA:1129:C:C1' | 1:AA:1130:A:OP2 | 2.62 | 0.42 |
| 1:CA:197:A:N6 | 1:CA:221:C:H5' | 2.34 | 0.42 |
| 1:CA:68:G:C6 | 1:CA:69:G:C5 | 3.07 | 0.42 |
| 36:BN:50:HIS:C | 36:BN:50:HIS:CD2 | 2.92 | 0.42 |
| 23:DA:738:G:H2' | 23:DA:739:G:C8 | 2.54 | 0.42 |
| 1:CA:1060:C:C2 | 1:CA:1198:G:C2 | 3.07 | 0.42 |
| 23:BA:2101:G:N2 | 23:BA:2189:U:C2 | 2.87 | 0.42 |
| 1:AA:976:G:H8 | 1:AA:1358:U:H2' | 1.83 | 0.42 |
| 23:DA:2188:C:C4 | 23:DA:2189:U:C6 | 3.07 | 0.42 |
| 7:CG:126:ASP:HB3 | 7:CG:131:LYS:O | 2.19 | 0.42 |
| 23:BA:1871:A:H2' | 23:BA:1872:A:H8 | 1.80 | 0.42 |
| 44:DV:24:LEU:HB3 | 44:DV:41:LEU:HG | 2.00 | 0.42 |
| 23:BA:333:G:C6 | 23:BA:334:C:C4 | 3.07 | 0.42 |
| 34:BL:115:LEU:HA | 34:BL:134:ALA:HB2 | 2.01 | 0.42 |
| 1:CA:570:G:H2' | 1:CA:571:U:C6 | 2.54 | 0.42 |
| 1:CA:861:G:O2' | 1:CA:862:C:H5' | 2.19 | 0.42 |
| 23:BA:302:C:O2' | 23:BA:303:U:H5' | 2.19 | 0.42 |
| 1:AA:922:G:C6 | 1:AA:923:A:N6 | 2.86 | 0.42 |
| 1:AA:542:G:H5' | 4:AD:41:GLY:HA3 | 2.00 | 0.42 |
| 18:AR:44:LEU:HG | 18:AR:50:ILE:HD13 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:AC:73:PRO:C | 3:AC:75:VAL:H | 2.22 | 0.42 |
| 23:DA:566:U:H2' | 23:DA:567:A:O4' | 2.18 | 0.42 |
| 23:BA:570:G:C5 | 23:BA:2030:A:C2 | 3.07 | 0.42 |
| 23:BA:758:C:O2 | 23:BA:1981:A:H2 | 2.02 | 0.42 |
| 36:DN:52:ILE:HG21 | 36:DN:94:TYR:CB | 2.49 | 0.42 |
| 23:BA:2737:G:C6 | 23:BA:2738:A:N7 | 2.86 | 0.42 |
| 10:AJ:6:ILE:HG12 | 10:AJ:72:VAL:O | 2.19 | 0.42 |
| 23:DA:2836:U:H2' | 23:DA:2837:G:H8 | 1.84 | 0.42 |
| 9:AI:95:LYS:HD3 | 9:AI:95:LYS:C | 2.39 | 0.42 |
| 23:DA:958:U:O2' | 23:DA:959:A:OP2 | 2.35 | 0.42 |
| 23:BA:2506:U:H5 | 23:BA:2507:C:H5 | 1.60 | 0.42 |
| 23:BA:1991:U:H2' | 23:BA:1992:G:C5' | 2.48 | 0.42 |
| 23:DA:553:U:O4 | 23:DA:554:U:O4 | 2.37 | 0.42 |
| 28:DF:137:GLU:HB3 | 28:DF:139:LEU:HG | 2.01 | 0.42 |
| 23:BA:880:G:H1 | 23:BA:897:C:N4 | 2.17 | 0.42 |
| 23:DA:1126:A:O5' | 23:DA:1126:A:C8 | 2.71 | 0.42 |
| 23:BA:2836:U:H2' | 23:BA:2837:G:H8 | 1.84 | 0.42 |
| 28:BF:137:GLU:HB3 | 28:BF:139:LEU:HG | 2.01 | 0.42 |
| 2:AB:17:PHE:CD1 | 2:AB:44:LEU:HD11 | 2.54 | 0.42 |
| 23:DA:1625:C:H2' | 23:DA:1626:G:O4' | 2.19 | 0.42 |
| 40:BR:75:PHE:O | 40:BR:75:PHE:CD1 | 2.72 | 0.42 |
| 10:AJ:30:SER:HB2 | 10:AJ:80:LYS:HG2 | 2.01 | 0.42 |
| 32:DJ:32:VAL:CG1 | 32:DJ:33:GLU:N | 2.82 | 0.42 |
| 30:DH:76:THR:HG22 | 30:DH:141:LYS:CB | 2.49 | 0.42 |
| 5:AE:107:ARG:HG2 | 5:AE:108:ALA:N | 2.34 | 0.42 |
| 23:DA:2703:C:C2' | 23:DA:2704:C:H5' | 2.48 | 0.42 |
| 23:BA:447:A:C4 | 23:BA:473:G:C8 | 3.07 | 0.42 |
| 23:DA:1686:C:N4 | 23:DA:1687:G:C6 | 2.87 | 0.42 |
| 23:DA:724:U:H2' | 23:DA:725:G:O4' | 2.18 | 0.42 |
| 23:DA:2552:U:H2' | 23:DA:2554:U:OP2 | 2.19 | 0.42 |
| 44:BV:70:LEU:CD2 | 44:BV:70:LEU:N | 2.82 | 0.42 |
| 1:AA:581:G:O2' | 1:AA:582:U:H5' | 2.19 | 0.42 |
| 23:DA:876:C:H2' | 23:DA:877:U:H5' | 2.00 | 0.42 |
| 2:CB:149:LEU:O | 2:CB:151:GLY:N | 2.51 | 0.42 |
| 23:DA:2450:A:C2 | 23:DA:2451:A:C4 | 3.06 | 0.42 |
| 9:CI:30:GLY:O | 9:CI:31:GLN:O | 2.36 | 0.42 |
| 23:BA:69:C:O2' | 23:BA:70:G:H5' | 2.19 | 0.42 |
| 1:CA:1383:C:C6 | 1:CA:1384:C:H5 | 2.37 | 0.42 |
| 9:CI:127:LYS:O | 9:CI:128:ARG:O | 2.37 | 0.42 |
| 5:CE:47:LYS:HB2 | 5:CE:47:LYS:HE3 | 1.85 | 0.42 |
| 1:AA:906:G:O5' | 1:AA:906:G:H8 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:AG:60:LYS:HD2 | 7:AG:60:LYS:HA | 1.78 | 0.42 |
| 49:B1:48:ILE:H | 49:B1:48:ILE:HD12 | 1.83 | 0.42 |
| 1:AA:347:G:N2 | 1:AA:348:G:H1' | 2.34 | 0.42 |
| 23:DA:2881:C:C2 | 23:DA:2882:A:C8 | 3.07 | 0.42 |
| 44:BV:129:SER:OG | 44:BV:130:PRO:HD2 | 2.19 | 0.42 |
| 31:DI:15:GLU:HG3 | 31:DI:66:LEU:HG | 2.00 | 0.42 |
| 34:BL:62:LEU:HD21 | 53:B5:25:MET:O | 2.20 | 0.42 |
| 47:DY:1:MET:O | 47:DY:1:MET:SD | 2.77 | 0.42 |
| 26:DD:103:ASP:OD2 | 26:DD:168:MET:HE2 | 2.18 | 0.42 |
| 34:BL:107:LYS:O | 34:BL:109:GLY:N | 2.50 | 0.42 |
| 23:BA:805:G:H4' | 23:BA:806:C:OP2 | 2.19 | 0.42 |
| 23:DA:673:C:H4' | 27:DE:82:ILE:HD13 | 2.01 | 0.42 |
| 29:DG:101:ARG:NE | 29:DG:101:ARG:N | 2.43 | 0.42 |
| 16:CP:20:VAL:HG22 | 16:CP:21:VAL:N | 2.34 | 0.42 |
| 23:DA:2295:C:C4 | 23:DA:2296:U:H5 | 2.37 | 0.42 |
| 4:AD:106:TYR:HE1 | 4:AD:113:SER:HA | 1.83 | 0.42 |
| 11:AK:26:ASN:O | 11:AK:27:ASN:HB2 | 2.19 | 0.42 |
| 23:DA:71:A:H4' | 23:DA:72:U:H5'' | 2.00 | 0.42 |
| 13:CM:37:THR:OG1 | 13:CM:39:ILE:HG12 | 2.19 | 0.42 |
| 30:DH:114:LEU:HD21 | 30:DH:128:LEU:HD13 | 2.00 | 0.42 |
| 36:BN:107:ASP:OD2 | 36:BN:108:GLY:N | 2.52 | 0.42 |
| 23:BA:1591:G:H2' | 23:BA:1592:C:C6 | 2.54 | 0.42 |
| 44:DV:30:ASN:HB3 | 44:DV:90:VAL:HB | 2.00 | 0.42 |
| 17:CQ:51:TYR:CE1 | 17:CQ:73:VAL:HG11 | 2.54 | 0.42 |
| 5:CE:139:LEU:O | 5:CE:142:LEU:HD12 | 2.19 | 0.42 |
| 5:CE:65:ASN:O | 5:CE:66:MET:HG3 | 2.20 | 0.42 |
| 23:DA:1284:A:H2' | 23:DA:1285:G:O4' | 2.18 | 0.42 |
| 48:BZ:40:THR:HG23 | 48:BZ:43:ILE:CD1 | 2.49 | 0.42 |
| 46:DX:13:ILE:O | 46:DX:13:ILE:HD12 | 2.19 | 0.42 |
| 4:AD:153:ARG:HD3 | 4:AD:181:MET:HE3 | 2.00 | 0.42 |
| 20:CT:57:ARG:HH12 | 20:CT:102:GLY:HA2 | 1.75 | 0.42 |
| 35:DM:68:ILE:HG23 | 35:DM:103:MET:HA | 2.01 | 0.42 |
| 18:CR:35:ARG:O | 18:CR:37:VAL:N | 2.46 | 0.42 |
| 1:CA:583:A:H61 | 1:CA:758:G:H1' | 1.84 | 0.42 |
| 1:AA:1329:A:N7 | 21:AU:7:ARG:NH2 | 2.63 | 0.42 |
| 4:CD:159:ARG:HA | 4:CD:162:LEU:HB2 | 2.00 | 0.42 |
| 1:AA:318:G:C2 | 1:AA:319:G:C5 | 3.08 | 0.42 |
| 1:AA:1237:C:C5 | 1:AA:1336:C:C4 | 3.07 | 0.42 |
| 23:BA:1586:A:H2' | 23:BA:1587:A:H5' | 2.01 | 0.42 |
| 23:BA:2753:A:C2' | 23:BA:2754:U:H5' | 2.49 | 0.42 |
| 35:BM:16:ARG:O | 35:BM:17:LEU:HD23 | 2.18 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 42:BT:21:PHE:O | 42:BT:23:GLU:O | 2.37 | 0.42 |
| 1:CA:1279:A:H62 | 3:CC:26:LYS:HE2 | 1.84 | 0.42 |
| 23:BA:8:A:C6 | 23:BA:9:U:O4 | 2.72 | 0.42 |
| 30:DH:62:LYS:CB | 30:DH:133:HIS:CE1 | 3.00 | 0.42 |
| 1:AA:616:G:N3 | 1:AA:625:G:C2 | 2.88 | 0.42 |
| 28:BF:133:LEU:CD2 | 28:BF:133:LEU:N | 2.83 | 0.42 |
| 42:BT:41:ASN:N | 42:BT:41:ASN:HD22 | 2.17 | 0.42 |
| 23:DA:997:G:H2' | 23:DA:998:C:H5' | 2.00 | 0.42 |
| 1:AA:197:A:N6 | 1:AA:221:C:H5' | 2.35 | 0.42 |
| 23:BA:1480:G:C2 | 23:BA:1481:U:C2 | 3.07 | 0.42 |
| 36:BN:48:VAL:HA | 36:BN:51:LEU:HD12 | 2.02 | 0.42 |
| 23:DA:257:A:C8 | 23:DA:257:A:H3' | 2.54 | 0.42 |
| 25:BC:182:LEU:HB3 | 25:BC:271:ILE:HG13 | 2.01 | 0.42 |
| 1:AA:710:G:C4 | 1:AA:711:G:C8 | 3.07 | 0.42 |
| 23:BA:2591:C:H2' | 23:BA:2592:G:C8 | 2.54 | 0.42 |
| 23:BA:2471:C:H2' | 23:BA:2472:G:O4' | 2.18 | 0.42 |
| 50:D2:33:CYS:SG | 50:D2:40:LYS:HE3 | 2.59 | 0.42 |
| 50:D2:40:LYS:HE2 | 50:D2:46:CYS:HB3 | 2.01 | 0.42 |
| 23:DA:1434:A:C2 | 23:DA:1435:G:C4 | 3.08 | 0.42 |
| 21:AU:22:ARG:HA | 21:AU:23:PRO:HD3 | 1.83 | 0.42 |
| 23:BA:864:G:C6 | 23:BA:865:C:N4 | 2.87 | 0.42 |
| 23:DA:2821:A:OP2 | 36:DN:5:LYS:NZ | 2.46 | 0.42 |
| 34:BL:85:LEU:CA | 34:BL:88:LEU:HB2 | 2.45 | 0.42 |
| 23:BA:2640:G:H2' | 23:BA:2641:G:O4' | 2.19 | 0.42 |
| 36:BN:79:LEU:HA | 36:BN:83:ILE:HG13 | 2.00 | 0.42 |
| 23:BA:2402:C:C3' | 23:BA:2403:C:H5' | 2.49 | 0.42 |
| 23:BA:1003:G:O2' | 23:BA:1010:A:N1 | 2.45 | 0.42 |
| 12:AL:7:ASN:HA | 12:AL:10:VAL:HG23 | 2.00 | 0.42 |
| 35:DM:45:GLN:H | 35:DM:45:GLN:CD | 2.21 | 0.42 |
| 1:CA:414:A:C5 | 1:CA:431:A:C2 | 3.07 | 0.42 |
| 7:AG:51:GLN:HA | 7:AG:54:THR:O | 2.18 | 0.42 |
| 51:B3:18:ARG:HH22 | 51:B3:44:ARG:HB2 | 1.83 | 0.42 |
| 23:DA:189:G:H1' | 23:DA:207:A:H61 | 1.84 | 0.42 |
| 23:DA:646:A:H5' | 23:DA:646:A:N3 | 2.34 | 0.42 |
| 23:BA:2737:G:C4 | 23:BA:2738:A:C8 | 3.07 | 0.42 |
| 23:DA:2019:A:O4' | 39:DQ:34:LYS:HD2 | 2.19 | 0.42 |
| 23:BA:2718:G:C2' | 23:BA:2719:G:O5' | 2.67 | 0.42 |
| 14:CN:40:CYS:O | 14:CN:44:LEU:HB3 | 2.19 | 0.42 |
| 5:AE:36:ASP:CG | 5:AE:37:ARG:N | 2.73 | 0.42 |
| 1:CA:1501:C:C6 | 1:CA:1504:G:N7 | 2.87 | 0.42 |
| 1:AA:1184:G:C5 | 1:AA:1185:G:N7 | 2.87 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:1360:A:H3' | 1:CA:1361:G:C8 | 2.55 | 0.42 |
| 1:AA:1464:G:C2' | 1:AA:1465:C:H5' | 2.48 | 0.42 |
| 23:BA:1443:G:H1 | 23:BA:1548:C:H42 | 1.67 | 0.42 |
| 38:BP:82:LEU:N | 38:BP:82:LEU:HD23 | 2.34 | 0.42 |
| 5:CE:36:ASP:CG | 5:CE:37:ARG:N | 2.72 | 0.42 |
| 23:BA:1005:C:O2' | 32:BJ:51:THR:HG21 | 2.19 | 0.42 |
| 23:BA:2744:G:N2 | 23:BA:2761:G:C5 | 2.88 | 0.42 |
| 23:BA:719:C:H6 | 23:BA:719:C:O5' | 2.02 | 0.42 |
| 1:AA:619:U:H2' | 4:AD:135:LEU:CD2 | 2.49 | 0.42 |
| 40:DR:75:PHE:HD1 | 40:DR:75:PHE:O | 2.02 | 0.42 |
| 52:B4:36:GLN:CG | 52:B4:36:GLN:O | 2.68 | 0.42 |
| 4:CD:190:ASP:O | 4:CD:194:LEU:CD2 | 2.67 | 0.42 |
| 23:BA:2016:U:H1' | 50:B2:6:VAL:HG13 | 2.01 | 0.42 |
| 41:BS:10:VAL:HG23 | 41:BS:101:SER:O | 2.18 | 0.42 |
| 1:CA:102(B):C:N4 | 1:CA:102(C):C:H41 | 2.17 | 0.42 |
| 11:AK:99:GLN:OE1 | 11:AK:99:GLN:HA | 2.20 | 0.42 |
| 20:CT:24:LEU:H | 20:CT:24:LEU:HD22 | 1.84 | 0.42 |
| 23:BA:517:C:OP1 | 50:B2:16:ARG:NH2 | 2.52 | 0.42 |
| 1:CA:1141:C:H2' | 1:CA:1142:G:H8 | 1.84 | 0.42 |
| 25:BC:147:LEU:HD13 | 25:BC:155:LEU:CD1 | 2.50 | 0.42 |
| 1:CA:1366:C:N4 | 1:CA:1367:C:N4 | 2.67 | 0.42 |
| 1:CA:1371:G:H5'' | 9:CI:69:GLY:N | 2.33 | 0.42 |
| 2:CB:164:VAL:O | 2:CB:186:ALA:HB1 | 2.19 | 0.42 |
| 23:DA:1971:A:N3 | 25:DC:241:PRO:HD3 | 2.35 | 0.42 |
| 23:BA:1019:U:O2' | 23:BA:1021:A:C2 | 2.70 | 0.42 |
| 39:DQ:105:VAL:CG1 | 40:DR:40:LEU:HD13 | 2.50 | 0.42 |
| 23:DA:194:G:C2' | 23:DA:195:A:H5' | 2.49 | 0.42 |
| 32:DJ:112:LYS:O | 32:DJ:116:THR:CG2 | 2.67 | 0.42 |
| 34:BL:49:ARG:HG3 | 53:B5:60:LEU:CD2 | 2.47 | 0.42 |
| 25:BC:35:LYS:H | 25:BC:36:PRO:HD2 | 1.84 | 0.42 |
| 47:DY:6:VAL:C | 47:DY:10:LEU:HG | 2.39 | 0.42 |
| 40:DR:78:LYS:O | 40:DR:78:LYS:HG3 | 2.19 | 0.42 |
| 23:DA:546:C:N4 | 23:DA:547:A:C6 | 2.87 | 0.42 |
| 23:BA:1409:C:C2 | 23:BA:1594:G:N2 | 2.88 | 0.42 |
| 24:BB:43:C:H2' | 24:BB:44:G:H5'' | 2.01 | 0.42 |
| 29:BG:72:ILE:O | 29:BG:75:ALA:N | 2.52 | 0.42 |
| 44:BV:48:PHE:CE1 | 44:BV:52:SER:HA | 2.55 | 0.42 |
| 1:AA:191(G):G:O2' | 20:AT:102:GLY:O | 2.37 | 0.42 |
| 1:AA:1077:G:C2 | 1:AA:1081:G:C5 | 3.08 | 0.42 |
| 7:AG:9:VAL:HG12 | 7:AG:10:ARG:N | 2.33 | 0.42 |
| 19:AS:63:THR:HG23 | 19:AS:65:ASN:N | 2.33 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:AM:4:ILE:HG12 | 13:AM:10:PRO:HD2 | 2.00 | 0.42 |
| 1:CA:878:G:C6 | 1:CA:879:C:N4 | 2.88 | 0.42 |
| 36:BN:2:ARG:O | 36:BN:3:HIS:CD2 | 2.72 | 0.42 |
| 33:BK:23:ARG:HG3 | 33:BK:24:VAL:N | 2.33 | 0.42 |
| 23:BA:2809:A:N1 | 23:BA:2892:A:C4 | 2.88 | 0.42 |
| 23:DA:1487:G:C2 | 23:DA:1488:G:C8 | 3.07 | 0.42 |
| 6:CF:75:LEU:HD21 | 6:CF:79:LEU:HD11 | 2.01 | 0.42 |
| 1:AA:668:G:H2' | 1:AA:669:U:H6 | 1.82 | 0.42 |
| 37:BO:51:ALA:HB3 | 37:BO:73:LEU:HG | 2.01 | 0.42 |
| 33:DK:35:VAL:HG23 | 33:DK:65:THR:CG2 | 2.42 | 0.42 |
| 23:BA:953:A:C2' | 23:BA:954:G:H5' | 2.50 | 0.42 |
| 23:BA:1285:G:O6 | 23:BA:1329:U:C2 | 2.73 | 0.42 |
| 33:DK:102:VAL:HG21 | 33:DK:118:ALA:CB | 2.49 | 0.42 |
| 1:AA:555:C:C2 | 1:AA:556:C:C5 | 3.07 | 0.42 |
| 1:AA:1314:C:H5 | 19:AS:6:LYS:NZ | 2.17 | 0.42 |
| 1:AA:101:A:H2' | 1:AA:102:G:H8 | 1.85 | 0.42 |
| 29:DG:90:LYS:O | 29:DG:94:TYR:HB2 | 2.19 | 0.42 |
| 1:CA:1067:A:N3 | 1:CA:1068:G:C1' | 2.82 | 0.42 |
| 27:DE:205:ARG:C | 27:DE:206:ILE:HG13 | 2.40 | 0.42 |
| 27:BE:34:TRP:CE3 | 27:BE:35:GLU:HG2 | 2.53 | 0.42 |
| 23:BA:483:A:H1' | 43:BU:47:LYS:O | 2.19 | 0.42 |
| 35:DM:66:ILE:HG22 | 35:DM:104:PHE:HD2 | 1.79 | 0.42 |
| 44:BV:60:GLU:OE1 | 44:BV:66:SER:HB3 | 2.19 | 0.42 |
| 50:D2:35:GLU:HB2 | 50:D2:49:CYS:SG | 2.58 | 0.42 |
| 33:BK:22:ILE:HD13 | 33:BK:22:ILE:HA | 1.46 | 0.42 |
| 23:BA:2208:U:O4' | 25:BC:151:LYS:HE3 | 2.19 | 0.42 |
| 17:AQ:31:LEU:HG | 17:AQ:31:LEU:O | 2.19 | 0.42 |
| 46:BX:23:LYS:HE2 | 46:BX:23:LYS:HB3 | 1.74 | 0.42 |
| 46:BX:23:LYS:HB3 | 46:BX:37:ILE:CG1 | 2.49 | 0.42 |
| 27:DE:32:LEU:O | 27:DE:36:VAL:HG23 | 2.19 | 0.42 |
| 23:DA:2467:C:C5' | 35:DM:123:HIS:CE1 | 3.02 | 0.42 |
| 1:CA:564:C:N3 | 17:CQ:31:LEU:HD11 | 2.33 | 0.42 |
| 1:AA:1441:G:H5'' | 1:AA:1442:G:O5' | 2.20 | 0.42 |
| 1:CA:1357:A:N6 | 1:CA:1358:U:H3 | 2.17 | 0.42 |
| 23:DA:838:C:C4 | 23:DA:839:U:C5 | 3.07 | 0.42 |
| 23:DA:564:C:C2' | 23:DA:565:C:H5' | 2.49 | 0.42 |
| 1:CA:1378:C:C5 | 1:CA:1379:G:N9 | 2.87 | 0.42 |
| 2:CB:20:GLU:OE1 | 2:CB:20:GLU:HA | 2.19 | 0.42 |
| 5:CE:140:ARG:CG | 5:CE:140:ARG:O | 2.66 | 0.42 |
| 23:DA:2861:G:C4 | 23:DA:2862:G:C8 | 3.08 | 0.42 |
| 14:CN:26:ARG:HD2 | 14:CN:47:LEU:HD11 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:DA:646:A:C2' | 23:DA:647:G:O5' | 2.67 | 0.42 |
| 1:AA:21:G:C2 | 1:AA:22:G:C6 | 3.07 | 0.42 |
| 23:BA:205:G:O2' | 23:BA:206:U:OP2 | 2.34 | 0.42 |
| 18:CR:19:LYS:O | 18:CR:20:ALA:CB | 2.67 | 0.42 |
| 19:AS:11:VAL:HG22 | 19:AS:12:ASP:N | 2.33 | 0.42 |
| 1:AA:179:A:C5 | 1:AA:180:U:C4 | 3.07 | 0.42 |
| 41:DS:45:TYR:HD2 | 41:DS:46:PHE:CE1 | 2.37 | 0.42 |
| 23:BA:399:G:H2' | 23:BA:400:G:C5' | 2.50 | 0.42 |
| 23:DA:2618:G:O2' | 26:DD:149:ARG:HG3 | 2.20 | 0.42 |
| 1:AA:55:A:C5 | 1:AA:56:U:C5 | 3.06 | 0.42 |
| 18:CR:53:ARG:HH21 | 18:CR:60:ALA:N | 2.16 | 0.42 |
| 23:DA:1464:C:H2' | 23:DA:1465:G:H8 | 1.84 | 0.42 |
| 7:AG:31:MET:HG3 | 7:AG:35:LYS:H | 1.85 | 0.42 |
| 23:BA:89:G:C5 | 23:BA:90:U:C5 | 3.08 | 0.42 |
| 23:BA:1647:G:P | 23:BA:1647:G:H3' | 2.59 | 0.42 |
| 4:CD:199:ASN:HD22 | 4:CD:202:LEU:HG | 1.83 | 0.42 |
| 23:DA:466:A:C3' | 23:DA:467:G:H5' | 2.49 | 0.42 |
| 23:DA:450:G:O6 | 23:DA:453:C:OP1 | 2.38 | 0.42 |
| 1:AA:134:A:N1 | 16:AP:25:ARG:NH1 | 2.67 | 0.42 |
| 1:CA:32:A:C2 | 1:CA:33:A:C4 | 3.07 | 0.42 |
| 19:CS:52:TYR:HA | 19:CS:56:GLN:O | 2.19 | 0.42 |
| 4:CD:189:PRO:CB | 4:CD:194:LEU:HD21 | 2.50 | 0.42 |
| 23:BA:32:C:C2' | 23:BA:33:U:H5' | 2.49 | 0.42 |
| 39:DQ:53:ARG:HA | 39:DQ:56:ASP:HB2 | 2.02 | 0.42 |
| 23:DA:2523:G:C2' | 23:DA:2524:G:H5' | 2.49 | 0.42 |
| 23:DA:273(B):G:C2 | 23:DA:364:C:C2 | 3.08 | 0.42 |
| 37:DO:78:LEU:C | 37:DO:80:LEU:H | 2.22 | 0.42 |
| 23:BA:1668:A:C8 | 23:BA:1674:G:C6 | 3.07 | 0.42 |
| 23:DA:608:A:C6 | 23:DA:609(A):A:C6 | 3.07 | 0.42 |
| 23:BA:443:A:N7 | 27:BE:45:ARG:HG2 | 2.34 | 0.42 |
| 23:BA:2666:C:H5'' | 23:BA:2667:C:OP2 | 2.18 | 0.42 |
| 1:AA:1217:C:H5'' | 14:AN:9:LYS:NZ | 2.34 | 0.42 |
| 23:DA:1320:C:H4' | 23:DA:1321:A:OP1 | 2.18 | 0.42 |
| 23:BA:1297:C:H2' | 23:BA:1298:C:H6 | 1.83 | 0.42 |
| 1:CA:1213:A:O2' | 1:CA:1215:G:N7 | 2.47 | 0.42 |
| 2:AB:60:ASP:O | 2:AB:64:ARG:CG | 2.68 | 0.42 |
| 1:AA:135:C:H2' | 1:AA:136:C:H5' | 2.01 | 0.42 |
| 23:DA:1461:G:C2' | 23:DA:1462:C:H5' | 2.50 | 0.42 |
| 1:CA:680:C:H2' | 1:CA:681:C:C6 | 2.54 | 0.42 |
| 48:BZ:12:PRO:O | 48:BZ:14:GLY:N | 2.52 | 0.42 |
| 41:DS:63:ASP:OD2 | 41:DS:63:ASP:C | 2.58 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 13:AM:98:VAL:HG12 | 13:AM:98:VAL:O | 2.20 | 0.42 |
| 36:DN:34:ILE:HD13 | 36:DN:34:ILE:HA | 1.83 | 0.42 |
| 7:AG:75:VAL:HG23 | 7:AG:75:VAL:O | 2.19 | 0.42 |
| 29:BG:103:LEU:HG | 29:BG:103:LEU:O | 2.18 | 0.42 |
| 6:CF:2:ARG:HG3 | 6:CF:2:ARG:H | 1.69 | 0.42 |
| 8:CH:37:ARG:O | 8:CH:37:ARG:HG2 | 2.18 | 0.42 |
| 35:DM:112:GLU:H | 35:DM:112:GLU:CD | 2.23 | 0.42 |
| 22:AV:6179:U:H2' | 22:AV:6180:U:C6 | 2.55 | 0.42 |
| 48:DZ:55:ARG:HD3 | 48:DZ:55:ARG:HA | 1.50 | 0.42 |
| 23:DA:2393:A:C5' | 34:DL:62:LEU:HD12 | 2.41 | 0.42 |
| 25:BC:147:LEU:HD12 | 25:BC:147:LEU:HA | 1.77 | 0.42 |
| 32:DJ:54:ALA:O | 32:DJ:57:LEU:N | 2.52 | 0.42 |
| 1:AA:363:A:N6 | 1:AA:364:A:C6 | 2.87 | 0.42 |
| 27:DE:68:LYS:HG3 | 27:DE:68:LYS:O | 2.19 | 0.42 |
| 23:BA:2342:C:O2 | 23:BA:2374:C:H4' | 2.19 | 0.42 |
| 23:DA:1191:G:OP1 | 34:DL:35:HIS:CE1 | 2.72 | 0.42 |
| 23:DA:1970:A:H4' | 23:DA:1971:A:OP1 | 2.19 | 0.42 |
| 24:DB:83:G:N2 | 24:DB:84:C:H1' | 2.33 | 0.42 |
| 32:DJ:89:LYS:O | 32:DJ:91:GLU:N | 2.52 | 0.42 |
| 1:CA:376:G:C2 | 1:CA:389:A:C2 | 3.07 | 0.42 |
| 39:BQ:79:PHE:CE2 | 39:BQ:106:PHE:CE1 | 3.07 | 0.42 |
| 40:BR:4:ILE:CD1 | 40:BR:13:ARG:HA | 2.49 | 0.42 |
| 23:DA:2727:G:C2 | 23:DA:2728:U:C5 | 3.07 | 0.42 |
| 25:DC:181:GLU:HA | 25:DC:272:ALA:CB | 2.49 | 0.42 |
| 4:CD:104:VAL:CG1 | 4:CD:146:ILE:HG21 | 2.50 | 0.42 |
| 30:DH:82:ARG:CA | 30:DH:89:TYR:HB2 | 2.49 | 0.42 |
| 8:CH:125:ARG:O | 8:CH:128:GLY:N | 2.51 | 0.42 |
| 23:DA:1188:U:H2' | 23:DA:1189:A:O5' | 2.19 | 0.42 |
| 26:BD:52:LEU:O | 26:BD:75:VAL:HA | 2.19 | 0.42 |
| 23:DA:1210:A:C8 | 23:DA:1210:A:H5' | 2.52 | 0.42 |
| 4:CD:29:PRO:O | 4:CD:30:LYS:HB3 | 2.18 | 0.42 |
| 47:DY:53:LEU:O | 47:DY:56:GLN:HB2 | 2.19 | 0.42 |
| 44:BV:72:ARG:HD3 | 44:BV:72:ARG:HA | 1.78 | 0.42 |
| 41:BS:8:ARG:NH1 | 41:BS:9:TYR:HE2 | 2.16 | 0.42 |
| 1:AA:1085:U:C6 | 1:AA:1094:G:N1 | 2.88 | 0.42 |
| 10:AJ:32:ALA:HB3 | 10:AJ:76:ASN:CB | 2.38 | 0.42 |
| 29:DG:44:VAL:CG1 | 29:DG:45:VAL:H | 2.24 | 0.42 |
| 1:CA:585:G:C2' | 1:CA:586:C:H5' | 2.50 | 0.42 |
| 23:BA:2304:G:H5' | 23:BA:2305:A:OP2 | 2.19 | 0.42 |
| 1:CA:1205:U:H1' | 3:CC:195:VAL:CG2 | 2.50 | 0.42 |
| 1:CA:721:G:O4' | 1:CA:722:A:C4 | 2.73 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:DA:1504:C:O2' | 23:DA:1505:C:H6 | 2.02 | 0.42 |
| 23:DA:1510:A:C2 | 23:DA:1511:A:C4 | 3.08 | 0.42 |
| 25:BC:120:GLY:HA2 | 25:BC:121:PRO:HD3 | 1.79 | 0.42 |
| 1:AA:725:G:C4 | 1:AA:726:C:C5 | 3.07 | 0.42 |
| 23:DA:2776:A:C2 | 23:DA:2778:A:C4 | 3.07 | 0.42 |
| 23:BA:1372:U:H2' | 23:BA:1373:A:H8 | 1.85 | 0.42 |
| 19:AS:7:LYS:HB2 | 19:AS:7:LYS:HE3 | 1.84 | 0.42 |
| 23:DA:1359:A:N7 | 23:DA:1372:U:C4 | 2.87 | 0.42 |
| 1:CA:556:C:O2 | 1:CA:557:G:C8 | 2.71 | 0.42 |
| 32:DJ:69:VAL:CG1 | 32:DJ:71:MET:HG3 | 2.45 | 0.42 |
| 30:BH:8:PRO:HD3 | 30:BH:15:VAL:CG2 | 2.50 | 0.42 |
| 23:BA:1475:G:C2 | 23:BA:1476:C:C2 | 3.08 | 0.42 |
| 23:BA:1434:A:C5 | 23:BA:1560:G:N2 | 2.87 | 0.42 |
| 23:DA:2285:C:H5 | 51:D3:27:LYS:HZ2 | 1.68 | 0.42 |
| 11:CK:21:ILE:HD13 | 11:CK:84:VAL:HG12 | 2.02 | 0.42 |
| 23:DA:1517:G:C2 | 23:DA:1518:C:C2 | 3.07 | 0.42 |
| 39:DQ:101:ARG:HG3 | 39:DQ:101:ARG:H | 1.70 | 0.42 |
| 23:BA:582:G:H2' | 23:BA:583:G:C8 | 2.54 | 0.42 |
| 1:AA:711:G:N2 | 1:AA:712:A:C4 | 2.87 | 0.42 |
| 33:BK:32:TYR:CD1 | 33:BK:32:TYR:N | 2.87 | 0.42 |
| 24:DB:48:A:H2' | 24:DB:49:C:C6 | 2.54 | 0.42 |
| 17:AQ:32:TYR:O | 17:AQ:34:LYS:N | 2.49 | 0.42 |
| 23:DA:2101:G:C6 | 23:DA:2102:U:C4 | 3.06 | 0.42 |
| 44:DV:74:VAL:HG22 | 44:DV:86:VAL:CG1 | 2.49 | 0.42 |
| 23:BA:1775:U:C2' | 23:BA:1776:G:O5' | 2.67 | 0.42 |
| 41:DS:25:ARG:NH1 | 41:DS:25:ARG:HB2 | 2.34 | 0.42 |
| 23:BA:828:U:H4' | 23:BA:831:G:C2 | 2.55 | 0.42 |
| 1:AA:1342:C:O3' | 9:AI:125:TYR:HB3 | 2.19 | 0.42 |
| 23:BA:991:C:C6 | 23:BA:1185:C:N3 | 2.86 | 0.42 |
| 1:CA:939:G:N1 | 1:CA:940:C:N4 | 2.67 | 0.42 |
| 3:CC:83:ARG:O | 3:CC:86:VAL:HG22 | 2.19 | 0.42 |
| 13:CM:79:LYS:HB2 | 13:CM:79:LYS:HE3 | 1.78 | 0.42 |
| 23:BA:2433:A:H5" | 23:BA:2434:A:OP2 | 2.18 | 0.42 |
| 13:AM:24:GLY:HA2 | 13:AM:70:LEU:HD13 | 2.01 | 0.42 |
| 18:AR:74:ARG:HB2 | 18:AR:81:PHE:CZ | 2.55 | 0.42 |
| 28:BF:20:ILE:O | 28:BF:24:GLY:HA2 | 2.19 | 0.42 |
| 7:CG:27:ILE:CD1 | 7:CG:43:PHE:CD2 | 3.01 | 0.42 |
| 23:BA:1754:C:P | 38:BP:96:ARG:HH12 | 2.40 | 0.42 |
| 7:AG:27:ILE:CD1 | 7:AG:43:PHE:CD2 | 3.03 | 0.42 |
| 1:AA:1328:C:H5" | 13:AM:28:ALA:HB3 | 2.01 | 0.42 |
| 1:AA:505:G:N3 | 1:AA:506:G:C8 | 2.88 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:BQ:17:ILE:HA | 39:BQ:20:LEU:CD2 | 2.50 | 0.42 |
| 6:AF:12:PRO:HB3 | 6:AF:58:GLY:N | 2.34 | 0.42 |
| 7:AG:148:ASN:C | 7:AG:150:ALA:N | 2.72 | 0.42 |
| 23:DA:2737:G:C4 | 23:DA:2738:A:C8 | 3.08 | 0.42 |
| 1:CA:1182:G:H4' | 1:CA:1183:A:O5' | 2.19 | 0.42 |
| 25:BC:123:ALA:HB1 | 25:BC:124:PRO:HD2 | 2.02 | 0.42 |
| 24:BB:116:G:O5' | 24:BB:116:G:H8 | 2.02 | 0.42 |
| 19:CS:12:ASP:O | 19:CS:16:LEU:HD13 | 2.20 | 0.42 |
| 1:AA:179:A:C6 | 1:AA:180:U:C4 | 3.08 | 0.42 |
| 1:AA:1048:G:OP1 | 14:AN:4:LYS:HB2 | 2.19 | 0.42 |
| 41:BS:5:ALA:HB2 | 41:BS:54:ALA:HA | 2.00 | 0.42 |
| 19:CS:40:ILE:CD1 | 19:CS:62:ILE:HD11 | 2.50 | 0.42 |
| 9:AI:81:ILE:O | 9:AI:85:LEU:HG | 2.19 | 0.42 |
| 1:CA:497:U:C2' | 1:CA:497:U:O2 | 2.66 | 0.42 |
| 1:AA:778:G:O2' | 11:AK:120:ARG:O | 2.30 | 0.42 |
| 23:BA:2024:G:H2' | 23:BA:2025:C:H6 | 1.85 | 0.42 |
| 1:CA:292:G:N7 | 1:CA:293:G:H1' | 2.34 | 0.42 |
| 10:AJ:30:SER:HB2 | 10:AJ:80:LYS:HG3 | 2.00 | 0.42 |
| 44:BV:76:LEU:HD12 | 44:BV:76:LEU:H | 1.83 | 0.42 |
| 38:BP:50:ILE:HD12 | 38:BP:50:ILE:HA | 1.83 | 0.42 |
| 1:AA:1402:C:C5 | 1:AA:1403:C:C4 | 3.07 | 0.42 |
| 30:BH:9:LEU:HB3 | 30:BH:12:LEU:HD23 | 2.01 | 0.42 |
| 1:AA:1272:G:H2' | 1:AA:1273:G:H8 | 1.84 | 0.42 |
| 23:BA:768:G:C4 | 23:BA:769:G:C8 | 3.08 | 0.42 |
| 37:DO:30:ARG:HB3 | 37:DO:35:ILE:HD12 | 2.02 | 0.42 |
| 30:DH:37:VAL:CG1 | 30:DH:38:LEU:N | 2.83 | 0.42 |
| 23:DA:2248:C:C2' | 23:DA:2249:U:H5' | 2.49 | 0.42 |
| 1:AA:604:G:N7 | 1:AA:605:U:C5 | 2.87 | 0.42 |
| 36:DN:36:THR:HG23 | 36:DN:41:ALA:HB2 | 2.01 | 0.42 |
| 1:AA:1001:G:H2' | 1:AA:1002:G:O4' | 2.18 | 0.42 |
| 17:AQ:76:LEU:HD12 | 17:AQ:77:VAL:H | 1.84 | 0.42 |
| 1:CA:27:G:H2' | 1:CA:28:G:O4' | 2.19 | 0.42 |
| 11:AK:50:TYR:O | 11:AK:51:LYS:HG3 | 2.19 | 0.42 |
| 23:BA:1225:G:OP1 | 40:BR:86:GLY:HA3 | 2.20 | 0.42 |
| 48:DZ:3:ARG:NH1 | 48:DZ:59:VAL:HG11 | 2.34 | 0.42 |
| 39:DQ:73:GLY:O | 39:DQ:74:LEU:HB3 | 2.19 | 0.42 |
| 5:CE:26:PHE:N | 5:CE:26:PHE:CD1 | 2.87 | 0.42 |
| 23:DA:2501:C:H6 | 23:DA:2501:C:H2' | 1.68 | 0.42 |
| 2:AB:169:LYS:C | 2:AB:169:LYS:HE2 | 2.39 | 0.42 |
| 16:CP:69:THR:OG1 | 16:CP:69:THR:O | 2.37 | 0.42 |
| 42:BT:8:ILE:N | 42:BT:8:ILE:HD12 | 2.34 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 22:CV:6212:U:O2 | 22:CV:6212:U:H2' | 2.18 | 0.42 |
| 23:DA:1049:C:O2 | 23:DA:1113:U:H4' | 2.19 | 0.42 |
| 1:CA:792:A:H4' | 1:CA:793:U:O5' | 2.19 | 0.42 |
| 16:AP:64:ALA:O | 16:AP:65:GLN:C | 2.58 | 0.42 |
| 34:DL:112:LEU:HD22 | 34:DL:127:ALA:CB | 2.50 | 0.42 |
| 23:BA:2496:C:OP1 | 35:BM:81:VAL:HG12 | 2.19 | 0.42 |
| 35:DM:81:VAL:C | 35:DM:82:ARG:HG2 | 2.32 | 0.42 |
| 26:DD:11:MET:CE | 26:DD:186:GLY:HA2 | 2.48 | 0.42 |
| 32:BJ:126:VAL:O | 32:BJ:127:LYS:C | 2.58 | 0.42 |
| 23:BA:2267:A:H5'' | 23:BA:2268:A:H5'' | 1.95 | 0.42 |
| 9:CI:112:LYS:HE3 | 9:CI:116:LYS:O | 2.20 | 0.42 |
| 38:BP:51:ARG:CD | 38:BP:62:THR:HG23 | 2.48 | 0.42 |
| 51:B3:25:LYS:HD3 | 53:B5:34:TRP:HZ3 | 1.83 | 0.42 |
| 23:BA:2392:A:OP2 | 53:B5:31:HIS:HE1 | 2.03 | 0.42 |
| 32:BJ:142:ARG:HH11 | 32:BJ:142:ARG:CG | 2.21 | 0.42 |
| 23:DA:197:A:N6 | 23:DA:2430:A:H2' | 2.34 | 0.42 |
| 3:AC:18:TRP:O | 3:AC:19:GLU:C | 2.57 | 0.42 |
| 53:B5:60:LEU:O | 53:B5:61:LEU:C | 2.57 | 0.42 |
| 26:BD:34:VAL:HG11 | 26:BD:78:LEU:CD1 | 2.49 | 0.42 |
| 23:DA:1493:C:N4 | 23:DA:2210:G:O2' | 2.53 | 0.42 |
| 23:BA:2712:U:HO2' | 23:BA:712(B):A:H5'' | 1.83 | 0.42 |
| 26:DD:2:LYS:CE | 26:DD:95:ILE:O | 2.65 | 0.42 |
| 24:BB:73:A:C5 | 24:BB:104:A:N3 | 2.88 | 0.42 |
| 24:BB:10:C:N4 | 24:BB:11:C:N4 | 2.68 | 0.42 |
| 24:BB:13:A:N6 | 24:BB:70:C:H5' | 2.35 | 0.42 |
| 5:AE:78:HIS:N | 5:AE:78:HIS:ND1 | 2.68 | 0.42 |
| 4:AD:196:LEU:C | 4:AD:198:VAL:H | 2.22 | 0.42 |
| 25:BC:223:GLY:HA3 | 25:BC:231:HIS:ND1 | 2.34 | 0.42 |
| 37:DO:51:ALA:HB3 | 37:DO:73:LEU:HG | 2.02 | 0.42 |
| 26:DD:59:VAL:C | 26:DD:61:ARG:N | 2.73 | 0.42 |
| 23:BA:2542:A:O2' | 23:BA:2543:G:OP2 | 2.31 | 0.42 |
| 52:B4:19:ARG:CB | 52:B4:19:ARG:NH1 | 2.83 | 0.42 |
| 1:CA:1309:G:N2 | 1:CA:1329:A:H1' | 2.32 | 0.42 |
| 11:CK:26:ASN:O | 11:CK:27:ASN:HB2 | 2.19 | 0.42 |
| 1:AA:57:G:H2' | 1:AA:58:C:O4' | 2.20 | 0.42 |
| 3:CC:195:VAL:CG1 | 3:CC:196:LEU:N | 2.65 | 0.42 |
| 23:BA:2722:G:H2' | 23:BA:2723:C:C6 | 2.55 | 0.42 |
| 23:BA:1999:C:OP1 | 23:BA:2723:C:O2' | 2.36 | 0.42 |
| 46:BX:46:LEU:HD23 | 46:BX:46:LEU:O | 2.19 | 0.42 |
| 23:BA:2396:G:C2 | 23:BA:2421:G:C2 | 3.07 | 0.42 |
| 23:BA:2755:C:O2' | 23:BA:2756:U:H6 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BA:1504:C:O2' | 23:BA:1505:C:C6 | 2.72 | 0.42 |
| 11:CK:40:ILE:HG22 | 11:CK:75:TYR:CD2 | 2.54 | 0.42 |
| 24:DB:10:C:N4 | 24:DB:11:C:N4 | 2.67 | 0.42 |
| 4:AD:79:PHE:CD1 | 4:AD:207:TYR:HD1 | 2.38 | 0.42 |
| 1:CA:627:G:H2' | 1:CA:628:G:H8 | 1.84 | 0.42 |
| 34:BL:70:GLN:O | 34:BL:73:GLY:N | 2.52 | 0.42 |
| 36:BN:51:LEU:HD22 | 36:BN:70:LEU:HD11 | 2.00 | 0.42 |
| 23:BA:581:C:H2' | 23:BA:582:G:C8 | 2.53 | 0.42 |
| 1:AA:711:G:N2 | 1:AA:712:A:N3 | 2.67 | 0.42 |
| 23:DA:497:A:C5 | 23:DA:498:G:C8 | 3.07 | 0.42 |
| 43:DU:20:TYR:CD1 | 43:DU:20:TYR:N | 2.87 | 0.42 |
| 32:BJ:135:LEU:O | 32:BJ:136:GLY:C | 2.56 | 0.42 |
| 23:DA:581:C:H2' | 23:DA:582:G:C8 | 2.55 | 0.42 |
| 1:CA:516:U:C5 | 1:CA:517:G:O6 | 2.72 | 0.42 |
| 1:CA:538:G:O2' | 1:CA:539:A:H5' | 2.20 | 0.42 |
| 9:AI:125:TYR:CD1 | 9:AI:126:SER:N | 2.87 | 0.42 |
| 1:CA:1232:U:N3 | 1:CA:1233:G:C8 | 2.87 | 0.42 |
| 1:AA:651:C:O2' | 1:AA:652:U:H5' | 2.20 | 0.42 |
| 23:BA:442:G:O4' | 27:BE:46:ARG:HD3 | 2.19 | 0.42 |
| 13:AM:24:GLY:CA | 13:AM:70:LEU:HD13 | 2.49 | 0.42 |
| 1:AA:909:A:H3' | 1:AA:910:C:C6 | 2.55 | 0.42 |
| 19:CS:29:ARG:HB2 | 19:CS:48:THR:H | 1.85 | 0.42 |
| 27:DE:112:MET:HA | 27:DE:115:ALA:HB3 | 2.01 | 0.42 |
| 23:DA:957:A:N6 | 23:DA:2459:A:C8 | 2.88 | 0.42 |
| 1:AA:538:G:O2' | 1:AA:539:A:H5' | 2.19 | 0.42 |
| 23:BA:2617:C:O2' | 23:BA:2618:G:H5' | 2.18 | 0.42 |
| 1:AA:1210:C:H4' | 1:AA:1214:C:C5 | 2.54 | 0.42 |
| 23:DA:1223:G:C6 | 23:DA:1227:G:C6 | 3.08 | 0.42 |
| 23:DA:1445:C:C2 | 23:DA:1446:C:H5 | 2.37 | 0.42 |
| 7:CG:78:ARG:HH11 | 7:CG:154:TYR:HB3 | 1.83 | 0.42 |
| 37:BO:30:ARG:HD2 | 37:BO:30:ARG:C | 2.39 | 0.42 |
| 23:BA:646:A:C2' | 23:BA:647:G:O5' | 2.68 | 0.42 |
| 32:BJ:32:VAL:CG1 | 32:BJ:33:GLU:N | 2.83 | 0.42 |
| 35:BM:34:LEU:HD11 | 35:BM:129:THR:HB | 2.02 | 0.42 |
| 1:AA:619:U:C2 | 4:AD:135:LEU:HD21 | 2.54 | 0.42 |
| 1:CA:149:A:H8 | 1:CA:149:A:O5' | 2.03 | 0.42 |
| 23:BA:1928:A:H5'' | 23:BA:1929:G:OP2 | 2.20 | 0.42 |
| 23:BA:1864:U:OP1 | 23:BA:2410:G:O2' | 2.36 | 0.42 |
| 26:BD:3:GLY:HA3 | 26:BD:81:ILE:HG21 | 2.02 | 0.42 |
| 23:BA:2690:C:OP2 | 36:BN:14:SER:HB3 | 2.19 | 0.42 |
| 23:DA:723:G:C6 | 23:DA:724:U:C4 | 3.07 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 15:AO:70:LEU:HD11 | 15:AO:77:ARG:HG3 | 2.02 | 0.42 |
| 30:DH:30:LEU:O | 30:DH:31:LEU:C | 2.58 | 0.42 |
| 16:CP:81:ARG:HD3 | 16:CP:83:GLU:OE1 | 2.19 | 0.42 |
| 23:DA:2666:C:H5'' | 23:DA:2667:C:OP2 | 2.19 | 0.42 |
| 52:B4:30:VAL:O | 52:B4:34:ARG:HG2 | 2.19 | 0.42 |
| 23:DA:2088:G:H2' | 23:DA:2089:U:O4' | 2.20 | 0.42 |
| 23:DA:11:G:H2' | 23:DA:12:U:O4' | 2.19 | 0.42 |
| 51:B3:14:THR:HG22 | 51:B3:51:GLU:O | 2.20 | 0.42 |
| 44:DV:10:ARG:HH21 | 44:DV:26:GLY:H | 1.65 | 0.42 |
| 23:BA:1958:C:C2' | 23:BA:1959:G:H5' | 2.50 | 0.42 |
| 10:CJ:61:GLU:OE2 | 14:CN:45:ARG:NH1 | 2.51 | 0.42 |
| 11:CK:50:TYR:O | 11:CK:51:LYS:HG3 | 2.20 | 0.42 |
| 3:CC:48:TYR:O | 3:CC:51:GLY:N | 2.52 | 0.42 |
| 1:CA:1027:C:H2' | 1:CA:102(A):C:O4' | 2.19 | 0.42 |
| 26:BD:64:LYS:HA | 26:BD:64:LYS:HD2 | 1.85 | 0.42 |
| 2:CB:221:LEU:HD22 | 2:CB:221:LEU:HA | 1.85 | 0.42 |
| 1:AA:1015:A:O5' | 1:AA:1015:A:H8 | 2.03 | 0.42 |
| 42:DT:54:VAL:C | 42:DT:55:ASN:HD22 | 2.21 | 0.42 |
| 23:BA:876:C:H2' | 23:BA:877:U:H5' | 2.01 | 0.42 |
| 24:DB:109:G:H2' | 24:DB:110:G:H8 | 1.85 | 0.42 |
| 23:BA:631:A:OP2 | 53:B5:47:LYS:NZ | 2.39 | 0.42 |
| 1:AA:969:A:OP1 | 10:AJ:55:LYS:NZ | 2.52 | 0.42 |
| 25:BC:10:THR:CG2 | 25:BC:13:ARG:HB3 | 2.23 | 0.42 |
| 27:DE:63:LYS:CE | 27:DE:67:GLN:HB3 | 2.49 | 0.42 |
| 23:BA:2293:C:H2' | 23:BA:2294:C:C6 | 2.54 | 0.42 |
| 23:BA:1021:A:N6 | 23:BA:1141:U:C2 | 2.88 | 0.42 |
| 23:DA:1158:C:H2' | 23:DA:1159:U:H5' | 2.01 | 0.42 |
| 39:DQ:95:LEU:C | 39:DQ:97:ASP:H | 2.23 | 0.42 |
| 34:DL:47:ASP:CB | 34:DL:51:PHE:CB | 2.98 | 0.42 |
| 30:BH:123:LEU:HD11 | 30:BH:145:VAL:OXT | 2.19 | 0.42 |
| 23:DA:2293:C:H2' | 23:DA:2294:C:C6 | 2.55 | 0.42 |
| 1:AA:375:U:H2' | 1:AA:376:G:H5' | 2.01 | 0.42 |
| 25:DC:145:VAL:HB | 25:DC:155:LEU:HB2 | 2.01 | 0.42 |
| 23:DA:676:A:N1 | 23:DA:802:A:N1 | 2.67 | 0.42 |
| 4:AD:100:ARG:NH2 | 4:AD:118:ARG:NH1 | 2.63 | 0.42 |
| 12:AL:118:LYS:C | 12:AL:119:TYR:CD1 | 2.93 | 0.42 |
| 4:CD:64:LEU:HD11 | 4:CD:97:LEU:CD1 | 2.50 | 0.42 |
| 42:DT:28:PHE:HE1 | 42:DT:81:VAL:HG22 | 1.84 | 0.42 |
| 16:AP:28:ARG:HG2 | 16:AP:28:ARG:NH1 | 2.11 | 0.42 |
| 23:BA:94:G:C2 | 47:BY:47:ASN:ND2 | 2.88 | 0.42 |
| 20:CT:22:ARG:O | 20:CT:26:ASN:ND2 | 2.52 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:DC:244:ARG:HB2 | 25:DC:245:PRO:HD3 | 2.02 | 0.42 |
| 24:BB:42:C:O2 | 28:BF:93:THR:N | 2.47 | 0.42 |
| 4:AD:108:LEU:O | 4:AD:110:PHE:CD2 | 2.72 | 0.42 |
| 24:DB:70:C:H2' | 24:DB:71:C:C6 | 2.45 | 0.42 |
| 26:BD:59:VAL:C | 26:BD:61:ARG:N | 2.71 | 0.42 |
| 23:DA:138:G:O2' | 23:DA:139:G:H5' | 2.19 | 0.42 |
| 39:DQ:54:LYS:O | 39:DQ:55:ARG:C | 2.57 | 0.42 |
| 5:CE:76:ILE:HG23 | 5:CE:78:HIS:H | 1.84 | 0.42 |
| 44:BV:92:SER:HB2 | 44:BV:94:GLU:OE1 | 2.19 | 0.42 |
| 1:AA:1104:G:N3 | 1:AA:1105:A:C8 | 2.87 | 0.42 |
| 1:CA:41:G:C6 | 1:CA:42:G:C5 | 3.07 | 0.42 |
| 23:BA:2306:C:C4 | 23:BA:2311:A:N6 | 2.87 | 0.42 |
| 47:DY:50:ILE:O | 47:DY:51:ARG:C | 2.57 | 0.42 |
| 23:BA:1495:A:C4 | 23:BA:1496:A:C2 | 3.07 | 0.42 |
| 25:BC:24:ILE:HD13 | 25:BC:84:TYR:HB2 | 2.00 | 0.42 |
| 1:CA:709:G:O2' | 1:CA:710:G:H5' | 2.20 | 0.42 |
| 24:DB:9:G:C6 | 24:DB:10:C:C4 | 3.07 | 0.42 |
| 23:BA:390:A:N6 | 34:BL:71:VAL:HG22 | 2.35 | 0.42 |
| 36:DN:99:LYS:HG2 | 50:D2:43:HIS:O | 2.19 | 0.42 |
| 23:DA:285:C:H2' | 23:DA:286:C:C6 | 2.55 | 0.42 |
| 44:BV:39:VAL:HG21 | 44:BV:44:PHE:CD2 | 2.55 | 0.42 |
| 7:AG:126:ASP:HB3 | 7:AG:131:LYS:O | 2.18 | 0.42 |
| 18:CR:70:ILE:HG23 | 18:CR:79:LEU:CD1 | 2.49 | 0.42 |
| 9:CI:114:TYR:HD1 | 10:CJ:60:ARG:HG2 | 1.84 | 0.42 |
| 38:DP:105:LEU:HD23 | 38:DP:105:LEU:HA | 1.72 | 0.42 |
| 17:CQ:10:VAL:CG1 | 17:CQ:53:LEU:HA | 2.50 | 0.42 |
| 23:BA:912:C:C2 | 23:BA:913:U:C5 | 3.08 | 0.42 |
| 1:CA:1206:G:O4' | 3:CC:194:GLY:N | 2.53 | 0.42 |
| 40:BR:93:GLU:O | 40:BR:94:LEU:HD23 | 2.20 | 0.42 |
| 23:DA:988:A:C5 | 48:DZ:13:ILE:HD12 | 2.55 | 0.42 |
| 1:CA:1022:G:C4 | 1:CA:1023:G:N7 | 2.88 | 0.42 |
| 41:BS:66:GLU:O | 41:BS:68:ARG:N | 2.52 | 0.42 |
| 51:D3:30:THR:CG2 | 51:D3:31:PRO:HD2 | 2.48 | 0.42 |
| 1:AA:587:G:C2 | 1:AA:755:G:C5 | 3.07 | 0.42 |
| 23:BA:17:G:H2' | 23:BA:18:C:H6 | 1.85 | 0.42 |
| 1:AA:565:U:C5 | 1:AA:566:G:C5 | 3.08 | 0.42 |
| 1:CA:382:A:H2' | 1:CA:383:A:H8 | 1.84 | 0.42 |
| 23:BA:1833:U:H2' | 23:BA:1834:U:H5' | 2.01 | 0.42 |
| 44:BV:9:TYR:CE1 | 44:BV:61:LEU:HD13 | 2.54 | 0.42 |
| 1:AA:160:A:H1' | 1:AA:344:A:N7 | 2.35 | 0.42 |
| 23:BA:2465:C:C2 | 23:BA:2486:G:C2 | 3.07 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:DA:2436:G:C4 | 23:DA:2437:U:C5 | 3.07 | 0.42 |
| 23:BA:1517:G:C2 | 23:BA:1518:C:C2 | 3.07 | 0.42 |
| 1:AA:180:U:C2' | 1:AA:181:G:H5' | 2.49 | 0.42 |
| 1:AA:303:A:H2' | 1:AA:304:U:O4' | 2.19 | 0.42 |
| 23:BA:496:G:C1' | 41:BS:61:ASN:HD21 | 2.31 | 0.42 |
| 14:AN:7:ILE:HD12 | 14:AN:8:GLU:N | 2.34 | 0.42 |
| 1:AA:439:A:C8 | 1:AA:440:A:C8 | 3.08 | 0.42 |
| 23:DA:963:U:H2' | 23:DA:964:C:C6 | 2.54 | 0.42 |
| 4:CD:53:ASP:OD2 | 5:CE:107:ARG:HD2 | 2.20 | 0.42 |
| 9:CI:81:ILE:O | 9:CI:85:LEU:HG | 2.19 | 0.42 |
| 1:AA:761:G:C5 | 1:AA:762:C:C5 | 3.08 | 0.42 |
| 10:CJ:30:SER:HB2 | 10:CJ:80:LYS:HG2 | 2.00 | 0.42 |
| 29:DG:38:SER:OG | 29:DG:39:PRO:HD2 | 2.19 | 0.42 |
| 51:B3:11:LEU:HG | 51:B3:26:ASN:HB2 | 2.01 | 0.42 |
| 1:CA:32:A:C6 | 1:CA:33:A:C6 | 3.07 | 0.42 |
| 23:BA:1465:G:C2 | 23:BA:1466:G:N9 | 2.88 | 0.42 |
| 1:AA:149:A:H2' | 1:AA:150:C:H6 | 1.84 | 0.42 |
| 4:AD:199:ASN:HD22 | 4:AD:202:LEU:HG | 1.83 | 0.42 |
| 23:DA:1665:A:H2' | 23:DA:1666:G:O4' | 2.20 | 0.42 |
| 8:CH:107:LEU:H | 8:CH:107:LEU:HD23 | 1.84 | 0.42 |
| 36:DN:65:LEU:HD12 | 36:DN:65:LEU:HA | 1.40 | 0.42 |
| 52:D4:18:PHE:CD2 | 52:D4:18:PHE:C | 2.93 | 0.42 |
| 23:BA:2017:U:O2 | 50:B2:10:LYS:HB2 | 2.20 | 0.42 |
| 23:DA:876:C:C2' | 23:DA:877:U:H5' | 2.50 | 0.42 |
| 23:DA:869:G:H2' | 23:DA:870:A:H8 | 1.85 | 0.42 |
| 23:DA:1421:G:C2 | 23:DA:1422:G:C8 | 3.08 | 0.42 |
| 23:DA:1480:G:C2 | 23:DA:1481:U:C2 | 3.07 | 0.42 |
| 49:B1:36:VAL:HB | 49:B1:37:PRO:HD2 | 2.02 | 0.42 |
| 8:CH:68:ARG:HG2 | 8:CH:69:ARG:N | 2.34 | 0.42 |
| 1:CA:568:G:O6 | 12:CL:4:PRO:HD3 | 2.19 | 0.42 |
| 23:BA:1049:C:O2 | 23:BA:1113:U:H4' | 2.19 | 0.42 |
| 23:DA:468:G:H5'' | 27:DE:60:SER:HB2 | 2.02 | 0.42 |
| 23:DA:1193:G:O2' | 23:DA:1194:A:H5' | 2.19 | 0.42 |
| 39:BQ:22:LYS:HA | 39:BQ:22:LYS:HD3 | 1.56 | 0.42 |
| 23:BA:1362:C:C6 | 23:BA:1362:C:H3' | 2.54 | 0.42 |
| 23:DA:1769:G:O2' | 23:DA:1958:C:OP1 | 2.26 | 0.42 |
| 30:BH:37:VAL:CG1 | 30:BH:38:LEU:N | 2.82 | 0.42 |
| 23:BA:11:G:H2' | 23:BA:12:U:O4' | 2.19 | 0.42 |
| 34:DL:62:LEU:HD21 | 53:D5:25:MET:O | 2.18 | 0.42 |
| 43:BU:71:LYS:NZ | 43:BU:71:LYS:CB | 2.83 | 0.42 |
| 23:BA:860:U:HO2' | 23:BA:861:A:H5' | 1.80 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 45:BW:25:ARG:HD2 | 45:BW:29:GLN:OE1 | 2.19 | 0.42 |
| 23:BA:1542:G:H4' | 23:BA:1543:A:O4' | 2.19 | 0.42 |
| 9:CI:10:ARG:O | 9:CI:11:LYS:HB2 | 2.20 | 0.42 |
| 28:BF:60:LEU:HA | 28:BF:63:ILE:CG1 | 2.49 | 0.42 |
| 22:CV:6193:U:H2' | 22:CV:6194:C:H5' | 2.02 | 0.42 |
| 23:DA:1190:G:H2' | 23:DA:1191:G:C8 | 2.55 | 0.42 |
| 34:DL:36:LYS:HB3 | 34:DL:36:LYS:HE3 | 1.81 | 0.42 |
| 32:BJ:36:TRP:HB2 | 32:BJ:156:GLN:HB2 | 2.01 | 0.42 |
| 26:BD:132:HIS:NE2 | 26:BD:135:HIS:NE2 | 2.66 | 0.42 |
| 23:BA:1021:A:H3' | 23:BA:1022:G:H5'' | 2.01 | 0.42 |
| 23:BA:114(B):A:N3 | 23:BA:1144:G:C8 | 2.87 | 0.42 |
| 42:DT:50:LYS:N | 42:DT:87:GLN:HE22 | 1.92 | 0.42 |
| 39:DQ:79:PHE:HE2 | 39:DQ:106:PHE:CE1 | 2.36 | 0.42 |
| 25:BC:143:HIS:CD2 | 25:BC:143:HIS:C | 2.92 | 0.42 |
| 23:DA:861:A:H2' | 23:DA:862:G:O4' | 2.19 | 0.42 |
| 39:BQ:95:LEU:O | 39:BQ:98:LEU:HG | 2.20 | 0.42 |
| 40:BR:47:VAL:HG12 | 40:BR:49:THR:O | 2.20 | 0.42 |
| 23:DA:2682:U:O4 | 23:DA:2728:U:H1' | 2.20 | 0.42 |
| 37:DO:11:LYS:CG | 37:DO:12:PHE:N | 2.69 | 0.42 |
| 25:DC:143:HIS:CD2 | 25:DC:144:ALA:CB | 2.99 | 0.42 |
| 4:CD:49:ARG:HD2 | 4:CD:49:ARG:HA | 1.76 | 0.42 |
| 1:AA:407:G:H2' | 1:AA:408:A:H8 | 1.84 | 0.42 |
| 4:AD:29:PRO:O | 4:AD:30:LYS:HB3 | 2.19 | 0.42 |
| 23:DA:2713:A:C3' | 23:DA:2714:G:C5' | 2.98 | 0.42 |
| 23:BA:549:G:H2' | 23:BA:550:G:O4' | 2.20 | 0.42 |
| 23:BA:1592:C:H2' | 23:BA:1593:G:C8 | 2.53 | 0.42 |
| 1:CA:189:U:C4 | 17:CQ:72:ARG:NH2 | 2.88 | 0.42 |
| 45:BW:70:GLN:HG2 | 45:BW:72:ARG:HG2 | 2.01 | 0.42 |
| 5:AE:135:THR:O | 5:AE:138:ALA:HB3 | 2.19 | 0.42 |
| 5:AE:41:VAL:O | 5:AE:66:MET:HA | 2.20 | 0.42 |
| 1:AA:1062:U:H2' | 1:AA:1063:C:C6 | 2.54 | 0.42 |
| 41:DS:75:TYR:CD2 | 41:DS:104:THR:HB | 2.52 | 0.42 |
| 36:DN:59:ASP:N | 36:DN:59:ASP:OD2 | 2.52 | 0.42 |
| 43:DU:81:LYS:HD2 | 43:DU:96:ILE:HG13 | 2.01 | 0.42 |
| 43:BU:96:ILE:HD11 | 43:BU:99:CYS:SG | 2.60 | 0.42 |
| 6:CF:33:TYR:HE1 | 6:CF:75:LEU:HA | 1.78 | 0.42 |
| 23:BA:952:G:C6 | 23:BA:966:G:C6 | 3.08 | 0.42 |
| 16:CP:71:ARG:C | 16:CP:73:LEU:H | 2.23 | 0.42 |
| 40:DR:58:VAL:HB | 40:DR:98:GLU:HB2 | 2.01 | 0.42 |
| 1:CA:625:G:C6 | 1:CA:626:U:C4 | 3.08 | 0.42 |
| 23:BA:2687:U:N3 | 23:BA:2688:U:C6 | 2.86 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DA:270(I):C:C2' | 23:DA:270(I):C:O2 | 2.65 | 0.42 |
| 11:AK:38:ASN:HA | 11:AK:39:PRO:HD2 | 1.77 | 0.42 |
| 23:BA:1799:G:O2' | 25:BC:181:GLU:OE2 | 2.37 | 0.42 |
| 28:BF:106:LEU:O | 28:BF:111:LEU:HG | 2.20 | 0.42 |
| 17:AQ:29:HIS:CE1 | 17:AQ:32:TYR:HD1 | 2.37 | 0.42 |
| 23:BA:1006:C:O2' | 23:BA:1007:C:H5' | 2.19 | 0.42 |
| 1:CA:1443:G:N2 | 38:DP:119:LYS:CB | 2.83 | 0.42 |
| 1:CA:649:G:N3 | 1:CA:650:G:C8 | 2.88 | 0.42 |
| 17:CQ:29:HIS:HA | 17:CQ:30:PRO:HD2 | 1.68 | 0.42 |
| 1:CA:731:G:OP1 | 1:CA:766:A:H1' | 2.19 | 0.42 |
| 1:CA:763:G:C4 | 1:CA:764:C:C5 | 3.08 | 0.42 |
| 1:CA:939:G:C2 | 1:CA:940:C:C4 | 3.08 | 0.42 |
| 36:BN:79:LEU:HD23 | 36:BN:83:ILE:HG13 | 2.01 | 0.42 |
| 13:AM:79:LYS:HB2 | 13:AM:79:LYS:HE3 | 1.79 | 0.42 |
| 23:BA:998:C:H2' | 23:BA:999:U:O4' | 2.19 | 0.42 |
| 23:BA:987:G:C6 | 23:BA:988:A:C4 | 3.08 | 0.42 |
| 1:CA:1378:C:H5 | 1:CA:1379:G:C8 | 2.38 | 0.42 |
| 7:CG:27:ILE:CD1 | 7:CG:43:PHE:HD2 | 2.30 | 0.42 |
| 23:DA:2035:G:H4' | 23:DA:2036:C:OP2 | 2.19 | 0.42 |
| 12:AL:74:HIS:HB2 | 12:AL:76:LEU:HD23 | 2.01 | 0.42 |
| 17:AQ:51:TYR:CE1 | 17:AQ:73:VAL:HG11 | 2.55 | 0.42 |
| 23:DA:176:G:H2' | 23:DA:177:G:H5' | 1.99 | 0.42 |
| 35:BM:43:THR:HA | 35:BM:94:VAL:HG12 | 2.02 | 0.42 |
| 8:AH:31:PHE:CE2 | 8:AH:35:ILE:HD11 | 2.55 | 0.42 |
| 23:DA:1431:U:H2' | 23:DA:1432:C:C6 | 2.55 | 0.42 |
| 23:DA:2854:G:C4 | 23:DA:2864:G:N2 | 2.88 | 0.42 |
| 23:DA:1919:A:H5'' | 23:DA:1920:C:OP2 | 2.20 | 0.42 |
| 1:CA:1504:G:H4' | 1:CA:1505:G:O4' | 2.19 | 0.42 |
| 1:CA:179:A:C5 | 1:CA:180:U:C4 | 3.07 | 0.42 |
| 38:BP:112:ARG:HB2 | 38:BP:112:ARG:HE | 1.42 | 0.42 |
| 23:BA:1442:G:C2 | 23:BA:1443:G:C4 | 3.08 | 0.42 |
| 1:CA:928:G:C2 | 1:CA:1390:U:C2 | 3.06 | 0.42 |
| 1:AA:1048:G:C2 | 1:AA:1210:C:N3 | 2.87 | 0.42 |
| 23:DA:1338:G:H2' | 23:DA:1339:G:H5' | 2.00 | 0.42 |
| 2:AB:212:GLN:HG3 | 2:AB:235:SER:HB2 | 2.01 | 0.42 |
| 2:AB:74:LYS:HD3 | 2:AB:76:GLN:OE1 | 2.20 | 0.42 |
| 23:DA:234:C:H2' | 23:DA:235:U:C6 | 2.55 | 0.42 |
| 1:CA:166:G:O2' | 1:CA:167:G:H5' | 2.20 | 0.42 |
| 23:BA:1127:A:H2' | 23:BA:1128:A:C5' | 2.49 | 0.42 |
| 23:DA:2752:C:C2' | 23:DA:2753:A:H5' | 2.49 | 0.42 |
| 23:DA:1360:A:C5' | 23:DA:1361:G:OP2 | 2.68 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DA:1854:A:H62 | 23:DA:1888:G:H8 | 1.68 | 0.42 |
| 32:DJ:58:ARG:HB2 | 32:DJ:60:LYS:HB2 | 2.01 | 0.42 |
| 23:DA:374:A:H3' | 23:DA:375:C:C6 | 2.55 | 0.42 |
| 23:BA:259:G:C2 | 23:BA:260:G:C8 | 3.07 | 0.42 |
| 23:DA:1984:G:H2' | 23:DA:1985:G:O5' | 2.20 | 0.42 |
| 52:D4:21:ARG:HB3 | 52:D4:31:LEU:HD22 | 2.02 | 0.42 |
| 23:BA:265:A:H1' | 23:BA:266:G:O4' | 2.19 | 0.42 |
| 23:BA:35:G:H1' | 23:BA:454:A:N3 | 2.35 | 0.42 |
| 23:BA:1278:A:O3' | 36:BN:34:ILE:HD12 | 2.19 | 0.42 |
| 32:BJ:61:HIS:CE1 | 32:BJ:73:ASP:OD2 | 2.73 | 0.42 |
| 35:BM:112:GLU:CD | 35:BM:112:GLU:H | 2.23 | 0.42 |
| 11:CK:99:GLN:HA | 11:CK:99:GLN:OE1 | 2.20 | 0.42 |
| 23:BA:2587:A:H8 | 23:BA:2587:A:O5' | 2.02 | 0.42 |
| 30:DH:35:LEU:N | 30:DH:35:LEU:HD23 | 2.33 | 0.42 |
| 25:BC:4:LYS:CB | 25:BC:4:LYS:NZ | 2.82 | 0.42 |
| 1:CA:398:C:H6 | 1:CA:398:C:O5' | 2.03 | 0.42 |
| 11:CK:121:PRO:O | 11:CK:122:LYS:O | 2.37 | 0.42 |
| 23:DA:595:C:H2' | 23:DA:596:G:O4' | 2.19 | 0.42 |
| 44:BV:46:LYS:O | 44:BV:50:GLN:OE1 | 2.38 | 0.42 |
| 35:BM:81:VAL:O | 35:BM:81:VAL:HG12 | 2.19 | 0.42 |
| 23:BA:2361:A:H5' | 53:B5:27:THR:OG1 | 2.20 | 0.42 |
| 23:BA:587:C:O2 | 34:BL:33:ARG:HD3 | 2.19 | 0.42 |
| 1:CA:1226:C:O2' | 13:CM:111:LYS:NZ | 2.53 | 0.42 |
| 23:DA:729:G:H5' | 23:DA:730:C:H5'' | 2.01 | 0.42 |
| 4:AD:104:VAL:CG1 | 4:AD:146:ILE:HG21 | 2.50 | 0.42 |
| 12:AL:123:LYS:HA | 12:AL:124:PRO:HD3 | 1.93 | 0.42 |
| 25:BC:33:LEU:CD2 | 25:BC:33:LEU:N | 2.81 | 0.42 |
| 23:DA:1813:G:O2' | 25:DC:50:THR:HG21 | 2.19 | 0.42 |
| 23:BA:547:A:C5 | 23:BA:548:A:C6 | 3.08 | 0.42 |
| 23:BA:2885:C:H2' | 23:BA:2886:G:O5' | 2.19 | 0.42 |
| 3:AC:29:TYR:HE1 | 3:AC:33:LEU:HD22 | 1.85 | 0.42 |
| 27:BE:167:ALA:O | 27:BE:168:ARG:C | 2.58 | 0.42 |
| 26:DD:1:MET:HA | 26:DD:1:MET:CE | 2.50 | 0.42 |
| 24:BB:73:A:C8 | 24:BB:74:U:C5 | 3.08 | 0.42 |
| 44:BV:97:GLU:O | 44:BV:98:MET:HB3 | 2.19 | 0.42 |
| 1:AA:15:G:C5 | 1:AA:16:A:N7 | 2.88 | 0.42 |
| 48:BZ:26:LEU:HD13 | 48:BZ:47:VAL:HG22 | 2.02 | 0.42 |
| 45:BW:66:VAL:O | 45:BW:81:VAL:HA | 2.19 | 0.42 |
| 27:BE:9:ILE:O | 27:BE:9:ILE:HD13 | 2.19 | 0.42 |
| 44:DV:136:PHE:O | 44:DV:137:ILE:HD12 | 2.19 | 0.42 |
| 44:DV:137:ILE:CD1 | 44:DV:137:ILE:N | 2.83 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:505:G:O2' | 1:CA:506:G:H5' | 2.20 | 0.42 |
| 1:CA:448:A:OP2 | 1:CA:485:G:N2 | 2.48 | 0.42 |
| 4:CD:108:LEU:CB | 4:CD:110:PHE:HE2 | 2.29 | 0.42 |
| 29:BG:144:VAL:CA | 29:BG:147:ASN:HB2 | 2.48 | 0.42 |
| 35:BM:8:LYS:CG | 35:BM:9:TYR:N | 2.78 | 0.42 |
| 23:BA:911:A:C2' | 35:BM:9:TYR:OH | 2.65 | 0.42 |
| 11:AK:92:GLU:CD | 11:AK:93:GLN:N | 2.73 | 0.42 |
| 35:DM:8:LYS:CG | 35:DM:9:TYR:N | 2.81 | 0.42 |
| 23:BA:1359:A:N7 | 23:BA:1372:U:C4 | 2.87 | 0.42 |
| 40:DR:99:ILE:HD13 | 40:DR:99:ILE:N | 2.34 | 0.42 |
| 25:DC:14:ARG:HG2 | 25:DC:15:PHE:CD1 | 2.55 | 0.42 |
| 23:DA:255:A:O2' | 23:DA:384:U:OP1 | 2.34 | 0.42 |
| 11:CK:110:ASP:HB3 | 18:CR:85:LEU:HB3 | 2.02 | 0.42 |
| 27:DE:34:TRP:CE3 | 27:DE:35:GLU:HG2 | 2.54 | 0.42 |
| 24:DB:77:U:O2' | 24:DB:78:A:H5' | 2.20 | 0.42 |
| 17:CQ:70:ARG:HD2 | 17:CQ:70:ARG:N | 2.35 | 0.42 |
| 23:DA:498:G:C6 | 23:DA:499:U:C4 | 3.08 | 0.42 |
| 23:DA:481:G:C2 | 23:DA:507:A:C4 | 3.08 | 0.42 |
| 23:DA:1434:A:C5 | 23:DA:1560:G:N2 | 2.87 | 0.42 |
| 38:DP:107:ASP:H | 38:DP:110:ILE:HG13 | 1.83 | 0.42 |
| 23:DA:2101:G:N2 | 23:DA:2189:U:C2 | 2.88 | 0.42 |
| 23:DA:2188:C:H2' | 23:DA:2189:U:C1' | 2.50 | 0.42 |
| 35:BM:21:THR:C | 35:BM:23:GLY:H | 2.22 | 0.42 |
| 1:CA:518:C:C6 | 1:CA:530:G:N3 | 2.88 | 0.42 |
| 23:DA:2476:A:N1 | 23:DA:2477:C:C5 | 2.87 | 0.42 |
| 17:AQ:59:ILE:HG23 | 17:AQ:71:PHE:HD1 | 1.82 | 0.42 |
| 23:DA:2636:U:H2' | 23:DA:2637:U:C6 | 2.55 | 0.42 |
| 23:DA:2662:A:C5 | 23:DA:2663:G:H1' | 2.55 | 0.42 |
| 23:BA:1856:G:C2 | 23:BA:1887:C:C2 | 3.08 | 0.42 |
| 6:CF:3:ARG:CG | 6:CF:66:GLU:HG2 | 2.45 | 0.42 |
| 28:DF:173:LEU:HB2 | 28:DF:180:PHE:HZ | 1.84 | 0.42 |
| 6:AF:50:TYR:O | 6:AF:50:TYR:CD2 | 2.73 | 0.42 |
| 6:CF:12:PRO:HB3 | 6:CF:58:GLY:N | 2.35 | 0.42 |
| 23:BA:1862:G:C2 | 23:BA:1863:G:C5 | 3.08 | 0.42 |
| 23:BA:2322:A:H3' | 23:BA:2323:G:C8 | 2.48 | 0.42 |
| 23:DA:1946:U:C2 | 23:DA:1947:C:C5 | 3.08 | 0.42 |
| 7:CG:23:VAL:CG1 | 7:CG:43:PHE:HE2 | 2.33 | 0.42 |
| 1:AA:433:C:C5 | 1:AA:434:U:H5 | 2.38 | 0.42 |
| 1:CA:498:A:C4' | 1:CA:500:G:OP1 | 2.67 | 0.42 |
| 40:BR:22:VAL:CG1 | 40:BR:23:GLU:H | 2.33 | 0.42 |
| 1:AA:565:U:C4 | 1:AA:566:G:C5 | 3.08 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1262:C:C2 | 1:CA:1263:C:C5 | 3.08 | 0.42 |
| 23:BA:692:C:C2' | 23:BA:693:C:H5' | 2.50 | 0.42 |
| 29:BG:169:VAL:O | 29:BG:170:ARG:HB2 | 2.19 | 0.42 |
| 1:CA:44:G:OP2 | 16:CP:12:LYS:HE3 | 2.20 | 0.42 |
| 1:AA:685:G:O2' | 1:AA:686:U:H5' | 2.20 | 0.42 |
| 23:DA:1638:C:H4' | 23:DA:2710:C:O2 | 2.20 | 0.42 |
| 23:BA:1547:C:H2' | 23:BA:1548:C:C6 | 2.52 | 0.42 |
| 1:CA:1386:G:H2' | 1:CA:1387:G:H8 | 1.85 | 0.42 |
| 1:AA:312:C:H2' | 1:AA:313:A:C8 | 2.55 | 0.42 |
| 1:AA:1386:G:H2' | 1:AA:1387:G:H8 | 1.85 | 0.42 |
| 23:BA:459:U:H4' | 52:B4:40:TRP:CH2 | 2.55 | 0.42 |
| 29:DG:121:ILE:O | 29:DG:122:THR:HG23 | 2.20 | 0.42 |
| 1:AA:504:C:H2' | 1:AA:504:C:O2 | 2.19 | 0.42 |
| 23:BA:262:A:C2' | 23:BA:263:C:H5' | 2.48 | 0.42 |
| 23:BA:1716:U:O2' | 23:BA:1717:G:H5' | 2.20 | 0.42 |
| 46:DX:48:LYS:HZ3 | 46:DX:50:ARG:NH1 | 2.17 | 0.42 |
| 23:BA:2583:G:H3' | 23:BA:2584:U:C5 | 2.55 | 0.42 |
| 1:AA:759:A:H2' | 1:AA:760:G:H5' | 2.02 | 0.42 |
| 1:AA:1384:C:C2 | 1:AA:1385:G:C8 | 3.07 | 0.42 |
| 23:BA:1625:C:H2' | 23:BA:1626:G:O4' | 2.19 | 0.42 |
| 15:CO:70:LEU:HD11 | 15:CO:77:ARG:HG3 | 2.01 | 0.42 |
| 23:BA:869:G:H2' | 23:BA:870:A:H8 | 1.84 | 0.42 |
| 1:AA:245:C:O2 | 1:AA:283:C:N3 | 2.53 | 0.42 |
| 16:AP:81:ARG:HD3 | 16:AP:83:GLU:OE1 | 2.20 | 0.42 |
| 31:BI:15:GLU:HG3 | 31:BI:66:LEU:HG | 2.02 | 0.42 |
| 23:BA:2692:C:H2' | 23:BA:2693:A:O4' | 2.20 | 0.42 |
| 49:D1:48:ILE:HD12 | 49:D1:48:ILE:H | 1.85 | 0.42 |
| 48:BZ:49:LYS:HA | 48:BZ:49:LYS:HD3 | 1.43 | 0.42 |
| 30:DH:61:ARG:O | 30:DH:61:ARG:HG2 | 2.19 | 0.42 |
| 23:DA:2419:U:OP2 | 53:D5:41:ILE:CD1 | 2.67 | 0.42 |
| 34:DL:112:LEU:C | 34:DL:112:LEU:HD23 | 2.40 | 0.42 |
| 34:DL:86:LYS:HB3 | 34:DL:117:GLU:O | 2.19 | 0.42 |
| 26:DD:188:VAL:HG23 | 26:DD:189:PRO:HD2 | 2.00 | 0.42 |
| 34:BL:126:VAL:HG23 | 34:BL:145:PRO:CG | 2.50 | 0.42 |
| 1:CA:1371:G:C2 | 1:CA:1372:U:C2 | 3.08 | 0.42 |
| 9:CI:15:ALA:HA | 9:CI:65:VAL:HA | 2.02 | 0.42 |
| 1:AA:946:A:N1 | 1:AA:1236:A:C2 | 2.87 | 0.42 |
| 10:AJ:58:ASP:C | 10:AJ:60:ARG:H | 2.23 | 0.42 |
| 1:AA:1320:C:O2 | 19:AS:72:GLY:C | 2.57 | 0.42 |
| 26:BD:12:THR:O | 26:BD:23:VAL:O | 2.38 | 0.42 |
| 22:AV:6192:G:H2' | 22:AV:6193:U:H6 | 1.82 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:CV:6183:G:C6 | 22:CV:6184:A:C5 | 3.08 | 0.42 |
| 1:CA:1324:A:O2' | 1:CA:136(A):C:H5'' | 2.19 | 0.42 |
| 23:BA:2846:G:N7 | 23:BA:2847:U:C5 | 2.88 | 0.42 |
| 38:BP:57:PHE:C | 38:BP:59:THR:H | 2.22 | 0.42 |
| 38:BP:73:GLU:OE2 | 38:BP:103:ARG:NE | 2.51 | 0.42 |
| 1:CA:503:C:N3 | 1:CA:504:C:C5 | 2.87 | 0.42 |
| 23:BA:2320:A:C5 | 23:BA:2333:A:C5 | 3.08 | 0.42 |
| 32:BJ:77:VAL:HG12 | 32:BJ:78:VAL:N | 2.35 | 0.42 |
| 40:BR:77:ALA:O | 40:BR:79:VAL:HB | 2.20 | 0.42 |
| 40:BR:13:ARG:HG3 | 40:BR:13:ARG:NH1 | 2.35 | 0.42 |
| 3:AC:182:ILE:HA | 3:AC:202:ILE:O | 2.20 | 0.42 |
| 3:CC:120:VAL:HG21 | 3:CC:137:ALA:CB | 2.50 | 0.42 |
| 24:DB:42:C:O2 | 28:DF:93:THR:N | 2.48 | 0.42 |
| 28:DF:5:LEU:O | 28:DF:8:LYS:HB3 | 2.20 | 0.42 |
| 23:BA:546:C:N4 | 23:BA:547:A:C6 | 2.88 | 0.42 |
| 47:DY:28:LYS:HA | 47:DY:28:LYS:HD3 | 1.78 | 0.42 |
| 35:BM:141:GLN:OXT | 44:BV:53:ILE:O | 2.37 | 0.42 |
| 28:BF:5:LEU:O | 28:BF:8:LYS:HB3 | 2.20 | 0.42 |
| 1:AA:1072:G:C5 | 1:AA:1073:U:C4 | 3.07 | 0.42 |
| 41:DS:75:TYR:C | 41:DS:75:TYR:HD2 | 2.23 | 0.42 |
| 1:CA:406:G:H5'' | 4:CD:5:ILE:CG2 | 2.50 | 0.42 |
| 37:DO:84:GLN:O | 37:DO:86:ALA:N | 2.53 | 0.42 |
| 35:DM:55:VAL:O | 35:DM:58:PHE:N | 2.53 | 0.42 |
| 1:AA:10:A:O2' | 1:AA:11:G:H5' | 2.20 | 0.42 |
| 12:CL:43:THR:HA | 12:CL:44:PRO:HD3 | 1.79 | 0.42 |
| 23:BA:528:A:H2' | 23:BA:529:A:O5' | 2.20 | 0.42 |
| 1:CA:9:G:H5'' | 5:CE:122:GLU:OE1 | 2.20 | 0.42 |
| 1:CA:9:G:O2' | 1:CA:10:A:H5' | 2.19 | 0.42 |
| 1:CA:986:A:C4 | 1:CA:1220:G:N2 | 2.88 | 0.42 |
| 5:CE:50:GLU:HB3 | 5:CE:53:LEU:HD11 | 2.01 | 0.42 |
| 41:BS:40:ASN:C | 41:BS:41:LYS:HG2 | 2.40 | 0.42 |
| 23:DA:933:A:H2' | 23:DA:934:G:O5' | 2.20 | 0.42 |
| 1:AA:821:G:C6 | 1:AA:822:C:N4 | 2.88 | 0.42 |
| 23:BA:1512:G:C5 | 23:BA:1513:C:C4 | 3.08 | 0.42 |
| 31:BI:4:LYS:HG3 | 31:BI:7:VAL:HB | 2.02 | 0.42 |
| 44:DV:151:HIS:HA | 44:DV:170:THR:HA | 2.02 | 0.42 |
| 40:BR:58:VAL:HB | 40:BR:98:GLU:HB2 | 2.01 | 0.42 |
| 1:CA:29:G:C4 | 1:CA:30:U:H5 | 2.38 | 0.42 |
| 23:BA:1478:G:C2 | 23:BA:1479:G:N7 | 2.88 | 0.42 |
| 23:DA:9:U:C2 | 23:DA:2629:A:N6 | 2.88 | 0.42 |
| 23:DA:256:A:H2' | 23:DA:257:A:H5' | 1.96 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BA:1799:G:C8 | 25:BC:181:GLU:CD | 2.93 | 0.42 |
| 29:BG:92:ILE:HG22 | 29:BG:93:GLY:H | 1.80 | 0.42 |
| 38:DP:88:ILE:CG1 | 38:DP:89:VAL:N | 2.82 | 0.42 |
| 23:BA:1468:C:H2' | 23:BA:1469:A:H8 | 1.84 | 0.42 |
| 35:BM:39:PRO:O | 35:BM:40:ALA:HB2 | 2.20 | 0.42 |
| 44:DV:24:LEU:HD12 | 44:DV:85:HIS:HA | 2.00 | 0.42 |
| 46:DX:23:LYS:HB3 | 46:DX:37:ILE:HG12 | 2.01 | 0.42 |
| 23:BA:2641:G:OP1 | 32:BJ:97:ARG:CD | 2.67 | 0.42 |
| 23:DA:1743:G:H2' | 23:DA:1746:G:H8 | 1.85 | 0.42 |
| 1:CA:255:G:O3' | 17:CQ:17:LYS:HD3 | 2.19 | 0.42 |
| 3:CC:73:PRO:C | 3:CC:75:VAL:H | 2.23 | 0.42 |
| 23:BA:2433:A:H5'' | 23:BA:2434:A:OP1 | 2.20 | 0.42 |
| 23:BA:519:U:H5'' | 41:BS:25:ARG:HH21 | 1.85 | 0.42 |
| 2:CB:112:VAL:O | 2:CB:115:LEU:HB3 | 2.20 | 0.42 |
| 23:DA:1709:U:N3 | 23:DA:1750:G:C2 | 2.88 | 0.42 |
| 23:DA:2350:C:H5'' | 53:D5:42:ARG:HD3 | 2.00 | 0.42 |
| 1:AA:1378:C:C5 | 1:AA:1379:G:N9 | 2.87 | 0.42 |
| 1:CA:357:G:H2' | 1:CA:358:U:H6 | 1.84 | 0.42 |
| 30:DH:86:THR:C | 30:DH:87:LYS:HG3 | 2.39 | 0.42 |
| 11:CK:124:LYS:HB3 | 11:CK:125:PHE:CD1 | 2.55 | 0.42 |
| 23:DA:270(Q):C:O2' | 23:DA:270(R):C:O5' | 2.38 | 0.42 |
| 46:BX:68:PRO:O | 46:BX:69:LYS:C | 2.57 | 0.42 |
| 23:BA:1901:A:C2' | 23:BA:1901:A:N3 | 2.81 | 0.42 |
| 1:AA:465:A:O2' | 1:AA:466:G:H5'' | 2.20 | 0.42 |
| 23:BA:171:G:N3 | 23:BA:171:G:H2' | 2.34 | 0.42 |
| 1:AA:358:U:O2 | 1:AA:358:U:H2' | 2.20 | 0.42 |
| 8:CH:50:ARG:H | 8:CH:50:ARG:HD3 | 1.85 | 0.42 |
| 9:CI:86:VAL:CG2 | 9:CI:93:ARG:HB2 | 2.49 | 0.42 |
| 23:DA:1253:A:C3' | 23:DA:1254:A:H5' | 2.50 | 0.42 |
| 23:BA:1203:G:O6 | 23:BA:1204:A:N6 | 2.53 | 0.42 |
| 3:CC:186:PHE:CG | 3:CC:187:ALA:N | 2.88 | 0.42 |
| 19:CS:46:GLY:HA2 | 19:CS:61:TYR:OH | 2.20 | 0.42 |
| 9:AI:86:VAL:CG2 | 9:AI:93:ARG:HB2 | 2.50 | 0.42 |
| 1:AA:827:U:H2' | 1:AA:870:U:O4 | 2.19 | 0.42 |
| 34:DL:100:LEU:HD22 | 34:DL:100:LEU:N | 2.34 | 0.42 |
| 23:DA:1930:G:HO2' | 23:DA:1931:U:P | 2.43 | 0.42 |
| 23:BA:231:C:C5 | 23:BA:232:G:C6 | 3.08 | 0.42 |
| 1:AA:5:U:O2' | 1:AA:6:G:C4 | 2.73 | 0.42 |
| 23:BA:2405:G:O2' | 23:BA:2411:A:N6 | 2.52 | 0.42 |
| 1:AA:897:C:H5'' | 1:AA:898:G:OP2 | 2.20 | 0.42 |
| 19:AS:52:TYR:HA | 19:AS:56:GLN:O | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:AD:189:PRO:CB | 4:AD:194:LEU:HD21 | 2.50 | 0.42 |
| 37:DO:30:ARG:HD2 | 37:DO:30:ARG:C | 2.40 | 0.42 |
| 46:BX:92:LYS:HD2 | 46:BX:92:LYS:HA | 1.92 | 0.42 |
| 23:BA:1581:G:O5' | 23:BA:1581:G:H8 | 2.03 | 0.42 |
| 24:BB:37:C:C5 | 24:BB:38:C:C4 | 3.08 | 0.42 |
| 36:BN:34:ILE:HD13 | 36:BN:34:ILE:HA | 1.84 | 0.42 |
| 23:DA:239:U:O2' | 23:DA:240:G:H5' | 2.20 | 0.42 |
| 23:BA:1835:G:C4 | 23:BA:1836:C:C5 | 3.08 | 0.42 |
| 1:CA:1092:A:C8 | 1:CA:1093:A:N7 | 2.88 | 0.42 |
| 23:DA:41:C:H2' | 23:DA:43:G:O4' | 2.20 | 0.42 |
| 24:DB:38:C:H2' | 24:DB:39:A:H8 | 1.84 | 0.42 |
| 25:BC:215:LEU:HD23 | 25:BC:215:LEU:HA | 1.61 | 0.42 |
| 53:B5:4:MET:HG2 | 53:B5:4:MET:H | 1.61 | 0.42 |
| 23:DA:417:C:O5' | 23:DA:417:C:H6 | 2.03 | 0.42 |
| 34:DL:122:PRO:HA | 34:DL:141:ALA:O | 2.19 | 0.42 |
| 26:DD:103:ASP:OD1 | 26:DD:169:ASN:N | 2.51 | 0.42 |
| 23:DA:1653:G:O6 | 36:DN:11:ASN:HB2 | 2.20 | 0.42 |
| 38:DP:47:GLY:C | 38:DP:63:VAL:HG12 | 2.40 | 0.42 |
| 13:AM:106:ASN:HB2 | 13:AM:107:ALA:H | 1.56 | 0.42 |
| 22:AV:6188:G:O2' | 22:AV:6189:G:H5' | 2.20 | 0.42 |
| 23:BA:2845:G:C2 | 23:BA:2846:G:C5 | 3.07 | 0.42 |
| 23:BA:2846:G:C8 | 23:BA:2847:U:C5 | 3.08 | 0.42 |
| 32:BJ:36:TRP:HB2 | 32:BJ:156:GLN:CB | 2.50 | 0.42 |
| 23:BA:1022:G:C5 | 23:BA:1140:C:N4 | 2.88 | 0.42 |
| 34:DL:47:ASP:HB3 | 34:DL:51:PHE:CB | 2.50 | 0.42 |
| 1:AA:376:G:H2' | 1:AA:377:G:O5' | 2.19 | 0.42 |
| 25:DC:142:VAL:CG2 | 25:DC:192:THR:O | 2.68 | 0.42 |
| 47:BY:28:LYS:HD3 | 47:BY:28:LYS:HA | 1.84 | 0.42 |
| 20:AT:73:HIS:O | 20:AT:74:LYS:C | 2.59 | 0.42 |
| 25:DC:161:THR:O | 25:DC:162:SER:HB2 | 2.19 | 0.42 |
| 23:BA:139:G:N3 | 23:BA:141(A):A:N1 | 2.68 | 0.42 |
| 23:DA:1208:C:C4 | 23:DA:1209:G:C8 | 3.08 | 0.42 |
| 5:CE:14:ARG:CZ | 5:CE:129:ILE:HD11 | 2.49 | 0.42 |
| 23:BA:1787:A:N3 | 23:BA:1787:A:H2' | 2.34 | 0.42 |
| 48:BZ:43:ILE:O | 48:BZ:47:VAL:HG23 | 2.20 | 0.42 |
| 2:AB:204:ASN:CG | 2:AB:205:ASP:H | 2.23 | 0.42 |
| 1:AA:1369:C:O2' | 1:AA:1370:G:O4' | 2.36 | 0.42 |
| 1:AA:1371:G:N1 | 1:AA:1372:U:N3 | 2.68 | 0.42 |
| 9:AI:117:HIS:C | 9:AI:118:LYS:HG3 | 2.40 | 0.42 |
| 9:AI:16:ARG:O | 9:AI:63:ILE:HG23 | 2.20 | 0.42 |
| 44:DV:103:ARG:HG3 | 44:DV:136:PHE:CD1 | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 41:BS:69:LEU:HA | 41:BS:108:GLY:O | 2.19 | 0.42 |
| 23:DA:317:G:C6 | 23:DA:318:C:C4 | 3.07 | 0.42 |
| 5:AE:126:ARG:HG3 | 5:AE:126:ARG:HH11 | 1.75 | 0.42 |
| 43:BU:81:LYS:HD3 | 43:BU:96:ILE:HG13 | 2.01 | 0.42 |
| 1:CA:825:G:H21 | 8:CH:11:THR:HG21 | 1.84 | 0.42 |
| 1:AA:658:G:H5'' | 15:AO:31:LEU:HD21 | 2.00 | 0.42 |
| 8:AH:25:ASP:O | 8:AH:26:VAL:HG12 | 2.20 | 0.42 |
| 16:AP:9:PHE:HB2 | 16:AP:16:HIS:O | 2.20 | 0.42 |
| 53:B5:22:VAL:CG2 | 53:B5:54:GLU:HG3 | 2.50 | 0.42 |
| 40:BR:34:GLU:O | 40:BR:36:PRO:CD | 2.63 | 0.42 |
| 13:AM:23:TYR:CE1 | 13:AM:71:ARG:HD3 | 2.53 | 0.42 |
| 23:BA:390:A:C6 | 34:BL:71:VAL:CG2 | 3.03 | 0.42 |
| 29:BG:77:LYS:HA | 29:BG:80:SER:CB | 2.47 | 0.42 |
| 29:DG:95:ARG:HH12 | 29:DG:97:ARG:HE | 1.67 | 0.42 |
| 1:CA:751:U:H2' | 1:CA:751:U:O2 | 2.19 | 0.42 |
| 23:BA:1467:C:O2' | 23:BA:1468:C:H5' | 2.20 | 0.42 |
| 23:DA:278:A:O2' | 23:DA:279:C:C1' | 2.68 | 0.42 |
| 3:CC:163:ALA:O | 3:CC:164:ARG:HB2 | 2.19 | 0.42 |
| 32:BJ:160:LYS:C | 32:BJ:161:LEU:HD23 | 2.40 | 0.42 |
| 23:DA:1717:G:C5 | 23:DA:1743:G:N1 | 2.88 | 0.42 |
| 1:CA:1076:C:H2' | 1:CA:1077:G:H5' | 2.02 | 0.42 |
| 23:BA:2350:C:H5'' | 53:B5:42:ARG:HD3 | 2.00 | 0.42 |
| 23:DA:817:C:O2' | 23:DA:839:U:H5'' | 2.20 | 0.42 |
| 18:AR:70:ILE:HG23 | 18:AR:79:LEU:CD1 | 2.49 | 0.42 |
| 1:CA:936:C:H2' | 1:CA:937:A:O4' | 2.19 | 0.42 |
| 8:AH:39:LEU:HD13 | 8:AH:39:LEU:HA | 1.72 | 0.42 |
| 2:CB:142:LEU:HG | 2:CB:146:GLN:HG3 | 2.01 | 0.42 |
| 43:BU:68:HIS:ND1 | 43:BU:70:SER:HB3 | 2.35 | 0.42 |
| 8:AH:119:LEU:CD1 | 8:AH:124:ALA:HA | 2.50 | 0.42 |
| 8:AH:119:LEU:H | 8:AH:119:LEU:HG | 1.55 | 0.42 |
| 23:DA:1268:A:C2 | 23:DA:2013:A:C4 | 3.08 | 0.42 |
| 1:AA:445:G:C5 | 1:AA:446:G:N7 | 2.88 | 0.42 |
| 24:BB:93:C:C2 | 24:BB:94:C:C5 | 3.07 | 0.42 |
| 2:AB:143:GLU:O | 2:AB:147:LYS:HB2 | 2.19 | 0.42 |
| 23:DA:2705:A:H2' | 23:DA:2706:G:O4' | 2.18 | 0.42 |
| 23:DA:1127:A:O2' | 23:DA:1128:A:H5'' | 2.20 | 0.42 |
| 38:DP:82:LEU:HD23 | 38:DP:82:LEU:N | 2.34 | 0.42 |
| 23:BA:2183:C:C2' | 23:BA:2183:C:O2 | 2.67 | 0.42 |
| 19:CS:11:VAL:HG22 | 19:CS:12:ASP:N | 2.34 | 0.42 |
| 24:DB:111:U:H2' | 24:DB:112:G:H8 | 1.84 | 0.42 |
| 23:DA:1203:G:H3' | 23:DA:1204:A:H5'' | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1166:G:N2 | 1:CA:1170:A:OP2 | 2.52 | 0.42 |
| 23:DA:1336:A:H2' | 23:DA:1337:G:H8 | 1.84 | 0.42 |
| 23:DA:2300:G:C6 | 23:DA:2301:C:C4 | 3.08 | 0.42 |
| 23:DA:2770:G:H5'' | 23:DA:2771:C:OP2 | 2.19 | 0.42 |
| 2:CB:37:ASN:HA | 2:CB:37:ASN:HD22 | 1.68 | 0.42 |
| 1:AA:763:G:C4 | 1:AA:764:C:C5 | 3.07 | 0.42 |
| 35:DM:84:GLY:HA3 | 45:DW:10:THR:HG23 | 2.01 | 0.42 |
| 51:D3:11:LEU:HG | 51:D3:26:ASN:HB2 | 2.02 | 0.42 |
| 1:AA:165:C:O2' | 1:AA:166:G:H5' | 2.20 | 0.42 |
| 1:AA:450:G:N7 | 1:AA:481:G:C6 | 2.88 | 0.42 |
| 23:DA:1345:C:C2' | 23:DA:1346:G:H5' | 2.50 | 0.42 |
| 23:BA:1983:C:O2' | 23:BA:1984:G:H5' | 2.20 | 0.42 |
| 23:BA:2258:C:H4' | 23:BA:2259:G:OP2 | 2.19 | 0.42 |
| 23:BA:1975:G:H2' | 23:BA:1976:U:C6 | 2.55 | 0.42 |
| 1:CA:1340:A:H2' | 1:CA:1341:U:O4' | 2.20 | 0.42 |
| 15:CO:17:ARG:HB3 | 15:CO:17:ARG:CZ | 2.48 | 0.42 |
| 26:DD:116:VAL:CG1 | 26:DD:122:PHE:CD2 | 3.03 | 0.42 |
| 23:DA:663:G:O3' | 34:DL:21:ARG:NH1 | 2.52 | 0.42 |
| 23:BA:1461:G:C2' | 23:BA:1462:C:H5' | 2.49 | 0.42 |
| 23:BA:1835:G:N3 | 23:BA:1835:G:H2' | 2.35 | 0.42 |
| 1:CA:1419:G:C6 | 1:CA:1420:C:C4 | 3.08 | 0.42 |
| 48:BZ:48:GLU:O | 48:BZ:51:ALA:HB2 | 2.19 | 0.42 |
| 23:BA:563:G:C4 | 23:BA:2018:G:C2 | 3.08 | 0.42 |
| 51:D3:14:THR:HG22 | 51:D3:51:GLU:O | 2.20 | 0.42 |
| 23:BA:449:A:C2' | 23:BA:450:G:H5' | 2.50 | 0.42 |
| 33:DK:13:ASN:C | 33:DK:15:GLY:N | 2.73 | 0.42 |
| 23:BA:132:G:C2' | 23:BA:133:C:H5' | 2.50 | 0.42 |
| 47:BY:32:LEU:HA | 47:BY:32:LEU:HD23 | 1.71 | 0.42 |
| 25:BC:214:TRP:C | 25:BC:216:GLY:H | 2.21 | 0.42 |
| 35:BM:110:THR:OG1 | 35:BM:113:GLN:HB2 | 2.20 | 0.42 |
| 4:CD:58:LEU:HD13 | 4:CD:59:ARG:N | 2.34 | 0.42 |
| 23:DA:2415:G:H4' | 34:DL:66:GLY:HA3 | 1.99 | 0.41 |
| 23:DA:2415:G:O2' | 23:DA:2416:C:H5' | 2.20 | 0.41 |
| 34:DL:111:ARG:HG3 | 34:DL:128:HIS:HB2 | 2.02 | 0.41 |
| 53:B5:23:VAL:HG11 | 53:B5:47:LYS:HD3 | 2.01 | 0.41 |
| 23:BA:2415:G:H2' | 23:BA:2416:C:C6 | 2.54 | 0.41 |
| 52:B4:10:ARG:HG3 | 52:B4:14:LYS:HD2 | 2.02 | 0.41 |
| 23:BA:1170:G:N2 | 23:BA:1180:C:N3 | 2.68 | 0.41 |
| 23:DA:1545:A:O2' | 23:DA:1546:A:H5' | 2.20 | 0.41 |
| 43:DU:12:THR:HG22 | 43:DU:13:VAL:N | 2.35 | 0.41 |
| 2:AB:154:LEU:C | 2:AB:154:LEU:HD22 | 2.39 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:DJ:140:PHE:CD2 | 32:DJ:140:PHE:O | 2.73 | 0.41 |
| 2:CB:111:ARG:NH1 | 2:CB:111:ARG:HA | 2.35 | 0.41 |
| 1:CA:978:A:H5'' | 1:CA:979:C:OP2 | 2.20 | 0.41 |
| 1:AA:1229:A:H2' | 1:AA:1230:C:H6 | 1.82 | 0.41 |
| 1:AA:953:G:O6 | 1:AA:1228:C:N4 | 2.53 | 0.41 |
| 1:CA:363:A:N6 | 1:CA:364:A:C6 | 2.88 | 0.41 |
| 23:BA:577:G:O6 | 23:BA:578:A:N6 | 2.53 | 0.41 |
| 23:BA:1188:U:C4' | 40:BR:79:VAL:HG22 | 2.50 | 0.41 |
| 25:BC:242:ARG:H | 25:BC:242:ARG:HH11 | 1.67 | 0.41 |
| 23:DA:1121:C:H2' | 23:DA:1122:G:O4' | 2.19 | 0.41 |
| 23:DA:2727:G:C6 | 23:DA:2728:U:C5 | 3.08 | 0.41 |
| 25:DC:67:PHE:HB3 | 25:DC:153:ALA:H | 1.85 | 0.41 |
| 23:DA:2579:C:O4' | 26:DD:134:ILE:HG12 | 2.19 | 0.41 |
| 47:BY:25:VAL:HG21 | 47:BY:61:LEU:HD13 | 2.02 | 0.41 |
| 30:DH:114:LEU:HA | 30:DH:130:TYR:CD1 | 2.55 | 0.41 |
| 30:DH:92:VAL:HG22 | 30:DH:93:THR:O | 2.20 | 0.41 |
| 40:DR:77:ALA:C | 40:DR:79:VAL:N | 2.72 | 0.41 |
| 28:BF:161:THR:CG2 | 28:BF:172:LEU:HD23 | 2.48 | 0.41 |
| 23:BA:2884:U:H2' | 23:BA:2885:C:H5' | 2.02 | 0.41 |
| 44:BV:163:LEU:HD23 | 44:BV:163:LEU:H | 1.84 | 0.41 |
| 1:CA:1070:U:O2 | 1:CA:1106:G:C2 | 2.73 | 0.41 |
| 41:BS:9:TYR:N | 41:BS:102:HIS:CD2 | 2.83 | 0.41 |
| 1:AA:1067:A:N3 | 1:AA:1068:G:N9 | 2.68 | 0.41 |
| 4:CD:3:ARG:O | 4:CD:5:ILE:N | 2.52 | 0.41 |
| 45:BW:32:ARG:HA | 45:BW:64:ASP:HB3 | 2.02 | 0.41 |
| 23:DA:2376:A:H2' | 23:DA:2377:A:O4' | 2.20 | 0.41 |
| 37:DO:23:ARG:HB3 | 37:DO:24:LEU:HG | 2.02 | 0.41 |
| 26:BD:49:LEU:N | 26:BD:49:LEU:HD13 | 2.35 | 0.41 |
| 9:AI:111:ARG:O | 9:AI:113:LYS:HE3 | 2.20 | 0.41 |
| 1:AA:1151:A:OP1 | 10:AJ:41:PRO:HA | 2.19 | 0.41 |
| 12:CL:44:PRO:HG2 | 12:CL:50:ALA:N | 2.35 | 0.41 |
| 23:BA:2842:G:H2' | 23:BA:2843:G:O4' | 2.20 | 0.41 |
| 23:BA:526:A:O2' | 23:BA:2043:C:O2 | 2.34 | 0.41 |
| 35:BM:6:ARG:HB2 | 35:BM:6:ARG:HE | 1.60 | 0.41 |
| 23:BA:2305:A:H1' | 28:BF:135:LEU:O | 2.20 | 0.41 |
| 43:BU:81:LYS:CE | 43:BU:97:ARG:HD3 | 2.50 | 0.41 |
| 1:CA:448:A:C4 | 1:CA:487:A:C2 | 3.08 | 0.41 |
| 23:BA:1496:A:C8 | 23:BA:1498:C:C4 | 3.08 | 0.41 |
| 25:BC:133:LEU:HG | 25:BC:189:CYS:O | 2.19 | 0.41 |
| 23:DA:2330:G:H1' | 45:DW:41:ARG:CB | 2.50 | 0.41 |
| 1:CA:350:G:C2' | 1:CA:351:G:H5' | 2.49 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:DE:101:LEU:O | 27:DE:106:ARG:HD3 | 2.19 | 0.41 |
| 23:BA:662:G:H5' | 34:BL:18:ARG:HA | 2.01 | 0.41 |
| 31:DI:4:LYS:HG3 | 31:DI:7:VAL:HB | 2.01 | 0.41 |
| 1:CA:555:C:C2 | 1:CA:556:C:C5 | 3.08 | 0.41 |
| 1:AA:67:C:H2' | 1:AA:68:G:C8 | 2.55 | 0.41 |
| 23:DA:1519:G:O2' | 23:DA:1520:U:H5' | 2.19 | 0.41 |
| 27:DE:204:ASN:C | 27:DE:206:ILE:N | 2.73 | 0.41 |
| 1:CA:105:G:C5 | 1:CA:106:C:C5 | 3.08 | 0.41 |
| 36:DN:99:LYS:HA | 36:DN:112:ALA:HB2 | 2.00 | 0.41 |
| 43:DU:50:ARG:CD | 43:DU:51:VAL:H | 2.27 | 0.41 |
| 23:DA:1131:G:N2 | 23:DA:1132:A:N3 | 2.68 | 0.41 |
| 50:D2:40:LYS:CE | 50:D2:46:CYS:HB3 | 2.50 | 0.41 |
| 43:BU:43:ASN:OD1 | 43:BU:64:GLU:HA | 2.19 | 0.41 |
| 23:DA:865:C:H4' | 23:DA:866:A:OP1 | 2.19 | 0.41 |
| 23:DA:909:A:H2' | 23:DA:912:C:H5 | 1.85 | 0.41 |
| 17:CQ:85:VAL:O | 17:CQ:86:GLU:C | 2.55 | 0.41 |
| 23:BA:559:G:H22 | 39:BQ:49:HIS:CD2 | 2.38 | 0.41 |
| 1:CA:216:G:C6 | 1:CA:217:C:N4 | 2.87 | 0.41 |
| 1:CA:1446:A:O2' | 1:CA:1447:G:C8 | 2.73 | 0.41 |
| 6:AF:3:ARG:CG | 6:AF:66:GLU:HG2 | 2.47 | 0.41 |
| 34:BL:86:LYS:HB3 | 34:BL:117:GLU:O | 2.20 | 0.41 |
| 23:BA:637:A:OP1 | 34:BL:133:SER:CB | 2.68 | 0.41 |
| 1:CA:922:G:H4' | 5:CE:20:GLN:HA | 2.01 | 0.41 |
| 5:CE:20:GLN:O | 5:CE:23:GLY:O | 2.38 | 0.41 |
| 23:BA:1164:G:C5 | 23:BA:1165:U:C4 | 3.08 | 0.41 |
| 1:CA:256:U:C2 | 1:CA:257:G:C8 | 3.08 | 0.41 |
| 28:DF:173:LEU:HD22 | 28:DF:178:PHE:CE1 | 2.55 | 0.41 |
| 1:AA:542:G:H2' | 1:AA:543:C:H6 | 1.85 | 0.41 |
| 4:AD:8:VAL:HG11 | 4:AD:115:ARG:NH1 | 2.34 | 0.41 |
| 12:AL:7:ASN:O | 12:AL:11:ARG:HG3 | 2.20 | 0.41 |
| 23:DA:2631:G:C6 | 23:DA:2632:A:C5 | 3.08 | 0.41 |
| 23:BA:540:G:C4 | 23:BA:541:C:C5 | 3.08 | 0.41 |
| 7:CG:51:GLN:HA | 7:CG:54:THR:O | 2.20 | 0.41 |
| 23:DA:797:C:O2' | 23:DA:798:G:H5' | 2.20 | 0.41 |
| 23:BA:2749:A:H4' | 29:BG:62:LYS:HB3 | 2.01 | 0.41 |
| 23:BA:855:G:C6 | 23:BA:856:C:C4 | 3.08 | 0.41 |
| 23:BA:2663:G:C5 | 23:BA:2664:G:N7 | 2.88 | 0.41 |
| 3:AC:122:GLU:OE2 | 3:AC:126:ARG:NH2 | 2.53 | 0.41 |
| 38:DP:84:GLN:HG3 | 38:DP:85:LYS:CG | 2.50 | 0.41 |
| 2:CB:182:ILE:HG22 | 2:CB:182:ILE:O | 2.18 | 0.41 |
| 1:CA:1262:C:OP2 | 21:CU:25:LYS:HD3 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 39:BQ:20:LEU:H | 39:BQ:20:LEU:HD22 | 1.85 | 0.41 |
| 23:DA:1128:A:N7 | 23:DA:2489:G:O2' | 2.51 | 0.41 |
| 23:DA:2737:G:C6 | 23:DA:2738:A:N7 | 2.88 | 0.41 |
| 23:DA:270(Q):C:O2' | 23:DA:270(R):C:P | 2.78 | 0.41 |
| 23:BA:1526:G:H2' | 23:BA:1527:G:C8 | 2.55 | 0.41 |
| 23:BA:137(A):C:H2' | 23:BA:137(A):C:O2 | 2.19 | 0.41 |
| 1:CA:1399:C:C4 | 1:CA:1502:A:C2 | 3.08 | 0.41 |
| 40:DR:15:GLU:HB3 | 40:DR:16:PRO:HD2 | 2.02 | 0.41 |
| 18:AR:84:LYS:HG2 | 18:AR:84:LYS:H | 1.33 | 0.41 |
| 5:AE:79:GLU:N | 5:AE:79:GLU:CD | 2.73 | 0.41 |
| 26:BD:144:ARG:HB3 | 26:BD:145:LYS:H | 1.50 | 0.41 |
| 42:DT:40:LYS:C | 42:DT:42:ALA:H | 2.23 | 0.41 |
| 23:BA:1444:G:C2 | 23:BA:1548:C:C2 | 3.08 | 0.41 |
| 23:DA:2369:A:H2' | 23:DA:2370:G:C8 | 2.55 | 0.41 |
| 1:AA:313:A:H2' | 1:AA:314:C:C6 | 2.55 | 0.41 |
| 1:CA:312:C:H2' | 1:CA:313:A:C8 | 2.54 | 0.41 |
| 23:BA:1773:A:N7 | 23:BA:1829:A:H1' | 2.35 | 0.41 |
| 15:CO:50:HIS:O | 15:CO:51:HIS:C | 2.57 | 0.41 |
| 14:AN:4:LYS:HD2 | 14:AN:7:ILE:HD11 | 2.03 | 0.41 |
| 39:BQ:27:LEU:O | 39:BQ:27:LEU:HD23 | 2.20 | 0.41 |
| 23:BA:1317:A:C6 | 23:BA:1318:C:N4 | 2.88 | 0.41 |
| 23:DA:503:A:C4 | 23:DA:506:G:N7 | 2.88 | 0.41 |
| 23:BA:2357:U:OP1 | 45:BW:20:ARG:HD3 | 2.20 | 0.41 |
| 1:CA:269:C:H2' | 1:CA:270:A:H8 | 1.85 | 0.41 |
| 2:AB:74:LYS:HB2 | 2:AB:74:LYS:HZ2 | 1.83 | 0.41 |
| 23:BA:2436:G:C4 | 23:BA:2437:U:C6 | 3.08 | 0.41 |
| 23:BA:1635:G:H2' | 23:BA:1636:C:C6 | 2.55 | 0.41 |
| 23:DA:465:G:C2 | 23:DA:466:A:C2 | 3.08 | 0.41 |
| 32:BJ:30:LYS:O | 32:BJ:32:VAL:HG23 | 2.20 | 0.41 |
| 20:AT:32:ALA:O | 20:AT:33:ILE:C | 2.58 | 0.41 |
| 23:BA:2063:C:O2 | 23:BA:2450:A:N1 | 2.53 | 0.41 |
| 15:CO:3:ILE:HG21 | 15:CO:34:LEU:HD23 | 2.01 | 0.41 |
| 23:BA:1983:C:C2' | 23:BA:1984:G:H5' | 2.50 | 0.41 |
| 42:BT:40:LYS:C | 42:BT:42:ALA:N | 2.73 | 0.41 |
| 33:BK:6:THR:O | 33:BK:20:MET:HA | 2.20 | 0.41 |
| 24:DB:95:U:N3 | 24:DB:96:G:N7 | 2.67 | 0.41 |
| 1:CA:1384:C:H2' | 1:CA:1385:G:H8 | 1.84 | 0.41 |
| 8:CH:68:ARG:HG2 | 8:CH:69:ARG:H | 1.84 | 0.41 |
| 8:AH:103:VAL:HB | 8:AH:108:GLY:C | 2.40 | 0.41 |
| 1:CA:1455:G:H2' | 1:CA:1459:C:C6 | 2.55 | 0.41 |
| 23:DA:623:G:H2' | 23:DA:624:C:C6 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:BK:122:LEU:HD23 | 33:BK:122:LEU:HA | 1.80 | 0.41 |
| 34:BL:77:ARG:HG3 | 34:BL:77:ARG:O | 2.20 | 0.41 |
| 38:DP:16:ARG:HD3 | 38:DP:16:ARG:HA | 1.91 | 0.41 |
| 32:DJ:130:LEU:HD23 | 32:DJ:130:LEU:HA | 1.85 | 0.41 |
| 28:DF:67:LYS:HG3 | 28:DF:67:LYS:H | 1.70 | 0.41 |
| 23:DA:1377:G:H8 | 23:DA:1377:G:O5' | 2.03 | 0.41 |
| 9:AI:30:GLY:O | 9:AI:31:GLN:O | 2.37 | 0.41 |
| 36:DN:32:GLY:C | 36:DN:33:ARG:HD2 | 2.39 | 0.41 |
| 52:D4:11:LYS:HD2 | 52:D4:15:THR:HG23 | 1.99 | 0.41 |
| 25:BC:70:TRP:O | 25:BC:70:TRP:CD1 | 2.72 | 0.41 |
| 23:DA:1173:G:C8 | 23:DA:1173:G:OP2 | 2.74 | 0.41 |
| 23:DA:1173:G:H3' | 23:DA:1174:A:H5'' | 2.02 | 0.41 |
| 32:DJ:139:LEU:O | 32:DJ:140:PHE:C | 2.58 | 0.41 |
| 38:DP:57:PHE:C | 38:DP:59:THR:H | 2.22 | 0.41 |
| 12:CL:32:ARG:O | 12:CL:84:ILE:CD1 | 2.64 | 0.41 |
| 1:CA:363:A:H5'' | 12:CL:33:ARG:HB2 | 2.02 | 0.41 |
| 28:BF:72:ARG:HG2 | 28:BF:87:PRO:O | 2.20 | 0.41 |
| 1:CA:1250:A:H4' | 9:CI:68:GLY:N | 2.34 | 0.41 |
| 40:DR:4:ILE:HD13 | 40:DR:13:ARG:HA | 2.02 | 0.41 |
| 30:BH:92:VAL:HG22 | 30:BH:93:THR:O | 2.20 | 0.41 |
| 23:BA:993:G:C6 | 23:BA:994:C:C5 | 3.08 | 0.41 |
| 37:DO:13:ARG:HG3 | 37:DO:14:VAL:H | 1.85 | 0.41 |
| 37:DO:25:ARG:NH2 | 37:DO:42:ASP:OD2 | 2.53 | 0.41 |
| 23:DA:2293:C:H5'' | 37:DO:89:ARG:HH12 | 1.85 | 0.41 |
| 16:AP:58:TYR:HE2 | 16:AP:59:TRP:CZ3 | 2.39 | 0.41 |
| 25:BC:35:LYS:HA | 25:BC:64:ILE:HD12 | 2.01 | 0.41 |
| 30:DH:77:LEU:O | 30:DH:79:ILE:HG12 | 2.20 | 0.41 |
| 23:DA:1408:C:C2 | 23:DA:1595:G:N2 | 2.88 | 0.41 |
| 27:BE:173:VAL:CG1 | 27:BE:174:VAL:N | 2.82 | 0.41 |
| 23:BA:2712:U:O2' | 23:BA:712(B):A:C5' | 2.67 | 0.41 |
| 23:DA:1786:A:C4' | 23:DA:1787:A:OP2 | 2.67 | 0.41 |
| 44:BV:30:ASN:CG | 44:BV:90:VAL:HB | 2.41 | 0.41 |
| 5:AE:75:THR:HG23 | 5:AE:76:ILE:H | 1.85 | 0.41 |
| 23:DA:2634:G:H5' | 26:DD:61:ARG:NH1 | 2.35 | 0.41 |
| 23:DA:1285:G:O6 | 23:DA:1329:U:C2 | 2.73 | 0.41 |
| 1:AA:1107:C:N4 | 1:AA:1108:G:N7 | 2.68 | 0.41 |
| 2:AB:203:GLY:O | 2:AB:204:ASN:O | 2.38 | 0.41 |
| 12:CL:69:ILE:HA | 12:CL:70:PRO:HD3 | 1.69 | 0.41 |
| 1:AA:1350:A:C6 | 1:AA:1351:U:N3 | 2.88 | 0.41 |
| 36:BN:21:TYR:OH | 36:BN:43:GLU:HG2 | 2.21 | 0.41 |
| 1:CA:520:A:N1 | 1:CA:536:C:H1' | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:59:A:H2' | 1:CA:59:A:N3 | 2.34 | 0.41 |
| 36:BN:55:ALA:CA | 36:BN:80:PHE:CE1 | 2.94 | 0.41 |
| 41:BS:29:LEU:HG | 41:BS:29:LEU:O | 2.19 | 0.41 |
| 1:CA:61:G:OP2 | 20:CT:10:LEU:HD13 | 2.19 | 0.41 |
| 23:BA:528:A:C2 | 23:BA:2043:C:O5' | 2.73 | 0.41 |
| 12:AL:50:ALA:O | 12:AL:51:LEU:C | 2.57 | 0.41 |
| 1:CA:1205:U:H3' | 1:CA:1205:U:H6 | 1.84 | 0.41 |
| 6:AF:61:LEU:HD12 | 6:AF:61:LEU:N | 2.35 | 0.41 |
| 23:DA:1496:A:C8 | 23:DA:1498:C:C4 | 3.08 | 0.41 |
| 25:BC:137:PRO:O | 25:BC:138:VAL:C | 2.58 | 0.41 |
| 23:DA:2331:G:H8 | 23:DA:2331:G:O5' | 2.03 | 0.41 |
| 23:DA:529:A:N6 | 23:DA:2041:U:C2 | 2.89 | 0.41 |
| 23:BA:2746:U:H2' | 23:BA:2747:G:C5' | 2.50 | 0.41 |
| 15:AO:18:PHE:O | 15:AO:21:ASP:HB3 | 2.20 | 0.41 |
| 1:CA:618:C:H5'' | 1:CA:619:U:H5'' | 2.02 | 0.41 |
| 37:BO:66:ALA:HA | 37:BO:69:VAL:HG13 | 2.01 | 0.41 |
| 37:BO:69:VAL:HA | 37:BO:72:ALA:HB2 | 2.02 | 0.41 |
| 1:AA:956:U:O2' | 1:AA:957:U:H5' | 2.21 | 0.41 |
| 8:CH:112:LEU:HA | 8:CH:134:ILE:H | 1.85 | 0.41 |
| 45:DW:70:GLN:HG2 | 45:DW:72:ARG:CG | 2.51 | 0.41 |
| 1:AA:833:U:C2 | 1:AA:834:C:C5 | 3.08 | 0.41 |
| 1:AA:99:C:O2' | 1:AA:101:A:H8 | 2.03 | 0.41 |
| 30:BH:14:ASP:H | 30:BH:17:GLN:NE2 | 2.17 | 0.41 |
| 1:CA:987:G:H2' | 1:CA:988:G:C8 | 2.54 | 0.41 |
| 1:AA:1145:C:H1' | 1:AA:1147:C:N4 | 2.35 | 0.41 |
| 1:CA:625:G:O2' | 1:CA:626:U:H5' | 2.20 | 0.41 |
| 25:BC:28:GLU:HB3 | 25:BC:29:PRO:CD | 2.46 | 0.41 |
| 25:BC:140:THR:O | 25:BC:165:ILE:HD12 | 2.19 | 0.41 |
| 11:AK:38:ASN:O | 11:AK:40:ILE:HD13 | 2.20 | 0.41 |
| 33:BK:88:ASN:O | 33:BK:91:LEU:HA | 2.20 | 0.41 |
| 18:CR:64:ARG:O | 18:CR:66:LEU:N | 2.53 | 0.41 |
| 23:BA:2287:A:HO2' | 23:BA:2288:A:C5' | 2.32 | 0.41 |
| 23:BA:286:C:H6 | 23:BA:286:C:O5' | 2.02 | 0.41 |
| 23:DA:1568:G:H5'' | 25:DC:61:LEU:HD22 | 2.01 | 0.41 |
| 32:BJ:62:ARG:HA | 32:BJ:63:PRO:HD3 | 1.89 | 0.41 |
| 1:CA:1195:C:H5'' | 1:CA:1196:U:OP2 | 2.20 | 0.41 |
| 23:BA:1348:G:H1 | 23:BA:1598:C:H42 | 1.67 | 0.41 |
| 1:CA:20:U:H2' | 1:CA:21:G:O4' | 2.20 | 0.41 |
| 23:BA:781:A:C2 | 23:BA:1776:G:N3 | 2.85 | 0.41 |
| 23:DA:581:C:H2' | 23:DA:582:G:H8 | 1.85 | 0.41 |
| 10:AJ:16:LEU:HD21 | 10:AJ:94:VAL:HG13 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:AR:44:LEU:O | 18:AR:45:SER:O | 2.38 | 0.41 |
| 6:CF:47:ARG:CZ | 6:CF:47:ARG:HB3 | 2.49 | 0.41 |
| 1:AA:769:G:H4' | 1:AA:1513:A:H4' | 2.01 | 0.41 |
| 23:DA:2741:A:H2' | 23:DA:2742:C:O4' | 2.21 | 0.41 |
| 20:CT:60:GLU:OE1 | 20:CT:85:MET:HE1 | 2.20 | 0.41 |
| 43:DU:37:VAL:HG13 | 43:DU:69:ALA:HA | 2.01 | 0.41 |
| 7:AG:57:GLU:O | 7:AG:61:VAL:HG23 | 2.20 | 0.41 |
| 2:AB:31:TYR:HE1 | 2:AB:200:ILE:HG21 | 1.85 | 0.41 |
| 2:AB:28:PHE:O | 2:AB:32:ILE:HD13 | 2.20 | 0.41 |
| 41:BS:35:ILE:O | 41:BS:36:LEU:C | 2.58 | 0.41 |
| 43:DU:91:GLU:HB3 | 43:DU:92:ASN:H | 1.67 | 0.41 |
| 24:BB:111:U:H2' | 24:BB:112:G:H8 | 1.84 | 0.41 |
| 19:CS:53:ASN:C | 19:CS:55:LYS:H | 2.24 | 0.41 |
| 26:BD:96:PHE:O | 26:BD:175:VAL:HG11 | 2.19 | 0.41 |
| 12:AL:61:SER:O | 12:AL:63:TYR:N | 2.52 | 0.41 |
| 27:BE:107:LYS:O | 27:BE:108:LYS:C | 2.59 | 0.41 |
| 9:AI:46:ALA:HB2 | 9:AI:74:ILE:HG22 | 2.02 | 0.41 |
| 38:BP:41:ARG:NH1 | 38:BP:41:ARG:HB2 | 2.35 | 0.41 |
| 14:CN:4:LYS:HD2 | 14:CN:7:ILE:HD11 | 2.02 | 0.41 |
| 37:BO:30:ARG:HB3 | 37:BO:35:ILE:HD12 | 2.02 | 0.41 |
| 5:AE:27:ARG:C | 5:AE:28:PHE:CD1 | 2.94 | 0.41 |
| 25:DC:52:ARG:CB | 25:DC:53:PHE:CD2 | 3.02 | 0.41 |
| 36:BN:65:LEU:HA | 36:BN:65:LEU:HD12 | 1.38 | 0.41 |
| 1:AA:451:A:H61 | 1:AA:481:G:C5' | 2.33 | 0.41 |
| 23:DA:1686:C:C4 | 23:DA:1687:G:C5 | 3.08 | 0.41 |
| 24:BB:95:U:N3 | 24:BB:96:G:N7 | 2.68 | 0.41 |
| 24:BB:95:U:C2 | 24:BB:96:G:N7 | 2.88 | 0.41 |
| 15:CO:17:ARG:HG3 | 15:CO:17:ARG:HH11 | 1.85 | 0.41 |
| 1:CA:680:C:H2' | 1:CA:681:C:H6 | 1.85 | 0.41 |
| 30:BH:3:VAL:HG12 | 30:BH:37:VAL:O | 2.20 | 0.41 |
| 1:CA:612:C:OP1 | 4:CD:84:LYS:HE3 | 2.19 | 0.41 |
| 23:BA:822:U:O2' | 23:BA:823:G:H5' | 2.20 | 0.41 |
| 29:BG:142:GLY:O | 29:BG:145:ALA:HB3 | 2.20 | 0.41 |
| 32:DJ:55:THR:O | 32:DJ:55:THR:HG22 | 2.20 | 0.41 |
| 25:DC:215:LEU:HD23 | 25:DC:215:LEU:HA | 1.55 | 0.41 |
| 38:BP:19:LEU:H | 38:BP:19:LEU:HG | 1.29 | 0.41 |
| 23:BA:1690:A:H5'' | 23:BA:1691:C:OP2 | 2.20 | 0.41 |
| 11:AK:87:THR:HA | 11:AK:91:ARG:HH21 | 1.84 | 0.41 |
| 23:DA:2415:G:H2' | 23:DA:2416:C:C6 | 2.56 | 0.41 |
| 23:BA:1309:G:H8 | 23:BA:1309:G:O5' | 2.03 | 0.41 |
| 26:BD:103:ASP:OD2 | 26:BD:168:MET:HE2 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 32:BJ:143:LEU:HD13 | 32:BJ:144:LYS:N | 2.35 | 0.41 |
| 23:BA:1541:U:O2 | 23:BA:1541:U:C2' | 2.66 | 0.41 |
| 32:DJ:120:ARG:O | 32:DJ:121:VAL:C | 2.58 | 0.41 |
| 1:CA:1349:A:H2' | 1:CA:1350:A:C8 | 2.55 | 0.41 |
| 9:CI:117:HIS:C | 9:CI:118:LYS:HG3 | 2.40 | 0.41 |
| 26:BD:188:VAL:HG23 | 26:BD:189:PRO:HD2 | 2.02 | 0.41 |
| 22:AV:6193:U:C4 | 22:AV:6194:C:C4 | 3.07 | 0.41 |
| 1:CA:946:A:N1 | 1:CA:1236:A:C2 | 2.88 | 0.41 |
| 27:DE:65:TRP:CZ3 | 27:DE:73:ALA:O | 2.72 | 0.41 |
| 32:BJ:156:GLN:O | 32:BJ:157:ARG:CB | 2.68 | 0.41 |
| 23:BA:1826:G:P | 25:BC:233:HIS:HD2 | 2.43 | 0.41 |
| 23:DA:1019:U:H5' | 23:DA:1121:C:H1' | 2.03 | 0.41 |
| 32:DJ:90:LEU:HA | 32:DJ:110:LEU:HB3 | 2.03 | 0.41 |
| 1:CA:375:U:H4' | 16:CP:17:TYR:CE2 | 2.54 | 0.41 |
| 30:BH:86:THR:C | 30:BH:87:LYS:HG3 | 2.40 | 0.41 |
| 28:DF:126:ASP:O | 28:DF:128:ARG:N | 2.46 | 0.41 |
| 1:AA:376:G:N3 | 1:AA:377:G:C8 | 2.88 | 0.41 |
| 16:AP:68:ASP:C | 16:AP:70:ALA:H | 2.22 | 0.41 |
| 2:CB:86:GLU:C | 2:CB:88:ALA:H | 2.24 | 0.41 |
| 44:DV:56:VAL:O | 44:DV:57:ILE:HD12 | 2.19 | 0.41 |
| 3:CC:36:ASP:HA | 3:CC:39:ILE:HD12 | 2.02 | 0.41 |
| 23:BA:2711:A:OP1 | 23:BA:712(B):A:P | 2.79 | 0.41 |
| 5:CE:41:VAL:O | 5:CE:66:MET:HA | 2.19 | 0.41 |
| 23:DA:2768:C:N4 | 23:DA:2769:C:C4 | 2.89 | 0.41 |
| 46:DX:13:ILE:HG23 | 46:DX:14:VAL:N | 2.33 | 0.41 |
| 35:DM:47:ILE:HD11 | 35:DM:68:ILE:CD1 | 2.51 | 0.41 |
| 1:CA:587:G:H4' | 8:CH:3:THR:O | 2.21 | 0.41 |
| 36:BN:3:HIS:C | 36:BN:5:LYS:N | 2.72 | 0.41 |
| 47:DY:49:LYS:CD | 47:DY:49:LYS:H | 2.33 | 0.41 |
| 23:DA:528:A:C2' | 23:DA:529:A:O5' | 2.69 | 0.41 |
| 23:BA:1510:A:C2 | 23:BA:1511:A:C4 | 3.08 | 0.41 |
| 42:DT:41:ASN:N | 42:DT:41:ASN:HD22 | 2.18 | 0.41 |
| 1:CA:475:G:C2 | 1:CA:476:G:C4 | 3.09 | 0.41 |
| 23:DA:379:G:C5 | 23:DA:380:U:C6 | 3.07 | 0.41 |
| 1:AA:510:A:H5'' | 1:AA:511:C:OP2 | 2.21 | 0.41 |
| 23:DA:2287:A:H62 | 23:DA:2344:U:H3 | 1.68 | 0.41 |
| 1:CA:101:A:H2' | 1:CA:102:G:H8 | 1.84 | 0.41 |
| 29:BG:73:ALA:O | 29:BG:76:VAL:HB | 2.20 | 0.41 |
| 43:BU:2:ARG:CG | 43:BU:3:VAL:N | 2.83 | 0.41 |
| 21:CU:22:ARG:HA | 21:CU:23:PRO:HD3 | 1.82 | 0.41 |
| 23:BA:2477:C:HO2' | 23:BA:2478:A:P | 2.40 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 18:CR:64:ARG:C | 18:CR:66:LEU:N | 2.73 | 0.41 |
| 44:BV:179:ASP:O | 44:BV:182:LYS:HB2 | 2.20 | 0.41 |
| 23:BA:2864:G:C2 | 23:BA:2865:U:O2 | 2.73 | 0.41 |
| 23:BA:815:C:H2' | 23:BA:816:C:C6 | 2.56 | 0.41 |
| 23:BA:814:C:H5 | 34:BL:27:HIS:CD2 | 2.39 | 0.41 |
| 1:CA:589:C:H42 | 1:CA:650:G:H1 | 1.69 | 0.41 |
| 8:AH:97:VAL:C | 8:AH:99:GLU:N | 2.73 | 0.41 |
| 1:CA:764:C:C2 | 1:CA:765:G:C8 | 3.08 | 0.41 |
| 23:DA:987:G:O6 | 23:DA:988:A:C2 | 2.74 | 0.41 |
| 23:BA:278:A:O2' | 23:BA:279:C:O4' | 2.35 | 0.41 |
| 1:CA:1357:A:C5 | 1:CA:1358:U:C4 | 3.09 | 0.41 |
| 1:AA:542:G:P | 4:AD:10:ARG:NH2 | 2.93 | 0.41 |
| 1:AA:1410:G:H2' | 1:AA:1411:C:H6 | 1.84 | 0.41 |
| 5:CE:144:THR:HG23 | 5:CE:147:ASP:OD1 | 2.21 | 0.41 |
| 7:AG:46:ALA:HB2 | 7:AG:117:ALA:O | 2.19 | 0.41 |
| 25:BC:245:PRO:HA | 25:BC:246:PRO:HD3 | 1.89 | 0.41 |
| 23:DA:2880:C:O3' | 36:DN:90:ARG:NH1 | 2.53 | 0.41 |
| 1:AA:1428:A:H2' | 1:AA:1429:C:C6 | 2.55 | 0.41 |
| 41:BS:36:LEU:CD1 | 41:BS:47:VAL:HB | 2.49 | 0.41 |
| 23:DA:189:G:H1' | 23:DA:207:A:N6 | 2.35 | 0.41 |
| 1:AA:112:G:C2 | 1:AA:113:G:C8 | 3.08 | 0.41 |
| 6:AF:11:ASN:HA | 6:AF:12:PRO:HD2 | 1.94 | 0.41 |
| 7:AG:148:ASN:C | 7:AG:150:ALA:H | 2.24 | 0.41 |
| 23:BA:693:C:C2' | 23:BA:694:U:O5' | 2.69 | 0.41 |
| 23:BA:2737:G:C5 | 23:BA:2738:A:N7 | 2.88 | 0.41 |
| 23:DA:1997:G:O2' | 23:DA:1998:G:H5' | 2.21 | 0.41 |
| 23:BA:2717:G:C6 | 23:BA:2718:G:N7 | 2.89 | 0.41 |
| 5:AE:36:ASP:OD2 | 5:AE:38:GLN:N | 2.53 | 0.41 |
| 1:CA:180:U:C2' | 1:CA:181:G:H5' | 2.50 | 0.41 |
| 23:DA:1833:U:N3 | 23:DA:1834:U:C5 | 2.88 | 0.41 |
| 23:DA:1403:C:H5'' | 23:DA:1471:A:O4' | 2.20 | 0.41 |
| 23:DA:781:A:C2 | 23:DA:1776:G:H2' | 2.56 | 0.41 |
| 23:DA:781:A:C2 | 23:DA:1776:G:N3 | 2.86 | 0.41 |
| 38:BP:77:PRO:HB2 | 38:BP:80:SER:HB2 | 2.01 | 0.41 |
| 2:CB:212:GLN:HG3 | 2:CB:235:SER:HB2 | 2.01 | 0.41 |
| 23:BA:2816:C:O2 | 23:BA:2883:A:O2' | 2.38 | 0.41 |
| 23:DA:1335:U:H2' | 23:DA:1336:A:O5' | 2.19 | 0.41 |
| 1:CA:1479:C:H2' | 1:CA:1480:G:H8 | 1.86 | 0.41 |
| 1:CA:636:U:H5' | 17:CQ:2:PRO:HG3 | 2.02 | 0.41 |
| 33:DK:18:LYS:HG3 | 33:DK:45:GLU:OE2 | 2.20 | 0.41 |
| 11:AK:103:LEU:HA | 11:AK:103:LEU:HD12 | 1.79 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BA:2521:C:O2' | 23:BA:2564:A:N3 | 2.47 | 0.41 |
| 1:CA:874:G:C6 | 1:CA:875:C:C4 | 3.08 | 0.41 |
| 23:BA:2743:C:H2' | 23:BA:2744:G:O4' | 2.20 | 0.41 |
| 30:BH:76:THR:HG22 | 30:BH:141:LYS:CB | 2.49 | 0.41 |
| 23:BA:46:C:N4 | 23:BA:179:G:H1 | 2.18 | 0.41 |
| 28:DF:110:ALA:O | 28:DF:140:ILE:HD12 | 2.19 | 0.41 |
| 23:BA:30:G:C5 | 23:BA:31:C:C4 | 3.08 | 0.41 |
| 26:BD:3:GLY:C | 26:BD:81:ILE:HD13 | 2.40 | 0.41 |
| 23:BA:2358:G:C5 | 23:BA:2359:C:C5 | 3.08 | 0.41 |
| 23:BA:1686:C:N4 | 23:BA:1687:G:C6 | 2.88 | 0.41 |
| 23:BA:2523:G:H2' | 23:BA:2524:G:H5' | 2.02 | 0.41 |
| 1:CA:604:G:H2' | 1:CA:605:U:H5' | 2.02 | 0.41 |
| 23:BA:75:G:H4' | 47:BY:55:ARG:NH2 | 2.35 | 0.41 |
| 23:DA:1889:A:H2' | 23:DA:1890:A:O4' | 2.20 | 0.41 |
| 23:BA:1824:G:C2' | 23:BA:1825:A:H5' | 2.51 | 0.41 |
| 53:D5:37:SER:OG | 53:D5:40:GLU:HG2 | 2.20 | 0.41 |
| 6:CF:99:ALA:HB3 | 18:CR:29:PHE:CE1 | 2.56 | 0.41 |
| 30:BH:136:VAL:HG12 | 30:BH:136:VAL:O | 2.20 | 0.41 |
| 30:BH:95:LYS:O | 30:BH:99:GLU:N | 2.46 | 0.41 |
| 23:DA:2676:C:C2' | 23:DA:2677:G:H5' | 2.50 | 0.41 |
| 7:AG:21:VAL:HG23 | 7:AG:22:LEU:N | 2.35 | 0.41 |
| 23:DA:2684:U:O2' | 23:DA:2685:G:H5' | 2.20 | 0.41 |
| 23:BA:122(A):C:H2' | 23:BA:1222:C:H6 | 1.85 | 0.41 |
| 17:AQ:16:GLN:HB3 | 17:AQ:16:GLN:HE21 | 1.76 | 0.41 |
| 30:DH:95:LYS:O | 30:DH:99:GLU:HB2 | 2.21 | 0.41 |
| 23:BA:468:G:H5'' | 27:BE:60:SER:HB2 | 2.00 | 0.41 |
| 27:DE:184:TYR:O | 27:DE:188:ARG:HB2 | 2.19 | 0.41 |
| 1:AA:1122:U:H2' | 1:AA:1123:A:C8 | 2.56 | 0.41 |
| 7:CG:108:ALA:O | 7:CG:119:ARG:HD2 | 2.20 | 0.41 |
| 23:DA:84:A:H4' | 23:DA:85:G:O5' | 2.20 | 0.41 |
| 32:DJ:49:LEU:O | 32:DJ:49:LEU:HD12 | 2.21 | 0.41 |
| 1:AA:977:A:H2' | 1:AA:978:A:H5'' | 2.02 | 0.41 |
| 1:AA:986:A:C2 | 1:AA:1220:G:C2 | 3.08 | 0.41 |
| 10:CJ:48:THR:HG22 | 10:CJ:62:HIS:CG | 2.53 | 0.41 |
| 13:CM:91:ARG:NH2 | 13:CM:96:LEU:HB3 | 2.35 | 0.41 |
| 27:DE:64:ILE:C | 27:DE:65:TRP:CD1 | 2.93 | 0.41 |
| 42:DT:62:LYS:C | 42:DT:63:LYS:HD3 | 2.40 | 0.41 |
| 23:DA:1971:A:C4 | 25:DC:241:PRO:HG3 | 2.54 | 0.41 |
| 23:BA:1121:C:H2' | 23:BA:1122:G:O4' | 2.20 | 0.41 |
| 32:BJ:90:LEU:HA | 32:BJ:110:LEU:HB3 | 2.01 | 0.41 |
| 28:BF:84:LYS:O | 28:BF:87:PRO:HD3 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 53:D5:62:LEU:HA | 53:D5:62:LEU:HD23 | 1.29 | 0.41 |
| 23:DA:1141:U:H5'' | 23:DA:114(B):A:O4' | 2.21 | 0.41 |
| 16:CP:5:ARG:HB2 | 16:CP:67:THR:HG1 | 1.85 | 0.41 |
| 24:DB:7:G:H5'' | 37:DO:29:PHE:CZ | 2.56 | 0.41 |
| 1:AA:374:A:C6 | 1:AA:375:U:C4 | 3.08 | 0.41 |
| 1:AA:386:C:H2' | 1:AA:387:U:C4' | 2.51 | 0.41 |
| 25:DC:143:HIS:NE2 | 25:DC:192:THR:OG1 | 2.53 | 0.41 |
| 23:DA:603:A:C2 | 23:DA:655:A:C2 | 3.08 | 0.41 |
| 1:CA:367:U:C6 | 1:CA:394:G:C2 | 3.08 | 0.41 |
| 4:CD:111:ALA:HB1 | 4:CD:116:GLN:CG | 2.50 | 0.41 |
| 47:BY:61:LEU:HD12 | 47:BY:61:LEU:HA | 1.49 | 0.41 |
| 24:DB:41:U:H5 | 28:DF:70:VAL:H | 1.67 | 0.41 |
| 20:CT:32:ALA:O | 20:CT:33:ILE:C | 2.58 | 0.41 |
| 4:AD:108:LEU:CB | 4:AD:110:PHE:HE2 | 2.23 | 0.41 |
| 44:DV:31:ARG:CZ | 44:DV:94:GLU:HG3 | 2.51 | 0.41 |
| 26:BD:5:LEU:CB | 26:BD:51:PHE:HD2 | 2.17 | 0.41 |
| 26:BD:55:ASN:C | 26:BD:57:LYS:N | 2.74 | 0.41 |
| 23:DA:2722:G:H2' | 23:DA:2723:C:C6 | 2.55 | 0.41 |
| 5:AE:76:ILE:CG1 | 5:AE:77:PRO:HD2 | 2.41 | 0.41 |
| 37:DO:56:LEU:HG | 37:DO:57:LYS:N | 2.35 | 0.41 |
| 23:BA:2769:C:O2 | 23:BA:2769:C:H2' | 2.20 | 0.41 |
| 7:AG:107:ALA:CB | 7:AG:134:ALA:HB2 | 2.38 | 0.41 |
| 45:BW:81:VAL:O | 45:BW:83:PRO:HD3 | 2.20 | 0.41 |
| 1:AA:1202:G:H4' | 14:AN:29:ARG:HD3 | 2.03 | 0.41 |
| 9:AI:112:LYS:HE3 | 9:AI:116:LYS:O | 2.21 | 0.41 |
| 9:AI:28:VAL:CG2 | 9:AI:63:ILE:HB | 2.46 | 0.41 |
| 8:AH:21:LYS:O | 8:AH:65:TYR:OH | 2.29 | 0.41 |
| 1:CA:506:G:H2' | 1:CA:507:C:H6 | 1.86 | 0.41 |
| 23:DA:2747:G:C6 | 23:DA:2754:U:C6 | 3.09 | 0.41 |
| 23:BA:83:G:N2 | 23:BA:84:A:H62 | 2.19 | 0.41 |
| 23:BA:2562:U:H2' | 23:BA:2563:U:C5' | 2.50 | 0.41 |
| 1:CA:448:A:C2 | 1:CA:487:A:C2 | 3.08 | 0.41 |
| 46:BX:31:GLY:O | 46:BX:32:LYS:CB | 2.63 | 0.41 |
| 23:DA:1486:A:N1 | 23:DA:1504:C:C4 | 2.87 | 0.41 |
| 23:DA:2330:G:C2' | 23:DA:2331:G:H5' | 2.51 | 0.41 |
| 37:BO:34:HIS:HB3 | 37:BO:36:TYR:CE1 | 2.55 | 0.41 |
| 1:CA:1238:A:C5 | 1:CA:1303:C:H1' | 2.53 | 0.41 |
| 1:CA:1237:C:C5 | 1:CA:1336:C:C4 | 3.08 | 0.41 |
| 8:CH:31:PHE:CE2 | 8:CH:35:ILE:HD11 | 2.55 | 0.41 |
| 23:DA:910:A:H2' | 23:DA:2264:C:O2' | 2.20 | 0.41 |
| 23:BA:686:G:O6 | 52:B4:12:ARG:NH1 | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 43:DU:2:ARG:HG3 | 43:DU:2:ARG:HH11 | 1.85 | 0.41 |
| 30:DH:4:ILE:HD12 | 30:DH:5:LEU:N | 2.35 | 0.41 |
| 23:DA:732:C:C2' | 23:DA:733:G:H5' | 2.50 | 0.41 |
| 19:CS:7:LYS:HE3 | 19:CS:7:LYS:HB2 | 1.88 | 0.41 |
| 23:DA:497:A:C6 | 23:DA:498:G:C5 | 3.08 | 0.41 |
| 33:BK:114:ILE:O | 33:BK:118:ALA:N | 2.52 | 0.41 |
| 23:DA:1434:A:H2' | 23:DA:1435:G:C8 | 2.55 | 0.41 |
| 23:BA:947:G:N2 | 23:BA:971:C:C2 | 2.89 | 0.41 |
| 17:CQ:54:GLY:HA3 | 17:CQ:82:MET:HE1 | 2.01 | 0.41 |
| 1:CA:523:A:N1 | 12:CL:91:ASP:HB2 | 2.35 | 0.41 |
| 2:CB:74:LYS:HZ3 | 2:CB:166:ASP:HB2 | 1.85 | 0.41 |
| 33:DK:2:ILE:HD11 | 33:DK:82:ASN:ND2 | 2.35 | 0.41 |
| 1:CA:914:A:OP2 | 1:CA:914:A:O4' | 2.37 | 0.41 |
| 33:DK:19:ILE:HA | 33:DK:42:SER:O | 2.20 | 0.41 |
| 46:DX:23:LYS:HE2 | 46:DX:23:LYS:HB3 | 1.74 | 0.41 |
| 1:AA:277:C:OP1 | 17:AQ:41:LYS:HE3 | 2.20 | 0.41 |
| 1:CA:542:G:C4 | 1:CA:543:C:C5 | 3.09 | 0.41 |
| 1:CA:542:G:H2' | 1:CA:543:C:H6 | 1.85 | 0.41 |
| 23:DA:2663:G:C4 | 23:DA:2664:G:C8 | 3.08 | 0.41 |
| 32:DJ:160:LYS:C | 32:DJ:161:LEU:HD23 | 2.41 | 0.41 |
| 1:CA:909:A:H3' | 1:CA:910:C:C6 | 2.55 | 0.41 |
| 4:AD:6:GLY:O | 4:AD:8:VAL:HG12 | 2.20 | 0.41 |
| 23:DA:2244:U:H1' | 23:DA:2434:A:C4 | 2.55 | 0.41 |
| 10:AJ:16:LEU:HD22 | 10:AJ:94:VAL:HG22 | 2.03 | 0.41 |
| 10:AJ:16:LEU:O | 10:AJ:70:ARG:HD2 | 2.19 | 0.41 |
| 1:AA:1089:G:C6 | 1:AA:1090:U:C5 | 3.09 | 0.41 |
| 1:AA:334:C:C2' | 1:AA:335:C:H5' | 2.51 | 0.41 |
| 23:BA:2663:G:C6 | 23:BA:2664:G:C5 | 3.08 | 0.41 |
| 12:CL:5:THR:CG2 | 12:CL:8:GLN:HG3 | 2.46 | 0.41 |
| 23:DA:956:G:H2' | 23:DA:957:A:H2' | 2.01 | 0.41 |
| 23:DA:2738:A:C2 | 23:DA:2739:U:H1' | 2.55 | 0.41 |
| 44:DV:120:ILE:N | 44:DV:120:ILE:CD1 | 2.83 | 0.41 |
| 23:BA:1356:G:C6 | 23:BA:1357:U:C4 | 3.07 | 0.41 |
| 9:CI:95:LYS:HD3 | 9:CI:95:LYS:C | 2.41 | 0.41 |
| 1:AA:993:G:H4' | 1:AA:994:A:OP2 | 2.19 | 0.41 |
| 13:AM:15:VAL:HG13 | 13:AM:43:THR:O | 2.20 | 0.41 |
| 23:DA:2078:C:H2' | 23:DA:2079:U:C6 | 2.54 | 0.41 |
| 23:BA:1798:U:C5' | 25:BC:259:THR:O | 2.69 | 0.41 |
| 23:DA:718:A:C8 | 23:DA:719:C:C6 | 3.08 | 0.41 |
| 1:AA:269:C:H2' | 1:AA:270:A:H8 | 1.84 | 0.41 |
| 1:AA:1505:G:H4' | 1:AA:1506:U:H5'' | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DA:1381:G:C2' | 23:DA:1382:G:H5' | 2.49 | 0.41 |
| 41:BS:71:VAL:HA | 41:BS:107:LEU:HD12 | 2.03 | 0.41 |
| 23:DA:2771:C:O2 | 23:DA:2771:C:C2' | 2.67 | 0.41 |
| 23:BA:2025:C:N3 | 23:BA:2026:C:C4 | 2.89 | 0.41 |
| 35:BM:84:GLY:HA3 | 45:BW:10:THR:HG23 | 2.02 | 0.41 |
| 23:DA:1230:C:H2' | 23:DA:1231:G:H8 | 1.84 | 0.41 |
| 33:BK:3:GLN:CG | 33:BK:4:PRO:HD2 | 2.50 | 0.41 |
| 42:BT:27:THR:HA | 42:BT:80:ILE:HA | 2.02 | 0.41 |
| 42:DT:18:TYR:O | 42:DT:19:ALA:C | 2.58 | 0.41 |
| 23:BA:2194:G:C5 | 23:BA:2195:C:C5 | 3.08 | 0.41 |
| 8:AH:107:LEU:HD23 | 8:AH:107:LEU:H | 1.84 | 0.41 |
| 23:DA:2795:G:H3' | 23:DA:2797:U:H5'' | 2.03 | 0.41 |
| 23:DA:575:A:OP2 | 23:DA:2499:C:O2' | 2.34 | 0.41 |
| 44:BV:77:ASP:HB2 | 44:BV:84:GLU:CG | 2.50 | 0.41 |
| 23:BA:1366:A:H2' | 23:BA:1367:A:O4' | 2.20 | 0.41 |
| 23:BA:394:A:O2' | 23:BA:395:U:H5' | 2.20 | 0.41 |
| 1:CA:1109:C:H2' | 1:CA:1110:A:O4' | 2.20 | 0.41 |
| 23:BA:14:A:H8 | 23:BA:14:A:O5' | 2.03 | 0.41 |
| 39:BQ:60:LEU:HD13 | 39:BQ:60:LEU:C | 2.41 | 0.41 |
| 1:AA:1433:A:N1 | 1:AA:1434:A:C2 | 2.89 | 0.41 |
| 25:BC:98:VAL:HG23 | 25:BC:99:ASP:N | 2.35 | 0.41 |
| 23:BA:2056:G:C8 | 23:BA:2577:A:C6 | 3.08 | 0.41 |
| 32:BJ:122:LEU:HD22 | 32:BJ:122:LEU:HA | 1.88 | 0.41 |
| 1:CA:1371:G:N1 | 1:CA:1372:U:N3 | 2.68 | 0.41 |
| 9:CI:117:HIS:O | 9:CI:118:LYS:HG3 | 2.20 | 0.41 |
| 34:BL:32:THR:CA | 34:BL:36:LYS:HE2 | 2.51 | 0.41 |
| 5:CE:102:ALA:HB2 | 5:CE:120:THR:HG21 | 2.00 | 0.41 |
| 22:CV:6193:U:C2' | 22:CV:6194:C:H5' | 2.50 | 0.41 |
| 23:DA:2257:U:O2' | 23:DA:2258:C:H5' | 2.20 | 0.41 |
| 1:CA:960:U:C5 | 1:CA:1225:A:C8 | 3.09 | 0.41 |
| 13:CM:106:ASN:O | 13:CM:107:ALA:CB | 2.67 | 0.41 |
| 13:CM:106:ASN:HB2 | 13:CM:107:ALA:H | 1.54 | 0.41 |
| 23:BA:2846:G:C4 | 23:BA:2847:U:C5 | 3.09 | 0.41 |
| 1:AA:1227:A:OP1 | 13:AM:94:ARG:NH2 | 2.54 | 0.41 |
| 25:DC:35:LYS:HA | 25:DC:64:ILE:HD12 | 2.01 | 0.41 |
| 25:BC:143:HIS:CD2 | 25:BC:144:ALA:N | 2.88 | 0.41 |
| 11:AK:115:PRO:C | 11:AK:117:ASN:H | 2.22 | 0.41 |
| 30:BH:98:ALA:HA | 30:BH:109:ILE:HG13 | 2.01 | 0.41 |
| 39:BQ:83:LEU:H | 39:BQ:83:LEU:HD12 | 1.86 | 0.41 |
| 40:BR:38:LEU:HD23 | 40:BR:39:LEU:H | 1.84 | 0.41 |
| 40:BR:49:THR:HB | 40:BR:50:PRO:CD | 2.48 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 16:AP:32:TYR:C | 16:AP:32:TYR:CD2 | 2.94 | 0.41 |
| 16:AP:4:ILE:HB | 16:AP:66:PRO:CB | 2.47 | 0.41 |
| 1:AA:32:A:C6 | 1:AA:33:A:C6 | 3.08 | 0.41 |
| 1:AA:688:G:C4 | 1:AA:689:C:C5 | 3.09 | 0.41 |
| 42:DT:10:ALA:HB1 | 42:DT:11:PRO:HD2 | 2.02 | 0.41 |
| 1:AA:1252:A:H2' | 1:AA:1253:G:O4' | 2.21 | 0.41 |
| 23:BA:1413:G:C2' | 23:BA:1414:G:H5' | 2.50 | 0.41 |
| 44:DV:163:LEU:N | 44:DV:163:LEU:HD23 | 2.35 | 0.41 |
| 35:BM:47:ILE:O | 35:BM:50:ALA:N | 2.52 | 0.41 |
| 26:BD:4:ILE:HG13 | 26:BD:5:LEU:N | 2.36 | 0.41 |
| 23:BA:2697:G:H2' | 23:BA:2698:U:O4' | 2.20 | 0.41 |
| 24:BB:73:A:N6 | 24:BB:104:A:H1' | 2.35 | 0.41 |
| 5:AE:110:LEU:O | 5:AE:115:VAL:HG23 | 2.20 | 0.41 |
| 1:CA:1098:C:H2' | 1:CA:1099:G:O4' | 2.20 | 0.41 |
| 1:CA:1105:A:N3 | 1:CA:1106:G:C8 | 2.88 | 0.41 |
| 1:CA:1106:G:C4 | 1:CA:1107:C:C5 | 3.08 | 0.41 |
| 1:CA:1107:C:N4 | 1:CA:1108:G:N7 | 2.69 | 0.41 |
| 44:BV:103:ARG:HG3 | 44:BV:136:PHE:CD1 | 2.54 | 0.41 |
| 13:CM:4:ILE:HG12 | 13:CM:10:PRO:HD2 | 2.03 | 0.41 |
| 1:AA:1104:G:C2 | 1:AA:1105:A:C4 | 3.09 | 0.41 |
| 1:CA:407:G:N2 | 1:CA:436:C:C2 | 2.88 | 0.41 |
| 1:CA:408:A:N3 | 1:CA:409:G:C8 | 2.88 | 0.41 |
| 46:DX:9:GLY:O | 46:DX:10:LYS:O | 2.38 | 0.41 |
| 12:CL:68:TYR:HB3 | 12:CL:98:HIS:HD2 | 1.86 | 0.41 |
| 1:CA:692:U:O4 | 11:CK:52:GLY:C | 2.59 | 0.41 |
| 1:AA:1366:C:N4 | 1:AA:1367:C:N4 | 2.68 | 0.41 |
| 4:AD:126:ILE:CG2 | 4:AD:127:THR:N | 2.79 | 0.41 |
| 1:CA:822:C:H42 | 1:CA:878:G:H1 | 1.69 | 0.41 |
| 23:DA:2306:C:N4 | 23:DA:2311:A:N6 | 2.68 | 0.41 |
| 6:AF:89:MET:CE | 18:AR:76:LEU:HD21 | 2.51 | 0.41 |
| 23:BA:1497:U:O4' | 23:BA:1497:U:O2 | 2.38 | 0.41 |
| 4:CD:110:PHE:CE1 | 4:CD:148:VAL:HG23 | 2.56 | 0.41 |
| 19:AS:22:LEU:HD13 | 19:AS:27:GLU:CB | 2.51 | 0.41 |
| 25:BC:120:GLY:O | 25:BC:131:LEU:HB3 | 2.19 | 0.41 |
| 8:AH:112:LEU:HB3 | 8:AH:133:LEU:HA | 2.02 | 0.41 |
| 1:AA:725:G:H2' | 1:AA:726:C:H6 | 1.85 | 0.41 |
| 23:BA:1285:G:C5 | 23:BA:1329:U:C4 | 3.08 | 0.41 |
| 23:DA:911:A:C5 | 35:DM:9:TYR:CE1 | 3.09 | 0.41 |
| 23:DA:910:A:N7 | 35:DM:12:GLN:HG3 | 2.36 | 0.41 |
| 1:CA:706:A:H2' | 1:CA:707:C:H5' | 2.02 | 0.41 |
| 3:CC:68:VAL:HG12 | 3:CC:70:VAL:CG2 | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:27:G:H2' | 1:AA:28:G:O4' | 2.20 | 0.41 |
| 23:DA:2209:C:C2 | 23:DA:2216:G:N1 | 2.89 | 0.41 |
| 1:AA:853:G:C4 | 1:AA:854:G:C8 | 3.08 | 0.41 |
| 23:DA:1152:C:O2' | 23:DA:1153:C:H5' | 2.21 | 0.41 |
| 23:DA:104:U:C5 | 23:DA:105:C:C4 | 3.09 | 0.41 |
| 43:DU:2:ARG:HG3 | 43:DU:2:ARG:NH1 | 2.36 | 0.41 |
| 1:CA:102:G:C6 | 1:CA:103:C:N4 | 2.88 | 0.41 |
| 1:CA:170:U:C2' | 1:CA:171:A:H5' | 2.50 | 0.41 |
| 10:AJ:34:VAL:CG2 | 10:AJ:74:ILE:HG22 | 2.50 | 0.41 |
| 43:BU:2:ARG:HG3 | 43:BU:2:ARG:HH11 | 1.85 | 0.41 |
| 15:CO:39:LEU:HD13 | 15:CO:56:LEU:HB2 | 2.00 | 0.41 |
| 7:AG:131:LYS:HE3 | 7:AG:136:LYS:HZ1 | 1.80 | 0.41 |
| 23:BA:2470:G:C2 | 23:BA:2471:C:C6 | 3.09 | 0.41 |
| 23:BA:2188:C:H2' | 23:BA:2189:U:C1' | 2.51 | 0.41 |
| 35:BM:60:ARG:H | 44:BV:179:ASP:HB2 | 1.85 | 0.41 |
| 1:CA:1056:U:H5 | 1:CA:1200:C:C4 | 2.38 | 0.41 |
| 4:CD:79:PHE:CD2 | 4:CD:79:PHE:C | 2.93 | 0.41 |
| 1:AA:1206:G:C6 | 1:AA:1207:G:C5 | 3.09 | 0.41 |
| 23:BA:998:C:OP2 | 39:BQ:93:LYS:NZ | 2.53 | 0.41 |
| 4:AD:6:GLY:O | 4:AD:8:VAL:CG1 | 2.69 | 0.41 |
| 32:DJ:83:ILE:H | 32:DJ:83:ILE:HG13 | 1.59 | 0.41 |
| 14:AN:40:CYS:O | 14:AN:44:LEU:HB3 | 2.20 | 0.41 |
| 23:BA:571:A:C5 | 23:BA:575:A:C8 | 3.08 | 0.41 |
| 36:DN:84:ALA:N | 36:DN:85:PRO:CD | 2.84 | 0.41 |
| 1:AA:937:A:C2 | 1:AA:1379:G:C6 | 3.08 | 0.41 |
| 23:DA:978:G:H2' | 23:DA:979:G:H5' | 2.02 | 0.41 |
| 5:CE:137:GLU:OE2 | 5:CE:137:GLU:O | 2.37 | 0.41 |
| 1:CA:356:A:H1' | 1:CA:368:U:O2' | 2.20 | 0.41 |
| 23:BA:693:C:H2' | 23:BA:694:U:H6 | 1.85 | 0.41 |
| 8:AH:50:ARG:CG | 8:AH:50:ARG:HH11 | 2.33 | 0.41 |
| 23:BA:2039:C:C2 | 23:BA:2040:C:C6 | 3.09 | 0.41 |
| 1:AA:1466:C:H2' | 1:AA:1467:G:O4' | 2.21 | 0.41 |
| 23:DA:880:G:H1 | 23:DA:897:C:N4 | 2.18 | 0.41 |
| 13:CM:15:VAL:HG13 | 13:CM:43:THR:O | 2.20 | 0.41 |
| 2:CB:143:GLU:O | 2:CB:147:LYS:HB2 | 2.20 | 0.41 |
| 23:BA:464:U:C4' | 52:B4:5:TRP:CZ3 | 3.03 | 0.41 |
| 23:DA:464:U:C4' | 52:D4:5:TRP:CZ3 | 3.03 | 0.41 |
| 2:CB:17:PHE:CD1 | 2:CB:44:LEU:HD11 | 2.56 | 0.41 |
| 23:DA:1761:C:H5'' | 23:DA:1762:A:OP2 | 2.21 | 0.41 |
| 1:CA:285:G:C2' | 1:CA:286:G:H5' | 2.50 | 0.41 |
| 32:BJ:52:LYS:O | 32:BJ:55:THR:N | 2.54 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1088:G:C4 | 1:CA:1089:G:C8 | 3.09 | 0.41 |
| 1:AA:515:G:H2' | 1:AA:516:U:O4' | 2.20 | 0.41 |
| 28:BF:52:ILE:HG23 | 28:BF:153:ARG:HH22 | 1.84 | 0.41 |
| 4:AD:23:GLY:HA3 | 4:AD:112:VAL:CG1 | 2.50 | 0.41 |
| 1:AA:763:G:H2' | 1:AA:764:C:H6 | 1.84 | 0.41 |
| 27:DE:179:GLU:CD | 27:DE:179:GLU:N | 2.74 | 0.41 |
| 1:CA:897:C:O2 | 1:CA:897:C:H2' | 2.21 | 0.41 |
| 1:CA:1270:C:H2' | 1:CA:1271:G:O4' | 2.20 | 0.41 |
| 32:DJ:30:LYS:O | 32:DJ:32:VAL:HG23 | 2.21 | 0.41 |
| 1:CA:1403:C:H6 | 1:CA:1403:C:O5' | 2.04 | 0.41 |
| 23:BA:30:G:C6 | 23:BA:31:C:C4 | 3.09 | 0.41 |
| 32:BJ:151:HIS:CD2 | 32:BJ:152:PRO:C | 2.94 | 0.41 |
| 23:BA:2194:G:H2' | 23:BA:2195:C:H6 | 1.86 | 0.41 |
| 1:AA:1186:G:H4' | 9:AI:110:GLU:CD | 2.41 | 0.41 |
| 23:DA:660:G:H5' | 27:DE:99:TYR:CD2 | 2.55 | 0.41 |
| 44:DV:70:LEU:CD2 | 44:DV:70:LEU:N | 2.82 | 0.41 |
| 1:CA:604:G:C2' | 1:CA:605:U:H5' | 2.49 | 0.41 |
| 39:BQ:60:LEU:HD22 | 39:BQ:60:LEU:O | 2.20 | 0.41 |
| 23:DA:2567:G:H2' | 23:DA:2568:C:C6 | 2.56 | 0.41 |
| 50:D2:30:LEU:HD23 | 50:D2:30:LEU:HA | 1.89 | 0.41 |
| 13:CM:98:VAL:HG12 | 13:CM:98:VAL:O | 2.20 | 0.41 |
| 23:BA:1772:G:N1 | 23:BA:1980:G:C6 | 2.89 | 0.41 |
| 15:CO:42:HIS:CD2 | 15:CO:43:LEU:HD23 | 2.54 | 0.41 |
| 53:D5:50:LEU:HD23 | 53:D5:50:LEU:HA | 1.87 | 0.41 |
| 34:DL:125:VAL:O | 34:DL:125:VAL:HG13 | 2.21 | 0.41 |
| 34:DL:83:VAL:O | 34:DL:114:ILE:HA | 2.20 | 0.41 |
| 23:BA:2262:U:H4' | 23:BA:2328:A:C2 | 2.55 | 0.41 |
| 43:BU:8:LYS:NZ | 43:BU:8:LYS:N | 2.62 | 0.41 |
| 26:DD:102:VAL:HB | 26:DD:198:VAL:HG12 | 2.02 | 0.41 |
| 32:BJ:121:VAL:HG23 | 32:BJ:122:LEU:N | 2.36 | 0.41 |
| 48:BZ:52:HIS:H | 48:BZ:52:HIS:HD2 | 1.64 | 0.41 |
| 23:DA:103:A:O5' | 23:DA:103:A:C8 | 2.74 | 0.41 |
| 33:DK:77:ILE:HD12 | 38:DP:73:GLU:O | 2.20 | 0.41 |
| 2:AB:61:LEU:O | 2:AB:61:LEU:HD12 | 2.20 | 0.41 |
| 34:BL:91:PHE:CE2 | 34:BL:95:VAL:HG12 | 2.56 | 0.41 |
| 1:CA:46:G:OP1 | 1:CA:307:C:H4' | 2.21 | 0.41 |
| 23:DA:577:G:C6 | 23:DA:578:A:C6 | 3.08 | 0.41 |
| 23:BA:1019:U:H5' | 23:BA:1121:C:H1' | 2.01 | 0.41 |
| 32:BJ:45:THR:HB | 32:BJ:48:ARG:HG3 | 2.02 | 0.41 |
| 40:DR:35:LEU:C | 40:DR:37:VAL:N | 2.74 | 0.41 |
| 40:DR:44:LYS:HB3 | 40:DR:46:VAL:CG1 | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:376:G:H2' | 1:CA:377:G:O5' | 2.21 | 0.41 |
| 16:CP:21:VAL:HG11 | 16:CP:59:TRP:CD1 | 2.56 | 0.41 |
| 30:BH:97:ILE:HG21 | 30:BH:114:LEU:HD11 | 2.01 | 0.41 |
| 30:BH:79:ILE:HG22 | 30:BH:81:VAL:CG2 | 2.45 | 0.41 |
| 30:BH:82:ARG:CB | 30:BH:89:TYR:HB2 | 2.50 | 0.41 |
| 39:BQ:53:ARG:HA | 39:BQ:56:ASP:HB2 | 2.02 | 0.41 |
| 39:BQ:54:LYS:O | 39:BQ:56:ASP:N | 2.53 | 0.41 |
| 4:AD:49:ARG:HD2 | 4:AD:49:ARG:HA | 1.76 | 0.41 |
| 23:BA:194:G:C2' | 23:BA:195:A:H5' | 2.50 | 0.41 |
| 23:DA:2337:G:N3 | 23:DA:2337:G:H2' | 2.36 | 0.41 |
| 25:DC:177:LEU:HD12 | 25:DC:181:GLU:HB3 | 2.03 | 0.41 |
| 4:AD:31:CYS:C | 4:AD:33:MET:H | 2.23 | 0.41 |
| 4:CD:146:ILE:O | 4:CD:146:ILE:HG22 | 2.20 | 0.41 |
| 23:DA:547:A:C5 | 23:DA:548:A:C6 | 3.08 | 0.41 |
| 2:CB:54:THR:HG21 | 2:CB:201:ILE:CD1 | 2.46 | 0.41 |
| 26:DD:85:ASN:HA | 26:DD:86:PRO:HD3 | 1.76 | 0.41 |
| 4:CD:31:CYS:O | 4:CD:32:ALA:CB | 2.69 | 0.41 |
| 35:BM:141:GLN:HA | 44:BV:72:ARG:HA | 2.02 | 0.41 |
| 44:BV:56:VAL:O | 44:BV:57:ILE:HD12 | 2.20 | 0.41 |
| 5:AE:80:ILE:HD11 | 5:AE:91:LEU:HD12 | 2.02 | 0.41 |
| 37:DO:51:ALA:O | 37:DO:52:SER:O | 2.39 | 0.41 |
| 26:DD:55:ASN:C | 26:DD:57:LYS:N | 2.74 | 0.41 |
| 1:AA:1084:G:H5' | 1:AA:1102:A:OP2 | 2.20 | 0.41 |
| 1:AA:17:U:N3 | 1:AA:18:C:C4 | 2.88 | 0.41 |
| 27:BE:124:LEU:CD1 | 27:BE:125:LEU:O | 2.68 | 0.41 |
| 43:DU:86:ARG:NH1 | 43:DU:95:LYS:HE3 | 2.35 | 0.41 |
| 6:CF:45:LEU:O | 6:CF:46:ARG:HG2 | 2.20 | 0.41 |
| 1:CA:317:G:C4 | 1:CA:318:G:C8 | 3.08 | 0.41 |
| 23:DA:2306:C:C4 | 23:DA:2311:A:N6 | 2.88 | 0.41 |
| 23:DA:2308:G:O2' | 23:DA:2310:A:P | 2.78 | 0.41 |
| 23:DA:95:G:N2 | 23:DA:96:G:H1' | 2.36 | 0.41 |
| 23:DA:1504:C:O2' | 23:DA:1505:C:C6 | 2.72 | 0.41 |
| 6:CF:8:ILE:HG22 | 6:CF:9:VAL:N | 2.34 | 0.41 |
| 23:BA:1323:U:C2' | 23:BA:1324:G:H5' | 2.50 | 0.41 |
| 16:AP:39:TYR:CD2 | 16:AP:39:TYR:C | 2.94 | 0.41 |
| 23:DA:911:A:C6 | 35:DM:9:TYR:CE1 | 3.09 | 0.41 |
| 15:AO:50:HIS:O | 15:AO:51:HIS:C | 2.58 | 0.41 |
| 1:AA:69:G:H2' | 1:AA:73:G:C8 | 2.54 | 0.41 |
| 23:BA:1479:G:C4 | 23:BA:1480:G:C8 | 3.08 | 0.41 |
| 33:DK:23:ARG:HG3 | 33:DK:24:VAL:N | 2.35 | 0.41 |
| 1:CA:1085:U:O4' | 1:CA:1094:G:C2 | 2.73 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:DA:225:A:N6 | 23:DA:226:G:C6 | 2.89 | 0.41 |
| 23:BA:2287:A:C6 | 23:BA:2289:G:C5 | 3.09 | 0.41 |
| 23:BA:2861:G:C4 | 23:BA:2862:G:C8 | 3.08 | 0.41 |
| 23:DA:1389:G:C2 | 23:DA:1399:C:O2 | 2.73 | 0.41 |
| 2:CB:223:ILE:C | 2:CB:225:ALA:N | 2.73 | 0.41 |
| 2:CB:223:ILE:HA | 2:CB:226:ARG:HB3 | 2.03 | 0.41 |
| 1:CA:649:G:C4 | 1:CA:650:G:C8 | 3.09 | 0.41 |
| 1:AA:1056:U:C5 | 1:AA:1200:C:C4 | 3.09 | 0.41 |
| 23:BA:781:A:C2 | 23:BA:1776:G:H2' | 2.55 | 0.41 |
| 23:DA:1270:C:H5'' | 23:DA:1271:G:H5' | 2.03 | 0.41 |
| 1:CA:538:G:N2 | 1:CA:539:A:H1' | 2.36 | 0.41 |
| 1:AA:949:A:OP1 | 13:AM:101:GLN:HB3 | 2.21 | 0.41 |
| 1:AA:1022:G:C4 | 1:AA:1023:G:N7 | 2.88 | 0.41 |
| 8:AH:97:VAL:O | 8:AH:99:GLU:N | 2.52 | 0.41 |
| 23:DA:988:A:N7 | 48:DZ:13:ILE:HD12 | 2.36 | 0.41 |
| 36:BN:79:LEU:HD23 | 36:BN:83:ILE:CB | 2.51 | 0.41 |
| 23:DA:1248:G:C5 | 39:DQ:3:ARG:HB2 | 2.55 | 0.41 |
| 35:BM:111:GLU:OE2 | 35:BM:133:ARG:NH2 | 2.54 | 0.41 |
| 1:CA:565:U:C4 | 1:CA:566:G:C6 | 3.08 | 0.41 |
| 23:BA:2705:A:H3' | 23:BA:2706:G:H8 | 1.85 | 0.41 |
| 50:D2:4:HIS:CB | 50:D2:5:PRO:CD | 2.95 | 0.41 |
| 24:DB:3:C:H2' | 24:DB:4:C:C6 | 2.54 | 0.41 |
| 1:AA:186(F):C:H42 | 1:AA:191(B):G:H1 | 1.67 | 0.41 |
| 6:CF:14:LEU:HD21 | 6:CF:19:LEU:N | 2.36 | 0.41 |
| 23:BA:1131:G:N2 | 23:BA:1132:A:N3 | 2.69 | 0.41 |
| 1:AA:774:G:N2 | 1:AA:806:C:C6 | 2.89 | 0.41 |
| 23:BA:2213:U:H6 | 23:BA:2213:U:O5' | 2.03 | 0.41 |
| 1:AA:925:G:C4 | 1:AA:1392:G:N2 | 2.88 | 0.41 |
| 37:BO:44:LYS:CB | 37:BO:44:LYS:NZ | 2.83 | 0.41 |
| 23:BA:1230:C:H2' | 23:BA:1231:G:C8 | 2.56 | 0.41 |
| 23:DA:1441:G:H2' | 23:DA:1442:G:H8 | 1.86 | 0.41 |
| 23:DA:1547:C:H2' | 23:DA:1548:C:C6 | 2.51 | 0.41 |
| 23:BA:1355:G:H2' | 23:BA:1356:G:O4' | 2.20 | 0.41 |
| 23:BA:1800:C:OP2 | 25:BC:183:ARG:NH2 | 2.54 | 0.41 |
| 19:AS:12:ASP:O | 19:AS:16:LEU:HD13 | 2.20 | 0.41 |
| 12:CL:89:VAL:O | 12:CL:90:LYS:C | 2.58 | 0.41 |
| 2:CB:16:HIS:HB3 | 2:CB:210:SER:HA | 2.03 | 0.41 |
| 23:DA:914:C:C3' | 23:DA:914:C:C6 | 3.03 | 0.41 |
| 2:CB:95:GLN:HA | 2:CB:95:GLN:OE1 | 2.20 | 0.41 |
| 25:BC:53:PHE:CE1 | 25:BC:220:HIS:HA | 2.56 | 0.41 |
| 39:DQ:17:ILE:HA | 39:DQ:20:LEU:HD23 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BA:2837:G:C6 | 23:BA:2838:G:N7 | 2.89 | 0.41 |
| 1:AA:270:A:C5 | 1:AA:271:C:C5 | 3.09 | 0.41 |
| 5:CE:36:ASP:OD2 | 5:CE:38:GLN:N | 2.53 | 0.41 |
| 38:DP:109:GLU:HA | 38:DP:112:ARG:CG | 2.50 | 0.41 |
| 26:DD:70:ALA:O | 26:DD:72:VAL:HG23 | 2.21 | 0.41 |
| 35:DM:10:ARG:HA | 35:DM:10:ARG:HD3 | 1.67 | 0.41 |
| 1:AA:760:G:H2' | 1:AA:761:G:C5' | 2.50 | 0.41 |
| 44:BV:91:LEU:CD2 | 44:BV:96:VAL:HG11 | 2.49 | 0.41 |
| 23:BA:646:A:N3 | 23:BA:646:A:H5' | 2.36 | 0.41 |
| 1:CA:261:U:C5 | 20:CT:79:ARG:CZ | 3.03 | 0.41 |
| 39:DQ:40:PHE:HA | 39:DQ:40:PHE:HD2 | 1.71 | 0.41 |
| 41:DS:71:VAL:HA | 41:DS:107:LEU:HD12 | 2.02 | 0.41 |
| 32:DJ:151:HIS:CD2 | 32:DJ:152:PRO:C | 2.94 | 0.41 |
| 1:AA:838:G:H8 | 1:AA:838:G:O5' | 2.04 | 0.41 |
| 1:AA:141:A:C5 | 1:AA:142:G:N7 | 2.88 | 0.41 |
| 25:DC:89:SER:HB2 | 25:DC:159:ALA:CB | 2.50 | 0.41 |
| 23:DA:2760:C:C2' | 23:DA:2760:C:O2 | 2.68 | 0.41 |
| 23:DA:1985:G:O2' | 23:DA:1986:A:H5' | 2.20 | 0.41 |
| 51:B3:13:CYS:HB2 | 51:B3:22:ALA:HB3 | 2.03 | 0.41 |
| 23:BA:1888:G:N3 | 23:BA:1888:G:H5'' | 2.36 | 0.41 |
| 23:DA:2881:C:C2' | 23:DA:2882:A:H5' | 2.49 | 0.41 |
| 1:AA:283:C:H2' | 1:AA:284:G:O4' | 2.20 | 0.41 |
| 23:BA:2523:G:C2' | 23:BA:2524:G:H5' | 2.51 | 0.41 |
| 30:BH:136:VAL:N | 30:BH:137:PRO:HD3 | 2.36 | 0.41 |
| 5:CE:127:ASN:O | 5:CE:128:PRO:C | 2.59 | 0.41 |
| 23:DA:1718:G:N2 | 23:DA:1742:C:C2 | 2.88 | 0.41 |
| 35:BM:108:GLY:O | 35:BM:109:VAL:HG13 | 2.21 | 0.41 |
| 43:BU:39:VAL:O | 43:BU:40:GLU:CD | 2.59 | 0.41 |
| 23:BA:1320:C:H4' | 23:BA:1321:A:OP1 | 2.21 | 0.41 |
| 23:DA:280:C:C2' | 23:DA:281:G:H5' | 2.50 | 0.41 |
| 23:BA:2441:C:H4' | 23:BA:2441:C:OP1 | 2.20 | 0.41 |
| 23:BA:2088:G:H2' | 23:BA:2089:U:O4' | 2.20 | 0.41 |
| 6:AF:83:ASP:N | 6:AF:83:ASP:OD1 | 2.54 | 0.41 |
| 6:AF:25:ILE:HD13 | 6:AF:25:ILE:HA | 1.80 | 0.41 |
| 3:CC:69:HIS:HA | 3:CC:104:GLN:O | 2.20 | 0.41 |
| 23:BA:1173:G:H3' | 23:BA:1174:A:H5'' | 2.02 | 0.41 |
| 24:BB:82:G:H2' | 24:BB:83:G:H8 | 1.85 | 0.41 |
| 23:DA:328:U:C2' | 23:DA:329:G:OP1 | 2.68 | 0.41 |
| 38:DP:61:PHE:CE2 | 38:DP:76:PHE:HB2 | 2.56 | 0.41 |
| 1:AA:977:A:H8 | 1:AA:1223:C:C4 | 2.38 | 0.41 |
| 26:BD:104:VAL:HG22 | 26:BD:198:VAL:HG13 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:AV:6191:A:C6 | 22:AV:6192:G:C5 | 3.08 | 0.41 |
| 23:DA:673:C:H2' | 23:DA:674:G:H5' | 2.02 | 0.41 |
| 23:DA:1900:A:C2 | 23:DA:1970:A:C4 | 3.09 | 0.41 |
| 23:DA:577:G:O6 | 23:DA:578:A:N6 | 2.54 | 0.41 |
| 25:DC:211:ARG:HD2 | 25:DC:211:ARG:HH11 | 1.74 | 0.41 |
| 32:BJ:110:LEU:O | 32:BJ:110:LEU:CD2 | 2.68 | 0.41 |
| 23:BA:603:A:H2 | 23:BA:655:A:C2 | 2.38 | 0.41 |
| 28:DF:72:ARG:HG2 | 28:DF:87:PRO:O | 2.21 | 0.41 |
| 3:AC:18:TRP:HE3 | 3:AC:18:TRP:H | 1.69 | 0.41 |
| 40:BR:35:LEU:C | 40:BR:37:VAL:N | 2.73 | 0.41 |
| 1:AA:437:U:O4 | 1:AA:438:G:C6 | 2.74 | 0.41 |
| 12:AL:26:LEU:HD22 | 12:AL:27:LYS:H | 1.85 | 0.41 |
| 1:AA:427:U:O4 | 1:AA:428:G:N1 | 2.54 | 0.41 |
| 11:AK:52:GLY:H | 11:AK:55:LYS:HE2 | 1.85 | 0.41 |
| 23:DA:142:G:H2' | 23:DA:143:C:C6 | 2.56 | 0.41 |
| 26:BD:84:PHE:CG | 26:BD:84:PHE:O | 2.74 | 0.41 |
| 26:BD:87:GLU:O | 26:BD:88:GLY:C | 2.54 | 0.41 |
| 23:BA:1589:C:C2' | 23:BA:1589:C:O2 | 2.69 | 0.41 |
| 44:DV:48:PHE:CE1 | 44:DV:52:SER:HA | 2.56 | 0.41 |
| 35:DM:140:ALA:HB1 | 44:DV:99:TYR:HB2 | 2.02 | 0.41 |
| 4:CD:31:CYS:C | 4:CD:33:MET:N | 2.74 | 0.41 |
| 24:BB:69:G:C6 | 24:BB:70:C:C4 | 3.09 | 0.41 |
| 45:BW:72:ARG:CZ | 45:BW:75:LEU:CD1 | 2.96 | 0.41 |
| 5:AE:11:ILE:N | 5:AE:31:LEU:O | 2.51 | 0.41 |
| 1:AA:192:U:O2' | 1:AA:193:C:H5' | 2.21 | 0.41 |
| 1:CA:1072:G:O6 | 1:CA:1104:G:C6 | 2.73 | 0.41 |
| 2:CB:97:TRP:HH2 | 2:CB:176:GLU:CD | 2.24 | 0.41 |
| 23:BA:71:A:H4' | 23:BA:72:U:H5'' | 2.01 | 0.41 |
| 23:BA:2768:C:N4 | 23:BA:2769:C:C4 | 2.88 | 0.41 |
| 1:AA:1070:U:OP1 | 5:AE:25:ARG:NH1 | 2.53 | 0.41 |
| 1:AA:1104:G:N1 | 1:AA:1105:A:C5 | 2.88 | 0.41 |
| 1:CA:42:G:C2 | 1:CA:401:C:O2 | 2.74 | 0.41 |
| 45:BW:50:ASN:HD22 | 45:BW:83:PRO:HD3 | 1.85 | 0.41 |
| 14:AN:23:ARG:HG3 | 14:AN:24:CYS:N | 2.36 | 0.41 |
| 4:AD:159:ARG:O | 4:AD:162:LEU:N | 2.54 | 0.41 |
| 23:BA:2310:A:H2' | 23:BA:2311:A:H5' | 2.03 | 0.41 |
| 46:DX:90:ILE:O | 46:DX:94:LEU:HD22 | 2.20 | 0.41 |
| 23:BA:2819:G:H2' | 23:BA:2821:A:N7 | 2.34 | 0.41 |
| 23:DA:1512:G:C2 | 23:DA:1513:C:C2 | 3.09 | 0.41 |
| 25:BC:168:ARG:HA | 25:BC:173:VAL:HA | 2.01 | 0.41 |
| 8:CH:137:VAL:HG12 | 8:CH:138:TRP:N | 2.36 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BA:2753:A:H2' | 23:BA:2754:U:C5' | 2.51 | 0.41 |
| 1:AA:751:U:H2' | 1:AA:751:U:O2 | 2.21 | 0.41 |
| 37:BO:51:ALA:O | 37:BO:52:SER:O | 2.38 | 0.41 |
| 1:AA:781:A:C3' | 1:AA:782:A:C5' | 2.91 | 0.41 |
| 1:AA:616:G:C2 | 1:AA:617:G:N7 | 2.89 | 0.41 |
| 1:AA:627:G:H2' | 1:AA:628:G:H8 | 1.85 | 0.41 |
| 1:CA:710:G:C6 | 1:CA:711:G:N7 | 2.89 | 0.41 |
| 23:DA:753:C:H2' | 23:DA:754:C:H6 | 1.85 | 0.41 |
| 36:DN:101:ALA:HB2 | 50:D2:44:THR:CB | 2.51 | 0.41 |
| 23:BA:1434:A:H2' | 23:BA:1435:G:H8 | 1.86 | 0.41 |
| 1:CA:781:A:C3' | 1:CA:782:A:C5' | 2.93 | 0.41 |
| 36:DN:100:LEU:H | 36:DN:112:ALA:HA | 1.85 | 0.41 |
| 11:AK:40:ILE:HG22 | 11:AK:75:TYR:CD2 | 2.55 | 0.41 |
| 36:BN:67:LEU:HD22 | 36:BN:67:LEU:HA | 1.91 | 0.41 |
| 50:D2:50:GLY:O | 50:D2:51:TYR:HB2 | 2.20 | 0.41 |
| 1:AA:976:G:H8 | 1:AA:1358:U:O2' | 2.04 | 0.41 |
| 25:DC:61:LEU:HD13 | 25:DC:61:LEU:HA | 1.53 | 0.41 |
| 44:BV:182:LYS:O | 44:BV:186:GLU:HB2 | 2.21 | 0.41 |
| 23:BA:2861:G:O2' | 23:BA:2862:G:H5' | 2.20 | 0.41 |
| 1:CA:915:A:N7 | 1:CA:916:G:C8 | 2.89 | 0.41 |
| 3:CC:17:ASP:HB3 | 3:CC:21:ARG:HH22 | 1.84 | 0.41 |
| 1:CA:759:A:H2' | 1:CA:760:G:H5' | 2.03 | 0.41 |
| 1:CA:1342:C:O2' | 1:CA:1343:G:H5' | 2.21 | 0.41 |
| 36:BN:53:HIS:HB2 | 36:BN:94:TYR:CE1 | 2.56 | 0.41 |
| 23:DA:1717:G:O6 | 23:DA:1743:G:C6 | 2.74 | 0.41 |
| 1:AA:1446:A:O2' | 1:AA:1447:G:C8 | 2.74 | 0.41 |
| 39:BQ:76:TYR:O | 39:BQ:80:ILE:HB | 2.19 | 0.41 |
| 29:BG:16:SER:HB2 | 29:BG:27:LYS:HB2 | 2.01 | 0.41 |
| 23:BA:479:A:N3 | 23:BA:481:G:H5'' | 2.36 | 0.41 |
| 1:CA:444:C:C4 | 1:CA:491:G:N1 | 2.89 | 0.41 |
| 36:BN:85:PRO:C | 36:BN:87:TYR:N | 2.74 | 0.41 |
| 15:AO:37:ASN:HD22 | 15:AO:37:ASN:N | 2.14 | 0.41 |
| 19:AS:29:ARG:HB2 | 19:AS:48:THR:H | 1.86 | 0.41 |
| 1:CA:186(F):C:H42 | 1:CA:191(B):G:H1 | 1.67 | 0.41 |
| 12:CL:5:THR:HG23 | 12:CL:8:GLN:CG | 2.49 | 0.41 |
| 35:DM:69:PHE:CG | 35:DM:70:PRO:HD2 | 2.55 | 0.41 |
| 1:AA:924:C:H2' | 1:AA:925:G:C8 | 2.56 | 0.41 |
| 23:DA:2854:G:C6 | 23:DA:2864:G:N1 | 2.89 | 0.41 |
| 7:CG:30:ILE:HD12 | 7:CG:120:ILE:HD11 | 2.03 | 0.41 |
| 23:DA:2737:G:C5 | 23:DA:2738:A:N7 | 2.89 | 0.41 |
| 23:BA:2738:A:C2 | 23:BA:2739:U:C1' | 3.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:577:G:C1' | 1:CA:816:A:C4 | 3.03 | 0.41 |
| 1:CA:816:A:OP2 | 1:CA:1527:C:C4' | 2.68 | 0.41 |
| 23:DA:880:G:H1 | 23:DA:897:C:H42 | 1.67 | 0.41 |
| 23:DA:26:G:H1' | 23:DA:514:A:H61 | 1.86 | 0.41 |
| 23:DA:1775:U:C2' | 23:DA:1776:G:O5' | 2.68 | 0.41 |
| 23:DA:89:G:C5 | 23:DA:90:U:C5 | 3.08 | 0.41 |
| 42:DT:65:ARG:HE | 42:DT:65:ARG:N | 2.19 | 0.41 |
| 23:BA:1203:G:C6 | 23:BA:1204:A:C6 | 3.08 | 0.41 |
| 23:BA:1116:C:H2' | 23:BA:1117:G:O4' | 2.21 | 0.41 |
| 30:DH:9:LEU:O | 30:DH:10:GLU:C | 2.59 | 0.41 |
| 1:CA:269:C:H2' | 1:CA:270:A:C8 | 2.55 | 0.41 |
| 34:DL:135:LEU:O | 34:DL:139:LYS:HB2 | 2.20 | 0.41 |
| 37:BO:99:LYS:O | 37:BO:100:ALA:C | 2.58 | 0.41 |
| 23:DA:537:C:H2' | 23:DA:539:G:O4' | 2.20 | 0.41 |
| 30:BH:73:GLU:C | 30:BH:75:LEU:H | 2.23 | 0.41 |
| 23:DA:2290:G:C2 | 23:DA:2343:C:O2 | 2.74 | 0.41 |
| 23:BA:269:U:C4 | 23:BA:271(A):U:C2 | 3.09 | 0.41 |
| 23:DA:2238:G:N3 | 23:DA:2238:G:H2' | 2.36 | 0.41 |
| 15:CO:17:ARG:NH1 | 15:CO:77:ARG:NH1 | 2.69 | 0.41 |
| 32:DJ:41:ALA:O | 32:DJ:44:LYS:HG2 | 2.21 | 0.41 |
| 23:DA:32:C:C2' | 23:DA:33:U:H5' | 2.50 | 0.41 |
| 1:AA:604:G:C5 | 1:AA:605:U:C5 | 3.08 | 0.41 |
| 23:DA:1035:U:H2' | 23:DA:1036:G:C8 | 2.56 | 0.41 |
| 23:DA:822:U:O2' | 23:DA:823:G:H5' | 2.19 | 0.41 |
| 23:DA:1370:C:H2' | 23:DA:1371:G:C5' | 2.51 | 0.41 |
| 38:DP:19:LEU:HG | 38:DP:19:LEU:H | 1.33 | 0.41 |
| 23:BA:239:U:O2' | 23:BA:240:G:H5' | 2.20 | 0.41 |
| 23:BA:1583:A:O5' | 23:BA:1583:A:H8 | 2.04 | 0.41 |
| 1:AA:997:U:C4 | 1:AA:998(A):G:N7 | 2.89 | 0.41 |
| 23:DA:1949:G:H2' | 23:DA:1950:G:O4' | 2.20 | 0.41 |
| 23:DA:1491:G:C5 | 23:DA:1500:G:N2 | 2.89 | 0.41 |
| 38:DP:10:VAL:C | 38:DP:12:SER:N | 2.74 | 0.41 |
| 23:DA:2393:A:H5'' | 34:DL:62:LEU:CD1 | 2.41 | 0.41 |
| 23:DA:2393:A:N6 | 23:DA:2422:A:C2 | 2.89 | 0.41 |
| 23:BA:306:U:H3' | 23:BA:306:U:H6 | 1.86 | 0.41 |
| 25:BC:150:LYS:HE3 | 25:BC:150:LYS:HA | 2.01 | 0.41 |
| 23:DA:310:A:P | 43:DU:18:GLY:HA2 | 2.60 | 0.41 |
| 2:AB:159:PRO:HB3 | 2:AB:161:ALA:O | 2.21 | 0.41 |
| 32:DJ:157:ARG:O | 32:DJ:157:ARG:CG | 2.67 | 0.41 |
| 32:DJ:36:TRP:HB2 | 32:DJ:156:GLN:HB2 | 2.02 | 0.41 |
| 41:DS:17:VAL:O | 41:DS:20:VAL:N | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 40:BR:47:VAL:CG1 | 40:BR:50:PRO:O | 2.69 | 0.41 |
| 23:BA:748:G:C8 | 23:BA:750:A:C8 | 3.09 | 0.41 |
| 1:CA:673:G:C6 | 1:CA:674:G:C6 | 3.09 | 0.41 |
| 4:CD:94:LEU:HD23 | 4:CD:97:LEU:HD12 | 2.01 | 0.41 |
| 1:AA:324:G:P | 20:AT:22:ARG:HG2 | 2.61 | 0.41 |
| 1:CA:232:G:H2' | 1:CA:233:C:O4' | 2.20 | 0.41 |
| 36:DN:103:ARG:HH12 | 36:DN:110:PRO:HG3 | 1.84 | 0.41 |
| 24:BB:41:U:H5 | 28:BF:70:VAL:H | 1.68 | 0.41 |
| 4:AD:110:PHE:CE1 | 4:AD:148:VAL:HG23 | 2.56 | 0.41 |
| 24:DB:70:C:C2 | 24:DB:71:C:C6 | 3.09 | 0.41 |
| 3:CC:91:LEU:HD12 | 3:CC:101:LEU:HD21 | 2.01 | 0.41 |
| 1:AA:367:U:C5 | 1:AA:394:G:N1 | 2.89 | 0.41 |
| 27:BE:167:ALA:O | 27:BE:170:LEU:HB2 | 2.21 | 0.41 |
| 45:BW:70:GLN:HG2 | 45:BW:72:ARG:CG | 2.51 | 0.41 |
| 5:AE:76:ILE:HG23 | 5:AE:78:HIS:H | 1.86 | 0.41 |
| 23:DA:2542:A:C8 | 23:DA:2544:G:O6 | 2.73 | 0.41 |
| 1:CA:1072:G:C6 | 1:CA:1104:G:N1 | 2.89 | 0.41 |
| 1:AA:1063:C:C5 | 1:AA:1064:G:C4 | 3.09 | 0.41 |
| 1:AA:1071:C:O2 | 1:AA:1072:G:C8 | 2.73 | 0.41 |
| 25:DC:172:TYR:CD1 | 25:DC:185:VAL:C | 2.91 | 0.41 |
| 2:CB:138:LEU:HA | 2:CB:141:GLU:HG3 | 2.02 | 0.41 |
| 6:CF:62:TRP:CD2 | 6:CF:62:TRP:O | 2.74 | 0.41 |
| 23:BA:528:A:N1 | 23:BA:2043:C:O5' | 2.54 | 0.41 |
| 23:DA:2755:C:H6 | 23:DA:2755:C:O5' | 2.03 | 0.41 |
| 5:CE:50:GLU:HB3 | 5:CE:53:LEU:CD1 | 2.51 | 0.41 |
| 1:AA:738:C:C2 | 1:AA:739:C:C5 | 3.09 | 0.41 |
| 23:BA:2752:C:C2' | 23:BA:2753:A:H5' | 2.51 | 0.41 |
| 1:AA:658:G:N1 | 1:AA:749:C:C4 | 2.88 | 0.41 |
| 23:BA:1105:U:C2' | 23:BA:1106:G:H5' | 2.50 | 0.41 |
| 9:CI:16:ARG:O | 9:CI:63:ILE:HG23 | 2.20 | 0.41 |
| 16:AP:72:ARG:O | 16:AP:72:ARG:HG2 | 2.20 | 0.41 |
| 8:CH:134:ILE:O | 8:CH:135:CYS:HB3 | 2.21 | 0.41 |
| 25:BC:7:LYS:HG3 | 25:BC:8:PRO:HD2 | 2.03 | 0.41 |
| 23:DA:1669:A:H2' | 23:DA:1670:C:H5' | 2.02 | 0.41 |
| 37:DO:34:HIS:CB | 37:DO:36:TYR:HE1 | 2.33 | 0.41 |
| 3:AC:50:ALA:HB1 | 3:AC:70:VAL:HG11 | 2.03 | 0.41 |
| 3:AC:58:GLU:C | 3:AC:59:ARG:HG3 | 2.41 | 0.41 |
| 1:AA:69:G:C6 | 1:AA:101:A:N6 | 2.88 | 0.41 |
| 29:DG:87:LEU:CD2 | 29:DG:164:TYR:CD1 | 3.03 | 0.41 |
| 2:AB:165:VAL:HG23 | 2:AB:166:ASP:N | 2.35 | 0.41 |
| 28:BF:106:LEU:HA | 28:BF:110:ALA:HB3 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:DR:93:GLU:O | 40:DR:94:LEU:HD23 | 2.21 | 0.41 |
| 50:D2:40:LYS:HE2 | 50:D2:46:CYS:SG | 2.60 | 0.41 |
| 32:BJ:136:GLY:O | 32:BJ:139:LEU:HB2 | 2.20 | 0.41 |
| 23:BA:333:G:C2' | 23:BA:334:C:H5' | 2.51 | 0.41 |
| 23:BA:2631:G:C6 | 23:BA:2632:A:C5 | 3.08 | 0.41 |
| 33:DK:48:PRO:C | 33:DK:49:ARG:HG2 | 2.41 | 0.41 |
| 23:BA:301:G:OP1 | 23:BA:301:G:H4' | 2.20 | 0.41 |
| 23:BA:304:G:H2' | 23:BA:305:U:O4' | 2.21 | 0.41 |
| 36:BN:52:ILE:HD12 | 36:BN:79:LEU:HD21 | 2.02 | 0.41 |
| 1:CA:976:G:H8 | 1:CA:1358:U:O2' | 2.03 | 0.41 |
| 41:BS:65:LEU:HB2 | 41:BS:68:ARG:NE | 2.27 | 0.41 |
| 1:CA:630:G:H2' | 1:CA:631:G:O4' | 2.21 | 0.41 |
| 12:AL:7:ASN:CA | 12:AL:10:VAL:HG23 | 2.51 | 0.41 |
| 8:AH:64:LYS:CB | 8:AH:79:VAL:HG21 | 2.51 | 0.41 |
| 35:DM:111:GLU:OE2 | 35:DM:133:ARG:CZ | 2.68 | 0.41 |
| 13:CM:24:GLY:CA | 13:CM:70:LEU:HD13 | 2.50 | 0.41 |
| 23:BA:2870:C:H2' | 23:BA:2871:C:O4' | 2.21 | 0.41 |
| 1:AA:560:U:O5' | 1:AA:566:G:N2 | 2.54 | 0.41 |
| 35:BM:45:GLN:O | 35:BM:49:ALA:HB2 | 2.21 | 0.41 |
| 15:AO:6:GLU:HG2 | 15:AO:7:GLU:N | 2.35 | 0.41 |
| 23:DA:189:G:C2' | 23:DA:190:A:O5' | 2.69 | 0.41 |
| 6:AF:47:ARG:HH11 | 6:AF:47:ARG:CG | 2.32 | 0.41 |
| 24:BB:112:G:N3 | 24:BB:112:G:H2' | 2.36 | 0.41 |
| 23:BA:2621:A:H5' | 26:BD:119:ARG:HH22 | 1.85 | 0.41 |
| 23:BA:1515:C:O2 | 23:BA:1515:C:H2' | 2.21 | 0.41 |
| 1:CA:55:A:C4 | 1:CA:56:U:C5 | 3.08 | 0.41 |
| 23:DA:524:U:H4' | 23:DA:554:U:H4' | 2.03 | 0.41 |
| 3:AC:120:VAL:HG21 | 3:AC:137:ALA:CB | 2.50 | 0.41 |
| 23:DA:161:U:O2 | 23:DA:165:U:O4 | 2.39 | 0.41 |
| 23:BA:914:C:C6 | 23:BA:914:C:C3' | 3.04 | 0.41 |
| 15:AO:67:LEU:HD23 | 15:AO:78:TYR:CE1 | 2.55 | 0.41 |
| 3:AC:186:PHE:CG | 3:AC:187:ALA:N | 2.88 | 0.41 |
| 1:CA:636:U:C5' | 17:CQ:2:PRO:HG3 | 2.50 | 0.41 |
| 23:DA:621:A:H5' | 23:DA:622:G:OP2 | 2.20 | 0.41 |
| 23:BA:260:G:C2 | 23:BA:261:G:H1' | 2.56 | 0.41 |
| 23:BA:2615:U:N1 | 50:B2:7:PRO:HA | 2.35 | 0.41 |
| 1:CA:1384:C:C2 | 1:CA:1385:G:C8 | 3.09 | 0.41 |
| 1:AA:572:A:H5'' | 1:AA:917:G:H4' | 2.03 | 0.41 |
| 7:CG:41:ARG:O | 7:CG:45:ASP:N | 2.42 | 0.41 |
| 33:BK:13:ASN:C | 33:BK:15:GLY:N | 2.74 | 0.41 |
| 1:CA:1163:C:C2 | 1:CA:1174:G:C2 | 3.08 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 29:DG:34:GLU:O | 29:DG:36:PRO:HD3 | 2.19 | 0.41 |
| 1:AA:296:U:H2' | 1:AA:297:G:C8 | 2.56 | 0.41 |
| 23:BA:41:C:H2' | 23:BA:43:G:O4' | 2.20 | 0.41 |
| 30:BH:78:THR:O | 30:BH:80:PRO:HD3 | 2.21 | 0.41 |
| 7:CG:111:ARG:CZ | 7:CG:122:HIS:HB3 | 2.50 | 0.41 |
| 23:BA:2446:G:N2 | 23:BA:2449:U:O2 | 2.53 | 0.41 |
| 40:DR:8:GLY:O | 40:DR:10:LYS:HG3 | 2.21 | 0.41 |
| 36:BN:116:LEU:HD23 | 36:BN:116:LEU:HA | 1.68 | 0.41 |
| 2:AB:172:ILE:HG13 | 2:AB:172:ILE:H | 1.57 | 0.41 |
| 23:BA:1801:G:H2' | 23:BA:1801:G:N3 | 2.36 | 0.41 |
| 28:BF:107:LEU:HD13 | 28:BF:177:GLY:O | 2.21 | 0.41 |
| 23:DA:2415:G:H4' | 34:DL:67:MET:N | 2.36 | 0.41 |
| 23:BA:2415:G:C2 | 23:BA:2416:C:C2 | 3.09 | 0.41 |
| 23:BA:2415:G:H4' | 34:BL:66:GLY:HA3 | 2.01 | 0.41 |
| 47:BY:1:MET:HE1 | 47:BY:4:SER:HB2 | 2.02 | 0.41 |
| 23:BA:1173:G:C8 | 23:BA:1173:G:OP2 | 2.73 | 0.41 |
| 32:BJ:120:ARG:O | 32:BJ:121:VAL:C | 2.58 | 0.41 |
| 23:DA:857:C:C2 | 23:DA:858:U:C5 | 3.09 | 0.41 |
| 38:DP:62:THR:HA | 38:DP:74:ARG:O | 2.20 | 0.41 |
| 2:AB:61:LEU:HG | 2:AB:68:ILE:HG13 | 2.02 | 0.41 |
| 7:CG:9:VAL:HG12 | 7:CG:10:ARG:N | 2.35 | 0.41 |
| 1:AA:950:U:H4' | 1:AA:971:G:H22 | 1.81 | 0.41 |
| 1:AA:962:C:N4 | 1:AA:973:G:H1 | 2.19 | 0.41 |
| 1:CA:1251:A:H1' | 1:CA:1369:C:O2' | 2.20 | 0.41 |
| 5:CE:101:ILE:CD1 | 5:CE:119:LEU:HD23 | 2.24 | 0.41 |
| 23:DA:674:G:H4' | 27:DE:74:ARG:HG3 | 2.02 | 0.41 |
| 23:DA:674:G:H2' | 23:DA:804:A:H61 | 1.86 | 0.41 |
| 1:CA:365:U:O4' | 1:CA:365:U:O2 | 2.32 | 0.41 |
| 1:CA:504:C:H2' | 1:CA:504:C:O2 | 2.21 | 0.41 |
| 23:BA:2292:C:O5' | 23:BA:2292:C:H6 | 2.04 | 0.41 |
| 23:BA:2293:C:H2' | 23:BA:2294:C:H6 | 1.85 | 0.41 |
| 37:BO:28:VAL:HG21 | 37:BO:87:PHE:HE1 | 1.86 | 0.41 |
| 23:BA:2291:U:H2' | 23:BA:2292:C:C6 | 2.56 | 0.41 |
| 32:BJ:36:TRP:CH2 | 32:BJ:74:PHE:CD2 | 3.09 | 0.41 |
| 23:BA:1188:U:H2' | 23:BA:1189:A:H5' | 2.01 | 0.41 |
| 28:BF:72:ARG:HG2 | 28:BF:86:MET:O | 2.21 | 0.41 |
| 34:DL:40:SER:O | 34:DL:41:ARG:CD | 2.49 | 0.41 |
| 42:BT:49:VAL:HG21 | 42:BT:83:VAL:CG1 | 2.45 | 0.41 |
| 42:BT:83:VAL:O | 42:BT:84:ALA:C | 2.58 | 0.41 |
| 30:BH:77:LEU:HD23 | 30:BH:105:HIS:HE1 | 1.86 | 0.41 |
| 39:BQ:79:PHE:CE2 | 39:BQ:106:PHE:CZ | 3.09 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 39:BQ:107:ALA:O | 39:BQ:110:VAL:HB | 2.20 | 0.41 |
| 23:DA:2292:C:O5' | 23:DA:2292:C:H6 | 2.03 | 0.41 |
| 37:DO:29:PHE:CD2 | 37:DO:92:TYR:OH | 2.74 | 0.41 |
| 1:AA:482:A:C2' | 1:AA:482:A:N3 | 2.81 | 0.41 |
| 1:AA:61:G:H2' | 1:AA:62:U:O4' | 2.20 | 0.41 |
| 25:DC:70:TRP:CD1 | 25:DC:70:TRP:O | 2.73 | 0.41 |
| 1:AA:438:G:C4' | 4:AD:123:HIS:ND1 | 2.82 | 0.41 |
| 4:CD:67:ILE:HG22 | 4:CD:68:TYR:CE1 | 2.56 | 0.41 |
| 1:CA:393:A:O2' | 1:CA:394:G:H5' | 2.21 | 0.41 |
| 30:DH:104:GLN:HE21 | 30:DH:104:GLN:HB3 | 1.68 | 0.41 |
| 23:DA:2712:U:O2' | 23:DA:2713:A:H5' | 2.21 | 0.41 |
| 1:CA:90:C:H2' | 1:CA:91:C:O4' | 2.21 | 0.41 |
| 3:CC:152:ILE:O | 3:CC:152:ILE:HG22 | 2.21 | 0.41 |
| 26:BD:4:ILE:HG13 | 26:BD:5:LEU:O | 2.21 | 0.41 |
| 1:CA:190:G:H8 | 1:CA:190:G:OP1 | 2.03 | 0.41 |
| 26:DD:86:PRO:HB2 | 26:DD:87:GLU:H | 1.43 | 0.41 |
| 24:BB:13:A:H8 | 45:BW:74:ARG:NH2 | 2.19 | 0.41 |
| 45:BW:72:ARG:O | 45:BW:73:GLY:C | 2.60 | 0.41 |
| 23:DA:2885:C:H2' | 23:DA:2886:G:O5' | 2.21 | 0.41 |
| 26:DD:50:GLY:HA3 | 26:DD:75:VAL:HG11 | 2.01 | 0.41 |
| 23:DA:1323:U:C2' | 23:DA:1324:G:H5' | 2.50 | 0.41 |
| 3:AC:4:LYS:O | 3:AC:5:ILE:C | 2.58 | 0.41 |
| 1:CA:407:G:H2' | 1:CA:408:A:H8 | 1.86 | 0.41 |
| 2:AB:86:GLU:C | 2:AB:88:ALA:H | 2.25 | 0.41 |
| 2:AB:88:ALA:HB2 | 2:AB:219:VAL:HG13 | 2.02 | 0.41 |
| 10:CJ:3:LYS:N | 10:CJ:75:ILE:HA | 2.35 | 0.41 |
| 1:CA:318:G:C2 | 1:CA:319:G:C5 | 3.09 | 0.41 |
| 1:CA:61:G:H2' | 1:CA:62:U:O4' | 2.21 | 0.41 |
| 23:DA:2743:C:H2' | 23:DA:2744:G:O4' | 2.21 | 0.41 |
| 29:DG:140:LYS:HB2 | 29:DG:140:LYS:HE3 | 1.88 | 0.41 |
| 23:DA:2758:A:C2 | 23:DA:2759:G:C1' | 3.04 | 0.41 |
| 23:BA:2306:C:N4 | 23:BA:2311:A:N6 | 2.68 | 0.41 |
| 23:DA:1423:G:N2 | 23:DA:1576:U:H1' | 2.35 | 0.41 |
| 1:CA:986:A:C2 | 1:CA:1220:G:C2 | 3.08 | 0.41 |
| 1:CA:448:A:OP2 | 1:CA:485:G:N1 | 2.52 | 0.41 |
| 23:DA:96:G:C4' | 47:DY:48:HIS:CE1 | 2.96 | 0.41 |
| 1:AA:818:G:N3 | 1:AA:820:U:C5 | 2.89 | 0.41 |
| 40:DR:64:HIS:HA | 40:DR:92:THR:HA | 2.03 | 0.41 |
| 11:CK:69:ALA:O | 11:CK:72:ALA:HB3 | 2.21 | 0.41 |
| 23:DA:1884:A:N1 | 23:DA:1885:A:C5 | 2.89 | 0.41 |
| 27:BE:65:TRP:CH2 | 27:BE:75:HIS:HD2 | 2.38 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 41:DS:41:LYS:O | 41:DS:42:ARG:C | 2.60 | 0.41 |
| 1:AA:628:G:O2' | 1:AA:629:G:H5' | 2.20 | 0.41 |
| 27:DE:89:VAL:C | 27:DE:91:GLY:H | 2.24 | 0.41 |
| 23:DA:911:A:C2' | 35:DM:9:TYR:OH | 2.62 | 0.41 |
| 23:BA:761:A:C8 | 23:BA:761:A:C3' | 3.04 | 0.41 |
| 23:DA:753:C:OP1 | 52:D4:1:MET:CE | 2.67 | 0.41 |
| 15:CO:85:LEU:HA | 15:CO:85:LEU:HD23 | 1.83 | 0.41 |
| 23:DA:2790:A:H2' | 23:DA:2791:C:C5' | 2.40 | 0.41 |
| 1:AA:1270:C:H2' | 1:AA:1271:G:O4' | 2.21 | 0.41 |
| 13:CM:67:GLU:HG3 | 13:CM:68:GLY:N | 2.27 | 0.41 |
| 13:AM:67:GLU:HG3 | 13:AM:68:GLY:N | 2.27 | 0.41 |
| 23:DA:2842:G:H2' | 23:DA:2843:G:O4' | 2.21 | 0.41 |
| 25:BC:25:THR:O | 25:BC:27:THR:CB | 2.68 | 0.41 |
| 23:DA:385:C:HO2' | 23:DA:390:A:H2 | 1.69 | 0.41 |
| 4:AD:82:ALA:CB | 4:AD:89:THR:HG23 | 2.50 | 0.41 |
| 25:DC:28:GLU:HB3 | 25:DC:29:PRO:CD | 2.44 | 0.41 |
| 1:CA:1067:A:N3 | 1:CA:1068:G:H1' | 2.36 | 0.41 |
| 1:AA:106:C:H2' | 1:AA:107:G:H5' | 2.00 | 0.41 |
| 1:CA:104:G:C2 | 1:CA:105:G:C5 | 3.09 | 0.41 |
| 1:CA:66:G:C4' | 1:CA:173:U:C5 | 3.02 | 0.41 |
| 28:BF:111:LEU:N | 28:BF:112:PRO:CD | 2.84 | 0.41 |
| 44:BV:85:HIS:C | 44:BV:85:HIS:HD1 | 2.24 | 0.41 |
| 50:D2:51:TYR:CZ | 50:D2:52:TYR:CE1 | 3.09 | 0.41 |
| 50:B2:29:ILE:O | 50:B2:42:PRO:HD3 | 2.21 | 0.41 |
| 50:B2:42:PRO:HB2 | 50:B2:43:HIS:CD2 | 2.55 | 0.41 |
| 18:CR:43:PHE:C | 18:CR:44:LEU:HD12 | 2.41 | 0.41 |
| 23:BA:2188:C:C4 | 23:BA:2189:U:C6 | 3.09 | 0.41 |
| 1:CA:658:G:C4 | 1:CA:659:U:C5 | 3.08 | 0.41 |
| 46:BX:23:LYS:HB3 | 46:BX:37:ILE:HG12 | 2.02 | 0.41 |
| 23:BA:2287:A:C4 | 23:BA:2289:G:N7 | 2.89 | 0.41 |
| 23:BA:284:U:H2' | 23:BA:285:C:H6 | 1.85 | 0.41 |
| 1:AA:216:G:C6 | 1:AA:217:C:N4 | 2.89 | 0.41 |
| 32:BJ:66:THR:HB | 32:BJ:69:VAL:CG1 | 2.50 | 0.41 |
| 23:DA:559:G:H22 | 39:DQ:49:HIS:CD2 | 2.38 | 0.41 |
| 50:B2:40:LYS:NZ | 50:B2:49:CYS:CB | 2.81 | 0.41 |
| 23:DA:2639:A:H2' | 23:DA:2640:G:C5' | 2.46 | 0.41 |
| 23:BA:2346:A:H5'' | 23:BA:2383:G:O4' | 2.20 | 0.41 |
| 29:DG:55:PRO:HG2 | 29:DG:61:HIS:ND1 | 2.36 | 0.41 |
| 1:CA:922:G:H3' | 1:CA:923:A:H8 | 1.85 | 0.41 |
| 16:AP:43:LYS:HA | 16:AP:48:TRP:CB | 2.51 | 0.41 |
| 23:BA:991:C:O2 | 23:BA:991:C:H2' | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:939:G:C6 | 1:CA:940:C:N4 | 2.89 | 0.41 |
| 1:CA:254:G:H2' | 1:CA:255:G:C8 | 2.53 | 0.41 |
| 1:CA:909:A:C8 | 1:CA:910:C:C5 | 3.08 | 0.41 |
| 23:BA:278:A:C2 | 23:BA:279:C:C2 | 3.09 | 0.41 |
| 23:BA:278:A:O2' | 23:BA:279:C:C1' | 2.69 | 0.41 |
| 1:AA:918:A:C2 | 1:AA:919:A:C4 | 3.09 | 0.41 |
| 1:CA:15:G:N3 | 1:CA:16:A:C8 | 2.89 | 0.41 |
| 5:AE:144:THR:HG23 | 5:AE:147:ASP:OD1 | 2.21 | 0.41 |
| 13:AM:79:LYS:O | 13:AM:82:MET:HB3 | 2.20 | 0.41 |
| 4:AD:8:VAL:O | 4:AD:11:LEU:HG | 2.21 | 0.41 |
| 23:BA:1946:U:C2 | 23:BA:1947:C:C5 | 3.09 | 0.41 |
| 1:AA:720:C:H5' | 18:AR:50:ILE:O | 2.21 | 0.41 |
| 23:DA:2869:G:C6 | 23:DA:2870:C:C4 | 3.08 | 0.41 |
| 1:AA:522:C:O2' | 1:AA:523:A:H5' | 2.21 | 0.41 |
| 8:AH:64:LYS:HB3 | 8:AH:79:VAL:HG21 | 2.02 | 0.41 |
| 4:AD:70:ILE:HG12 | 4:AD:71:SER:H | 1.84 | 0.41 |
| 35:DM:134:ARG:O | 35:DM:135:ASP:C | 2.59 | 0.41 |
| 7:CG:15:ASP:HB3 | 7:CG:19:GLY:H | 1.86 | 0.41 |
| 8:AH:39:LEU:C | 8:AH:45:ILE:HG12 | 2.41 | 0.41 |
| 43:BU:46:LYS:C | 43:BU:48:ALA:N | 2.74 | 0.41 |
| 12:CL:7:ASN:CA | 12:CL:10:VAL:HG23 | 2.50 | 0.41 |
| 12:AL:74:HIS:CD2 | 12:AL:76:LEU:HB2 | 2.56 | 0.41 |
| 25:BC:257:LEU:HD23 | 25:BC:258:LYS:N | 2.36 | 0.41 |
| 23:DA:2190:G:O2' | 23:DA:2191:G:H5' | 2.21 | 0.41 |
| 1:AA:1109:C:H2' | 1:AA:1110:A:O4' | 2.21 | 0.41 |
| 40:DR:72:VAL:HG23 | 40:DR:85:LYS:HB3 | 2.03 | 0.41 |
| 44:BV:120:ILE:H | 44:BV:172:ALA:HA | 1.86 | 0.41 |
| 23:DA:1217:C:OP1 | 39:DQ:15:LYS:HE2 | 2.20 | 0.41 |
| 1:CA:186(E):C:H2' | 1:CA:186(F):C:H6 | 1.86 | 0.41 |
| 23:BA:1131:G:C2 | 23:BA:1132:A:C4 | 3.09 | 0.41 |
| 43:DU:89:PHE:HA | 43:DU:89:PHE:HD1 | 1.68 | 0.41 |
| 6:CF:74:ASP:HA | 6:CF:77:ARG:NH1 | 2.36 | 0.41 |
| 23:DA:2085:C:H2' | 23:DA:2086:U:O4' | 2.21 | 0.41 |
| 23:BA:1335:U:H2' | 23:BA:1336:A:O5' | 2.21 | 0.41 |
| 23:DA:2459:A:C4 | 23:DA:2460:U:C6 | 3.08 | 0.41 |
| 23:BA:1232:G:H2' | 23:BA:1233:C:C6 | 2.51 | 0.41 |
| 23:DA:2853:C:H2' | 23:DA:2854:G:C8 | 2.49 | 0.41 |
| 23:DA:1444:G:C2 | 23:DA:1548:C:C2 | 3.08 | 0.41 |
| 44:DV:120:ILE:HG12 | 44:DV:172:ALA:HA | 2.03 | 0.41 |
| 33:BK:60:ALA:HB2 | 33:BK:86:ILE:HA | 2.02 | 0.41 |
| 23:BA:189:G:H1' | 23:BA:207:A:H61 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 38:BP:126:ALA:C | 38:BP:128:GLU:H | 2.23 | 0.41 |
| 1:AA:145:G:N2 | 1:AA:178:C:N3 | 2.69 | 0.41 |
| 21:CU:9:ARG:HG3 | 21:CU:10:ARG:N | 2.36 | 0.41 |
| 23:DA:24:G:C6 | 23:DA:25:U:C4 | 3.09 | 0.41 |
| 23:BA:414:C:O2' | 23:BA:415:A:H5' | 2.20 | 0.41 |
| 3:AC:16:ARG:HH11 | 3:AC:16:ARG:HB2 | 1.83 | 0.41 |
| 2:AB:37:ASN:HA | 2:AB:37:ASN:HD22 | 1.67 | 0.41 |
| 23:DA:1993:U:H4' | 26:DD:128:SER:HB2 | 2.03 | 0.41 |
| 23:DA:171:G:N3 | 23:DA:171:G:H2' | 2.35 | 0.41 |
| 1:AA:1165:C:C2' | 1:AA:1166:G:H5' | 2.51 | 0.41 |
| 28:BF:139:LEU:HA | 28:BF:144:ILE:HG21 | 2.03 | 0.41 |
| 14:CN:7:ILE:HD12 | 14:CN:8:GLU:N | 2.36 | 0.41 |
| 29:BG:117:PRO:HA | 29:BG:118:PRO:HD2 | 1.90 | 0.41 |
| 1:CA:259:G:OP2 | 20:CT:83:ARG:HD3 | 2.21 | 0.41 |
| 23:BA:503:A:C6 | 23:BA:506:G:C6 | 3.09 | 0.41 |
| 35:BM:29:PHE:N | 35:BM:105:GLU:OE2 | 2.53 | 0.41 |
| 37:BO:98:VAL:HG23 | 37:BO:99:LYS:N | 2.36 | 0.41 |
| 23:DA:1281:G:C4 | 23:DA:1282:U:C6 | 3.09 | 0.41 |
| 23:BA:1993:U:H4' | 26:BD:128:SER:HB2 | 2.03 | 0.41 |
| 1:CA:425:G:O2' | 1:CA:426:G:H5' | 2.20 | 0.41 |
| 23:DA:1234:U:H2' | 23:DA:1235:G:O4' | 2.21 | 0.41 |
| 4:CD:23:GLY:HA3 | 4:CD:112:VAL:CG1 | 2.51 | 0.41 |
| 1:CA:1464:G:C2' | 1:CA:1465:C:H5' | 2.51 | 0.41 |
| 37:BO:79:ALA:C | 37:BO:80:LEU:HD23 | 2.41 | 0.41 |
| 1:AA:157:G:C2 | 1:AA:165:C:N3 | 2.89 | 0.41 |
| 30:BH:30:LEU:O | 30:BH:31:LEU:C | 2.58 | 0.41 |
| 1:AA:619:U:O2 | 4:AD:135:LEU:HD22 | 2.20 | 0.41 |
| 1:CA:450:G:H2' | 1:CA:451:A:OP1 | 2.21 | 0.41 |
| 23:BA:1464:C:H2' | 23:BA:1465:G:H8 | 1.85 | 0.41 |
| 12:CL:51:LEU:H | 12:CL:51:LEU:HD12 | 1.85 | 0.41 |
| 44:BV:157:LEU:HA | 44:BV:158:PRO:HD2 | 1.92 | 0.41 |
| 23:DA:2694:G:C4 | 23:DA:2695:C:C5 | 3.09 | 0.41 |
| 1:AA:385:C:H3' | 1:AA:385:C:C6 | 2.54 | 0.41 |
| 32:BJ:151:HIS:O | 32:BJ:151:HIS:CG | 2.73 | 0.41 |
| 23:BA:768:G:C6 | 23:BA:769:G:C5 | 3.08 | 0.41 |
| 35:BM:72:LYS:O | 35:BM:93:TYR:HA | 2.20 | 0.41 |
| 23:BA:2230:G:O3' | 46:BX:43:TYR:HB2 | 2.21 | 0.41 |
| 18:AR:65:ILE:H | 18:AR:65:ILE:HG12 | 1.52 | 0.41 |
| 23:BA:876:C:C2' | 23:BA:877:U:H5' | 2.51 | 0.41 |
| 1:CA:157:G:H2' | 1:CA:158:G:H8 | 1.85 | 0.41 |
| 23:BA:2489:G:O2' | 23:BA:2518:A:N6 | 2.52 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DA:2818:G:O2' | 23:DA:2819:G:H5' | 2.20 | 0.41 |
| 23:BA:660:G:H5' | 27:BE:99:TYR:CD2 | 2.56 | 0.41 |
| 1:CA:360:A:H2' | 1:CA:361:G:C8 | 2.55 | 0.41 |
| 2:AB:51:LEU:HB3 | 2:AB:55:PHE:CE2 | 2.56 | 0.41 |
| 23:DA:2052:G:O4' | 26:DD:142:GLY:HA3 | 2.21 | 0.41 |
| 23:DA:872:A:C6 | 23:DA:906:G:C2 | 3.09 | 0.41 |
| 6:AF:100:ASN:C | 6:AF:100:ASN:HD22 | 2.24 | 0.41 |
| 17:AQ:43:LEU:HA | 17:AQ:43:LEU:HD12 | 1.54 | 0.41 |
| 23:BA:618(B):C:H2' | 23:BA:618(B):C:O2 | 2.20 | 0.41 |
| 26:DD:64:LYS:HA | 26:DD:64:LYS:HD2 | 1.81 | 0.41 |
| 33:BK:47:ILE:HA | 33:BK:47:ILE:HD12 | 1.61 | 0.41 |
| 40:BR:99:ILE:HD13 | 40:BR:99:ILE:N | 2.36 | 0.41 |
| 1:CA:135:C:H2' | 1:CA:136:C:H5' | 2.01 | 0.41 |
| 36:BN:105:ARG:HG2 | 36:BN:106:GLY:N | 2.34 | 0.41 |
| 23:BA:2515:C:O2 | 23:BA:2570:G:C2 | 2.74 | 0.41 |
| 1:AA:930:C:C4 | 1:AA:931:C:C5 | 3.08 | 0.41 |
| 44:DV:129:SER:OG | 44:DV:130:PRO:HD2 | 2.21 | 0.41 |
| 6:AF:24:GLU:O | 6:AF:27:GLN:HB2 | 2.21 | 0.41 |
| 43:BU:52:SER:HA | 43:BU:53:PRO:HD3 | 1.92 | 0.41 |
| 2:CB:51:LEU:HB3 | 2:CB:55:PHE:CE2 | 2.56 | 0.41 |
| 42:BT:92:LEU:HD23 | 42:BT:92:LEU:HA | 1.91 | 0.41 |
| 40:BR:10:LYS:HB2 | 40:BR:10:LYS:HE3 | 1.83 | 0.41 |
| 48:BZ:55:ARG:HA | 48:BZ:55:ARG:HD3 | 1.45 | 0.41 |
| 1:AA:102(A):C:H6 | 1:AA:102(A):C:O5' | 2.04 | 0.41 |
| 1:AA:1114:C:H6 | 1:AA:1114:C:O5' | 2.03 | 0.41 |
| 26:BD:183:LEU:HA | 26:BD:183:LEU:HD12 | 1.79 | 0.41 |
| 23:DA:1914:C:O4' | 23:DA:1914:C:O2 | 2.39 | 0.41 |
| 53:D5:13:ARG:O | 53:D5:14:VAL:HG23 | 2.20 | 0.41 |
| 34:DL:101:VAL:C | 34:DL:103:ALA:N | 2.75 | 0.41 |
| 45:BW:26:TYR:HB2 | 45:BW:29:GLN:NE2 | 2.37 | 0.41 |
| 34:BL:148:LEU:H | 34:BL:148:LEU:HD13 | 1.86 | 0.41 |
| 9:CI:118:LYS:C | 9:CI:120:ARG:H | 2.24 | 0.41 |
| 22:AV:6183:G:C6 | 22:AV:6184:A:C5 | 3.09 | 0.41 |
| 34:BL:36:LYS:HE3 | 34:BL:36:LYS:HB3 | 1.84 | 0.41 |
| 53:B5:32:LEU:CD2 | 53:B5:33:ASN:N | 2.82 | 0.41 |
| 1:CA:1122:U:H2' | 1:CA:1123:A:C8 | 2.56 | 0.41 |
| 39:DQ:72:HIS:ND1 | 39:DQ:110:VAL:HG21 | 2.36 | 0.41 |
| 39:DQ:69:CYS:HB3 | 39:DQ:79:PHE:CD2 | 2.56 | 0.41 |
| 23:DA:1144:G:C6 | 23:DA:1145:C:C4 | 3.09 | 0.41 |
| 30:BH:88:ILE:HG12 | 30:BH:122:GLU:C | 2.42 | 0.41 |
| 39:BQ:92:ARG:HD3 | 39:BQ:94:ASN:CB | 2.49 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:AD:55:ALA:O | 4:AD:58:LEU:HB3 | 2.21 | 0.41 |
| 37:DO:25:ARG:CG | 37:DO:88:ASP:HB2 | 2.51 | 0.41 |
| 2:CB:88:ALA:HB2 | 2:CB:219:VAL:HG13 | 2.02 | 0.41 |
| 5:AE:14:ARG:CZ | 5:AE:129:ILE:HD11 | 2.50 | 0.41 |
| 1:CA:1102:A:C6 | 1:CA:1103:C:C4 | 3.09 | 0.41 |
| 23:DA:1439:A:C2 | 23:DA:1553:A:C4 | 3.09 | 0.41 |
| 1:AA:1085:U:O4' | 1:AA:1094:G:C2 | 2.74 | 0.41 |
| 1:AA:255:G:O6 | 1:AA:266:G:O6 | 2.39 | 0.41 |
| 1:AA:1281:U:H3' | 1:AA:1282:C:C6 | 2.56 | 0.41 |
| 1:AA:1371:G:C6 | 1:AA:1372:U:C4 | 3.08 | 0.41 |
| 23:BA:1652:A:OP1 | 36:BN:9:LYS:HD2 | 2.21 | 0.41 |
| 19:AS:62:ILE:C | 19:AS:66:MET:HE3 | 2.41 | 0.41 |
| 1:CA:52:G:O2' | 1:CA:53:A:H5' | 2.21 | 0.41 |
| 23:BA:528:A:C2 | 23:BA:2043:C:C4' | 3.04 | 0.41 |
| 33:BK:35:VAL:HG23 | 33:BK:65:THR:CG2 | 2.41 | 0.41 |
| 41:DS:9:TYR:N | 41:DS:102:HIS:HD2 | 2.04 | 0.41 |
| 23:BA:2786:U:OP1 | 26:BD:69:LYS:HE3 | 2.21 | 0.41 |
| 23:BA:1577:C:H2' | 23:BA:1578:U:C1' | 2.51 | 0.41 |
| 23:BA:1884:A:N3 | 23:BA:1885:A:C8 | 2.89 | 0.41 |
| 6:CF:29:ALA:O | 6:CF:30:LEU:C | 2.59 | 0.41 |
| 23:BA:1586:A:C2' | 23:BA:1587:A:H5' | 2.50 | 0.41 |
| 23:BA:2755:C:H6 | 23:BA:2755:C:O5' | 2.04 | 0.41 |
| 29:BG:21:PRO:HB2 | 29:BG:22:GLY:H | 1.71 | 0.41 |
| 1:CA:642:A:C1' | 8:CH:113:SER:OG | 2.69 | 0.41 |
| 11:CK:22:HIS:HB3 | 11:CK:29:ILE:HG12 | 2.03 | 0.41 |
| 27:BE:130:ALA:O | 27:BE:132:VAL:N | 2.54 | 0.41 |
| 1:CA:29:G:C4 | 1:CA:30:U:C5 | 3.09 | 0.41 |
| 40:DR:99:ILE:HD13 | 40:DR:99:ILE:H | 1.86 | 0.41 |
| 23:DA:379:G:C6 | 23:DA:380:U:C5 | 3.09 | 0.41 |
| 23:DA:2285:C:C2' | 23:DA:2286:A:H5'' | 2.46 | 0.41 |
| 23:BA:1684:C:C2 | 23:BA:1705:G:C2 | 3.08 | 0.41 |
| 1:CA:67:C:H2' | 1:CA:68:G:C8 | 2.56 | 0.41 |
| 11:AK:69:ALA:O | 11:AK:72:ALA:HB3 | 2.21 | 0.41 |
| 15:CO:56:LEU:HD23 | 15:CO:60:VAL:CG2 | 2.51 | 0.41 |
| 27:BE:37:VAL:HG22 | 27:BE:184:TYR:HA | 2.03 | 0.41 |
| 23:BA:1418:G:C8 | 23:BA:1418:G:O5' | 2.61 | 0.41 |
| 29:DG:92:ILE:H | 29:DG:92:ILE:CD1 | 2.34 | 0.41 |
| 23:BA:2428:G:H5'' | 23:BA:2429:G:O5' | 2.20 | 0.41 |
| 1:AA:1342:C:O2' | 1:AA:1343:G:H5' | 2.21 | 0.41 |
| 23:BA:304:G:N2 | 23:BA:314:A:C4 | 2.89 | 0.41 |
| 1:CA:941:G:C2 | 1:CA:942:G:C8 | 3.09 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BA:641:C:O2' | 23:BA:2350:C:OP1 | 2.30 | 0.41 |
| 3:AC:22:TRP:HZ3 | 3:AC:24:ALA:HB2 | 1.85 | 0.41 |
| 8:CH:64:LYS:CB | 8:CH:79:VAL:HG21 | 2.52 | 0.41 |
| 4:AD:13:ARG:O | 4:AD:39:PRO:HA | 2.21 | 0.41 |
| 23:DA:1006:C:O2' | 23:DA:1007:C:H5' | 2.21 | 0.41 |
| 8:AH:36:LEU:C | 8:AH:38:ILE:H | 2.23 | 0.41 |
| 1:AA:559:A:H4' | 1:AA:560:U:C3' | 2.51 | 0.41 |
| 23:DA:1894:C:N3 | 23:DA:1895:C:C5 | 2.89 | 0.41 |
| 1:AA:1095:U:H5' | 1:AA:1109:C:O2 | 2.21 | 0.41 |
| 23:BA:572:A:H2' | 23:BA:573:G:O4' | 2.21 | 0.41 |
| 43:BU:89:PHE:HD1 | 43:BU:89:PHE:HA | 1.68 | 0.41 |
| 2:CB:35:GLU:HG3 | 2:CB:40:HIS:HA | 2.03 | 0.41 |
| 44:BV:107:THR:HA | 44:BV:108:PRO:HD3 | 1.77 | 0.41 |
| 23:DA:2461:C:H42 | 23:DA:2489:G:H1 | 1.67 | 0.41 |
| 1:AA:1262:C:C2 | 1:AA:1263:C:C5 | 3.09 | 0.41 |
| 1:AA:638:G:H2' | 1:AA:639:G:C5' | 2.50 | 0.41 |
| 1:AA:20:U:H2' | 1:AA:21:G:O4' | 2.21 | 0.41 |
| 26:BD:96:PHE:HA | 26:BD:100:GLU:OE1 | 2.20 | 0.41 |
| 1:CA:145:G:N2 | 1:CA:178:C:N3 | 2.68 | 0.41 |
| 19:CS:16:LEU:HD12 | 19:CS:16:LEU:H | 1.86 | 0.41 |
| 23:BA:2097:C:O5' | 23:BA:2097:C:H6 | 2.04 | 0.41 |
| 18:AR:53:ARG:C | 18:AR:55:ARG:N | 2.73 | 0.41 |
| 1:CA:1480:G:C6 | 1:CA:1481:U:C4 | 3.09 | 0.41 |
| 29:BG:121:ILE:O | 29:BG:122:THR:HG23 | 2.21 | 0.41 |
| 1:AA:576:G:N2 | 1:AA:759:A:OP1 | 2.53 | 0.41 |
| 23:BA:718:A:H2' | 23:BA:719:C:H5' | 2.03 | 0.41 |
| 23:BA:245:G:C4 | 23:BA:246:C:C6 | 3.09 | 0.41 |
| 30:BH:54:GLN:HA | 30:BH:57:ARG:HB3 | 2.03 | 0.41 |
| 23:BA:1838:C:HO2' | 23:BA:1898:U:H5 | 1.68 | 0.41 |
| 32:DJ:151:HIS:NE2 | 32:DJ:153:HIS:HA | 2.36 | 0.41 |
| 1:AA:838:G:N2 | 1:AA:849:C:C4 | 2.89 | 0.41 |
| 1:CA:1438:G:H2' | 1:CA:1439:C:H6 | 1.86 | 0.41 |
| 1:AA:897:C:H42 | 1:AA:902:G:H1 | 1.69 | 0.41 |
| 23:BA:1416:G:O2' | 23:BA:1417:C:P | 2.78 | 0.41 |
| 23:BA:663:G:O3' | 34:BL:21:ARG:NH1 | 2.53 | 0.41 |
| 23:DA:2448:A:OP1 | 23:DA:2499:C:OP1 | 2.39 | 0.41 |
| 44:DV:77:ASP:HB2 | 44:DV:84:GLU:CG | 2.51 | 0.41 |
| 44:BV:129:SER:HA | 44:BV:130:PRO:HD3 | 1.90 | 0.41 |
| 25:BC:98:VAL:CG2 | 25:BC:99:ASP:N | 2.84 | 0.41 |
| 22:CV:6179:U:H2' | 22:CV:6180:U:C6 | 2.56 | 0.41 |
| 1:AA:298:A:H2' | 1:AA:299:G:O4' | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 43:DU:31:LEU:HA | 43:DU:32:PRO:HD3 | 1.80 | 0.41 |
| 27:DE:114:VAL:HG11 | 27:DE:202:PHE:CZ | 2.55 | 0.41 |
| 23:BA:2626:C:H2' | 23:BA:2627:G:O4' | 2.21 | 0.41 |
| 23:DA:1632:A:C6 | 23:DA:1633:G:C6 | 3.09 | 0.41 |
| 23:DA:2859:G:O2' | 23:DA:2860:A:H5' | 2.21 | 0.41 |
| 4:AD:120:LEU:O | 4:AD:125:HIS:HB2 | 2.21 | 0.41 |
| 25:DC:4:LYS:NZ | 25:DC:4:LYS:CB | 2.84 | 0.41 |
| 23:DA:97:C:H2' | 23:DA:97:C:O2 | 2.19 | 0.41 |
| 6:CF:100:ASN:C | 6:CF:100:ASN:HD22 | 2.24 | 0.41 |
| 23:BA:196:A:N3 | 23:BA:196:A:H2' | 2.36 | 0.41 |
| 17:AQ:98:LEU:HD23 | 17:AQ:98:LEU:HA | 1.70 | 0.41 |
| 9:CI:56:LEU:C | 9:CI:56:LEU:HD23 | 2.41 | 0.41 |
| 26:BD:68:ALA:C | 26:BD:70:ALA:H | 2.25 | 0.41 |
| 6:CF:41:GLU:O | 6:CF:43:LEU:N | 2.54 | 0.41 |
| 34:DL:80:TYR:CZ | 34:DL:111:ARG:HG2 | 2.55 | 0.40 |
| 23:BA:960:A:H2 | 23:BA:2495:G:N3 | 2.19 | 0.40 |
| 34:BL:59:LEU:O | 34:BL:59:LEU:HD23 | 2.20 | 0.40 |
| 47:DY:2:LYS:O | 47:DY:5:GLU:CD | 2.59 | 0.40 |
| 23:BA:2013:A:N6 | 23:BA:2014:A:C6 | 2.89 | 0.40 |
| 23:DA:1541:U:H3' | 23:DA:1542:G:C2' | 2.50 | 0.40 |
| 23:BA:1448:G:N2 | 23:BA:149(B):A:N6 | 2.69 | 0.40 |
| 23:BA:1541:U:H5'' | 23:BA:1543:A:OP2 | 2.19 | 0.40 |
| 23:DA:1178:C:H2' | 23:DA:1179:C:H6 | 1.86 | 0.40 |
| 2:AB:182:ILE:O | 2:AB:183:PRO:C | 2.59 | 0.40 |
| 2:AB:184:VAL:H | 2:AB:198:ASP:HB2 | 1.86 | 0.40 |
| 1:CA:1351:U:C2' | 1:CA:1352:C:H5' | 2.50 | 0.40 |
| 23:BA:1191:G:OP1 | 34:BL:35:HIS:CE1 | 2.74 | 0.40 |
| 38:BP:62:THR:HA | 38:BP:74:ARG:O | 2.20 | 0.40 |
| 2:CB:61:LEU:O | 2:CB:61:LEU:HD12 | 2.21 | 0.40 |
| 23:DA:743:G:O2' | 23:DA:744:G:H5' | 2.21 | 0.40 |
| 16:CP:4:ILE:HA | 16:CP:20:VAL:O | 2.21 | 0.40 |
| 1:AA:551:U:H5' | 12:AL:118:LYS:HZ3 | 1.86 | 0.40 |
| 1:AA:429:U:H1' | 1:AA:430:A:H5'' | 2.03 | 0.40 |
| 47:BY:29:LYS:HD3 | 47:BY:57:ILE:HG21 | 2.02 | 0.40 |
| 47:BY:60:LEU:C | 47:BY:62:THR:N | 2.74 | 0.40 |
| 20:AT:30:LYS:HA | 20:AT:30:LYS:HD3 | 1.93 | 0.40 |
| 23:DA:1299:G:H3' | 23:DA:1639:U:O4 | 2.22 | 0.40 |
| 23:DA:1640:C:H5' | 23:DA:1640:C:H6 | 1.85 | 0.40 |
| 24:DB:41:U:OP1 | 24:DB:42:C:H5 | 2.04 | 0.40 |
| 24:DB:73:A:C8 | 24:DB:74:U:C5 | 3.09 | 0.40 |
| 26:BD:34:VAL:HG11 | 26:BD:78:LEU:HD12 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:1201:A:C2' | 1:CA:1202:G:OP2 | 2.68 | 0.40 |
| 5:CE:109:ILE:O | 5:CE:113:ALA:HB2 | 2.20 | 0.40 |
| 36:DN:21:TYR:OH | 36:DN:43:GLU:HG2 | 2.21 | 0.40 |
| 44:BV:30:ASN:O | 44:BV:33:LEU:N | 2.53 | 0.40 |
| 4:AD:195:ALA:C | 4:AD:196:LEU:HD12 | 2.41 | 0.40 |
| 23:DA:1286:A:O2' | 23:DA:1288:U:P | 2.79 | 0.40 |
| 42:BT:31:HIS:HA | 42:BT:32:PRO:HD3 | 1.92 | 0.40 |
| 48:DZ:40:THR:HG23 | 48:DZ:43:ILE:CD1 | 2.50 | 0.40 |
| 25:DC:172:TYR:CD1 | 25:DC:185:VAL:O | 2.67 | 0.40 |
| 12:AL:44:PRO:HB3 | 12:AL:91:ASP:OD1 | 2.21 | 0.40 |
| 23:DA:2310:A:H2' | 23:DA:2311:A:H5' | 2.03 | 0.40 |
| 47:DY:48:HIS:C | 47:DY:50:ILE:N | 2.72 | 0.40 |
| 23:DA:1486:A:C2 | 23:DA:1487:G:C5 | 3.09 | 0.40 |
| 27:BE:106:ARG:HG2 | 27:BE:106:ARG:H | 1.46 | 0.40 |
| 27:BE:39:TRP:CH2 | 27:BE:106:ARG:NE | 2.89 | 0.40 |
| 23:BA:2776:A:C2 | 23:BA:2778:A:C4 | 3.09 | 0.40 |
| 23:BA:732:C:H2' | 23:BA:733:G:C5' | 2.51 | 0.40 |
| 1:AA:828:A:C5' | 1:AA:859:A:C2 | 2.96 | 0.40 |
| 23:DA:2207:C:H2' | 23:DA:2208:U:O4' | 2.22 | 0.40 |
| 33:DK:88:ASN:N | 33:DK:92:GLU:O | 2.40 | 0.40 |
| 40:DR:99:ILE:HD13 | 40:DR:100:ARG:H | 1.86 | 0.40 |
| 43:DU:3:VAL:C | 43:DU:5:MET:H | 2.23 | 0.40 |
| 25:BC:81:ALA:O | 25:BC:93:ALA:HA | 2.20 | 0.40 |
| 23:DA:2562:U:H2' | 23:DA:2563:U:C5' | 2.50 | 0.40 |
| 1:CA:1085:U:O4' | 1:CA:1094:G:N1 | 2.54 | 0.40 |
| 3:CC:4:LYS:O | 3:CC:5:ILE:C | 2.58 | 0.40 |
| 25:BC:165:ILE:C | 25:BC:166:GLN:HE21 | 2.24 | 0.40 |
| 23:DA:256:A:HO2' | 23:DA:257:A:H5' | 1.84 | 0.40 |
| 1:CA:658:G:C4' | 15:CO:22:THR:HB | 2.51 | 0.40 |
| 23:BA:1386:C:C2 | 23:BA:1387:C:C5 | 3.08 | 0.40 |
| 23:BA:1389:G:N2 | 23:BA:1390:U:C2 | 2.89 | 0.40 |
| 1:CA:1056:U:C5 | 1:CA:1200:C:N4 | 2.88 | 0.40 |
| 27:BE:89:VAL:CG1 | 27:BE:90:PHE:H | 2.28 | 0.40 |
| 23:BA:1728:G:C8 | 23:BA:1728:G:C3' | 3.04 | 0.40 |
| 23:BA:2840:C:H5" | 36:BN:53:HIS:CG | 2.56 | 0.40 |
| 23:DA:1248:G:N7 | 39:DQ:3:ARG:HB2 | 2.36 | 0.40 |
| 13:CM:76:ALA:CA | 13:CM:79:LYS:HE2 | 2.45 | 0.40 |
| 8:CH:64:LYS:HB3 | 8:CH:79:VAL:HG21 | 2.02 | 0.40 |
| 1:CA:973:G:OP1 | 10:CJ:57:LYS:HE2 | 2.21 | 0.40 |
| 1:CA:973:G:OP1 | 10:CJ:57:LYS:CE | 2.69 | 0.40 |
| 13:CM:24:GLY:HA2 | 13:CM:70:LEU:HD13 | 2.02 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:433:C:C5 | 1:CA:434:U:H5 | 2.39 | 0.40 |
| 23:BA:978:G:H2' | 23:BA:979:G:H5' | 1.99 | 0.40 |
| 7:CG:23:VAL:HG13 | 7:CG:43:PHE:CE2 | 2.56 | 0.40 |
| 23:BA:737:C:O2' | 23:BA:738:G:H5' | 2.21 | 0.40 |
| 8:CH:39:LEU:HA | 8:CH:39:LEU:HD13 | 1.77 | 0.40 |
| 7:AG:23:VAL:CG1 | 7:AG:43:PHE:HE2 | 2.34 | 0.40 |
| 23:DA:1709:U:C2 | 23:DA:1750:G:N2 | 2.88 | 0.40 |
| 23:BA:1833:U:H2' | 23:BA:1834:U:H6 | 1.86 | 0.40 |
| 12:CL:5:THR:O | 12:CL:9:LEU:HD12 | 2.21 | 0.40 |
| 37:BO:13:ARG:HG3 | 37:BO:14:VAL:H | 1.85 | 0.40 |
| 23:BA:2280:G:C2' | 23:BA:2281:C:H5' | 2.52 | 0.40 |
| 23:BA:2738:A:H2' | 23:BA:2739:U:O5' | 2.21 | 0.40 |
| 23:BA:136:G:C4 | 23:BA:137(A):C:C6 | 3.10 | 0.40 |
| 19:AS:12:ASP:HB2 | 19:AS:15:LEU:HD23 | 2.03 | 0.40 |
| 43:DU:61:ILE:HG12 | 43:DU:61:ILE:H | 1.54 | 0.40 |
| 23:DA:1797:C:O2' | 25:DC:259:THR:CG2 | 2.69 | 0.40 |
| 25:BC:162:SER:HB2 | 25:BC:195:ALA:CB | 2.51 | 0.40 |
| 9:CI:46:ALA:HB2 | 9:CI:74:ILE:HG22 | 2.03 | 0.40 |
| 23:DA:1242:A:C8 | 23:DA:1243:G:C8 | 3.08 | 0.40 |
| 35:DM:30:GLY:HA2 | 35:DM:107:ALA:HB2 | 2.02 | 0.40 |
| 24:BB:100:G:H2' | 24:BB:101:A:O4' | 2.21 | 0.40 |
| 3:CC:16:ARG:HB2 | 3:CC:16:ARG:HH11 | 1.86 | 0.40 |
| 12:AL:125:LYS:HD2 | 12:AL:125:LYS:HA | 1.84 | 0.40 |
| 23:BA:466:A:C3' | 23:BA:467:G:H5' | 2.50 | 0.40 |
| 23:BA:608:A:C4 | 23:BA:621:A:C6 | 3.09 | 0.40 |
| 23:BA:273(B):G:N2 | 23:BA:364:C:C2 | 2.89 | 0.40 |
| 36:DN:18:LEU:HD11 | 36:DN:22:ARG:CZ | 2.50 | 0.40 |
| 23:BA:878:A:C6 | 23:BA:900:A:N7 | 2.89 | 0.40 |
| 23:DA:265:A:C8 | 23:DA:266:G:H1' | 2.56 | 0.40 |
| 23:BA:1465:G:H21 | 23:BA:1466:G:H1' | 1.85 | 0.40 |
| 23:DA:2812:G:H2' | 23:DA:2813:A:O5' | 2.21 | 0.40 |
| 1:AA:892:A:O2' | 1:AA:1415:G:H4' | 2.21 | 0.40 |
| 23:BA:1769:G:C6 | 23:BA:1984:G:C6 | 3.09 | 0.40 |
| 23:BA:270(X):G:O2' | 23:BA:270(Y):G:H5' | 2.21 | 0.40 |
| 23:BA:1416:G:O2' | 23:BA:1417:C:H6 | 2.04 | 0.40 |
| 33:BK:7:TYR:CZ | 33:BK:44:LYS:HG3 | 2.56 | 0.40 |
| 34:DL:23:PRO:O | 34:DL:29:LYS:O | 2.38 | 0.40 |
| 15:CO:66:LEU:H | 15:CO:66:LEU:HD13 | 1.86 | 0.40 |
| 40:BR:99:ILE:HD13 | 40:BR:99:ILE:H | 1.86 | 0.40 |
| 46:DX:34:THR:C | 46:DX:35:THR:HG23 | 2.41 | 0.40 |
| 1:CA:340:U:H2' | 1:CA:341:C:C6 | 2.56 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DA:1107:G:H2' | 23:DA:1108:U:H6 | 1.86 | 0.40 |
| 8:AH:74:PRO:O | 8:AH:76:PRO:HD3 | 2.21 | 0.40 |
| 28:DF:97:ASP:HA | 28:DF:100:TRP:HD1 | 1.86 | 0.40 |
| 23:BA:1484:G:H2' | 23:BA:1485:G:H8 | 1.85 | 0.40 |
| 23:BA:2508:G:H2' | 23:BA:2509:G:O4' | 2.20 | 0.40 |
| 25:DC:248:SER:HB2 | 25:DC:250:TRP:CE3 | 2.56 | 0.40 |
| 23:BA:180:G:N1 | 23:BA:214:G:N7 | 2.62 | 0.40 |
| 36:DN:28:LEU:HD23 | 36:DN:28:LEU:HA | 1.70 | 0.40 |
| 23:BA:2006:C:H6 | 23:BA:2006:C:O5' | 2.04 | 0.40 |
| 23:BA:144:C:H2' | 23:BA:145:G:H8 | 1.86 | 0.40 |
| 23:BA:2760:C:H2' | 23:BA:2760:C:O2 | 2.21 | 0.40 |
| 27:BE:140:LEU:HA | 27:BE:140:LEU:HD12 | 1.90 | 0.40 |
| 2:CB:169:LYS:HE2 | 2:CB:169:LYS:C | 2.41 | 0.40 |
| 23:DA:2380:C:H6 | 23:DA:2380:C:O5' | 2.03 | 0.40 |
| 39:DQ:59:ARG:HB2 | 39:DQ:59:ARG:HE | 1.50 | 0.40 |
| 2:AB:122:PHE:O | 2:AB:122:PHE:CD2 | 2.74 | 0.40 |
| 23:DA:1733:G:H8 | 23:DA:1733:G:O5' | 2.03 | 0.40 |
| 3:AC:136:GLN:O | 3:AC:140:ARG:N | 2.54 | 0.40 |
| 43:BU:73:ARG:HH22 | 43:BU:82:PRO:HD3 | 1.86 | 0.40 |
| 53:D5:53:PRO:HA | 53:D5:56:GLU:HB2 | 2.04 | 0.40 |
| 23:BA:2388:A:H8 | 23:BA:2389:G:C5 | 2.40 | 0.40 |
| 23:BA:1448:G:H1' | 23:BA:1528:A:N1 | 2.36 | 0.40 |
| 34:BL:90:ARG:C | 34:BL:91:PHE:HD1 | 2.24 | 0.40 |
| 23:DA:2846:G:C4 | 23:DA:2847:U:C5 | 3.09 | 0.40 |
| 2:CB:61:LEU:HD21 | 2:CB:161:ALA:CB | 2.51 | 0.40 |
| 2:CB:61:LEU:HG | 2:CB:68:ILE:HG13 | 2.03 | 0.40 |
| 42:BT:63:LYS:HZ1 | 42:BT:72:LYS:HB3 | 1.85 | 0.40 |
| 34:DL:51:PHE:O | 34:DL:52:GLU:C | 2.59 | 0.40 |
| 53:B5:7:HIS:CD2 | 53:B5:60:LEU:HD13 | 2.56 | 0.40 |
| 3:CC:18:TRP:HE3 | 3:CC:18:TRP:H | 1.68 | 0.40 |
| 4:CD:68:TYR:N | 4:CD:68:TYR:CD1 | 2.88 | 0.40 |
| 1:AA:690:G:C5 | 1:AA:691:G:C6 | 3.09 | 0.40 |
| 23:DA:72:U:H1' | 47:DY:58:ALA:CB | 2.52 | 0.40 |
| 30:DH:97:ILE:HG21 | 30:DH:114:LEU:HD11 | 2.04 | 0.40 |
| 13:AM:56:LEU:HD13 | 13:AM:56:LEU:O | 2.21 | 0.40 |
| 1:AA:1098:C:H2' | 1:AA:1099:G:O4' | 2.21 | 0.40 |
| 49:D1:59:VAL:CG1 | 49:D1:60:GLU:H | 2.15 | 0.40 |
| 36:DN:103:ARG:NH1 | 36:DN:108:GLY:O | 2.55 | 0.40 |
| 24:DB:72:G:N2 | 24:DB:103:U:C5 | 2.89 | 0.40 |
| 26:BD:61:ARG:HB2 | 26:BD:63:LEU:HB2 | 2.04 | 0.40 |
| 27:DE:123:LEU:HD11 | 27:DE:125:LEU:HD23 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:CQ:63:ARG:HG2 | 17:CQ:64:PRO:CD | 2.52 | 0.40 |
| 5:CE:79:GLU:CG | 5:CE:92:LYS:HG3 | 2.52 | 0.40 |
| 24:BB:16:G:O6 | 24:BB:69:G:C2 | 2.74 | 0.40 |
| 23:DA:1332:G:H22 | 23:DA:1610:A:H8 | 1.68 | 0.40 |
| 1:CA:1102:A:N6 | 1:CA:1103:C:N4 | 2.70 | 0.40 |
| 2:AB:100:GLY:N | 2:AB:176:GLU:OE2 | 2.41 | 0.40 |
| 1:AA:1151:A:O2' | 1:AA:1152:A:O4' | 2.39 | 0.40 |
| 1:AA:1292:U:O5' | 1:AA:1292:U:H6 | 2.04 | 0.40 |
| 36:BN:59:ASP:N | 36:BN:59:ASP:OD2 | 2.53 | 0.40 |
| 27:DE:167:ALA:O | 27:DE:168:ARG:C | 2.60 | 0.40 |
| 23:DA:2396:G:N3 | 23:DA:2421:G:C2 | 2.89 | 0.40 |
| 23:DA:2305:A:H5'' | 28:DF:134:GLY:CA | 2.48 | 0.40 |
| 1:CA:448:A:C6 | 1:CA:487:A:N3 | 2.89 | 0.40 |
| 23:BA:2792:G:C6 | 23:BA:2805:G:N1 | 2.90 | 0.40 |
| 23:BA:380:U:O2 | 23:BA:381:G:C8 | 2.74 | 0.40 |
| 6:CF:29:ALA:HA | 6:CF:32:ASN:OD1 | 2.21 | 0.40 |
| 23:BA:1509:A:O3' | 23:BA:1510:A:O4' | 2.39 | 0.40 |
| 6:AF:91:VAL:HG13 | 18:AR:72:ARG:HH21 | 1.87 | 0.40 |
| 1:AA:1118:C:H5'' | 9:AI:104:ARG:HG2 | 2.04 | 0.40 |
| 37:DO:34:HIS:HB3 | 37:DO:36:TYR:HE1 | 1.86 | 0.40 |
| 23:DA:2208:U:C1' | 25:DC:151:LYS:HE3 | 2.51 | 0.40 |
| 18:CR:40:LEU:HA | 18:CR:40:LEU:HD23 | 1.88 | 0.40 |
| 23:DA:998:C:OP2 | 39:DQ:93:LYS:NZ | 2.55 | 0.40 |
| 1:AA:102:G:C5 | 1:AA:103:C:C5 | 3.09 | 0.40 |
| 25:DC:205:VAL:O | 25:DC:205:VAL:CG1 | 2.68 | 0.40 |
| 23:DA:283:A:H4' | 23:DA:284:U:OP2 | 2.21 | 0.40 |
| 50:B2:31:VAL:HG13 | 50:B2:42:PRO:HG3 | 2.02 | 0.40 |
| 46:BX:23:LYS:HE2 | 46:BX:37:ILE:HD11 | 2.03 | 0.40 |
| 23:BA:2285:C:H5 | 51:B3:27:LYS:HZ2 | 1.69 | 0.40 |
| 2:CB:74:LYS:HB2 | 2:CB:74:LYS:NZ | 2.36 | 0.40 |
| 3:CC:21:ARG:O | 3:CC:22:TRP:HB3 | 2.21 | 0.40 |
| 17:AQ:3:LYS:O | 17:AQ:5:VAL:HG23 | 2.21 | 0.40 |
| 26:DD:110:GLY:CA | 26:DD:162:ALA:HB2 | 2.52 | 0.40 |
| 23:DA:2749:A:H4' | 29:DG:62:LYS:HB3 | 2.02 | 0.40 |
| 1:CA:862:C:C5 | 1:CA:863:U:C5 | 3.09 | 0.40 |
| 44:BV:36:LYS:C | 44:BV:37:VAL:CG1 | 2.88 | 0.40 |
| 23:BA:1607:C:N4 | 23:BA:1621:U:C3' | 2.84 | 0.40 |
| 8:AH:17:THR:O | 8:AH:78:GLN:NE2 | 2.54 | 0.40 |
| 14:CN:36:PHE:CD1 | 14:CN:36:PHE:C | 2.94 | 0.40 |
| 6:CF:55:ASP:OD1 | 6:CF:56:PRO:HD2 | 2.22 | 0.40 |
| 23:DA:855:G:C6 | 23:DA:856:C:C4 | 3.10 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:BD:158:GLY:O | 26:BD:159:HIS:O | 2.38 | 0.40 |
| 1:CA:638:G:H2' | 1:CA:639:G:C5' | 2.51 | 0.40 |
| 23:DA:902:C:H2' | 23:DA:903:C:C6 | 2.56 | 0.40 |
| 15:CO:63:ARG:O | 15:CO:67:LEU:HD12 | 2.21 | 0.40 |
| 19:AS:53:ASN:C | 19:AS:55:LYS:H | 2.24 | 0.40 |
| 1:AA:540:G:C6 | 1:AA:541:G:C5 | 3.09 | 0.40 |
| 23:DA:692:C:C2' | 23:DA:693:C:H5' | 2.52 | 0.40 |
| 23:BA:958:U:C2' | 23:BA:959:A:OP2 | 2.69 | 0.40 |
| 23:DA:415:A:C5 | 23:DA:416:C:C5 | 3.09 | 0.40 |
| 23:DA:415:A:H2' | 23:DA:416:C:O4' | 2.22 | 0.40 |
| 30:BH:27:ARG:HD2 | 46:BX:71:TYR:CE1 | 2.56 | 0.40 |
| 23:DA:2299:G:O6 | 23:DA:2318:G:N2 | 2.54 | 0.40 |
| 44:DV:9:TYR:CD2 | 44:DV:35:ARG:CZ | 3.03 | 0.40 |
| 38:DP:126:ALA:C | 38:DP:128:GLU:H | 2.24 | 0.40 |
| 23:BA:2575:C:H5' | 26:BD:144:ARG:HG2 | 2.02 | 0.40 |
| 23:DA:2183:C:C2' | 23:DA:2183:C:O2 | 2.67 | 0.40 |
| 23:DA:288:C:O2' | 23:DA:289:A:H5' | 2.21 | 0.40 |
| 1:AA:562:C:H1' | 12:AL:14:ARG:HD2 | 2.02 | 0.40 |
| 1:CA:562:C:N3 | 1:CA:884:U:C5 | 2.89 | 0.40 |
| 23:DA:2039:C:H2' | 23:DA:2040:C:C6 | 2.54 | 0.40 |
| 2:AB:52:GLU:HG2 | 2:AB:56:ARG:HE | 1.86 | 0.40 |
| 41:BS:107:LEU:N | 41:BS:107:LEU:HD13 | 2.36 | 0.40 |
| 18:CR:53:ARG:C | 18:CR:55:ARG:N | 2.74 | 0.40 |
| 30:DH:9:LEU:HB3 | 30:DH:12:LEU:HD23 | 2.04 | 0.40 |
| 35:BM:83:MET:CG | 35:BM:83:MET:O | 2.70 | 0.40 |
| 2:AB:74:LYS:NZ | 2:AB:74:LYS:HB2 | 2.36 | 0.40 |
| 23:DA:769:G:O2' | 23:DA:770:G:H5' | 2.21 | 0.40 |
| 23:BA:2823:A:OP1 | 26:BD:113:PHE:HB2 | 2.21 | 0.40 |
| 23:DA:2197:U:H1' | 23:DA:2198:A:C8 | 2.56 | 0.40 |
| 1:AA:450:G:H5'' | 16:AP:41:PRO:O | 2.22 | 0.40 |
| 1:AA:451:A:H1' | 1:AA:452:A:N7 | 2.37 | 0.40 |
| 23:BA:1926:U:O2 | 23:BA:1929:G:C2 | 2.75 | 0.40 |
| 1:CA:614:A:H2' | 1:CA:615:C:C6 | 2.56 | 0.40 |
| 27:BE:144:LYS:O | 27:BE:146:ALA:N | 2.44 | 0.40 |
| 23:DA:1416:G:O2' | 23:DA:1417:C:H6 | 2.03 | 0.40 |
| 1:AA:245:C:C2 | 1:AA:284:G:C2 | 3.09 | 0.40 |
| 1:CA:604:G:N7 | 1:CA:605:U:C5 | 2.89 | 0.40 |
| 15:CO:43:LEU:HD23 | 15:CO:43:LEU:HA | 1.87 | 0.40 |
| 23:DA:1632:A:H8 | 23:DA:1632:A:O5' | 2.04 | 0.40 |
| 36:DN:105:ARG:HG2 | 36:DN:106:GLY:N | 2.37 | 0.40 |
| 12:AL:36:CYS:SG | 12:AL:80:SER:HB2 | 2.61 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BA:455:C:N3 | 23:BA:472:A:H2' | 2.36 | 0.40 |
| 3:AC:48:TYR:O | 3:AC:51:GLY:N | 2.51 | 0.40 |
| 23:DA:2464:C:C2 | 23:DA:2487:G:N2 | 2.90 | 0.40 |
| 23:BA:2052:G:O4' | 26:BD:142:GLY:HA3 | 2.21 | 0.40 |
| 23:DA:1555:G:O2' | 23:DA:1556:C:H5' | 2.21 | 0.40 |
| 1:AA:700:G:H4' | 1:AA:704:A:H1' | 2.04 | 0.40 |
| 45:DW:55:ARG:NH1 | 45:DW:55:ARG:HB3 | 2.36 | 0.40 |
| 7:CG:75:VAL:O | 7:CG:75:VAL:HG23 | 2.21 | 0.40 |
| 23:BA:2415:G:H4' | 34:BL:67:MET:H | 1.86 | 0.40 |
| 24:BB:83:G:N2 | 24:BB:84:C:H1' | 2.36 | 0.40 |
| 23:DA:857:C:N3 | 23:DA:858:U:C4 | 2.89 | 0.40 |
| 23:BA:674:G:H2' | 23:BA:804:A:H61 | 1.85 | 0.40 |
| 1:CA:1371:G:H4' | 9:CI:69:GLY:HA3 | 2.04 | 0.40 |
| 9:AI:127:LYS:O | 9:AI:128:ARG:O | 2.38 | 0.40 |
| 34:BL:32:THR:C | 34:BL:36:LYS:HE2 | 2.36 | 0.40 |
| 1:CA:977:A:H8 | 1:CA:1223:C:C4 | 2.40 | 0.40 |
| 1:AA:953:G:C6 | 1:AA:954:G:C4 | 3.10 | 0.40 |
| 23:BA:578:A:H5' | 23:BA:1254:A:OP1 | 2.21 | 0.40 |
| 42:BT:62:LYS:C | 42:BT:63:LYS:HD3 | 2.42 | 0.40 |
| 39:DQ:106:PHE:O | 39:DQ:109:LEU:HB2 | 2.21 | 0.40 |
| 25:DC:32:SER:HA | 25:DC:36:PRO:HG3 | 2.03 | 0.40 |
| 35:DM:74:TYR:N | 35:DM:92:GLY:O | 2.45 | 0.40 |
| 23:DA:1614:A:C6 | 41:DS:87:PRO:HB3 | 2.56 | 0.40 |
| 23:DA:114(B):A:N3 | 23:DA:1144:G:C8 | 2.90 | 0.40 |
| 30:BH:79:ILE:H | 30:BH:145:VAL:HG23 | 1.87 | 0.40 |
| 39:BQ:79:PHE:CE1 | 39:BQ:83:LEU:HD13 | 2.57 | 0.40 |
| 23:BA:748:G:OP2 | 41:BS:88:ARG:HG3 | 2.21 | 0.40 |
| 23:BA:2727:G:C6 | 23:BA:2728:U:C5 | 3.08 | 0.40 |
| 23:BA:2682:U:O4 | 23:BA:2728:U:H1' | 2.21 | 0.40 |
| 16:AP:6:LEU:HB3 | 16:AP:17:TYR:HD2 | 1.85 | 0.40 |
| 25:DC:147:LEU:HD13 | 25:DC:155:LEU:HD13 | 2.03 | 0.40 |
| 25:DC:130:ALA:CB | 25:DC:192:THR:HA | 2.51 | 0.40 |
| 12:AL:100:VAL:HG12 | 12:AL:103:VAL:HG23 | 2.03 | 0.40 |
| 42:DT:35:THR:O | 42:DT:39:ILE:CG1 | 2.61 | 0.40 |
| 23:BA:1411:C:O2' | 23:BA:1412:A:H5' | 2.21 | 0.40 |
| 8:AH:120:THR:O | 8:AH:121:ASP:C | 2.60 | 0.40 |
| 1:AA:92:G:H2' | 1:AA:93:U:O4' | 2.22 | 0.40 |
| 26:BD:6:GLY:CA | 26:BD:51:PHE:HE2 | 2.33 | 0.40 |
| 3:AC:172:ARG:O | 3:AC:173:VAL:CG2 | 2.56 | 0.40 |
| 23:DA:1596:A:O2' | 23:DA:1597:A:H5' | 2.22 | 0.40 |
| 34:DL:16:ARG:O | 34:DL:18:ARG:N | 2.55 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:AC:33:LEU:HD12 | 3:AC:33:LEU:O | 2.21 | 0.40 |
| 1:CA:130:A:H5'' | 1:CA:190:G:O2' | 2.21 | 0.40 |
| 26:DD:2:LYS:CD | 26:DD:95:ILE:O | 2.69 | 0.40 |
| 26:DD:47:VAL:HG21 | 26:DD:85:ASN:HA | 2.02 | 0.40 |
| 39:DQ:60:LEU:HD13 | 39:DQ:60:LEU:C | 2.41 | 0.40 |
| 5:CE:136:MET:O | 5:CE:139:LEU:N | 2.54 | 0.40 |
| 23:DA:1652:A:OP1 | 36:DN:9:LYS:HD2 | 2.21 | 0.40 |
| 5:AE:12:LEU:O | 5:AE:12:LEU:HD22 | 2.22 | 0.40 |
| 5:AE:77:PRO:CD | 5:AE:142:LEU:HD22 | 2.45 | 0.40 |
| 1:AA:184:G:N2 | 1:AA:194:C:C2 | 2.90 | 0.40 |
| 26:DD:34:VAL:HG11 | 26:DD:78:LEU:CD1 | 2.52 | 0.40 |
| 5:AE:51:VAL:O | 5:AE:52:PRO:C | 2.57 | 0.40 |
| 42:BT:7:VAL:HG13 | 42:BT:30:VAL:HG13 | 2.02 | 0.40 |
| 1:AA:1066:C:H3' | 1:AA:1067:A:C8 | 2.56 | 0.40 |
| 41:DS:6:ILE:HG12 | 41:DS:104:THR:OG1 | 2.21 | 0.40 |
| 1:CA:402:G:H2' | 1:CA:403:C:H5' | 2.03 | 0.40 |
| 1:AA:448:A:C2 | 1:AA:487:A:C2 | 3.08 | 0.40 |
| 23:BA:2378:A:H4' | 37:BO:84:GLN:NE2 | 2.35 | 0.40 |
| 25:DC:185:VAL:HG12 | 25:DC:186:HIS:H | 1.85 | 0.40 |
| 20:CT:55:ILE:C | 20:CT:57:ARG:N | 2.74 | 0.40 |
| 20:CT:15:ARG:HD3 | 20:CT:15:ARG:HA | 1.89 | 0.40 |
| 23:DA:2755:C:O2' | 23:DA:2756:U:H6 | 2.03 | 0.40 |
| 27:DE:154:VAL:O | 27:DE:174:VAL:HG23 | 2.21 | 0.40 |
| 23:BA:2305:A:C5' | 28:BF:134:GLY:HA3 | 2.48 | 0.40 |
| 23:BA:2722:G:O2' | 36:BN:5:LYS:HB2 | 2.22 | 0.40 |
| 23:DA:1401:G:C5 | 23:DA:1402:C:C4 | 3.09 | 0.40 |
| 6:CF:88:VAL:CG1 | 6:CF:89:MET:N | 2.83 | 0.40 |
| 23:DA:1105:U:C2' | 23:DA:1106:G:H5' | 2.51 | 0.40 |
| 15:AO:45:VAL:HG22 | 15:AO:46:HIS:N | 2.36 | 0.40 |
| 23:BA:1649:G:C6 | 23:BA:2009:G:C6 | 3.09 | 0.40 |
| 23:DA:528:A:H2' | 23:DA:529:A:O5' | 2.21 | 0.40 |
| 23:BA:2746:U:C2' | 23:BA:2747:G:O5' | 2.69 | 0.40 |
| 27:DE:101:LEU:CD1 | 27:DE:102:PRO:HD2 | 2.42 | 0.40 |
| 8:AH:111:ILE:O | 8:AH:112:LEU:CB | 2.70 | 0.40 |
| 1:AA:658:G:C4 | 1:AA:659:U:C5 | 3.10 | 0.40 |
| 1:AA:658:G:O2' | 1:AA:659:U:H5' | 2.22 | 0.40 |
| 25:DC:133:LEU:HG | 25:DC:189:CYS:O | 2.20 | 0.40 |
| 1:AA:781:A:H3' | 1:AA:782:A:C5' | 2.50 | 0.40 |
| 1:AA:59:A:C2 | 1:AA:354:G:C4 | 3.10 | 0.40 |
| 1:AA:53:A:C2 | 1:AA:54:C:C1' | 3.04 | 0.40 |
| 1:AA:630:G:H2' | 1:AA:631:G:O4' | 2.22 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 33:DK:114:ILE:O | 33:DK:118:ALA:N | 2.49 | 0.40 |
| 25:BC:8:PRO:CB | 25:BC:14:ARG:HB2 | 2.42 | 0.40 |
| 33:DK:119:PRO:HB2 | 38:DP:68:TYR:HE1 | 1.76 | 0.40 |
| 1:CA:69:G:H2' | 1:CA:73:G:C8 | 2.56 | 0.40 |
| 15:AO:85:LEU:HD23 | 15:AO:85:LEU:HA | 1.83 | 0.40 |
| 23:DA:2592:G:C5 | 23:DA:2593:U:C5 | 3.09 | 0.40 |
| 50:D2:51:TYR:CZ | 50:D2:52:TYR:CZ | 3.09 | 0.40 |
| 1:CA:1060:C:H5'' | 10:CJ:51:ARG:HG2 | 2.03 | 0.40 |
| 35:DM:54:MET:CG | 35:DM:64:ILE:HD13 | 2.46 | 0.40 |
| 23:BA:865:C:C4' | 23:BA:866:A:N7 | 2.82 | 0.40 |
| 35:BM:127:ILE:HG23 | 35:BM:128:LYS:N | 2.36 | 0.40 |
| 23:BA:588:U:C2 | 27:BE:90:PHE:CE1 | 3.10 | 0.40 |
| 23:BA:588:U:H1' | 27:BE:90:PHE:HB3 | 2.04 | 0.40 |
| 23:BA:2861:G:C2 | 23:BA:2862:G:C8 | 3.09 | 0.40 |
| 1:CA:20:U:O2 | 1:CA:916:G:C2 | 2.75 | 0.40 |
| 23:BA:830:G:C8 | 23:BA:2448:A:C2 | 3.09 | 0.40 |
| 23:DA:2661:G:H2' | 23:DA:2662:A:O4' | 2.21 | 0.40 |
| 1:CA:1077:G:C6 | 1:CA:1081:G:C6 | 3.10 | 0.40 |
| 23:BA:2244:U:H1' | 23:BA:2434:A:C4 | 2.55 | 0.40 |
| 1:CA:1410:G:H2' | 1:CA:1411:C:C6 | 2.57 | 0.40 |
| 1:AA:731:G:C6 | 1:AA:732:C:C4 | 3.09 | 0.40 |
| 23:DA:814:C:H41 | 34:DL:27:HIS:HD2 | 1.64 | 0.40 |
| 23:DA:2242:G:H2' | 23:DA:2243:U:O4' | 2.21 | 0.40 |
| 1:AA:754:C:H1' | 15:AO:69:TYR:CG | 2.56 | 0.40 |
| 1:CA:972:C:OP2 | 10:CJ:57:LYS:HD2 | 2.22 | 0.40 |
| 43:DU:63:LYS:CG | 43:DU:64:GLU:N | 2.84 | 0.40 |
| 23:DA:2036:C:C6 | 23:DA:2036:C:C5' | 2.99 | 0.40 |
| 12:CL:6:ILE:O | 12:CL:7:ASN:C | 2.60 | 0.40 |
| 1:AA:560:U:H4' | 1:AA:561:U:O5' | 2.21 | 0.40 |
| 1:AA:565:U:C4 | 1:AA:566:G:C6 | 3.09 | 0.40 |
| 23:DA:1856:G:C2 | 23:DA:1857:G:H1' | 2.56 | 0.40 |
| 24:BB:3:C:H2' | 24:BB:4:C:C6 | 2.57 | 0.40 |
| 23:BA:1335:U:OP2 | 42:BT:65:ARG:NH1 | 2.54 | 0.40 |
| 1:AA:538:G:O3' | 12:AL:113:LYS:HG3 | 2.22 | 0.40 |
| 34:BL:122:PRO:O | 34:BL:123:LEU:HB3 | 2.22 | 0.40 |
| 20:AT:78:ALA:O | 20:AT:79:ARG:C | 2.60 | 0.40 |
| 1:CA:465:A:O2' | 1:CA:466:G:H5'' | 2.21 | 0.40 |
| 23:BA:1051:G:C5 | 23:BA:1052:C:N3 | 2.89 | 0.40 |
| 41:DS:45:TYR:CD2 | 41:DS:46:PHE:CE1 | 3.10 | 0.40 |
| 26:BD:67:PHE:HB3 | 26:BD:72:VAL:O | 2.20 | 0.40 |
| 2:AB:16:HIS:HB3 | 2:AB:210:SER:HA | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 47:DY:36:ARG:HA | 47:DY:39:ALA:HB2 | 2.02 | 0.40 |
| 2:CB:52:GLU:HG2 | 2:CB:56:ARG:HE | 1.86 | 0.40 |
| 1:CA:1048:G:C2 | 1:CA:1210:C:N3 | 2.88 | 0.40 |
| 40:BR:15:GLU:HB3 | 40:BR:16:PRO:HD2 | 2.04 | 0.40 |
| 36:DN:13:HIS:CE1 | 36:DN:15:SER:HB3 | 2.56 | 0.40 |
| 5:CE:104:ALA:O | 5:CE:107:ARG:HB3 | 2.21 | 0.40 |
| 1:AA:425:G:C6 | 1:AA:426:G:C5 | 3.10 | 0.40 |
| 39:DQ:47:TYR:CE1 | 40:DR:74:LYS:HE3 | 2.56 | 0.40 |
| 23:DA:770:G:C2' | 23:DA:771:G:O5' | 2.69 | 0.40 |
| 23:DA:900:A:C5 | 23:DA:901:A:C8 | 3.10 | 0.40 |
| 1:CA:897:C:H5'' | 1:CA:898:G:OP2 | 2.21 | 0.40 |
| 1:CA:451:A:H61 | 1:CA:481:G:C5' | 2.34 | 0.40 |
| 23:DA:1881:C:O2' | 23:DA:1882:C:H5' | 2.21 | 0.40 |
| 33:BK:18:LYS:HG3 | 33:BK:45:GLU:OE2 | 2.22 | 0.40 |
| 23:DA:1314:C:H2' | 23:DA:1315:C:H5' | 2.04 | 0.40 |
| 35:DM:34:LEU:HB2 | 35:DM:118:LEU:HD13 | 2.02 | 0.40 |
| 38:DP:34:VAL:O | 38:DP:40:THR:HA | 2.21 | 0.40 |
| 23:BA:1687:G:H2' | 23:BA:1688:U:C6 | 2.56 | 0.40 |
| 23:DA:1416:G:O2' | 23:DA:1417:C:P | 2.78 | 0.40 |
| 23:DA:1417:C:N4 | 23:DA:1581:G:H1 | 2.20 | 0.40 |
| 38:BP:113:LYS:O | 38:BP:114:LEU:HD23 | 2.21 | 0.40 |
| 23:BA:2615:U:C2 | 50:B2:7:PRO:HA | 2.56 | 0.40 |
| 23:DA:2063:C:O2 | 23:DA:2450:A:N1 | 2.54 | 0.40 |
| 8:CH:69:ARG:HD3 | 8:CH:69:ARG:HA | 1.80 | 0.40 |
| 23:DA:1718:G:H2' | 23:DA:1725:G:H8 | 1.87 | 0.40 |
| 23:BA:799:G:N1 | 23:BA:800:A:N6 | 2.70 | 0.40 |
| 23:DA:791:C:H4' | 23:DA:792:G:OP1 | 2.21 | 0.40 |
| 1:CA:900:A:H2' | 1:CA:901:A:C8 | 2.56 | 0.40 |
| 25:DC:98:VAL:HG23 | 25:DC:99:ASP:N | 2.36 | 0.40 |
| 23:DA:1805:U:H2' | 23:DA:1806:C:C6 | 2.56 | 0.40 |
| 18:CR:65:ILE:O | 18:CR:69:THR:HG23 | 2.21 | 0.40 |
| 1:CA:772:U:C2' | 1:CA:773:G:H5' | 2.51 | 0.40 |
| 34:BL:6:LEU:HD12 | 34:BL:8:PRO:HD2 | 2.01 | 0.40 |
| 23:BA:2552:U:H6 | 23:BA:2552:U:O5' | 2.04 | 0.40 |
| 8:AH:2:LEU:HD23 | 8:AH:2:LEU:HA | 1.88 | 0.40 |
| 13:CM:93:ARG:HE | 13:CM:93:ARG:HA | 1.87 | 0.40 |
| 5:AE:127:ASN:HB3 | 5:AE:130:ASN:HB2 | 2.04 | 0.40 |
| 23:DA:1599:C:H2' | 23:DA:1600:C:C6 | 2.57 | 0.40 |
| 26:DD:24:THR:CB | 26:DD:186:GLY:HA2 | 2.50 | 0.40 |
| 23:DA:1448:G:H1' | 23:DA:1528:A:N1 | 2.35 | 0.40 |
| 34:BL:107:LYS:C | 34:BL:108:LYS:HG2 | 2.41 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 34:BL:112:LEU:HD23 | 34:BL:112:LEU:C | 2.42 | 0.40 |
| 1:CA:1371:G:C6 | 1:CA:1372:U:C4 | 3.10 | 0.40 |
| 9:CI:111:ARG:O | 9:CI:113:LYS:HE3 | 2.20 | 0.40 |
| 25:BC:206:LEU:HA | 25:BC:211:ARG:HE | 1.86 | 0.40 |
| 23:DA:2846:G:N7 | 23:DA:2847:U:C5 | 2.90 | 0.40 |
| 37:BO:26:LEU:HD23 | 37:BO:38:GLN:O | 2.21 | 0.40 |
| 32:BJ:91:GLU:HA | 32:BJ:111:GLU:OE2 | 2.21 | 0.40 |
| 23:DA:1263:U:O4' | 50:D2:10:LYS:HG3 | 2.22 | 0.40 |
| 24:DB:81:G:C5 | 24:DB:82:G:N7 | 2.90 | 0.40 |
| 16:CP:18:ARG:O | 16:CP:19:ILE:C | 2.59 | 0.40 |
| 23:BA:243:U:OP1 | 53:B5:6:THR:CG2 | 2.70 | 0.40 |
| 28:DF:25:TYR:HD1 | 28:DF:30:GLU:HB3 | 1.79 | 0.40 |
| 23:DA:2295:C:N3 | 23:DA:2296:U:C5 | 2.89 | 0.40 |
| 16:AP:32:TYR:C | 16:AP:32:TYR:HD2 | 2.25 | 0.40 |
| 25:DC:70:TRP:CH2 | 25:DC:150:LYS:CA | 3.03 | 0.40 |
| 4:AD:146:ILE:HG22 | 4:AD:146:ILE:O | 2.21 | 0.40 |
| 3:CC:141:VAL:HG11 | 3:CC:202:ILE:HG23 | 2.04 | 0.40 |
| 1:AA:690:G:C6 | 1:AA:691:G:N1 | 2.89 | 0.40 |
| 30:DH:129:THR:HG22 | 30:DH:130:TYR:H | 1.87 | 0.40 |
| 13:AM:33:ALA:HB1 | 13:AM:56:LEU:CD2 | 2.47 | 0.40 |
| 20:CT:23:ARG:O | 20:CT:26:ASN:ND2 | 2.55 | 0.40 |
| 28:BF:41:GLN:HG2 | 28:BF:155:MET:CB | 2.48 | 0.40 |
| 44:DV:48:PHE:CE2 | 44:DV:71:VAL:HG21 | 2.57 | 0.40 |
| 44:DV:56:VAL:C | 44:DV:57:ILE:HD12 | 2.41 | 0.40 |
| 47:DY:35:LEU:HD12 | 47:DY:53:LEU:CD1 | 2.35 | 0.40 |
| 23:DA:1999:C:O2 | 23:DA:2687:U:O2' | 2.29 | 0.40 |
| 24:BB:72:G:N2 | 24:BB:103:U:C5 | 2.90 | 0.40 |
| 25:BC:232:PRO:HG3 | 25:BC:248:SER:O | 2.21 | 0.40 |
| 23:DA:2766:G:C2 | 23:DA:2767:C:C5 | 3.10 | 0.40 |
| 1:CA:39:G:N1 | 1:CA:40:C:C5 | 2.90 | 0.40 |
| 4:AD:156:GLU:O | 4:AD:160:GLN:HG3 | 2.21 | 0.40 |
| 41:BS:29:LEU:HD21 | 41:BS:33:ARG:NH2 | 2.36 | 0.40 |
| 1:CA:725:G:H2' | 1:CA:726:C:C6 | 2.56 | 0.40 |
| 26:BD:9:VAL:CG2 | 26:BD:10:GLY:N | 2.85 | 0.40 |
| 23:BA:2791:C:H2' | 23:BA:2791:C:O2 | 2.21 | 0.40 |
| 23:BA:379:G:N2 | 46:BX:20:ARG:NH2 | 2.70 | 0.40 |
| 23:BA:380:U:C2' | 46:BX:20:ARG:HE | 2.35 | 0.40 |
| 2:CB:83:MET:HE2 | 2:CB:234:PRO:HG2 | 2.04 | 0.40 |
| 11:CK:13:GLN:HG3 | 11:CK:75:TYR:C | 2.42 | 0.40 |
| 37:BO:73:LEU:O | 37:BO:77:ALA:N | 2.54 | 0.40 |
| 27:BE:64:ILE:HG23 | 27:BE:65:TRP:NE1 | 2.36 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:724:G:N3 | 1:AA:725:G:C8 | 2.89 | 0.40 |
| 23:BA:953:A:O2' | 23:BA:954:G:H5' | 2.21 | 0.40 |
| 11:AK:93:GLN:HA | 11:AK:96:ARG:HB2 | 2.04 | 0.40 |
| 25:DC:26:LYS:HB2 | 25:DC:26:LYS:HE3 | 1.68 | 0.40 |
| 23:DA:1952:A:C6 | 33:DK:22:ILE:HD12 | 2.55 | 0.40 |
| 1:AA:853:G:H2' | 1:AA:854:G:H5' | 2.03 | 0.40 |
| 25:DC:205:VAL:O | 25:DC:206:LEU:C | 2.57 | 0.40 |
| 1:CA:1129:C:C1' | 1:CA:1130:A:OP2 | 2.63 | 0.40 |
| 1:CA:1139:G:N2 | 1:CA:1143:G:N1 | 2.70 | 0.40 |
| 43:BU:2:ARG:HG3 | 43:BU:2:ARG:NH1 | 2.35 | 0.40 |
| 15:AO:81:LEU:HD12 | 15:AO:81:LEU:O | 2.20 | 0.40 |
| 23:BA:1679:U:C3' | 23:BA:1680:U:H5' | 2.52 | 0.40 |
| 1:AA:336:C:H2' | 1:AA:337:C:C6 | 2.56 | 0.40 |
| 50:D2:33:CYS:SG | 50:D2:38:ALA:HB3 | 2.62 | 0.40 |
| 1:CA:719:C:O2' | 18:CR:49:LYS:HB3 | 2.21 | 0.40 |
| 23:BA:1389:G:H2' | 23:BA:1390:U:H6 | 1.85 | 0.40 |
| 23:BA:286:C:C2 | 23:BA:287:C:C5 | 3.09 | 0.40 |
| 23:DA:1388:G:C4 | 23:DA:1389:G:C8 | 3.10 | 0.40 |
| 50:B2:51:TYR:CZ | 50:B2:52:TYR:CE1 | 3.09 | 0.40 |
| 23:BA:814:C:H41 | 34:BL:27:HIS:HD2 | 1.64 | 0.40 |
| 34:BL:131:SER:HB3 | 34:BL:134:ALA:H | 1.86 | 0.40 |
| 1:CA:1233:G:OP1 | 9:CI:123:PRO:HA | 2.21 | 0.40 |
| 1:AA:650:G:C2' | 1:AA:651:C:H5' | 2.51 | 0.40 |
| 36:BN:45:ARG:HG3 | 36:BN:95:THR:CG2 | 2.51 | 0.40 |
| 13:CM:79:LYS:O | 13:CM:82:MET:HB3 | 2.22 | 0.40 |
| 1:AA:728:A:C6 | 15:AO:54:ARG:HD2 | 2.57 | 0.40 |
| 23:DA:826:U:O2 | 23:DA:832:G:C2 | 2.75 | 0.40 |
| 35:DM:138:ASP:HB3 | 35:DM:139:GLU:H | 1.53 | 0.40 |
| 23:DA:2322:A:H3' | 23:DA:2323:G:C8 | 2.48 | 0.40 |
| 36:BN:84:ALA:N | 36:BN:85:PRO:CD | 2.84 | 0.40 |
| 1:AA:186(D):G:C6 | 1:AA:186(E):C:C4 | 3.09 | 0.40 |
| 1:AA:505:G:OP2 | 1:AA:534:U:H2' | 2.21 | 0.40 |
| 7:AG:95:ARG:CZ | 7:AG:99:LEU:HD11 | 2.50 | 0.40 |
| 1:CA:357:G:H8 | 1:CA:357:G:O5' | 2.04 | 0.40 |
| 39:DQ:8:VAL:O | 39:DQ:9:VAL:C | 2.59 | 0.40 |
| 6:AF:96:PRO:HB3 | 18:AR:30:ASP:OD2 | 2.21 | 0.40 |
| 39:DQ:34:LYS:HE3 | 39:DQ:37:GLU:OE1 | 2.21 | 0.40 |
| 23:DA:2837:G:N1 | 23:DA:2838:G:C5 | 2.90 | 0.40 |
| 23:BA:189:G:H1' | 23:BA:207:A:N6 | 2.36 | 0.40 |
| 23:DA:553:U:C4 | 23:DA:554:U:C4 | 3.10 | 0.40 |
| 23:DA:2370:G:O2' | 51:D3:45:LYS:HE3 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:DX:67:ILE:N | 46:DX:68:PRO:CD | 2.83 | 0.40 |
| 1:CA:311:C:OP1 | 16:CP:26:ARG:NH2 | 2.45 | 0.40 |
| 12:CL:64:GLU:OE1 | 12:CL:64:GLU:C | 2.59 | 0.40 |
| 23:DA:1798:U:C5' | 25:DC:259:THR:O | 2.70 | 0.40 |
| 23:DA:1116:C:H2' | 23:DA:1117:G:O4' | 2.22 | 0.40 |
| 3:AC:146:ALA:HA | 3:AC:204:LEU:HD23 | 2.04 | 0.40 |
| 23:BA:2436:G:C4 | 23:BA:2437:U:C5 | 3.10 | 0.40 |
| 23:BA:1234:U:H2' | 23:BA:1235:G:O4' | 2.22 | 0.40 |
| 1:CA:1466:C:H2' | 1:CA:1467:G:O4' | 2.22 | 0.40 |
| 23:BA:337:C:C2' | 23:BA:338:G:O5' | 2.70 | 0.40 |
| 23:DA:1314:C:O2' | 23:DA:1315:C:H5' | 2.21 | 0.40 |
| 44:DV:146:ILE:HG12 | 44:DV:146:ILE:H | 1.62 | 0.40 |
| 1:CA:654:G:C2 | 1:CA:753:A:C4 | 3.08 | 0.40 |
| 23:DA:2358:G:C5 | 23:DA:2359:C:C5 | 3.10 | 0.40 |
| 23:BA:2075:U:C4 | 23:BA:2238:G:C6 | 3.09 | 0.40 |
| 52:D4:31:LEU:HD12 | 52:D4:31:LEU:HA | 1.84 | 0.40 |
| 23:DA:1889:A:C6 | 23:DA:1890:A:C6 | 3.09 | 0.40 |
| 28:BF:96:ARG:HB2 | 28:BF:97:ASP:H | 1.63 | 0.40 |
| 3:AC:56:ASP:HB3 | 3:AC:67:THR:HB | 2.04 | 0.40 |
| 23:DA:53:A:H2' | 23:DA:54:G:O4' | 2.22 | 0.40 |
| 23:DA:1497:U:O4' | 23:DA:1497:U:O2 | 2.38 | 0.40 |
| 30:BH:35:LEU:N | 30:BH:35:LEU:HD23 | 2.36 | 0.40 |
| 4:CD:78:LEU:HD23 | 4:CD:78:LEU:HA | 1.93 | 0.40 |
| 30:DH:136:VAL:N | 30:DH:137:PRO:HD3 | 2.37 | 0.40 |
| 3:CC:61:ALA:O | 3:CC:62:ASP:HB2 | 2.22 | 0.40 |
| 23:BA:1341:U:H4' | 42:BT:56:THR:O | 2.21 | 0.40 |
| 34:DL:88:LEU:CD2 | 34:DL:114:ILE:HG21 | 2.51 | 0.40 |
| 47:DY:1:MET:O | 47:DY:1:MET:HE2 | 2.22 | 0.40 |
| 26:DD:103:ASP:OD2 | 26:DD:201:THR:HA | 2.21 | 0.40 |
| 23:DA:1542:G:H4' | 23:DA:1543:A:O4' | 2.21 | 0.40 |
| 24:BB:80:U:C2 | 24:BB:81:G:N2 | 2.90 | 0.40 |
| 1:AA:979:C:P | 1:AA:981:U:O4 | 2.80 | 0.40 |
| 9:AI:128:ARG:CZ | 22:AV:6184:A:OP2 | 2.69 | 0.40 |
| 1:CA:979:C:P | 1:CA:981:U:O4 | 2.80 | 0.40 |
| 33:BK:75:SER:HB2 | 38:BP:75:ILE:O | 2.21 | 0.40 |
| 38:BP:57:PHE:CD2 | 38:BP:58:ASN:N | 2.89 | 0.40 |
| 34:DL:33:ARG:NE | 34:DL:36:LYS:CD | 2.77 | 0.40 |
| 42:BT:62:LYS:O | 42:BT:63:LYS:HD3 | 2.22 | 0.40 |
| 39:DQ:69:CYS:SG | 39:DQ:79:PHE:CD2 | 3.14 | 0.40 |
| 40:DR:49:THR:HB | 40:DR:50:PRO:CD | 2.51 | 0.40 |
| 1:AA:675:A:O2' | 11:AK:114:VAL:O | 2.38 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BA:1615:C:O2' | 23:BA:1617:C:H5'' | 2.22 | 0.40 |
| 53:B5:62:LEU:HA | 53:B5:62:LEU:HD23 | 1.32 | 0.40 |
| 37:DO:90:GLY:O | 37:DO:92:TYR:O | 2.40 | 0.40 |
| 23:DA:1799:G:O2' | 25:DC:181:GLU:OE2 | 2.38 | 0.40 |
| 1:AA:407:G:N3 | 1:AA:408:A:C8 | 2.90 | 0.40 |
| 23:DA:71:A:C2 | 42:DT:31:HIS:HE1 | 2.36 | 0.40 |
| 1:CA:80:G:H8 | 1:CA:80:G:OP2 | 2.04 | 0.40 |
| 35:BM:74:TYR:CE2 | 35:BM:91:GLU:HB2 | 2.52 | 0.40 |
| 20:CT:72:LEU:HD23 | 20:CT:72:LEU:C | 2.42 | 0.40 |
| 2:CB:80:ILE:HG22 | 2:CB:80:ILE:O | 2.22 | 0.40 |
| 24:BB:41:U:O4 | 28:BF:71:THR:HA | 2.21 | 0.40 |
| 4:AD:108:LEU:HD23 | 4:AD:110:PHE:CE2 | 2.56 | 0.40 |
| 24:DB:73:A:C5 | 24:DB:74:U:C6 | 3.10 | 0.40 |
| 44:DV:30:ASN:O | 44:DV:31:ARG:C | 2.59 | 0.40 |
| 44:DV:92:SER:HB2 | 44:DV:94:GLU:OE1 | 2.22 | 0.40 |
| 14:CN:23:ARG:HG3 | 14:CN:24:CYS:N | 2.36 | 0.40 |
| 5:CE:41:VAL:HG23 | 5:CE:67:VAL:HG13 | 2.04 | 0.40 |
| 1:CA:1252:A:H2' | 1:CA:1253:G:O4' | 2.22 | 0.40 |
| 1:CA:737:A:C5 | 1:CA:738:C:C5 | 3.09 | 0.40 |
| 23:BA:2516:G:C6 | 23:BA:2517:C:C4 | 3.09 | 0.40 |
| 23:BA:2517:C:C5 | 23:BA:2542:A:C2 | 3.10 | 0.40 |
| 23:BA:848:G:N9 | 23:BA:933:A:C8 | 2.89 | 0.40 |
| 43:DU:96:ILE:HD11 | 43:DU:99:CYS:HB2 | 2.03 | 0.40 |
| 1:CA:1292:U:O5' | 1:CA:1292:U:H6 | 2.04 | 0.40 |
| 41:DS:23:LEU:HD12 | 41:DS:23:LEU:HA | 1.79 | 0.40 |
| 41:DS:24:ILE:CG2 | 41:DS:36:LEU:CD2 | 3.00 | 0.40 |
| 6:AF:62:TRP:CD1 | 18:AR:35:ARG:NH1 | 2.89 | 0.40 |
| 26:BD:37:ARG:NH1 | 26:BD:42:ASP:OD1 | 2.55 | 0.40 |
| 5:CE:51:VAL:O | 5:CE:52:PRO:C | 2.60 | 0.40 |
| 25:BC:121:PRO:CB | 25:BC:135:PHE:CE2 | 3.00 | 0.40 |
| 25:DC:165:ILE:C | 25:DC:166:GLN:HE21 | 2.24 | 0.40 |
| 23:BA:2758:A:C2 | 23:BA:2759:G:C1' | 3.05 | 0.40 |
| 23:BA:1503:U:H2' | 23:BA:1504:C:H6 | 1.87 | 0.40 |
| 1:AA:658:G:O4' | 15:AO:22:THR:HB | 2.22 | 0.40 |
| 35:BM:85:LYS:HD2 | 35:BM:86:GLY:H | 1.85 | 0.40 |
| 23:DA:588:U:H1' | 27:DE:90:PHE:CG | 2.56 | 0.40 |
| 33:DK:112:MET:HA | 33:DK:115:VAL:HG13 | 2.03 | 0.40 |
| 18:CR:40:LEU:C | 18:CR:42:ARG:N | 2.74 | 0.40 |
| 23:DA:295:G:C5 | 23:DA:296:C:C5 | 3.09 | 0.40 |
| 30:DH:8:PRO:HA | 30:DH:14:ASP:HA | 2.03 | 0.40 |
| 43:BU:41:GLY:O | 43:BU:42:VAL:C | 2.60 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:914:A:OP2 | 1:AA:914:A:O4' | 2.39 | 0.40 |
| 1:AA:39:G:N2 | 1:AA:40:C:N1 | 2.69 | 0.40 |
| 23:DA:1478:G:C2 | 23:DA:1479:G:N7 | 2.90 | 0.40 |
| 18:CR:74:ARG:H | 18:CR:74:ARG:HG3 | 1.50 | 0.40 |
| 25:DC:176:ARG:CG | 25:DC:176:ARG:NH1 | 2.83 | 0.40 |
| 23:BA:2284:C:H1' | 23:BA:2325:G:N2 | 2.37 | 0.40 |
| 23:BA:1270:C:H5'' | 23:BA:1271:G:H5' | 2.04 | 0.40 |
| 21:AU:9:ARG:HG3 | 21:AU:10:ARG:N | 2.37 | 0.40 |
| 1:CA:1053:G:C5 | 1:CA:1199:U:C6 | 3.09 | 0.40 |
| 50:B2:40:LYS:HE2 | 50:B2:46:CYS:HB3 | 2.04 | 0.40 |
| 27:BE:199:TRP:CZ3 | 27:BE:203:GLN:HG3 | 2.57 | 0.40 |
| 27:BE:203:GLN:OE1 | 27:BE:207:GLY:CA | 2.69 | 0.40 |
| 28:BF:178:PHE:HA | 28:BF:179:PRO:HD3 | 1.68 | 0.40 |
| 28:BF:173:LEU:HB2 | 28:BF:180:PHE:HZ | 1.87 | 0.40 |
| 1:CA:922:G:H3' | 1:CA:923:A:C8 | 2.56 | 0.40 |
| 23:BA:774:A:C2' | 23:BA:775:G:OP2 | 2.68 | 0.40 |
| 1:AA:941:G:C2 | 1:AA:942:G:C8 | 3.09 | 0.40 |
| 1:AA:1232:U:H5'' | 9:AI:124:GLN:O | 2.21 | 0.40 |
| 23:DA:1747:G:C2 | 23:DA:1748:G:C8 | 3.10 | 0.40 |
| 23:BA:998:C:C2' | 23:BA:999:U:O5' | 2.69 | 0.40 |
| 23:DA:815:C:H2' | 23:DA:816:C:C6 | 2.56 | 0.40 |
| 23:DA:2872:G:C2 | 23:DA:2873:A:N6 | 2.89 | 0.40 |
| 35:BM:138:ASP:HB3 | 35:BM:139:GLU:H | 1.55 | 0.40 |
| 28:BF:11:TYR:HE2 | 28:BF:16:ARG:HH21 | 1.69 | 0.40 |
| 23:BA:1162:G:O4' | 40:BR:23:GLU:HG3 | 2.21 | 0.40 |
| 1:CA:490:G:H2' | 1:CA:491:G:H8 | 1.86 | 0.40 |
| 41:DS:65:LEU:HD23 | 41:DS:65:LEU:HA | 1.76 | 0.40 |
| 23:BA:2811:G:C6 | 23:BA:2891:G:N2 | 2.90 | 0.40 |
| 1:CA:754:C:O5' | 15:CO:72:ARG:NH2 | 2.55 | 0.40 |
| 23:DA:991:C:H2' | 23:DA:991:C:O2 | 2.22 | 0.40 |
| 1:AA:806:C:O2' | 1:AA:807:A:H5' | 2.21 | 0.40 |
| 24:BB:28:C:H3' | 24:BB:28:C:C6 | 2.57 | 0.40 |
| 41:BS:44:ALA:O | 41:BS:46:PHE:N | 2.54 | 0.40 |
| 23:DA:1442:G:C2 | 23:DA:1443:G:C4 | 3.09 | 0.40 |
| 23:BA:136:G:C6 | 23:BA:137(A):C:C5 | 3.10 | 0.40 |
| 23:BA:460:A:H2' | 23:BA:461:C:O4' | 2.21 | 0.40 |
| 1:AA:1166:G:N2 | 1:AA:1170:A:OP2 | 2.54 | 0.40 |
| 23:BA:270(Q):C:O2' | 23:BA:270(R):C:P | 2.79 | 0.40 |
| 1:AA:1501:C:C6 | 1:AA:1504:G:N7 | 2.90 | 0.40 |
| 1:AA:1399:C:N3 | 1:AA:1502:A:N1 | 2.69 | 0.40 |
| 44:DV:91:LEU:HD21 | 44:DV:96:VAL:HG11 | 2.02 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:425:G:C2' | 1:CA:426:G:H5' | 2.52 | 0.40 |
| 28:BF:15:VAL:HG22 | 28:BF:175:LEU:HB3 | 2.03 | 0.40 |
| 23:BA:2695:C:H2' | 23:BA:2696:U:C6 | 2.55 | 0.40 |
| 23:BA:245:G:N3 | 23:BA:246:C:C6 | 2.89 | 0.40 |
| 1:CA:892:A:O2' | 1:CA:1415:G:H4' | 2.22 | 0.40 |
| 23:DA:2194:G:C5 | 23:DA:2195:C:C5 | 3.09 | 0.40 |
| 23:BA:1632:A:N6 | 23:BA:1633:G:N1 | 2.70 | 0.40 |
| 17:AQ:14:LYS:H | 17:AQ:14:LYS:CD | 2.34 | 0.40 |
| 1:AA:929:G:C6 | 1:AA:930:C:C4 | 3.10 | 0.40 |
| 23:DA:1987:G:H2' | 23:DA:1988:C:H6 | 1.85 | 0.40 |
| 1:AA:702:A:O4' | 23:BA:1848:A:H1' | 2.22 | 0.40 |
| 23:BA:2404:C:C4 | 23:BA:2414:G:N1 | 2.89 | 0.40 |
| 1:CA:298:A:H2' | 1:CA:299:G:O4' | 2.22 | 0.40 |
| 1:AA:1419:G:C6 | 1:AA:1420:C:C4 | 3.09 | 0.40 |
| 38:BP:10:VAL:C | 38:BP:12:SER:N | 2.75 | 0.40 |
| 23:DA:14:A:H8 | 23:DA:14:A:O5' | 2.03 | 0.40 |
| 23:DA:1362:C:H3' | 23:DA:1362:C:C6 | 2.57 | 0.40 |
| 24:BB:1:U:O2 | 24:BB:1:U:H2' | 2.21 | 0.40 |
| 26:DD:152:LYS:HE3 | 26:DD:152:LYS:HB3 | 1.77 | 0.40 |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------------|--------------------------|-------------------|
| 6:AF:15:ASP:OD1 | 4:CD:20:TYR:OH[4_555] | 2.18 | 0.02 |

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|-----|-------|---------------|-----------|----------|----------|--------------------|
| 2 | AB | 232/234 (99%) | 172 (74%) | 40 (17%) | 20 (9%) | 1 10 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 2 | CB | 232/234 (99%) | 173 (75%) | 38 (16%) | 21 (9%) | 1 | 9 |
| 3 | AC | 204/206 (99%) | 136 (67%) | 43 (21%) | 25 (12%) | 0 | 5 |
| 3 | CC | 204/206 (99%) | 134 (66%) | 45 (22%) | 25 (12%) | 0 | 5 |
| 4 | AD | 206/208 (99%) | 152 (74%) | 38 (18%) | 16 (8%) | 1 | 12 |
| 4 | CD | 206/208 (99%) | 151 (73%) | 40 (19%) | 15 (7%) | 1 | 14 |
| 5 | AE | 149/151 (99%) | 103 (69%) | 34 (23%) | 12 (8%) | 1 | 11 |
| 5 | CE | 149/151 (99%) | 104 (70%) | 34 (23%) | 11 (7%) | 1 | 14 |
| 6 | AF | 99/101 (98%) | 71 (72%) | 17 (17%) | 11 (11%) | 0 | 6 |
| 6 | CF | 99/101 (98%) | 71 (72%) | 18 (18%) | 10 (10%) | 1 | 7 |
| 7 | AG | 153/155 (99%) | 121 (79%) | 27 (18%) | 5 (3%) | 5 | 37 |
| 7 | CG | 153/155 (99%) | 121 (79%) | 27 (18%) | 5 (3%) | 5 | 37 |
| 8 | AH | 136/138 (99%) | 97 (71%) | 29 (21%) | 10 (7%) | 1 | 14 |
| 8 | CH | 136/138 (99%) | 98 (72%) | 28 (21%) | 10 (7%) | 1 | 14 |
| 9 | AI | 125/127 (98%) | 91 (73%) | 31 (25%) | 3 (2%) | 7 | 44 |
| 9 | CI | 125/127 (98%) | 89 (71%) | 32 (26%) | 4 (3%) | 5 | 38 |
| 10 | AJ | 96/98 (98%) | 72 (75%) | 20 (21%) | 4 (4%) | 3 | 29 |
| 10 | CJ | 96/98 (98%) | 74 (77%) | 18 (19%) | 4 (4%) | 3 | 29 |
| 11 | AK | 117/119 (98%) | 83 (71%) | 29 (25%) | 5 (4%) | 3 | 29 |
| 11 | CK | 117/119 (98%) | 82 (70%) | 30 (26%) | 5 (4%) | 3 | 29 |
| 12 | AL | 122/124 (98%) | 78 (64%) | 28 (23%) | 16 (13%) | 0 | 4 |
| 12 | CL | 122/124 (98%) | 80 (66%) | 27 (22%) | 15 (12%) | 0 | 5 |
| 13 | AM | 114/116 (98%) | 93 (82%) | 17 (15%) | 4 (4%) | 4 | 35 |
| 13 | CM | 114/116 (98%) | 93 (82%) | 17 (15%) | 4 (4%) | 4 | 35 |
| 14 | AN | 58/60 (97%) | 46 (79%) | 9 (16%) | 3 (5%) | 2 | 23 |
| 14 | CN | 58/60 (97%) | 46 (79%) | 9 (16%) | 3 (5%) | 2 | 23 |
| 15 | AO | 86/88 (98%) | 62 (72%) | 17 (20%) | 7 (8%) | 1 | 11 |
| 15 | CO | 86/88 (98%) | 61 (71%) | 19 (22%) | 6 (7%) | 1 | 15 |
| 16 | AP | 81/83 (98%) | 46 (57%) | 24 (30%) | 11 (14%) | 0 | 3 |
| 16 | CP | 81/83 (98%) | 46 (57%) | 25 (31%) | 10 (12%) | 0 | 5 |
| 17 | AQ | 97/99 (98%) | 74 (76%) | 16 (16%) | 7 (7%) | 1 | 14 |
| 17 | CQ | 97/99 (98%) | 75 (77%) | 16 (16%) | 6 (6%) | 2 | 18 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 18 | AR | 68/70 (97%) | 40 (59%) | 19 (28%) | 9 (13%) | 0 | 4 |
| 18 | CR | 68/70 (97%) | 41 (60%) | 18 (26%) | 9 (13%) | 0 | 4 |
| 19 | AS | 76/78 (97%) | 51 (67%) | 21 (28%) | 4 (5%) | 2 | 22 |
| 19 | CS | 76/78 (97%) | 50 (66%) | 21 (28%) | 5 (7%) | 1 | 16 |
| 20 | AT | 97/99 (98%) | 67 (69%) | 23 (24%) | 7 (7%) | 1 | 14 |
| 20 | CT | 97/99 (98%) | 67 (69%) | 23 (24%) | 7 (7%) | 1 | 14 |
| 21 | AU | 22/24 (92%) | 13 (59%) | 8 (36%) | 1 (4%) | 3 | 27 |
| 21 | CU | 22/24 (92%) | 13 (59%) | 8 (36%) | 1 (4%) | 3 | 27 |
| 25 | BC | 269/271 (99%) | 213 (79%) | 36 (13%) | 20 (7%) | 1 | 14 |
| 25 | DC | 269/271 (99%) | 210 (78%) | 39 (14%) | 20 (7%) | 1 | 14 |
| 26 | BD | 202/204 (99%) | 154 (76%) | 34 (17%) | 14 (7%) | 1 | 15 |
| 26 | DD | 202/204 (99%) | 155 (77%) | 32 (16%) | 15 (7%) | 1 | 14 |
| 27 | BE | 200/202 (99%) | 152 (76%) | 32 (16%) | 16 (8%) | 1 | 12 |
| 27 | DE | 200/202 (99%) | 155 (78%) | 30 (15%) | 15 (8%) | 1 | 13 |
| 28 | BF | 179/181 (99%) | 136 (76%) | 31 (17%) | 12 (7%) | 1 | 16 |
| 28 | DF | 179/181 (99%) | 136 (76%) | 31 (17%) | 12 (7%) | 1 | 16 |
| 29 | BG | 157/159 (99%) | 112 (71%) | 35 (22%) | 10 (6%) | 2 | 17 |
| 29 | DG | 157/159 (99%) | 111 (71%) | 36 (23%) | 10 (6%) | 2 | 17 |
| 30 | BH | 143/145 (99%) | 95 (66%) | 29 (20%) | 19 (13%) | 0 | 4 |
| 30 | DH | 143/145 (99%) | 91 (64%) | 31 (22%) | 21 (15%) | 0 | 3 |
| 31 | BI | 28/65 (43%) | 25 (89%) | 3 (11%) | 0 | 100 | 100 |
| 31 | DI | 28/65 (43%) | 25 (89%) | 3 (11%) | 0 | 100 | 100 |
| 32 | BJ | 135/137 (98%) | 97 (72%) | 26 (19%) | 12 (9%) | 1 | 9 |
| 32 | DJ | 135/137 (98%) | 97 (72%) | 24 (18%) | 14 (10%) | 1 | 7 |
| 33 | BK | 120/122 (98%) | 100 (83%) | 11 (9%) | 9 (8%) | 1 | 13 |
| 33 | DK | 120/122 (98%) | 98 (82%) | 14 (12%) | 8 (7%) | 1 | 16 |
| 34 | BL | 144/146 (99%) | 87 (60%) | 31 (22%) | 26 (18%) | 0 | 1 |
| 34 | DL | 144/146 (99%) | 86 (60%) | 35 (24%) | 23 (16%) | 0 | 2 |
| 35 | BM | 134/136 (98%) | 86 (64%) | 28 (21%) | 20 (15%) | 0 | 2 |
| 35 | DM | 134/136 (98%) | 86 (64%) | 30 (22%) | 18 (13%) | 0 | 4 |
| 36 | BN | 115/117 (98%) | 91 (79%) | 13 (11%) | 11 (10%) | 1 | 8 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 36 | DN | 115/117 (98%) | 90 (78%) | 15 (13%) | 10 (9%) | 1 | 10 |
| 37 | BO | 96/98 (98%) | 57 (59%) | 23 (24%) | 16 (17%) | 0 | 2 |
| 37 | DO | 96/98 (98%) | 54 (56%) | 25 (26%) | 17 (18%) | 0 | 2 |
| 38 | BP | 135/137 (98%) | 101 (75%) | 18 (13%) | 16 (12%) | 0 | 5 |
| 38 | DP | 135/137 (98%) | 100 (74%) | 19 (14%) | 16 (12%) | 0 | 5 |
| 39 | BQ | 114/116 (98%) | 78 (68%) | 22 (19%) | 14 (12%) | 0 | 5 |
| 39 | DQ | 114/116 (98%) | 82 (72%) | 20 (18%) | 12 (10%) | 1 | 7 |
| 40 | BR | 99/101 (98%) | 70 (71%) | 20 (20%) | 9 (9%) | 1 | 9 |
| 40 | DR | 99/101 (98%) | 70 (71%) | 20 (20%) | 9 (9%) | 1 | 9 |
| 41 | BS | 110/112 (98%) | 88 (80%) | 17 (16%) | 5 (4%) | 3 | 27 |
| 41 | DS | 110/112 (98%) | 87 (79%) | 17 (16%) | 6 (6%) | 2 | 21 |
| 42 | BT | 90/92 (98%) | 69 (77%) | 16 (18%) | 5 (6%) | 2 | 21 |
| 42 | DT | 90/92 (98%) | 67 (74%) | 18 (20%) | 5 (6%) | 2 | 21 |
| 43 | BU | 98/100 (98%) | 55 (56%) | 24 (24%) | 19 (19%) | 0 | 1 |
| 43 | DU | 98/100 (98%) | 58 (59%) | 21 (21%) | 19 (19%) | 0 | 1 |
| 44 | BV | 186/188 (99%) | 135 (73%) | 34 (18%) | 17 (9%) | 1 | 9 |
| 44 | DV | 186/188 (99%) | 135 (73%) | 34 (18%) | 17 (9%) | 1 | 9 |
| 45 | BW | 74/76 (97%) | 61 (82%) | 10 (14%) | 3 (4%) | 3 | 30 |
| 45 | DW | 74/76 (97%) | 60 (81%) | 10 (14%) | 4 (5%) | 2 | 22 |
| 46 | BX | 86/88 (98%) | 57 (66%) | 16 (19%) | 13 (15%) | 0 | 2 |
| 46 | DX | 86/88 (98%) | 54 (63%) | 19 (22%) | 13 (15%) | 0 | 2 |
| 47 | BY | 60/62 (97%) | 45 (75%) | 8 (13%) | 7 (12%) | 0 | 5 |
| 47 | DY | 60/62 (97%) | 41 (68%) | 12 (20%) | 7 (12%) | 0 | 5 |
| 48 | BZ | 57/59 (97%) | 49 (86%) | 7 (12%) | 1 (2%) | 11 | 50 |
| 48 | DZ | 57/59 (97%) | 50 (88%) | 6 (10%) | 1 (2%) | 11 | 50 |
| 49 | B1 | 28/30 (93%) | 15 (54%) | 7 (25%) | 6 (21%) | 0 | 1 |
| 49 | D1 | 28/30 (93%) | 15 (54%) | 7 (25%) | 6 (21%) | 0 | 1 |
| 50 | B2 | 50/52 (96%) | 40 (80%) | 6 (12%) | 4 (8%) | 1 | 12 |
| 50 | D2 | 50/52 (96%) | 39 (78%) | 7 (14%) | 4 (8%) | 1 | 12 |
| 51 | B3 | 42/44 (96%) | 26 (62%) | 11 (26%) | 5 (12%) | 0 | 5 |
| 51 | D3 | 42/44 (96%) | 26 (62%) | 11 (26%) | 5 (12%) | 0 | 5 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|------------|------------|----------|-------------|----|
| 52 | B4 | 46/48 (96%) | 42 (91%) | 3 (6%) | 1 (2%) | 8 | 46 |
| 52 | D4 | 46/48 (96%) | 42 (91%) | 3 (6%) | 1 (2%) | 8 | 46 |
| 53 | B5 | 61/63 (97%) | 43 (70%) | 12 (20%) | 6 (10%) | 1 | 8 |
| 53 | D5 | 61/63 (97%) | 44 (72%) | 10 (16%) | 7 (12%) | 0 | 5 |
| All | All | 11192/11458 (98%) | 8080 (72%) | 2125 (19%) | 987 (9%) | 1 | 10 |

All (987) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 204 | ASN |
| 3 | AC | 189 | ALA |
| 3 | AC | 196 | LEU |
| 4 | AD | 28 | SER |
| 4 | AD | 30 | LYS |
| 5 | AE | 37 | ARG |
| 5 | AE | 140 | ARG |
| 6 | AF | 6 | VAL |
| 6 | AF | 36 | ARG |
| 6 | AF | 39 | LYS |
| 6 | AF | 42 | GLU |
| 6 | AF | 87 | ARG |
| 10 | AJ | 92 | THR |
| 11 | AK | 27 | ASN |
| 12 | AL | 50 | ALA |
| 12 | AL | 63 | TYR |
| 12 | AL | 117 | SER |
| 13 | AM | 106 | ASN |
| 15 | AO | 29 | VAL |
| 16 | AP | 11 | SER |
| 16 | AP | 19 | ILE |
| 17 | AQ | 79 | SER |
| 17 | AQ | 99 | SER |
| 18 | AR | 20 | ALA |
| 19 | AS | 28 | LYS |
| 20 | AT | 71 | THR |
| 20 | AT | 99 | LEU |
| 25 | BC | 26 | LYS |
| 25 | BC | 33 | LEU |
| 25 | BC | 34 | VAL |
| 25 | BC | 236 | GLY |
| 25 | BC | 237 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | BC | 271 | ILE |
| 26 | BD | 2 | LYS |
| 26 | BD | 17 | ASP |
| 27 | BE | 89 | VAL |
| 27 | BE | 128 | ALA |
| 27 | BE | 168 | ARG |
| 28 | BF | 86 | MET |
| 28 | BF | 87 | PRO |
| 29 | BG | 92 | ILE |
| 29 | BG | 165 | ALA |
| 30 | BH | 10 | GLU |
| 30 | BH | 82 | ARG |
| 30 | BH | 132 | PRO |
| 30 | BH | 142 | VAL |
| 30 | BH | 143 | SER |
| 32 | BJ | 149 | PRO |
| 32 | BJ | 155 | ALA |
| 32 | BJ | 157 | ARG |
| 33 | BK | 4 | PRO |
| 33 | BK | 27 | GLY |
| 33 | BK | 29 | ASN |
| 33 | BK | 91 | LEU |
| 33 | BK | 101 | PRO |
| 34 | BL | 11 | GLY |
| 34 | BL | 15 | ARG |
| 34 | BL | 17 | LYS |
| 34 | BL | 36 | LYS |
| 34 | BL | 39 | LYS |
| 34 | BL | 49 | ARG |
| 34 | BL | 50 | ARG |
| 34 | BL | 65 | ARG |
| 34 | BL | 110 | TYR |
| 34 | BL | 141 | ALA |
| 34 | BL | 147 | LEU |
| 35 | BM | 8 | LYS |
| 35 | BM | 13 | GLN |
| 35 | BM | 18 | LYS |
| 35 | BM | 21 | THR |
| 35 | BM | 25 | ASP |
| 35 | BM | 30 | GLY |
| 35 | BM | 82 | ARG |
| 35 | BM | 134 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35 | BM | 135 | ASP |
| 36 | BN | 3 | HIS |
| 36 | BN | 5 | LYS |
| 36 | BN | 6 | SER |
| 36 | BN | 12 | ARG |
| 36 | BN | 86 | ARG |
| 37 | BO | 12 | PHE |
| 37 | BO | 35 | ILE |
| 37 | BO | 44 | LYS |
| 37 | BO | 52 | SER |
| 37 | BO | 53 | SER |
| 37 | BO | 59 | LYS |
| 38 | BP | 58 | ASN |
| 38 | BP | 89 | VAL |
| 38 | BP | 90 | GLN |
| 38 | BP | 107 | ASP |
| 38 | BP | 136 | GLN |
| 39 | BQ | 9 | VAL |
| 39 | BQ | 31 | SER |
| 39 | BQ | 33 | ARG |
| 39 | BQ | 99 | ALA |
| 40 | BR | 35 | LEU |
| 40 | BR | 78 | LYS |
| 43 | BU | 7 | VAL |
| 43 | BU | 49 | VAL |
| 43 | BU | 76 | CYS |
| 43 | BU | 88 | LYS |
| 44 | BV | 31 | ARG |
| 44 | BV | 93 | ASP |
| 44 | BV | 177 | PRO |
| 45 | BW | 47 | PRO |
| 46 | BX | 10 | LYS |
| 46 | BX | 11 | ARG |
| 46 | BX | 32 | LYS |
| 46 | BX | 85 | LEU |
| 47 | BY | 3 | LEU |
| 47 | BY | 44 | LEU |
| 48 | BZ | 13 | ILE |
| 49 | B1 | 44 | CYS |
| 49 | B1 | 52 | SER |
| 50 | B2 | 4 | HIS |
| 50 | B2 | 35 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50 | B2 | 49 | CYS |
| 51 | B3 | 28 | ARG |
| 51 | B3 | 51 | GLU |
| 53 | B5 | 31 | HIS |
| 53 | B5 | 34 | TRP |
| 53 | B5 | 51 | ALA |
| 53 | B5 | 62 | LEU |
| 2 | CB | 204 | ASN |
| 3 | CC | 189 | ALA |
| 3 | CC | 196 | LEU |
| 4 | CD | 30 | LYS |
| 5 | CE | 37 | ARG |
| 5 | CE | 140 | ARG |
| 6 | CF | 6 | VAL |
| 6 | CF | 36 | ARG |
| 6 | CF | 39 | LYS |
| 6 | CF | 42 | GLU |
| 6 | CF | 87 | ARG |
| 10 | CJ | 92 | THR |
| 11 | CK | 27 | ASN |
| 11 | CK | 122 | LYS |
| 12 | CL | 50 | ALA |
| 12 | CL | 63 | TYR |
| 12 | CL | 117 | SER |
| 13 | CM | 106 | ASN |
| 15 | CO | 29 | VAL |
| 16 | CP | 11 | SER |
| 16 | CP | 19 | ILE |
| 17 | CQ | 79 | SER |
| 17 | CQ | 99 | SER |
| 18 | CR | 20 | ALA |
| 19 | CS | 28 | LYS |
| 20 | CT | 71 | THR |
| 20 | CT | 99 | LEU |
| 25 | DC | 26 | LYS |
| 25 | DC | 33 | LEU |
| 25 | DC | 34 | VAL |
| 25 | DC | 271 | ILE |
| 26 | DD | 2 | LYS |
| 26 | DD | 17 | ASP |
| 26 | DD | 86 | PRO |
| 27 | DE | 68 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27 | DE | 89 | VAL |
| 27 | DE | 128 | ALA |
| 27 | DE | 168 | ARG |
| 28 | DF | 86 | MET |
| 28 | DF | 87 | PRO |
| 29 | DG | 92 | ILE |
| 29 | DG | 165 | ALA |
| 30 | DH | 10 | GLU |
| 30 | DH | 15 | VAL |
| 30 | DH | 82 | ARG |
| 30 | DH | 132 | PRO |
| 30 | DH | 142 | VAL |
| 30 | DH | 143 | SER |
| 32 | DJ | 81 | ASP |
| 32 | DJ | 149 | PRO |
| 32 | DJ | 155 | ALA |
| 32 | DJ | 157 | ARG |
| 33 | DK | 27 | GLY |
| 33 | DK | 29 | ASN |
| 33 | DK | 101 | PRO |
| 34 | DL | 15 | ARG |
| 34 | DL | 17 | LYS |
| 34 | DL | 36 | LYS |
| 34 | DL | 39 | LYS |
| 34 | DL | 49 | ARG |
| 34 | DL | 50 | ARG |
| 34 | DL | 65 | ARG |
| 34 | DL | 110 | TYR |
| 34 | DL | 141 | ALA |
| 34 | DL | 147 | LEU |
| 35 | DM | 8 | LYS |
| 35 | DM | 13 | GLN |
| 35 | DM | 21 | THR |
| 35 | DM | 25 | ASP |
| 35 | DM | 30 | GLY |
| 35 | DM | 82 | ARG |
| 35 | DM | 134 | ARG |
| 36 | DN | 3 | HIS |
| 36 | DN | 5 | LYS |
| 36 | DN | 6 | SER |
| 36 | DN | 12 | ARG |
| 36 | DN | 86 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 37 | DO | 12 | PHE |
| 37 | DO | 35 | ILE |
| 37 | DO | 44 | LYS |
| 37 | DO | 52 | SER |
| 37 | DO | 53 | SER |
| 37 | DO | 59 | LYS |
| 38 | DP | 58 | ASN |
| 38 | DP | 89 | VAL |
| 38 | DP | 90 | GLN |
| 38 | DP | 97 | ALA |
| 38 | DP | 107 | ASP |
| 38 | DP | 136 | GLN |
| 39 | DQ | 9 | VAL |
| 39 | DQ | 31 | SER |
| 39 | DQ | 33 | ARG |
| 39 | DQ | 99 | ALA |
| 40 | DR | 35 | LEU |
| 40 | DR | 78 | LYS |
| 43 | DU | 7 | VAL |
| 43 | DU | 17 | SER |
| 43 | DU | 49 | VAL |
| 43 | DU | 76 | CYS |
| 43 | DU | 88 | LYS |
| 44 | DV | 31 | ARG |
| 44 | DV | 93 | ASP |
| 44 | DV | 177 | PRO |
| 45 | DW | 47 | PRO |
| 45 | DW | 74 | ARG |
| 46 | DX | 11 | ARG |
| 46 | DX | 13 | ILE |
| 46 | DX | 32 | LYS |
| 46 | DX | 85 | LEU |
| 47 | DY | 3 | LEU |
| 47 | DY | 44 | LEU |
| 48 | DZ | 13 | ILE |
| 49 | D1 | 44 | CYS |
| 49 | D1 | 52 | SER |
| 50 | D2 | 4 | HIS |
| 50 | D2 | 35 | GLU |
| 50 | D2 | 49 | CYS |
| 51 | D3 | 28 | ARG |
| 51 | D3 | 51 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53 | D5 | 31 | HIS |
| 53 | D5 | 34 | TRP |
| 53 | D5 | 51 | ALA |
| 53 | D5 | 62 | LEU |
| 2 | AB | 14 | GLY |
| 2 | AB | 19 | HIS |
| 2 | AB | 24 | TRP |
| 2 | AB | 129 | GLU |
| 2 | AB | 176 | GLU |
| 2 | AB | 205 | ASP |
| 2 | AB | 229 | VAL |
| 3 | AC | 14 | ILE |
| 3 | AC | 22 | TRP |
| 3 | AC | 56 | ASP |
| 3 | AC | 100 | ALA |
| 3 | AC | 144 | SER |
| 3 | AC | 188 | LEU |
| 4 | AD | 4 | TYR |
| 4 | AD | 110 | PHE |
| 4 | AD | 145 | GLU |
| 4 | AD | 171 | GLY |
| 6 | AF | 2 | ARG |
| 6 | AF | 89 | MET |
| 7 | AG | 4 | ARG |
| 8 | AH | 2 | LEU |
| 8 | AH | 133 | LEU |
| 9 | AI | 31 | GLN |
| 10 | AJ | 59 | SER |
| 11 | AK | 122 | LYS |
| 12 | AL | 22 | LYS |
| 12 | AL | 27 | LYS |
| 12 | AL | 64 | GLU |
| 15 | AO | 6 | GLU |
| 15 | AO | 19 | PRO |
| 16 | AP | 10 | GLY |
| 16 | AP | 16 | HIS |
| 16 | AP | 26 | ARG |
| 16 | AP | 48 | TRP |
| 16 | AP | 64 | ALA |
| 18 | AR | 45 | SER |
| 18 | AR | 54 | ARG |
| 18 | AR | 57 | GLY |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 19 | AS | 11 | VAL |
| 20 | AT | 11 | SER |
| 20 | AT | 42 | GLN |
| 20 | AT | 74 | LYS |
| 21 | AU | 9 | ARG |
| 25 | BC | 169 | GLU |
| 25 | BC | 261 | LYS |
| 25 | BC | 268 | ARG |
| 26 | BD | 29 | GLY |
| 26 | BD | 86 | PRO |
| 27 | BE | 19 | GLU |
| 27 | BE | 68 | LYS |
| 27 | BE | 132 | VAL |
| 28 | BF | 26 | GLN |
| 28 | BF | 96 | ARG |
| 28 | BF | 115 | ARG |
| 29 | BG | 21 | PRO |
| 29 | BG | 138 | LYS |
| 30 | BH | 15 | VAL |
| 30 | BH | 16 | GLY |
| 30 | BH | 74 | ASN |
| 30 | BH | 91 | SER |
| 30 | BH | 92 | VAL |
| 32 | BJ | 81 | ASP |
| 32 | BJ | 89 | LYS |
| 34 | BL | 32 | THR |
| 34 | BL | 137 | LYS |
| 35 | BM | 47 | ILE |
| 35 | BM | 136 | ALA |
| 35 | BM | 140 | ALA |
| 36 | BN | 8 | ARG |
| 37 | BO | 57 | LYS |
| 37 | BO | 82 | ILE |
| 37 | BO | 90 | GLY |
| 37 | BO | 95 | HIS |
| 38 | BP | 2 | ASN |
| 38 | BP | 36 | GLU |
| 38 | BP | 57 | PHE |
| 38 | BP | 97 | ALA |
| 38 | BP | 106 | SER |
| 38 | BP | 115 | ARG |
| 38 | BP | 126 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38 | BP | 127 | ALA |
| 39 | BQ | 54 | LYS |
| 39 | BQ | 98 | LEU |
| 39 | BQ | 117 | GLN |
| 40 | BR | 46 | VAL |
| 40 | BR | 100 | ARG |
| 41 | BS | 61 | ASN |
| 41 | BS | 63 | ASP |
| 43 | BU | 3 | VAL |
| 43 | BU | 11 | ASP |
| 43 | BU | 17 | SER |
| 43 | BU | 69 | ALA |
| 43 | BU | 98 | VAL |
| 44 | BV | 80 | ARG |
| 44 | BV | 135 | GLU |
| 44 | BV | 178 | GLU |
| 45 | BW | 74 | ARG |
| 46 | BX | 13 | ILE |
| 47 | BY | 43 | GLN |
| 47 | BY | 61 | LEU |
| 2 | CB | 14 | GLY |
| 2 | CB | 18 | GLY |
| 2 | CB | 19 | HIS |
| 2 | CB | 24 | TRP |
| 2 | CB | 129 | GLU |
| 2 | CB | 176 | GLU |
| 2 | CB | 205 | ASP |
| 2 | CB | 229 | VAL |
| 3 | CC | 14 | ILE |
| 3 | CC | 22 | TRP |
| 3 | CC | 56 | ASP |
| 3 | CC | 100 | ALA |
| 3 | CC | 144 | SER |
| 3 | CC | 188 | LEU |
| 4 | CD | 4 | TYR |
| 4 | CD | 28 | SER |
| 4 | CD | 110 | PHE |
| 4 | CD | 145 | GLU |
| 4 | CD | 171 | GLY |
| 5 | CE | 85 | GLY |
| 6 | CF | 2 | ARG |
| 6 | CF | 89 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | CG | 4 | ARG |
| 8 | CH | 2 | LEU |
| 8 | CH | 133 | LEU |
| 9 | CI | 31 | GLN |
| 10 | CJ | 57 | LYS |
| 10 | CJ | 59 | SER |
| 12 | CL | 22 | LYS |
| 12 | CL | 27 | LYS |
| 12 | CL | 64 | GLU |
| 12 | CL | 78 | GLU |
| 13 | CM | 4 | ILE |
| 15 | CO | 6 | GLU |
| 16 | CP | 10 | GLY |
| 16 | CP | 16 | HIS |
| 16 | CP | 26 | ARG |
| 16 | CP | 48 | TRP |
| 16 | CP | 64 | ALA |
| 18 | CR | 54 | ARG |
| 18 | CR | 57 | GLY |
| 19 | CS | 11 | VAL |
| 20 | CT | 11 | SER |
| 21 | CU | 9 | ARG |
| 25 | DC | 43 | ARG |
| 25 | DC | 125 | ILE |
| 25 | DC | 134 | ARG |
| 25 | DC | 169 | GLU |
| 25 | DC | 236 | GLY |
| 25 | DC | 237 | GLU |
| 25 | DC | 261 | LYS |
| 25 | DC | 268 | ARG |
| 26 | DD | 29 | GLY |
| 27 | DE | 19 | GLU |
| 27 | DE | 132 | VAL |
| 28 | DF | 26 | GLN |
| 28 | DF | 96 | ARG |
| 28 | DF | 115 | ARG |
| 29 | DG | 21 | PRO |
| 29 | DG | 138 | LYS |
| 30 | DH | 16 | GLY |
| 30 | DH | 74 | ASN |
| 30 | DH | 91 | SER |
| 30 | DH | 92 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 32 | DJ | 89 | LYS |
| 33 | DK | 91 | LEU |
| 34 | DL | 11 | GLY |
| 34 | DL | 42 | SER |
| 34 | DL | 52 | GLU |
| 34 | DL | 136 | GLU |
| 34 | DL | 137 | LYS |
| 35 | DM | 18 | LYS |
| 35 | DM | 47 | ILE |
| 35 | DM | 135 | ASP |
| 35 | DM | 136 | ALA |
| 35 | DM | 140 | ALA |
| 37 | DO | 57 | LYS |
| 37 | DO | 82 | ILE |
| 37 | DO | 85 | VAL |
| 37 | DO | 89 | ARG |
| 37 | DO | 90 | GLY |
| 37 | DO | 95 | HIS |
| 38 | DP | 2 | ASN |
| 38 | DP | 4 | GLY |
| 38 | DP | 36 | GLU |
| 38 | DP | 57 | PHE |
| 38 | DP | 106 | SER |
| 38 | DP | 115 | ARG |
| 38 | DP | 126 | ALA |
| 38 | DP | 127 | ALA |
| 39 | DQ | 117 | GLN |
| 40 | DR | 46 | VAL |
| 40 | DR | 100 | ARG |
| 41 | DS | 48 | ALA |
| 41 | DS | 61 | ASN |
| 43 | DU | 3 | VAL |
| 43 | DU | 98 | VAL |
| 44 | DV | 80 | ARG |
| 44 | DV | 135 | GLU |
| 44 | DV | 178 | GLU |
| 45 | DW | 57 | PHE |
| 46 | DX | 10 | LYS |
| 46 | DX | 38 | SER |
| 47 | DY | 43 | GLN |
| 47 | DY | 61 | LEU |
| 2 | AB | 18 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 88 | ALA |
| 2 | AB | 130 | ARG |
| 2 | AB | 183 | PRO |
| 2 | AB | 206 | ASP |
| 2 | AB | 235 | SER |
| 3 | AC | 15 | THR |
| 3 | AC | 47 | LEU |
| 3 | AC | 60 | ALA |
| 3 | AC | 81 | GLY |
| 3 | AC | 91 | LEU |
| 3 | AC | 127 | ARG |
| 4 | AD | 105 | VAL |
| 5 | AE | 21 | ALA |
| 5 | AE | 49 | PRO |
| 5 | AE | 85 | GLY |
| 7 | AG | 14 | PRO |
| 8 | AH | 77 | GLU |
| 8 | AH | 98 | LYS |
| 8 | AH | 112 | LEU |
| 8 | AH | 119 | LEU |
| 10 | AJ | 57 | LYS |
| 12 | AL | 11 | ARG |
| 12 | AL | 61 | SER |
| 12 | AL | 78 | GLU |
| 12 | AL | 88 | ARG |
| 13 | AM | 4 | ILE |
| 15 | AO | 21 | ASP |
| 16 | AP | 77 | ALA |
| 17 | AQ | 78 | GLU |
| 17 | AQ | 80 | GLY |
| 20 | AT | 84 | LEU |
| 25 | BC | 35 | LYS |
| 25 | BC | 42 | GLY |
| 25 | BC | 43 | ARG |
| 25 | BC | 115 | GLN |
| 25 | BC | 125 | ILE |
| 25 | BC | 134 | ARG |
| 26 | BD | 159 | HIS |
| 27 | BE | 66 | PRO |
| 27 | BE | 86 | GLY |
| 27 | BE | 145 | GLU |
| 27 | BE | 176 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28 | BF | 14 | GLU |
| 28 | BF | 148 | MET |
| 29 | BG | 80 | SER |
| 29 | BG | 155 | SER |
| 30 | BH | 30 | LEU |
| 30 | BH | 77 | LEU |
| 30 | BH | 99 | GLU |
| 30 | BH | 144 | VAL |
| 32 | BJ | 152 | PRO |
| 34 | BL | 12 | ALA |
| 34 | BL | 42 | SER |
| 34 | BL | 43 | GLY |
| 34 | BL | 52 | GLU |
| 34 | BL | 90 | ARG |
| 34 | BL | 136 | GLU |
| 35 | BM | 10 | ARG |
| 35 | BM | 22 | LYS |
| 35 | BM | 54 | MET |
| 36 | BN | 32 | GLY |
| 37 | BO | 83 | LYS |
| 37 | BO | 85 | VAL |
| 37 | BO | 89 | ARG |
| 37 | BO | 91 | PRO |
| 39 | BQ | 93 | LYS |
| 39 | BQ | 96 | ALA |
| 40 | BR | 61 | VAL |
| 42 | BT | 72 | LYS |
| 43 | BU | 42 | VAL |
| 43 | BU | 90 | LEU |
| 43 | BU | 99 | CYS |
| 44 | BV | 38 | TYR |
| 44 | BV | 117 | LEU |
| 44 | BV | 142 | SER |
| 44 | BV | 153 | SER |
| 45 | BW | 57 | PHE |
| 46 | BX | 56 | GLN |
| 46 | BX | 83 | GLU |
| 47 | BY | 17 | SER |
| 50 | B2 | 46 | CYS |
| 51 | B3 | 31 | PRO |
| 51 | B3 | 32 | ASN |
| 51 | B3 | 46 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53 | B5 | 3 | LYS |
| 2 | CB | 88 | ALA |
| 2 | CB | 130 | ARG |
| 2 | CB | 150 | SER |
| 2 | CB | 206 | ASP |
| 2 | CB | 235 | SER |
| 3 | CC | 15 | THR |
| 3 | CC | 47 | LEU |
| 3 | CC | 60 | ALA |
| 3 | CC | 81 | GLY |
| 3 | CC | 105 | GLU |
| 3 | CC | 127 | ARG |
| 5 | CE | 72 | GLN |
| 5 | CE | 128 | PRO |
| 7 | CG | 14 | PRO |
| 8 | CH | 87 | SER |
| 8 | CH | 98 | LYS |
| 8 | CH | 112 | LEU |
| 8 | CH | 119 | LEU |
| 12 | CL | 61 | SER |
| 14 | CN | 18 | VAL |
| 15 | CO | 19 | PRO |
| 15 | CO | 21 | ASP |
| 16 | CP | 77 | ALA |
| 17 | CQ | 78 | GLU |
| 17 | CQ | 80 | GLY |
| 18 | CR | 45 | SER |
| 20 | CT | 42 | GLN |
| 20 | CT | 74 | LYS |
| 25 | DC | 35 | LYS |
| 25 | DC | 37 | LEU |
| 25 | DC | 42 | GLY |
| 25 | DC | 239 | ARG |
| 26 | DD | 69 | LYS |
| 26 | DD | 159 | HIS |
| 26 | DD | 185 | LYS |
| 27 | DE | 86 | GLY |
| 27 | DE | 134 | GLY |
| 27 | DE | 145 | GLU |
| 27 | DE | 176 | LEU |
| 28 | DF | 14 | GLU |
| 28 | DF | 148 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29 | DG | 80 | SER |
| 29 | DG | 155 | SER |
| 30 | DH | 30 | LEU |
| 30 | DH | 39 | ALA |
| 30 | DH | 77 | LEU |
| 30 | DH | 99 | GLU |
| 32 | DJ | 124 | HIS |
| 32 | DJ | 152 | PRO |
| 33 | DK | 4 | PRO |
| 34 | DL | 108 | LYS |
| 35 | DM | 10 | ARG |
| 35 | DM | 62 | GLY |
| 36 | DN | 8 | ARG |
| 39 | DQ | 8 | VAL |
| 39 | DQ | 54 | LYS |
| 39 | DQ | 96 | ALA |
| 39 | DQ | 98 | LEU |
| 40 | DR | 53 | GLU |
| 40 | DR | 61 | VAL |
| 41 | DS | 49 | LYS |
| 41 | DS | 64 | MET |
| 42 | DT | 41 | ASN |
| 42 | DT | 87 | GLN |
| 43 | DU | 11 | ASP |
| 43 | DU | 39 | VAL |
| 43 | DU | 42 | VAL |
| 43 | DU | 69 | ALA |
| 43 | DU | 90 | LEU |
| 43 | DU | 99 | CYS |
| 44 | DV | 38 | TYR |
| 44 | DV | 39 | VAL |
| 44 | DV | 117 | LEU |
| 44 | DV | 142 | SER |
| 44 | DV | 153 | SER |
| 46 | DX | 9 | GLY |
| 46 | DX | 56 | GLN |
| 46 | DX | 83 | GLU |
| 47 | DY | 17 | SER |
| 47 | DY | 47 | ASN |
| 49 | D1 | 62 | CYS |
| 50 | D2 | 46 | CYS |
| 51 | D3 | 31 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51 | D3 | 32 | ASN |
| 51 | D3 | 46 | HIS |
| 53 | D5 | 3 | LYS |
| 2 | AB | 150 | SER |
| 2 | AB | 182 | ILE |
| 2 | AB | 224 | GLN |
| 3 | AC | 18 | TRP |
| 3 | AC | 45 | LYS |
| 3 | AC | 61 | ALA |
| 3 | AC | 105 | GLU |
| 3 | AC | 145 | GLY |
| 4 | AD | 10 | ARG |
| 5 | AE | 62 | ALA |
| 5 | AE | 72 | GLN |
| 5 | AE | 104 | ALA |
| 5 | AE | 128 | PRO |
| 6 | AF | 38 | GLU |
| 10 | AJ | 78 | ASN |
| 11 | AK | 39 | PRO |
| 12 | AL | 28 | GLY |
| 12 | AL | 86 | GLY |
| 13 | AM | 116 | THR |
| 14 | AN | 18 | VAL |
| 15 | AO | 23 | GLY |
| 17 | AQ | 33 | GLY |
| 17 | AQ | 34 | LYS |
| 18 | AR | 41 | LYS |
| 19 | AS | 25 | LYS |
| 25 | BC | 37 | LEU |
| 25 | BC | 224 | ALA |
| 25 | BC | 239 | ARG |
| 25 | BC | 256 | GLY |
| 26 | BD | 60 | ASN |
| 26 | BD | 87 | GLU |
| 26 | BD | 178 | GLU |
| 26 | BD | 185 | LYS |
| 27 | BE | 48 | THR |
| 27 | BE | 127 | GLU |
| 28 | BF | 24 | GLY |
| 28 | BF | 25 | TYR |
| 28 | BF | 46 | ALA |
| 29 | BG | 107 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 30 | BH | 7 | GLU |
| 30 | BH | 60 | GLU |
| 32 | BJ | 156 | GLN |
| 32 | BJ | 158 | PRO |
| 33 | BK | 21 | CYS |
| 33 | BK | 97 | ARG |
| 34 | BL | 47 | ASP |
| 34 | BL | 70 | GLN |
| 34 | BL | 109 | GLY |
| 37 | BO | 62 | LYS |
| 38 | BP | 4 | GLY |
| 40 | BR | 48 | GLY |
| 40 | BR | 53 | GLU |
| 41 | BS | 48 | ALA |
| 41 | BS | 64 | MET |
| 42 | BT | 40 | LYS |
| 42 | BT | 41 | ASN |
| 42 | BT | 87 | GLN |
| 43 | BU | 39 | VAL |
| 43 | BU | 80 | GLY |
| 44 | BV | 39 | VAL |
| 44 | BV | 101 | PRO |
| 46 | BX | 9 | GLY |
| 49 | B1 | 41 | ILE |
| 49 | B1 | 54 | LYS |
| 49 | B1 | 62 | CYS |
| 52 | B4 | 47 | ARG |
| 53 | B5 | 61 | LEU |
| 2 | CB | 224 | GLN |
| 3 | CC | 18 | TRP |
| 3 | CC | 61 | ALA |
| 3 | CC | 91 | LEU |
| 3 | CC | 145 | GLY |
| 3 | CC | 164 | ARG |
| 4 | CD | 147 | ALA |
| 5 | CE | 49 | PRO |
| 5 | CE | 104 | ALA |
| 5 | CE | 107 | ARG |
| 6 | CF | 38 | GLU |
| 8 | CH | 77 | GLU |
| 11 | CK | 39 | PRO |
| 12 | CL | 11 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | CL | 28 | GLY |
| 12 | CL | 86 | GLY |
| 13 | CM | 116 | THR |
| 14 | CN | 58 | LYS |
| 15 | CO | 23 | GLY |
| 17 | CQ | 34 | LYS |
| 18 | CR | 36 | ASN |
| 19 | CS | 25 | LYS |
| 20 | CT | 84 | LEU |
| 25 | DC | 115 | GLN |
| 25 | DC | 256 | GLY |
| 26 | DD | 60 | ASN |
| 26 | DD | 87 | GLU |
| 26 | DD | 94 | GLU |
| 26 | DD | 127 | ASP |
| 26 | DD | 178 | GLU |
| 27 | DE | 127 | GLU |
| 28 | DF | 24 | GLY |
| 28 | DF | 25 | TYR |
| 29 | DG | 107 | VAL |
| 30 | DH | 7 | GLU |
| 30 | DH | 86 | THR |
| 30 | DH | 144 | VAL |
| 32 | DJ | 133 | GLY |
| 32 | DJ | 158 | PRO |
| 33 | DK | 21 | CYS |
| 33 | DK | 22 | ILE |
| 33 | DK | 97 | ARG |
| 34 | DL | 43 | GLY |
| 34 | DL | 47 | ASP |
| 34 | DL | 109 | GLY |
| 35 | DM | 22 | LYS |
| 37 | DO | 62 | LYS |
| 37 | DO | 83 | LYS |
| 37 | DO | 91 | PRO |
| 38 | DP | 14 | TYR |
| 39 | DQ | 58 | ARG |
| 41 | DS | 63 | ASP |
| 42 | DT | 40 | LYS |
| 42 | DT | 72 | LYS |
| 43 | DU | 80 | GLY |
| 49 | D1 | 41 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49 | D1 | 54 | LYS |
| 52 | D4 | 47 | ARG |
| 53 | D5 | 61 | LEU |
| 4 | AD | 75 | PHE |
| 4 | AD | 146 | ILE |
| 4 | AD | 147 | ALA |
| 4 | AD | 168 | ARG |
| 5 | AE | 11 | ILE |
| 5 | AE | 107 | ARG |
| 8 | AH | 37 | ARG |
| 8 | AH | 68 | ARG |
| 9 | AI | 10 | ARG |
| 9 | AI | 127 | LYS |
| 11 | AK | 80 | VAL |
| 12 | AL | 79 | HIS |
| 13 | AM | 3 | ARG |
| 14 | AN | 58 | LYS |
| 16 | AP | 72 | ARG |
| 17 | AQ | 30 | PRO |
| 18 | AR | 64 | ARG |
| 18 | AR | 87 | ARG |
| 19 | AS | 29 | ARG |
| 26 | BD | 69 | LYS |
| 26 | BD | 94 | GLU |
| 27 | BE | 134 | GLY |
| 29 | BG | 15 | VAL |
| 29 | BG | 90 | LYS |
| 30 | BH | 86 | THR |
| 30 | BH | 93 | THR |
| 32 | BJ | 75 | VAL |
| 32 | BJ | 105 | LEU |
| 32 | BJ | 106 | LYS |
| 33 | BK | 120 | GLU |
| 34 | BL | 108 | LYS |
| 35 | BM | 117 | ALA |
| 36 | BN | 10 | LEU |
| 36 | BN | 45 | ARG |
| 36 | BN | 85 | PRO |
| 38 | BP | 14 | TYR |
| 39 | BQ | 58 | ARG |
| 39 | BQ | 86 | ALA |
| 41 | BS | 67 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 43 | BU | 47 | LYS |
| 44 | BV | 140 | ASP |
| 46 | BX | 36 | GLY |
| 46 | BX | 38 | SER |
| 46 | BX | 53 | VAL |
| 47 | BY | 47 | ASN |
| 2 | CB | 182 | ILE |
| 2 | CB | 183 | PRO |
| 2 | CB | 228 | GLY |
| 3 | CC | 45 | LYS |
| 4 | CD | 10 | ARG |
| 4 | CD | 48 | ALA |
| 4 | CD | 105 | VAL |
| 4 | CD | 146 | ILE |
| 5 | CE | 11 | ILE |
| 5 | CE | 62 | ALA |
| 5 | CE | 129 | ILE |
| 6 | CF | 11 | ASN |
| 8 | CH | 73 | ASP |
| 9 | CI | 10 | ARG |
| 9 | CI | 124 | GLN |
| 9 | CI | 127 | LYS |
| 10 | CJ | 78 | ASN |
| 11 | CK | 80 | VAL |
| 12 | CL | 79 | HIS |
| 13 | CM | 3 | ARG |
| 16 | CP | 78 | GLY |
| 18 | CR | 41 | LYS |
| 18 | CR | 64 | ARG |
| 18 | CR | 87 | ARG |
| 19 | CS | 29 | ARG |
| 25 | DC | 224 | ALA |
| 26 | DD | 201 | THR |
| 27 | DE | 144 | LYS |
| 27 | DE | 160 | ASN |
| 28 | DF | 46 | ALA |
| 29 | DG | 15 | VAL |
| 30 | DH | 60 | GLU |
| 30 | DH | 76 | THR |
| 30 | DH | 93 | THR |
| 30 | DH | 115 | ALA |
| 32 | DJ | 75 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | DJ | 90 | LEU |
| 32 | DJ | 105 | LEU |
| 32 | DJ | 156 | GLN |
| 34 | DL | 70 | GLN |
| 34 | DL | 90 | ARG |
| 35 | DM | 23 | GLY |
| 36 | DN | 45 | ARG |
| 36 | DN | 85 | PRO |
| 37 | DO | 101 | LEU |
| 39 | DQ | 86 | ALA |
| 40 | DR | 48 | GLY |
| 41 | DS | 110 | LYS |
| 43 | DU | 47 | LYS |
| 44 | DV | 101 | PRO |
| 44 | DV | 140 | ASP |
| 45 | DW | 55 | ARG |
| 47 | DY | 15 | LYS |
| 53 | D5 | 40 | GLU |
| 2 | AB | 228 | GLY |
| 3 | AC | 5 | ILE |
| 3 | AC | 74 | GLY |
| 3 | AC | 96 | GLY |
| 3 | AC | 117 | ALA |
| 4 | AD | 48 | ALA |
| 6 | AF | 11 | ASN |
| 6 | AF | 90 | VAL |
| 7 | AG | 17 | VAL |
| 8 | AH | 73 | ASP |
| 11 | AK | 112 | THR |
| 12 | AL | 94 | GLY |
| 16 | AP | 63 | GLY |
| 16 | AP | 78 | GLY |
| 18 | AR | 36 | ASN |
| 20 | AT | 98 | PRO |
| 26 | BD | 201 | THR |
| 27 | BE | 144 | LYS |
| 30 | BH | 76 | THR |
| 33 | BK | 22 | ILE |
| 35 | BM | 62 | GLY |
| 37 | BO | 101 | LEU |
| 44 | BV | 114 | GLY |
| 44 | BV | 133 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44 | BV | 134 | PRO |
| 2 | CB | 191 | ASP |
| 3 | CC | 96 | GLY |
| 4 | CD | 63 | LYS |
| 4 | CD | 189 | PRO |
| 7 | CG | 17 | VAL |
| 8 | CH | 37 | ARG |
| 11 | CK | 112 | THR |
| 14 | CN | 42 | ILE |
| 17 | CQ | 30 | PRO |
| 19 | CS | 27 | GLU |
| 20 | CT | 98 | PRO |
| 26 | DD | 61 | ARG |
| 27 | DE | 66 | PRO |
| 29 | DG | 139 | GLN |
| 32 | DJ | 106 | LYS |
| 35 | DM | 54 | MET |
| 43 | DU | 41 | GLY |
| 44 | DV | 133 | ILE |
| 44 | DV | 134 | PRO |
| 46 | DX | 53 | VAL |
| 3 | AC | 173 | VAL |
| 4 | AD | 189 | PRO |
| 7 | AG | 82 | GLY |
| 12 | AL | 62 | GLY |
| 14 | AN | 42 | ILE |
| 18 | AR | 27 | GLY |
| 26 | BD | 61 | ARG |
| 27 | BE | 206 | ILE |
| 32 | BJ | 133 | GLY |
| 34 | BL | 19 | VAL |
| 35 | BM | 23 | GLY |
| 39 | BQ | 26 | GLY |
| 39 | BQ | 65 | ILE |
| 44 | BV | 37 | VAL |
| 3 | CC | 5 | ILE |
| 3 | CC | 74 | GLY |
| 3 | CC | 173 | VAL |
| 7 | CG | 82 | GLY |
| 12 | CL | 94 | GLY |
| 15 | CO | 87 | ILE |
| 16 | CP | 63 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26 | DD | 30 | PRO |
| 27 | DE | 206 | ILE |
| 40 | DR | 50 | PRO |
| 42 | DT | 84 | ALA |
| 43 | DU | 18 | GLY |
| 43 | DU | 96 | ILE |
| 44 | DV | 114 | GLY |
| 46 | DX | 36 | GLY |
| 15 | AO | 36 | ILE |
| 15 | AO | 87 | ILE |
| 43 | BU | 18 | GLY |
| 43 | BU | 41 | GLY |
| 43 | BU | 55 | TYR |
| 43 | BU | 96 | ILE |
| 46 | BX | 31 | GLY |
| 2 | CB | 159 | PRO |
| 3 | CC | 39 | ILE |
| 4 | CD | 197 | PRO |
| 36 | DN | 73 | VAL |
| 38 | DP | 81 | PRO |
| 2 | AB | 159 | PRO |
| 2 | AB | 194 | PRO |
| 4 | AD | 197 | PRO |
| 6 | AF | 40 | VAL |
| 25 | BC | 123 | ALA |
| 26 | BD | 30 | PRO |
| 27 | BE | 25 | PRO |
| 36 | BN | 58 | GLY |
| 38 | BP | 81 | PRO |
| 40 | BR | 50 | PRO |
| 42 | BT | 84 | ALA |
| 2 | CB | 194 | PRO |
| 12 | CL | 62 | GLY |
| 36 | DN | 58 | GLY |
| 40 | DR | 17 | GLY |
| 44 | DV | 37 | VAL |
| 3 | AC | 39 | ILE |
| 4 | AD | 56 | VAL |
| 5 | AE | 129 | ILE |
| 8 | AH | 103 | VAL |
| 12 | AL | 17 | VAL |
| 28 | BF | 109 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 28 | BF | 142 | PRO |
| 34 | BL | 10 | PRO |
| 35 | BM | 81 | VAL |
| 35 | BM | 92 | GLY |
| 39 | BQ | 8 | VAL |
| 40 | BR | 17 | GLY |
| 47 | BY | 50 | ILE |
| 4 | CD | 56 | VAL |
| 6 | CF | 90 | VAL |
| 7 | CG | 70 | LYS |
| 8 | CH | 51 | VAL |
| 12 | CL | 17 | VAL |
| 29 | DG | 52 | VAL |
| 34 | DL | 10 | PRO |
| 35 | DM | 81 | VAL |
| 39 | DQ | 65 | ILE |
| 43 | DU | 55 | TYR |
| 46 | DX | 14 | VAL |
| 46 | DX | 31 | GLY |
| 7 | AG | 70 | LYS |
| 29 | BG | 52 | VAL |
| 34 | BL | 125 | VAL |
| 46 | BX | 14 | VAL |
| 49 | B1 | 47 | VAL |
| 18 | CR | 50 | ILE |
| 25 | DC | 10 | THR |
| 28 | DF | 109 | VAL |
| 28 | DF | 142 | PRO |
| 34 | DL | 19 | VAL |
| 37 | DO | 60 | GLY |
| 49 | D1 | 47 | VAL |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2 | AB | 202/202 (100%) | 178 (88%) | 24 (12%) | 6 | 29 |
| 2 | CB | 202/202 (100%) | 179 (89%) | 23 (11%) | 7 | 31 |
| 3 | AC | 160/160 (100%) | 146 (91%) | 14 (9%) | 12 | 46 |
| 3 | CC | 160/160 (100%) | 145 (91%) | 15 (9%) | 11 | 42 |
| 4 | AD | 180/180 (100%) | 150 (83%) | 30 (17%) | 3 | 14 |
| 4 | CD | 180/180 (100%) | 150 (83%) | 30 (17%) | 3 | 14 |
| 5 | AE | 116/116 (100%) | 92 (79%) | 24 (21%) | 1 | 7 |
| 5 | CE | 116/116 (100%) | 94 (81%) | 22 (19%) | 2 | 9 |
| 6 | AF | 90/90 (100%) | 82 (91%) | 8 (9%) | 12 | 45 |
| 6 | CF | 90/90 (100%) | 83 (92%) | 7 (8%) | 16 | 52 |
| 7 | AG | 126/126 (100%) | 121 (96%) | 5 (4%) | 38 | 75 |
| 7 | CG | 126/126 (100%) | 121 (96%) | 5 (4%) | 38 | 75 |
| 8 | AH | 119/119 (100%) | 102 (86%) | 17 (14%) | 4 | 22 |
| 8 | CH | 119/119 (100%) | 104 (87%) | 15 (13%) | 5 | 27 |
| 9 | AI | 98/98 (100%) | 88 (90%) | 10 (10%) | 9 | 38 |
| 9 | CI | 98/98 (100%) | 88 (90%) | 10 (10%) | 9 | 38 |
| 10 | AJ | 88/88 (100%) | 78 (89%) | 10 (11%) | 7 | 31 |
| 10 | CJ | 88/88 (100%) | 78 (89%) | 10 (11%) | 7 | 31 |
| 11 | AK | 90/90 (100%) | 75 (83%) | 15 (17%) | 3 | 14 |
| 11 | CK | 90/90 (100%) | 76 (84%) | 14 (16%) | 3 | 18 |
| 12 | AL | 104/104 (100%) | 83 (80%) | 21 (20%) | 1 | 7 |
| 12 | CL | 104/104 (100%) | 83 (80%) | 21 (20%) | 1 | 7 |
| 13 | AM | 94/94 (100%) | 87 (93%) | 7 (7%) | 17 | 55 |
| 13 | CM | 94/94 (100%) | 87 (93%) | 7 (7%) | 17 | 55 |
| 14 | AN | 49/49 (100%) | 45 (92%) | 4 (8%) | 14 | 50 |
| 14 | CN | 49/49 (100%) | 45 (92%) | 4 (8%) | 14 | 50 |
| 15 | AO | 79/79 (100%) | 69 (87%) | 10 (13%) | 5 | 26 |
| 15 | CO | 79/79 (100%) | 69 (87%) | 10 (13%) | 5 | 26 |
| 16 | AP | 72/72 (100%) | 57 (79%) | 15 (21%) | 1 | 6 |
| 16 | CP | 72/72 (100%) | 56 (78%) | 16 (22%) | 1 | 5 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 17 | AQ | 94/94 (100%) | 78 (83%) | 16 (17%) | 2 | 14 |
| 17 | CQ | 94/94 (100%) | 79 (84%) | 15 (16%) | 3 | 16 |
| 18 | AR | 61/61 (100%) | 58 (95%) | 3 (5%) | 31 | 70 |
| 18 | CR | 61/61 (100%) | 58 (95%) | 3 (5%) | 31 | 70 |
| 19 | AS | 69/69 (100%) | 60 (87%) | 9 (13%) | 5 | 25 |
| 19 | CS | 69/69 (100%) | 60 (87%) | 9 (13%) | 5 | 25 |
| 20 | AT | 76/76 (100%) | 65 (86%) | 11 (14%) | 4 | 21 |
| 20 | CT | 76/76 (100%) | 65 (86%) | 11 (14%) | 4 | 21 |
| 21 | AU | 19/19 (100%) | 19 (100%) | 0 | 100 | 100 |
| 21 | CU | 19/19 (100%) | 19 (100%) | 0 | 100 | 100 |
| 25 | BC | 213/213 (100%) | 164 (77%) | 49 (23%) | 1 | 4 |
| 25 | DC | 213/213 (100%) | 162 (76%) | 51 (24%) | 1 | 4 |
| 26 | BD | 165/165 (100%) | 129 (78%) | 36 (22%) | 1 | 6 |
| 26 | DD | 165/165 (100%) | 129 (78%) | 36 (22%) | 1 | 6 |
| 27 | BE | 161/161 (100%) | 124 (77%) | 37 (23%) | 1 | 4 |
| 27 | DE | 161/161 (100%) | 124 (77%) | 37 (23%) | 1 | 4 |
| 28 | BF | 155/155 (100%) | 132 (85%) | 23 (15%) | 4 | 20 |
| 28 | DF | 155/155 (100%) | 134 (86%) | 21 (14%) | 5 | 24 |
| 29 | BG | 132/132 (100%) | 108 (82%) | 24 (18%) | 2 | 11 |
| 29 | DG | 132/132 (100%) | 107 (81%) | 25 (19%) | 2 | 9 |
| 30 | BH | 122/122 (100%) | 103 (84%) | 19 (16%) | 3 | 18 |
| 30 | DH | 122/122 (100%) | 103 (84%) | 19 (16%) | 3 | 18 |
| 31 | BI | 27/53 (51%) | 25 (93%) | 2 (7%) | 17 | 55 |
| 31 | DI | 27/53 (51%) | 25 (93%) | 2 (7%) | 17 | 55 |
| 32 | BJ | 116/116 (100%) | 84 (72%) | 32 (28%) | 0 | 3 |
| 32 | DJ | 116/116 (100%) | 85 (73%) | 31 (27%) | 0 | 3 |
| 33 | BK | 100/100 (100%) | 78 (78%) | 22 (22%) | 1 | 5 |
| 33 | DK | 100/100 (100%) | 78 (78%) | 22 (22%) | 1 | 5 |
| 34 | BL | 112/112 (100%) | 75 (67%) | 37 (33%) | 0 | 2 |
| 34 | DL | 112/112 (100%) | 76 (68%) | 36 (32%) | 0 | 2 |
| 35 | BM | 106/106 (100%) | 82 (77%) | 24 (23%) | 1 | 5 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 35 | DM | 106/106 (100%) | 81 (76%) | 25 (24%) | 1 | 4 |
| 36 | BN | 100/100 (100%) | 75 (75%) | 25 (25%) | 1 | 4 |
| 36 | DN | 100/100 (100%) | 76 (76%) | 24 (24%) | 1 | 4 |
| 37 | BO | 77/77 (100%) | 63 (82%) | 14 (18%) | 2 | 11 |
| 37 | DO | 77/77 (100%) | 63 (82%) | 14 (18%) | 2 | 11 |
| 38 | BP | 121/121 (100%) | 96 (79%) | 25 (21%) | 1 | 7 |
| 38 | DP | 121/121 (100%) | 94 (78%) | 27 (22%) | 1 | 5 |
| 39 | BQ | 92/92 (100%) | 71 (77%) | 21 (23%) | 1 | 5 |
| 39 | DQ | 92/92 (100%) | 71 (77%) | 21 (23%) | 1 | 5 |
| 40 | BR | 82/82 (100%) | 63 (77%) | 19 (23%) | 1 | 4 |
| 40 | DR | 82/82 (100%) | 61 (74%) | 21 (26%) | 0 | 3 |
| 41 | BS | 91/91 (100%) | 65 (71%) | 26 (29%) | 0 | 2 |
| 41 | DS | 91/91 (100%) | 65 (71%) | 26 (29%) | 0 | 2 |
| 42 | BT | 74/74 (100%) | 60 (81%) | 14 (19%) | 2 | 9 |
| 42 | DT | 74/74 (100%) | 60 (81%) | 14 (19%) | 2 | 9 |
| 43 | BU | 84/84 (100%) | 66 (79%) | 18 (21%) | 1 | 6 |
| 43 | DU | 84/84 (100%) | 67 (80%) | 17 (20%) | 1 | 7 |
| 44 | BV | 163/163 (100%) | 142 (87%) | 21 (13%) | 5 | 26 |
| 44 | DV | 163/163 (100%) | 141 (86%) | 22 (14%) | 5 | 24 |
| 45 | BW | 61/61 (100%) | 52 (85%) | 9 (15%) | 4 | 20 |
| 45 | DW | 61/61 (100%) | 53 (87%) | 8 (13%) | 5 | 25 |
| 46 | BX | 73/73 (100%) | 50 (68%) | 23 (32%) | 0 | 2 |
| 46 | DX | 73/73 (100%) | 50 (68%) | 23 (32%) | 0 | 2 |
| 47 | BY | 58/58 (100%) | 46 (79%) | 12 (21%) | 1 | 7 |
| 47 | DY | 58/58 (100%) | 46 (79%) | 12 (21%) | 1 | 7 |
| 48 | BZ | 51/51 (100%) | 43 (84%) | 8 (16%) | 3 | 18 |
| 48 | DZ | 51/51 (100%) | 43 (84%) | 8 (16%) | 3 | 18 |
| 49 | B1 | 27/27 (100%) | 26 (96%) | 1 (4%) | 41 | 77 |
| 49 | D1 | 27/27 (100%) | 26 (96%) | 1 (4%) | 41 | 77 |
| 50 | B2 | 45/45 (100%) | 40 (89%) | 5 (11%) | 8 | 33 |
| 50 | D2 | 45/45 (100%) | 39 (87%) | 6 (13%) | 5 | 24 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|------------|-------------|----|
| 51 | B3 | 43/43 (100%) | 38 (88%) | 5 (12%) | 7 | 31 |
| 51 | D3 | 43/43 (100%) | 38 (88%) | 5 (12%) | 7 | 31 |
| 52 | B4 | 41/41 (100%) | 29 (71%) | 12 (29%) | 0 | 2 |
| 52 | D4 | 41/41 (100%) | 28 (68%) | 13 (32%) | 0 | 2 |
| 53 | B5 | 53/53 (100%) | 42 (79%) | 11 (21%) | 1 | 6 |
| 53 | D5 | 53/53 (100%) | 43 (81%) | 10 (19%) | 2 | 9 |
| All | All | 9462/9514 (100%) | 7811 (83%) | 1651 (17%) | 2 | 13 |

All (1651) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 16 | HIS |
| 2 | AB | 27 | LYS |
| 2 | AB | 28 | PHE |
| 2 | AB | 60 | ASP |
| 2 | AB | 61 | LEU |
| 2 | AB | 71 | VAL |
| 2 | AB | 75 | LYS |
| 2 | AB | 76 | GLN |
| 2 | AB | 87 | ARG |
| 2 | AB | 93 | VAL |
| 2 | AB | 111 | ARG |
| 2 | AB | 117 | GLU |
| 2 | AB | 127 | ILE |
| 2 | AB | 128 | GLU |
| 2 | AB | 130 | ARG |
| 2 | AB | 142 | LEU |
| 2 | AB | 153 | ARG |
| 2 | AB | 154 | LEU |
| 2 | AB | 158 | LEU |
| 2 | AB | 164 | VAL |
| 2 | AB | 169 | LYS |
| 2 | AB | 178 | ARG |
| 2 | AB | 187 | LEU |
| 2 | AB | 221 | LEU |
| 3 | AC | 3 | ASN |
| 3 | AC | 5 | ILE |
| 3 | AC | 11 | ARG |
| 3 | AC | 16 | ARG |
| 3 | AC | 29 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | AC | 79 | ARG |
| 3 | AC | 95 | THR |
| 3 | AC | 115 | LEU |
| 3 | AC | 131 | ARG |
| 3 | AC | 152 | ILE |
| 3 | AC | 165 | THR |
| 3 | AC | 167 | TRP |
| 3 | AC | 196 | LEU |
| 3 | AC | 202 | ILE |
| 4 | AD | 3 | ARG |
| 4 | AD | 4 | TYR |
| 4 | AD | 8 | VAL |
| 4 | AD | 9 | CYS |
| 4 | AD | 11 | LEU |
| 4 | AD | 21 | LEU |
| 4 | AD | 45 | GLN |
| 4 | AD | 49 | ARG |
| 4 | AD | 59 | ARG |
| 4 | AD | 72 | GLU |
| 4 | AD | 76 | ARG |
| 4 | AD | 92 | VAL |
| 4 | AD | 96 | LEU |
| 4 | AD | 103 | ASN |
| 4 | AD | 108 | LEU |
| 4 | AD | 110 | PHE |
| 4 | AD | 114 | ARG |
| 4 | AD | 119 | GLN |
| 4 | AD | 122 | ARG |
| 4 | AD | 129 | ASN |
| 4 | AD | 131 | ARG |
| 4 | AD | 135 | LEU |
| 4 | AD | 141 | ARG |
| 4 | AD | 144 | ASP |
| 4 | AD | 154 | ASN |
| 4 | AD | 155 | LEU |
| 4 | AD | 158 | ILE |
| 4 | AD | 166 | LYS |
| 4 | AD | 203 | VAL |
| 4 | AD | 208 | SER |
| 5 | AE | 8 | GLU |
| 5 | AE | 12 | LEU |
| 5 | AE | 16 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | AE | 18 | ARG |
| 5 | AE | 20 | GLN |
| 5 | AE | 28 | PHE |
| 5 | AE | 31 | LEU |
| 5 | AE | 43 | LEU |
| 5 | AE | 47 | LYS |
| 5 | AE | 53 | LEU |
| 5 | AE | 55 | VAL |
| 5 | AE | 60 | TYR |
| 5 | AE | 64 | ARG |
| 5 | AE | 71 | LEU |
| 5 | AE | 73 | ASN |
| 5 | AE | 76 | ILE |
| 5 | AE | 78 | HIS |
| 5 | AE | 79 | GLU |
| 5 | AE | 110 | LEU |
| 5 | AE | 116 | THR |
| 5 | AE | 120 | THR |
| 5 | AE | 126 | ARG |
| 5 | AE | 144 | THR |
| 5 | AE | 147 | ASP |
| 6 | AF | 43 | LEU |
| 6 | AF | 46 | ARG |
| 6 | AF | 48 | LEU |
| 6 | AF | 63 | TYR |
| 6 | AF | 69 | GLU |
| 6 | AF | 72 | VAL |
| 6 | AF | 89 | MET |
| 6 | AF | 100 | ASN |
| 7 | AG | 67 | GLU |
| 7 | AG | 91 | VAL |
| 7 | AG | 104 | LEU |
| 7 | AG | 118 | VAL |
| 7 | AG | 148 | ASN |
| 8 | AH | 1 | MET |
| 8 | AH | 8 | ASP |
| 8 | AH | 25 | ASP |
| 8 | AH | 26 | VAL |
| 8 | AH | 39 | LEU |
| 8 | AH | 50 | ARG |
| 8 | AH | 52 | ASP |
| 8 | AH | 54 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | AH | 73 | ASP |
| 8 | AH | 80 | ILE |
| 8 | AH | 91 | ARG |
| 8 | AH | 104 | ARG |
| 8 | AH | 107 | LEU |
| 8 | AH | 111 | ILE |
| 8 | AH | 119 | LEU |
| 8 | AH | 127 | LEU |
| 8 | AH | 136 | GLU |
| 9 | AI | 10 | ARG |
| 9 | AI | 14 | VAL |
| 9 | AI | 88 | TYR |
| 9 | AI | 95 | LYS |
| 9 | AI | 99 | LEU |
| 9 | AI | 104 | ARG |
| 9 | AI | 109 | VAL |
| 9 | AI | 114 | TYR |
| 9 | AI | 121 | ARG |
| 9 | AI | 124 | GLN |
| 10 | AJ | 16 | LEU |
| 10 | AJ | 22 | LYS |
| 10 | AJ | 49 | VAL |
| 10 | AJ | 55 | LYS |
| 10 | AJ | 62 | HIS |
| 10 | AJ | 63 | PHE |
| 10 | AJ | 66 | ARG |
| 10 | AJ | 74 | ILE |
| 10 | AJ | 92 | THR |
| 10 | AJ | 96 | ILE |
| 11 | AK | 14 | VAL |
| 11 | AK | 29 | ILE |
| 11 | AK | 32 | ILE |
| 11 | AK | 33 | THR |
| 11 | AK | 34 | ASP |
| 11 | AK | 40 | ILE |
| 11 | AK | 48 | ILE |
| 11 | AK | 53 | SER |
| 11 | AK | 80 | VAL |
| 11 | AK | 81 | ASP |
| 11 | AK | 92 | GLU |
| 11 | AK | 103 | LEU |
| 11 | AK | 114 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | AK | 117 | ASN |
| 11 | AK | 126 | ARG |
| 12 | AL | 5 | THR |
| 12 | AL | 6 | ILE |
| 12 | AL | 9 | LEU |
| 12 | AL | 10 | VAL |
| 12 | AL | 19 | LYS |
| 12 | AL | 31 | PHE |
| 12 | AL | 35 | VAL |
| 12 | AL | 40 | ARG |
| 12 | AL | 41 | THR |
| 12 | AL | 42 | VAL |
| 12 | AL | 43 | THR |
| 12 | AL | 52 | ARG |
| 12 | AL | 59 | LEU |
| 12 | AL | 61 | SER |
| 12 | AL | 65 | VAL |
| 12 | AL | 69 | ILE |
| 12 | AL | 83 | LEU |
| 12 | AL | 84 | ILE |
| 12 | AL | 95 | VAL |
| 12 | AL | 99 | ILE |
| 12 | AL | 109 | VAL |
| 13 | AM | 58 | GLU |
| 13 | AM | 64 | TRP |
| 13 | AM | 87 | TYR |
| 13 | AM | 93 | ARG |
| 13 | AM | 105 | THR |
| 13 | AM | 106 | ASN |
| 13 | AM | 115 | LYS |
| 14 | AN | 16 | PHE |
| 14 | AN | 41 | ARG |
| 14 | AN | 42 | ILE |
| 14 | AN | 44 | LEU |
| 15 | AO | 5 | LYS |
| 15 | AO | 17 | ARG |
| 15 | AO | 34 | LEU |
| 15 | AO | 39 | LEU |
| 15 | AO | 44 | LYS |
| 15 | AO | 45 | VAL |
| 15 | AO | 63 | ARG |
| 15 | AO | 66 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15 | AO | 67 | LEU |
| 15 | AO | 82 | ILE |
| 16 | AP | 1 | MET |
| 16 | AP | 2 | VAL |
| 16 | AP | 16 | HIS |
| 16 | AP | 20 | VAL |
| 16 | AP | 27 | LYS |
| 16 | AP | 28 | ARG |
| 16 | AP | 32 | TYR |
| 16 | AP | 47 | ASP |
| 16 | AP | 61 | SER |
| 16 | AP | 65 | GLN |
| 16 | AP | 69 | THR |
| 16 | AP | 72 | ARG |
| 16 | AP | 74 | LEU |
| 16 | AP | 82 | GLN |
| 16 | AP | 83 | GLU |
| 17 | AQ | 4 | LYS |
| 17 | AQ | 7 | THR |
| 17 | AQ | 9 | VAL |
| 17 | AQ | 10 | VAL |
| 17 | AQ | 11 | VAL |
| 17 | AQ | 15 | MET |
| 17 | AQ | 19 | VAL |
| 17 | AQ | 23 | VAL |
| 17 | AQ | 38 | ARG |
| 17 | AQ | 43 | LEU |
| 17 | AQ | 52 | LYS |
| 17 | AQ | 57 | VAL |
| 17 | AQ | 59 | ILE |
| 17 | AQ | 70 | ARG |
| 17 | AQ | 74 | LEU |
| 17 | AQ | 85 | VAL |
| 18 | AR | 65 | ILE |
| 18 | AR | 84 | LYS |
| 18 | AR | 88 | LYS |
| 19 | AS | 6 | LYS |
| 19 | AS | 7 | LYS |
| 19 | AS | 22 | LEU |
| 19 | AS | 27 | GLU |
| 19 | AS | 29 | ARG |
| 19 | AS | 37 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19 | AS | 44 | MET |
| 19 | AS | 49 | ILE |
| 19 | AS | 53 | ASN |
| 20 | AT | 9 | ASN |
| 20 | AT | 10 | LEU |
| 20 | AT | 22 | ARG |
| 20 | AT | 26 | ASN |
| 20 | AT | 30 | LYS |
| 20 | AT | 55 | ILE |
| 20 | AT | 57 | ARG |
| 20 | AT | 62 | LEU |
| 20 | AT | 73 | HIS |
| 20 | AT | 93 | GLU |
| 20 | AT | 100 | ILE |
| 25 | BC | 10 | THR |
| 25 | BC | 13 | ARG |
| 25 | BC | 14 | ARG |
| 25 | BC | 16 | MET |
| 25 | BC | 33 | LEU |
| 25 | BC | 38 | LYS |
| 25 | BC | 44 | ASN |
| 25 | BC | 61 | LEU |
| 25 | BC | 68 | LYS |
| 25 | BC | 69 | ARG |
| 25 | BC | 73 | VAL |
| 25 | BC | 87 | ASN |
| 25 | BC | 94 | LEU |
| 25 | BC | 95 | LEU |
| 25 | BC | 99 | ASP |
| 25 | BC | 102 | LYS |
| 25 | BC | 103 | ARG |
| 25 | BC | 105 | ILE |
| 25 | BC | 111 | LEU |
| 25 | BC | 112 | GLN |
| 25 | BC | 125 | ILE |
| 25 | BC | 126 | GLN |
| 25 | BC | 131 | LEU |
| 25 | BC | 134 | ARG |
| 25 | BC | 138 | VAL |
| 25 | BC | 141 | VAL |
| 25 | BC | 150 | LYS |
| 25 | BC | 154 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | BC | 155 | LEU |
| 25 | BC | 166 | GLN |
| 25 | BC | 171 | ASP |
| 25 | BC | 174 | ILE |
| 25 | BC | 192 | THR |
| 25 | BC | 193 | VAL |
| 25 | BC | 198 | ASN |
| 25 | BC | 204 | ILE |
| 25 | BC | 205 | VAL |
| 25 | BC | 211 | ARG |
| 25 | BC | 212 | SER |
| 25 | BC | 218 | ARG |
| 25 | BC | 226 | MET |
| 25 | BC | 227 | ASN |
| 25 | BC | 229 | VAL |
| 25 | BC | 237 | GLU |
| 25 | BC | 242 | ARG |
| 25 | BC | 244 | ARG |
| 25 | BC | 259 | THR |
| 25 | BC | 270 | ILE |
| 25 | BC | 271 | ILE |
| 26 | BD | 1 | MET |
| 26 | BD | 4 | ILE |
| 26 | BD | 5 | LEU |
| 26 | BD | 9 | VAL |
| 26 | BD | 16 | ARG |
| 26 | BD | 18 | ASP |
| 26 | BD | 33 | VAL |
| 26 | BD | 34 | VAL |
| 26 | BD | 40 | GLU |
| 26 | BD | 45 | THR |
| 26 | BD | 49 | LEU |
| 26 | BD | 54 | GLN |
| 26 | BD | 57 | LYS |
| 26 | BD | 76 | ARG |
| 26 | BD | 77 | ILE |
| 26 | BD | 79 | ARG |
| 26 | BD | 84 | PHE |
| 26 | BD | 95 | ILE |
| 26 | BD | 116 | VAL |
| 26 | BD | 121 | ASN |
| 26 | BD | 141 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26 | BD | 145 | LYS |
| 26 | BD | 152 | LYS |
| 26 | BD | 154 | LYS |
| 26 | BD | 156 | MET |
| 26 | BD | 160 | TYR |
| 26 | BD | 167 | VAL |
| 26 | BD | 169 | ASN |
| 26 | BD | 170 | LEU |
| 26 | BD | 171 | GLU |
| 26 | BD | 173 | VAL |
| 26 | BD | 175 | VAL |
| 26 | BD | 176 | ILE |
| 26 | BD | 181 | LEU |
| 26 | BD | 184 | VAL |
| 26 | BD | 197 | ILE |
| 27 | BE | 6 | MET |
| 27 | BE | 8 | GLN |
| 27 | BE | 9 | ILE |
| 27 | BE | 24 | LEU |
| 27 | BE | 33 | LEU |
| 27 | BE | 46 | ARG |
| 27 | BE | 48 | THR |
| 27 | BE | 50 | SER |
| 27 | BE | 53 | THR |
| 27 | BE | 64 | ILE |
| 27 | BE | 65 | TRP |
| 27 | BE | 67 | GLN |
| 27 | BE | 68 | LYS |
| 27 | BE | 70 | THR |
| 27 | BE | 74 | ARG |
| 27 | BE | 78 | ILE |
| 27 | BE | 82 | ILE |
| 27 | BE | 88 | VAL |
| 27 | BE | 98 | SER |
| 27 | BE | 100 | THR |
| 27 | BE | 106 | ARG |
| 27 | BE | 122 | LYS |
| 27 | BE | 125 | LEU |
| 27 | BE | 127 | GLU |
| 27 | BE | 129 | PHE |
| 27 | BE | 136 | THR |
| 27 | BE | 158 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27 | BE | 160 | ASN |
| 27 | BE | 164 | ARG |
| 27 | BE | 165 | ARG |
| 27 | BE | 174 | VAL |
| 27 | BE | 175 | THR |
| 27 | BE | 181 | LEU |
| 27 | BE | 183 | VAL |
| 27 | BE | 192 | LEU |
| 27 | BE | 194 | MET |
| 27 | BE | 197 | ASP |
| 28 | BF | 5 | LEU |
| 28 | BF | 8 | LYS |
| 28 | BF | 26 | GLN |
| 28 | BF | 33 | ARG |
| 28 | BF | 35 | GLU |
| 28 | BF | 47 | LYS |
| 28 | BF | 78 | SER |
| 28 | BF | 86 | MET |
| 28 | BF | 90 | LEU |
| 28 | BF | 93 | THR |
| 28 | BF | 94 | LEU |
| 28 | BF | 97 | ASP |
| 28 | BF | 98 | ARG |
| 28 | BF | 107 | LEU |
| 28 | BF | 115 | ARG |
| 28 | BF | 128 | ARG |
| 28 | BF | 132 | ASN |
| 28 | BF | 143 | GLU |
| 28 | BF | 155 | MET |
| 28 | BF | 157 | ILE |
| 28 | BF | 159 | VAL |
| 28 | BF | 161 | THR |
| 28 | BF | 166 | ASP |
| 29 | BG | 13 | LYS |
| 29 | BG | 23 | ARG |
| 29 | BG | 34 | GLU |
| 29 | BG | 37 | VAL |
| 29 | BG | 57 | ASP |
| 29 | BG | 60 | ARG |
| 29 | BG | 71 | LEU |
| 29 | BG | 90 | LYS |
| 29 | BG | 94 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29 | BG | 101 | ARG |
| 29 | BG | 116 | GLU |
| 29 | BG | 122 | THR |
| 29 | BG | 123 | PHE |
| 29 | BG | 124 | GLU |
| 29 | BG | 129 | THR |
| 29 | BG | 133 | VAL |
| 29 | BG | 136 | ILE |
| 29 | BG | 139 | GLN |
| 29 | BG | 140 | LYS |
| 29 | BG | 147 | ASN |
| 29 | BG | 151 | ILE |
| 29 | BG | 158 | HIS |
| 29 | BG | 162 | ILE |
| 29 | BG | 163 | TYR |
| 30 | BH | 3 | VAL |
| 30 | BH | 4 | ILE |
| 30 | BH | 5 | LEU |
| 30 | BH | 6 | LEU |
| 30 | BH | 14 | ASP |
| 30 | BH | 20 | ASP |
| 30 | BH | 21 | VAL |
| 30 | BH | 33 | ARG |
| 30 | BH | 40 | THR |
| 30 | BH | 50 | ARG |
| 30 | BH | 67 | ARG |
| 30 | BH | 68 | LEU |
| 30 | BH | 73 | GLU |
| 30 | BH | 77 | LEU |
| 30 | BH | 89 | TYR |
| 30 | BH | 91 | SER |
| 30 | BH | 109 | ILE |
| 30 | BH | 135 | GLU |
| 30 | BH | 142 | VAL |
| 31 | BI | 3 | ASN |
| 31 | BI | 58 | LEU |
| 32 | BJ | 38 | LEU |
| 32 | BJ | 39 | ILE |
| 32 | BJ | 42 | GLU |
| 32 | BJ | 46 | LEU |
| 32 | BJ | 51 | THR |
| 32 | BJ | 56 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 32 | BJ | 57 | LEU |
| 32 | BJ | 68 | ASN |
| 32 | BJ | 71 | MET |
| 32 | BJ | 81 | ASP |
| 32 | BJ | 83 | ILE |
| 32 | BJ | 86 | THR |
| 32 | BJ | 92 | GLN |
| 32 | BJ | 105 | LEU |
| 32 | BJ | 106 | LYS |
| 32 | BJ | 110 | LEU |
| 32 | BJ | 112 | LYS |
| 32 | BJ | 113 | MET |
| 32 | BJ | 116 | THR |
| 32 | BJ | 117 | HIS |
| 32 | BJ | 122 | LEU |
| 32 | BJ | 126 | VAL |
| 32 | BJ | 129 | MET |
| 32 | BJ | 132 | LYS |
| 32 | BJ | 137 | ARG |
| 32 | BJ | 142 | ARG |
| 32 | BJ | 143 | LEU |
| 32 | BJ | 144 | LYS |
| 32 | BJ | 146 | TYR |
| 32 | BJ | 154 | GLN |
| 32 | BJ | 160 | LYS |
| 32 | BJ | 161 | LEU |
| 33 | BK | 2 | ILE |
| 33 | BK | 3 | GLN |
| 33 | BK | 4 | PRO |
| 33 | BK | 19 | ILE |
| 33 | BK | 22 | ILE |
| 33 | BK | 23 | ARG |
| 33 | BK | 24 | VAL |
| 33 | BK | 26 | LYS |
| 33 | BK | 31 | LYS |
| 33 | BK | 32 | TYR |
| 33 | BK | 47 | ILE |
| 33 | BK | 52 | VAL |
| 33 | BK | 65 | THR |
| 33 | BK | 78 | ARG |
| 33 | BK | 87 | ILE |
| 33 | BK | 89 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33 | BK | 90 | GLN |
| 33 | BK | 91 | LEU |
| 33 | BK | 98 | VAL |
| 33 | BK | 99 | PHE |
| 33 | BK | 102 | VAL |
| 33 | BK | 115 | VAL |
| 34 | BL | 9 | ASN |
| 34 | BL | 15 | ARG |
| 34 | BL | 16 | ARG |
| 34 | BL | 18 | ARG |
| 34 | BL | 19 | VAL |
| 34 | BL | 29 | LYS |
| 34 | BL | 33 | ARG |
| 34 | BL | 39 | LYS |
| 34 | BL | 40 | SER |
| 34 | BL | 41 | ARG |
| 34 | BL | 42 | SER |
| 34 | BL | 49 | ARG |
| 34 | BL | 50 | ARG |
| 34 | BL | 51 | PHE |
| 34 | BL | 52 | GLU |
| 34 | BL | 55 | ARG |
| 34 | BL | 56 | SER |
| 34 | BL | 57 | THR |
| 34 | BL | 59 | LEU |
| 34 | BL | 61 | ARG |
| 34 | BL | 62 | LEU |
| 34 | BL | 67 | MET |
| 34 | BL | 75 | ILE |
| 34 | BL | 81 | GLN |
| 34 | BL | 83 | VAL |
| 34 | BL | 85 | LEU |
| 34 | BL | 88 | LEU |
| 34 | BL | 91 | PHE |
| 34 | BL | 105 | LEU |
| 34 | BL | 111 | ARG |
| 34 | BL | 114 | ILE |
| 34 | BL | 123 | LEU |
| 34 | BL | 135 | LEU |
| 34 | BL | 144 | GLU |
| 34 | BL | 146 | VAL |
| 34 | BL | 147 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | BL | 148 | LEU |
| 35 | BM | 6 | ARG |
| 35 | BM | 9 | TYR |
| 35 | BM | 11 | LYS |
| 35 | BM | 13 | GLN |
| 35 | BM | 22 | LYS |
| 35 | BM | 25 | ASP |
| 35 | BM | 43 | THR |
| 35 | BM | 45 | GLN |
| 35 | BM | 52 | VAL |
| 35 | BM | 58 | PHE |
| 35 | BM | 59 | ARG |
| 35 | BM | 63 | LYS |
| 35 | BM | 66 | ILE |
| 35 | BM | 79 | LEU |
| 35 | BM | 80 | GLU |
| 35 | BM | 81 | VAL |
| 35 | BM | 83 | MET |
| 35 | BM | 89 | ASN |
| 35 | BM | 103 | MET |
| 35 | BM | 109 | VAL |
| 35 | BM | 115 | MET |
| 35 | BM | 119 | ARG |
| 35 | BM | 132 | VAL |
| 35 | BM | 135 | ASP |
| 36 | BN | 2 | ARG |
| 36 | BN | 8 | ARG |
| 36 | BN | 10 | LEU |
| 36 | BN | 12 | ARG |
| 36 | BN | 15 | SER |
| 36 | BN | 17 | ARG |
| 36 | BN | 18 | LEU |
| 36 | BN | 28 | LEU |
| 36 | BN | 35 | THR |
| 36 | BN | 37 | THR |
| 36 | BN | 44 | LEU |
| 36 | BN | 52 | ILE |
| 36 | BN | 54 | LEU |
| 36 | BN | 60 | LEU |
| 36 | BN | 63 | ARG |
| 36 | BN | 67 | LEU |
| 36 | BN | 70 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36 | BN | 75 | LEU |
| 36 | BN | 79 | LEU |
| 36 | BN | 95 | THR |
| 36 | BN | 98 | LEU |
| 36 | BN | 99 | LYS |
| 36 | BN | 104 | ARG |
| 36 | BN | 107 | ASP |
| 36 | BN | 111 | LEU |
| 37 | BO | 12 | PHE |
| 37 | BO | 13 | ARG |
| 37 | BO | 26 | LEU |
| 37 | BO | 30 | ARG |
| 37 | BO | 36 | TYR |
| 37 | BO | 40 | ILE |
| 37 | BO | 44 | LYS |
| 37 | BO | 48 | LEU |
| 37 | BO | 54 | LEU |
| 37 | BO | 63 | THR |
| 37 | BO | 69 | VAL |
| 37 | BO | 92 | TYR |
| 37 | BO | 93 | LYS |
| 37 | BO | 101 | LEU |
| 38 | BP | 15 | VAL |
| 38 | BP | 19 | LEU |
| 38 | BP | 23 | ARG |
| 38 | BP | 28 | VAL |
| 38 | BP | 30 | VAL |
| 38 | BP | 41 | ARG |
| 38 | BP | 50 | ILE |
| 38 | BP | 51 | ARG |
| 38 | BP | 53 | ARG |
| 38 | BP | 54 | ARG |
| 38 | BP | 58 | ASN |
| 38 | BP | 61 | PHE |
| 38 | BP | 63 | VAL |
| 38 | BP | 75 | ILE |
| 38 | BP | 84 | GLN |
| 38 | BP | 85 | LYS |
| 38 | BP | 86 | ILE |
| 38 | BP | 87 | ASP |
| 38 | BP | 88 | ILE |
| 38 | BP | 89 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38 | BP | 99 | LEU |
| 38 | BP | 100 | TYR |
| 38 | BP | 112 | ARG |
| 38 | BP | 113 | LYS |
| 38 | BP | 115 | ARG |
| 39 | BQ | 8 | VAL |
| 39 | BQ | 14 | HIS |
| 39 | BQ | 18 | LEU |
| 39 | BQ | 20 | LEU |
| 39 | BQ | 27 | LEU |
| 39 | BQ | 34 | LYS |
| 39 | BQ | 40 | PHE |
| 39 | BQ | 52 | ARG |
| 39 | BQ | 55 | ARG |
| 39 | BQ | 62 | ILE |
| 39 | BQ | 64 | ARG |
| 39 | BQ | 70 | ARG |
| 39 | BQ | 74 | LEU |
| 39 | BQ | 76 | TYR |
| 39 | BQ | 79 | PHE |
| 39 | BQ | 80 | ILE |
| 39 | BQ | 92 | ARG |
| 39 | BQ | 97 | ASP |
| 39 | BQ | 101 | ARG |
| 39 | BQ | 108 | GLU |
| 39 | BQ | 112 | ARG |
| 40 | BR | 5 | VAL |
| 40 | BR | 10 | LYS |
| 40 | BR | 12 | TYR |
| 40 | BR | 13 | ARG |
| 40 | BR | 18 | LEU |
| 40 | BR | 20 | LEU |
| 40 | BR | 21 | ARG |
| 40 | BR | 37 | VAL |
| 40 | BR | 39 | LEU |
| 40 | BR | 44 | LYS |
| 40 | BR | 53 | GLU |
| 40 | BR | 57 | VAL |
| 40 | BR | 72 | VAL |
| 40 | BR | 78 | LYS |
| 40 | BR | 79 | VAL |
| 40 | BR | 80 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40 | BR | 88 | ARG |
| 40 | BR | 98 | GLU |
| 40 | BR | 99 | ILE |
| 41 | BS | 1 | MET |
| 41 | BS | 8 | ARG |
| 41 | BS | 10 | VAL |
| 41 | BS | 11 | ARG |
| 41 | BS | 15 | ARG |
| 41 | BS | 17 | VAL |
| 41 | BS | 19 | LEU |
| 41 | BS | 23 | LEU |
| 41 | BS | 28 | SER |
| 41 | BS | 36 | LEU |
| 41 | BS | 39 | THR |
| 41 | BS | 47 | VAL |
| 41 | BS | 51 | LEU |
| 41 | BS | 53 | SER |
| 41 | BS | 60 | ASN |
| 41 | BS | 61 | ASN |
| 41 | BS | 69 | LEU |
| 41 | BS | 75 | TYR |
| 41 | BS | 76 | VAL |
| 41 | BS | 78 | GLU |
| 41 | BS | 84 | ARG |
| 41 | BS | 92 | ARG |
| 41 | BS | 96 | ILE |
| 41 | BS | 100 | THR |
| 41 | BS | 105 | VAL |
| 41 | BS | 107 | LEU |
| 42 | BT | 9 | LEU |
| 42 | BT | 12 | VAL |
| 42 | BT | 28 | PHE |
| 42 | BT | 39 | ILE |
| 42 | BT | 45 | THR |
| 42 | BT | 49 | VAL |
| 42 | BT | 52 | VAL |
| 42 | BT | 57 | LEU |
| 42 | BT | 62 | LYS |
| 42 | BT | 65 | ARG |
| 42 | BT | 68 | ARG |
| 42 | BT | 70 | LEU |
| 42 | BT | 80 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42 | BT | 81 | VAL |
| 43 | BU | 4 | LYS |
| 43 | BU | 6 | HIS |
| 43 | BU | 8 | LYS |
| 43 | BU | 9 | LYS |
| 43 | BU | 30 | VAL |
| 43 | BU | 31 | LEU |
| 43 | BU | 32 | PRO |
| 43 | BU | 60 | PHE |
| 43 | BU | 61 | ILE |
| 43 | BU | 62 | GLU |
| 43 | BU | 63 | LYS |
| 43 | BU | 67 | LEU |
| 43 | BU | 71 | LYS |
| 43 | BU | 76 | CYS |
| 43 | BU | 89 | PHE |
| 43 | BU | 90 | LEU |
| 43 | BU | 97 | ARG |
| 43 | BU | 98 | VAL |
| 44 | BV | 3 | TYR |
| 44 | BV | 24 | LEU |
| 44 | BV | 27 | VAL |
| 44 | BV | 31 | ARG |
| 44 | BV | 35 | ARG |
| 44 | BV | 39 | VAL |
| 44 | BV | 42 | VAL |
| 44 | BV | 70 | LEU |
| 44 | BV | 72 | ARG |
| 44 | BV | 82 | ARG |
| 44 | BV | 85 | HIS |
| 44 | BV | 86 | VAL |
| 44 | BV | 89 | PHE |
| 44 | BV | 94 | GLU |
| 44 | BV | 98 | MET |
| 44 | BV | 118 | GLN |
| 44 | BV | 140 | ASP |
| 44 | BV | 146 | ILE |
| 44 | BV | 150 | LEU |
| 44 | BV | 161 | VAL |
| 44 | BV | 163 | LEU |
| 45 | BW | 14 | ARG |
| 45 | BW | 20 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45 | BW | 21 | LEU |
| 45 | BW | 38 | VAL |
| 45 | BW | 53 | MET |
| 45 | BW | 63 | VAL |
| 45 | BW | 64 | ASP |
| 45 | BW | 80 | HIS |
| 45 | BW | 84 | LEU |
| 46 | BX | 8 | SER |
| 46 | BX | 13 | ILE |
| 46 | BX | 17 | SER |
| 46 | BX | 18 | ILE |
| 46 | BX | 21 | ARG |
| 46 | BX | 25 | LYS |
| 46 | BX | 27 | GLU |
| 46 | BX | 37 | ILE |
| 46 | BX | 38 | SER |
| 46 | BX | 40 | ARG |
| 46 | BX | 41 | ARG |
| 46 | BX | 45 | ASN |
| 46 | BX | 46 | LEU |
| 46 | BX | 51 | VAL |
| 46 | BX | 58 | ILE |
| 46 | BX | 60 | PHE |
| 46 | BX | 70 | VAL |
| 46 | BX | 72 | GLU |
| 46 | BX | 73 | LEU |
| 46 | BX | 75 | GLU |
| 46 | BX | 80 | LEU |
| 46 | BX | 88 | LYS |
| 46 | BX | 95 | LEU |
| 47 | BY | 1 | MET |
| 47 | BY | 2 | LYS |
| 47 | BY | 3 | LEU |
| 47 | BY | 5 | GLU |
| 47 | BY | 19 | VAL |
| 47 | BY | 21 | LEU |
| 47 | BY | 24 | LEU |
| 47 | BY | 32 | LEU |
| 47 | BY | 35 | LEU |
| 47 | BY | 57 | ILE |
| 47 | BY | 61 | LEU |
| 47 | BY | 62 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48 | BZ | 1 | MET |
| 48 | BZ | 8 | LEU |
| 48 | BZ | 37 | LEU |
| 48 | BZ | 40 | THR |
| 48 | BZ | 43 | ILE |
| 48 | BZ | 52 | HIS |
| 48 | BZ | 55 | ARG |
| 48 | BZ | 56 | VAL |
| 49 | B1 | 60 | GLU |
| 50 | B2 | 3 | LYS |
| 50 | B2 | 4 | HIS |
| 50 | B2 | 11 | THR |
| 50 | B2 | 25 | LEU |
| 50 | B2 | 52 | TYR |
| 51 | B3 | 12 | GLU |
| 51 | B3 | 29 | ASN |
| 51 | B3 | 30 | THR |
| 51 | B3 | 34 | LEU |
| 51 | B3 | 42 | TRP |
| 52 | B4 | 4 | THR |
| 52 | B4 | 8 | ASN |
| 52 | B4 | 9 | ARG |
| 52 | B4 | 15 | THR |
| 52 | B4 | 19 | ARG |
| 52 | B4 | 24 | THR |
| 52 | B4 | 31 | LEU |
| 52 | B4 | 34 | ARG |
| 52 | B4 | 36 | GLN |
| 52 | B4 | 41 | ARG |
| 52 | B4 | 42 | LEU |
| 52 | B4 | 46 | VAL |
| 53 | B5 | 4 | MET |
| 53 | B5 | 11 | LYS |
| 53 | B5 | 19 | SER |
| 53 | B5 | 30 | ARG |
| 53 | B5 | 31 | HIS |
| 53 | B5 | 33 | ASN |
| 53 | B5 | 41 | ILE |
| 53 | B5 | 57 | ARG |
| 53 | B5 | 60 | LEU |
| 53 | B5 | 62 | LEU |
| 53 | B5 | 64 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | CB | 16 | HIS |
| 2 | CB | 27 | LYS |
| 2 | CB | 28 | PHE |
| 2 | CB | 60 | ASP |
| 2 | CB | 61 | LEU |
| 2 | CB | 71 | VAL |
| 2 | CB | 75 | LYS |
| 2 | CB | 76 | GLN |
| 2 | CB | 87 | ARG |
| 2 | CB | 93 | VAL |
| 2 | CB | 111 | ARG |
| 2 | CB | 117 | GLU |
| 2 | CB | 127 | ILE |
| 2 | CB | 128 | GLU |
| 2 | CB | 142 | LEU |
| 2 | CB | 153 | ARG |
| 2 | CB | 154 | LEU |
| 2 | CB | 158 | LEU |
| 2 | CB | 164 | VAL |
| 2 | CB | 169 | LYS |
| 2 | CB | 178 | ARG |
| 2 | CB | 187 | LEU |
| 2 | CB | 221 | LEU |
| 3 | CC | 3 | ASN |
| 3 | CC | 5 | ILE |
| 3 | CC | 11 | ARG |
| 3 | CC | 16 | ARG |
| 3 | CC | 29 | TYR |
| 3 | CC | 79 | ARG |
| 3 | CC | 95 | THR |
| 3 | CC | 111 | LEU |
| 3 | CC | 115 | LEU |
| 3 | CC | 131 | ARG |
| 3 | CC | 152 | ILE |
| 3 | CC | 165 | THR |
| 3 | CC | 167 | TRP |
| 3 | CC | 196 | LEU |
| 3 | CC | 202 | ILE |
| 4 | CD | 3 | ARG |
| 4 | CD | 4 | TYR |
| 4 | CD | 8 | VAL |
| 4 | CD | 9 | CYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | CD | 11 | LEU |
| 4 | CD | 21 | LEU |
| 4 | CD | 45 | GLN |
| 4 | CD | 49 | ARG |
| 4 | CD | 59 | ARG |
| 4 | CD | 72 | GLU |
| 4 | CD | 76 | ARG |
| 4 | CD | 92 | VAL |
| 4 | CD | 96 | LEU |
| 4 | CD | 103 | ASN |
| 4 | CD | 108 | LEU |
| 4 | CD | 110 | PHE |
| 4 | CD | 114 | ARG |
| 4 | CD | 119 | GLN |
| 4 | CD | 122 | ARG |
| 4 | CD | 129 | ASN |
| 4 | CD | 131 | ARG |
| 4 | CD | 135 | LEU |
| 4 | CD | 141 | ARG |
| 4 | CD | 144 | ASP |
| 4 | CD | 154 | ASN |
| 4 | CD | 155 | LEU |
| 4 | CD | 158 | ILE |
| 4 | CD | 166 | LYS |
| 4 | CD | 203 | VAL |
| 4 | CD | 208 | SER |
| 5 | CE | 8 | GLU |
| 5 | CE | 12 | LEU |
| 5 | CE | 16 | THR |
| 5 | CE | 18 | ARG |
| 5 | CE | 20 | GLN |
| 5 | CE | 31 | LEU |
| 5 | CE | 43 | LEU |
| 5 | CE | 47 | LYS |
| 5 | CE | 53 | LEU |
| 5 | CE | 55 | VAL |
| 5 | CE | 60 | TYR |
| 5 | CE | 64 | ARG |
| 5 | CE | 71 | LEU |
| 5 | CE | 73 | ASN |
| 5 | CE | 76 | ILE |
| 5 | CE | 78 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | CE | 79 | GLU |
| 5 | CE | 110 | LEU |
| 5 | CE | 116 | THR |
| 5 | CE | 120 | THR |
| 5 | CE | 126 | ARG |
| 5 | CE | 147 | ASP |
| 6 | CF | 43 | LEU |
| 6 | CF | 46 | ARG |
| 6 | CF | 48 | LEU |
| 6 | CF | 63 | TYR |
| 6 | CF | 69 | GLU |
| 6 | CF | 89 | MET |
| 6 | CF | 100 | ASN |
| 7 | CG | 67 | GLU |
| 7 | CG | 91 | VAL |
| 7 | CG | 104 | LEU |
| 7 | CG | 118 | VAL |
| 7 | CG | 148 | ASN |
| 8 | CH | 1 | MET |
| 8 | CH | 8 | ASP |
| 8 | CH | 25 | ASP |
| 8 | CH | 26 | VAL |
| 8 | CH | 50 | ARG |
| 8 | CH | 52 | ASP |
| 8 | CH | 54 | ASP |
| 8 | CH | 73 | ASP |
| 8 | CH | 80 | ILE |
| 8 | CH | 91 | ARG |
| 8 | CH | 104 | ARG |
| 8 | CH | 107 | LEU |
| 8 | CH | 119 | LEU |
| 8 | CH | 127 | LEU |
| 8 | CH | 136 | GLU |
| 9 | CI | 10 | ARG |
| 9 | CI | 14 | VAL |
| 9 | CI | 88 | TYR |
| 9 | CI | 95 | LYS |
| 9 | CI | 99 | LEU |
| 9 | CI | 104 | ARG |
| 9 | CI | 109 | VAL |
| 9 | CI | 114 | TYR |
| 9 | CI | 121 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | CI | 124 | GLN |
| 10 | CJ | 16 | LEU |
| 10 | CJ | 22 | LYS |
| 10 | CJ | 49 | VAL |
| 10 | CJ | 55 | LYS |
| 10 | CJ | 62 | HIS |
| 10 | CJ | 63 | PHE |
| 10 | CJ | 66 | ARG |
| 10 | CJ | 74 | ILE |
| 10 | CJ | 92 | THR |
| 10 | CJ | 96 | ILE |
| 11 | CK | 14 | VAL |
| 11 | CK | 29 | ILE |
| 11 | CK | 32 | ILE |
| 11 | CK | 33 | THR |
| 11 | CK | 34 | ASP |
| 11 | CK | 40 | ILE |
| 11 | CK | 48 | ILE |
| 11 | CK | 80 | VAL |
| 11 | CK | 81 | ASP |
| 11 | CK | 92 | GLU |
| 11 | CK | 103 | LEU |
| 11 | CK | 114 | VAL |
| 11 | CK | 117 | ASN |
| 11 | CK | 126 | ARG |
| 12 | CL | 5 | THR |
| 12 | CL | 6 | ILE |
| 12 | CL | 9 | LEU |
| 12 | CL | 10 | VAL |
| 12 | CL | 19 | LYS |
| 12 | CL | 31 | PHE |
| 12 | CL | 35 | VAL |
| 12 | CL | 40 | ARG |
| 12 | CL | 41 | THR |
| 12 | CL | 42 | VAL |
| 12 | CL | 43 | THR |
| 12 | CL | 52 | ARG |
| 12 | CL | 59 | LEU |
| 12 | CL | 61 | SER |
| 12 | CL | 65 | VAL |
| 12 | CL | 69 | ILE |
| 12 | CL | 83 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | CL | 84 | ILE |
| 12 | CL | 95 | VAL |
| 12 | CL | 99 | ILE |
| 12 | CL | 109 | VAL |
| 13 | CM | 58 | GLU |
| 13 | CM | 64 | TRP |
| 13 | CM | 87 | TYR |
| 13 | CM | 93 | ARG |
| 13 | CM | 105 | THR |
| 13 | CM | 106 | ASN |
| 13 | CM | 115 | LYS |
| 14 | CN | 16 | PHE |
| 14 | CN | 41 | ARG |
| 14 | CN | 42 | ILE |
| 14 | CN | 44 | LEU |
| 15 | CO | 5 | LYS |
| 15 | CO | 17 | ARG |
| 15 | CO | 34 | LEU |
| 15 | CO | 39 | LEU |
| 15 | CO | 44 | LYS |
| 15 | CO | 45 | VAL |
| 15 | CO | 63 | ARG |
| 15 | CO | 66 | LEU |
| 15 | CO | 67 | LEU |
| 15 | CO | 82 | ILE |
| 16 | CP | 1 | MET |
| 16 | CP | 2 | VAL |
| 16 | CP | 16 | HIS |
| 16 | CP | 17 | TYR |
| 16 | CP | 20 | VAL |
| 16 | CP | 27 | LYS |
| 16 | CP | 28 | ARG |
| 16 | CP | 32 | TYR |
| 16 | CP | 47 | ASP |
| 16 | CP | 61 | SER |
| 16 | CP | 65 | GLN |
| 16 | CP | 69 | THR |
| 16 | CP | 72 | ARG |
| 16 | CP | 74 | LEU |
| 16 | CP | 82 | GLN |
| 16 | CP | 83 | GLU |
| 17 | CQ | 4 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17 | CQ | 7 | THR |
| 17 | CQ | 9 | VAL |
| 17 | CQ | 10 | VAL |
| 17 | CQ | 11 | VAL |
| 17 | CQ | 19 | VAL |
| 17 | CQ | 23 | VAL |
| 17 | CQ | 38 | ARG |
| 17 | CQ | 43 | LEU |
| 17 | CQ | 52 | LYS |
| 17 | CQ | 57 | VAL |
| 17 | CQ | 59 | ILE |
| 17 | CQ | 70 | ARG |
| 17 | CQ | 74 | LEU |
| 17 | CQ | 85 | VAL |
| 18 | CR | 65 | ILE |
| 18 | CR | 84 | LYS |
| 18 | CR | 88 | LYS |
| 19 | CS | 6 | LYS |
| 19 | CS | 7 | LYS |
| 19 | CS | 22 | LEU |
| 19 | CS | 27 | GLU |
| 19 | CS | 29 | ARG |
| 19 | CS | 37 | ARG |
| 19 | CS | 44 | MET |
| 19 | CS | 49 | ILE |
| 19 | CS | 53 | ASN |
| 20 | CT | 9 | ASN |
| 20 | CT | 10 | LEU |
| 20 | CT | 22 | ARG |
| 20 | CT | 26 | ASN |
| 20 | CT | 30 | LYS |
| 20 | CT | 55 | ILE |
| 20 | CT | 57 | ARG |
| 20 | CT | 62 | LEU |
| 20 | CT | 73 | HIS |
| 20 | CT | 93 | GLU |
| 20 | CT | 100 | ILE |
| 25 | DC | 10 | THR |
| 25 | DC | 13 | ARG |
| 25 | DC | 14 | ARG |
| 25 | DC | 16 | MET |
| 25 | DC | 33 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | DC | 38 | LYS |
| 25 | DC | 44 | ASN |
| 25 | DC | 61 | LEU |
| 25 | DC | 68 | LYS |
| 25 | DC | 69 | ARG |
| 25 | DC | 73 | VAL |
| 25 | DC | 87 | ASN |
| 25 | DC | 94 | LEU |
| 25 | DC | 95 | LEU |
| 25 | DC | 99 | ASP |
| 25 | DC | 102 | LYS |
| 25 | DC | 103 | ARG |
| 25 | DC | 105 | ILE |
| 25 | DC | 111 | LEU |
| 25 | DC | 112 | GLN |
| 25 | DC | 125 | ILE |
| 25 | DC | 126 | GLN |
| 25 | DC | 131 | LEU |
| 25 | DC | 134 | ARG |
| 25 | DC | 138 | VAL |
| 25 | DC | 141 | VAL |
| 25 | DC | 150 | LYS |
| 25 | DC | 154 | LYS |
| 25 | DC | 155 | LEU |
| 25 | DC | 166 | GLN |
| 25 | DC | 171 | ASP |
| 25 | DC | 174 | ILE |
| 25 | DC | 192 | THR |
| 25 | DC | 193 | VAL |
| 25 | DC | 198 | ASN |
| 25 | DC | 200 | ASP |
| 25 | DC | 204 | ILE |
| 25 | DC | 205 | VAL |
| 25 | DC | 211 | ARG |
| 25 | DC | 212 | SER |
| 25 | DC | 217 | ARG |
| 25 | DC | 218 | ARG |
| 25 | DC | 226 | MET |
| 25 | DC | 227 | ASN |
| 25 | DC | 229 | VAL |
| 25 | DC | 237 | GLU |
| 25 | DC | 242 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | DC | 244 | ARG |
| 25 | DC | 254 | THR |
| 25 | DC | 259 | THR |
| 25 | DC | 271 | ILE |
| 26 | DD | 1 | MET |
| 26 | DD | 4 | ILE |
| 26 | DD | 9 | VAL |
| 26 | DD | 16 | ARG |
| 26 | DD | 18 | ASP |
| 26 | DD | 33 | VAL |
| 26 | DD | 34 | VAL |
| 26 | DD | 40 | GLU |
| 26 | DD | 45 | THR |
| 26 | DD | 49 | LEU |
| 26 | DD | 54 | GLN |
| 26 | DD | 57 | LYS |
| 26 | DD | 76 | ARG |
| 26 | DD | 77 | ILE |
| 26 | DD | 78 | LEU |
| 26 | DD | 79 | ARG |
| 26 | DD | 84 | PHE |
| 26 | DD | 95 | ILE |
| 26 | DD | 116 | VAL |
| 26 | DD | 121 | ASN |
| 26 | DD | 122 | PHE |
| 26 | DD | 141 | ILE |
| 26 | DD | 144 | ARG |
| 26 | DD | 145 | LYS |
| 26 | DD | 152 | LYS |
| 26 | DD | 154 | LYS |
| 26 | DD | 156 | MET |
| 26 | DD | 160 | TYR |
| 26 | DD | 169 | ASN |
| 26 | DD | 170 | LEU |
| 26 | DD | 171 | GLU |
| 26 | DD | 173 | VAL |
| 26 | DD | 175 | VAL |
| 26 | DD | 176 | ILE |
| 26 | DD | 181 | LEU |
| 26 | DD | 184 | VAL |
| 27 | DE | 6 | MET |
| 27 | DE | 8 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27 | DE | 9 | ILE |
| 27 | DE | 24 | LEU |
| 27 | DE | 33 | LEU |
| 27 | DE | 46 | ARG |
| 27 | DE | 48 | THR |
| 27 | DE | 50 | SER |
| 27 | DE | 53 | THR |
| 27 | DE | 62 | ARG |
| 27 | DE | 64 | ILE |
| 27 | DE | 65 | TRP |
| 27 | DE | 67 | GLN |
| 27 | DE | 68 | LYS |
| 27 | DE | 70 | THR |
| 27 | DE | 74 | ARG |
| 27 | DE | 78 | ILE |
| 27 | DE | 82 | ILE |
| 27 | DE | 88 | VAL |
| 27 | DE | 98 | SER |
| 27 | DE | 100 | THR |
| 27 | DE | 106 | ARG |
| 27 | DE | 122 | LYS |
| 27 | DE | 127 | GLU |
| 27 | DE | 129 | PHE |
| 27 | DE | 136 | THR |
| 27 | DE | 158 | THR |
| 27 | DE | 160 | ASN |
| 27 | DE | 164 | ARG |
| 27 | DE | 165 | ARG |
| 27 | DE | 174 | VAL |
| 27 | DE | 175 | THR |
| 27 | DE | 181 | LEU |
| 27 | DE | 183 | VAL |
| 27 | DE | 192 | LEU |
| 27 | DE | 194 | MET |
| 27 | DE | 197 | ASP |
| 28 | DF | 5 | LEU |
| 28 | DF | 8 | LYS |
| 28 | DF | 26 | GLN |
| 28 | DF | 33 | ARG |
| 28 | DF | 35 | GLU |
| 28 | DF | 47 | LYS |
| 28 | DF | 78 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28 | DF | 86 | MET |
| 28 | DF | 90 | LEU |
| 28 | DF | 93 | THR |
| 28 | DF | 94 | LEU |
| 28 | DF | 98 | ARG |
| 28 | DF | 107 | LEU |
| 28 | DF | 115 | ARG |
| 28 | DF | 128 | ARG |
| 28 | DF | 143 | GLU |
| 28 | DF | 155 | MET |
| 28 | DF | 157 | ILE |
| 28 | DF | 159 | VAL |
| 28 | DF | 161 | THR |
| 28 | DF | 166 | ASP |
| 29 | DG | 13 | LYS |
| 29 | DG | 23 | ARG |
| 29 | DG | 34 | GLU |
| 29 | DG | 37 | VAL |
| 29 | DG | 52 | VAL |
| 29 | DG | 57 | ASP |
| 29 | DG | 60 | ARG |
| 29 | DG | 71 | LEU |
| 29 | DG | 90 | LYS |
| 29 | DG | 94 | TYR |
| 29 | DG | 101 | ARG |
| 29 | DG | 116 | GLU |
| 29 | DG | 122 | THR |
| 29 | DG | 123 | PHE |
| 29 | DG | 124 | GLU |
| 29 | DG | 129 | THR |
| 29 | DG | 133 | VAL |
| 29 | DG | 136 | ILE |
| 29 | DG | 139 | GLN |
| 29 | DG | 140 | LYS |
| 29 | DG | 147 | ASN |
| 29 | DG | 151 | ILE |
| 29 | DG | 158 | HIS |
| 29 | DG | 162 | ILE |
| 29 | DG | 163 | TYR |
| 30 | DH | 3 | VAL |
| 30 | DH | 4 | ILE |
| 30 | DH | 5 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30 | DH | 6 | LEU |
| 30 | DH | 14 | ASP |
| 30 | DH | 20 | ASP |
| 30 | DH | 21 | VAL |
| 30 | DH | 33 | ARG |
| 30 | DH | 40 | THR |
| 30 | DH | 50 | ARG |
| 30 | DH | 67 | ARG |
| 30 | DH | 68 | LEU |
| 30 | DH | 73 | GLU |
| 30 | DH | 77 | LEU |
| 30 | DH | 89 | TYR |
| 30 | DH | 91 | SER |
| 30 | DH | 109 | ILE |
| 30 | DH | 135 | GLU |
| 30 | DH | 142 | VAL |
| 31 | DI | 3 | ASN |
| 31 | DI | 58 | LEU |
| 32 | DJ | 38 | LEU |
| 32 | DJ | 39 | ILE |
| 32 | DJ | 42 | GLU |
| 32 | DJ | 46 | LEU |
| 32 | DJ | 51 | THR |
| 32 | DJ | 56 | LEU |
| 32 | DJ | 57 | LEU |
| 32 | DJ | 71 | MET |
| 32 | DJ | 83 | ILE |
| 32 | DJ | 86 | THR |
| 32 | DJ | 92 | GLN |
| 32 | DJ | 96 | THR |
| 32 | DJ | 105 | LEU |
| 32 | DJ | 106 | LYS |
| 32 | DJ | 110 | LEU |
| 32 | DJ | 112 | LYS |
| 32 | DJ | 113 | MET |
| 32 | DJ | 116 | THR |
| 32 | DJ | 117 | HIS |
| 32 | DJ | 122 | LEU |
| 32 | DJ | 126 | VAL |
| 32 | DJ | 129 | MET |
| 32 | DJ | 132 | LYS |
| 32 | DJ | 137 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | DJ | 142 | ARG |
| 32 | DJ | 143 | LEU |
| 32 | DJ | 144 | LYS |
| 32 | DJ | 146 | TYR |
| 32 | DJ | 154 | GLN |
| 32 | DJ | 160 | LYS |
| 32 | DJ | 161 | LEU |
| 33 | DK | 2 | ILE |
| 33 | DK | 3 | GLN |
| 33 | DK | 4 | PRO |
| 33 | DK | 19 | ILE |
| 33 | DK | 22 | ILE |
| 33 | DK | 23 | ARG |
| 33 | DK | 24 | VAL |
| 33 | DK | 26 | LYS |
| 33 | DK | 31 | LYS |
| 33 | DK | 32 | TYR |
| 33 | DK | 47 | ILE |
| 33 | DK | 52 | VAL |
| 33 | DK | 65 | THR |
| 33 | DK | 78 | ARG |
| 33 | DK | 87 | ILE |
| 33 | DK | 89 | ASN |
| 33 | DK | 90 | GLN |
| 33 | DK | 91 | LEU |
| 33 | DK | 98 | VAL |
| 33 | DK | 99 | PHE |
| 33 | DK | 102 | VAL |
| 33 | DK | 115 | VAL |
| 34 | DL | 6 | LEU |
| 34 | DL | 9 | ASN |
| 34 | DL | 15 | ARG |
| 34 | DL | 16 | ARG |
| 34 | DL | 18 | ARG |
| 34 | DL | 19 | VAL |
| 34 | DL | 29 | LYS |
| 34 | DL | 33 | ARG |
| 34 | DL | 39 | LYS |
| 34 | DL | 40 | SER |
| 34 | DL | 42 | SER |
| 34 | DL | 49 | ARG |
| 34 | DL | 50 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 34 | DL | 51 | PHE |
| 34 | DL | 52 | GLU |
| 34 | DL | 55 | ARG |
| 34 | DL | 56 | SER |
| 34 | DL | 57 | THR |
| 34 | DL | 59 | LEU |
| 34 | DL | 61 | ARG |
| 34 | DL | 62 | LEU |
| 34 | DL | 67 | MET |
| 34 | DL | 75 | ILE |
| 34 | DL | 81 | GLN |
| 34 | DL | 85 | LEU |
| 34 | DL | 88 | LEU |
| 34 | DL | 91 | PHE |
| 34 | DL | 105 | LEU |
| 34 | DL | 111 | ARG |
| 34 | DL | 114 | ILE |
| 34 | DL | 123 | LEU |
| 34 | DL | 135 | LEU |
| 34 | DL | 144 | GLU |
| 34 | DL | 146 | VAL |
| 34 | DL | 147 | LEU |
| 34 | DL | 148 | LEU |
| 35 | DM | 6 | ARG |
| 35 | DM | 9 | TYR |
| 35 | DM | 11 | LYS |
| 35 | DM | 13 | GLN |
| 35 | DM | 22 | LYS |
| 35 | DM | 25 | ASP |
| 35 | DM | 43 | THR |
| 35 | DM | 45 | GLN |
| 35 | DM | 52 | VAL |
| 35 | DM | 58 | PHE |
| 35 | DM | 59 | ARG |
| 35 | DM | 63 | LYS |
| 35 | DM | 66 | ILE |
| 35 | DM | 79 | LEU |
| 35 | DM | 80 | GLU |
| 35 | DM | 81 | VAL |
| 35 | DM | 83 | MET |
| 35 | DM | 89 | ASN |
| 35 | DM | 103 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35 | DM | 106 | VAL |
| 35 | DM | 109 | VAL |
| 35 | DM | 115 | MET |
| 35 | DM | 119 | ARG |
| 35 | DM | 132 | VAL |
| 35 | DM | 135 | ASP |
| 36 | DN | 2 | ARG |
| 36 | DN | 10 | LEU |
| 36 | DN | 15 | SER |
| 36 | DN | 17 | ARG |
| 36 | DN | 28 | LEU |
| 36 | DN | 35 | THR |
| 36 | DN | 37 | THR |
| 36 | DN | 40 | LYS |
| 36 | DN | 44 | LEU |
| 36 | DN | 48 | VAL |
| 36 | DN | 52 | ILE |
| 36 | DN | 54 | LEU |
| 36 | DN | 60 | LEU |
| 36 | DN | 63 | ARG |
| 36 | DN | 67 | LEU |
| 36 | DN | 70 | LEU |
| 36 | DN | 75 | LEU |
| 36 | DN | 79 | LEU |
| 36 | DN | 95 | THR |
| 36 | DN | 98 | LEU |
| 36 | DN | 99 | LYS |
| 36 | DN | 104 | ARG |
| 36 | DN | 107 | ASP |
| 36 | DN | 111 | LEU |
| 37 | DO | 12 | PHE |
| 37 | DO | 13 | ARG |
| 37 | DO | 26 | LEU |
| 37 | DO | 30 | ARG |
| 37 | DO | 36 | TYR |
| 37 | DO | 40 | ILE |
| 37 | DO | 44 | LYS |
| 37 | DO | 48 | LEU |
| 37 | DO | 54 | LEU |
| 37 | DO | 63 | THR |
| 37 | DO | 69 | VAL |
| 37 | DO | 92 | TYR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 37 | DO | 93 | LYS |
| 37 | DO | 101 | LEU |
| 38 | DP | 15 | VAL |
| 38 | DP | 19 | LEU |
| 38 | DP | 23 | ARG |
| 38 | DP | 28 | VAL |
| 38 | DP | 30 | VAL |
| 38 | DP | 39 | ARG |
| 38 | DP | 41 | ARG |
| 38 | DP | 50 | ILE |
| 38 | DP | 51 | ARG |
| 38 | DP | 53 | ARG |
| 38 | DP | 54 | ARG |
| 38 | DP | 58 | ASN |
| 38 | DP | 63 | VAL |
| 38 | DP | 64 | ARG |
| 38 | DP | 75 | ILE |
| 38 | DP | 84 | GLN |
| 38 | DP | 85 | LYS |
| 38 | DP | 86 | ILE |
| 38 | DP | 87 | ASP |
| 38 | DP | 88 | ILE |
| 38 | DP | 89 | VAL |
| 38 | DP | 99 | LEU |
| 38 | DP | 100 | TYR |
| 38 | DP | 104 | ASN |
| 38 | DP | 112 | ARG |
| 38 | DP | 113 | LYS |
| 38 | DP | 115 | ARG |
| 39 | DQ | 8 | VAL |
| 39 | DQ | 14 | HIS |
| 39 | DQ | 18 | LEU |
| 39 | DQ | 20 | LEU |
| 39 | DQ | 27 | LEU |
| 39 | DQ | 34 | LYS |
| 39 | DQ | 40 | PHE |
| 39 | DQ | 47 | TYR |
| 39 | DQ | 52 | ARG |
| 39 | DQ | 55 | ARG |
| 39 | DQ | 62 | ILE |
| 39 | DQ | 64 | ARG |
| 39 | DQ | 70 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39 | DQ | 76 | TYR |
| 39 | DQ | 79 | PHE |
| 39 | DQ | 80 | ILE |
| 39 | DQ | 92 | ARG |
| 39 | DQ | 97 | ASP |
| 39 | DQ | 101 | ARG |
| 39 | DQ | 108 | GLU |
| 39 | DQ | 112 | ARG |
| 40 | DR | 5 | VAL |
| 40 | DR | 10 | LYS |
| 40 | DR | 12 | TYR |
| 40 | DR | 13 | ARG |
| 40 | DR | 18 | LEU |
| 40 | DR | 20 | LEU |
| 40 | DR | 21 | ARG |
| 40 | DR | 33 | VAL |
| 40 | DR | 37 | VAL |
| 40 | DR | 39 | LEU |
| 40 | DR | 44 | LYS |
| 40 | DR | 53 | GLU |
| 40 | DR | 57 | VAL |
| 40 | DR | 66 | ARG |
| 40 | DR | 72 | VAL |
| 40 | DR | 78 | LYS |
| 40 | DR | 79 | VAL |
| 40 | DR | 80 | GLN |
| 40 | DR | 88 | ARG |
| 40 | DR | 98 | GLU |
| 40 | DR | 99 | ILE |
| 41 | DS | 1 | MET |
| 41 | DS | 8 | ARG |
| 41 | DS | 10 | VAL |
| 41 | DS | 11 | ARG |
| 41 | DS | 15 | ARG |
| 41 | DS | 17 | VAL |
| 41 | DS | 19 | LEU |
| 41 | DS | 23 | LEU |
| 41 | DS | 28 | SER |
| 41 | DS | 33 | ARG |
| 41 | DS | 36 | LEU |
| 41 | DS | 39 | THR |
| 41 | DS | 47 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41 | DS | 51 | LEU |
| 41 | DS | 53 | SER |
| 41 | DS | 60 | ASN |
| 41 | DS | 61 | ASN |
| 41 | DS | 69 | LEU |
| 41 | DS | 75 | TYR |
| 41 | DS | 76 | VAL |
| 41 | DS | 78 | GLU |
| 41 | DS | 84 | ARG |
| 41 | DS | 92 | ARG |
| 41 | DS | 100 | THR |
| 41 | DS | 105 | VAL |
| 41 | DS | 107 | LEU |
| 42 | DT | 9 | LEU |
| 42 | DT | 12 | VAL |
| 42 | DT | 28 | PHE |
| 42 | DT | 39 | ILE |
| 42 | DT | 45 | THR |
| 42 | DT | 49 | VAL |
| 42 | DT | 52 | VAL |
| 42 | DT | 57 | LEU |
| 42 | DT | 62 | LYS |
| 42 | DT | 65 | ARG |
| 42 | DT | 68 | ARG |
| 42 | DT | 70 | LEU |
| 42 | DT | 80 | ILE |
| 42 | DT | 81 | VAL |
| 43 | DU | 4 | LYS |
| 43 | DU | 6 | HIS |
| 43 | DU | 8 | LYS |
| 43 | DU | 9 | LYS |
| 43 | DU | 30 | VAL |
| 43 | DU | 31 | LEU |
| 43 | DU | 32 | PRO |
| 43 | DU | 60 | PHE |
| 43 | DU | 61 | ILE |
| 43 | DU | 62 | GLU |
| 43 | DU | 63 | LYS |
| 43 | DU | 71 | LYS |
| 43 | DU | 76 | CYS |
| 43 | DU | 89 | PHE |
| 43 | DU | 90 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 43 | DU | 97 | ARG |
| 43 | DU | 98 | VAL |
| 44 | DV | 3 | TYR |
| 44 | DV | 24 | LEU |
| 44 | DV | 27 | VAL |
| 44 | DV | 31 | ARG |
| 44 | DV | 35 | ARG |
| 44 | DV | 39 | VAL |
| 44 | DV | 42 | VAL |
| 44 | DV | 70 | LEU |
| 44 | DV | 72 | ARG |
| 44 | DV | 81 | ARG |
| 44 | DV | 82 | ARG |
| 44 | DV | 85 | HIS |
| 44 | DV | 86 | VAL |
| 44 | DV | 89 | PHE |
| 44 | DV | 94 | GLU |
| 44 | DV | 98 | MET |
| 44 | DV | 118 | GLN |
| 44 | DV | 140 | ASP |
| 44 | DV | 146 | ILE |
| 44 | DV | 150 | LEU |
| 44 | DV | 161 | VAL |
| 44 | DV | 163 | LEU |
| 45 | DW | 17 | GLN |
| 45 | DW | 20 | ARG |
| 45 | DW | 21 | LEU |
| 45 | DW | 38 | VAL |
| 45 | DW | 53 | MET |
| 45 | DW | 63 | VAL |
| 45 | DW | 64 | ASP |
| 45 | DW | 84 | LEU |
| 46 | DX | 8 | SER |
| 46 | DX | 13 | ILE |
| 46 | DX | 17 | SER |
| 46 | DX | 18 | ILE |
| 46 | DX | 21 | ARG |
| 46 | DX | 25 | LYS |
| 46 | DX | 27 | GLU |
| 46 | DX | 37 | ILE |
| 46 | DX | 38 | SER |
| 46 | DX | 40 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46 | DX | 41 | ARG |
| 46 | DX | 45 | ASN |
| 46 | DX | 46 | LEU |
| 46 | DX | 51 | VAL |
| 46 | DX | 58 | ILE |
| 46 | DX | 60 | PHE |
| 46 | DX | 70 | VAL |
| 46 | DX | 72 | GLU |
| 46 | DX | 73 | LEU |
| 46 | DX | 75 | GLU |
| 46 | DX | 80 | LEU |
| 46 | DX | 88 | LYS |
| 46 | DX | 95 | LEU |
| 47 | DY | 1 | MET |
| 47 | DY | 2 | LYS |
| 47 | DY | 3 | LEU |
| 47 | DY | 5 | GLU |
| 47 | DY | 19 | VAL |
| 47 | DY | 21 | LEU |
| 47 | DY | 24 | LEU |
| 47 | DY | 32 | LEU |
| 47 | DY | 35 | LEU |
| 47 | DY | 57 | ILE |
| 47 | DY | 61 | LEU |
| 47 | DY | 62 | THR |
| 48 | DZ | 1 | MET |
| 48 | DZ | 8 | LEU |
| 48 | DZ | 37 | LEU |
| 48 | DZ | 40 | THR |
| 48 | DZ | 43 | ILE |
| 48 | DZ | 52 | HIS |
| 48 | DZ | 55 | ARG |
| 48 | DZ | 56 | VAL |
| 49 | D1 | 60 | GLU |
| 50 | D2 | 3 | LYS |
| 50 | D2 | 4 | HIS |
| 50 | D2 | 11 | THR |
| 50 | D2 | 25 | LEU |
| 50 | D2 | 49 | CYS |
| 50 | D2 | 52 | TYR |
| 51 | D3 | 12 | GLU |
| 51 | D3 | 29 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 51 | D3 | 30 | THR |
| 51 | D3 | 34 | LEU |
| 51 | D3 | 42 | TRP |
| 52 | D4 | 1 | MET |
| 52 | D4 | 4 | THR |
| 52 | D4 | 8 | ASN |
| 52 | D4 | 9 | ARG |
| 52 | D4 | 15 | THR |
| 52 | D4 | 19 | ARG |
| 52 | D4 | 24 | THR |
| 52 | D4 | 31 | LEU |
| 52 | D4 | 34 | ARG |
| 52 | D4 | 36 | GLN |
| 52 | D4 | 41 | ARG |
| 52 | D4 | 42 | LEU |
| 52 | D4 | 46 | VAL |
| 53 | D5 | 4 | MET |
| 53 | D5 | 11 | LYS |
| 53 | D5 | 19 | SER |
| 53 | D5 | 30 | ARG |
| 53 | D5 | 31 | HIS |
| 53 | D5 | 33 | ASN |
| 53 | D5 | 41 | ILE |
| 53 | D5 | 57 | ARG |
| 53 | D5 | 60 | LEU |
| 53 | D5 | 62 | LEU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (245) such sidechains are listed below:

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | AB | 37 | ASN |
| 2 | AB | 40 | HIS |
| 2 | AB | 110 | GLN |
| 2 | AB | 135 | GLN |
| 2 | AB | 212 | GLN |
| 3 | AC | 28 | GLN |
| 3 | AC | 31 | HIS |
| 3 | AC | 69 | HIS |
| 3 | AC | 136 | GLN |
| 3 | AC | 170 | GLN |
| 3 | AC | 176 | HIS |
| 4 | AD | 42 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | AD | 62 | GLN |
| 6 | AF | 100 | ASN |
| 7 | AG | 13 | GLN |
| 7 | AG | 96 | GLN |
| 8 | AH | 82 | HIS |
| 9 | AI | 23 | ASN |
| 9 | AI | 73 | GLN |
| 9 | AI | 117 | HIS |
| 9 | AI | 124 | GLN |
| 10 | AJ | 56 | HIS |
| 10 | AJ | 78 | ASN |
| 11 | AK | 26 | ASN |
| 12 | AL | 48 | ASN |
| 12 | AL | 74 | HIS |
| 12 | AL | 79 | HIS |
| 13 | AM | 101 | GLN |
| 15 | AO | 37 | ASN |
| 15 | AO | 46 | HIS |
| 15 | AO | 53 | HIS |
| 16 | AP | 82 | GLN |
| 19 | AS | 14 | HIS |
| 19 | AS | 53 | ASN |
| 19 | AS | 57 | HIS |
| 19 | AS | 65 | ASN |
| 20 | AT | 18 | GLN |
| 20 | AT | 26 | ASN |
| 25 | BC | 58 | HIS |
| 25 | BC | 87 | ASN |
| 25 | BC | 116 | GLN |
| 25 | BC | 126 | GLN |
| 25 | BC | 166 | GLN |
| 25 | BC | 186 | HIS |
| 25 | BC | 198 | ASN |
| 25 | BC | 220 | HIS |
| 25 | BC | 227 | ASN |
| 25 | BC | 231 | HIS |
| 25 | BC | 233 | HIS |
| 26 | BD | 60 | ASN |
| 26 | BD | 66 | HIS |
| 26 | BD | 85 | ASN |
| 26 | BD | 132 | HIS |
| 26 | BD | 143 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 26 | BD | 169 | ASN |
| 26 | BD | 192 | ASN |
| 27 | BE | 67 | GLN |
| 27 | BE | 75 | HIS |
| 27 | BE | 160 | ASN |
| 27 | BE | 169 | ASN |
| 28 | BF | 58 | GLN |
| 28 | BF | 108 | ASN |
| 28 | BF | 121 | ASN |
| 28 | BF | 132 | ASN |
| 29 | BG | 65 | HIS |
| 29 | BG | 147 | ASN |
| 30 | BH | 17 | GLN |
| 30 | BH | 104 | GLN |
| 30 | BH | 133 | HIS |
| 31 | BI | 3 | ASN |
| 31 | BI | 56 | ASN |
| 32 | BJ | 61 | HIS |
| 32 | BJ | 68 | ASN |
| 32 | BJ | 79 | ASN |
| 32 | BJ | 151 | HIS |
| 32 | BJ | 153 | HIS |
| 32 | BJ | 154 | GLN |
| 33 | BK | 82 | ASN |
| 34 | BL | 70 | GLN |
| 35 | BM | 45 | GLN |
| 36 | BN | 3 | HIS |
| 36 | BN | 16 | HIS |
| 36 | BN | 53 | HIS |
| 36 | BN | 61 | HIS |
| 36 | BN | 71 | GLN |
| 36 | BN | 91 | GLN |
| 38 | BP | 58 | ASN |
| 38 | BP | 84 | GLN |
| 38 | BP | 90 | GLN |
| 39 | BQ | 14 | HIS |
| 39 | BQ | 49 | HIS |
| 39 | BQ | 72 | HIS |
| 39 | BQ | 75 | ASN |
| 40 | BR | 11 | GLN |
| 40 | BR | 64 | HIS |
| 40 | BR | 87 | HIS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 41 | BS | 34 | ASN |
| 41 | BS | 57 | ASN |
| 41 | BS | 61 | ASN |
| 41 | BS | 102 | HIS |
| 42 | BT | 31 | HIS |
| 42 | BT | 41 | ASN |
| 42 | BT | 55 | ASN |
| 42 | BT | 82 | GLN |
| 42 | BT | 87 | GLN |
| 43 | BU | 6 | HIS |
| 44 | BV | 73 | GLN |
| 44 | BV | 121 | HIS |
| 45 | BW | 35 | ASN |
| 45 | BW | 50 | ASN |
| 46 | BX | 45 | ASN |
| 46 | BX | 56 | GLN |
| 46 | BX | 66 | HIS |
| 47 | BY | 47 | ASN |
| 47 | BY | 56 | GLN |
| 48 | BZ | 19 | GLN |
| 48 | BZ | 46 | ASN |
| 48 | BZ | 52 | HIS |
| 50 | B2 | 22 | HIS |
| 50 | B2 | 23 | HIS |
| 50 | B2 | 43 | HIS |
| 51 | B3 | 29 | ASN |
| 52 | B4 | 8 | ASN |
| 53 | B5 | 33 | ASN |
| 2 | CB | 37 | ASN |
| 2 | CB | 40 | HIS |
| 2 | CB | 110 | GLN |
| 2 | CB | 135 | GLN |
| 2 | CB | 212 | GLN |
| 3 | CC | 28 | GLN |
| 3 | CC | 31 | HIS |
| 3 | CC | 69 | HIS |
| 3 | CC | 170 | GLN |
| 4 | CD | 62 | GLN |
| 4 | CD | 123 | HIS |
| 4 | CD | 161 | ASN |
| 6 | CF | 100 | ASN |
| 7 | CG | 13 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | CG | 96 | GLN |
| 8 | CH | 15 | ASN |
| 8 | CH | 82 | HIS |
| 9 | CI | 23 | ASN |
| 9 | CI | 117 | HIS |
| 9 | CI | 124 | GLN |
| 10 | CJ | 56 | HIS |
| 10 | CJ | 78 | ASN |
| 11 | CK | 26 | ASN |
| 12 | CL | 48 | ASN |
| 12 | CL | 74 | HIS |
| 12 | CL | 79 | HIS |
| 13 | CM | 101 | GLN |
| 15 | CO | 37 | ASN |
| 15 | CO | 46 | HIS |
| 15 | CO | 53 | HIS |
| 16 | CP | 82 | GLN |
| 19 | CS | 14 | HIS |
| 19 | CS | 53 | ASN |
| 19 | CS | 57 | HIS |
| 19 | CS | 65 | ASN |
| 20 | CT | 18 | GLN |
| 20 | CT | 26 | ASN |
| 25 | DC | 58 | HIS |
| 25 | DC | 87 | ASN |
| 25 | DC | 116 | GLN |
| 25 | DC | 126 | GLN |
| 25 | DC | 143 | HIS |
| 25 | DC | 166 | GLN |
| 25 | DC | 186 | HIS |
| 25 | DC | 198 | ASN |
| 25 | DC | 220 | HIS |
| 25 | DC | 227 | ASN |
| 25 | DC | 231 | HIS |
| 25 | DC | 233 | HIS |
| 26 | DD | 60 | ASN |
| 26 | DD | 66 | HIS |
| 26 | DD | 85 | ASN |
| 26 | DD | 143 | ASN |
| 26 | DD | 169 | ASN |
| 26 | DD | 192 | ASN |
| 27 | DE | 67 | GLN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 27 | DE | 75 | HIS |
| 27 | DE | 160 | ASN |
| 27 | DE | 169 | ASN |
| 28 | DF | 58 | GLN |
| 28 | DF | 108 | ASN |
| 28 | DF | 121 | ASN |
| 28 | DF | 132 | ASN |
| 29 | DG | 65 | HIS |
| 29 | DG | 147 | ASN |
| 30 | DH | 17 | GLN |
| 30 | DH | 104 | GLN |
| 30 | DH | 133 | HIS |
| 31 | DI | 3 | ASN |
| 31 | DI | 56 | ASN |
| 32 | DJ | 61 | HIS |
| 32 | DJ | 68 | ASN |
| 32 | DJ | 79 | ASN |
| 32 | DJ | 151 | HIS |
| 32 | DJ | 154 | GLN |
| 33 | DK | 82 | ASN |
| 34 | DL | 70 | GLN |
| 36 | DN | 3 | HIS |
| 36 | DN | 16 | HIS |
| 36 | DN | 61 | HIS |
| 36 | DN | 71 | GLN |
| 36 | DN | 91 | GLN |
| 38 | DP | 58 | ASN |
| 38 | DP | 84 | GLN |
| 38 | DP | 90 | GLN |
| 39 | DQ | 14 | HIS |
| 39 | DQ | 49 | HIS |
| 39 | DQ | 72 | HIS |
| 39 | DQ | 75 | ASN |
| 40 | DR | 11 | GLN |
| 40 | DR | 87 | HIS |
| 41 | DS | 34 | ASN |
| 41 | DS | 57 | ASN |
| 41 | DS | 61 | ASN |
| 41 | DS | 102 | HIS |
| 42 | DT | 31 | HIS |
| 42 | DT | 41 | ASN |
| 42 | DT | 55 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42 | DT | 82 | GLN |
| 42 | DT | 87 | GLN |
| 43 | DU | 6 | HIS |
| 44 | DV | 73 | GLN |
| 44 | DV | 121 | HIS |
| 45 | DW | 35 | ASN |
| 45 | DW | 50 | ASN |
| 46 | DX | 45 | ASN |
| 46 | DX | 56 | GLN |
| 46 | DX | 66 | HIS |
| 47 | DY | 47 | ASN |
| 47 | DY | 56 | GLN |
| 48 | DZ | 19 | GLN |
| 48 | DZ | 46 | ASN |
| 48 | DZ | 52 | HIS |
| 50 | D2 | 22 | HIS |
| 50 | D2 | 23 | HIS |
| 50 | D2 | 43 | HIS |
| 51 | D3 | 29 | ASN |
| 51 | D3 | 49 | HIS |
| 52 | D4 | 8 | ASN |
| 53 | D5 | 31 | HIS |
| 53 | D5 | 33 | ASN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | AA | 1505/1506 (99%) | 293 (19%) | 14 (0%) |
| 1 | CA | 1505/1506 (99%) | 294 (19%) | 14 (0%) |
| 22 | AV | 32/43 (74%) | 3 (9%) | 0 |
| 22 | CV | 32/43 (74%) | 3 (9%) | 0 |
| 23 | BA | 2755/2879 (95%) | 584 (21%) | 27 (0%) |
| 23 | DA | 2757/2879 (95%) | 589 (21%) | 29 (1%) |
| 24 | BB | 118/119 (99%) | 26 (22%) | 0 |
| 24 | DB | 118/119 (99%) | 27 (22%) | 0 |
| All | All | 8822/9094 (97%) | 1819 (20%) | 84 (0%) |

All (1819) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 6 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 7 | G |
| 1 | AA | 9 | G |
| 1 | AA | 13 | U |
| 1 | AA | 14 | U |
| 1 | AA | 15 | G |
| 1 | AA | 32 | A |
| 1 | AA | 33 | A |
| 1 | AA | 39 | G |
| 1 | AA | 41 | G |
| 1 | AA | 42 | G |
| 1 | AA | 47 | C |
| 1 | AA | 48 | C |
| 1 | AA | 50 | A |
| 1 | AA | 51 | A |
| 1 | AA | 59 | A |
| 1 | AA | 61 | G |
| 1 | AA | 88 | C |
| 1 | AA | 97 | U |
| 1 | AA | 99 | C |
| 1 | AA | 110 | C |
| 1 | AA | 115 | G |
| 1 | AA | 116 | A |
| 1 | AA | 120 | A |
| 1 | AA | 121 | C |
| 1 | AA | 131 | C |
| 1 | AA | 144 | G |
| 1 | AA | 151 | A |
| 1 | AA | 163 | C |
| 1 | AA | 171 | A |
| 1 | AA | 182 | U |
| 1 | AA | 183 | G |
| 1 | AA | 189 | U |
| 1 | AA | 190 | G |
| 1 | AA | 195 | A |
| 1 | AA | 196 | A |
| 1 | AA | 197 | A |
| 1 | AA | 201 | C |
| 1 | AA | 209 | U |
| 1 | AA | 210 | U |
| 1 | AA | 231 | G |
| 1 | AA | 240 | C |
| 1 | AA | 247 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 250 | A |
| 1 | AA | 251 | G |
| 1 | AA | 252 | U |
| 1 | AA | 258 | G |
| 1 | AA | 266 | G |
| 1 | AA | 267 | C |
| 1 | AA | 280 | C |
| 1 | AA | 281 | G |
| 1 | AA | 289 | G |
| 1 | AA | 298 | A |
| 1 | AA | 305 | G |
| 1 | AA | 306 | G |
| 1 | AA | 320 | C |
| 1 | AA | 321 | A |
| 1 | AA | 328 | C |
| 1 | AA | 330 | C |
| 1 | AA | 332 | G |
| 1 | AA | 345 | C |
| 1 | AA | 347 | G |
| 1 | AA | 351 | G |
| 1 | AA | 352 | C |
| 1 | AA | 353 | A |
| 1 | AA | 354 | G |
| 1 | AA | 358 | U |
| 1 | AA | 364 | A |
| 1 | AA | 365 | U |
| 1 | AA | 366 | C |
| 1 | AA | 367 | U |
| 1 | AA | 372 | C |
| 1 | AA | 373 | A |
| 1 | AA | 382 | A |
| 1 | AA | 384 | G |
| 1 | AA | 387 | U |
| 1 | AA | 388 | G |
| 1 | AA | 397 | A |
| 1 | AA | 398 | C |
| 1 | AA | 406 | G |
| 1 | AA | 410 | G |
| 1 | AA | 412 | A |
| 1 | AA | 413 | G |
| 1 | AA | 414 | A |
| 1 | AA | 422 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 423 | G |
| 1 | AA | 427 | U |
| 1 | AA | 429 | U |
| 1 | AA | 439 | A |
| 1 | AA | 452 | A |
| 1 | AA | 453 | A |
| 1 | AA | 457 | C |
| 1 | AA | 464 | G |
| 1 | AA | 465 | A |
| 1 | AA | 466 | G |
| 1 | AA | 467 | G |
| 1 | AA | 484 | G |
| 1 | AA | 485 | G |
| 1 | AA | 486 | U |
| 1 | AA | 496 | A |
| 1 | AA | 497 | U |
| 1 | AA | 500 | G |
| 1 | AA | 509 | A |
| 1 | AA | 511 | C |
| 1 | AA | 512 | U |
| 1 | AA | 518 | C |
| 1 | AA | 523 | A |
| 1 | AA | 527 | G |
| 1 | AA | 531 | U |
| 1 | AA | 532 | A |
| 1 | AA | 533 | A |
| 1 | AA | 547 | A |
| 1 | AA | 558 | G |
| 1 | AA | 559 | A |
| 1 | AA | 560 | U |
| 1 | AA | 561 | U |
| 1 | AA | 562 | C |
| 1 | AA | 567 | G |
| 1 | AA | 572 | A |
| 1 | AA | 573 | A |
| 1 | AA | 575 | G |
| 1 | AA | 576 | G |
| 1 | AA | 577 | G |
| 1 | AA | 580 | U |
| 1 | AA | 581 | G |
| 1 | AA | 596 | C |
| 1 | AA | 607 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | AA | 653 | A |
| 1 | AA | 665 | A |
| 1 | AA | 687 | A |
| 1 | AA | 688 | G |
| 1 | AA | 690 | G |
| 1 | AA | 693 | G |
| 1 | AA | 702 | A |
| 1 | AA | 718 | G |
| 1 | AA | 731 | G |
| 1 | AA | 733 | A |
| 1 | AA | 753 | A |
| 1 | AA | 777 | A |
| 1 | AA | 782 | A |
| 1 | AA | 792 | A |
| 1 | AA | 793 | U |
| 1 | AA | 794 | A |
| 1 | AA | 800 | G |
| 1 | AA | 810 | C |
| 1 | AA | 816 | A |
| 1 | AA | 817 | C |
| 1 | AA | 818 | G |
| 1 | AA | 819 | A |
| 1 | AA | 828 | A |
| 1 | AA | 829 | G |
| 1 | AA | 833 | U |
| 1 | AA | 841 | U |
| 1 | AA | 842 | C |
| 1 | AA | 843 | U |
| 1 | AA | 849 | C |
| 1 | AA | 859 | A |
| 1 | AA | 870 | U |
| 1 | AA | 873 | A |
| 1 | AA | 876 | G |
| 1 | AA | 884 | U |
| 1 | AA | 897 | C |
| 1 | AA | 902 | G |
| 1 | AA | 914 | A |
| 1 | AA | 916 | G |
| 1 | AA | 921 | U |
| 1 | AA | 922 | G |
| 1 | AA | 927 | G |
| 1 | AA | 934 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | AA | 935 | A |
| 1 | AA | 945 | G |
| 1 | AA | 951 | G |
| 1 | AA | 960 | U |
| 1 | AA | 961 | U |
| 1 | AA | 968 | A |
| 1 | AA | 969 | A |
| 1 | AA | 971 | G |
| 1 | AA | 972 | C |
| 1 | AA | 974 | A |
| 1 | AA | 976 | G |
| 1 | AA | 977 | A |
| 1 | AA | 980 | C |
| 1 | AA | 981 | U |
| 1 | AA | 982 | U |
| 1 | AA | 992 | U |
| 1 | AA | 993 | G |
| 1 | AA | 1004 | A |
| 1 | AA | 1006 | C |
| 1 | AA | 1009 | G |
| 1 | AA | 1025 | U |
| 1 | AA | 1045 | C |
| 1 | AA | 1054 | C |
| 1 | AA | 1055 | A |
| 1 | AA | 1065 | U |
| 1 | AA | 1067 | A |
| 1 | AA | 1068 | G |
| 1 | AA | 1080 | A |
| 1 | AA | 1081 | G |
| 1 | AA | 1094 | G |
| 1 | AA | 1095 | U |
| 1 | AA | 1101 | A |
| 1 | AA | 1117 | G |
| 1 | AA | 1118 | C |
| 1 | AA | 1124 | G |
| 1 | AA | 1125 | U |
| 1 | AA | 1126 | U |
| 1 | AA | 1129 | C |
| 1 | AA | 1130 | A |
| 1 | AA | 1131 | G |
| 1 | AA | 1136 | U |
| 1 | AA | 1137 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | AA | 1139 | G |
| 1 | AA | 1151 | A |
| 1 | AA | 1152 | A |
| 1 | AA | 1159 | U |
| 1 | AA | 1160 | G |
| 1 | AA | 1181 | G |
| 1 | AA | 1183 | A |
| 1 | AA | 1189 | C |
| 1 | AA | 1193 | G |
| 1 | AA | 1196 | U |
| 1 | AA | 1197 | G |
| 1 | AA | 1202 | G |
| 1 | AA | 1212 | U |
| 1 | AA | 1213 | A |
| 1 | AA | 1214 | C |
| 1 | AA | 1218 | C |
| 1 | AA | 1224 | G |
| 1 | AA | 1225 | A |
| 1 | AA | 1226 | C |
| 1 | AA | 1227 | A |
| 1 | AA | 1228 | C |
| 1 | AA | 1238 | A |
| 1 | AA | 1240 | U |
| 1 | AA | 1241 | G |
| 1 | AA | 1245 | A |
| 1 | AA | 1256 | A |
| 1 | AA | 1257 | U |
| 1 | AA | 1262 | C |
| 1 | AA | 1270 | C |
| 1 | AA | 1277 | C |
| 1 | AA | 1280 | A |
| 1 | AA | 1281 | U |
| 1 | AA | 1287 | A |
| 1 | AA | 1300 | G |
| 1 | AA | 1301 | U |
| 1 | AA | 1302 | U |
| 1 | AA | 1305 | G |
| 1 | AA | 1317 | C |
| 1 | AA | 1320 | C |
| 1 | AA | 1322 | C |
| 1 | AA | 1323 | G |
| 1 | AA | 1326 | C |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | AA | 1331 | G |
| 1 | AA | 1335 | C |
| 1 | AA | 1337 | G |
| 1 | AA | 1346 | A |
| 1 | AA | 1347 | G |
| 1 | AA | 1353 | G |
| 1 | AA | 136(B) | C |
| 1 | AA | 1363 | A |
| 1 | AA | 1364 | U |
| 1 | AA | 1366 | C |
| 1 | AA | 1378 | C |
| 1 | AA | 1379 | G |
| 1 | AA | 1397 | C |
| 1 | AA | 1401 | G |
| 1 | AA | 1419 | G |
| 1 | AA | 1440 | C |
| 1 | AA | 1442 | G |
| 1 | AA | 1443 | G |
| 1 | AA | 1446 | A |
| 1 | AA | 1447 | G |
| 1 | AA | 1451 | A |
| 1 | AA | 1452 | C |
| 1 | AA | 1454 | G |
| 1 | AA | 1469 | G |
| 1 | AA | 1483 | A |
| 1 | AA | 1487 | G |
| 1 | AA | 1492 | A |
| 1 | AA | 1494 | G |
| 1 | AA | 1497 | G |
| 1 | AA | 1502 | A |
| 1 | AA | 1503 | A |
| 1 | AA | 1504 | G |
| 1 | AA | 1506 | U |
| 1 | AA | 1514 | C |
| 1 | AA | 1517 | G |
| 1 | AA | 1519 | A |
| 1 | AA | 1520 | G |
| 1 | AA | 1528 | U |
| 1 | AA | 1529 | G |
| 1 | AA | 1530 | G |
| 22 | AV | 6182 | A |
| 22 | AV | 6187 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 22 | AV | 6194 | C |
| 23 | BA | 10 | G |
| 23 | BA | 11 | G |
| 23 | BA | 34 | C |
| 23 | BA | 35 | G |
| 23 | BA | 46 | C |
| 23 | BA | 64 | A |
| 23 | BA | 71 | A |
| 23 | BA | 72 | U |
| 23 | BA | 74 | A |
| 23 | BA | 75 | G |
| 23 | BA | 84 | A |
| 23 | BA | 96 | G |
| 23 | BA | 97 | C |
| 23 | BA | 101 | G |
| 23 | BA | 102 | G |
| 23 | BA | 116 | C |
| 23 | BA | 118 | A |
| 23 | BA | 119 | A |
| 23 | BA | 120 | U |
| 23 | BA | 125 | G |
| 23 | BA | 135 | G |
| 23 | BA | 138 | G |
| 23 | BA | 139 | G |
| 23 | BA | 140 | A |
| 23 | BA | 181 | A |
| 23 | BA | 192 | C |
| 23 | BA | 195 | A |
| 23 | BA | 196 | A |
| 23 | BA | 197 | A |
| 23 | BA | 198 | C |
| 23 | BA | 199 | A |
| 23 | BA | 205 | G |
| 23 | BA | 215 | G |
| 23 | BA | 216 | A |
| 23 | BA | 218 | A |
| 23 | BA | 221 | A |
| 23 | BA | 222 | A |
| 23 | BA | 225 | A |
| 23 | BA | 228 | A |
| 23 | BA | 229 | A |
| 23 | BA | 230 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 23 | BA | 244 | A |
| 23 | BA | 248 | G |
| 23 | BA | 249 | C |
| 23 | BA | 252 | G |
| 23 | BA | 257 | A |
| 23 | BA | 258 | G |
| 23 | BA | 265 | A |
| 23 | BA | 269 | U |
| 23 | BA | 270(K) | G |
| 23 | BA | 270(L) | C |
| 23 | BA | 270(M) | U |
| 23 | BA | 270(N) | U |
| 23 | BA | 270(O) | G |
| 23 | BA | 270(Q) | C |
| 23 | BA | 270(R) | C |
| 23 | BA | 271(D) | U |
| 23 | BA | 271 | G |
| 23 | BA | 274 | G |
| 23 | BA | 275 | G |
| 23 | BA | 276 | A |
| 23 | BA | 277 | C |
| 23 | BA | 278 | A |
| 23 | BA | 283 | A |
| 23 | BA | 302 | C |
| 23 | BA | 304 | G |
| 23 | BA | 311 | A |
| 23 | BA | 323 | G |
| 23 | BA | 324 | A |
| 23 | BA | 329 | G |
| 23 | BA | 330 | A |
| 23 | BA | 334 | C |
| 23 | BA | 335 | C |
| 23 | BA | 345 | A |
| 23 | BA | 352 | G |
| 23 | BA | 353 | G |
| 23 | BA | 360 | G |
| 23 | BA | 363(A) | G |
| 23 | BA | 372 | G |
| 23 | BA | 386 | G |
| 23 | BA | 396 | G |
| 23 | BA | 405 | U |
| 23 | BA | 406 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 23 | BA | 407 | G |
| 23 | BA | 411 | G |
| 23 | BA | 416 | C |
| 23 | BA | 421 | U |
| 23 | BA | 444 | C |
| 23 | BA | 455 | C |
| 23 | BA | 456 | C |
| 23 | BA | 457 | A |
| 23 | BA | 464 | U |
| 23 | BA | 467 | G |
| 23 | BA | 480 | A |
| 23 | BA | 481 | G |
| 23 | BA | 483 | A |
| 23 | BA | 491 | G |
| 23 | BA | 504 | U |
| 23 | BA | 505 | A |
| 23 | BA | 508 | G |
| 23 | BA | 509 | C |
| 23 | BA | 530 | G |
| 23 | BA | 531 | C |
| 23 | BA | 532 | A |
| 23 | BA | 533 | G |
| 23 | BA | 546 | C |
| 23 | BA | 547 | A |
| 23 | BA | 548 | A |
| 23 | BA | 558 | G |
| 23 | BA | 563 | G |
| 23 | BA | 566 | U |
| 23 | BA | 573 | G |
| 23 | BA | 575 | A |
| 23 | BA | 580 | C |
| 23 | BA | 586 | A |
| 23 | BA | 593 | G |
| 23 | BA | 595 | C |
| 23 | BA | 599 | G |
| 23 | BA | 603 | A |
| 23 | BA | 609(A) | A |
| 23 | BA | 615 | G |
| 23 | BA | 617 | G |
| 23 | BA | 620 | G |
| 23 | BA | 627 | A |
| 23 | BA | 632 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 23 | BA | 637 | A |
| 23 | BA | 645 | C |
| 23 | BA | 646 | A |
| 23 | BA | 654 | U |
| 23 | BA | 655 | A |
| 23 | BA | 682 | G |
| 23 | BA | 686 | G |
| 23 | BA | 694 | U |
| 23 | BA | 695 | G |
| 23 | BA | 717 | G |
| 23 | BA | 730 | C |
| 23 | BA | 739 | G |
| 23 | BA | 746 | A |
| 23 | BA | 747 | U |
| 23 | BA | 775 | G |
| 23 | BA | 776 | G |
| 23 | BA | 777 | A |
| 23 | BA | 782 | A |
| 23 | BA | 784 | A |
| 23 | BA | 785 | G |
| 23 | BA | 787 | U |
| 23 | BA | 792 | G |
| 23 | BA | 805 | G |
| 23 | BA | 812 | C |
| 23 | BA | 819 | A |
| 23 | BA | 822 | U |
| 23 | BA | 827 | U |
| 23 | BA | 828 | U |
| 23 | BA | 832 | G |
| 23 | BA | 846 | C |
| 23 | BA | 855 | G |
| 23 | BA | 857 | C |
| 23 | BA | 859 | G |
| 23 | BA | 868 | U |
| 23 | BA | 869 | G |
| 23 | BA | 878 | A |
| 23 | BA | 887 | A |
| 23 | BA | 889 | C |
| 23 | BA | 890 | A |
| 23 | BA | 896 | A |
| 23 | BA | 897 | C |
| 23 | BA | 910 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 23 | BA | 914 | C |
| 23 | BA | 915 | C |
| 23 | BA | 917 | A |
| 23 | BA | 919 | G |
| 23 | BA | 932 | G |
| 23 | BA | 933 | A |
| 23 | BA | 934 | G |
| 23 | BA | 938 | G |
| 23 | BA | 941 | A |
| 23 | BA | 946 | G |
| 23 | BA | 948 | G |
| 23 | BA | 957 | A |
| 23 | BA | 958 | U |
| 23 | BA | 959 | A |
| 23 | BA | 961 | C |
| 23 | BA | 964 | C |
| 23 | BA | 974(A) | G |
| 23 | BA | 974(B) | C |
| 23 | BA | 975 | G |
| 23 | BA | 979 | G |
| 23 | BA | 983 | A |
| 23 | BA | 989 | G |
| 23 | BA | 990 | A |
| 23 | BA | 991 | C |
| 23 | BA | 996 | A |
| 23 | BA | 1005 | C |
| 23 | BA | 1009 | A |
| 23 | BA | 1010 | A |
| 23 | BA | 1011 | G |
| 23 | BA | 1012 | U |
| 23 | BA | 1013 | C |
| 23 | BA | 1020 | A |
| 23 | BA | 1022 | G |
| 23 | BA | 1023 | U |
| 23 | BA | 1025 | G |
| 23 | BA | 1026 | U |
| 23 | BA | 1030 | G |
| 23 | BA | 1033 | U |
| 23 | BA | 1046 | A |
| 23 | BA | 1047 | G |
| 23 | BA | 1053 | C |
| 23 | BA | 1105 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 23 | BA | 1110 | G |
| 23 | BA | 1112 | G |
| 23 | BA | 1122 | G |
| 23 | BA | 1126 | A |
| 23 | BA | 1129 | A |
| 23 | BA | 1130 | U |
| 23 | BA | 1135 | C |
| 23 | BA | 1136 | G |
| 23 | BA | 1139 | G |
| 23 | BA | 1142 | U |
| 23 | BA | 114(B) | A |
| 23 | BA | 1143 | A |
| 23 | BA | 1144 | G |
| 23 | BA | 1151 | G |
| 23 | BA | 1155 | A |
| 23 | BA | 1156 | A |
| 23 | BA | 1174 | A |
| 23 | BA | 1175 | U |
| 23 | BA | 1177 | A |
| 23 | BA | 1178 | C |
| 23 | BA | 1190 | G |
| 23 | BA | 1205 | U |
| 23 | BA | 1210 | A |
| 23 | BA | 1211 | U |
| 23 | BA | 1212 | G |
| 23 | BA | 1220 | A |
| 23 | BA | 1221 | C |
| 23 | BA | 1227 | G |
| 23 | BA | 1236 | G |
| 23 | BA | 1248 | G |
| 23 | BA | 1253 | A |
| 23 | BA | 1256 | G |
| 23 | BA | 1269 | A |
| 23 | BA | 1271 | G |
| 23 | BA | 1272 | A |
| 23 | BA | 1273 | U |
| 23 | BA | 1287 | A |
| 23 | BA | 1288 | U |
| 23 | BA | 1289 | C |
| 23 | BA | 1300 | U |
| 23 | BA | 1301 | A |
| 23 | BA | 1310 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 23 | BA | 1313 | U |
| 23 | BA | 1314 | C |
| 23 | BA | 1317 | A |
| 23 | BA | 1329 | U |
| 23 | BA | 1332 | G |
| 23 | BA | 1338 | G |
| 23 | BA | 1343 | G |
| 23 | BA | 1344 | G |
| 23 | BA | 1345 | C |
| 23 | BA | 1349 | A |
| 23 | BA | 1352 | U |
| 23 | BA | 1359 | A |
| 23 | BA | 1360 | A |
| 23 | BA | 1365 | A |
| 23 | BA | 1368 | G |
| 23 | BA | 1380 | G |
| 23 | BA | 1384 | A |
| 23 | BA | 1385 | G |
| 23 | BA | 1396 | U |
| 23 | BA | 1405 | U |
| 23 | BA | 1416 | G |
| 23 | BA | 1417 | C |
| 23 | BA | 1420 | U |
| 23 | BA | 1427 | A |
| 23 | BA | 1428 | C |
| 23 | BA | 1434 | A |
| 23 | BA | 144(B) | A |
| 23 | BA | 1453 | A |
| 23 | BA | 1458 | C |
| 23 | BA | 1459 | G |
| 23 | BA | 1467 | C |
| 23 | BA | 1469 | A |
| 23 | BA | 1483 | G |
| 23 | BA | 1490 | A |
| 23 | BA | 1493 | C |
| 23 | BA | 1494 | A |
| 23 | BA | 1495 | A |
| 23 | BA | 1496 | A |
| 23 | BA | 1497 | U |
| 23 | BA | 1505 | C |
| 23 | BA | 1509 | A |
| 23 | BA | 1510 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 23 | BA | 1519 | G |
| 23 | BA | 1535 | U |
| 23 | BA | 1537 | C |
| 23 | BA | 1542 | G |
| 23 | BA | 1543 | A |
| 23 | BA | 1544 | C |
| 23 | BA | 1545 | A |
| 23 | BA | 1547 | C |
| 23 | BA | 1558 | A |
| 23 | BA | 1559 | G |
| 23 | BA | 1565 | C |
| 23 | BA | 1566 | A |
| 23 | BA | 1569 | A |
| 23 | BA | 1578 | U |
| 23 | BA | 1585 | C |
| 23 | BA | 1586 | A |
| 23 | BA | 1588 | C |
| 23 | BA | 1598 | C |
| 23 | BA | 1599 | C |
| 23 | BA | 1608 | A |
| 23 | BA | 1609 | A |
| 23 | BA | 1610 | A |
| 23 | BA | 1616 | A |
| 23 | BA | 1617 | C |
| 23 | BA | 1618 | A |
| 23 | BA | 1631 | A |
| 23 | BA | 1639 | U |
| 23 | BA | 1640 | C |
| 23 | BA | 1644 | C |
| 23 | BA | 1647 | G |
| 23 | BA | 1648 | C |
| 23 | BA | 1651 | G |
| 23 | BA | 1654 | A |
| 23 | BA | 1669 | A |
| 23 | BA | 1674 | G |
| 23 | BA | 1677 | A |
| 23 | BA | 1680 | U |
| 23 | BA | 1681 | G |
| 23 | BA | 1690 | A |
| 23 | BA | 1696 | G |
| 23 | BA | 1703 | G |
| 23 | BA | 1727 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 23 | BA | 1729 | A |
| 23 | BA | 1743 | G |
| 23 | BA | 1750 | G |
| 23 | BA | 1756 | G |
| 23 | BA | 1761 | C |
| 23 | BA | 1763 | G |
| 23 | BA | 1764 | G |
| 23 | BA | 1767 | C |
| 23 | BA | 1773 | A |
| 23 | BA | 1778 | U |
| 23 | BA | 1787 | A |
| 23 | BA | 1791 | A |
| 23 | BA | 1800 | C |
| 23 | BA | 1801 | G |
| 23 | BA | 1811 | G |
| 23 | BA | 1813 | G |
| 23 | BA | 1816 | G |
| 23 | BA | 1829 | A |
| 23 | BA | 1835 | G |
| 23 | BA | 1838 | C |
| 23 | BA | 1840 | G |
| 23 | BA | 1847 | A |
| 23 | BA | 1870 | C |
| 23 | BA | 1887 | C |
| 23 | BA | 1888 | G |
| 23 | BA | 1889 | A |
| 23 | BA | 1896 | G |
| 23 | BA | 1900 | A |
| 23 | BA | 1902 | C |
| 23 | BA | 1903 | G |
| 23 | BA | 1906 | G |
| 23 | BA | 1913 | A |
| 23 | BA | 1914 | C |
| 23 | BA | 1929 | G |
| 23 | BA | 1930 | G |
| 23 | BA | 1936 | A |
| 23 | BA | 1938 | A |
| 23 | BA | 1939 | U |
| 23 | BA | 1955 | U |
| 23 | BA | 1956 | U |
| 23 | BA | 1960 | A |
| 23 | BA | 1963 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 23 | BA | 1964 | G |
| 23 | BA | 1966 | A |
| 23 | BA | 1967 | C |
| 23 | BA | 1970 | A |
| 23 | BA | 1971 | A |
| 23 | BA | 1972 | A |
| 23 | BA | 1974 | C |
| 23 | BA | 1975 | G |
| 23 | BA | 1981 | A |
| 23 | BA | 1982 | C |
| 23 | BA | 1985 | G |
| 23 | BA | 1991 | U |
| 23 | BA | 1992 | G |
| 23 | BA | 1993 | U |
| 23 | BA | 1997 | G |
| 23 | BA | 2007 | C |
| 23 | BA | 2010 | G |
| 23 | BA | 2020 | A |
| 23 | BA | 2023 | G |
| 23 | BA | 2031 | A |
| 23 | BA | 2032 | G |
| 23 | BA | 2033 | A |
| 23 | BA | 2034 | U |
| 23 | BA | 2036 | C |
| 23 | BA | 2043 | C |
| 23 | BA | 2049 | G |
| 23 | BA | 2051 | A |
| 23 | BA | 2055 | C |
| 23 | BA | 2056 | G |
| 23 | BA | 2060 | A |
| 23 | BA | 2061 | G |
| 23 | BA | 2062 | A |
| 23 | BA | 2063 | C |
| 23 | BA | 2067 | G |
| 23 | BA | 2069 | G |
| 23 | BA | 2079 | U |
| 23 | BA | 2080 | G |
| 23 | BA | 2086 | U |
| 23 | BA | 2099 | U |
| 23 | BA | 2183 | C |
| 23 | BA | 2189 | U |
| 23 | BA | 2190 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 23 | BA | 2198 | A |
| 23 | BA | 2211 | G |
| 23 | BA | 2212 | A |
| 23 | BA | 2213 | U |
| 23 | BA | 2215 | G |
| 23 | BA | 2225 | A |
| 23 | BA | 2226 | C |
| 23 | BA | 2227 | A |
| 23 | BA | 2228 | G |
| 23 | BA | 2235 | G |
| 23 | BA | 2238 | G |
| 23 | BA | 2239 | G |
| 23 | BA | 2267 | A |
| 23 | BA | 2268 | A |
| 23 | BA | 2269 | A |
| 23 | BA | 2272 | U |
| 23 | BA | 2273 | A |
| 23 | BA | 2275 | C |
| 23 | BA | 2278 | A |
| 23 | BA | 2283 | C |
| 23 | BA | 2287 | A |
| 23 | BA | 2288 | A |
| 23 | BA | 2305 | A |
| 23 | BA | 2306 | C |
| 23 | BA | 2307 | G |
| 23 | BA | 2309 | A |
| 23 | BA | 2310 | A |
| 23 | BA | 2319 | G |
| 23 | BA | 2320 | A |
| 23 | BA | 2322 | A |
| 23 | BA | 2325 | G |
| 23 | BA | 2334 | G |
| 23 | BA | 2336 | A |
| 23 | BA | 2343 | C |
| 23 | BA | 2346 | A |
| 23 | BA | 2347 | C |
| 23 | BA | 2350 | C |
| 23 | BA | 2358 | G |
| 23 | BA | 2361 | A |
| 23 | BA | 2365 | G |
| 23 | BA | 2379 | G |
| 23 | BA | 2383 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 23 | BA | 2384 | G |
| 23 | BA | 2385 | C |
| 23 | BA | 2388 | A |
| 23 | BA | 2389 | G |
| 23 | BA | 2394 | C |
| 23 | BA | 2402 | C |
| 23 | BA | 2403 | C |
| 23 | BA | 2405 | G |
| 23 | BA | 2406 | U |
| 23 | BA | 2410 | G |
| 23 | BA | 2413 | G |
| 23 | BA | 2414 | G |
| 23 | BA | 2422 | A |
| 23 | BA | 2423 | U |
| 23 | BA | 2424 | C |
| 23 | BA | 2425 | A |
| 23 | BA | 2429 | G |
| 23 | BA | 2430 | A |
| 23 | BA | 2431 | U |
| 23 | BA | 2434 | A |
| 23 | BA | 2436 | G |
| 23 | BA | 2439 | A |
| 23 | BA | 2440 | C |
| 23 | BA | 2441 | C |
| 23 | BA | 2448 | A |
| 23 | BA | 2468 | G |
| 23 | BA | 2469 | A |
| 23 | BA | 2470 | G |
| 23 | BA | 2474 | C |
| 23 | BA | 2476 | A |
| 23 | BA | 2477 | C |
| 23 | BA | 2478 | A |
| 23 | BA | 2484 | G |
| 23 | BA | 2491 | U |
| 23 | BA | 2496 | C |
| 23 | BA | 2502 | G |
| 23 | BA | 2503 | A |
| 23 | BA | 2505 | G |
| 23 | BA | 2515 | C |
| 23 | BA | 2518 | A |
| 23 | BA | 2520 | C |
| 23 | BA | 2525 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 23 | BA | 2529 | G |
| 23 | BA | 2532 | G |
| 23 | BA | 2535 | G |
| 23 | BA | 2541 | A |
| 23 | BA | 2542 | A |
| 23 | BA | 2543 | G |
| 23 | BA | 2550 | G |
| 23 | BA | 2554 | U |
| 23 | BA | 2566 | A |
| 23 | BA | 2567 | G |
| 23 | BA | 2574 | G |
| 23 | BA | 2585 | U |
| 23 | BA | 2593 | U |
| 23 | BA | 2599 | G |
| 23 | BA | 2602 | A |
| 23 | BA | 2603 | G |
| 23 | BA | 2604 | U |
| 23 | BA | 2609 | U |
| 23 | BA | 2612 | C |
| 23 | BA | 2613 | U |
| 23 | BA | 2615 | U |
| 23 | BA | 2617 | C |
| 23 | BA | 2621 | A |
| 23 | BA | 2636 | U |
| 23 | BA | 2637 | U |
| 23 | BA | 2638 | G |
| 23 | BA | 2647 | U |
| 23 | BA | 2657 | A |
| 23 | BA | 2660 | A |
| 23 | BA | 2665 | A |
| 23 | BA | 2679 | A |
| 23 | BA | 2682 | U |
| 23 | BA | 2683 | C |
| 23 | BA | 2684 | U |
| 23 | BA | 2689 | U |
| 23 | BA | 2691 | C |
| 23 | BA | 2693 | A |
| 23 | BA | 2700 | C |
| 23 | BA | 2702 | U |
| 23 | BA | 2703 | C |
| 23 | BA | 2705 | A |
| 23 | BA | 2707 | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 23 | BA | 2712 | U |
| 23 | BA | 712(B) | A |
| 23 | BA | 2713 | A |
| 23 | BA | 2714 | G |
| 23 | BA | 2719 | G |
| 23 | BA | 2724 | C |
| 23 | BA | 2726 | U |
| 23 | BA | 2730 | C |
| 23 | BA | 2731 | G |
| 23 | BA | 2733 | A |
| 23 | BA | 2748 | A |
| 23 | BA | 2751 | G |
| 23 | BA | 2755 | C |
| 23 | BA | 2757 | A |
| 23 | BA | 2758 | A |
| 23 | BA | 2764 | A |
| 23 | BA | 2765 | A |
| 23 | BA | 2766 | G |
| 23 | BA | 2768 | C |
| 23 | BA | 2778 | A |
| 23 | BA | 2779 | U |
| 23 | BA | 2781 | A |
| 23 | BA | 2790 | A |
| 23 | BA | 2791 | C |
| 23 | BA | 2792 | G |
| 23 | BA | 2808 | U |
| 23 | BA | 2818 | G |
| 23 | BA | 2820 | A |
| 23 | BA | 2821 | A |
| 23 | BA | 2825 | U |
| 23 | BA | 2833 | G |
| 23 | BA | 2834 | G |
| 23 | BA | 2835 | A |
| 23 | BA | 2836 | U |
| 23 | BA | 2872 | G |
| 23 | BA | 2874 | C |
| 23 | BA | 2886 | G |
| 23 | BA | 2892 | A |
| 23 | BA | 2894 | G |
| 24 | BB | 5 | C |
| 24 | BB | 9 | G |
| 24 | BB | 12 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 24 | BB | 13 | A |
| 24 | BB | 15 | A |
| 24 | BB | 16 | G |
| 24 | BB | 23 | G |
| 24 | BB | 24 | G |
| 24 | BB | 41 | U |
| 24 | BB | 42 | C |
| 24 | BB | 44 | G |
| 24 | BB | 47 | C |
| 24 | BB | 65 | C |
| 24 | BB | 66 | A |
| 24 | BB | 73 | A |
| 24 | BB | 84 | C |
| 24 | BB | 88 | C |
| 24 | BB | 89(A) | G |
| 24 | BB | 89(B) | A |
| 24 | BB | 90 | C |
| 24 | BB | 96 | G |
| 24 | BB | 100 | G |
| 24 | BB | 105 | G |
| 24 | BB | 107 | U |
| 24 | BB | 109 | G |
| 24 | BB | 110 | G |
| 1 | CA | 6 | G |
| 1 | CA | 7 | G |
| 1 | CA | 9 | G |
| 1 | CA | 13 | U |
| 1 | CA | 14 | U |
| 1 | CA | 15 | G |
| 1 | CA | 32 | A |
| 1 | CA | 33 | A |
| 1 | CA | 39 | G |
| 1 | CA | 41 | G |
| 1 | CA | 42 | G |
| 1 | CA | 47 | C |
| 1 | CA | 48 | C |
| 1 | CA | 50 | A |
| 1 | CA | 51 | A |
| 1 | CA | 59 | A |
| 1 | CA | 61 | G |
| 1 | CA | 88 | C |
| 1 | CA | 97 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | CA | 99 | C |
| 1 | CA | 110 | C |
| 1 | CA | 115 | G |
| 1 | CA | 116 | A |
| 1 | CA | 120 | A |
| 1 | CA | 121 | C |
| 1 | CA | 131 | C |
| 1 | CA | 144 | G |
| 1 | CA | 151 | A |
| 1 | CA | 163 | C |
| 1 | CA | 171 | A |
| 1 | CA | 182 | U |
| 1 | CA | 183 | G |
| 1 | CA | 189 | U |
| 1 | CA | 190 | G |
| 1 | CA | 195 | A |
| 1 | CA | 196 | A |
| 1 | CA | 197 | A |
| 1 | CA | 201 | C |
| 1 | CA | 209 | U |
| 1 | CA | 210 | U |
| 1 | CA | 231 | G |
| 1 | CA | 240 | C |
| 1 | CA | 247 | G |
| 1 | CA | 250 | A |
| 1 | CA | 251 | G |
| 1 | CA | 252 | U |
| 1 | CA | 258 | G |
| 1 | CA | 266 | G |
| 1 | CA | 267 | C |
| 1 | CA | 280 | C |
| 1 | CA | 281 | G |
| 1 | CA | 289 | G |
| 1 | CA | 298 | A |
| 1 | CA | 305 | G |
| 1 | CA | 306 | G |
| 1 | CA | 320 | C |
| 1 | CA | 321 | A |
| 1 | CA | 328 | C |
| 1 | CA | 329 | A |
| 1 | CA | 330 | C |
| 1 | CA | 332 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | CA | 345 | C |
| 1 | CA | 347 | G |
| 1 | CA | 351 | G |
| 1 | CA | 352 | C |
| 1 | CA | 353 | A |
| 1 | CA | 354 | G |
| 1 | CA | 358 | U |
| 1 | CA | 364 | A |
| 1 | CA | 365 | U |
| 1 | CA | 366 | C |
| 1 | CA | 367 | U |
| 1 | CA | 372 | C |
| 1 | CA | 373 | A |
| 1 | CA | 382 | A |
| 1 | CA | 384 | G |
| 1 | CA | 387 | U |
| 1 | CA | 388 | G |
| 1 | CA | 397 | A |
| 1 | CA | 398 | C |
| 1 | CA | 406 | G |
| 1 | CA | 412 | A |
| 1 | CA | 413 | G |
| 1 | CA | 414 | A |
| 1 | CA | 422 | C |
| 1 | CA | 423 | G |
| 1 | CA | 427 | U |
| 1 | CA | 429 | U |
| 1 | CA | 439 | A |
| 1 | CA | 452 | A |
| 1 | CA | 453 | A |
| 1 | CA | 457 | C |
| 1 | CA | 464 | G |
| 1 | CA | 465 | A |
| 1 | CA | 466 | G |
| 1 | CA | 467 | G |
| 1 | CA | 484 | G |
| 1 | CA | 485 | G |
| 1 | CA | 486 | U |
| 1 | CA | 496 | A |
| 1 | CA | 497 | U |
| 1 | CA | 500 | G |
| 1 | CA | 511 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | CA | 512 | U |
| 1 | CA | 518 | C |
| 1 | CA | 523 | A |
| 1 | CA | 527 | G |
| 1 | CA | 531 | U |
| 1 | CA | 532 | A |
| 1 | CA | 533 | A |
| 1 | CA | 547 | A |
| 1 | CA | 558 | G |
| 1 | CA | 559 | A |
| 1 | CA | 560 | U |
| 1 | CA | 561 | U |
| 1 | CA | 562 | C |
| 1 | CA | 567 | G |
| 1 | CA | 572 | A |
| 1 | CA | 573 | A |
| 1 | CA | 575 | G |
| 1 | CA | 576 | G |
| 1 | CA | 577 | G |
| 1 | CA | 580 | U |
| 1 | CA | 581 | G |
| 1 | CA | 596 | C |
| 1 | CA | 607 | A |
| 1 | CA | 653 | A |
| 1 | CA | 665 | A |
| 1 | CA | 687 | A |
| 1 | CA | 688 | G |
| 1 | CA | 690 | G |
| 1 | CA | 693 | G |
| 1 | CA | 702 | A |
| 1 | CA | 724 | G |
| 1 | CA | 731 | G |
| 1 | CA | 733 | A |
| 1 | CA | 753 | A |
| 1 | CA | 777 | A |
| 1 | CA | 782 | A |
| 1 | CA | 792 | A |
| 1 | CA | 793 | U |
| 1 | CA | 794 | A |
| 1 | CA | 800 | G |
| 1 | CA | 810 | C |
| 1 | CA | 816 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | CA | 817 | C |
| 1 | CA | 818 | G |
| 1 | CA | 819 | A |
| 1 | CA | 828 | A |
| 1 | CA | 829 | G |
| 1 | CA | 833 | U |
| 1 | CA | 841 | U |
| 1 | CA | 842 | C |
| 1 | CA | 843 | U |
| 1 | CA | 849 | C |
| 1 | CA | 859 | A |
| 1 | CA | 870 | U |
| 1 | CA | 873 | A |
| 1 | CA | 876 | G |
| 1 | CA | 884 | U |
| 1 | CA | 897 | C |
| 1 | CA | 902 | G |
| 1 | CA | 914 | A |
| 1 | CA | 916 | G |
| 1 | CA | 921 | U |
| 1 | CA | 922 | G |
| 1 | CA | 927 | G |
| 1 | CA | 934 | C |
| 1 | CA | 935 | A |
| 1 | CA | 945 | G |
| 1 | CA | 951 | G |
| 1 | CA | 960 | U |
| 1 | CA | 961 | U |
| 1 | CA | 968 | A |
| 1 | CA | 969 | A |
| 1 | CA | 971 | G |
| 1 | CA | 972 | C |
| 1 | CA | 974 | A |
| 1 | CA | 976 | G |
| 1 | CA | 977 | A |
| 1 | CA | 980 | C |
| 1 | CA | 981 | U |
| 1 | CA | 982 | U |
| 1 | CA | 992 | U |
| 1 | CA | 993 | G |
| 1 | CA | 1004 | A |
| 1 | CA | 1006 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | CA | 1009 | G |
| 1 | CA | 1025 | U |
| 1 | CA | 103(A) | A |
| 1 | CA | 1033 | G |
| 1 | CA | 1045 | C |
| 1 | CA | 1054 | C |
| 1 | CA | 1055 | A |
| 1 | CA | 1065 | U |
| 1 | CA | 1067 | A |
| 1 | CA | 1068 | G |
| 1 | CA | 1080 | A |
| 1 | CA | 1081 | G |
| 1 | CA | 1094 | G |
| 1 | CA | 1095 | U |
| 1 | CA | 1101 | A |
| 1 | CA | 1117 | G |
| 1 | CA | 1118 | C |
| 1 | CA | 1124 | G |
| 1 | CA | 1125 | U |
| 1 | CA | 1126 | U |
| 1 | CA | 1129 | C |
| 1 | CA | 1130 | A |
| 1 | CA | 1131 | G |
| 1 | CA | 1136 | U |
| 1 | CA | 1137 | C |
| 1 | CA | 1139 | G |
| 1 | CA | 1151 | A |
| 1 | CA | 1152 | A |
| 1 | CA | 1159 | U |
| 1 | CA | 1160 | G |
| 1 | CA | 1181 | G |
| 1 | CA | 1183 | A |
| 1 | CA | 1189 | C |
| 1 | CA | 1193 | G |
| 1 | CA | 1196 | U |
| 1 | CA | 1197 | G |
| 1 | CA | 1202 | G |
| 1 | CA | 1212 | U |
| 1 | CA | 1213 | A |
| 1 | CA | 1214 | C |
| 1 | CA | 1218 | C |
| 1 | CA | 1224 | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | CA | 1225 | A |
| 1 | CA | 1226 | C |
| 1 | CA | 1227 | A |
| 1 | CA | 1228 | C |
| 1 | CA | 1238 | A |
| 1 | CA | 1240 | U |
| 1 | CA | 1241 | G |
| 1 | CA | 1245 | A |
| 1 | CA | 1256 | A |
| 1 | CA | 1257 | U |
| 1 | CA | 1262 | C |
| 1 | CA | 1270 | C |
| 1 | CA | 1277 | C |
| 1 | CA | 1280 | A |
| 1 | CA | 1281 | U |
| 1 | CA | 1287 | A |
| 1 | CA | 1300 | G |
| 1 | CA | 1301 | U |
| 1 | CA | 1302 | U |
| 1 | CA | 1305 | G |
| 1 | CA | 1317 | C |
| 1 | CA | 1320 | C |
| 1 | CA | 1322 | C |
| 1 | CA | 1323 | G |
| 1 | CA | 1326 | C |
| 1 | CA | 1331 | G |
| 1 | CA | 1335 | C |
| 1 | CA | 1337 | G |
| 1 | CA | 1346 | A |
| 1 | CA | 1347 | G |
| 1 | CA | 1353 | G |
| 1 | CA | 136(B) | C |
| 1 | CA | 1363 | A |
| 1 | CA | 1364 | U |
| 1 | CA | 1366 | C |
| 1 | CA | 1378 | C |
| 1 | CA | 1379 | G |
| 1 | CA | 1397 | C |
| 1 | CA | 1401 | G |
| 1 | CA | 1419 | G |
| 1 | CA | 1440 | C |
| 1 | CA | 1442 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | CA | 1443 | G |
| 1 | CA | 1446 | A |
| 1 | CA | 1447 | G |
| 1 | CA | 1451 | A |
| 1 | CA | 1452 | C |
| 1 | CA | 1454 | G |
| 1 | CA | 1469 | G |
| 1 | CA | 1483 | A |
| 1 | CA | 1487 | G |
| 1 | CA | 1492 | A |
| 1 | CA | 1494 | G |
| 1 | CA | 1497 | G |
| 1 | CA | 1502 | A |
| 1 | CA | 1503 | A |
| 1 | CA | 1504 | G |
| 1 | CA | 1506 | U |
| 1 | CA | 1514 | C |
| 1 | CA | 1517 | G |
| 1 | CA | 1519 | A |
| 1 | CA | 1520 | G |
| 1 | CA | 1528 | U |
| 1 | CA | 1529 | G |
| 1 | CA | 1530 | G |
| 22 | CV | 6182 | A |
| 22 | CV | 6187 | A |
| 22 | CV | 6194 | C |
| 23 | DA | 10 | G |
| 23 | DA | 11 | G |
| 23 | DA | 34 | C |
| 23 | DA | 35 | G |
| 23 | DA | 46 | C |
| 23 | DA | 60 | G |
| 23 | DA | 61 | G |
| 23 | DA | 64 | A |
| 23 | DA | 71 | A |
| 23 | DA | 72 | U |
| 23 | DA | 74 | A |
| 23 | DA | 75 | G |
| 23 | DA | 84 | A |
| 23 | DA | 96 | G |
| 23 | DA | 97 | C |
| 23 | DA | 101 | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 23 | DA | 102 | G |
| 23 | DA | 110 | G |
| 23 | DA | 116 | C |
| 23 | DA | 117 | G |
| 23 | DA | 118 | A |
| 23 | DA | 119 | A |
| 23 | DA | 120 | U |
| 23 | DA | 125 | G |
| 23 | DA | 129 | C |
| 23 | DA | 135 | G |
| 23 | DA | 138 | G |
| 23 | DA | 139 | G |
| 23 | DA | 140 | A |
| 23 | DA | 181 | A |
| 23 | DA | 192 | C |
| 23 | DA | 195 | A |
| 23 | DA | 196 | A |
| 23 | DA | 197 | A |
| 23 | DA | 199 | A |
| 23 | DA | 205 | G |
| 23 | DA | 215 | G |
| 23 | DA | 216 | A |
| 23 | DA | 218 | A |
| 23 | DA | 221 | A |
| 23 | DA | 222 | A |
| 23 | DA | 225 | A |
| 23 | DA | 228 | A |
| 23 | DA | 229 | A |
| 23 | DA | 230 | U |
| 23 | DA | 233 | A |
| 23 | DA | 244 | A |
| 23 | DA | 248 | G |
| 23 | DA | 249 | C |
| 23 | DA | 252 | G |
| 23 | DA | 257 | A |
| 23 | DA | 258 | G |
| 23 | DA | 265 | A |
| 23 | DA | 269 | U |
| 23 | DA | 270(K) | G |
| 23 | DA | 270(L) | C |
| 23 | DA | 270(M) | U |
| 23 | DA | 270(N) | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 23 | DA | 270(O) | G |
| 23 | DA | 270(Q) | C |
| 23 | DA | 270(R) | C |
| 23 | DA | 271(D) | U |
| 23 | DA | 271 | G |
| 23 | DA | 274 | G |
| 23 | DA | 275 | G |
| 23 | DA | 276 | A |
| 23 | DA | 277 | C |
| 23 | DA | 278 | A |
| 23 | DA | 283 | A |
| 23 | DA | 301 | G |
| 23 | DA | 302 | C |
| 23 | DA | 304 | G |
| 23 | DA | 311 | A |
| 23 | DA | 323 | G |
| 23 | DA | 324 | A |
| 23 | DA | 329 | G |
| 23 | DA | 330 | A |
| 23 | DA | 334 | C |
| 23 | DA | 335 | C |
| 23 | DA | 345 | A |
| 23 | DA | 352 | G |
| 23 | DA | 353 | G |
| 23 | DA | 360 | G |
| 23 | DA | 363(A) | G |
| 23 | DA | 372 | G |
| 23 | DA | 386 | G |
| 23 | DA | 396 | G |
| 23 | DA | 405 | U |
| 23 | DA | 406 | G |
| 23 | DA | 407 | G |
| 23 | DA | 411 | G |
| 23 | DA | 416 | C |
| 23 | DA | 421 | U |
| 23 | DA | 444 | C |
| 23 | DA | 455 | C |
| 23 | DA | 456 | C |
| 23 | DA | 457 | A |
| 23 | DA | 463 | G |
| 23 | DA | 464 | U |
| 23 | DA | 467 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 23 | DA | 480 | A |
| 23 | DA | 481 | G |
| 23 | DA | 483 | A |
| 23 | DA | 491 | G |
| 23 | DA | 504 | U |
| 23 | DA | 505 | A |
| 23 | DA | 508 | G |
| 23 | DA | 509 | C |
| 23 | DA | 530 | G |
| 23 | DA | 531 | C |
| 23 | DA | 532 | A |
| 23 | DA | 533 | G |
| 23 | DA | 546 | C |
| 23 | DA | 547 | A |
| 23 | DA | 548 | A |
| 23 | DA | 558 | G |
| 23 | DA | 563 | G |
| 23 | DA | 566 | U |
| 23 | DA | 573 | G |
| 23 | DA | 575 | A |
| 23 | DA | 580 | C |
| 23 | DA | 586 | A |
| 23 | DA | 593 | G |
| 23 | DA | 595 | C |
| 23 | DA | 599 | G |
| 23 | DA | 603 | A |
| 23 | DA | 609(A) | A |
| 23 | DA | 615 | G |
| 23 | DA | 617 | G |
| 23 | DA | 620 | G |
| 23 | DA | 627 | A |
| 23 | DA | 632 | A |
| 23 | DA | 637 | A |
| 23 | DA | 645 | C |
| 23 | DA | 646 | A |
| 23 | DA | 647 | G |
| 23 | DA | 654 | U |
| 23 | DA | 655 | A |
| 23 | DA | 664 | C |
| 23 | DA | 682 | G |
| 23 | DA | 686 | G |
| 23 | DA | 694 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 23 | DA | 695 | G |
| 23 | DA | 717 | G |
| 23 | DA | 730 | C |
| 23 | DA | 739 | G |
| 23 | DA | 746 | A |
| 23 | DA | 747 | U |
| 23 | DA | 761 | A |
| 23 | DA | 775 | G |
| 23 | DA | 776 | G |
| 23 | DA | 777 | A |
| 23 | DA | 782 | A |
| 23 | DA | 784 | A |
| 23 | DA | 785 | G |
| 23 | DA | 787 | U |
| 23 | DA | 792 | G |
| 23 | DA | 805 | G |
| 23 | DA | 812 | C |
| 23 | DA | 819 | A |
| 23 | DA | 822 | U |
| 23 | DA | 826 | U |
| 23 | DA | 827 | U |
| 23 | DA | 828 | U |
| 23 | DA | 832 | G |
| 23 | DA | 846 | C |
| 23 | DA | 855 | G |
| 23 | DA | 857 | C |
| 23 | DA | 858 | U |
| 23 | DA | 859 | G |
| 23 | DA | 869 | G |
| 23 | DA | 878 | A |
| 23 | DA | 887 | A |
| 23 | DA | 889 | C |
| 23 | DA | 890 | A |
| 23 | DA | 896 | A |
| 23 | DA | 897 | C |
| 23 | DA | 910 | A |
| 23 | DA | 914 | C |
| 23 | DA | 915 | C |
| 23 | DA | 917 | A |
| 23 | DA | 919 | G |
| 23 | DA | 932 | G |
| 23 | DA | 933 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 23 | DA | 934 | G |
| 23 | DA | 938 | G |
| 23 | DA | 941 | A |
| 23 | DA | 946 | G |
| 23 | DA | 957 | A |
| 23 | DA | 958 | U |
| 23 | DA | 959 | A |
| 23 | DA | 961 | C |
| 23 | DA | 964 | C |
| 23 | DA | 974(A) | G |
| 23 | DA | 974(B) | C |
| 23 | DA | 975 | G |
| 23 | DA | 979 | G |
| 23 | DA | 983 | A |
| 23 | DA | 989 | G |
| 23 | DA | 990 | A |
| 23 | DA | 991 | C |
| 23 | DA | 996 | A |
| 23 | DA | 1005 | C |
| 23 | DA | 1009 | A |
| 23 | DA | 1010 | A |
| 23 | DA | 1011 | G |
| 23 | DA | 1012 | U |
| 23 | DA | 1013 | C |
| 23 | DA | 1020 | A |
| 23 | DA | 1022 | G |
| 23 | DA | 1023 | U |
| 23 | DA | 1025 | G |
| 23 | DA | 1026 | U |
| 23 | DA | 1030 | G |
| 23 | DA | 1033 | U |
| 23 | DA | 1046 | A |
| 23 | DA | 1047 | G |
| 23 | DA | 1053 | C |
| 23 | DA | 1105 | U |
| 23 | DA | 1110 | G |
| 23 | DA | 1112 | G |
| 23 | DA | 1122 | G |
| 23 | DA | 1126 | A |
| 23 | DA | 1129 | A |
| 23 | DA | 1130 | U |
| 23 | DA | 1135 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 23 | DA | 1136 | G |
| 23 | DA | 1139 | G |
| 23 | DA | 1142 | U |
| 23 | DA | 114(B) | A |
| 23 | DA | 1143 | A |
| 23 | DA | 1151 | G |
| 23 | DA | 1155 | A |
| 23 | DA | 1156 | A |
| 23 | DA | 1174 | A |
| 23 | DA | 1175 | U |
| 23 | DA | 1177 | A |
| 23 | DA | 1178 | C |
| 23 | DA | 1190 | G |
| 23 | DA | 1205 | U |
| 23 | DA | 1210 | A |
| 23 | DA | 1211 | U |
| 23 | DA | 1212 | G |
| 23 | DA | 1220 | A |
| 23 | DA | 1221 | C |
| 23 | DA | 1227 | G |
| 23 | DA | 1236 | G |
| 23 | DA | 1241 | A |
| 23 | DA | 1253 | A |
| 23 | DA | 1256 | G |
| 23 | DA | 1269 | A |
| 23 | DA | 1271 | G |
| 23 | DA | 1272 | A |
| 23 | DA | 1273 | U |
| 23 | DA | 1287 | A |
| 23 | DA | 1288 | U |
| 23 | DA | 1289 | C |
| 23 | DA | 1300 | U |
| 23 | DA | 1301 | A |
| 23 | DA | 1310 | G |
| 23 | DA | 1313 | U |
| 23 | DA | 1314 | C |
| 23 | DA | 1329 | U |
| 23 | DA | 1332 | G |
| 23 | DA | 1338 | G |
| 23 | DA | 1343 | G |
| 23 | DA | 1344 | G |
| 23 | DA | 1345 | C |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 23 | DA | 1349 | A |
| 23 | DA | 1352 | U |
| 23 | DA | 1359 | A |
| 23 | DA | 1360 | A |
| 23 | DA | 1365 | A |
| 23 | DA | 1368 | G |
| 23 | DA | 1380 | G |
| 23 | DA | 1384 | A |
| 23 | DA | 1385 | G |
| 23 | DA | 1386 | C |
| 23 | DA | 1396 | U |
| 23 | DA | 1416 | G |
| 23 | DA | 1417 | C |
| 23 | DA | 1420 | U |
| 23 | DA | 1427 | A |
| 23 | DA | 1428 | C |
| 23 | DA | 1434 | A |
| 23 | DA | 144(B) | A |
| 23 | DA | 1453 | A |
| 23 | DA | 1459 | G |
| 23 | DA | 1467 | C |
| 23 | DA | 1469 | A |
| 23 | DA | 1483 | G |
| 23 | DA | 1490 | A |
| 23 | DA | 1493 | C |
| 23 | DA | 1494 | A |
| 23 | DA | 1495 | A |
| 23 | DA | 1496 | A |
| 23 | DA | 1497 | U |
| 23 | DA | 1505 | C |
| 23 | DA | 1509 | A |
| 23 | DA | 1510 | A |
| 23 | DA | 1519 | G |
| 23 | DA | 1535 | U |
| 23 | DA | 1537 | C |
| 23 | DA | 1542 | G |
| 23 | DA | 1543 | A |
| 23 | DA | 1544 | C |
| 23 | DA | 1545 | A |
| 23 | DA | 1547 | C |
| 23 | DA | 1558 | A |
| 23 | DA | 1559 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 23 | DA | 1565 | C |
| 23 | DA | 1566 | A |
| 23 | DA | 1569 | A |
| 23 | DA | 1578 | U |
| 23 | DA | 1585 | C |
| 23 | DA | 1586 | A |
| 23 | DA | 1587 | A |
| 23 | DA | 1588 | C |
| 23 | DA | 1598 | C |
| 23 | DA | 1599 | C |
| 23 | DA | 1608 | A |
| 23 | DA | 1609 | A |
| 23 | DA | 1610 | A |
| 23 | DA | 1617 | C |
| 23 | DA | 1618 | A |
| 23 | DA | 1631 | A |
| 23 | DA | 1639 | U |
| 23 | DA | 1640 | C |
| 23 | DA | 1644 | C |
| 23 | DA | 1647 | G |
| 23 | DA | 1648 | C |
| 23 | DA | 1651 | G |
| 23 | DA | 1654 | A |
| 23 | DA | 1674 | G |
| 23 | DA | 1677 | A |
| 23 | DA | 1680 | U |
| 23 | DA | 1681 | G |
| 23 | DA | 1690 | A |
| 23 | DA | 1696 | G |
| 23 | DA | 1703 | G |
| 23 | DA | 1727 | U |
| 23 | DA | 1729 | A |
| 23 | DA | 1743 | G |
| 23 | DA | 1750 | G |
| 23 | DA | 1756 | G |
| 23 | DA | 1763 | G |
| 23 | DA | 1764 | G |
| 23 | DA | 1767 | C |
| 23 | DA | 1773 | A |
| 23 | DA | 1778 | U |
| 23 | DA | 1787 | A |
| 23 | DA | 1788 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 23 | DA | 1791 | A |
| 23 | DA | 1800 | C |
| 23 | DA | 1801 | G |
| 23 | DA | 1811 | G |
| 23 | DA | 1813 | G |
| 23 | DA | 1816 | G |
| 23 | DA | 1829 | A |
| 23 | DA | 1835 | G |
| 23 | DA | 1838 | C |
| 23 | DA | 1840 | G |
| 23 | DA | 1847 | A |
| 23 | DA | 1870 | C |
| 23 | DA | 1887 | C |
| 23 | DA | 1888 | G |
| 23 | DA | 1889 | A |
| 23 | DA | 1896 | G |
| 23 | DA | 1900 | A |
| 23 | DA | 1902 | C |
| 23 | DA | 1903 | G |
| 23 | DA | 1906 | G |
| 23 | DA | 1913 | A |
| 23 | DA | 1914 | C |
| 23 | DA | 1929 | G |
| 23 | DA | 1936 | A |
| 23 | DA | 1938 | A |
| 23 | DA | 1939 | U |
| 23 | DA | 1955 | U |
| 23 | DA | 1956 | U |
| 23 | DA | 1960 | A |
| 23 | DA | 1963 | U |
| 23 | DA | 1964 | G |
| 23 | DA | 1966 | A |
| 23 | DA | 1967 | C |
| 23 | DA | 1970 | A |
| 23 | DA | 1971 | A |
| 23 | DA | 1972 | A |
| 23 | DA | 1974 | C |
| 23 | DA | 1975 | G |
| 23 | DA | 1981 | A |
| 23 | DA | 1982 | C |
| 23 | DA | 1985 | G |
| 23 | DA | 1991 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 23 | DA | 1992 | G |
| 23 | DA | 1993 | U |
| 23 | DA | 1997 | G |
| 23 | DA | 2007 | C |
| 23 | DA | 2010 | G |
| 23 | DA | 2020 | A |
| 23 | DA | 2023 | G |
| 23 | DA | 2031 | A |
| 23 | DA | 2032 | G |
| 23 | DA | 2033 | A |
| 23 | DA | 2034 | U |
| 23 | DA | 2036 | C |
| 23 | DA | 2043 | C |
| 23 | DA | 2049 | G |
| 23 | DA | 2051 | A |
| 23 | DA | 2055 | C |
| 23 | DA | 2056 | G |
| 23 | DA | 2060 | A |
| 23 | DA | 2061 | G |
| 23 | DA | 2062 | A |
| 23 | DA | 2069 | G |
| 23 | DA | 2079 | U |
| 23 | DA | 2080 | G |
| 23 | DA | 2086 | U |
| 23 | DA | 2099 | U |
| 23 | DA | 2183 | C |
| 23 | DA | 2189 | U |
| 23 | DA | 2190 | G |
| 23 | DA | 2196 | C |
| 23 | DA | 2198 | A |
| 23 | DA | 2205 | C |
| 23 | DA | 2211 | G |
| 23 | DA | 2212 | A |
| 23 | DA | 2213 | U |
| 23 | DA | 2215 | G |
| 23 | DA | 2225 | A |
| 23 | DA | 2226 | C |
| 23 | DA | 2227 | A |
| 23 | DA | 2228 | G |
| 23 | DA | 2235 | G |
| 23 | DA | 2238 | G |
| 23 | DA | 2239 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 23 | DA | 2267 | A |
| 23 | DA | 2268 | A |
| 23 | DA | 2269 | A |
| 23 | DA | 2272 | U |
| 23 | DA | 2273 | A |
| 23 | DA | 2275 | C |
| 23 | DA | 2278 | A |
| 23 | DA | 2283 | C |
| 23 | DA | 2287 | A |
| 23 | DA | 2288 | A |
| 23 | DA | 2305 | A |
| 23 | DA | 2306 | C |
| 23 | DA | 2307 | G |
| 23 | DA | 2309 | A |
| 23 | DA | 2310 | A |
| 23 | DA | 2319 | G |
| 23 | DA | 2320 | A |
| 23 | DA | 2322 | A |
| 23 | DA | 2325 | G |
| 23 | DA | 2334 | G |
| 23 | DA | 2336 | A |
| 23 | DA | 2343 | C |
| 23 | DA | 2346 | A |
| 23 | DA | 2347 | C |
| 23 | DA | 2350 | C |
| 23 | DA | 2358 | G |
| 23 | DA | 2360 | A |
| 23 | DA | 2361 | A |
| 23 | DA | 2365 | G |
| 23 | DA | 2379 | G |
| 23 | DA | 2383 | G |
| 23 | DA | 2384 | G |
| 23 | DA | 2385 | C |
| 23 | DA | 2388 | A |
| 23 | DA | 2389 | G |
| 23 | DA | 2394 | C |
| 23 | DA | 2402 | C |
| 23 | DA | 2403 | C |
| 23 | DA | 2405 | G |
| 23 | DA | 2406 | U |
| 23 | DA | 2410 | G |
| 23 | DA | 2413 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 23 | DA | 2414 | G |
| 23 | DA | 2422 | A |
| 23 | DA | 2423 | U |
| 23 | DA | 2424 | C |
| 23 | DA | 2425 | A |
| 23 | DA | 2429 | G |
| 23 | DA | 2430 | A |
| 23 | DA | 2434 | A |
| 23 | DA | 2436 | G |
| 23 | DA | 2439 | A |
| 23 | DA | 2440 | C |
| 23 | DA | 2441 | C |
| 23 | DA | 2448 | A |
| 23 | DA | 2468 | G |
| 23 | DA | 2469 | A |
| 23 | DA | 2470 | G |
| 23 | DA | 2474 | C |
| 23 | DA | 2476 | A |
| 23 | DA | 2477 | C |
| 23 | DA | 2478 | A |
| 23 | DA | 2484 | G |
| 23 | DA | 2491 | U |
| 23 | DA | 2496 | C |
| 23 | DA | 2502 | G |
| 23 | DA | 2503 | A |
| 23 | DA | 2505 | G |
| 23 | DA | 2515 | C |
| 23 | DA | 2518 | A |
| 23 | DA | 2520 | C |
| 23 | DA | 2525 | G |
| 23 | DA | 2529 | G |
| 23 | DA | 2532 | G |
| 23 | DA | 2535 | G |
| 23 | DA | 2542 | A |
| 23 | DA | 2543 | G |
| 23 | DA | 2554 | U |
| 23 | DA | 2566 | A |
| 23 | DA | 2567 | G |
| 23 | DA | 2574 | G |
| 23 | DA | 2584 | U |
| 23 | DA | 2585 | U |
| 23 | DA | 2599 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 23 | DA | 2602 | A |
| 23 | DA | 2603 | G |
| 23 | DA | 2604 | U |
| 23 | DA | 2609 | U |
| 23 | DA | 2612 | C |
| 23 | DA | 2613 | U |
| 23 | DA | 2615 | U |
| 23 | DA | 2617 | C |
| 23 | DA | 2621 | A |
| 23 | DA | 2636 | U |
| 23 | DA | 2637 | U |
| 23 | DA | 2638 | G |
| 23 | DA | 2647 | U |
| 23 | DA | 2657 | A |
| 23 | DA | 2660 | A |
| 23 | DA | 2665 | A |
| 23 | DA | 2679 | A |
| 23 | DA | 2680 | C |
| 23 | DA | 2682 | U |
| 23 | DA | 2683 | C |
| 23 | DA | 2684 | U |
| 23 | DA | 2689 | U |
| 23 | DA | 2691 | C |
| 23 | DA | 2693 | A |
| 23 | DA | 2700 | C |
| 23 | DA | 2702 | U |
| 23 | DA | 2705 | A |
| 23 | DA | 2707 | G |
| 23 | DA | 2711 | A |
| 23 | DA | 2712 | U |
| 23 | DA | 712(B) | A |
| 23 | DA | 2713 | A |
| 23 | DA | 2714 | G |
| 23 | DA | 2719 | G |
| 23 | DA | 2724 | C |
| 23 | DA | 2726 | U |
| 23 | DA | 2730 | C |
| 23 | DA | 2731 | G |
| 23 | DA | 2733 | A |
| 23 | DA | 2748 | A |
| 23 | DA | 2751 | G |
| 23 | DA | 2752 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 23 | DA | 2755 | C |
| 23 | DA | 2757 | A |
| 23 | DA | 2758 | A |
| 23 | DA | 2764 | A |
| 23 | DA | 2765 | A |
| 23 | DA | 2766 | G |
| 23 | DA | 2768 | C |
| 23 | DA | 2778 | A |
| 23 | DA | 2779 | U |
| 23 | DA | 2781 | A |
| 23 | DA | 2790 | A |
| 23 | DA | 2791 | C |
| 23 | DA | 2792 | G |
| 23 | DA | 2808 | U |
| 23 | DA | 2818 | G |
| 23 | DA | 2820 | A |
| 23 | DA | 2821 | A |
| 23 | DA | 2825 | U |
| 23 | DA | 2833 | G |
| 23 | DA | 2834 | G |
| 23 | DA | 2835 | A |
| 23 | DA | 2836 | U |
| 23 | DA | 2872 | G |
| 23 | DA | 2874 | C |
| 23 | DA | 2886 | G |
| 23 | DA | 2892 | A |
| 23 | DA | 2894 | G |
| 24 | DB | 5 | C |
| 24 | DB | 9 | G |
| 24 | DB | 12 | C |
| 24 | DB | 13 | A |
| 24 | DB | 15 | A |
| 24 | DB | 16 | G |
| 24 | DB | 23 | G |
| 24 | DB | 24 | G |
| 24 | DB | 41 | U |
| 24 | DB | 42 | C |
| 24 | DB | 44 | G |
| 24 | DB | 47 | C |
| 24 | DB | 65 | C |
| 24 | DB | 66 | A |
| 24 | DB | 73 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 24 | DB | 82 | G |
| 24 | DB | 88 | C |
| 24 | DB | 89(A) | G |
| 24 | DB | 89(B) | A |
| 24 | DB | 90 | C |
| 24 | DB | 96 | G |
| 24 | DB | 100 | G |
| 24 | DB | 101 | A |
| 24 | DB | 105 | G |
| 24 | DB | 107 | U |
| 24 | DB | 109 | G |
| 24 | DB | 110 | G |

All (84) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | AA | 251 | G |
| 1 | AA | 327 | A |
| 1 | AA | 364 | A |
| 1 | AA | 428 | G |
| 1 | AA | 560 | U |
| 1 | AA | 687 | A |
| 1 | AA | 793 | U |
| 1 | AA | 913 | A |
| 1 | AA | 1064 | G |
| 1 | AA | 1067 | A |
| 1 | AA | 1129 | C |
| 1 | AA | 1201 | A |
| 1 | AA | 1493 | A |
| 1 | AA | 1529 | G |
| 23 | BA | 196 | A |
| 23 | BA | 257 | A |
| 23 | BA | 385 | C |
| 23 | BA | 479 | A |
| 23 | BA | 685 | A |
| 23 | BA | 746 | A |
| 23 | BA | 791 | C |
| 23 | BA | 974(A) | G |
| 23 | BA | 1022 | G |
| 23 | BA | 1210 | A |
| 23 | BA | 1343 | G |
| 23 | BA | 1379 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 23 | BA | 1558 | A |
| 23 | BA | 1608 | A |
| 23 | BA | 1609 | A |
| 23 | BA | 1617 | C |
| 23 | BA | 1786 | A |
| 23 | BA | 1936 | A |
| 23 | BA | 2062 | A |
| 23 | BA | 2225 | A |
| 23 | BA | 2272 | U |
| 23 | BA | 2275 | C |
| 23 | BA | 2405 | G |
| 23 | BA | 2433 | A |
| 23 | BA | 2439 | A |
| 23 | BA | 2542 | A |
| 23 | BA | 2778 | A |
| 1 | CA | 251 | G |
| 1 | CA | 327 | A |
| 1 | CA | 364 | A |
| 1 | CA | 428 | G |
| 1 | CA | 560 | U |
| 1 | CA | 687 | A |
| 1 | CA | 793 | U |
| 1 | CA | 913 | A |
| 1 | CA | 1064 | G |
| 1 | CA | 1067 | A |
| 1 | CA | 1129 | C |
| 1 | CA | 1201 | A |
| 1 | CA | 1493 | A |
| 1 | CA | 1529 | G |
| 23 | DA | 60 | G |
| 23 | DA | 196 | A |
| 23 | DA | 257 | A |
| 23 | DA | 385 | C |
| 23 | DA | 479 | A |
| 23 | DA | 685 | A |
| 23 | DA | 746 | A |
| 23 | DA | 791 | C |
| 23 | DA | 858 | U |
| 23 | DA | 974(A) | G |
| 23 | DA | 1022 | G |
| 23 | DA | 1210 | A |
| 23 | DA | 1343 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 23 | DA | 1379 | A |
| 23 | DA | 1558 | A |
| 23 | DA | 1608 | A |
| 23 | DA | 1609 | A |
| 23 | DA | 1617 | C |
| 23 | DA | 1786 | A |
| 23 | DA | 1936 | A |
| 23 | DA | 2062 | A |
| 23 | DA | 2225 | A |
| 23 | DA | 2272 | U |
| 23 | DA | 2275 | C |
| 23 | DA | 2405 | G |
| 23 | DA | 2433 | A |
| 23 | DA | 2435 | A |
| 23 | DA | 2439 | A |
| 23 | DA | 2542 | A |

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1198 ligands modelled in this entry, 1198 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|------------------|--------|---------------|-----------------------|-------|
| 1 | AA | 1506/1506 (100%) | 0.40 | 63 (4%) 40 35 | 51, 122, 245, 498 | 0 |
| 1 | CA | 1506/1506 (100%) | 0.47 | 98 (6%) 22 21 | 51, 126, 251, 414 | 0 |
| 2 | AB | 234/234 (100%) | 1.11 | 46 (19%) 1 2 | 113, 174, 244, 298 | 0 |
| 2 | CB | 234/234 (100%) | 0.92 | 48 (20%) 1 1 | 111, 177, 259, 325 | 0 |
| 3 | AC | 206/206 (100%) | 0.82 | 30 (14%) 3 3 | 106, 160, 225, 263 | 0 |
| 3 | CC | 206/206 (100%) | 0.85 | 37 (17%) 2 2 | 105, 161, 226, 271 | 0 |
| 4 | AD | 208/208 (100%) | 0.56 | 17 (8%) 14 13 | 90, 142, 199, 247 | 0 |
| 4 | CD | 208/208 (100%) | 1.22 | 46 (22%) 1 1 | 94, 146, 220, 300 | 0 |
| 5 | AE | 151/151 (100%) | 0.40 | 8 (5%) 30 27 | 73, 114, 172, 272 | 0 |
| 5 | CE | 151/151 (100%) | 0.65 | 18 (11%) 6 6 | 73, 117, 188, 252 | 0 |
| 6 | AF | 101/101 (100%) | 0.82 | 17 (16%) 2 2 | 83, 135, 192, 270 | 0 |
| 6 | CF | 101/101 (100%) | 0.26 | 5 (4%) 32 29 | 79, 131, 184, 246 | 0 |
| 7 | AG | 155/155 (100%) | 1.31 | 48 (30%) 1 1 | 118, 187, 237, 333 | 0 |
| 7 | CG | 155/155 (100%) | 1.77 | 59 (38%) 0 1 | 119, 187, 237, 286 | 0 |
| 8 | AH | 138/138 (100%) | 0.53 | 11 (7%) 15 14 | 77, 121, 166, 199 | 0 |
| 8 | CH | 138/138 (100%) | 0.70 | 13 (9%) 11 11 | 81, 123, 167, 219 | 0 |
| 9 | AI | 127/127 (100%) | 1.70 | 40 (31%) 1 1 | 119, 225, 289, 345 | 0 |
| 9 | CI | 127/127 (100%) | 1.75 | 34 (26%) 1 1 | 121, 225, 286, 354 | 0 |
| 10 | AJ | 98/98 (100%) | 1.92 | 37 (37%) 0 1 | 118, 198, 278, 356 | 0 |
| 10 | CJ | 98/98 (100%) | 2.03 | 42 (42%) 0 0 | 122, 197, 264, 351 | 0 |
| 11 | AK | 119/119 (100%) | 0.71 | 19 (15%) 3 3 | 71, 111, 171, 263 | 0 |
| 11 | CK | 119/119 (100%) | 0.45 | 10 (8%) 14 13 | 74, 111, 178, 264 | 0 |
| 12 | AL | 124/124 (100%) | 0.52 | 6 (4%) 34 31 | 67, 107, 165, 268 | 0 |
| 12 | CL | 124/124 (100%) | 0.89 | 19 (15%) 3 3 | 70, 109, 178, 252 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 13 | AM | 116/116 (100%) | 1.29 | 34 (29%) 1 1 | 134, 213, 299, 335 | 0 |
| 13 | CM | 116/116 (100%) | 2.18 | 52 (44%) 0 0 | 135, 214, 309, 362 | 0 |
| 14 | AN | 60/60 (100%) | 1.49 | 15 (25%) 1 1 | 114, 166, 217, 235 | 0 |
| 14 | CN | 60/60 (100%) | 1.25 | 12 (20%) 1 2 | 116, 167, 227, 281 | 0 |
| 15 | AO | 88/88 (100%) | 0.17 | 1 (1%) 82 77 | 66, 108, 159, 227 | 0 |
| 15 | CO | 88/88 (100%) | 0.45 | 4 (4%) 37 33 | 67, 110, 166, 241 | 0 |
| 16 | AP | 83/83 (100%) | 0.63 | 6 (7%) 18 17 | 84, 118, 174, 214 | 0 |
| 16 | CP | 83/83 (100%) | 1.84 | 33 (39%) 0 0 | 87, 123, 177, 210 | 0 |
| 17 | AQ | 99/99 (100%) | 0.30 | 2 (2%) 68 62 | 78, 112, 169, 216 | 0 |
| 17 | CQ | 99/99 (100%) | 0.78 | 11 (11%) 7 7 | 79, 116, 166, 215 | 0 |
| 18 | AR | 70/70 (100%) | 1.01 | 14 (20%) 1 2 | 84, 128, 183, 284 | 0 |
| 18 | CR | 70/70 (100%) | 0.63 | 7 (10%) 9 9 | 82, 128, 192, 232 | 0 |
| 19 | AS | 78/78 (100%) | 2.97 | 47 (60%) 0 0 | 152, 210, 275, 321 | 0 |
| 19 | CS | 78/78 (100%) | 3.24 | 53 (67%) 0 0 | 151, 216, 291, 350 | 0 |
| 20 | AT | 99/99 (100%) | 0.62 | 5 (5%) 32 28 | 86, 134, 203, 241 | 0 |
| 20 | CT | 99/99 (100%) | 1.21 | 26 (26%) 1 1 | 92, 136, 212, 269 | 0 |
| 21 | AU | 24/24 (100%) | 2.89 | 16 (66%) 0 0 | 160, 225, 264, 322 | 0 |
| 21 | CU | 24/24 (100%) | 3.00 | 13 (54%) 0 0 | 163, 218, 265, 364 | 0 |
| 22 | AV | 34/43 (79%) | 1.59 | 12 (35%) 0 1 | 89, 196, 324, 362 | 0 |
| 22 | CV | 34/43 (79%) | 2.13 | 12 (35%) 0 1 | 92, 198, 333, 339 | 0 |
| 23 | BA | 2760/2879 (95%) | 0.03 | 55 (1%) 68 62 | 27, 65, 180, 398 | 0 |
| 23 | DA | 2760/2879 (95%) | 0.09 | 48 (1%) 73 67 | 25, 63, 178, 410 | 0 |
| 24 | BB | 119/119 (100%) | 0.24 | 5 (4%) 40 35 | 77, 129, 182, 232 | 0 |
| 24 | DB | 119/119 (100%) | 0.23 | 6 (5%) 32 29 | 78, 129, 184, 236 | 0 |
| 25 | BC | 271/271 (100%) | -0.06 | 3 (1%) 82 77 | 25, 58, 109, 175 | 0 |
| 25 | DC | 271/271 (100%) | -0.01 | 0 100 100 | 18, 57, 109, 177 | 0 |
| 26 | BD | 204/204 (100%) | 0.45 | 17 (8%) 14 13 | 36, 73, 146, 341 | 0 |
| 26 | DD | 204/204 (100%) | 0.45 | 9 (4%) 38 34 | 33, 71, 145, 347 | 0 |
| 27 | BE | 202/202 (100%) | -0.04 | 1 (0%) 91 89 | 31, 73, 155, 246 | 0 |
| 27 | DE | 202/202 (100%) | 0.20 | 5 (2%) 61 55 | 25, 73, 155, 192 | 0 |
| 28 | BF | 181/181 (100%) | 1.57 | 59 (32%) 1 1 | 102, 182, 254, 314 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 28 | DF | 181/181 (100%) | 1.55 | 62 (34%) 0 1 | 104, 185, 268, 331 | 0 |
| 29 | BG | 159/159 (100%) | 1.65 | 56 (35%) 0 1 | 85, 143, 221, 343 | 0 |
| 29 | DG | 159/159 (100%) | 0.61 | 9 (5%) 27 25 | 79, 136, 186, 235 | 0 |
| 30 | BH | 145/145 (100%) | 3.27 | 72 (49%) 0 0 | 67, 243, 391, 482 | 0 |
| 30 | DH | 145/145 (100%) | 1.90 | 49 (33%) 0 1 | 64, 236, 379, 480 | 0 |
| 31 | BI | 32/65 (49%) | 6.02 | 30 (93%) 0 0 | 171, 246, 347, 355 | 0 |
| 31 | DI | 32/65 (49%) | 3.39 | 24 (75%) 0 0 | 168, 253, 310, 334 | 0 |
| 32 | BJ | 137/137 (100%) | 0.15 | 3 (2%) 65 60 | 51, 81, 142, 201 | 0 |
| 32 | DJ | 137/137 (100%) | 0.07 | 1 (0%) 89 85 | 52, 81, 146, 194 | 0 |
| 33 | BK | 122/122 (100%) | 0.09 | 0 100 100 | 42, 70, 111, 150 | 0 |
| 33 | DK | 122/122 (100%) | 0.23 | 4 (3%) 50 45 | 41, 69, 111, 162 | 0 |
| 34 | BL | 146/146 (100%) | 0.65 | 15 (10%) 9 8 | 34, 97, 166, 309 | 0 |
| 34 | DL | 146/146 (100%) | 0.56 | 14 (9%) 10 10 | 32, 97, 163, 293 | 0 |
| 35 | BM | 136/136 (100%) | 0.35 | 8 (5%) 26 23 | 49, 89, 199, 370 | 0 |
| 35 | DM | 136/136 (100%) | 0.58 | 12 (8%) 12 12 | 48, 88, 205, 406 | 0 |
| 36 | BN | 117/117 (100%) | 0.35 | 1 (0%) 85 81 | 45, 73, 137, 249 | 0 |
| 36 | DN | 117/117 (100%) | 0.24 | 1 (0%) 85 81 | 43, 73, 134, 235 | 0 |
| 37 | BO | 98/98 (100%) | 1.31 | 26 (26%) 1 1 | 82, 137, 197, 223 | 0 |
| 37 | DO | 98/98 (100%) | 1.05 | 24 (24%) 1 1 | 80, 136, 190, 215 | 0 |
| 38 | BP | 137/137 (100%) | 0.16 | 6 (4%) 38 34 | 58, 93, 185, 250 | 0 |
| 38 | DP | 137/137 (100%) | 0.45 | 18 (13%) 5 4 | 55, 92, 190, 273 | 0 |
| 39 | BQ | 116/116 (100%) | -0.04 | 0 100 100 | 35, 75, 124, 239 | 0 |
| 39 | DQ | 116/116 (100%) | -0.19 | 1 (0%) 85 81 | 26, 74, 126, 248 | 0 |
| 40 | BR | 101/101 (100%) | 0.15 | 0 100 100 | 41, 105, 164, 264 | 0 |
| 40 | DR | 101/101 (100%) | 0.60 | 5 (4%) 32 29 | 41, 110, 156, 259 | 0 |
| 41 | BS | 112/112 (100%) | 0.10 | 2 (1%) 71 65 | 44, 59, 137, 254 | 0 |
| 41 | DS | 112/112 (100%) | 0.14 | 5 (4%) 37 33 | 43, 59, 134, 255 | 0 |
| 42 | BT | 92/92 (100%) | 0.03 | 2 (2%) 65 60 | 45, 77, 129, 170 | 0 |
| 42 | DT | 92/92 (100%) | 0.19 | 0 100 100 | 36, 73, 127, 169 | 0 |
| 43 | BU | 100/100 (100%) | 1.69 | 31 (31%) 1 1 | 62, 104, 257, 396 | 0 |
| 43 | DU | 100/100 (100%) | 1.43 | 13 (13%) 5 4 | 61, 102, 251, 408 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 44 | BV | 188/188 (100%) | 0.79 | 28 (14%) 3 3 | 83, 138, 195, 245 | 0 |
| 44 | DV | 188/188 (100%) | 0.32 | 4 (2%) 67 61 | 83, 139, 194, 230 | 0 |
| 45 | BW | 76/76 (100%) | 0.49 | 6 (7%) 15 14 | 58, 84, 139, 261 | 0 |
| 45 | DW | 76/76 (100%) | 0.62 | 4 (5%) 30 27 | 59, 84, 135, 256 | 0 |
| 46 | BX | 88/88 (100%) | 0.43 | 4 (4%) 37 33 | 37, 74, 153, 322 | 0 |
| 46 | DX | 88/88 (100%) | 0.49 | 3 (3%) 49 44 | 39, 70, 153, 326 | 0 |
| 47 | BY | 62/62 (100%) | 0.32 | 6 (9%) 10 10 | 57, 98, 209, 292 | 0 |
| 47 | DY | 62/62 (100%) | 0.85 | 7 (11%) 7 7 | 51, 96, 212, 328 | 0 |
| 48 | BZ | 59/59 (100%) | 0.85 | 5 (8%) 13 13 | 43, 81, 156, 299 | 0 |
| 48 | DZ | 59/59 (100%) | 1.08 | 6 (10%) 9 9 | 45, 85, 157, 305 | 0 |
| 49 | B1 | 30/30 (100%) | 2.79 | 20 (66%) 0 0 | 184, 253, 295, 311 | 0 |
| 49 | D1 | 30/30 (100%) | 2.09 | 12 (40%) 0 0 | 183, 261, 306, 358 | 0 |
| 50 | B2 | 52/52 (100%) | 0.50 | 8 (15%) 3 3 | 26, 71, 187, 233 | 0 |
| 50 | D2 | 52/52 (100%) | 0.03 | 3 (5%) 26 24 | 21, 72, 197, 229 | 0 |
| 51 | B3 | 44/44 (100%) | 8.21 | 39 (88%) 0 0 | 139, 249, 299, 320 | 0 |
| 51 | D3 | 44/44 (100%) | 9.38 | 38 (86%) 0 0 | 141, 245, 312, 333 | 0 |
| 52 | B4 | 48/48 (100%) | 0.09 | 1 (2%) 67 61 | 33, 43, 93, 194 | 0 |
| 52 | D4 | 48/48 (100%) | 0.02 | 1 (2%) 67 61 | 21, 41, 91, 200 | 0 |
| 53 | B5 | 63/63 (100%) | 0.17 | 1 (1%) 74 69 | 45, 68, 131, 215 | 0 |
| 53 | D5 | 63/63 (100%) | 0.29 | 4 (6%) 23 22 | 45, 70, 132, 216 | 0 |
| All | All | 20230/20552 (98%) | 0.58 | 2048 (10%) 9 9 | 18, 104, 241, 498 | 0 |

All (2048) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 51 | D3 | 47 | THR | 31.3 |
| 51 | B3 | 41 | PRO | 26.6 |
| 43 | DU | 52 | SER | 25.3 |
| 51 | B3 | 40 | CYS | 24.3 |
| 51 | B3 | 13 | CYS | 24.2 |
| 51 | D3 | 13 | CYS | 23.6 |
| 30 | DH | 90 | GLY | 22.9 |
| 51 | D3 | 49 | HIS | 21.9 |
| 1 | AA | 82 | U | 20.3 |
| 51 | D3 | 46 | HIS | 19.2 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 51 | D3 | 43 | CYS | 18.6 |
| 51 | B3 | 14 | THR | 18.6 |
| 51 | B3 | 47 | THR | 18.4 |
| 1 | AA | 85 | U | 18.2 |
| 30 | BH | 85 | GLU | 18.0 |
| 51 | D3 | 48 | VAL | 17.1 |
| 30 | BH | 111 | PRO | 16.7 |
| 51 | D3 | 20 | ASN | 16.6 |
| 30 | BH | 84 | GLY | 16.5 |
| 51 | D3 | 14 | THR | 16.4 |
| 30 | BH | 68 | LEU | 16.3 |
| 51 | D3 | 22 | ALA | 16.0 |
| 43 | BU | 53 | PRO | 15.8 |
| 51 | B3 | 39 | TYR | 15.8 |
| 43 | BU | 52 | SER | 15.4 |
| 51 | B3 | 49 | HIS | 15.4 |
| 51 | D3 | 21 | TYR | 15.3 |
| 43 | DU | 50 | ARG | 14.7 |
| 9 | CI | 8 | GLY | 14.5 |
| 51 | D3 | 41 | PRO | 14.3 |
| 30 | BH | 119 | PRO | 13.3 |
| 47 | DY | 16 | LEU | 13.0 |
| 43 | DU | 51 | VAL | 12.9 |
| 1 | AA | 84 | U | 12.8 |
| 28 | BF | 2 | PRO | 12.7 |
| 1 | AA | 86 | U | 12.7 |
| 30 | BH | 128 | LEU | 12.5 |
| 19 | CS | 48 | THR | 12.3 |
| 30 | BH | 91 | SER | 12.0 |
| 43 | DU | 59 | GLY | 11.9 |
| 51 | B3 | 42 | TRP | 11.9 |
| 51 | D3 | 15 | GLU | 11.9 |
| 31 | BI | 66 | LEU | 11.7 |
| 31 | BI | 8 | GLU | 11.7 |
| 51 | D3 | 52 | VAL | 11.6 |
| 51 | D3 | 39 | TYR | 11.6 |
| 51 | B3 | 46 | HIS | 11.0 |
| 51 | B3 | 21 | TYR | 11.0 |
| 51 | D3 | 37 | ARG | 11.0 |
| 19 | AS | 75 | ALA | 10.9 |
| 31 | BI | 67 | GLY | 10.6 |
| 30 | DH | 80 | PRO | 10.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 19 | CS | 41 | VAL | 10.5 |
| 30 | BH | 65 | ALA | 10.5 |
| 51 | D3 | 16 | CYS | 10.4 |
| 1 | AA | 81 | G | 10.4 |
| 35 | BM | 140 | ALA | 10.2 |
| 23 | BA | 2799 | A | 10.1 |
| 51 | D3 | 18 | ARG | 10.1 |
| 51 | D3 | 19 | ARG | 10.0 |
| 30 | BH | 93 | THR | 10.0 |
| 30 | BH | 100 | ALA | 10.0 |
| 35 | DM | 141 | GLN | 10.0 |
| 23 | BA | 2798 | C | 9.8 |
| 30 | BH | 110 | ASP | 9.8 |
| 23 | DA | 2798 | C | 9.8 |
| 30 | BH | 134 | PRO | 9.7 |
| 51 | B3 | 16 | CYS | 9.7 |
| 30 | BH | 72 | LEU | 9.6 |
| 51 | B3 | 43 | CYS | 9.5 |
| 1 | AA | 80 | G | 9.5 |
| 31 | BI | 9 | LEU | 9.5 |
| 30 | BH | 108 | THR | 9.4 |
| 51 | D3 | 36 | LEU | 9.3 |
| 43 | BU | 51 | VAL | 9.3 |
| 51 | D3 | 40 | CYS | 9.3 |
| 19 | AS | 77 | THR | 9.2 |
| 30 | BH | 140 | LEU | 9.0 |
| 51 | B3 | 44 | ARG | 9.0 |
| 31 | BI | 11 | ALA | 9.0 |
| 51 | D3 | 38 | LYS | 9.0 |
| 47 | DY | 15 | LYS | 9.0 |
| 7 | CG | 80 | VAL | 8.9 |
| 13 | CM | 30 | ALA | 8.9 |
| 51 | D3 | 17 | LYS | 8.9 |
| 35 | DM | 140 | ALA | 8.9 |
| 13 | CM | 117 | VAL | 8.8 |
| 31 | BI | 15 | GLU | 8.8 |
| 30 | BH | 112 | LYS | 8.7 |
| 30 | BH | 118 | LYS | 8.7 |
| 51 | D3 | 24 | GLU | 8.5 |
| 51 | B3 | 20 | ASN | 8.5 |
| 30 | DH | 63 | ALA | 8.5 |
| 23 | BA | 2797 | U | 8.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 51 | B3 | 26 | ASN | 8.5 |
| 30 | DH | 88 | ILE | 8.4 |
| 19 | CS | 47 | HIS | 8.4 |
| 23 | DA | 2801 | A | 8.4 |
| 51 | B3 | 48 | VAL | 8.4 |
| 13 | AM | 116 | THR | 8.4 |
| 51 | B3 | 22 | ALA | 8.4 |
| 2 | AB | 7 | VAL | 8.4 |
| 1 | AA | 1129 | C | 8.4 |
| 19 | AS | 74 | PHE | 8.3 |
| 35 | BM | 141 | GLN | 8.3 |
| 28 | BF | 85 | GLY | 8.3 |
| 46 | BX | 85 | LEU | 8.2 |
| 30 | BH | 137 | PRO | 8.2 |
| 51 | D3 | 45 | LYS | 8.2 |
| 9 | CI | 7 | THR | 8.2 |
| 19 | CS | 74 | PHE | 8.1 |
| 23 | DA | 2799 | A | 8.0 |
| 51 | D3 | 44 | ARG | 8.0 |
| 2 | CB | 188 | ALA | 8.0 |
| 20 | CT | 102 | GLY | 8.0 |
| 51 | D3 | 42 | TRP | 7.9 |
| 13 | CM | 116 | THR | 7.9 |
| 23 | BA | 888 | C | 7.9 |
| 19 | CS | 5 | LEU | 7.9 |
| 30 | BH | 94 | ALA | 7.9 |
| 3 | CC | 207 | VAL | 7.8 |
| 23 | BA | 2793 | G | 7.8 |
| 2 | AB | 19 | HIS | 7.8 |
| 51 | B3 | 52 | VAL | 7.8 |
| 51 | D3 | 11 | LEU | 7.8 |
| 30 | BH | 109 | ILE | 7.8 |
| 30 | BH | 86 | THR | 7.8 |
| 31 | BI | 12 | THR | 7.8 |
| 30 | BH | 129 | THR | 7.7 |
| 31 | BI | 6 | ASN | 7.7 |
| 21 | CU | 18 | TYR | 7.7 |
| 30 | BH | 1 | MET | 7.7 |
| 31 | BI | 63 | LEU | 7.6 |
| 51 | B3 | 38 | LYS | 7.6 |
| 20 | CT | 103 | GLY | 7.5 |
| 31 | BI | 64 | LYS | 7.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 30 | DH | 92 | VAL | 7.5 |
| 23 | DA | 2797 | U | 7.4 |
| 22 | CV | 6174 | G | 7.4 |
| 9 | AI | 62 | TYR | 7.4 |
| 31 | DI | 62 | ALA | 7.4 |
| 30 | BH | 120 | ILE | 7.3 |
| 30 | BH | 79 | ILE | 7.3 |
| 51 | B3 | 51 | GLU | 7.3 |
| 1 | AA | 1000 | A | 7.3 |
| 7 | CG | 82 | GLY | 7.3 |
| 51 | B3 | 15 | GLU | 7.3 |
| 9 | AI | 9 | ARG | 7.2 |
| 19 | AS | 81 | ARG | 7.2 |
| 3 | CC | 149 | ALA | 7.2 |
| 45 | DW | 85 | ALA | 7.1 |
| 34 | BL | 149 | GLU | 7.1 |
| 48 | BZ | 1 | MET | 7.1 |
| 30 | DH | 116 | LEU | 7.0 |
| 21 | CU | 5 | ASP | 7.0 |
| 21 | CU | 25 | LYS | 7.0 |
| 1 | CA | 1002 | G | 6.9 |
| 30 | DH | 106 | GLY | 6.9 |
| 29 | BG | 161 | GLY | 6.9 |
| 10 | AJ | 72 | VAL | 6.9 |
| 30 | BH | 121 | LYS | 6.9 |
| 19 | AS | 4 | SER | 6.9 |
| 30 | DH | 114 | LEU | 6.9 |
| 19 | CS | 37 | ARG | 6.9 |
| 10 | AJ | 34 | VAL | 6.9 |
| 51 | B3 | 50 | ARG | 6.8 |
| 28 | BF | 171 | ALA | 6.8 |
| 51 | B3 | 24 | GLU | 6.8 |
| 51 | D3 | 12 | GLU | 6.7 |
| 19 | AS | 41 | VAL | 6.7 |
| 1 | CA | 1000 | A | 6.7 |
| 43 | DU | 53 | PRO | 6.7 |
| 30 | BH | 122 | GLU | 6.7 |
| 23 | DA | 2803 | C | 6.6 |
| 23 | BA | 2801 | A | 6.6 |
| 19 | AS | 67 | VAL | 6.6 |
| 12 | CL | 28 | GLY | 6.5 |
| 28 | DF | 2 | PRO | 6.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 9 | AI | 64 | THR | 6.5 |
| 19 | AS | 49 | ILE | 6.5 |
| 44 | DV | 181 | GLU | 6.5 |
| 2 | AB | 40 | HIS | 6.5 |
| 13 | CM | 96 | LEU | 6.5 |
| 30 | BH | 64 | GLU | 6.5 |
| 37 | BO | 58 | LEU | 6.5 |
| 49 | B1 | 36 | VAL | 6.4 |
| 28 | DF | 87 | PRO | 6.4 |
| 21 | AU | 17 | THR | 6.4 |
| 14 | CN | 32 | SER | 6.4 |
| 16 | CP | 35 | LYS | 6.4 |
| 49 | D1 | 45 | GLY | 6.3 |
| 19 | AS | 5 | LEU | 6.3 |
| 19 | CS | 40 | ILE | 6.3 |
| 23 | BA | 1174 | A | 6.3 |
| 31 | BI | 14 | LYS | 6.3 |
| 30 | BH | 127 | VAL | 6.3 |
| 19 | AS | 44 | MET | 6.3 |
| 19 | AS | 60 | VAL | 6.3 |
| 19 | CS | 61 | TYR | 6.2 |
| 7 | CG | 62 | PHE | 6.2 |
| 28 | BF | 21 | ARG | 6.2 |
| 30 | BH | 103 | ARG | 6.2 |
| 31 | BI | 16 | ASN | 6.2 |
| 31 | DI | 20 | ALA | 6.2 |
| 19 | CS | 69 | HIS | 6.2 |
| 7 | AG | 80 | VAL | 6.2 |
| 13 | CM | 15 | VAL | 6.2 |
| 11 | AK | 12 | ARG | 6.1 |
| 30 | DH | 145 | VAL | 6.1 |
| 19 | CS | 66 | MET | 6.1 |
| 51 | D3 | 23 | THR | 6.1 |
| 21 | AU | 18 | TYR | 6.1 |
| 12 | CL | 127 | ALA | 6.1 |
| 31 | BI | 65 | GLU | 6.1 |
| 9 | AI | 18 | PHE | 6.1 |
| 16 | CP | 34 | GLU | 6.1 |
| 49 | B1 | 37 | PRO | 6.1 |
| 6 | AF | 101 | ALA | 6.1 |
| 30 | BH | 104 | GLN | 6.0 |
| 2 | CB | 132 | LYS | 6.0 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 34 | BL | 148 | LEU | 6.0 |
| 19 | CS | 49 | ILE | 6.0 |
| 8 | CH | 52 | ASP | 6.0 |
| 30 | BH | 114 | LEU | 6.0 |
| 1 | AA | 1138 | G | 6.0 |
| 31 | BI | 59 | ILE | 5.9 |
| 9 | CI | 128 | ARG | 5.9 |
| 49 | B1 | 55 | PRO | 5.9 |
| 49 | B1 | 50 | THR | 5.9 |
| 9 | CI | 12 | GLU | 5.9 |
| 13 | AM | 113 | PRO | 5.9 |
| 9 | AI | 82 | ALA | 5.9 |
| 4 | CD | 104 | VAL | 5.9 |
| 31 | BI | 4 | LYS | 5.9 |
| 30 | DH | 59 | ALA | 5.9 |
| 12 | AL | 127 | ALA | 5.8 |
| 19 | CS | 36 | ARG | 5.8 |
| 22 | AV | 6174 | G | 5.8 |
| 19 | CS | 81 | ARG | 5.8 |
| 21 | CU | 7 | ARG | 5.8 |
| 22 | CV | 6212 | U | 5.8 |
| 23 | BA | 2794 | C | 5.8 |
| 31 | BI | 21 | GLN | 5.8 |
| 28 | BF | 69 | ALA | 5.7 |
| 28 | DF | 80 | PHE | 5.7 |
| 13 | CM | 16 | ASP | 5.7 |
| 29 | DG | 169 | VAL | 5.7 |
| 19 | CS | 73 | GLU | 5.7 |
| 23 | DA | 1535 | U | 5.7 |
| 51 | B3 | 45 | LYS | 5.7 |
| 10 | CJ | 26 | ALA | 5.7 |
| 13 | CM | 85 | GLY | 5.7 |
| 49 | D1 | 65 | CYS | 5.6 |
| 21 | AU | 25 | LYS | 5.6 |
| 48 | DZ | 1 | MET | 5.6 |
| 9 | AI | 7 | THR | 5.6 |
| 13 | CM | 87 | TYR | 5.6 |
| 1 | CA | 84 | U | 5.6 |
| 1 | CA | 1286 | A | 5.6 |
| 31 | BI | 61 | LEU | 5.6 |
| 29 | BG | 32 | GLU | 5.6 |
| 10 | CJ | 38 | ILE | 5.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 9 | AI | 65 | VAL | 5.6 |
| 29 | BG | 43 | VAL | 5.6 |
| 21 | AU | 21 | TYR | 5.6 |
| 51 | B3 | 17 | LYS | 5.6 |
| 28 | DF | 85 | GLY | 5.6 |
| 1 | CA | 1533 | C | 5.6 |
| 13 | AM | 117 | VAL | 5.5 |
| 51 | D3 | 50 | ARG | 5.5 |
| 51 | B3 | 36 | LEU | 5.5 |
| 9 | CI | 33 | PHE | 5.5 |
| 1 | AA | 1001 | G | 5.5 |
| 49 | D1 | 37 | PRO | 5.5 |
| 16 | CP | 36 | ILE | 5.5 |
| 31 | DI | 59 | ILE | 5.5 |
| 13 | CM | 113 | PRO | 5.5 |
| 22 | CV | 6175 | G | 5.5 |
| 23 | BA | 2795 | G | 5.5 |
| 28 | DF | 146 | TYR | 5.5 |
| 28 | BF | 25 | TYR | 5.4 |
| 31 | BI | 56 | ASN | 5.4 |
| 23 | DA | 2804 | C | 5.4 |
| 9 | CI | 97 | LYS | 5.4 |
| 13 | CM | 112 | GLY | 5.4 |
| 9 | CI | 96 | LEU | 5.4 |
| 31 | BI | 7 | VAL | 5.4 |
| 19 | AS | 50 | ALA | 5.4 |
| 16 | CP | 21 | VAL | 5.4 |
| 51 | D3 | 31 | PRO | 5.4 |
| 28 | BF | 172 | LEU | 5.4 |
| 31 | BI | 13 | LEU | 5.4 |
| 28 | DF | 88 | ILE | 5.4 |
| 47 | BY | 3 | LEU | 5.3 |
| 31 | DI | 6 | ASN | 5.3 |
| 19 | CS | 39 | THR | 5.3 |
| 14 | AN | 13 | THR | 5.3 |
| 34 | DL | 150 | ALA | 5.3 |
| 37 | DO | 87 | PHE | 5.3 |
| 19 | CS | 71 | LEU | 5.3 |
| 49 | D1 | 44 | CYS | 5.3 |
| 51 | B3 | 23 | THR | 5.3 |
| 30 | DH | 78 | THR | 5.3 |
| 43 | BU | 50 | ARG | 5.2 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 31 | DI | 63 | LEU | 5.2 |
| 23 | DA | 888 | C | 5.2 |
| 51 | B3 | 37 | ARG | 5.2 |
| 28 | DF | 152 | LEU | 5.2 |
| 1 | CA | 999 | U | 5.2 |
| 30 | DH | 83 | ALA | 5.2 |
| 45 | DW | 61 | ALA | 5.2 |
| 1 | CA | 210 | U | 5.2 |
| 2 | AB | 165 | VAL | 5.2 |
| 29 | BG | 124 | GLU | 5.2 |
| 30 | BH | 117 | GLU | 5.2 |
| 29 | BG | 94 | TYR | 5.2 |
| 28 | DF | 52 | ILE | 5.2 |
| 51 | B3 | 19 | ARG | 5.1 |
| 23 | BA | 2211 | G | 5.1 |
| 3 | CC | 160 | ALA | 5.1 |
| 31 | BI | 5 | ARG | 5.1 |
| 3 | CC | 206 | GLU | 5.1 |
| 11 | AK | 129 | SER | 5.1 |
| 47 | DY | 12 | GLU | 5.1 |
| 10 | CJ | 6 | ILE | 5.1 |
| 9 | AI | 14 | VAL | 5.1 |
| 28 | BF | 77 | ILE | 5.1 |
| 9 | CI | 18 | PHE | 5.1 |
| 9 | CI | 13 | ALA | 5.1 |
| 9 | CI | 93 | ARG | 5.1 |
| 23 | BA | 1046 | A | 5.1 |
| 51 | B3 | 28 | ARG | 5.0 |
| 9 | AI | 101 | PHE | 5.0 |
| 30 | DH | 107 | ILE | 5.0 |
| 10 | CJ | 72 | VAL | 5.0 |
| 43 | DU | 17 | SER | 5.0 |
| 19 | AS | 69 | HIS | 5.0 |
| 44 | BV | 97 | GLU | 5.0 |
| 31 | DI | 18 | GLU | 5.0 |
| 19 | CS | 46 | GLY | 5.0 |
| 28 | DF | 82 | LEU | 5.0 |
| 20 | CT | 48 | LYS | 5.0 |
| 24 | DB | 52 | A | 5.0 |
| 47 | DY | 14 | ARG | 5.0 |
| 28 | DF | 137 | GLU | 5.0 |
| 14 | AN | 55 | GLY | 5.0 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 4 | CD | 169 | LYS | 5.0 |
| 1 | CA | 103(C) | G | 5.0 |
| 28 | BF | 23 | PHE | 5.0 |
| 30 | DH | 94 | ALA | 5.0 |
| 13 | CM | 97 | PRO | 5.0 |
| 16 | CP | 22 | THR | 4.9 |
| 3 | CC | 168 | ALA | 4.9 |
| 10 | CJ | 8 | LEU | 4.9 |
| 30 | BH | 131 | LYS | 4.9 |
| 16 | CP | 54 | GLU | 4.9 |
| 1 | CA | 103(B) | G | 4.9 |
| 22 | AV | 6212 | U | 4.9 |
| 41 | DS | 112 | GLY | 4.9 |
| 31 | DI | 12 | THR | 4.9 |
| 7 | AG | 15 | ASP | 4.9 |
| 7 | AG | 16 | LEU | 4.9 |
| 7 | CG | 22 | LEU | 4.9 |
| 10 | AJ | 27 | ALA | 4.9 |
| 28 | DF | 131 | TYR | 4.9 |
| 43 | BU | 54 | LYS | 4.9 |
| 10 | CJ | 71 | LEU | 4.9 |
| 10 | CJ | 95 | GLU | 4.9 |
| 34 | DL | 149 | GLU | 4.9 |
| 19 | CS | 38 | SER | 4.9 |
| 31 | DI | 14 | LYS | 4.9 |
| 21 | CU | 23 | PRO | 4.8 |
| 10 | CJ | 61 | GLU | 4.8 |
| 31 | BI | 10 | LEU | 4.8 |
| 31 | BI | 60 | ARG | 4.8 |
| 2 | CB | 101 | MET | 4.8 |
| 52 | B4 | 48 | LYS | 4.8 |
| 13 | AM | 112 | GLY | 4.8 |
| 21 | AU | 22 | ARG | 4.8 |
| 18 | AR | 31 | LEU | 4.8 |
| 19 | CS | 12 | ASP | 4.8 |
| 7 | CG | 16 | LEU | 4.8 |
| 4 | CD | 182 | LYS | 4.8 |
| 7 | CG | 31 | MET | 4.8 |
| 44 | BV | 159 | PRO | 4.8 |
| 1 | AA | 1287 | A | 4.8 |
| 23 | DA | 2107 | C | 4.8 |
| 13 | CM | 63 | THR | 4.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 12 | AL | 49 | SER | 4.8 |
| 20 | CT | 100 | ILE | 4.8 |
| 1 | AA | 1288 | A | 4.8 |
| 31 | BI | 19 | ARG | 4.8 |
| 38 | DP | 133 | GLU | 4.8 |
| 2 | CB | 28 | PHE | 4.7 |
| 26 | BD | 204 | ALA | 4.7 |
| 28 | BF | 34 | LEU | 4.7 |
| 13 | AM | 87 | TYR | 4.7 |
| 30 | DH | 87 | LYS | 4.7 |
| 10 | AJ | 67 | THR | 4.7 |
| 1 | CA | 1033 | G | 4.7 |
| 7 | CG | 83 | ALA | 4.7 |
| 7 | CG | 84 | ASN | 4.7 |
| 1 | CA | 1260 | C | 4.7 |
| 8 | AH | 94 | TYR | 4.7 |
| 4 | CD | 175 | SER | 4.7 |
| 29 | BG | 89 | ILE | 4.7 |
| 29 | BG | 105 | LEU | 4.7 |
| 10 | AJ | 33 | GLN | 4.7 |
| 2 | AB | 36 | ARG | 4.7 |
| 19 | AS | 51 | VAL | 4.7 |
| 3 | AC | 149 | ALA | 4.7 |
| 7 | AG | 37 | ASN | 4.7 |
| 18 | AR | 46 | GLU | 4.7 |
| 31 | DI | 5 | ARG | 4.7 |
| 16 | CP | 19 | ILE | 4.7 |
| 23 | BA | 2892 | A | 4.7 |
| 19 | AS | 70 | LYS | 4.7 |
| 13 | AM | 39 | ILE | 4.6 |
| 10 | AJ | 26 | ALA | 4.6 |
| 10 | CJ | 9 | ARG | 4.6 |
| 2 | CB | 29 | ALA | 4.6 |
| 9 | AI | 8 | GLY | 4.6 |
| 7 | CG | 134 | ALA | 4.6 |
| 37 | BO | 60 | GLY | 4.6 |
| 2 | CB | 138 | LEU | 4.6 |
| 21 | CU | 2 | GLY | 4.6 |
| 7 | CG | 58 | PRO | 4.6 |
| 1 | CA | 1289 | A | 4.6 |
| 22 | AV | 6175 | G | 4.6 |
| 43 | BU | 55 | TYR | 4.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | CA | 1243 | C | 4.6 |
| 30 | BH | 132 | PRO | 4.6 |
| 7 | CG | 26 | PHE | 4.6 |
| 30 | DH | 127 | VAL | 4.6 |
| 28 | DF | 48 | GLU | 4.6 |
| 44 | BV | 169 | GLU | 4.6 |
| 19 | CS | 33 | THR | 4.6 |
| 29 | BG | 106 | THR | 4.6 |
| 9 | CI | 127 | LYS | 4.5 |
| 20 | CT | 95 | ALA | 4.5 |
| 34 | DL | 89 | ALA | 4.5 |
| 31 | DI | 16 | ASN | 4.5 |
| 10 | CJ | 73 | ASP | 4.5 |
| 7 | CG | 32 | ARG | 4.5 |
| 9 | AI | 17 | VAL | 4.5 |
| 30 | DH | 89 | TYR | 4.5 |
| 19 | CS | 35 | SER | 4.5 |
| 51 | B3 | 30 | THR | 4.5 |
| 27 | DE | 6 | MET | 4.5 |
| 43 | BU | 2 | ARG | 4.5 |
| 10 | CJ | 36 | GLY | 4.5 |
| 12 | AL | 126 | GLU | 4.5 |
| 49 | B1 | 53 | THR | 4.5 |
| 7 | CG | 71 | PRO | 4.5 |
| 28 | DF | 81 | LYS | 4.5 |
| 4 | CD | 108 | LEU | 4.5 |
| 3 | AC | 151 | VAL | 4.4 |
| 8 | CH | 25 | ASP | 4.4 |
| 49 | D1 | 41 | ILE | 4.4 |
| 1 | CA | 1003 | G | 4.4 |
| 38 | DP | 136 | GLN | 4.4 |
| 29 | BG | 170 | ARG | 4.4 |
| 38 | BP | 2 | ASN | 4.4 |
| 7 | CG | 33 | ASP | 4.4 |
| 7 | CG | 12 | LEU | 4.4 |
| 19 | AS | 71 | LEU | 4.4 |
| 6 | AF | 63 | TYR | 4.4 |
| 14 | AN | 20 | ALA | 4.4 |
| 28 | DF | 39 | ILE | 4.4 |
| 30 | DH | 98 | ALA | 4.4 |
| 34 | BL | 150 | ALA | 4.4 |
| 49 | B1 | 49 | GLU | 4.4 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 28 | DF | 76 | SER | 4.4 |
| 44 | BV | 168 | GLU | 4.4 |
| 51 | B3 | 12 | GLU | 4.4 |
| 49 | B1 | 38 | ALA | 4.4 |
| 14 | AN | 8 | GLU | 4.4 |
| 48 | BZ | 58 | VAL | 4.3 |
| 51 | B3 | 32 | ASN | 4.3 |
| 18 | AR | 23 | LYS | 4.3 |
| 1 | CA | 998(B) | C | 4.3 |
| 10 | AJ | 28 | ARG | 4.3 |
| 9 | AI | 63 | ILE | 4.3 |
| 30 | DH | 105 | HIS | 4.3 |
| 44 | BV | 163 | LEU | 4.3 |
| 3 | CC | 185 | GLY | 4.3 |
| 12 | CL | 44 | PRO | 4.3 |
| 7 | CG | 81 | GLY | 4.3 |
| 9 | AI | 15 | ALA | 4.3 |
| 7 | CG | 101 | LEU | 4.3 |
| 1 | AA | 1036 | G | 4.3 |
| 9 | AI | 85 | LEU | 4.3 |
| 9 | CI | 102 | LEU | 4.3 |
| 11 | CK | 129 | SER | 4.3 |
| 29 | BG | 95 | ARG | 4.3 |
| 21 | CU | 4 | GLY | 4.3 |
| 37 | DO | 38 | GLN | 4.3 |
| 35 | BM | 91 | GLU | 4.3 |
| 51 | B3 | 29 | ASN | 4.3 |
| 24 | BB | 52 | A | 4.3 |
| 49 | B1 | 51 | TYR | 4.3 |
| 43 | BU | 62 | GLU | 4.3 |
| 13 | CM | 65 | LYS | 4.3 |
| 2 | CB | 133 | LYS | 4.3 |
| 13 | CM | 90 | LEU | 4.3 |
| 3 | CC | 151 | VAL | 4.2 |
| 29 | BG | 123 | PHE | 4.2 |
| 30 | BH | 58 | LEU | 4.2 |
| 10 | CJ | 10 | GLY | 4.2 |
| 4 | CD | 11 | LEU | 4.2 |
| 3 | AC | 197 | GLY | 4.2 |
| 13 | CM | 34 | LEU | 4.2 |
| 29 | BG | 55 | PRO | 4.2 |
| 48 | BZ | 2 | PRO | 4.2 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 28 | BF | 35 | GLU | 4.2 |
| 51 | D3 | 51 | GLU | 4.2 |
| 29 | BG | 29 | PRO | 4.2 |
| 41 | BS | 112 | GLY | 4.2 |
| 21 | AU | 23 | PRO | 4.2 |
| 24 | BB | 54 | G | 4.2 |
| 31 | DI | 66 | LEU | 4.2 |
| 31 | DI | 8 | GLU | 4.2 |
| 1 | AA | 1260 | C | 4.2 |
| 10 | CJ | 4 | ILE | 4.2 |
| 13 | CM | 82 | MET | 4.2 |
| 10 | CJ | 69 | ASN | 4.2 |
| 1 | CA | 1044 | A | 4.2 |
| 28 | DF | 41 | GLN | 4.2 |
| 4 | CD | 95 | GLY | 4.2 |
| 7 | AG | 26 | PHE | 4.2 |
| 23 | DA | 2802 | G | 4.2 |
| 28 | BF | 142 | PRO | 4.2 |
| 5 | AE | 19 | MET | 4.2 |
| 7 | AG | 34 | GLY | 4.1 |
| 14 | CN | 2 | ALA | 4.1 |
| 1 | CA | 1001 | G | 4.1 |
| 7 | AG | 85 | TYR | 4.1 |
| 19 | AS | 59 | PRO | 4.1 |
| 31 | DI | 13 | LEU | 4.1 |
| 1 | CA | 407 | G | 4.1 |
| 11 | CK | 128 | ALA | 4.1 |
| 8 | AH | 131 | GLY | 4.1 |
| 28 | BF | 82 | LEU | 4.1 |
| 2 | CB | 128 | GLU | 4.1 |
| 19 | AS | 40 | ILE | 4.1 |
| 29 | DG | 60 | ARG | 4.1 |
| 29 | BG | 25 | LYS | 4.1 |
| 8 | AH | 25 | ASP | 4.1 |
| 19 | AS | 35 | SER | 4.1 |
| 28 | BF | 87 | PRO | 4.1 |
| 10 | AJ | 98 | ILE | 4.1 |
| 19 | CS | 50 | ALA | 4.1 |
| 38 | DP | 137 | LYS | 4.1 |
| 16 | CP | 1 | MET | 4.1 |
| 23 | BA | 1535 | U | 4.1 |
| 16 | CP | 18 | ARG | 4.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 3 | AC | 152 | ILE | 4.0 |
| 19 | AS | 10 | PHE | 4.0 |
| 29 | BG | 96 | ALA | 4.0 |
| 30 | DH | 67 | ARG | 4.0 |
| 31 | BI | 20 | ALA | 4.0 |
| 23 | BA | 1045 | A | 4.0 |
| 29 | BG | 90 | LYS | 4.0 |
| 3 | CC | 204 | LEU | 4.0 |
| 47 | BY | 16 | LEU | 4.0 |
| 7 | AG | 78 | ARG | 4.0 |
| 19 | AS | 48 | THR | 4.0 |
| 10 | AJ | 70 | ARG | 4.0 |
| 30 | DH | 132 | PRO | 4.0 |
| 43 | BU | 44 | ILE | 4.0 |
| 11 | AK | 13 | GLN | 4.0 |
| 9 | CI | 94 | ALA | 4.0 |
| 10 | AJ | 68 | HIS | 4.0 |
| 18 | CR | 24 | ALA | 4.0 |
| 16 | CP | 9 | PHE | 4.0 |
| 3 | CC | 170 | GLN | 4.0 |
| 14 | AN | 14 | PRO | 4.0 |
| 51 | B3 | 31 | PRO | 4.0 |
| 13 | CM | 7 | VAL | 4.0 |
| 28 | DF | 133 | LEU | 4.0 |
| 31 | DI | 17 | LEU | 4.0 |
| 19 | CS | 44 | MET | 4.0 |
| 28 | DF | 27 | ASN | 4.0 |
| 23 | DA | 11 | G | 4.0 |
| 1 | AA | 87 | A | 4.0 |
| 29 | DG | 170 | ARG | 4.0 |
| 31 | DI | 4 | LYS | 4.0 |
| 3 | CC | 19 | GLU | 4.0 |
| 38 | DP | 132 | LYS | 3.9 |
| 13 | CM | 60 | VAL | 3.9 |
| 30 | BH | 71 | ILE | 3.9 |
| 9 | AI | 32 | ASP | 3.9 |
| 43 | DU | 2 | ARG | 3.9 |
| 13 | CM | 98 | VAL | 3.9 |
| 1 | AA | 1002 | G | 3.9 |
| 2 | AB | 122 | PHE | 3.9 |
| 29 | BG | 91 | GLY | 3.9 |
| 7 | CG | 5 | ARG | 3.9 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 31 | DI | 11 | ALA | 3.9 |
| 37 | BO | 37 | ALA | 3.9 |
| 10 | CJ | 65 | LEU | 3.9 |
| 49 | D1 | 55 | PRO | 3.9 |
| 51 | B3 | 27 | LYS | 3.9 |
| 28 | BF | 76 | SER | 3.9 |
| 4 | CD | 101 | LEU | 3.9 |
| 7 | AG | 79 | ARG | 3.9 |
| 2 | AB | 167 | PRO | 3.9 |
| 16 | CP | 59 | TRP | 3.9 |
| 19 | AS | 76 | PRO | 3.9 |
| 28 | BF | 26 | GLN | 3.9 |
| 28 | DF | 34 | LEU | 3.9 |
| 19 | CS | 59 | PRO | 3.9 |
| 29 | BG | 104 | GLU | 3.9 |
| 17 | CQ | 73 | VAL | 3.9 |
| 31 | DI | 19 | ARG | 3.9 |
| 50 | B2 | 46 | CYS | 3.9 |
| 30 | DH | 71 | ILE | 3.9 |
| 51 | B3 | 25 | LYS | 3.9 |
| 13 | AM | 94 | ARG | 3.9 |
| 23 | BA | 2802 | G | 3.9 |
| 28 | DF | 175 | LEU | 3.9 |
| 21 | AU | 2 | GLY | 3.9 |
| 19 | AS | 52 | TYR | 3.8 |
| 30 | BH | 97 | ILE | 3.8 |
| 13 | CM | 91 | ARG | 3.8 |
| 16 | CP | 37 | GLY | 3.8 |
| 29 | BG | 17 | VAL | 3.8 |
| 43 | BU | 87 | LYS | 3.8 |
| 10 | AJ | 73 | ASP | 3.8 |
| 28 | BF | 11 | TYR | 3.8 |
| 37 | BO | 68 | GLN | 3.8 |
| 11 | AK | 11 | LYS | 3.8 |
| 23 | BA | 1104 | C | 3.8 |
| 9 | AI | 21 | PRO | 3.8 |
| 1 | AA | 1025 | U | 3.8 |
| 5 | AE | 33 | VAL | 3.8 |
| 1 | AA | 1042 | G | 3.8 |
| 37 | BO | 35 | ILE | 3.8 |
| 7 | CG | 13 | GLN | 3.8 |
| 8 | CH | 61 | VAL | 3.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | AB | 101 | MET | 3.8 |
| 19 | CS | 80 | TYR | 3.8 |
| 13 | CM | 24 | GLY | 3.8 |
| 43 | BU | 47 | LYS | 3.8 |
| 1 | CA | 1353 | G | 3.8 |
| 7 | CG | 8 | GLU | 3.8 |
| 19 | AS | 39 | THR | 3.8 |
| 7 | AG | 31 | MET | 3.8 |
| 28 | DF | 147 | ASP | 3.8 |
| 3 | AC | 201 | TYR | 3.8 |
| 9 | AI | 3 | GLN | 3.8 |
| 2 | AB | 41 | ILE | 3.8 |
| 11 | CK | 12 | ARG | 3.8 |
| 19 | AS | 78 | ARG | 3.8 |
| 13 | AM | 82 | MET | 3.8 |
| 13 | CM | 5 | ALA | 3.8 |
| 28 | DF | 79 | ASN | 3.8 |
| 2 | AB | 160 | ASP | 3.8 |
| 29 | BG | 44 | VAL | 3.7 |
| 6 | CF | 55 | ASP | 3.7 |
| 28 | DF | 77 | ILE | 3.7 |
| 49 | B1 | 54 | LYS | 3.7 |
| 1 | AA | 1257 | U | 3.7 |
| 2 | AB | 237 | ALA | 3.7 |
| 28 | DF | 115 | ARG | 3.7 |
| 37 | BO | 52 | SER | 3.7 |
| 2 | AB | 166 | ASP | 3.7 |
| 10 | CJ | 15 | THR | 3.7 |
| 4 | CD | 200 | GLU | 3.7 |
| 31 | BI | 3 | ASN | 3.7 |
| 5 | CE | 77 | PRO | 3.7 |
| 9 | AI | 61 | ALA | 3.7 |
| 19 | AS | 34 | TRP | 3.7 |
| 23 | BA | 1509 | A | 3.7 |
| 28 | DF | 46 | ALA | 3.7 |
| 10 | AJ | 29 | ARG | 3.7 |
| 30 | DH | 140 | LEU | 3.7 |
| 22 | AV | 6201 | C | 3.7 |
| 30 | DH | 120 | ILE | 3.7 |
| 10 | CJ | 35 | SER | 3.7 |
| 3 | AC | 207 | VAL | 3.7 |
| 11 | CK | 127 | LYS | 3.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 18 | AR | 22 | VAL | 3.7 |
| 7 | AG | 12 | LEU | 3.7 |
| 19 | AS | 47 | HIS | 3.7 |
| 3 | CC | 101 | LEU | 3.7 |
| 7 | AG | 17 | VAL | 3.7 |
| 12 | CL | 29 | ALA | 3.7 |
| 13 | AM | 60 | VAL | 3.7 |
| 23 | DA | 2182 | G | 3.7 |
| 30 | DH | 133 | HIS | 3.7 |
| 30 | BH | 87 | LYS | 3.7 |
| 30 | BH | 139 | GLN | 3.7 |
| 1 | CA | 958 | A | 3.7 |
| 1 | AA | 999 | U | 3.7 |
| 13 | AM | 107 | ALA | 3.7 |
| 37 | DO | 28 | VAL | 3.7 |
| 38 | DP | 2 | ASN | 3.7 |
| 7 | CG | 125 | MET | 3.7 |
| 2 | AB | 226 | ARG | 3.7 |
| 4 | CD | 18 | LYS | 3.7 |
| 23 | DA | 887 | A | 3.7 |
| 13 | AM | 83 | ASP | 3.7 |
| 19 | AS | 38 | SER | 3.7 |
| 10 | AJ | 52 | GLY | 3.7 |
| 31 | DI | 21 | GLN | 3.7 |
| 31 | DI | 9 | LEU | 3.7 |
| 11 | CK | 65 | ALA | 3.7 |
| 30 | DH | 70 | GLU | 3.7 |
| 29 | BG | 101 | ARG | 3.7 |
| 16 | CP | 4 | ILE | 3.7 |
| 10 | AJ | 71 | LEU | 3.7 |
| 19 | AS | 36 | ARG | 3.7 |
| 19 | CS | 75 | ALA | 3.7 |
| 20 | CT | 106 | ALA | 3.7 |
| 49 | B1 | 48 | ILE | 3.7 |
| 1 | CA | 1111 | A | 3.6 |
| 5 | CE | 78 | HIS | 3.6 |
| 3 | AC | 56 | ASP | 3.6 |
| 9 | AI | 12 | GLU | 3.6 |
| 28 | DF | 176 | LEU | 3.6 |
| 50 | B2 | 37 | LYS | 3.6 |
| 19 | AS | 42 | PRO | 3.6 |
| 2 | CB | 187 | LEU | 3.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 21 | CU | 6 | ARG | 3.6 |
| 30 | BH | 62 | LYS | 3.6 |
| 8 | CH | 51 | VAL | 3.6 |
| 30 | DH | 125 | GLU | 3.6 |
| 20 | CT | 55 | ILE | 3.6 |
| 28 | DF | 73 | ALA | 3.6 |
| 4 | CD | 145 | GLU | 3.6 |
| 29 | BG | 159 | GLU | 3.6 |
| 26 | DD | 204 | ALA | 3.6 |
| 2 | AB | 163 | PHE | 3.6 |
| 37 | DO | 41 | ASP | 3.6 |
| 2 | AB | 12 | GLU | 3.6 |
| 31 | DI | 10 | LEU | 3.6 |
| 30 | DH | 108 | THR | 3.6 |
| 1 | CA | 1149 | C | 3.6 |
| 9 | AI | 128 | ARG | 3.6 |
| 3 | AC | 170 | GLN | 3.6 |
| 7 | AG | 104 | LEU | 3.6 |
| 10 | AJ | 25 | GLU | 3.6 |
| 16 | CP | 39 | TYR | 3.6 |
| 30 | BH | 81 | VAL | 3.6 |
| 10 | CJ | 19 | SER | 3.6 |
| 28 | BF | 88 | ILE | 3.6 |
| 30 | DH | 101 | LEU | 3.6 |
| 43 | BU | 5 | MET | 3.6 |
| 9 | AI | 92 | TYR | 3.6 |
| 28 | BF | 12 | TYR | 3.6 |
| 7 | CG | 9 | VAL | 3.6 |
| 4 | CD | 117 | ALA | 3.6 |
| 30 | BH | 95 | LYS | 3.6 |
| 6 | AF | 6 | VAL | 3.6 |
| 13 | AM | 106 | ASN | 3.6 |
| 19 | AS | 9 | VAL | 3.6 |
| 19 | AS | 53 | ASN | 3.6 |
| 22 | CV | 6213 | A | 3.6 |
| 10 | AJ | 35 | SER | 3.6 |
| 6 | AF | 91 | VAL | 3.5 |
| 11 | AK | 109 | VAL | 3.5 |
| 43 | BU | 42 | VAL | 3.5 |
| 1 | CA | 1031 | G | 3.5 |
| 10 | CJ | 33 | GLN | 3.5 |
| 23 | BA | 2792 | G | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 27 | DE | 27 | GLU | 3.5 |
| 11 | AK | 18 | ARG | 3.5 |
| 23 | DA | 2602 | A | 3.5 |
| 28 | DF | 90 | LEU | 3.5 |
| 37 | BO | 51 | ALA | 3.5 |
| 11 | AK | 17 | GLY | 3.5 |
| 11 | CK | 13 | GLN | 3.5 |
| 37 | DO | 26 | LEU | 3.5 |
| 7 | CG | 85 | TYR | 3.5 |
| 22 | CV | 6199 | G | 3.5 |
| 25 | BC | 2 | ALA | 3.5 |
| 14 | AN | 17 | LYS | 3.5 |
| 44 | BV | 160 | GLY | 3.5 |
| 7 | CG | 135 | VAL | 3.5 |
| 9 | AI | 26 | VAL | 3.5 |
| 1 | CA | 1112 | C | 3.5 |
| 13 | CM | 43 | THR | 3.5 |
| 19 | CS | 53 | ASN | 3.5 |
| 7 | CG | 20 | ASP | 3.5 |
| 1 | CA | 723 | U | 3.5 |
| 2 | CB | 7 | VAL | 3.5 |
| 19 | CS | 42 | PRO | 3.5 |
| 23 | DA | 2805 | G | 3.5 |
| 2 | AB | 132 | LYS | 3.5 |
| 50 | D2 | 48 | GLU | 3.5 |
| 13 | AM | 100 | GLY | 3.5 |
| 31 | BI | 62 | ALA | 3.5 |
| 37 | DO | 86 | ALA | 3.5 |
| 51 | B3 | 18 | ARG | 3.5 |
| 44 | BV | 126 | VAL | 3.5 |
| 9 | CI | 37 | PHE | 3.5 |
| 3 | CC | 66 | VAL | 3.5 |
| 8 | CH | 24 | THR | 3.5 |
| 28 | DF | 45 | GLU | 3.5 |
| 38 | DP | 129 | ARG | 3.5 |
| 28 | DF | 13 | GLU | 3.5 |
| 30 | DH | 66 | GLU | 3.5 |
| 7 | AG | 36 | LYS | 3.4 |
| 7 | AG | 81 | GLY | 3.4 |
| 44 | BV | 162 | GLU | 3.4 |
| 7 | CG | 79 | ARG | 3.4 |
| 14 | CN | 8 | GLU | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 23 | BA | 280 | C | 3.4 |
| 20 | CT | 96 | GLY | 3.4 |
| 23 | BA | 2894 | G | 3.4 |
| 9 | CI | 65 | VAL | 3.4 |
| 5 | CE | 118 | ILE | 3.4 |
| 2 | CB | 19 | HIS | 3.4 |
| 2 | CB | 72 | GLY | 3.4 |
| 43 | BU | 59 | GLY | 3.4 |
| 21 | CU | 8 | THR | 3.4 |
| 2 | AB | 137 | ARG | 3.4 |
| 7 | AG | 40 | ALA | 3.4 |
| 23 | BA | 2896 | C | 3.4 |
| 18 | CR | 29 | PHE | 3.4 |
| 13 | AM | 81 | LEU | 3.4 |
| 28 | BF | 90 | LEU | 3.4 |
| 34 | DL | 100 | LEU | 3.4 |
| 29 | BG | 34 | GLU | 3.4 |
| 13 | CM | 40 | ASN | 3.4 |
| 28 | DF | 157 | ILE | 3.4 |
| 28 | BF | 178 | PHE | 3.4 |
| 29 | DG | 61 | HIS | 3.4 |
| 5 | AE | 18 | ARG | 3.4 |
| 7 | AG | 28 | ASN | 3.4 |
| 2 | AB | 35 | GLU | 3.4 |
| 30 | BH | 61 | ARG | 3.4 |
| 13 | CM | 41 | PRO | 3.4 |
| 2 | CB | 228 | GLY | 3.4 |
| 35 | DM | 139 | GLU | 3.4 |
| 30 | DH | 4 | ILE | 3.4 |
| 1 | AA | 1130 | A | 3.4 |
| 14 | AN | 33 | VAL | 3.4 |
| 44 | BV | 27 | VAL | 3.4 |
| 21 | CU | 22 | ARG | 3.4 |
| 22 | AV | 6177 | U | 3.4 |
| 4 | AD | 23 | GLY | 3.4 |
| 28 | DF | 86 | MET | 3.4 |
| 29 | BG | 131 | VAL | 3.4 |
| 19 | AS | 72 | GLY | 3.3 |
| 43 | BU | 41 | GLY | 3.3 |
| 2 | CB | 31 | TYR | 3.3 |
| 30 | DH | 126 | TYR | 3.3 |
| 19 | CS | 63 | THR | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | AA | 210 | U | 3.3 |
| 4 | CD | 16 | GLY | 3.3 |
| 13 | CM | 89 | GLY | 3.3 |
| 19 | CS | 76 | PRO | 3.3 |
| 30 | BH | 145 | VAL | 3.3 |
| 23 | BA | 2108 | C | 3.3 |
| 8 | AH | 119 | LEU | 3.3 |
| 6 | AF | 100 | ASN | 3.3 |
| 23 | BA | 1420 | U | 3.3 |
| 29 | BG | 100 | GLY | 3.3 |
| 47 | BY | 13 | ALA | 3.3 |
| 22 | AV | 6199 | G | 3.3 |
| 43 | BU | 64 | GLU | 3.3 |
| 19 | CS | 15 | LEU | 3.3 |
| 9 | CI | 9 | ARG | 3.3 |
| 12 | CL | 111 | ASP | 3.3 |
| 30 | BH | 107 | ILE | 3.3 |
| 10 | AJ | 83 | GLU | 3.3 |
| 51 | D3 | 35 | GLU | 3.3 |
| 10 | AJ | 39 | PRO | 3.3 |
| 6 | CF | 95 | GLU | 3.3 |
| 32 | BJ | 59 | GLY | 3.3 |
| 35 | DM | 90 | VAL | 3.3 |
| 43 | BU | 45 | VAL | 3.3 |
| 5 | CE | 17 | ALA | 3.3 |
| 1 | AA | 1024 | G | 3.3 |
| 3 | CC | 153 | VAL | 3.3 |
| 26 | DD | 186 | GLY | 3.3 |
| 3 | AC | 54 | ARG | 3.3 |
| 34 | DL | 105 | LEU | 3.3 |
| 9 | CI | 14 | VAL | 3.3 |
| 22 | AV | 6176 | U | 3.3 |
| 37 | BO | 53 | SER | 3.3 |
| 10 | CJ | 79 | ARG | 3.3 |
| 14 | AN | 2 | ALA | 3.3 |
| 13 | CM | 6 | GLY | 3.3 |
| 23 | BA | 886 | C | 3.3 |
| 28 | BF | 13 | GLU | 3.3 |
| 1 | CA | 92 | G | 3.3 |
| 9 | CI | 17 | VAL | 3.3 |
| 28 | BF | 120 | LEU | 3.3 |
| 43 | DU | 5 | MET | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 23 | DA | 1174 | A | 3.2 |
| 1 | CA | 1030 | C | 3.2 |
| 16 | CP | 65 | GLN | 3.2 |
| 28 | DF | 26 | GLN | 3.2 |
| 38 | DP | 91 | ARG | 3.2 |
| 20 | CT | 9 | ASN | 3.2 |
| 28 | BF | 101 | ILE | 3.2 |
| 28 | BF | 143 | GLU | 3.2 |
| 2 | AB | 130 | ARG | 3.2 |
| 19 | CS | 43 | GLU | 3.2 |
| 1 | CA | 136(B) | C | 3.2 |
| 44 | BV | 164 | ALA | 3.2 |
| 20 | AT | 103 | GLY | 3.2 |
| 5 | CE | 73 | ASN | 3.2 |
| 7 | CG | 10 | ARG | 3.2 |
| 43 | BU | 92 | ASN | 3.2 |
| 2 | CB | 200 | ILE | 3.2 |
| 49 | D1 | 36 | VAL | 3.2 |
| 1 | CA | 1034 | G | 3.2 |
| 13 | AM | 80 | ARG | 3.2 |
| 45 | DW | 76 | GLY | 3.2 |
| 3 | AC | 87 | LEU | 3.2 |
| 29 | BG | 88 | LEU | 3.2 |
| 29 | BG | 168 | PRO | 3.2 |
| 18 | AR | 62 | GLU | 3.2 |
| 23 | BA | 2803 | C | 3.2 |
| 4 | CD | 168 | ARG | 3.2 |
| 19 | CS | 70 | LYS | 3.2 |
| 12 | CL | 31 | PHE | 3.2 |
| 13 | CM | 100 | GLY | 3.2 |
| 19 | AS | 45 | VAL | 3.2 |
| 28 | BF | 29 | TRP | 3.2 |
| 29 | BG | 26 | VAL | 3.2 |
| 37 | DO | 85 | VAL | 3.2 |
| 44 | BV | 128 | VAL | 3.2 |
| 7 | CG | 64 | GLN | 3.2 |
| 9 | CI | 50 | LEU | 3.2 |
| 13 | CM | 115 | LYS | 3.2 |
| 35 | BM | 139 | GLU | 3.2 |
| 44 | BV | 95 | PRO | 3.2 |
| 5 | CE | 109 | ILE | 3.2 |
| 7 | CG | 34 | GLY | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 20 | CT | 104 | LEU | 3.2 |
| 31 | DI | 3 | ASN | 3.2 |
| 3 | AC | 147 | LYS | 3.2 |
| 2 | AB | 43 | ASP | 3.2 |
| 31 | BI | 18 | GLU | 3.2 |
| 38 | DP | 1 | MET | 3.2 |
| 23 | DA | 1104 | C | 3.2 |
| 23 | DA | 2794 | C | 3.2 |
| 1 | CA | 87 | A | 3.2 |
| 1 | CA | 179 | A | 3.2 |
| 3 | CC | 56 | ASP | 3.2 |
| 2 | AB | 131 | PRO | 3.2 |
| 40 | DR | 16 | PRO | 3.2 |
| 44 | BV | 166 | SER | 3.2 |
| 26 | BD | 60 | ASN | 3.1 |
| 43 | BU | 43 | ASN | 3.1 |
| 23 | DA | 2309 | A | 3.1 |
| 34 | BL | 94 | GLU | 3.1 |
| 30 | BH | 92 | VAL | 3.1 |
| 4 | CD | 153 | ARG | 3.1 |
| 49 | B1 | 46 | ASN | 3.1 |
| 7 | CG | 61 | VAL | 3.1 |
| 30 | BH | 143 | SER | 3.1 |
| 30 | DH | 60 | GLU | 3.1 |
| 30 | DH | 122 | GLU | 3.1 |
| 49 | B1 | 56 | GLU | 3.1 |
| 16 | CP | 55 | ARG | 3.1 |
| 28 | BF | 3 | LEU | 3.1 |
| 28 | BF | 83 | ARG | 3.1 |
| 37 | DO | 45 | GLY | 3.1 |
| 23 | DA | 508 | G | 3.1 |
| 4 | AD | 38 | TYR | 3.1 |
| 10 | CJ | 41 | PRO | 3.1 |
| 16 | CP | 17 | TYR | 3.1 |
| 2 | CB | 27 | LYS | 3.1 |
| 10 | AJ | 88 | LEU | 3.1 |
| 51 | D3 | 30 | THR | 3.1 |
| 1 | CA | 81 | G | 3.1 |
| 9 | AI | 37 | PHE | 3.1 |
| 37 | BO | 87 | PHE | 3.1 |
| 7 | CG | 29 | LYS | 3.1 |
| 7 | CG | 156 | TRP | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | AA | 1030 | C | 3.1 |
| 1 | CA | 136 | C | 3.1 |
| 1 | CA | 1045 | C | 3.1 |
| 29 | BG | 169 | VAL | 3.1 |
| 50 | B2 | 29 | ILE | 3.1 |
| 12 | CL | 97 | TYR | 3.1 |
| 3 | AC | 57 | ILE | 3.1 |
| 10 | AJ | 38 | ILE | 3.1 |
| 13 | AM | 6 | GLY | 3.1 |
| 30 | BH | 69 | LYS | 3.1 |
| 30 | DH | 118 | LYS | 3.1 |
| 28 | DF | 143 | GLU | 3.1 |
| 37 | DO | 36 | TYR | 3.1 |
| 2 | AB | 121 | LEU | 3.1 |
| 28 | DF | 47 | LYS | 3.1 |
| 43 | DU | 3 | VAL | 3.1 |
| 4 | CD | 181 | MET | 3.1 |
| 5 | CE | 94 | ALA | 3.1 |
| 9 | CI | 4 | TYR | 3.1 |
| 37 | BO | 34 | HIS | 3.1 |
| 9 | CI | 44 | VAL | 3.1 |
| 13 | CM | 86 | CYS | 3.1 |
| 1 | CA | 66 | G | 3.1 |
| 1 | CA | 181 | G | 3.1 |
| 22 | CV | 6189 | G | 3.1 |
| 7 | AG | 18 | TYR | 3.1 |
| 29 | BG | 27 | LYS | 3.1 |
| 51 | D3 | 25 | LYS | 3.1 |
| 34 | BL | 85 | LEU | 3.1 |
| 21 | AU | 9 | ARG | 3.1 |
| 2 | AB | 48 | MET | 3.1 |
| 11 | CK | 19 | ALA | 3.1 |
| 28 | DF | 72 | ARG | 3.1 |
| 10 | CJ | 27 | ALA | 3.0 |
| 13 | CM | 80 | ARG | 3.0 |
| 23 | DA | 2310 | A | 3.0 |
| 28 | DF | 42 | GLY | 3.0 |
| 26 | BD | 73 | GLU | 3.0 |
| 31 | BI | 57 | THR | 3.0 |
| 14 | CN | 60 | SER | 3.0 |
| 34 | BL | 110 | TYR | 3.0 |
| 21 | CU | 12 | LYS | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 22 | AV | 6213 | A | 3.0 |
| 23 | BA | 2897 | U | 3.0 |
| 35 | BM | 135 | ASP | 3.0 |
| 5 | AE | 20 | GLN | 3.0 |
| 20 | CT | 18 | GLN | 3.0 |
| 23 | BA | 2895 | U | 3.0 |
| 35 | DM | 24 | GLY | 3.0 |
| 13 | CM | 61 | GLU | 3.0 |
| 29 | BG | 116 | GLU | 3.0 |
| 1 | AA | 1137 | C | 3.0 |
| 23 | BA | 2105 | C | 3.0 |
| 28 | BF | 22 | ARG | 3.0 |
| 15 | CO | 15 | PHE | 3.0 |
| 29 | BG | 24 | VAL | 3.0 |
| 44 | BV | 91 | LEU | 3.0 |
| 13 | AM | 114 | ARG | 3.0 |
| 28 | BF | 168 | GLU | 3.0 |
| 49 | D1 | 49 | GLU | 3.0 |
| 1 | AA | 79 | G | 3.0 |
| 7 | CG | 66 | VAL | 3.0 |
| 18 | AR | 24 | ALA | 3.0 |
| 44 | BV | 127 | LYS | 3.0 |
| 12 | CL | 91 | ASP | 3.0 |
| 1 | AA | 723 | U | 3.0 |
| 2 | CB | 96 | ARG | 3.0 |
| 23 | BA | 1175 | U | 3.0 |
| 29 | BG | 48 | GLY | 3.0 |
| 1 | AA | 1250 | A | 3.0 |
| 2 | AB | 118 | LEU | 3.0 |
| 7 | CG | 69 | VAL | 3.0 |
| 10 | AJ | 53 | PRO | 3.0 |
| 9 | AI | 27 | THR | 3.0 |
| 19 | CS | 60 | VAL | 3.0 |
| 1 | AA | 91 | C | 3.0 |
| 9 | AI | 33 | PHE | 3.0 |
| 5 | CE | 25 | ARG | 3.0 |
| 10 | AJ | 5 | ARG | 3.0 |
| 44 | BV | 161 | VAL | 3.0 |
| 1 | CA | 103(A) | A | 3.0 |
| 6 | AF | 4 | TYR | 3.0 |
| 1 | CA | 1027 | C | 3.0 |
| 3 | CC | 158 | GLY | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 37 | BO | 11 | LYS | 3.0 |
| 28 | BF | 155 | MET | 3.0 |
| 49 | D1 | 64 | LYS | 3.0 |
| 20 | CT | 51 | GLU | 3.0 |
| 38 | BP | 36 | GLU | 3.0 |
| 50 | B2 | 2 | ALA | 3.0 |
| 19 | CS | 4 | SER | 2.9 |
| 10 | AJ | 54 | PHE | 2.9 |
| 37 | BO | 48 | LEU | 2.9 |
| 1 | CA | 1036 | G | 2.9 |
| 7 | CG | 137 | LYS | 2.9 |
| 1 | AA | 1492 | A | 2.9 |
| 10 | AJ | 6 | ILE | 2.9 |
| 28 | DF | 29 | TRP | 2.9 |
| 13 | AM | 97 | PRO | 2.9 |
| 29 | BG | 19 | VAL | 2.9 |
| 30 | BH | 144 | VAL | 2.9 |
| 6 | CF | 69 | GLU | 2.9 |
| 21 | AU | 8 | THR | 2.9 |
| 23 | DA | 2795 | G | 2.9 |
| 26 | BD | 24 | THR | 2.9 |
| 7 | AG | 43 | PHE | 2.9 |
| 11 | CK | 11 | LYS | 2.9 |
| 16 | CP | 38 | TYR | 2.9 |
| 18 | AR | 78 | LEU | 2.9 |
| 21 | AU | 24 | ARG | 2.9 |
| 29 | BG | 41 | MET | 2.9 |
| 38 | BP | 1 | MET | 2.9 |
| 4 | CD | 142 | PRO | 2.9 |
| 10 | AJ | 8 | LEU | 2.9 |
| 10 | CJ | 39 | PRO | 2.9 |
| 20 | CT | 42 | GLN | 2.9 |
| 50 | B2 | 31 | VAL | 2.9 |
| 10 | CJ | 5 | ARG | 2.9 |
| 30 | BH | 113 | ARG | 2.9 |
| 30 | DH | 16 | GLY | 2.9 |
| 7 | CG | 68 | ASN | 2.9 |
| 2 | AB | 213 | LEU | 2.9 |
| 19 | AS | 79 | THR | 2.9 |
| 2 | AB | 136 | VAL | 2.9 |
| 12 | CL | 27 | LYS | 2.9 |
| 1 | CA | 1248 | A | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | CA | 610 | G | 2.9 |
| 20 | CT | 99 | LEU | 2.9 |
| 29 | BG | 61 | HIS | 2.9 |
| 22 | CV | 6180 | U | 2.9 |
| 1 | AA | 1026 | G | 2.9 |
| 1 | CA | 1274 | G | 2.9 |
| 3 | AC | 153 | VAL | 2.9 |
| 37 | DO | 44 | LYS | 2.9 |
| 1 | AA | 1041 | A | 2.9 |
| 28 | BF | 145 | THR | 2.9 |
| 29 | BG | 12 | PRO | 2.9 |
| 1 | CA | 91 | C | 2.9 |
| 1 | CA | 1043 | C | 2.9 |
| 13 | CM | 110 | ARG | 2.9 |
| 37 | DO | 27 | SER | 2.9 |
| 34 | DL | 101 | VAL | 2.9 |
| 7 | AG | 120 | ILE | 2.9 |
| 49 | B1 | 45 | GLY | 2.9 |
| 1 | AA | 1374 | A | 2.9 |
| 3 | AC | 172 | ARG | 2.9 |
| 4 | CD | 141 | ARG | 2.9 |
| 14 | CN | 22 | THR | 2.9 |
| 1 | CA | 1116 | C | 2.9 |
| 23 | DA | 277 | C | 2.9 |
| 23 | DA | 2183 | C | 2.9 |
| 30 | BH | 14 | ASP | 2.9 |
| 23 | DA | 10 | G | 2.9 |
| 49 | B1 | 47 | VAL | 2.9 |
| 37 | DO | 39 | ILE | 2.9 |
| 38 | DP | 125 | ARG | 2.9 |
| 11 | AK | 39 | PRO | 2.9 |
| 20 | CT | 56 | MET | 2.9 |
| 28 | BF | 36 | LYS | 2.9 |
| 44 | BV | 68 | PRO | 2.9 |
| 7 | AG | 101 | LEU | 2.9 |
| 2 | CB | 134 | GLU | 2.9 |
| 1 | CA | 75 | C | 2.9 |
| 28 | DF | 69 | ALA | 2.8 |
| 9 | AI | 102 | LEU | 2.8 |
| 7 | AG | 113 | GLU | 2.8 |
| 19 | AS | 61 | TYR | 2.8 |
| 1 | CA | 135 | C | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | AB | 154 | LEU | 2.8 |
| 23 | BA | 277 | C | 2.8 |
| 16 | CP | 2 | VAL | 2.8 |
| 29 | DG | 59 | ARG | 2.8 |
| 44 | BV | 96 | VAL | 2.8 |
| 1 | CA | 80 | G | 2.8 |
| 19 | CS | 32 | LYS | 2.8 |
| 35 | DM | 100 | GLY | 2.8 |
| 16 | CP | 6 | LEU | 2.8 |
| 1 | AA | 1035 | A | 2.8 |
| 1 | AA | 1451 | A | 2.8 |
| 2 | AB | 37 | ASN | 2.8 |
| 16 | CP | 15 | PRO | 2.8 |
| 23 | BA | 2402 | C | 2.8 |
| 28 | BF | 32 | PRO | 2.8 |
| 3 | CC | 191 | THR | 2.8 |
| 19 | AS | 31 | ILE | 2.8 |
| 1 | AA | 1224 | G | 2.8 |
| 7 | AG | 124 | LEU | 2.8 |
| 13 | AM | 96 | LEU | 2.8 |
| 49 | D1 | 56 | GLU | 2.8 |
| 11 | AK | 82 | VAL | 2.8 |
| 1 | CA | 63 | C | 2.8 |
| 1 | CA | 90 | C | 2.8 |
| 6 | AF | 8 | ILE | 2.8 |
| 12 | CL | 102 | GLY | 2.8 |
| 28 | BF | 39 | ILE | 2.8 |
| 37 | BO | 82 | ILE | 2.8 |
| 37 | DO | 82 | ILE | 2.8 |
| 2 | CB | 163 | PHE | 2.8 |
| 7 | CG | 59 | LEU | 2.8 |
| 7 | CG | 98 | SER | 2.8 |
| 20 | CT | 60 | GLU | 2.8 |
| 47 | DY | 9 | GLN | 2.8 |
| 23 | BA | 1483 | G | 2.8 |
| 4 | CD | 4 | TYR | 2.8 |
| 9 | CI | 5 | TYR | 2.8 |
| 19 | CS | 31 | ILE | 2.8 |
| 19 | CS | 72 | GLY | 2.8 |
| 30 | BH | 82 | ARG | 2.8 |
| 37 | DO | 11 | LYS | 2.8 |
| 2 | CB | 12 | GLU | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 7 | CG | 50 | ILE | 2.8 |
| 9 | CI | 6 | GLY | 2.8 |
| 13 | AM | 93 | ARG | 2.8 |
| 18 | CR | 31 | LEU | 2.8 |
| 23 | DA | 2211 | G | 2.8 |
| 37 | BO | 57 | LYS | 2.8 |
| 47 | BY | 10 | LEU | 2.8 |
| 4 | CD | 24 | GLU | 2.8 |
| 30 | BH | 36 | ALA | 2.8 |
| 37 | DO | 43 | GLU | 2.8 |
| 44 | BV | 186 | GLU | 2.8 |
| 7 | CG | 63 | LYS | 2.8 |
| 7 | CG | 77 | SER | 2.8 |
| 30 | DH | 69 | LYS | 2.8 |
| 1 | CA | 1285 | A | 2.8 |
| 13 | CM | 73 | GLU | 2.8 |
| 51 | B3 | 35 | GLU | 2.8 |
| 29 | BG | 107 | VAL | 2.8 |
| 4 | AD | 25 | ARG | 2.8 |
| 34 | BL | 137 | LYS | 2.8 |
| 38 | DP | 117 | ASP | 2.8 |
| 43 | BU | 58 | GLY | 2.8 |
| 9 | CI | 101 | PHE | 2.8 |
| 18 | AR | 26 | LEU | 2.8 |
| 3 | CC | 177 | THR | 2.8 |
| 2 | AB | 187 | LEU | 2.8 |
| 10 | CJ | 23 | ILE | 2.8 |
| 28 | DF | 65 | GLY | 2.8 |
| 29 | BG | 68 | THR | 2.8 |
| 30 | BH | 4 | ILE | 2.8 |
| 37 | BO | 54 | LEU | 2.8 |
| 5 | CE | 18 | ARG | 2.8 |
| 34 | BL | 125 | VAL | 2.8 |
| 24 | DB | 54 | G | 2.8 |
| 3 | AC | 2 | GLY | 2.7 |
| 3 | CC | 196 | LEU | 2.7 |
| 28 | BF | 157 | ILE | 2.7 |
| 43 | BU | 83 | THR | 2.7 |
| 1 | CA | 1025 | U | 2.7 |
| 10 | AJ | 66 | ARG | 2.7 |
| 29 | BG | 112 | PRO | 2.7 |
| 4 | CD | 17 | VAL | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 50 | D2 | 2 | ALA | 2.7 |
| 30 | DH | 109 | ILE | 2.7 |
| 43 | DU | 61 | ILE | 2.7 |
| 1 | AA | 1493 | A | 2.7 |
| 13 | CM | 8 | GLU | 2.7 |
| 23 | BA | 1051 | G | 2.7 |
| 29 | BG | 160 | LYS | 2.7 |
| 34 | DL | 110 | TYR | 2.7 |
| 4 | CD | 148 | VAL | 2.7 |
| 8 | AH | 129 | VAL | 2.7 |
| 30 | BH | 142 | VAL | 2.7 |
| 23 | DA | 1026 | U | 2.7 |
| 8 | CH | 43 | GLY | 2.7 |
| 20 | CT | 43 | LEU | 2.7 |
| 2 | CB | 229 | VAL | 2.7 |
| 3 | AC | 142 | MET | 2.7 |
| 9 | AI | 36 | TYR | 2.7 |
| 12 | CL | 23 | VAL | 2.7 |
| 30 | BH | 96 | ASP | 2.7 |
| 43 | BU | 65 | ALA | 2.7 |
| 4 | CD | 201 | GLN | 2.7 |
| 34 | DL | 85 | LEU | 2.7 |
| 47 | DY | 44 | LEU | 2.7 |
| 2 | CB | 166 | ASP | 2.7 |
| 37 | DO | 37 | ALA | 2.7 |
| 2 | CB | 234 | PRO | 2.7 |
| 20 | CT | 83 | ARG | 2.7 |
| 17 | CQ | 58 | GLU | 2.7 |
| 35 | DM | 91 | GLU | 2.7 |
| 37 | BO | 39 | ILE | 2.7 |
| 1 | CA | 975 | A | 2.7 |
| 22 | CV | 6198 | U | 2.7 |
| 23 | DA | 2897 | U | 2.7 |
| 8 | CH | 116 | LYS | 2.7 |
| 13 | CM | 27 | LYS | 2.7 |
| 4 | AD | 4 | TYR | 2.7 |
| 16 | CP | 53 | VAL | 2.7 |
| 9 | AI | 20 | ARG | 2.7 |
| 2 | CB | 26 | PRO | 2.7 |
| 3 | CC | 152 | ILE | 2.7 |
| 15 | CO | 7 | GLU | 2.7 |
| 21 | CU | 19 | GLY | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 29 | DG | 167 | GLU | 2.7 |
| 36 | BN | 83 | ILE | 2.7 |
| 46 | DX | 85 | LEU | 2.7 |
| 7 | CG | 23 | VAL | 2.7 |
| 29 | BG | 102 | ALA | 2.7 |
| 9 | AI | 69 | GLY | 2.7 |
| 21 | AU | 19 | GLY | 2.7 |
| 30 | BH | 123 | LEU | 2.7 |
| 9 | AI | 81 | ILE | 2.7 |
| 37 | BO | 36 | TYR | 2.7 |
| 4 | CD | 192 | GLU | 2.7 |
| 8 | AH | 96 | GLY | 2.7 |
| 28 | BF | 43 | LEU | 2.7 |
| 29 | BG | 67 | LEU | 2.7 |
| 30 | BH | 77 | LEU | 2.7 |
| 34 | DL | 119 | GLU | 2.7 |
| 23 | BA | 2107 | C | 2.7 |
| 3 | CC | 195 | VAL | 2.7 |
| 4 | CD | 88 | VAL | 2.7 |
| 7 | AG | 110 | GLN | 2.7 |
| 14 | AN | 25 | VAL | 2.7 |
| 17 | AQ | 95 | TYR | 2.7 |
| 5 | CE | 91 | LEU | 2.7 |
| 12 | CL | 72 | GLU | 2.7 |
| 13 | AM | 34 | LEU | 2.7 |
| 19 | CS | 10 | PHE | 2.7 |
| 37 | BO | 102 | ALA | 2.7 |
| 1 | AA | 1003 | G | 2.7 |
| 23 | BA | 2104 | G | 2.7 |
| 4 | CD | 8 | VAL | 2.7 |
| 16 | AP | 59 | TRP | 2.7 |
| 45 | BW | 79 | VAL | 2.7 |
| 5 | CE | 98 | THR | 2.7 |
| 18 | AR | 88 | LYS | 2.6 |
| 21 | AU | 3 | LYS | 2.6 |
| 24 | BB | 53 | A | 2.6 |
| 50 | B2 | 48 | GLU | 2.6 |
| 16 | CP | 33 | ILE | 2.6 |
| 30 | DH | 97 | ILE | 2.6 |
| 46 | DX | 81 | ARG | 2.6 |
| 1 | CA | 1042 | G | 2.6 |
| 8 | CH | 62 | TYR | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 19 | AS | 43 | GLU | 2.6 |
| 23 | BA | 34 | C | 2.6 |
| 29 | BG | 108 | GLY | 2.6 |
| 30 | DH | 115 | ALA | 2.6 |
| 43 | BU | 3 | VAL | 2.6 |
| 2 | AB | 128 | GLU | 2.6 |
| 7 | AG | 5 | ARG | 2.6 |
| 20 | CT | 47 | GLY | 2.6 |
| 10 | CJ | 74 | ILE | 2.6 |
| 23 | BA | 279 | C | 2.6 |
| 14 | CN | 14 | PRO | 2.6 |
| 23 | DA | 1509 | A | 2.6 |
| 30 | BH | 54 | GLN | 2.6 |
| 28 | BF | 131 | TYR | 2.6 |
| 30 | BH | 20 | ASP | 2.6 |
| 48 | DZ | 57 | GLU | 2.6 |
| 26 | BD | 26 | ILE | 2.6 |
| 13 | AM | 43 | THR | 2.6 |
| 19 | CS | 45 | VAL | 2.6 |
| 37 | DO | 52 | SER | 2.6 |
| 37 | BO | 73 | LEU | 2.6 |
| 34 | DL | 118 | GLY | 2.6 |
| 7 | CG | 91 | VAL | 2.6 |
| 28 | DF | 160 | VAL | 2.6 |
| 37 | DO | 47 | THR | 2.6 |
| 50 | B2 | 39 | MET | 2.6 |
| 44 | BV | 64 | GLY | 2.6 |
| 2 | AB | 201 | ILE | 2.6 |
| 6 | AF | 55 | ASP | 2.6 |
| 49 | B1 | 40 | ILE | 2.6 |
| 19 | AS | 58 | VAL | 2.6 |
| 23 | DA | 2793 | G | 2.6 |
| 4 | CD | 15 | GLU | 2.6 |
| 21 | CU | 17 | THR | 2.6 |
| 10 | CJ | 55 | LYS | 2.6 |
| 21 | AU | 20 | LYS | 2.6 |
| 34 | BL | 138 | LEU | 2.6 |
| 1 | AA | 998(B) | C | 2.6 |
| 7 | AG | 156 | TRP | 2.6 |
| 28 | BF | 97 | ASP | 2.6 |
| 41 | DS | 111 | HIS | 2.6 |
| 2 | CB | 238 | LEU | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 10 | CJ | 7 | LYS | 2.6 |
| 3 | AC | 81 | GLY | 2.6 |
| 23 | BA | 2790 | A | 2.6 |
| 10 | CJ | 96 | ILE | 2.6 |
| 11 | AK | 19 | ALA | 2.6 |
| 1 | AA | 1027 | C | 2.6 |
| 8 | AH | 95 | VAL | 2.6 |
| 9 | CI | 105 | ASP | 2.6 |
| 16 | CP | 29 | ASP | 2.6 |
| 28 | DF | 120 | LEU | 2.6 |
| 43 | BU | 6 | HIS | 2.6 |
| 48 | BZ | 57 | GLU | 2.6 |
| 41 | DS | 108 | GLY | 2.6 |
| 17 | CQ | 65 | ILE | 2.6 |
| 2 | CB | 77 | ALA | 2.6 |
| 19 | CS | 24 | ALA | 2.6 |
| 1 | AA | 1033 | G | 2.6 |
| 1 | CA | 1288 | A | 2.6 |
| 4 | CD | 105 | VAL | 2.6 |
| 19 | CS | 67 | VAL | 2.6 |
| 21 | AU | 5 | ASP | 2.6 |
| 28 | DF | 116 | ASP | 2.6 |
| 20 | CT | 46 | GLU | 2.6 |
| 4 | CD | 87 | GLY | 2.6 |
| 19 | CS | 78 | ARG | 2.6 |
| 14 | AN | 10 | ALA | 2.6 |
| 16 | CP | 7 | ALA | 2.6 |
| 28 | DF | 56 | ALA | 2.6 |
| 2 | CB | 131 | PRO | 2.6 |
| 1 | AA | 1363 | A | 2.6 |
| 1 | CA | 1231 | G | 2.6 |
| 2 | CB | 140 | HIS | 2.6 |
| 16 | CP | 13 | HIS | 2.6 |
| 7 | CG | 11 | GLN | 2.6 |
| 3 | AC | 169 | ALA | 2.6 |
| 9 | CI | 43 | ALA | 2.6 |
| 12 | CL | 50 | ALA | 2.6 |
| 18 | AR | 25 | THR | 2.6 |
| 30 | DH | 143 | SER | 2.6 |
| 1 | CA | 1240 | U | 2.6 |
| 5 | CE | 24 | ARG | 2.5 |
| 7 | AG | 3 | ARG | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 10 | CJ | 70 | ARG | 2.5 |
| 28 | DF | 150 | ASP | 2.5 |
| 30 | BH | 90 | GLY | 2.5 |
| 23 | DA | 2106 | G | 2.5 |
| 13 | AM | 56 | LEU | 2.5 |
| 28 | DF | 172 | LEU | 2.5 |
| 39 | DQ | 118 | GLY | 2.5 |
| 14 | CN | 7 | ILE | 2.5 |
| 1 | CA | 1035 | A | 2.5 |
| 7 | AG | 62 | PHE | 2.5 |
| 13 | CM | 94 | ARG | 2.5 |
| 29 | BG | 52 | VAL | 2.5 |
| 8 | CH | 63 | LEU | 2.5 |
| 1 | AA | 1116 | C | 2.5 |
| 14 | AN | 61 | TRP | 2.5 |
| 1 | CA | 85 | U | 2.5 |
| 28 | BF | 20 | ILE | 2.5 |
| 2 | AB | 87 | ARG | 2.5 |
| 7 | AG | 86 | GLN | 2.5 |
| 9 | AI | 5 | TYR | 2.5 |
| 11 | AK | 128 | ALA | 2.5 |
| 13 | CM | 33 | ALA | 2.5 |
| 10 | CJ | 63 | PHE | 2.5 |
| 13 | AM | 85 | GLY | 2.5 |
| 15 | AO | 89 | GLY | 2.5 |
| 17 | CQ | 8 | GLY | 2.5 |
| 29 | BG | 128 | PRO | 2.5 |
| 1 | CA | 1037 | C | 2.5 |
| 13 | CM | 62 | ASN | 2.5 |
| 14 | AN | 30 | ALA | 2.5 |
| 16 | CP | 14 | ASN | 2.5 |
| 3 | CC | 167 | TRP | 2.5 |
| 20 | AT | 37 | SER | 2.5 |
| 11 | AK | 27 | ASN | 2.5 |
| 16 | CP | 70 | ALA | 2.5 |
| 18 | AR | 43 | PHE | 2.5 |
| 30 | BH | 89 | TYR | 2.5 |
| 41 | DS | 109 | GLU | 2.5 |
| 49 | B1 | 65 | CYS | 2.5 |
| 1 | CA | 1026 | G | 2.5 |
| 4 | CD | 147 | ALA | 2.5 |
| 10 | CJ | 87 | THR | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 28 | DF | 97 | ASP | 2.5 |
| 2 | AB | 133 | LYS | 2.5 |
| 20 | CT | 87 | LYS | 2.5 |
| 37 | DO | 22 | GLY | 2.5 |
| 45 | BW | 76 | GLY | 2.5 |
| 37 | DO | 40 | ILE | 2.5 |
| 2 | CB | 73 | THR | 2.5 |
| 28 | BF | 33 | ARG | 2.5 |
| 30 | DH | 52 | ARG | 2.5 |
| 16 | CP | 23 | ASP | 2.5 |
| 1 | CA | 1370 | G | 2.5 |
| 2 | CB | 94 | ASN | 2.5 |
| 31 | DI | 22 | GLY | 2.5 |
| 7 | CG | 139 | GLU | 2.5 |
| 14 | AN | 12 | ARG | 2.5 |
| 34 | DL | 147 | LEU | 2.5 |
| 1 | CA | 1039 | C | 2.5 |
| 11 | AK | 31 | THR | 2.5 |
| 23 | BA | 2474 | C | 2.5 |
| 13 | CM | 25 | ILE | 2.5 |
| 13 | CM | 84 | ILE | 2.5 |
| 1 | AA | 92 | G | 2.5 |
| 1 | AA | 998(A) | G | 2.5 |
| 7 | AG | 88 | PRO | 2.5 |
| 13 | AM | 115 | LYS | 2.5 |
| 29 | DG | 12 | PRO | 2.5 |
| 1 | AA | 1006 | C | 2.5 |
| 4 | AD | 161 | ASN | 2.5 |
| 9 | AI | 29 | ASN | 2.5 |
| 13 | AM | 91 | ARG | 2.5 |
| 28 | BF | 109 | VAL | 2.5 |
| 28 | DF | 132 | ASN | 2.5 |
| 43 | BU | 91 | GLU | 2.5 |
| 2 | CB | 139 | LYS | 2.5 |
| 4 | AD | 30 | LYS | 2.5 |
| 28 | DF | 75 | LYS | 2.5 |
| 30 | BH | 5 | LEU | 2.5 |
| 3 | AC | 53 | ALA | 2.4 |
| 19 | AS | 24 | ALA | 2.4 |
| 1 | CA | 1351 | U | 2.4 |
| 2 | AB | 72 | GLY | 2.4 |
| 23 | BA | 2807 | G | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 23 | DA | 2308 | G | 2.4 |
| 1 | CA | 1493 | A | 2.4 |
| 2 | CB | 137 | ARG | 2.4 |
| 5 | CE | 10 | MET | 2.4 |
| 10 | CJ | 64 | GLU | 2.4 |
| 13 | CM | 32 | GLU | 2.4 |
| 29 | BG | 47 | GLU | 2.4 |
| 37 | BO | 41 | ASP | 2.4 |
| 10 | CJ | 94 | VAL | 2.4 |
| 17 | CQ | 22 | LEU | 2.4 |
| 28 | DF | 70 | VAL | 2.4 |
| 33 | DK | 51 | ALA | 2.4 |
| 2 | CB | 18 | GLY | 2.4 |
| 13 | AM | 102 | ARG | 2.4 |
| 26 | BD | 197 | ILE | 2.4 |
| 7 | CG | 17 | VAL | 2.4 |
| 10 | CJ | 54 | PHE | 2.4 |
| 16 | AP | 22 | THR | 2.4 |
| 18 | AR | 29 | PHE | 2.4 |
| 26 | DD | 27 | LEU | 2.4 |
| 7 | CG | 37 | ASN | 2.4 |
| 23 | DA | 2896 | C | 2.4 |
| 38 | BP | 129 | ARG | 2.4 |
| 3 | CC | 161 | GLU | 2.4 |
| 30 | DH | 138 | ILE | 2.4 |
| 23 | DA | 271(D) | U | 2.4 |
| 26 | DD | 159 | HIS | 2.4 |
| 3 | AC | 196 | LEU | 2.4 |
| 32 | DJ | 74 | PHE | 2.4 |
| 48 | BZ | 59 | VAL | 2.4 |
| 1 | CA | 216 | G | 2.4 |
| 1 | CA | 1190 | G | 2.4 |
| 8 | AH | 130 | GLY | 2.4 |
| 10 | CJ | 3 | LYS | 2.4 |
| 13 | CM | 101 | GLN | 2.4 |
| 33 | DK | 15 | GLY | 2.4 |
| 34 | DL | 82 | GLY | 2.4 |
| 2 | AB | 170 | GLU | 2.4 |
| 23 | BA | 1053 | C | 2.4 |
| 28 | DF | 145 | THR | 2.4 |
| 4 | CD | 107 | ARG | 2.4 |
| 28 | DF | 153 | ARG | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 7 | AG | 84 | ASN | 2.4 |
| 12 | CL | 48 | ASN | 2.4 |
| 7 | AG | 27 | ILE | 2.4 |
| 26 | BD | 14 | ILE | 2.4 |
| 26 | BD | 102 | VAL | 2.4 |
| 37 | BO | 85 | VAL | 2.4 |
| 1 | CA | 1029 | G | 2.4 |
| 53 | D5 | 34 | TRP | 2.4 |
| 19 | AS | 28 | LYS | 2.4 |
| 7 | AG | 83 | ALA | 2.4 |
| 37 | DO | 53 | SER | 2.4 |
| 45 | BW | 85 | ALA | 2.4 |
| 35 | BM | 24 | GLY | 2.4 |
| 28 | BF | 176 | LEU | 2.4 |
| 30 | BH | 19 | VAL | 2.4 |
| 51 | D3 | 34 | LEU | 2.4 |
| 22 | CV | 6200 | A | 2.4 |
| 20 | CT | 101 | GLY | 2.4 |
| 26 | BD | 174 | ASP | 2.4 |
| 1 | CA | 65 | U | 2.4 |
| 10 | AJ | 74 | ILE | 2.4 |
| 6 | AF | 9 | VAL | 2.4 |
| 7 | CG | 155 | ARG | 2.4 |
| 12 | CL | 30 | PRO | 2.4 |
| 28 | BF | 86 | MET | 2.4 |
| 37 | BO | 59 | LYS | 2.4 |
| 29 | BG | 46 | GLU | 2.4 |
| 35 | DM | 19 | GLY | 2.4 |
| 4 | CD | 20 | TYR | 2.4 |
| 10 | AJ | 42 | THR | 2.4 |
| 19 | AS | 80 | TYR | 2.4 |
| 34 | DL | 114 | ILE | 2.4 |
| 23 | DA | 654 | U | 2.4 |
| 30 | DH | 121 | LYS | 2.4 |
| 34 | BL | 51 | PHE | 2.4 |
| 3 | CC | 3 | ASN | 2.4 |
| 9 | CI | 98 | PRO | 2.4 |
| 3 | CC | 200 | ALA | 2.4 |
| 20 | AT | 44 | ALA | 2.4 |
| 2 | AB | 71 | VAL | 2.4 |
| 13 | AM | 109 | THR | 2.4 |
| 19 | CS | 11 | VAL | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 50 | B2 | 30 | LEU | 2.4 |
| 1 | CA | 488 | C | 2.4 |
| 4 | CD | 7 | PRO | 2.4 |
| 6 | AF | 89 | MET | 2.4 |
| 23 | BA | 2804 | C | 2.4 |
| 23 | BA | 887 | A | 2.4 |
| 23 | DA | 276 | A | 2.4 |
| 44 | BV | 98 | MET | 2.4 |
| 44 | BV | 167 | PRO | 2.4 |
| 1 | CA | 998(A) | G | 2.4 |
| 4 | AD | 169 | LYS | 2.4 |
| 7 | AG | 133 | GLY | 2.4 |
| 8 | CH | 21 | LYS | 2.4 |
| 26 | BD | 186 | GLY | 2.4 |
| 30 | BH | 60 | GLU | 2.4 |
| 7 | AG | 23 | VAL | 2.4 |
| 41 | BS | 38 | TYR | 2.4 |
| 44 | DV | 140 | ASP | 2.4 |
| 45 | BW | 75 | LEU | 2.4 |
| 5 | CE | 19 | MET | 2.4 |
| 1 | AA | 1005 | A | 2.4 |
| 3 | CC | 148 | GLY | 2.4 |
| 3 | CC | 179 | ARG | 2.4 |
| 13 | CM | 29 | ARG | 2.4 |
| 30 | BH | 10 | GLU | 2.4 |
| 30 | BH | 88 | ILE | 2.4 |
| 37 | BO | 49 | VAL | 2.4 |
| 2 | CB | 135 | GLN | 2.4 |
| 7 | CG | 97 | GLN | 2.4 |
| 23 | DA | 1421 | G | 2.3 |
| 8 | CH | 60 | ARG | 2.3 |
| 25 | BC | 262 | ARG | 2.3 |
| 29 | BG | 51 | ARG | 2.3 |
| 30 | BH | 125 | GLU | 2.3 |
| 1 | CA | 1257 | U | 2.3 |
| 1 | CA | 1352 | C | 2.3 |
| 9 | CI | 47 | LEU | 2.3 |
| 17 | CQ | 43 | LEU | 2.3 |
| 19 | AS | 57 | HIS | 2.3 |
| 23 | DA | 12 | U | 2.3 |
| 30 | DH | 12 | LEU | 2.3 |
| 1 | AA | 1346 | A | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 11 | AK | 77 | MET | 2.3 |
| 28 | BF | 166 | ASP | 2.3 |
| 5 | AE | 7 | GLU | 2.3 |
| 16 | AP | 41 | PRO | 2.3 |
| 1 | CA | 1356 | G | 2.3 |
| 7 | AG | 19 | GLY | 2.3 |
| 4 | AD | 5 | ILE | 2.3 |
| 26 | DD | 4 | ILE | 2.3 |
| 23 | DA | 1105 | U | 2.3 |
| 3 | CC | 131 | ARG | 2.3 |
| 7 | CG | 4 | ARG | 2.3 |
| 18 | AR | 61 | LYS | 2.3 |
| 1 | CA | 1110 | A | 2.3 |
| 28 | DF | 35 | GLU | 2.3 |
| 2 | CB | 227 | GLY | 2.3 |
| 7 | AG | 132 | GLY | 2.3 |
| 17 | AQ | 8 | GLY | 2.3 |
| 28 | BF | 93 | THR | 2.3 |
| 5 | AE | 109 | ILE | 2.3 |
| 43 | BU | 39 | VAL | 2.3 |
| 43 | DU | 47 | LYS | 2.3 |
| 46 | BX | 20 | ARG | 2.3 |
| 1 | AA | 1249 | C | 2.3 |
| 11 | AK | 81 | ASP | 2.3 |
| 35 | DM | 105 | GLU | 2.3 |
| 1 | AA | 1357 | A | 2.3 |
| 1 | CA | 1287 | A | 2.3 |
| 7 | AG | 2 | ALA | 2.3 |
| 7 | CG | 46 | ALA | 2.3 |
| 8 | CH | 44 | PHE | 2.3 |
| 10 | CJ | 59 | SER | 2.3 |
| 11 | AK | 107 | SER | 2.3 |
| 24 | DB | 53 | A | 2.3 |
| 37 | DO | 23 | ARG | 2.3 |
| 49 | B1 | 39 | ARG | 2.3 |
| 3 | AC | 184 | TYR | 2.3 |
| 22 | AV | 6198 | U | 2.3 |
| 2 | AB | 203 | GLY | 2.3 |
| 1 | AA | 103(B) | G | 2.3 |
| 1 | AA | 1370 | G | 2.3 |
| 3 | CC | 199 | LYS | 2.3 |
| 4 | AD | 110 | PHE | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 7 | AG | 99 | LEU | 2.3 |
| 9 | AI | 79 | LEU | 2.3 |
| 23 | BA | 1107 | G | 2.3 |
| 28 | BF | 169 | ALA | 2.3 |
| 2 | CB | 30 | ARG | 2.3 |
| 49 | B1 | 59 | VAL | 2.3 |
| 2 | CB | 148 | TYR | 2.3 |
| 13 | AM | 64 | TRP | 2.3 |
| 22 | CV | 6178 | A | 2.3 |
| 3 | AC | 206 | GLU | 2.3 |
| 1 | CA | 82 | U | 2.3 |
| 1 | CA | 1125 | U | 2.3 |
| 28 | DF | 84 | LYS | 2.3 |
| 4 | CD | 120 | LEU | 2.3 |
| 13 | CM | 81 | LEU | 2.3 |
| 17 | CQ | 63 | ARG | 2.3 |
| 14 | CN | 33 | VAL | 2.3 |
| 33 | DK | 12 | ASP | 2.3 |
| 1 | AA | 980 | C | 2.3 |
| 1 | AA | 1023 | G | 2.3 |
| 1 | CA | 68 | G | 2.3 |
| 1 | CA | 1259 | C | 2.3 |
| 4 | CD | 93 | PHE | 2.3 |
| 9 | AI | 80 | GLY | 2.3 |
| 19 | AS | 66 | MET | 2.3 |
| 5 | CE | 43 | LEU | 2.3 |
| 10 | CJ | 60 | ARG | 2.3 |
| 48 | DZ | 4 | LEU | 2.3 |
| 1 | CA | 1040 | U | 2.3 |
| 12 | AL | 63 | TYR | 2.3 |
| 41 | DS | 110 | LYS | 2.3 |
| 23 | DA | 645 | C | 2.3 |
| 29 | BG | 33 | LEU | 2.3 |
| 34 | DL | 130 | PHE | 2.3 |
| 6 | AF | 90 | VAL | 2.3 |
| 20 | CT | 64 | ASP | 2.3 |
| 30 | DH | 130 | TYR | 2.3 |
| 48 | DZ | 3 | ARG | 2.3 |
| 2 | CB | 54 | THR | 2.3 |
| 6 | AF | 61 | LEU | 2.3 |
| 18 | CR | 43 | PHE | 2.3 |
| 27 | DE | 194 | MET | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 40 | DR | 54 | GLY | 2.3 |
| 44 | BV | 125 | LEU | 2.3 |
| 4 | CD | 203 | VAL | 2.3 |
| 4 | CD | 204 | ILE | 2.3 |
| 7 | CG | 7 | ALA | 2.3 |
| 11 | CK | 82 | VAL | 2.3 |
| 53 | D5 | 33 | ASN | 2.3 |
| 12 | CL | 45 | LYS | 2.3 |
| 34 | BL | 139 | LYS | 2.3 |
| 3 | CC | 109 | PRO | 2.3 |
| 13 | AM | 32 | GLU | 2.3 |
| 29 | BG | 58 | GLU | 2.3 |
| 35 | DM | 99 | PRO | 2.3 |
| 23 | BA | 2808 | U | 2.3 |
| 23 | DA | 362 | U | 2.3 |
| 26 | BD | 31 | CYS | 2.3 |
| 40 | DR | 94 | LEU | 2.3 |
| 47 | DY | 10 | LEU | 2.3 |
| 48 | DZ | 28 | LEU | 2.3 |
| 14 | CN | 5 | ALA | 2.3 |
| 28 | DF | 159 | VAL | 2.3 |
| 2 | AB | 157 | ARG | 2.3 |
| 15 | CO | 26 | GLU | 2.3 |
| 49 | B1 | 58 | TYR | 2.3 |
| 1 | CA | 1041 | A | 2.3 |
| 10 | AJ | 21 | GLN | 2.3 |
| 17 | CQ | 53 | LEU | 2.3 |
| 19 | CS | 16 | LEU | 2.3 |
| 38 | DP | 92 | GLY | 2.3 |
| 22 | CV | 6191 | A | 2.3 |
| 23 | BA | 11 | G | 2.3 |
| 23 | DA | 1055 | G | 2.3 |
| 23 | DA | 1536 | A | 2.3 |
| 30 | DH | 144 | VAL | 2.3 |
| 43 | BU | 72 | VAL | 2.3 |
| 28 | BF | 27 | ASN | 2.2 |
| 1 | AA | 1395 | C | 2.2 |
| 3 | AC | 203 | PHE | 2.2 |
| 16 | CP | 32 | TYR | 2.2 |
| 2 | CB | 95 | GLN | 2.2 |
| 28 | BF | 75 | LYS | 2.2 |
| 30 | BH | 6 | LEU | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-------|------|------|
| 28 | BF | 96 | ARG | 2.2 |
| 24 | DB | 89(A) | G | 2.2 |
| 4 | AD | 183 | GLY | 2.2 |
| 20 | AT | 64 | ASP | 2.2 |
| 20 | CT | 91 | LEU | 2.2 |
| 30 | DH | 119 | PRO | 2.2 |
| 7 | AG | 87 | VAL | 2.2 |
| 9 | AI | 66 | ARG | 2.2 |
| 28 | BF | 66 | GLN | 2.2 |
| 28 | DF | 83 | ARG | 2.2 |
| 47 | BY | 9 | GLN | 2.2 |
| 1 | CA | 173 | U | 2.2 |
| 3 | AC | 146 | ALA | 2.2 |
| 31 | DI | 65 | GLU | 2.2 |
| 10 | AJ | 100 | THR | 2.2 |
| 7 | CG | 48 | LYS | 2.2 |
| 13 | AM | 36 | LYS | 2.2 |
| 9 | CI | 36 | TYR | 2.2 |
| 12 | CL | 92 | LEU | 2.2 |
| 23 | BA | 276 | A | 2.2 |
| 28 | BF | 173 | LEU | 2.2 |
| 35 | BM | 90 | VAL | 2.2 |
| 28 | BF | 167 | GLU | 2.2 |
| 29 | DG | 102 | ALA | 2.2 |
| 34 | BL | 9 | ASN | 2.2 |
| 1 | CA | 1350 | A | 2.2 |
| 3 | AC | 157 | ILE | 2.2 |
| 31 | DI | 7 | VAL | 2.2 |
| 6 | CF | 99 | ALA | 2.2 |
| 1 | CA | 293 | G | 2.2 |
| 17 | CQ | 69 | LYS | 2.2 |
| 20 | CT | 52 | ALA | 2.2 |
| 43 | BU | 28 | LYS | 2.2 |
| 19 | CS | 34 | TRP | 2.2 |
| 12 | AL | 61 | SER | 2.2 |
| 22 | CV | 6194 | C | 2.2 |
| 53 | D5 | 32 | LEU | 2.2 |
| 6 | AF | 68 | PRO | 2.2 |
| 10 | AJ | 99 | LYS | 2.2 |
| 50 | D2 | 47 | PRO | 2.2 |
| 3 | CC | 146 | ALA | 2.2 |
| 2 | CB | 97 | TRP | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 5 | CE | 142 | LEU | 2.2 |
| 3 | AC | 15 | THR | 2.2 |
| 3 | CC | 193 | TYR | 2.2 |
| 3 | CC | 202 | ILE | 2.2 |
| 35 | BM | 21 | THR | 2.2 |
| 10 | AJ | 76 | ASN | 2.2 |
| 16 | AP | 1 | MET | 2.2 |
| 28 | BF | 108 | ASN | 2.2 |
| 46 | DX | 27 | GLU | 2.2 |
| 51 | D3 | 32 | ASN | 2.2 |
| 9 | AI | 84 | ALA | 2.2 |
| 10 | AJ | 10 | GLY | 2.2 |
| 16 | CP | 3 | LYS | 2.2 |
| 17 | CQ | 59 | ILE | 2.2 |
| 26 | BD | 2 | LYS | 2.2 |
| 30 | BH | 37 | VAL | 2.2 |
| 6 | CF | 1 | MET | 2.2 |
| 17 | CQ | 20 | THR | 2.2 |
| 19 | CS | 79 | THR | 2.2 |
| 6 | AF | 35 | ALA | 2.2 |
| 7 | AG | 4 | ARG | 2.2 |
| 9 | AI | 10 | ARG | 2.2 |
| 1 | AA | 745 | C | 2.2 |
| 1 | CA | 74 | C | 2.2 |
| 1 | CA | 1187 | G | 2.2 |
| 2 | CB | 125 | PRO | 2.2 |
| 38 | DP | 90 | GLN | 2.2 |
| 1 | CA | 1242 | C | 2.2 |
| 23 | DA | 363(A) | G | 2.2 |
| 9 | CI | 100 | GLY | 2.2 |
| 44 | BV | 23 | LYS | 2.2 |
| 28 | BF | 140 | ILE | 2.2 |
| 10 | AJ | 59 | SER | 2.2 |
| 38 | DP | 36 | GLU | 2.2 |
| 38 | DP | 134 | GLU | 2.2 |
| 26 | BD | 48 | GLN | 2.2 |
| 4 | AD | 197 | PRO | 2.2 |
| 10 | CJ | 88 | LEU | 2.2 |
| 11 | AK | 98 | LEU | 2.2 |
| 16 | CP | 16 | HIS | 2.2 |
| 36 | DN | 59 | ASP | 2.2 |
| 1 | AA | 1034 | G | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 11 | AK | 14 | VAL | 2.2 |
| 23 | DA | 2181 | G | 2.2 |
| 7 | CG | 78 | ARG | 2.2 |
| 25 | BC | 183 | ARG | 2.2 |
| 28 | BF | 16 | ARG | 2.2 |
| 38 | BP | 11 | GLU | 2.2 |
| 7 | AG | 39 | ALA | 2.2 |
| 38 | BP | 130 | ALA | 2.2 |
| 4 | CD | 19 | LEU | 2.2 |
| 9 | AI | 19 | LEU | 2.2 |
| 12 | CL | 26 | LEU | 2.2 |
| 22 | AV | 6200 | A | 2.2 |
| 27 | BE | 181 | LEU | 2.2 |
| 27 | DE | 133 | ASN | 2.2 |
| 32 | BJ | 46 | LEU | 2.2 |
| 1 | AA | 1348 | U | 2.2 |
| 2 | CB | 43 | ASP | 2.2 |
| 34 | BL | 27 | HIS | 2.2 |
| 3 | AC | 79 | ARG | 2.2 |
| 29 | BG | 50 | VAL | 2.2 |
| 37 | BO | 97 | ARG | 2.2 |
| 1 | CA | 221 | C | 2.2 |
| 13 | AM | 86 | CYS | 2.2 |
| 2 | AB | 215 | LEU | 2.2 |
| 2 | CB | 98 | LEU | 2.2 |
| 4 | CD | 135 | LEU | 2.2 |
| 26 | DD | 187 | ALA | 2.2 |
| 4 | AD | 198 | VAL | 2.2 |
| 5 | AE | 117 | ASP | 2.2 |
| 26 | DD | 42 | ASP | 2.2 |
| 32 | BJ | 73 | ASP | 2.2 |
| 35 | DM | 63 | LYS | 2.1 |
| 45 | DW | 78 | TYR | 2.1 |
| 8 | AH | 112 | LEU | 2.1 |
| 14 | CN | 16 | PHE | 2.1 |
| 44 | BV | 155 | LEU | 2.1 |
| 1 | AA | 993 | G | 2.1 |
| 49 | B1 | 57 | ILE | 2.1 |
| 3 | CC | 184 | TYR | 2.1 |
| 12 | AL | 46 | LYS | 2.1 |
| 3 | AC | 32 | LEU | 2.1 |
| 3 | CC | 190 | ARG | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 4 | CD | 64 | LEU | 2.1 |
| 16 | AP | 7 | ALA | 2.1 |
| 26 | BD | 182 | LEU | 2.1 |
| 30 | DH | 5 | LEU | 2.1 |
| 1 | CA | 1115 | C | 2.1 |
| 6 | AF | 5 | GLU | 2.1 |
| 10 | AJ | 41 | PRO | 2.1 |
| 19 | CS | 27 | GLU | 2.1 |
| 53 | B5 | 54 | GLU | 2.1 |
| 19 | CS | 65 | ASN | 2.1 |
| 51 | D3 | 26 | ASN | 2.1 |
| 8 | CH | 20 | TYR | 2.1 |
| 1 | AA | 1164 | G | 2.1 |
| 1 | CA | 1302 | U | 2.1 |
| 3 | CC | 59 | ARG | 2.1 |
| 7 | CG | 73 | MET | 2.1 |
| 4 | CD | 32 | ALA | 2.1 |
| 7 | AG | 108 | ALA | 2.1 |
| 7 | AG | 134 | ALA | 2.1 |
| 4 | CD | 5 | ILE | 2.1 |
| 4 | CD | 29 | PRO | 2.1 |
| 19 | AS | 73 | GLU | 2.1 |
| 44 | BV | 39 | VAL | 2.1 |
| 44 | BV | 133 | ILE | 2.1 |
| 26 | DD | 60 | ASN | 2.1 |
| 29 | BG | 129 | THR | 2.1 |
| 2 | AB | 33 | TYR | 2.1 |
| 13 | CM | 104 | ARG | 2.1 |
| 18 | AR | 34 | TYR | 2.1 |
| 7 | CG | 99 | LEU | 2.1 |
| 26 | BD | 27 | LEU | 2.1 |
| 28 | DF | 53 | LEU | 2.1 |
| 10 | AJ | 32 | ALA | 2.1 |
| 22 | AV | 6193 | U | 2.1 |
| 1 | CA | 1220 | G | 2.1 |
| 19 | CS | 19 | VAL | 2.1 |
| 23 | BA | 1056 | G | 2.1 |
| 23 | BA | 1733 | G | 2.1 |
| 26 | BD | 104 | VAL | 2.1 |
| 3 | CC | 156 | ARG | 2.1 |
| 4 | AD | 209 | ARG | 2.1 |
| 10 | CJ | 56 | HIS | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 20 | AT | 72 | LEU | 2.1 |
| 37 | DO | 29 | PHE | 2.1 |
| 38 | DP | 22 | PHE | 2.1 |
| 2 | CB | 177 | ALA | 2.1 |
| 23 | DA | 2108 | C | 2.1 |
| 5 | AE | 100 | VAL | 2.1 |
| 53 | D5 | 54 | GLU | 2.1 |
| 14 | AN | 29 | ARG | 2.1 |
| 28 | DF | 32 | PRO | 2.1 |
| 45 | BW | 72 | ARG | 2.1 |
| 1 | CA | 1290 | G | 2.1 |
| 7 | AG | 122 | HIS | 2.1 |
| 37 | BO | 50 | SER | 2.1 |
| 23 | BA | 1534 | G | 2.1 |
| 43 | DU | 89 | PHE | 2.1 |
| 3 | CC | 181 | ASN | 2.1 |
| 49 | D1 | 46 | ASN | 2.1 |
| 16 | AP | 76 | GLN | 2.1 |
| 19 | AS | 68 | GLY | 2.1 |
| 26 | DD | 29 | GLY | 2.1 |
| 31 | BI | 22 | GLY | 2.1 |
| 7 | CG | 49 | ILE | 2.1 |
| 16 | CP | 51 | VAL | 2.1 |
| 28 | BF | 30 | GLU | 2.1 |
| 29 | BG | 53 | GLU | 2.1 |
| 42 | BT | 60 | ARG | 2.1 |
| 29 | BG | 103 | LEU | 2.1 |
| 44 | BV | 28 | MET | 2.1 |
| 44 | DV | 153 | SER | 2.1 |
| 4 | CD | 34 | GLU | 2.1 |
| 19 | CS | 26 | GLY | 2.1 |
| 1 | CA | 73 | G | 2.1 |
| 1 | CA | 1251 | A | 2.1 |
| 9 | CI | 51 | ARG | 2.1 |
| 43 | DU | 15 | VAL | 2.1 |
| 7 | AG | 63 | LYS | 2.1 |
| 7 | AG | 154 | TYR | 2.1 |
| 23 | BA | 1105 | U | 2.1 |
| 2 | AB | 231 | GLU | 2.1 |
| 5 | CE | 22 | GLY | 2.1 |
| 3 | AC | 68 | VAL | 2.1 |
| 9 | CI | 66 | ARG | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 14 | CN | 41 | ARG | 2.1 |
| 46 | BX | 19 | GLN | 2.1 |
| 44 | DV | 127 | LYS | 2.1 |
| 2 | AB | 28 | PHE | 2.1 |
| 23 | BA | 2893 | G | 2.1 |
| 34 | BL | 147 | LEU | 2.1 |
| 1 | AA | 995 | C | 2.1 |
| 1 | CA | 102(C) | C | 2.1 |
| 2 | CB | 170 | GLU | 2.1 |
| 7 | CG | 90 | GLU | 2.1 |
| 8 | AH | 124 | ALA | 2.1 |
| 19 | AS | 46 | GLY | 2.1 |
| 24 | BB | 55 | U | 2.1 |
| 28 | DF | 51 | ARG | 2.1 |
| 2 | AB | 139 | LYS | 2.1 |
| 45 | BW | 69 | PHE | 2.1 |
| 3 | AC | 23 | TYR | 2.1 |
| 13 | CM | 14 | ARG | 2.1 |
| 26 | BD | 56 | PRO | 2.1 |
| 38 | DP | 115 | ARG | 2.1 |
| 6 | AF | 99 | ALA | 2.1 |
| 13 | CM | 92 | HIS | 2.1 |
| 23 | DA | 2892 | A | 2.1 |
| 27 | DE | 207 | GLY | 2.1 |
| 28 | DF | 129 | GLY | 2.1 |
| 28 | DF | 177 | GLY | 2.1 |
| 29 | BG | 167 | GLU | 2.1 |
| 28 | BF | 92 | VAL | 2.1 |
| 29 | DG | 44 | VAL | 2.1 |
| 1 | AA | 1031 | G | 2.1 |
| 1 | CA | 1266 | G | 2.1 |
| 2 | AB | 214 | ILE | 2.1 |
| 4 | CD | 113 | SER | 2.1 |
| 19 | CS | 62 | ILE | 2.1 |
| 24 | DB | 88 | C | 2.1 |
| 28 | BF | 52 | ILE | 2.1 |
| 4 | AD | 135 | LEU | 2.1 |
| 9 | AI | 49 | PRO | 2.1 |
| 10 | CJ | 37 | PRO | 2.1 |
| 13 | AM | 35 | GLU | 2.1 |
| 43 | BU | 71 | LYS | 2.1 |
| 47 | BY | 15 | LYS | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 52 | D4 | 48 | LYS | 2.1 |
| 20 | CT | 70 | SER | 2.0 |
| 24 | DB | 57 | A | 2.0 |
| 38 | DP | 106 | SER | 2.0 |
| 4 | AD | 93 | PHE | 2.0 |
| 9 | CI | 64 | THR | 2.0 |
| 23 | BA | 508 | G | 2.0 |
| 24 | BB | 67 | G | 2.0 |
| 2 | CB | 141 | GLU | 2.0 |
| 9 | AI | 39 | GLY | 2.0 |
| 28 | DF | 25 | TYR | 2.0 |
| 2 | CB | 123 | ALA | 2.0 |
| 11 | AK | 80 | VAL | 2.0 |
| 15 | CO | 16 | ALA | 2.0 |
| 2 | CB | 42 | ILE | 2.0 |
| 5 | CE | 80 | ILE | 2.0 |
| 4 | AD | 36 | ARG | 2.0 |
| 18 | CR | 54 | ARG | 2.0 |
| 40 | DR | 20 | LEU | 2.0 |
| 13 | CM | 111 | LYS | 2.0 |
| 7 | CG | 28 | ASN | 2.0 |
| 12 | CL | 71 | GLY | 2.0 |
| 19 | CS | 54 | GLY | 2.0 |
| 30 | BH | 130 | TYR | 2.0 |
| 46 | BX | 84 | GLY | 2.0 |
| 14 | CN | 18 | VAL | 2.0 |
| 38 | DP | 135 | VAL | 2.0 |
| 49 | D1 | 58 | TYR | 2.0 |
| 1 | CA | 292 | G | 2.0 |
| 2 | AB | 202 | PRO | 2.0 |
| 10 | CJ | 53 | PRO | 2.0 |
| 40 | DR | 36 | PRO | 2.0 |
| 10 | AJ | 7 | LYS | 2.0 |
| 13 | CM | 31 | LYS | 2.0 |
| 18 | CR | 40 | LEU | 2.0 |
| 43 | BU | 17 | SER | 2.0 |
| 9 | CI | 23 | ASN | 2.0 |
| 37 | DO | 46 | VAL | 2.0 |
| 23 | BA | 229 | A | 2.0 |
| 43 | BU | 61 | ILE | 2.0 |
| 34 | BL | 124 | LYS | 2.0 |
| 42 | BT | 88 | LYS | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 48 | DZ | 2 | PRO | 2.0 |
| 8 | AH | 107 | LEU | 2.0 |
| 18 | CR | 79 | LEU | 2.0 |
| 1 | AA | 1358 | U | 2.0 |
| 4 | AD | 32 | ALA | 2.0 |
| 13 | AM | 4 | ILE | 2.0 |
| 33 | DK | 86 | ILE | 2.0 |
| 13 | CM | 19 | LEU | 2.0 |
| 11 | CK | 62 | GLN | 2.0 |
| 22 | AV | 6194 | C | 2.0 |
| 37 | BO | 95 | HIS | 2.0 |
| 2 | AB | 143 | GLU | 2.0 |
| 4 | CD | 71 | SER | 2.0 |
| 13 | CM | 83 | ASP | 2.0 |
| 14 | AN | 11 | LYS | 2.0 |
| 21 | AU | 14 | TRP | 2.0 |
| 6 | AF | 7 | ASN | 2.0 |
| 7 | AG | 152 | ALA | 2.0 |
| 21 | AU | 13 | ILE | 2.0 |
| 23 | BA | 1530 | G | 2.0 |
| 23 | DA | 352 | G | 2.0 |
| 35 | DM | 107 | ALA | 2.0 |

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 54 | MG | BA | 3222 | 1/1 | 0.92 | 1.17 | 87.35 | 91,91,91,91 | 0 |
| 54 | MG | CA | 1612 | 1/1 | 0.86 | 0.93 | 81.46 | 58,58,58,58 | 0 |
| 54 | MG | DA | 3223 | 1/1 | 0.85 | 0.61 | 56.85 | 45,45,45,45 | 0 |
| 54 | MG | BA | 3284 | 1/1 | 0.86 | 0.89 | 54.14 | 85,85,85,85 | 0 |
| 54 | MG | BA | 3046 | 1/1 | 0.98 | 0.92 | 45.19 | 87,87,87,87 | 0 |
| 54 | MG | DA | 3216 | 1/1 | 0.90 | 0.62 | 44.76 | 46,46,46,46 | 0 |
| 54 | MG | BA | 3019 | 1/1 | 0.75 | 0.65 | 44.61 | 58,58,58,58 | 0 |
| 54 | MG | CA | 1692 | 1/1 | 0.90 | 0.80 | 40.04 | 78,78,78,78 | 0 |
| 54 | MG | DA | 3191 | 1/1 | 0.99 | 0.48 | 35.59 | 24,24,24,24 | 0 |
| 54 | MG | AA | 1752 | 1/1 | 0.87 | 0.93 | 35.09 | 81,81,81,81 | 0 |
| 54 | MG | DA | 2932 | 1/1 | 0.81 | 0.53 | 32.74 | 38,38,38,38 | 0 |
| 54 | MG | DA | 2934 | 1/1 | 0.94 | 0.44 | 29.96 | 25,25,25,25 | 0 |
| 54 | MG | DA | 3190 | 1/1 | 0.99 | 0.44 | 29.54 | 27,27,27,27 | 0 |
| 54 | MG | BA | 3268 | 1/1 | 0.81 | 0.77 | 29.22 | 58,58,58,58 | 0 |
| 54 | MG | DA | 3202 | 1/1 | 0.81 | 0.66 | 27.71 | 44,44,44,44 | 0 |
| 54 | MG | BA | 3027 | 1/1 | 0.71 | 0.51 | 26.34 | 62,62,62,62 | 0 |
| 54 | MG | AA | 1621 | 1/1 | 0.77 | 0.61 | 26.08 | 74,74,74,74 | 0 |
| 54 | MG | DA | 2955 | 1/1 | 0.95 | 0.45 | 24.73 | 40,40,40,40 | 0 |
| 54 | MG | BA | 2924 | 1/1 | 0.95 | 0.45 | 23.35 | 47,47,47,47 | 0 |
| 54 | MG | DA | 2999 | 1/1 | 0.57 | 0.43 | 23.14 | 76,76,76,76 | 0 |
| 54 | MG | DA | 2907 | 1/1 | 0.98 | 0.47 | 21.13 | 7,7,7,7 | 0 |
| 54 | MG | DA | 2911 | 1/1 | 0.96 | 0.40 | 21.11 | 7,7,7,7 | 0 |
| 54 | MG | DA | 3241 | 1/1 | 0.89 | 0.51 | 20.02 | 54,54,54,54 | 0 |
| 54 | MG | AA | 1630 | 1/1 | 0.91 | 0.37 | 19.13 | 70,70,70,70 | 0 |
| 54 | MG | DA | 2904 | 1/1 | 0.95 | 0.46 | 19.12 | 4,4,4,4 | 0 |
| 54 | MG | BA | 2941 | 1/1 | 0.95 | 0.64 | 18.77 | 50,50,50,50 | 0 |
| 54 | MG | BA | 3088 | 1/1 | 0.92 | 0.55 | 18.69 | 73,73,73,73 | 0 |
| 54 | MG | BA | 3185 | 1/1 | 0.95 | 0.24 | 18.51 | 56,56,56,56 | 0 |
| 54 | MG | DA | 3024 | 1/1 | 0.72 | 0.39 | 17.66 | 36,36,36,36 | 0 |
| 54 | MG | DA | 2902 | 1/1 | 0.98 | 0.40 | 17.51 | 10,10,10,10 | 0 |
| 54 | MG | BA | 2911 | 1/1 | 0.97 | 0.47 | 17.42 | 23,23,23,23 | 0 |
| 54 | MG | DA | 2905 | 1/1 | 0.95 | 0.38 | 17.19 | 9,9,9,9 | 0 |
| 54 | MG | BA | 2910 | 1/1 | 0.97 | 0.53 | 17.07 | 27,27,27,27 | 0 |
| 54 | MG | BA | 2903 | 1/1 | 0.99 | 0.39 | 16.87 | 14,14,14,14 | 0 |
| 54 | MG | BA | 2961 | 1/1 | 0.90 | 0.38 | 16.69 | 43,43,43,43 | 0 |
| 54 | MG | DA | 3228 | 1/1 | 0.85 | 0.46 | 16.56 | 51,51,51,51 | 0 |
| 54 | MG | DA | 2959 | 1/1 | 0.79 | 0.39 | 16.47 | 56,56,56,56 | 0 |
| 54 | MG | DA | 3208 | 1/1 | 0.96 | 0.41 | 16.45 | 49,49,49,49 | 0 |
| 54 | MG | BA | 3182 | 1/1 | 0.96 | 0.51 | 15.84 | 20,20,20,20 | 0 |
| 54 | MG | BA | 2952 | 1/1 | 0.97 | 0.28 | 15.70 | 38,38,38,38 | 0 |
| 54 | MG | BA | 2970 | 1/1 | 0.90 | 0.58 | 15.47 | 45,45,45,45 | 0 |
| 54 | MG | DA | 2933 | 1/1 | 0.95 | 0.47 | 15.32 | 30,30,30,30 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 54 | MG | BA | 2920 | 1/1 | 0.95 | 0.35 | 15.19 | 28,28,28,28 | 0 |
| 54 | MG | BA | 2921 | 1/1 | 0.94 | 0.39 | 15.18 | 21,21,21,21 | 0 |
| 54 | MG | BA | 2918 | 1/1 | 0.98 | 0.35 | 15.07 | 17,17,17,17 | 0 |
| 54 | MG | BA | 3006 | 1/1 | 0.58 | 0.51 | 14.92 | 77,77,77,77 | 0 |
| 54 | MG | DA | 3165 | 1/1 | 0.80 | 0.62 | 14.88 | 71,71,71,71 | 0 |
| 54 | MG | DA | 3274 | 1/1 | 0.85 | 0.39 | 14.87 | 62,62,62,62 | 0 |
| 54 | MG | AA | 1682 | 1/1 | 0.84 | 0.40 | 14.64 | 85,85,85,85 | 0 |
| 54 | MG | BA | 2931 | 1/1 | 0.87 | 0.47 | 14.53 | 32,32,32,32 | 0 |
| 54 | MG | DA | 3324 | 1/1 | 0.58 | 0.51 | 14.33 | 78,78,78,78 | 0 |
| 54 | MG | BA | 3004 | 1/1 | 0.71 | 1.27 | 13.59 | 74,74,74,74 | 0 |
| 54 | MG | BA | 2909 | 1/1 | 0.95 | 0.41 | 13.58 | 24,24,24,24 | 0 |
| 54 | MG | BA | 3192 | 1/1 | 0.94 | 0.58 | 13.48 | 52,52,52,52 | 0 |
| 54 | MG | DA | 3251 | 1/1 | 0.72 | 0.37 | 13.33 | 63,63,63,63 | 0 |
| 54 | MG | AA | 1622 | 1/1 | 0.97 | 0.81 | 13.23 | 88,88,88,88 | 0 |
| 54 | MG | DA | 3259 | 1/1 | 0.85 | 0.53 | 13.20 | 108,108,108,108 | 0 |
| 54 | MG | BA | 3220 | 1/1 | 0.81 | 0.33 | 13.11 | 56,56,56,56 | 0 |
| 54 | MG | BA | 2967 | 1/1 | 0.95 | 0.41 | 13.10 | 24,24,24,24 | 0 |
| 54 | MG | DA | 3012 | 1/1 | 0.84 | 0.38 | 13.02 | 45,45,45,45 | 0 |
| 54 | MG | BA | 2968 | 1/1 | 0.87 | 0.47 | 12.76 | 51,51,51,51 | 0 |
| 54 | MG | DA | 3232 | 1/1 | 0.95 | 0.34 | 12.74 | 39,39,39,39 | 0 |
| 54 | MG | DA | 2915 | 1/1 | 0.91 | 0.47 | 12.72 | 14,14,14,14 | 0 |
| 54 | MG | BA | 3188 | 1/1 | 0.77 | 0.38 | 12.69 | 45,45,45,45 | 0 |
| 54 | MG | DA | 3149 | 1/1 | 0.81 | 0.45 | 12.64 | 74,74,74,74 | 0 |
| 54 | MG | DA | 3188 | 1/1 | 0.98 | 0.51 | 12.31 | 9,9,9,9 | 0 |
| 54 | MG | DA | 3047 | 1/1 | 0.84 | 0.34 | 12.26 | 66,66,66,66 | 0 |
| 54 | MG | DA | 3066 | 1/1 | 0.89 | 0.47 | 12.23 | 85,85,85,85 | 0 |
| 54 | MG | DA | 2921 | 1/1 | 0.98 | 0.42 | 12.17 | 17,17,17,17 | 0 |
| 54 | MG | BA | 3232 | 1/1 | 0.97 | 0.40 | 12.04 | 24,24,24,24 | 0 |
| 54 | MG | AA | 1679 | 1/1 | 0.85 | 0.58 | 11.91 | 78,78,78,78 | 0 |
| 54 | MG | DA | 2906 | 1/1 | 0.98 | 0.41 | 11.68 | 27,27,27,27 | 0 |
| 54 | MG | AA | 1742 | 1/1 | 0.93 | 0.42 | 11.66 | 87,87,87,87 | 0 |
| 54 | MG | BA | 2901 | 1/1 | 0.98 | 0.40 | 11.46 | 23,23,23,23 | 0 |
| 54 | MG | BA | 2917 | 1/1 | 0.97 | 0.41 | 11.32 | 8,8,8,8 | 0 |
| 54 | MG | DA | 3000 | 1/1 | 0.97 | 0.36 | 11.30 | 35,35,35,35 | 0 |
| 54 | MG | DA | 2943 | 1/1 | 0.95 | 0.41 | 11.26 | 32,32,32,32 | 0 |
| 54 | MG | DA | 2909 | 1/1 | 0.97 | 0.41 | 11.21 | 5,5,5,5 | 0 |
| 54 | MG | BA | 3256 | 1/1 | 0.89 | 0.39 | 10.99 | 79,79,79,79 | 0 |
| 54 | MG | DA | 3272 | 1/1 | 0.87 | 0.43 | 10.87 | 41,41,41,41 | 0 |
| 54 | MG | DA | 3174 | 1/1 | 0.64 | 0.51 | 10.81 | 42,42,42,42 | 0 |
| 54 | MG | BA | 3179 | 1/1 | 0.96 | 0.48 | 10.76 | 19,19,19,19 | 0 |
| 54 | MG | AA | 1728 | 1/1 | 0.94 | 0.89 | 10.71 | 105,105,105,105 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 54 | MG | BA | 3270 | 1/1 | 0.92 | 0.30 | 10.63 | 61,61,61,61 | 0 |
| 54 | MG | DA | 2976 | 1/1 | 0.98 | 0.30 | 10.61 | 37,37,37,37 | 0 |
| 54 | MG | BA | 2914 | 1/1 | 0.93 | 0.43 | 10.61 | 31,31,31,31 | 0 |
| 54 | MG | AA | 1601 | 1/1 | 0.96 | 0.44 | 10.38 | 31,31,31,31 | 0 |
| 54 | MG | BA | 3091 | 1/1 | 0.83 | 0.40 | 10.23 | 56,56,56,56 | 0 |
| 54 | MG | DA | 2918 | 1/1 | 0.99 | 0.35 | 10.22 | 15,15,15,15 | 0 |
| 54 | MG | AA | 1723 | 1/1 | 0.79 | 0.51 | 10.19 | 81,81,81,81 | 0 |
| 54 | MG | BA | 2943 | 1/1 | 0.97 | 0.37 | 10.14 | 42,42,42,42 | 0 |
| 54 | MG | DA | 3215 | 1/1 | 0.94 | 0.45 | 10.10 | 39,39,39,39 | 0 |
| 54 | MG | DA | 3079 | 1/1 | 0.90 | 0.33 | 9.98 | 38,38,38,38 | 0 |
| 54 | MG | BA | 3226 | 1/1 | 0.76 | 0.42 | 9.84 | 81,81,81,81 | 0 |
| 54 | MG | DA | 2989 | 1/1 | 0.94 | 0.34 | 9.62 | 45,45,45,45 | 0 |
| 54 | MG | BA | 3097 | 1/1 | 0.89 | 0.30 | 9.42 | 53,53,53,53 | 0 |
| 54 | MG | DA | 2914 | 1/1 | 0.94 | 0.46 | 9.41 | 27,27,27,27 | 0 |
| 54 | MG | DA | 3198 | 1/1 | 0.97 | 0.29 | 9.38 | 26,26,26,26 | 0 |
| 54 | MG | BA | 3181 | 1/1 | 0.98 | 0.53 | 9.30 | 22,22,22,22 | 0 |
| 54 | MG | CA | 1715 | 1/1 | 0.88 | 0.36 | 9.25 | 74,74,74,74 | 0 |
| 54 | MG | BA | 2930 | 1/1 | 0.98 | 0.34 | 8.96 | 34,34,34,34 | 0 |
| 54 | MG | AA | 1603 | 1/1 | 0.93 | 0.32 | 8.81 | 35,35,35,35 | 0 |
| 54 | MG | AA | 1636 | 1/1 | 0.96 | 0.44 | 8.28 | 76,76,76,76 | 0 |
| 54 | MG | BA | 3184 | 1/1 | 0.96 | 0.32 | 8.16 | 42,42,42,42 | 0 |
| 54 | MG | AA | 1714 | 1/1 | 0.89 | 0.34 | 7.76 | 58,58,58,58 | 0 |
| 54 | MG | BA | 3151 | 1/1 | 0.97 | 0.71 | 7.54 | 56,56,56,56 | 0 |
| 54 | MG | DA | 3022 | 1/1 | 0.94 | 0.32 | 7.48 | 60,60,60,60 | 0 |
| 54 | MG | BA | 2904 | 1/1 | 0.97 | 0.39 | 7.46 | 13,13,13,13 | 0 |
| 54 | MG | DA | 3313 | 1/1 | 0.34 | 0.27 | 7.43 | 107,107,107,107 | 0 |
| 54 | MG | BA | 2940 | 1/1 | 0.96 | 0.30 | 7.40 | 29,29,29,29 | 0 |
| 54 | MG | CA | 1672 | 1/1 | 0.83 | 0.30 | 7.31 | 62,62,62,62 | 0 |
| 54 | MG | DA | 3039 | 1/1 | 0.97 | 0.29 | 7.29 | 48,48,48,48 | 0 |
| 54 | MG | BA | 3118 | 1/1 | 0.75 | 0.44 | 7.26 | 109,109,109,109 | 0 |
| 54 | MG | DA | 3306 | 1/1 | 0.89 | 0.31 | 7.15 | 51,51,51,51 | 0 |
| 54 | MG | BA | 3257 | 1/1 | 0.92 | 0.32 | 7.07 | 64,64,64,64 | 0 |
| 54 | MG | DA | 3082 | 1/1 | 0.84 | 0.41 | 6.92 | 70,70,70,70 | 0 |
| 54 | MG | BA | 3277 | 1/1 | 0.95 | 0.27 | 6.88 | 71,71,71,71 | 0 |
| 54 | MG | DA | 3101 | 1/1 | 0.76 | 0.76 | 6.77 | 72,72,72,72 | 0 |
| 54 | MG | DA | 3214 | 1/1 | 0.95 | 0.34 | 6.40 | 46,46,46,46 | 0 |
| 54 | MG | DA | 3083 | 1/1 | 0.91 | 0.24 | 6.32 | 67,67,67,67 | 0 |
| 54 | MG | DG | 201 | 1/1 | 0.07 | 0.44 | 6.32 | 101,101,101,101 | 0 |
| 54 | MG | CA | 1609 | 1/1 | 0.92 | 0.23 | 6.32 | 93,93,93,93 | 0 |
| 54 | MG | BA | 3204 | 1/1 | 0.81 | 0.35 | 6.29 | 74,74,74,74 | 0 |
| 54 | MG | BA | 2913 | 1/1 | 0.97 | 0.33 | 6.19 | 16,16,16,16 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | DA | 3033 | 1/1 | 0.46 | 0.46 | 6.11 | 101,101,101,101 | 0 |
| 54 | MG | AA | 1637 | 1/1 | 0.89 | 0.45 | 6.07 | 61,61,61,61 | 0 |
| 54 | MG | BA | 2925 | 1/1 | 0.99 | 0.27 | 5.97 | 29,29,29,29 | 0 |
| 54 | MG | DA | 2965 | 1/1 | 0.93 | 0.39 | 5.87 | 57,57,57,57 | 0 |
| 54 | MG | DA | 2944 | 1/1 | 0.97 | 0.36 | 5.77 | 35,35,35,35 | 0 |
| 54 | MG | DA | 3298 | 1/1 | 0.78 | 0.68 | 5.64 | 79,79,79,79 | 0 |
| 54 | MG | BA | 3242 | 1/1 | 0.85 | 0.35 | 5.60 | 44,44,44,44 | 0 |
| 54 | MG | BA | 2999 | 1/1 | 0.94 | 0.24 | 5.41 | 45,45,45,45 | 0 |
| 54 | MG | DA | 3003 | 1/1 | 0.85 | 0.36 | 5.28 | 41,41,41,41 | 0 |
| 54 | MG | BA | 2908 | 1/1 | 0.96 | 0.47 | 5.10 | 18,18,18,18 | 0 |
| 54 | MG | DA | 3154 | 1/1 | 0.88 | 0.33 | 5.10 | 94,94,94,94 | 0 |
| 54 | MG | DA | 2901 | 1/1 | 0.96 | 0.46 | 5.00 | 7,7,7,7 | 0 |
| 54 | MG | AA | 1695 | 1/1 | 0.78 | 0.38 | 4.93 | 83,83,83,83 | 0 |
| 54 | MG | DA | 3023 | 1/1 | 0.85 | 0.24 | 4.91 | 49,49,49,49 | 0 |
| 54 | MG | DA | 2968 | 1/1 | 0.95 | 0.27 | 4.86 | 56,56,56,56 | 0 |
| 54 | MG | CA | 1617 | 1/1 | 0.95 | 0.34 | 4.84 | 90,90,90,90 | 0 |
| 54 | MG | DA | 3105 | 1/1 | 0.47 | 0.52 | 4.62 | 75,75,75,75 | 0 |
| 54 | MG | DA | 2966 | 1/1 | 0.96 | 0.35 | 4.61 | 70,70,70,70 | 0 |
| 54 | MG | DA | 3304 | 1/1 | 0.95 | 0.25 | 4.57 | 59,59,59,59 | 0 |
| 54 | MG | BA | 2979 | 1/1 | 0.94 | 0.25 | 4.48 | 40,40,40,40 | 0 |
| 54 | MG | DA | 2927 | 1/1 | 0.91 | 0.23 | 4.44 | 22,22,22,22 | 0 |
| 54 | MG | BA | 3090 | 1/1 | 0.82 | 0.34 | 4.42 | 69,69,69,69 | 0 |
| 54 | MG | DA | 3070 | 1/1 | 0.88 | 0.27 | 4.40 | 70,70,70,70 | 0 |
| 54 | MG | DA | 3310 | 1/1 | 0.89 | 0.27 | 4.35 | 52,52,52,52 | 0 |
| 54 | MG | BA | 2922 | 1/1 | 0.97 | 0.46 | 4.21 | 25,25,25,25 | 0 |
| 54 | MG | AA | 1721 | 1/1 | 0.90 | 0.55 | 4.16 | 66,66,66,66 | 0 |
| 54 | MG | BA | 3180 | 1/1 | 0.97 | 0.27 | 4.13 | 26,26,26,26 | 0 |
| 54 | MG | BA | 2998 | 1/1 | 0.96 | 0.22 | 4.10 | 46,46,46,46 | 0 |
| 54 | MG | BA | 2916 | 1/1 | 0.95 | 0.43 | 4.07 | 38,38,38,38 | 0 |
| 54 | MG | DA | 3192 | 1/1 | 0.94 | 0.29 | 4.06 | 30,30,30,30 | 0 |
| 54 | MG | CA | 1607 | 1/1 | 0.87 | 0.27 | 4.01 | 52,52,52,52 | 0 |
| 54 | MG | BA | 2982 | 1/1 | 0.93 | 0.31 | 3.83 | 41,41,41,41 | 0 |
| 54 | MG | BA | 3186 | 1/1 | 0.97 | 0.32 | 3.81 | 52,52,52,52 | 0 |
| 54 | MG | DA | 2978 | 1/1 | 0.93 | 0.28 | 3.67 | 44,44,44,44 | 0 |
| 54 | MG | AA | 1624 | 1/1 | 0.96 | 0.36 | 3.64 | 67,67,67,67 | 0 |
| 54 | MG | BA | 3208 | 1/1 | 0.82 | 0.24 | 3.39 | 48,48,48,48 | 0 |
| 54 | MG | DA | 3034 | 1/1 | 0.84 | 0.29 | 3.37 | 65,65,65,65 | 0 |
| 54 | MG | AA | 1707 | 1/1 | 0.87 | 0.29 | 3.28 | 100,100,100,100 | 0 |
| 54 | MG | DA | 2971 | 1/1 | 0.97 | 0.23 | 3.25 | 47,47,47,47 | 0 |
| 54 | MG | CA | 1691 | 1/1 | 0.71 | 0.42 | 3.19 | 85,85,85,85 | 0 |
| 54 | MG | BA | 2980 | 1/1 | 0.91 | 0.26 | 3.09 | 40,40,40,40 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | CA | 1703 | 1/1 | 0.60 | 0.35 | 3.06 | 108,108,108,108 | 0 |
| 54 | MG | DA | 3072 | 1/1 | 0.79 | 0.60 | 2.99 | 73,73,73,73 | 0 |
| 54 | MG | BA | 3052 | 1/1 | 0.96 | 0.24 | 2.86 | 56,56,56,56 | 0 |
| 54 | MG | AA | 1713 | 1/1 | 0.73 | 0.30 | 2.70 | 93,93,93,93 | 0 |
| 54 | MG | DA | 3036 | 1/1 | 0.89 | 0.34 | 2.69 | 51,51,51,51 | 0 |
| 54 | MG | DA | 2950 | 1/1 | 0.92 | 0.20 | 2.53 | 29,29,29,29 | 0 |
| 54 | MG | AA | 1647 | 1/1 | 0.90 | 0.24 | 2.52 | 85,85,85,85 | 0 |
| 54 | MG | AA | 1731 | 1/1 | 0.86 | 0.27 | 2.42 | 76,76,76,76 | 0 |
| 54 | MG | BA | 3152 | 1/1 | 0.91 | 0.21 | 2.31 | 75,75,75,75 | 0 |
| 54 | MG | CA | 1698 | 1/1 | 0.75 | 0.30 | 2.31 | 117,117,117,117 | 0 |
| 54 | MG | CA | 1717 | 1/1 | 0.69 | 0.27 | 2.27 | 84,84,84,84 | 0 |
| 54 | MG | AA | 1650 | 1/1 | 0.88 | 0.29 | 2.26 | 103,103,103,103 | 0 |
| 54 | MG | DA | 2916 | 1/1 | 0.89 | 0.27 | 2.14 | 22,22,22,22 | 0 |
| 54 | MG | DA | 2908 | 1/1 | 0.98 | 0.26 | 2.14 | 24,24,24,24 | 0 |
| 54 | MG | DA | 2917 | 1/1 | 0.99 | 0.25 | 2.13 | 22,22,22,22 | 0 |
| 54 | MG | DA | 3201 | 1/1 | 0.85 | 0.44 | 1.88 | 72,72,72,72 | 0 |
| 54 | MG | BA | 3255 | 1/1 | 0.75 | 0.21 | 1.81 | 57,57,57,57 | 0 |
| 54 | MG | DA | 3277 | 1/1 | 0.89 | 0.31 | 1.76 | 52,52,52,52 | 0 |
| 54 | MG | DA | 3037 | 1/1 | 0.67 | 0.18 | 1.68 | 77,77,77,77 | 0 |
| 54 | MG | DA | 3195 | 1/1 | 0.98 | 0.26 | 1.66 | 51,51,51,51 | 0 |
| 54 | MG | BA | 3102 | 1/1 | 0.95 | 0.27 | 1.54 | 69,69,69,69 | 0 |
| 54 | MG | DA | 3007 | 1/1 | 0.89 | 0.19 | 1.50 | 43,43,43,43 | 0 |
| 54 | MG | BA | 2938 | 1/1 | 0.97 | 0.20 | 1.38 | 10,10,10,10 | 0 |
| 54 | MG | AA | 1755 | 1/1 | 0.83 | 0.32 | 1.32 | 103,103,103,103 | 0 |
| 54 | MG | AA | 1628 | 1/1 | 0.96 | 0.38 | 1.23 | 62,62,62,62 | 0 |
| 54 | MG | DA | 3067 | 1/1 | 0.96 | 0.20 | 1.22 | 63,63,63,63 | 0 |
| 54 | MG | BA | 3017 | 1/1 | 0.89 | 0.21 | 1.13 | 69,69,69,69 | 0 |
| 54 | MG | AA | 1740 | 1/1 | 0.87 | 0.34 | 1.08 | 80,80,80,80 | 0 |
| 54 | MG | CA | 1686 | 1/1 | 0.95 | 0.25 | 1.00 | 60,60,60,60 | 0 |
| 54 | MG | DA | 2967 | 1/1 | 0.94 | 0.35 | 0.97 | 54,54,54,54 | 0 |
| 54 | MG | CA | 1604 | 1/1 | 0.94 | 0.23 | 0.95 | 59,59,59,59 | 0 |
| 54 | MG | BA | 3234 | 1/1 | 0.95 | 0.22 | 0.79 | 61,61,61,61 | 0 |
| 54 | MG | BA | 3153 | 1/1 | 0.99 | 0.30 | 0.72 | 67,67,67,67 | 0 |
| 54 | MG | BA | 3065 | 1/1 | 0.92 | 0.20 | 0.68 | 61,61,61,61 | 0 |
| 54 | MG | DA | 2991 | 1/1 | 0.91 | 0.24 | 0.64 | 31,31,31,31 | 0 |
| 54 | MG | AA | 1612 | 1/1 | 0.81 | 0.25 | 0.63 | 64,64,64,64 | 0 |
| 54 | MG | DA | 2980 | 1/1 | 0.95 | 0.18 | 0.60 | 63,63,63,63 | 0 |
| 54 | MG | DA | 3025 | 1/1 | 0.92 | 0.16 | 0.59 | 69,69,69,69 | 0 |
| 54 | MG | AA | 1754 | 1/1 | 0.42 | 0.22 | 0.59 | 110,110,110,110 | 0 |
| 54 | MG | CA | 1603 | 1/1 | 0.94 | 0.27 | 0.58 | 48,48,48,48 | 0 |
| 54 | MG | D2 | 101 | 1/1 | 0.87 | 0.27 | 0.57 | 66,66,66,66 | 0 |
| 54 | MG | BA | 2986 | 1/1 | 0.63 | 0.23 | 0.56 | 67,67,67,67 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 54 | MG | CA | 1610 | 1/1 | 0.79 | 0.28 | 0.51 | 77,77,77,77 | 0 |
| 54 | MG | DA | 3118 | 1/1 | 0.93 | 0.25 | 0.50 | 62,62,62,62 | 0 |
| 54 | MG | BA | 3011 | 1/1 | 0.97 | 0.15 | 0.50 | 83,83,83,83 | 0 |
| 54 | MG | DA | 2984 | 1/1 | 0.98 | 0.20 | 0.48 | 66,66,66,66 | 0 |
| 54 | MG | CA | 1629 | 1/1 | 0.98 | 0.24 | 0.43 | 106,106,106,106 | 0 |
| 54 | MG | BA | 2949 | 1/1 | 0.94 | 0.18 | 0.38 | 47,47,47,47 | 0 |
| 54 | MG | BA | 2915 | 1/1 | 0.94 | 0.17 | 0.20 | 4,4,4,4 | 0 |
| 54 | MG | BA | 2995 | 1/1 | 0.91 | 0.20 | 0.14 | 47,47,47,47 | 0 |
| 54 | MG | BA | 3055 | 1/1 | 0.93 | 0.17 | 0.08 | 60,60,60,60 | 0 |
| 54 | MG | DA | 2939 | 1/1 | 0.92 | 0.17 | 0.07 | 40,40,40,40 | 0 |
| 54 | MG | DE | 301 | 1/1 | 0.88 | 0.24 | -0.01 | 44,44,44,44 | 0 |
| 54 | MG | BA | 2975 | 1/1 | 0.84 | 0.19 | -0.12 | 37,37,37,37 | 0 |
| 54 | MG | CA | 1664 | 1/1 | 0.94 | 0.20 | -0.16 | 82,82,82,82 | 0 |
| 54 | MG | BK | 201 | 1/1 | 0.68 | 0.19 | -0.19 | 91,91,91,91 | 0 |
| 54 | MG | DA | 3221 | 1/1 | 0.89 | 0.18 | -0.27 | 68,68,68,68 | 0 |
| 54 | MG | DA | 2964 | 1/1 | 0.94 | 0.20 | -0.32 | 34,34,34,34 | 0 |
| 54 | MG | CA | 1638 | 1/1 | 0.90 | 0.19 | -0.34 | 65,65,65,65 | 0 |
| 54 | MG | DA | 2990 | 1/1 | 0.97 | 0.20 | -0.37 | 35,35,35,35 | 0 |
| 54 | MG | BA | 3243 | 1/1 | 0.88 | 0.17 | -0.40 | 82,82,82,82 | 0 |
| 54 | MG | AA | 1615 | 1/1 | 0.95 | 0.15 | -0.51 | 42,42,42,42 | 0 |
| 54 | MG | DB | 203 | 1/1 | 0.84 | 0.19 | -0.55 | 82,82,82,82 | 0 |
| 54 | MG | AA | 1662 | 1/1 | 0.93 | 0.23 | -0.60 | 53,53,53,53 | 0 |
| 54 | MG | AA | 1619 | 1/1 | 0.95 | 0.16 | -0.64 | 80,80,80,80 | 0 |
| 54 | MG | AA | 1607 | 1/1 | 0.97 | 0.21 | -0.65 | 54,54,54,54 | 0 |
| 54 | MG | AA | 1652 | 1/1 | 0.93 | 0.20 | -0.69 | 89,89,89,89 | 0 |
| 55 | ZN | AD | 301 | 1/1 | 0.99 | 0.27 | -0.69 | 80,80,80,80 | 0 |
| 54 | MG | BA | 3010 | 1/1 | 0.95 | 0.15 | -0.72 | 37,37,37,37 | 0 |
| 54 | MG | DA | 2982 | 1/1 | 0.90 | 0.20 | -0.77 | 33,33,33,33 | 0 |
| 54 | MG | BA | 3030 | 1/1 | 0.86 | 0.15 | -0.77 | 57,57,57,57 | 0 |
| 54 | MG | AA | 1716 | 1/1 | 0.91 | 0.16 | -0.90 | 120,120,120,120 | 0 |
| 54 | MG | DA | 2994 | 1/1 | 0.87 | 0.13 | -0.97 | 67,67,67,67 | 0 |
| 54 | MG | BA | 2973 | 1/1 | 0.94 | 0.15 | -1.00 | 61,61,61,61 | 0 |
| 54 | MG | BA | 3227 | 1/1 | 0.95 | 0.15 | -1.06 | 48,48,48,48 | 0 |
| 54 | MG | CA | 1608 | 1/1 | 0.84 | 0.11 | -1.11 | 61,61,61,61 | 0 |
| 54 | MG | CA | 1725 | 1/1 | 0.31 | 0.17 | -1.12 | 105,105,105,105 | 0 |
| 54 | MG | BA | 3307 | 1/1 | 0.93 | 0.14 | -1.14 | 68,68,68,68 | 0 |
| 54 | MG | DA | 3018 | 1/1 | 0.90 | 0.13 | -1.20 | 73,73,73,73 | 0 |
| 54 | MG | DA | 2969 | 1/1 | 0.96 | 0.18 | -1.27 | 42,42,42,42 | 0 |
| 54 | MG | BA | 2962 | 1/1 | 0.90 | 0.17 | -1.28 | 17,17,17,17 | 0 |
| 54 | MG | AA | 1739 | 1/1 | 0.76 | 0.15 | -1.32 | 129,129,129,129 | 0 |
| 54 | MG | AD | 302 | 1/1 | 0.56 | 0.18 | -1.33 | 87,87,87,87 | 0 |
| 54 | MG | BA | 3263 | 1/1 | 0.45 | 0.23 | -1.42 | 80,80,80,80 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|--------|-----------------------------|-------|
| 54 | MG | AA | 1725 | 1/1 | 0.92 | 0.20 | -1.46 | 72,72,72,72 | 0 |
| 54 | MG | AA | 1632 | 1/1 | 0.92 | 0.11 | -1.48 | 68,68,68,68 | 0 |
| 54 | MG | DA | 2951 | 1/1 | 0.99 | 0.18 | -1.64 | 38,38,38,38 | 0 |
| 55 | ZN | CD | 301 | 1/1 | 0.96 | 0.24 | -1.75 | 131,131,131,131 | 0 |
| 55 | ZN | CN | 101 | 1/1 | 0.96 | 0.10 | -1.76 | 144,144,144,144 | 0 |
| 54 | MG | BA | 2991 | 1/1 | 0.88 | 0.16 | -1.76 | 36,36,36,36 | 0 |
| 54 | MG | BA | 3252 | 1/1 | 0.87 | 0.12 | -1.83 | 92,92,92,92 | 0 |
| 54 | MG | BB | 210 | 1/1 | 0.82 | 0.10 | -1.86 | 100,100,100,100 | 0 |
| 54 | MG | BA | 3138 | 1/1 | 0.83 | 0.14 | -1.91 | 100,100,100,100 | 0 |
| 54 | MG | CA | 1624 | 1/1 | 0.90 | 0.13 | -1.93 | 66,66,66,66 | 0 |
| 54 | MG | DB | 204 | 1/1 | 0.94 | 0.07 | -2.34 | 75,75,75,75 | 0 |
| 54 | MG | BA | 2969 | 1/1 | 0.80 | 0.15 | -2.37 | 37,37,37,37 | 0 |
| 54 | MG | AA | 1604 | 1/1 | 0.96 | 0.12 | -2.52 | 57,57,57,57 | 0 |
| 54 | MG | BB | 207 | 1/1 | 0.90 | 0.11 | -2.68 | 105,105,105,105 | 0 |
| 54 | MG | BA | 3251 | 1/1 | 0.96 | 0.10 | -2.70 | 64,64,64,64 | 0 |
| 54 | MG | CA | 1719 | 1/1 | 0.97 | 0.13 | -3.12 | 78,78,78,78 | 0 |
| 54 | MG | DA | 2975 | 1/1 | 0.89 | 0.07 | -3.50 | 58,58,58,58 | 0 |
| 54 | MG | AA | 1618 | 1/1 | 0.67 | 0.09 | -3.67 | 91,91,91,91 | 0 |
| 54 | MG | DA | 3006 | 1/1 | 0.87 | 0.12 | -3.88 | 74,74,74,74 | 0 |
| 54 | MG | DA | 2974 | 1/1 | 0.92 | 0.08 | -3.91 | 46,46,46,46 | 0 |
| 54 | MG | CA | 1666 | 1/1 | 0.93 | 0.08 | -3.92 | 116,116,116,116 | 0 |
| 54 | MG | AA | 1736 | 1/1 | 0.97 | 0.13 | -5.40 | 79,79,79,79 | 0 |
| 54 | MG | DA | 2958 | 1/1 | 0.96 | 0.16 | -6.56 | 2,2,2,2 | 0 |
| 54 | MG | DA | 3026 | 1/1 | 0.92 | 0.08 | -10.63 | 48,48,48,48 | 0 |
| 54 | MG | AA | 1654 | 1/1 | 0.90 | 0.30 | - | 76,76,76,76 | 0 |
| 54 | MG | DA | 3276 | 1/1 | 0.84 | 0.17 | - | 128,128,128,128 | 0 |
| 54 | MG | DB | 212 | 1/1 | 0.64 | 0.14 | - | 70,70,70,70 | 0 |
| 54 | MG | AA | 1741 | 1/1 | 0.95 | 0.13 | - | 74,74,74,74 | 0 |
| 54 | MG | DA | 3205 | 1/1 | 0.82 | 0.32 | - | 48,48,48,48 | 0 |
| 54 | MG | AA | 1668 | 1/1 | 0.94 | 0.08 | - | 90,90,90,90 | 0 |
| 54 | MG | DA | 3094 | 1/1 | 0.72 | 0.30 | - | 76,76,76,76 | 0 |
| 54 | MG | DA | 3312 | 1/1 | 0.72 | 0.54 | - | 66,66,66,66 | 0 |
| 54 | MG | DA | 3252 | 1/1 | 0.97 | 0.10 | - | 44,44,44,44 | 0 |
| 54 | MG | CA | 1705 | 1/1 | 0.66 | 0.24 | - | 54,54,54,54 | 0 |
| 54 | MG | DA | 2995 | 1/1 | 0.85 | 0.55 | - | 48,48,48,48 | 0 |
| 54 | MG | DA | 3020 | 1/1 | 0.94 | 0.17 | - | 63,63,63,63 | 0 |
| 54 | MG | DA | 3123 | 1/1 | 0.99 | 0.07 | - | 59,59,59,59 | 0 |
| 54 | MG | BA | 3114 | 1/1 | 0.70 | 0.67 | - | 78,78,78,78 | 0 |
| 54 | MG | DA | 3281 | 1/1 | 0.78 | 0.29 | - | 73,73,73,73 | 0 |
| 54 | MG | DA | 3004 | 1/1 | 0.85 | 0.33 | - | 67,67,67,67 | 0 |
| 54 | MG | DA | 2993 | 1/1 | 0.78 | 0.08 | - | 69,69,69,69 | 0 |
| 54 | MG | BA | 3249 | 1/1 | 0.92 | 0.24 | - | 37,37,37,37 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | DA | 3234 | 1/1 | 0.94 | 0.10 | - | 130,130,130,130 | 0 |
| 54 | MG | DA | 3099 | 1/1 | 0.89 | 0.18 | - | 81,81,81,81 | 0 |
| 54 | MG | BA | 3022 | 1/1 | 0.88 | 0.14 | - | 77,77,77,77 | 0 |
| 54 | MG | AA | 1672 | 1/1 | 0.98 | 0.46 | - | 101,101,101,101 | 0 |
| 54 | MG | BA | 2951 | 1/1 | 0.98 | 0.38 | - | 28,28,28,28 | 0 |
| 54 | MG | DA | 3109 | 1/1 | 0.87 | 0.31 | - | 54,54,54,54 | 0 |
| 54 | MG | DA | 2936 | 1/1 | 0.90 | 0.36 | - | 27,27,27,27 | 0 |
| 54 | MG | DA | 3226 | 1/1 | 0.59 | 0.49 | - | 80,80,80,80 | 0 |
| 54 | MG | BA | 3200 | 1/1 | 0.88 | 0.33 | - | 64,64,64,64 | 0 |
| 54 | MG | CA | 1648 | 1/1 | 0.41 | 0.34 | - | 64,64,64,64 | 0 |
| 54 | MG | BA | 3142 | 1/1 | 0.93 | 0.09 | - | 89,89,89,89 | 0 |
| 54 | MG | BA | 3302 | 1/1 | 0.79 | 0.30 | - | 121,121,121,121 | 0 |
| 54 | MG | BA | 3167 | 1/1 | 0.98 | 0.14 | - | 50,50,50,50 | 0 |
| 54 | MG | BA | 3209 | 1/1 | 0.94 | 0.27 | - | 69,69,69,69 | 0 |
| 54 | MG | AA | 1631 | 1/1 | 0.90 | 0.31 | - | 70,70,70,70 | 0 |
| 54 | MG | AA | 1692 | 1/1 | 0.90 | 0.33 | - | 84,84,84,84 | 0 |
| 54 | MG | BA | 3223 | 1/1 | 0.90 | 0.23 | - | 54,54,54,54 | 0 |
| 54 | MG | CA | 1615 | 1/1 | 0.98 | 0.26 | - | 51,51,51,51 | 0 |
| 54 | MG | DA | 3053 | 1/1 | 0.96 | 0.27 | - | 61,61,61,61 | 0 |
| 54 | MG | BA | 3106 | 1/1 | 0.94 | 0.21 | - | 70,70,70,70 | 0 |
| 54 | MG | DA | 3189 | 1/1 | 0.86 | 0.25 | - | 37,37,37,37 | 0 |
| 54 | MG | BA | 3292 | 1/1 | 0.93 | 0.19 | - | 72,72,72,72 | 0 |
| 54 | MG | BA | 3293 | 1/1 | 0.96 | 0.20 | - | 86,86,86,86 | 0 |
| 54 | MG | CA | 1676 | 1/1 | 0.91 | 0.36 | - | 82,82,82,82 | 0 |
| 54 | MG | BA | 3043 | 1/1 | 0.93 | 0.30 | - | 70,70,70,70 | 0 |
| 54 | MG | DA | 3144 | 1/1 | 0.96 | 0.16 | - | 72,72,72,72 | 0 |
| 54 | MG | AA | 1735 | 1/1 | 0.90 | 0.20 | - | 104,104,104,104 | 0 |
| 54 | MG | DA | 3142 | 1/1 | 0.80 | 0.18 | - | 109,109,109,109 | 0 |
| 54 | MG | DA | 3128 | 1/1 | 0.85 | 0.20 | - | 114,114,114,114 | 0 |
| 54 | MG | DA | 3284 | 1/1 | 0.05 | 0.33 | - | 134,134,134,134 | 0 |
| 54 | MG | AA | 1719 | 1/1 | 0.80 | 0.28 | - | 78,78,78,78 | 0 |
| 54 | MG | AA | 1620 | 1/1 | 0.98 | 0.23 | - | 56,56,56,56 | 0 |
| 54 | MG | BB | 201 | 1/1 | 0.90 | 0.35 | - | 56,56,56,56 | 0 |
| 54 | MG | AA | 1697 | 1/1 | 0.86 | 0.36 | - | 80,80,80,80 | 0 |
| 54 | MG | BA | 3197 | 1/1 | 0.86 | 0.37 | - | 57,57,57,57 | 0 |
| 54 | MG | DA | 3235 | 1/1 | 0.53 | 0.62 | - | 90,90,90,90 | 0 |
| 54 | MG | AA | 1756 | 1/1 | 0.92 | 0.20 | - | 106,106,106,106 | 0 |
| 54 | MG | BA | 3175 | 1/1 | 0.82 | 0.35 | - | 85,85,85,85 | 0 |
| 54 | MG | DA | 3263 | 1/1 | 0.78 | 0.35 | - | 63,63,63,63 | 0 |
| 54 | MG | BA | 3266 | 1/1 | 0.84 | 0.19 | - | 98,98,98,98 | 0 |
| 54 | MG | DA | 2938 | 1/1 | 0.74 | 0.27 | - | 66,66,66,66 | 0 |
| 54 | MG | CA | 1620 | 1/1 | 0.86 | 0.11 | - | 79,79,79,79 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | DA | 3273 | 1/1 | 0.93 | 0.29 | - | 85,85,85,85 | 0 |
| 54 | MG | DA | 3222 | 1/1 | 0.67 | 0.54 | - | 70,70,70,70 | 0 |
| 54 | MG | DA | 3139 | 1/1 | 0.93 | 0.28 | - | 60,60,60,60 | 0 |
| 54 | MG | AA | 1655 | 1/1 | 0.87 | 0.72 | - | 72,72,72,72 | 0 |
| 54 | MG | BA | 2958 | 1/1 | 0.90 | 0.32 | - | 42,42,42,42 | 0 |
| 54 | MG | DA | 3238 | 1/1 | 0.62 | 0.29 | - | 58,58,58,58 | 0 |
| 54 | MG | BA | 3168 | 1/1 | 0.87 | 0.20 | - | 76,76,76,76 | 0 |
| 54 | MG | AA | 1685 | 1/1 | 0.81 | 0.16 | - | 106,106,106,106 | 0 |
| 54 | MG | BA | 2966 | 1/1 | 0.88 | 0.09 | - | 75,75,75,75 | 0 |
| 54 | MG | BA | 2987 | 1/1 | 0.92 | 0.28 | - | 59,59,59,59 | 0 |
| 54 | MG | BA | 3264 | 1/1 | 0.98 | 0.14 | - | 116,116,116,116 | 0 |
| 54 | MG | DB | 210 | 1/1 | 0.95 | 0.06 | - | 74,74,74,74 | 0 |
| 54 | MG | BA | 2953 | 1/1 | 0.98 | 0.16 | - | 37,37,37,37 | 0 |
| 54 | MG | BA | 3304 | 1/1 | 0.98 | 0.06 | - | 124,124,124,124 | 0 |
| 54 | MG | DA | 3078 | 1/1 | 0.58 | 0.60 | - | 79,79,79,79 | 0 |
| 54 | MG | BB | 212 | 1/1 | 0.89 | 0.14 | - | 89,89,89,89 | 0 |
| 54 | MG | DA | 3106 | 1/1 | 0.95 | 0.37 | - | 67,67,67,67 | 0 |
| 54 | MG | DA | 3200 | 1/1 | 0.56 | 0.11 | - | 87,87,87,87 | 0 |
| 54 | MG | DB | 202 | 1/1 | 0.97 | 0.59 | - | 64,64,64,64 | 0 |
| 54 | MG | CA | 1645 | 1/1 | 0.87 | 0.64 | - | 72,72,72,72 | 0 |
| 54 | MG | BB | 213 | 1/1 | 0.82 | 0.65 | - | 84,84,84,84 | 0 |
| 54 | MG | DA | 3293 | 1/1 | 0.97 | 0.10 | - | 67,67,67,67 | 0 |
| 54 | MG | DA | 3199 | 1/1 | 0.72 | 0.71 | - | 38,38,38,38 | 0 |
| 54 | MG | AA | 1711 | 1/1 | 0.93 | 0.56 | - | 53,53,53,53 | 0 |
| 54 | MG | DA | 2985 | 1/1 | 0.96 | 0.38 | - | 48,48,48,48 | 0 |
| 54 | MG | DA | 3315 | 1/1 | 0.92 | 0.16 | - | 52,52,52,52 | 0 |
| 54 | MG | BA | 3267 | 1/1 | 0.78 | 0.47 | - | 86,86,86,86 | 0 |
| 54 | MG | AV | 6302 | 1/1 | 0.79 | 0.48 | - | 121,121,121,121 | 0 |
| 54 | MG | CA | 1681 | 1/1 | 0.88 | 0.42 | - | 81,81,81,81 | 0 |
| 54 | MG | DA | 3233 | 1/1 | 0.95 | 0.42 | - | 57,57,57,57 | 0 |
| 54 | MG | BA | 3248 | 1/1 | 0.85 | 0.16 | - | 77,77,77,77 | 0 |
| 54 | MG | BA | 3214 | 1/1 | 0.98 | 0.41 | - | 53,53,53,53 | 0 |
| 54 | MG | DB | 213 | 1/1 | 0.95 | 0.45 | - | 63,63,63,63 | 0 |
| 54 | MG | BA | 3131 | 1/1 | 0.90 | 0.26 | - | 67,67,67,67 | 0 |
| 54 | MG | BA | 3093 | 1/1 | 0.76 | 0.34 | - | 83,83,83,83 | 0 |
| 54 | MG | DA | 2970 | 1/1 | 0.80 | 0.19 | - | 67,67,67,67 | 0 |
| 54 | MG | AA | 1681 | 1/1 | 0.84 | 0.16 | - | 99,99,99,99 | 0 |
| 54 | MG | BA | 3018 | 1/1 | 0.92 | 0.31 | - | 68,68,68,68 | 0 |
| 54 | MG | DA | 3320 | 1/1 | 0.87 | 0.41 | - | 58,58,58,58 | 0 |
| 54 | MG | DA | 3085 | 1/1 | 0.77 | 0.13 | - | 89,89,89,89 | 0 |
| 54 | MG | BA | 3083 | 1/1 | 0.74 | 0.30 | - | 87,87,87,87 | 0 |
| 54 | MG | BA | 3143 | 1/1 | 0.81 | 0.51 | - | 84,84,84,84 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | DA | 3197 | 1/1 | 0.96 | 0.34 | - | 28,28,28,28 | 0 |
| 54 | MG | BA | 3233 | 1/1 | 0.97 | 0.23 | - | 52,52,52,52 | 0 |
| 54 | MG | BB | 211 | 1/1 | 0.86 | 0.49 | - | 112,112,112,112 | 0 |
| 54 | MG | BA | 3007 | 1/1 | 0.91 | 0.19 | - | 55,55,55,55 | 0 |
| 54 | MG | BA | 3290 | 1/1 | 0.93 | 0.27 | - | 42,42,42,42 | 0 |
| 54 | MG | CA | 1647 | 1/1 | 0.91 | 0.28 | - | 77,77,77,77 | 0 |
| 54 | MG | AA | 1718 | 1/1 | 0.64 | 0.63 | - | 98,98,98,98 | 0 |
| 54 | MG | BA | 3273 | 1/1 | 0.96 | 0.16 | - | 83,83,83,83 | 0 |
| 54 | MG | DA | 2998 | 1/1 | 0.92 | 0.39 | - | 68,68,68,68 | 0 |
| 54 | MG | DA | 3264 | 1/1 | 0.89 | 0.24 | - | 61,61,61,61 | 0 |
| 54 | MG | BA | 3301 | 1/1 | 0.85 | 0.65 | - | 66,66,66,66 | 0 |
| 54 | MG | AA | 1634 | 1/1 | 0.91 | 0.19 | - | 70,70,70,70 | 0 |
| 54 | MG | BA | 3166 | 1/1 | 0.90 | 0.40 | - | 74,74,74,74 | 0 |
| 54 | MG | DA | 3131 | 1/1 | 0.82 | 0.45 | - | 66,66,66,66 | 0 |
| 54 | MG | AA | 1700 | 1/1 | 0.73 | 0.56 | - | 98,98,98,98 | 0 |
| 54 | MG | CA | 1738 | 1/1 | 0.86 | 0.51 | - | 81,81,81,81 | 0 |
| 54 | MG | DA | 3071 | 1/1 | 0.81 | 0.38 | - | 64,64,64,64 | 0 |
| 54 | MG | BA | 3135 | 1/1 | 0.91 | 0.23 | - | 77,77,77,77 | 0 |
| 54 | MG | BA | 2993 | 1/1 | 0.92 | 0.24 | - | 58,58,58,58 | 0 |
| 54 | MG | AA | 1724 | 1/1 | 0.96 | 0.29 | - | 85,85,85,85 | 0 |
| 54 | MG | DA | 3255 | 1/1 | 0.98 | 0.15 | - | 101,101,101,101 | 0 |
| 54 | MG | DA | 2961 | 1/1 | 0.98 | 0.15 | - | 29,29,29,29 | 0 |
| 54 | MG | DA | 3224 | 1/1 | 0.90 | 0.17 | - | 72,72,72,72 | 0 |
| 54 | MG | BA | 2976 | 1/1 | 0.88 | 0.47 | - | 70,70,70,70 | 0 |
| 54 | MG | DA | 3231 | 1/1 | 0.82 | 0.70 | - | 60,60,60,60 | 0 |
| 54 | MG | BA | 3172 | 1/1 | 0.65 | 0.68 | - | 102,102,102,102 | 0 |
| 54 | MG | DA | 3153 | 1/1 | 0.93 | 0.28 | - | 85,85,85,85 | 0 |
| 54 | MG | CA | 1706 | 1/1 | 0.84 | 0.53 | - | 101,101,101,101 | 0 |
| 54 | MG | AA | 1748 | 1/1 | 0.89 | 0.15 | - | 96,96,96,96 | 0 |
| 54 | MG | BA | 3297 | 1/1 | 0.91 | 0.52 | - | 67,67,67,67 | 0 |
| 54 | MG | BA | 3049 | 1/1 | 0.88 | 0.14 | - | 86,86,86,86 | 0 |
| 54 | MG | BA | 3230 | 1/1 | 0.92 | 0.51 | - | 44,44,44,44 | 0 |
| 54 | MG | BA | 3288 | 1/1 | 0.87 | 0.62 | - | 62,62,62,62 | 0 |
| 54 | MG | BA | 3021 | 1/1 | 0.95 | 0.19 | - | 60,60,60,60 | 0 |
| 54 | MG | DA | 3217 | 1/1 | 0.97 | 0.12 | - | 56,56,56,56 | 0 |
| 54 | MG | BA | 3199 | 1/1 | 0.93 | 0.63 | - | 68,68,68,68 | 0 |
| 54 | MG | AA | 1661 | 1/1 | 0.72 | 0.41 | - | 65,65,65,65 | 0 |
| 54 | MG | DA | 3145 | 1/1 | 0.88 | 0.42 | - | 70,70,70,70 | 0 |
| 54 | MG | DA | 2946 | 1/1 | 0.94 | 0.55 | - | 24,24,24,24 | 0 |
| 54 | MG | DA | 3302 | 1/1 | 0.60 | 0.56 | - | 77,77,77,77 | 0 |
| 54 | MG | DA | 3060 | 1/1 | 0.91 | 0.21 | - | 87,87,87,87 | 0 |
| 54 | MG | AA | 1626 | 1/1 | 0.76 | 0.15 | - | 62,62,62,62 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | DA | 3301 | 1/1 | 0.90 | 0.30 | - | 80,80,80,80 | 0 |
| 54 | MG | BA | 3241 | 1/1 | 0.88 | 0.25 | - | 60,60,60,60 | 0 |
| 54 | MG | BB | 216 | 1/1 | 0.84 | 0.18 | - | 79,79,79,79 | 0 |
| 54 | MG | DA | 2992 | 1/1 | 0.89 | 0.18 | - | 46,46,46,46 | 0 |
| 54 | MG | CA | 1700 | 1/1 | 0.81 | 0.50 | - | 65,65,65,65 | 0 |
| 54 | MG | DA | 3249 | 1/1 | 0.67 | 0.36 | - | 56,56,56,56 | 0 |
| 54 | MG | BA | 2956 | 1/1 | 0.98 | 0.45 | - | 35,35,35,35 | 0 |
| 54 | MG | BA | 3229 | 1/1 | 0.80 | 0.28 | - | 62,62,62,62 | 0 |
| 54 | MG | DA | 3311 | 1/1 | 0.79 | 0.15 | - | 95,95,95,95 | 0 |
| 54 | MG | BA | 3057 | 1/1 | 0.94 | 0.43 | - | 63,63,63,63 | 0 |
| 54 | MG | CA | 1626 | 1/1 | 0.97 | 0.33 | - | 65,65,65,65 | 0 |
| 54 | MG | BA | 3028 | 1/1 | 0.94 | 0.46 | - | 62,62,62,62 | 0 |
| 54 | MG | BB | 217 | 1/1 | 0.83 | 0.15 | - | 78,78,78,78 | 0 |
| 54 | MG | BA | 3269 | 1/1 | 0.93 | 0.23 | - | 63,63,63,63 | 0 |
| 54 | MG | CA | 1702 | 1/1 | 0.91 | 0.70 | - | 68,68,68,68 | 0 |
| 54 | MG | DA | 3250 | 1/1 | 0.92 | 0.37 | - | 74,74,74,74 | 0 |
| 54 | MG | DA | 3048 | 1/1 | 0.98 | 0.09 | - | 66,66,66,66 | 0 |
| 54 | MG | AA | 1657 | 1/1 | 0.89 | 0.31 | - | 101,101,101,101 | 0 |
| 54 | MG | BA | 3205 | 1/1 | 0.93 | 0.23 | - | 38,38,38,38 | 0 |
| 54 | MG | DA | 3056 | 1/1 | 0.96 | 0.19 | - | 48,48,48,48 | 0 |
| 54 | MG | DA | 3029 | 1/1 | 0.82 | 0.23 | - | 70,70,70,70 | 0 |
| 54 | MG | AA | 1758 | 1/1 | 0.87 | 0.14 | - | 73,73,73,73 | 0 |
| 54 | MG | BA | 3206 | 1/1 | 0.94 | 0.10 | - | 60,60,60,60 | 0 |
| 54 | MG | CA | 1644 | 1/1 | 0.98 | 0.45 | - | 77,77,77,77 | 0 |
| 54 | MG | CA | 1633 | 1/1 | 0.88 | 0.48 | - | 102,102,102,102 | 0 |
| 54 | MG | CA | 1730 | 1/1 | 0.95 | 0.08 | - | 122,122,122,122 | 0 |
| 54 | MG | DA | 3331 | 1/1 | 0.97 | 0.19 | - | 52,52,52,52 | 0 |
| 54 | MG | CA | 1614 | 1/1 | 0.75 | 0.33 | - | 89,89,89,89 | 0 |
| 54 | MG | DA | 3209 | 1/1 | 0.52 | 0.58 | - | 80,80,80,80 | 0 |
| 54 | MG | BA | 3189 | 1/1 | 0.65 | 0.44 | - | 88,88,88,88 | 0 |
| 54 | MG | DA | 3236 | 1/1 | 0.96 | 0.59 | - | 63,63,63,63 | 0 |
| 54 | MG | DA | 3084 | 1/1 | 0.93 | 0.11 | - | 146,146,146,146 | 0 |
| 54 | MG | BB | 202 | 1/1 | 0.97 | 0.24 | - | 75,75,75,75 | 0 |
| 54 | MG | DA | 3316 | 1/1 | 0.72 | 0.24 | - | 97,97,97,97 | 0 |
| 54 | MG | CA | 1670 | 1/1 | 0.96 | 0.47 | - | 128,128,128,128 | 0 |
| 54 | MG | CA | 1680 | 1/1 | 0.92 | 0.32 | - | 58,58,58,58 | 0 |
| 54 | MG | DA | 3146 | 1/1 | 0.91 | 0.13 | - | 95,95,95,95 | 0 |
| 54 | MG | BA | 3036 | 1/1 | 0.73 | 0.24 | - | 92,92,92,92 | 0 |
| 54 | MG | BA | 3201 | 1/1 | 0.86 | 0.20 | - | 80,80,80,80 | 0 |
| 54 | MG | CA | 1655 | 1/1 | 0.94 | 0.22 | - | 80,80,80,80 | 0 |
| 54 | MG | BA | 3296 | 1/1 | 0.98 | 0.16 | - | 47,47,47,47 | 0 |
| 54 | MG | BA | 3236 | 1/1 | 0.51 | 0.31 | - | 119,119,119,119 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | BA | 2964 | 1/1 | 0.90 | 0.47 | - | 30,30,30,30 | 0 |
| 54 | MG | DA | 3040 | 1/1 | 0.92 | 0.36 | - | 41,41,41,41 | 0 |
| 54 | MG | BA | 3219 | 1/1 | 0.69 | 0.80 | - | 66,66,66,66 | 0 |
| 54 | MG | CA | 1696 | 1/1 | 0.60 | 0.18 | - | 133,133,133,133 | 0 |
| 54 | MG | AA | 1703 | 1/1 | 0.94 | 0.15 | - | 83,83,83,83 | 0 |
| 54 | MG | AA | 1759 | 1/1 | 0.95 | 0.13 | - | 81,81,81,81 | 0 |
| 54 | MG | BA | 3144 | 1/1 | 0.90 | 0.34 | - | 75,75,75,75 | 0 |
| 54 | MG | AA | 1611 | 1/1 | 0.96 | 0.27 | - | 49,49,49,49 | 0 |
| 54 | MG | DA | 3134 | 1/1 | 0.77 | 0.16 | - | 71,71,71,71 | 0 |
| 54 | MG | BA | 3070 | 1/1 | 0.96 | 0.24 | - | 75,75,75,75 | 0 |
| 54 | MG | AA | 1644 | 1/1 | 0.85 | 0.27 | - | 53,53,53,53 | 0 |
| 54 | MG | BA | 3126 | 1/1 | 0.90 | 0.15 | - | 54,54,54,54 | 0 |
| 54 | MG | DA | 3180 | 1/1 | 0.90 | 0.26 | - | 77,77,77,77 | 0 |
| 54 | MG | BA | 3262 | 1/1 | 0.83 | 0.39 | - | 60,60,60,60 | 0 |
| 54 | MG | AA | 1704 | 1/1 | 0.84 | 0.20 | - | 81,81,81,81 | 0 |
| 54 | MG | DA | 3015 | 1/1 | 0.96 | 0.22 | - | 74,74,74,74 | 0 |
| 54 | MG | CA | 1684 | 1/1 | 0.80 | 0.14 | - | 117,117,117,117 | 0 |
| 54 | MG | DA | 3161 | 1/1 | 0.82 | 0.29 | - | 74,74,74,74 | 0 |
| 54 | MG | DA | 3074 | 1/1 | 0.81 | 0.31 | - | 64,64,64,64 | 0 |
| 54 | MG | BA | 3170 | 1/1 | 0.95 | 0.12 | - | 64,64,64,64 | 0 |
| 54 | MG | DA | 3148 | 1/1 | 0.91 | 0.23 | - | 99,99,99,99 | 0 |
| 54 | MG | BA | 2950 | 1/1 | 0.98 | 0.18 | - | 32,32,32,32 | 0 |
| 54 | MG | BA | 3124 | 1/1 | 0.89 | 0.30 | - | 89,89,89,89 | 0 |
| 54 | MG | AA | 1640 | 1/1 | 0.77 | 0.44 | - | 106,106,106,106 | 0 |
| 54 | MG | DA | 3046 | 1/1 | 0.91 | 0.09 | - | 76,76,76,76 | 0 |
| 54 | MG | CP | 101 | 1/1 | 0.78 | 0.17 | - | 96,96,96,96 | 0 |
| 54 | MG | CA | 1662 | 1/1 | 0.87 | 0.76 | - | 86,86,86,86 | 0 |
| 54 | MG | AA | 1751 | 1/1 | 0.90 | 0.18 | - | 72,72,72,72 | 0 |
| 54 | MG | DA | 3254 | 1/1 | 0.92 | 0.52 | - | 79,79,79,79 | 0 |
| 54 | MG | DA | 3156 | 1/1 | 0.98 | 0.18 | - | 78,78,78,78 | 0 |
| 54 | MG | DA | 3124 | 1/1 | 0.92 | 0.09 | - | 90,90,90,90 | 0 |
| 54 | MG | CA | 1699 | 1/1 | 0.85 | 0.72 | - | 71,71,71,71 | 0 |
| 54 | MG | DB | 205 | 1/1 | 0.92 | 0.10 | - | 79,79,79,79 | 0 |
| 54 | MG | BA | 3054 | 1/1 | 0.85 | 0.18 | - | 46,46,46,46 | 0 |
| 54 | MG | AA | 1753 | 1/1 | 0.80 | 0.34 | - | 102,102,102,102 | 0 |
| 54 | MG | AA | 1677 | 1/1 | 0.85 | 0.44 | - | 64,64,64,64 | 0 |
| 54 | MG | AA | 1649 | 1/1 | 0.80 | 0.37 | - | 89,89,89,89 | 0 |
| 54 | MG | BA | 3291 | 1/1 | 0.79 | 0.28 | - | 68,68,68,68 | 0 |
| 54 | MG | BB | 208 | 1/1 | 0.88 | 0.47 | - | 109,109,109,109 | 0 |
| 54 | MG | BA | 3213 | 1/1 | 0.61 | 0.25 | - | 101,101,101,101 | 0 |
| 54 | MG | DA | 3030 | 1/1 | 0.67 | 0.41 | - | 71,71,71,71 | 0 |
| 54 | MG | BA | 2965 | 1/1 | 0.99 | 0.27 | - | 47,47,47,47 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | DB | 211 | 1/1 | 0.94 | 0.15 | - | 109,109,109,109 | 0 |
| 54 | MG | BA | 3077 | 1/1 | 0.97 | 0.09 | - | 75,75,75,75 | 0 |
| 54 | MG | BA | 3287 | 1/1 | 0.78 | 0.44 | - | 74,74,74,74 | 0 |
| 54 | MG | AA | 1629 | 1/1 | 0.88 | 0.36 | - | 72,72,72,72 | 0 |
| 54 | MG | AA | 1669 | 1/1 | 0.64 | 0.33 | - | 110,110,110,110 | 0 |
| 54 | MG | DA | 3052 | 1/1 | 0.93 | 0.16 | - | 107,107,107,107 | 0 |
| 54 | MG | BA | 3271 | 1/1 | 0.52 | 0.17 | - | 91,91,91,91 | 0 |
| 54 | MG | BA | 3113 | 1/1 | 0.87 | 0.29 | - | 71,71,71,71 | 0 |
| 54 | MG | BA | 3087 | 1/1 | 0.96 | 0.10 | - | 69,69,69,69 | 0 |
| 54 | MG | BA | 3110 | 1/1 | 0.75 | 0.14 | - | 86,86,86,86 | 0 |
| 54 | MG | CA | 1735 | 1/1 | 0.84 | 0.27 | - | 61,61,61,61 | 0 |
| 54 | MG | DA | 3176 | 1/1 | 0.94 | 0.24 | - | 83,83,83,83 | 0 |
| 54 | MG | BA | 2972 | 1/1 | 0.95 | 0.35 | - | 49,49,49,49 | 0 |
| 54 | MG | BA | 3061 | 1/1 | 0.79 | 0.21 | - | 91,91,91,91 | 0 |
| 54 | MG | CA | 1630 | 1/1 | 0.95 | 0.33 | - | 70,70,70,70 | 0 |
| 54 | MG | BA | 3157 | 1/1 | 0.78 | 0.29 | - | 68,68,68,68 | 0 |
| 54 | MG | BA | 3014 | 1/1 | 0.90 | 0.20 | - | 47,47,47,47 | 0 |
| 54 | MG | AA | 1720 | 1/1 | 0.78 | 0.23 | - | 69,69,69,69 | 0 |
| 54 | MG | DA | 2949 | 1/1 | 0.97 | 0.54 | - | 41,41,41,41 | 0 |
| 54 | MG | DA | 3292 | 1/1 | 0.96 | 0.47 | - | 33,33,33,33 | 0 |
| 54 | MG | CA | 1605 | 1/1 | 0.96 | 0.21 | - | 56,56,56,56 | 0 |
| 54 | MG | BA | 2929 | 1/1 | 0.98 | 0.45 | - | 37,37,37,37 | 0 |
| 54 | MG | DA | 3282 | 1/1 | 0.88 | 0.14 | - | 96,96,96,96 | 0 |
| 54 | MG | DA | 2913 | 1/1 | 0.92 | 0.41 | - | 17,17,17,17 | 0 |
| 54 | MG | BA | 3278 | 1/1 | 0.69 | 0.29 | - | 115,115,115,115 | 0 |
| 54 | MG | DA | 3168 | 1/1 | 0.64 | 0.46 | - | 94,94,94,94 | 0 |
| 54 | MG | CA | 1634 | 1/1 | 0.87 | 0.26 | - | 60,60,60,60 | 0 |
| 54 | MG | AA | 1702 | 1/1 | 0.56 | 1.09 | - | 94,94,94,94 | 0 |
| 54 | MG | AA | 1743 | 1/1 | 0.98 | 0.47 | - | 83,83,83,83 | 0 |
| 54 | MG | BA | 2902 | 1/1 | 0.99 | 0.46 | - | 16,16,16,16 | 0 |
| 54 | MG | BA | 3058 | 1/1 | 0.94 | 0.12 | - | 114,114,114,114 | 0 |
| 54 | MG | BA | 3276 | 1/1 | 0.93 | 0.21 | - | 65,65,65,65 | 0 |
| 54 | MG | DA | 2928 | 1/1 | 0.95 | 0.22 | - | 43,43,43,43 | 0 |
| 54 | MG | CA | 1622 | 1/1 | 0.93 | 0.23 | - | 79,79,79,79 | 0 |
| 54 | MG | DA | 2926 | 1/1 | 0.97 | 0.23 | - | 43,43,43,43 | 0 |
| 54 | MG | DA | 3013 | 1/1 | 0.84 | 0.26 | - | 44,44,44,44 | 0 |
| 54 | MG | BA | 3041 | 1/1 | 0.87 | 0.23 | - | 67,67,67,67 | 0 |
| 54 | MG | DA | 3323 | 1/1 | 0.50 | 0.34 | - | 69,69,69,69 | 0 |
| 54 | MG | DA | 3050 | 1/1 | 0.71 | 0.09 | - | 105,105,105,105 | 0 |
| 54 | MG | DA | 2983 | 1/1 | 0.54 | 0.27 | - | 70,70,70,70 | 0 |
| 54 | MG | BA | 3001 | 1/1 | 0.90 | 0.30 | - | 59,59,59,59 | 0 |
| 54 | MG | CA | 1625 | 1/1 | 0.92 | 0.10 | - | 94,94,94,94 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|-------|------|------|-----------------------------|-------|
| 54 | MG | AA | 1676 | 1/1 | 0.84 | 0.15 | - | 63,63,63,63 | 0 |
| 54 | MG | DA | 3043 | 1/1 | 0.61 | 0.69 | - | 70,70,70,70 | 0 |
| 54 | MG | DA | 3151 | 1/1 | 0.95 | 0.37 | - | 82,82,82,82 | 0 |
| 54 | MG | DA | 2942 | 1/1 | 0.93 | 0.29 | - | 39,39,39,39 | 0 |
| 54 | MG | CA | 1688 | 1/1 | 0.53 | 0.35 | - | 99,99,99,99 | 0 |
| 54 | MG | DA | 3129 | 1/1 | 0.92 | 0.43 | - | 63,63,63,63 | 0 |
| 54 | MG | DA | 3260 | 1/1 | 0.87 | 0.50 | - | 102,102,102,102 | 0 |
| 54 | MG | CA | 1651 | 1/1 | 0.94 | 0.09 | - | 99,99,99,99 | 0 |
| 54 | MG | BA | 3237 | 1/1 | 0.94 | 0.14 | - | 60,60,60,60 | 0 |
| 54 | MG | BA | 3103 | 1/1 | 0.73 | 0.30 | - | 88,88,88,88 | 0 |
| 54 | MG | AA | 1613 | 1/1 | 0.96 | 0.15 | - | 47,47,47,47 | 0 |
| 54 | MG | DA | 3289 | 1/1 | 0.81 | 0.53 | - | 92,92,92,92 | 0 |
| 54 | MG | BA | 3169 | 1/1 | 0.87 | 0.51 | - | 75,75,75,75 | 0 |
| 54 | MG | DA | 3009 | 1/1 | 0.88 | 0.48 | - | 49,49,49,49 | 0 |
| 54 | MG | BA | 2971 | 1/1 | 0.84 | 0.34 | - | 65,65,65,65 | 0 |
| 54 | MG | BA | 3078 | 1/1 | 0.80 | 0.10 | - | 83,83,83,83 | 0 |
| 54 | MG | AA | 1667 | 1/1 | 0.83 | 0.51 | - | 61,61,61,61 | 0 |
| 54 | MG | DA | 3299 | 1/1 | 0.80 | 0.34 | - | 68,68,68,68 | 0 |
| 54 | MG | BA | 3100 | 1/1 | 0.85 | 0.07 | - | 77,77,77,77 | 0 |
| 54 | MG | DA | 3248 | 1/1 | 0.92 | 0.30 | - | 75,75,75,75 | 0 |
| 54 | MG | DA | 3054 | 1/1 | 0.94 | 0.32 | - | 75,75,75,75 | 0 |
| 54 | MG | BA | 3127 | 1/1 | 0.88 | 0.76 | - | 56,56,56,56 | 0 |
| 54 | MG | CA | 1623 | 1/1 | 0.92 | 0.48 | - | 99,99,99,99 | 0 |
| 54 | MG | AA | 1627 | 1/1 | 0.94 | 0.12 | - | 85,85,85,85 | 0 |
| 54 | MG | BA | 3053 | 1/1 | 0.97 | 0.20 | - | 67,67,67,67 | 0 |
| 54 | MG | CA | 1663 | 1/1 | 0.74 | 0.28 | - | 86,86,86,86 | 0 |
| 54 | MG | CA | 1671 | 1/1 | 0.81 | 0.24 | - | 74,74,74,74 | 0 |
| 54 | MG | CA | 1635 | 1/1 | 0.94 | 0.23 | - | 67,67,67,67 | 0 |
| 54 | MG | CA | 1658 | 1/1 | 0.79 | 0.42 | - | 110,110,110,110 | 0 |
| 54 | MG | BA | 3253 | 1/1 | 0.78 | 0.35 | - | 76,76,76,76 | 0 |
| 54 | MG | DA | 3230 | 1/1 | 0.84 | 0.21 | - | 63,63,63,63 | 0 |
| 54 | MG | DA | 3132 | 1/1 | 0.90 | 0.07 | - | 70,70,70,70 | 0 |
| 54 | MG | DA | 3076 | 1/1 | 0.90 | 0.16 | - | 63,63,63,63 | 0 |
| 54 | MG | BA | 3235 | 1/1 | 0.94 | 0.13 | - | 62,62,62,62 | 0 |
| 54 | MG | BA | 3174 | 1/1 | 0.98 | 0.20 | - | 84,84,84,84 | 0 |
| 54 | MG | DA | 3322 | 1/1 | -0.12 | 0.38 | - | 95,95,95,95 | 0 |
| 54 | MG | BA | 3259 | 1/1 | 0.71 | 0.38 | - | 75,75,75,75 | 0 |
| 54 | MG | DA | 3185 | 1/1 | 0.74 | 0.32 | - | 108,108,108,108 | 0 |
| 54 | MG | AA | 1763 | 1/1 | 0.76 | 0.13 | - | 96,96,96,96 | 0 |
| 54 | MG | DB | 216 | 1/1 | 0.72 | 0.36 | - | 88,88,88,88 | 0 |
| 54 | MG | BA | 3063 | 1/1 | 0.93 | 0.23 | - | 56,56,56,56 | 0 |
| 54 | MG | DA | 3314 | 1/1 | 0.93 | 0.54 | - | 102,102,102,102 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | DA | 3183 | 1/1 | 0.98 | 0.09 | - | 83,83,83,83 | 0 |
| 54 | MG | BA | 2945 | 1/1 | 0.98 | 0.22 | - | 72,72,72,72 | 0 |
| 54 | MG | BA | 3039 | 1/1 | 0.87 | 0.19 | - | 94,94,94,94 | 0 |
| 54 | MG | CA | 1685 | 1/1 | 0.72 | 0.60 | - | 106,106,106,106 | 0 |
| 54 | MG | BA | 3244 | 1/1 | 0.94 | 0.78 | - | 47,47,47,47 | 0 |
| 54 | MG | AA | 1684 | 1/1 | 0.88 | 0.38 | - | 95,95,95,95 | 0 |
| 54 | MG | DA | 3011 | 1/1 | 0.91 | 0.14 | - | 99,99,99,99 | 0 |
| 54 | MG | BA | 3173 | 1/1 | 0.87 | 0.51 | - | 80,80,80,80 | 0 |
| 54 | MG | CA | 1728 | 1/1 | 0.88 | 0.54 | - | 82,82,82,82 | 0 |
| 54 | MG | DA | 3096 | 1/1 | 0.97 | 0.37 | - | 40,40,40,40 | 0 |
| 54 | MG | DA | 2930 | 1/1 | 0.98 | 0.15 | - | 36,36,36,36 | 0 |
| 54 | MG | AA | 1674 | 1/1 | 0.85 | 0.49 | - | 79,79,79,79 | 0 |
| 54 | MG | DA | 3268 | 1/1 | 0.83 | 0.42 | - | 81,81,81,81 | 0 |
| 54 | MG | BA | 3089 | 1/1 | 0.95 | 0.29 | - | 59,59,59,59 | 0 |
| 54 | MG | AA | 1663 | 1/1 | 0.88 | 0.12 | - | 70,70,70,70 | 0 |
| 54 | MG | DA | 3001 | 1/1 | 0.94 | 0.12 | - | 56,56,56,56 | 0 |
| 54 | MG | BA | 3308 | 1/1 | 0.75 | 0.48 | - | 94,94,94,94 | 0 |
| 54 | MG | DA | 3055 | 1/1 | 0.09 | 0.85 | - | 93,93,93,93 | 0 |
| 54 | MG | DA | 2935 | 1/1 | 0.93 | 0.61 | - | 30,30,30,30 | 0 |
| 54 | MG | AA | 1690 | 1/1 | 0.88 | 0.09 | - | 117,117,117,117 | 0 |
| 54 | MG | AA | 1708 | 1/1 | 0.95 | 0.15 | - | 101,101,101,101 | 0 |
| 54 | MG | B2 | 101 | 1/1 | 0.86 | 0.54 | - | 64,64,64,64 | 0 |
| 54 | MG | DA | 3179 | 1/1 | 0.93 | 0.19 | - | 68,68,68,68 | 0 |
| 54 | MG | AA | 1664 | 1/1 | 0.84 | 0.61 | - | 103,103,103,103 | 0 |
| 54 | MG | CA | 1723 | 1/1 | 0.83 | 0.24 | - | 141,141,141,141 | 0 |
| 54 | MG | BA | 3282 | 1/1 | 0.85 | 0.37 | - | 62,62,62,62 | 0 |
| 54 | MG | BA | 3231 | 1/1 | 0.96 | 0.16 | - | 22,22,22,22 | 0 |
| 54 | MG | BA | 3306 | 1/1 | 0.77 | 0.38 | - | 74,74,74,74 | 0 |
| 54 | MG | BA | 3040 | 1/1 | 0.94 | 0.26 | - | 58,58,58,58 | 0 |
| 54 | MG | BA | 3245 | 1/1 | 0.98 | 0.29 | - | 54,54,54,54 | 0 |
| 54 | MG | BA | 3085 | 1/1 | 0.90 | 0.28 | - | 68,68,68,68 | 0 |
| 54 | MG | CA | 1643 | 1/1 | 0.95 | 0.13 | - | 58,58,58,58 | 0 |
| 54 | MG | DA | 3150 | 1/1 | 0.95 | 0.21 | - | 62,62,62,62 | 0 |
| 54 | MG | DA | 3294 | 1/1 | 0.87 | 0.28 | - | 61,61,61,61 | 0 |
| 54 | MG | DA | 2945 | 1/1 | 0.88 | 0.61 | - | 41,41,41,41 | 0 |
| 54 | MG | AA | 1609 | 1/1 | 0.92 | 0.63 | - | 70,70,70,70 | 0 |
| 54 | MG | BA | 3216 | 1/1 | 0.97 | 0.19 | - | 65,65,65,65 | 0 |
| 54 | MG | BA | 3218 | 1/1 | 0.75 | 0.67 | - | 75,75,75,75 | 0 |
| 54 | MG | DA | 3171 | 1/1 | 0.93 | 0.27 | - | 61,61,61,61 | 0 |
| 54 | MG | CA | 1695 | 1/1 | 0.97 | 0.37 | - | 80,80,80,80 | 0 |
| 54 | MG | CA | 1683 | 1/1 | 0.72 | 0.31 | - | 91,91,91,91 | 0 |
| 54 | MG | CA | 1613 | 1/1 | 0.95 | 0.24 | - | 87,87,87,87 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | BA | 3299 | 1/1 | 0.77 | 0.28 | - | 80,80,80,80 | 0 |
| 54 | MG | AA | 1639 | 1/1 | 0.86 | 0.35 | - | 79,79,79,79 | 0 |
| 54 | MG | CA | 1632 | 1/1 | 0.77 | 0.27 | - | 79,79,79,79 | 0 |
| 54 | MG | AA | 1643 | 1/1 | 0.86 | 0.33 | - | 70,70,70,70 | 0 |
| 54 | MG | CA | 1606 | 1/1 | 0.97 | 0.12 | - | 68,68,68,68 | 0 |
| 54 | MG | BA | 3080 | 1/1 | 0.89 | 0.14 | - | 73,73,73,73 | 0 |
| 54 | MG | DA | 2947 | 1/1 | 0.96 | 0.24 | - | 40,40,40,40 | 0 |
| 54 | MG | BA | 3139 | 1/1 | 0.75 | 0.31 | - | 78,78,78,78 | 0 |
| 54 | MG | DA | 3051 | 1/1 | 0.94 | 0.15 | - | 89,89,89,89 | 0 |
| 54 | MG | DA | 3041 | 1/1 | 0.88 | 0.17 | - | 51,51,51,51 | 0 |
| 54 | MG | BA | 3193 | 1/1 | 0.93 | 0.38 | - | 53,53,53,53 | 0 |
| 54 | MG | BA | 3191 | 1/1 | 0.72 | 0.37 | - | 76,76,76,76 | 0 |
| 54 | MG | CV | 6301 | 1/1 | 0.65 | 0.22 | - | 98,98,98,98 | 0 |
| 54 | MG | AA | 1738 | 1/1 | 0.83 | 0.28 | - | 70,70,70,70 | 0 |
| 54 | MG | DA | 2931 | 1/1 | 0.99 | 0.25 | - | 23,23,23,23 | 0 |
| 54 | MG | BA | 3163 | 1/1 | 0.54 | 0.49 | - | 72,72,72,72 | 0 |
| 54 | MG | DA | 3005 | 1/1 | 0.91 | 0.32 | - | 33,33,33,33 | 0 |
| 54 | MG | BA | 3203 | 1/1 | 0.98 | 0.19 | - | 41,41,41,41 | 0 |
| 54 | MG | AA | 1605 | 1/1 | 0.88 | 0.57 | - | 42,42,42,42 | 0 |
| 54 | MG | BA | 3003 | 1/1 | 0.93 | 0.28 | - | 48,48,48,48 | 0 |
| 54 | MG | AA | 1658 | 1/1 | 0.86 | 0.09 | - | 94,94,94,94 | 0 |
| 54 | MG | DA | 3059 | 1/1 | 0.83 | 0.21 | - | 67,67,67,67 | 0 |
| 54 | MG | DA | 3286 | 1/1 | 0.88 | 0.34 | - | 98,98,98,98 | 0 |
| 54 | MG | DA | 3112 | 1/1 | 0.91 | 0.20 | - | 60,60,60,60 | 0 |
| 54 | MG | BA | 3081 | 1/1 | 0.93 | 0.14 | - | 65,65,65,65 | 0 |
| 54 | MG | CA | 1619 | 1/1 | 0.97 | 0.34 | - | 61,61,61,61 | 0 |
| 54 | MG | CA | 1734 | 1/1 | 0.98 | 0.15 | - | 117,117,117,117 | 0 |
| 54 | MG | BA | 2957 | 1/1 | 0.95 | 0.57 | - | 35,35,35,35 | 0 |
| 54 | MG | AA | 1671 | 1/1 | 0.96 | 0.14 | - | 114,114,114,114 | 0 |
| 54 | MG | DA | 3290 | 1/1 | 0.58 | 0.17 | - | 85,85,85,85 | 0 |
| 54 | MG | DA | 3212 | 1/1 | 0.83 | 0.49 | - | 78,78,78,78 | 0 |
| 54 | MG | CA | 1646 | 1/1 | 0.87 | 0.15 | - | 78,78,78,78 | 0 |
| 54 | MG | BB | 204 | 1/1 | 0.98 | 0.12 | - | 87,87,87,87 | 0 |
| 54 | MG | DA | 2912 | 1/1 | 0.98 | 0.45 | - | 18,18,18,18 | 0 |
| 54 | MG | CA | 1731 | 1/1 | 0.88 | 0.13 | - | 90,90,90,90 | 0 |
| 54 | MG | DA | 3211 | 1/1 | 0.96 | 0.18 | - | 38,38,38,38 | 0 |
| 54 | MG | DA | 3088 | 1/1 | 0.83 | 0.10 | - | 70,70,70,70 | 0 |
| 54 | MG | AA | 1749 | 1/1 | 0.90 | 0.25 | - | 90,90,90,90 | 0 |
| 54 | MG | DA | 3275 | 1/1 | 0.93 | 0.17 | - | 78,78,78,78 | 0 |
| 54 | MG | DA | 3136 | 1/1 | 0.79 | 0.37 | - | 68,68,68,68 | 0 |
| 54 | MG | BA | 3111 | 1/1 | 0.87 | 0.54 | - | 46,46,46,46 | 0 |
| 54 | MG | AA | 1698 | 1/1 | 0.64 | 0.47 | - | 88,88,88,88 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | AV | 6301 | 1/1 | 0.85 | 0.10 | - | 72,72,72,72 | 0 |
| 54 | MG | BA | 3238 | 1/1 | 0.90 | 0.14 | - | 91,91,91,91 | 0 |
| 54 | MG | BA | 3161 | 1/1 | 0.97 | 0.26 | - | 62,62,62,62 | 0 |
| 54 | MG | DA | 2903 | 1/1 | 0.98 | 0.33 | - | 7,7,7,7 | 0 |
| 54 | MG | BA | 3260 | 1/1 | 0.97 | 0.13 | - | 62,62,62,62 | 0 |
| 54 | MG | DA | 3247 | 1/1 | 0.93 | 0.21 | - | 40,40,40,40 | 0 |
| 54 | MG | DA | 2923 | 1/1 | 0.98 | 0.23 | - | 17,17,17,17 | 0 |
| 54 | MG | CA | 1659 | 1/1 | 0.98 | 0.38 | - | 71,71,71,71 | 0 |
| 54 | MG | BA | 3095 | 1/1 | 0.77 | 0.14 | - | 83,83,83,83 | 0 |
| 54 | MG | DA | 3157 | 1/1 | 0.91 | 0.14 | - | 71,71,71,71 | 0 |
| 54 | MG | AA | 1717 | 1/1 | 0.86 | 0.35 | - | 81,81,81,81 | 0 |
| 54 | MG | DA | 3075 | 1/1 | 0.98 | 0.23 | - | 64,64,64,64 | 0 |
| 54 | MG | BA | 3012 | 1/1 | 0.86 | 0.16 | - | 91,91,91,91 | 0 |
| 54 | MG | AA | 1726 | 1/1 | 0.93 | 0.08 | - | 108,108,108,108 | 0 |
| 54 | MG | DA | 3014 | 1/1 | 0.60 | 0.40 | - | 69,69,69,69 | 0 |
| 54 | MG | BA | 3155 | 1/1 | 0.79 | 0.38 | - | 85,85,85,85 | 0 |
| 54 | MG | BA | 3034 | 1/1 | 0.84 | 0.87 | - | 102,102,102,102 | 0 |
| 54 | MG | DA | 2996 | 1/1 | 0.95 | 0.40 | - | 43,43,43,43 | 0 |
| 54 | MG | BA | 3289 | 1/1 | 0.88 | 0.25 | - | 65,65,65,65 | 0 |
| 54 | MG | CA | 1732 | 1/1 | 0.93 | 0.23 | - | 73,73,73,73 | 0 |
| 54 | MG | DA | 3245 | 1/1 | 0.91 | 0.55 | - | 54,54,54,54 | 0 |
| 54 | MG | BA | 3129 | 1/1 | 0.89 | 0.13 | - | 75,75,75,75 | 0 |
| 54 | MG | BA | 3294 | 1/1 | 0.92 | 0.17 | - | 64,64,64,64 | 0 |
| 54 | MG | DA | 3155 | 1/1 | 0.90 | 0.07 | - | 124,124,124,124 | 0 |
| 54 | MG | DA | 3278 | 1/1 | 0.49 | 0.34 | - | 75,75,75,75 | 0 |
| 54 | MG | DA | 3089 | 1/1 | 0.88 | 0.26 | - | 76,76,76,76 | 0 |
| 54 | MG | BA | 3024 | 1/1 | 0.96 | 0.53 | - | 67,67,67,67 | 0 |
| 54 | MG | DB | 206 | 1/1 | 0.78 | 0.29 | - | 99,99,99,99 | 0 |
| 54 | MG | DA | 3318 | 1/1 | 0.74 | 0.36 | - | 101,101,101,101 | 0 |
| 54 | MG | DA | 3288 | 1/1 | 0.87 | 0.43 | - | 78,78,78,78 | 0 |
| 54 | MG | CA | 1716 | 1/1 | 0.95 | 0.22 | - | 77,77,77,77 | 0 |
| 54 | MG | DA | 3303 | 1/1 | 0.89 | 0.15 | - | 66,66,66,66 | 0 |
| 54 | MG | DA | 3038 | 1/1 | 0.89 | 0.26 | - | 71,71,71,71 | 0 |
| 54 | MG | BA | 3013 | 1/1 | 0.73 | 0.10 | - | 90,90,90,90 | 0 |
| 54 | MG | DA | 3297 | 1/1 | 0.83 | 0.38 | - | 49,49,49,49 | 0 |
| 54 | MG | BA | 3136 | 1/1 | 0.72 | 0.22 | - | 87,87,87,87 | 0 |
| 54 | MG | CA | 1637 | 1/1 | 0.72 | 0.17 | - | 112,112,112,112 | 0 |
| 54 | MG | BA | 3098 | 1/1 | 0.84 | 0.19 | - | 78,78,78,78 | 0 |
| 54 | MG | BA | 2905 | 1/1 | 0.94 | 0.54 | - | 12,12,12,12 | 0 |
| 54 | MG | AA | 1617 | 1/1 | 0.98 | 0.19 | - | 77,77,77,77 | 0 |
| 54 | MG | BA | 2928 | 1/1 | 0.97 | 0.36 | - | 42,42,42,42 | 0 |
| 54 | MG | AA | 1625 | 1/1 | 0.88 | 1.01 | - | 88,88,88,88 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | DA | 3172 | 1/1 | 0.85 | 0.35 | - | 81,81,81,81 | 0 |
| 54 | MG | BA | 2947 | 1/1 | 0.98 | 0.30 | - | 14,14,14,14 | 0 |
| 54 | MG | AA | 1744 | 1/1 | 0.96 | 0.25 | - | 82,82,82,82 | 0 |
| 54 | MG | CA | 1677 | 1/1 | 0.92 | 0.28 | - | 85,85,85,85 | 0 |
| 54 | MG | BA | 2959 | 1/1 | 0.97 | 0.39 | - | 55,55,55,55 | 0 |
| 54 | MG | CA | 1711 | 1/1 | 0.78 | 0.36 | - | 87,87,87,87 | 0 |
| 54 | MG | DA | 3325 | 1/1 | 0.55 | 0.71 | - | 92,92,92,92 | 0 |
| 54 | MG | DA | 3133 | 1/1 | 0.91 | 0.13 | - | 89,89,89,89 | 0 |
| 54 | MG | BA | 3183 | 1/1 | 0.96 | 0.37 | - | 27,27,27,27 | 0 |
| 54 | MG | BA | 3281 | 1/1 | 0.76 | 0.33 | - | 84,84,84,84 | 0 |
| 54 | MG | BA | 3104 | 1/1 | 0.85 | 0.34 | - | 63,63,63,63 | 0 |
| 54 | MG | BA | 2906 | 1/1 | 1.00 | 0.22 | - | 5,5,5,5 | 0 |
| 54 | MG | DA | 3178 | 1/1 | 0.84 | 0.27 | - | 83,83,83,83 | 0 |
| 54 | MG | DA | 3147 | 1/1 | 0.92 | 0.14 | - | 78,78,78,78 | 0 |
| 54 | MG | DA | 3077 | 1/1 | 0.87 | 0.61 | - | 67,67,67,67 | 0 |
| 54 | MG | AA | 1653 | 1/1 | 0.84 | 0.32 | - | 89,89,89,89 | 0 |
| 54 | MG | AA | 1710 | 1/1 | 0.97 | 0.26 | - | 65,65,65,65 | 0 |
| 54 | MG | DA | 3182 | 1/1 | 0.95 | 0.59 | - | 86,86,86,86 | 0 |
| 54 | MG | DB | 215 | 1/1 | 0.48 | 0.44 | - | 103,103,103,103 | 0 |
| 54 | MG | BA | 2934 | 1/1 | 0.98 | 0.44 | - | 28,28,28,28 | 0 |
| 54 | MG | BA | 3082 | 1/1 | 0.92 | 0.18 | - | 61,61,61,61 | 0 |
| 54 | MG | BA | 3265 | 1/1 | 0.87 | 0.33 | - | 80,80,80,80 | 0 |
| 54 | MG | DA | 3069 | 1/1 | 0.88 | 0.17 | - | 81,81,81,81 | 0 |
| 54 | MG | BA | 3140 | 1/1 | 0.86 | 0.43 | - | 76,76,76,76 | 0 |
| 54 | MG | CA | 1674 | 1/1 | 0.84 | 0.15 | - | 74,74,74,74 | 0 |
| 54 | MG | AA | 1645 | 1/1 | 0.76 | 0.59 | - | 79,79,79,79 | 0 |
| 54 | MG | DA | 3204 | 1/1 | 0.99 | 0.14 | - | 54,54,54,54 | 0 |
| 54 | MG | DA | 3321 | 1/1 | 0.95 | 0.51 | - | 30,30,30,30 | 0 |
| 54 | MG | DA | 3328 | 1/1 | 0.98 | 0.10 | - | 45,45,45,45 | 0 |
| 54 | MG | BA | 3202 | 1/1 | 0.93 | 0.60 | - | 63,63,63,63 | 0 |
| 54 | MG | DA | 3035 | 1/1 | 0.90 | 0.42 | - | 77,77,77,77 | 0 |
| 54 | MG | CA | 1652 | 1/1 | 0.96 | 0.43 | - | 85,85,85,85 | 0 |
| 54 | MG | DA | 3087 | 1/1 | 0.70 | 0.29 | - | 67,67,67,67 | 0 |
| 54 | MG | CA | 1687 | 1/1 | 0.81 | 0.27 | - | 64,64,64,64 | 0 |
| 54 | MG | AA | 1760 | 1/1 | 0.91 | 0.16 | - | 84,84,84,84 | 0 |
| 54 | MG | DA | 3210 | 1/1 | 0.91 | 0.10 | - | 59,59,59,59 | 0 |
| 54 | MG | AA | 1750 | 1/1 | 0.94 | 0.46 | - | 109,109,109,109 | 0 |
| 54 | MG | DA | 3092 | 1/1 | 0.83 | 0.09 | - | 98,98,98,98 | 0 |
| 54 | MG | BA | 3032 | 1/1 | 0.91 | 0.26 | - | 59,59,59,59 | 0 |
| 54 | MG | BA | 3000 | 1/1 | 0.86 | 0.17 | - | 65,65,65,65 | 0 |
| 54 | MG | BA | 3120 | 1/1 | 0.96 | 0.30 | - | 57,57,57,57 | 0 |
| 54 | MG | DA | 3130 | 1/1 | 0.79 | 0.32 | - | 82,82,82,82 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | DA | 2910 | 1/1 | 0.98 | 0.30 | - | 6,6,6,6 | 0 |
| 54 | MG | DA | 2988 | 1/1 | 0.90 | 0.52 | - | 41,41,41,41 | 0 |
| 54 | MG | BA | 2919 | 1/1 | 0.97 | 0.41 | - | 24,24,24,24 | 0 |
| 54 | MG | DA | 3100 | 1/1 | 0.71 | 0.45 | - | 59,59,59,59 | 0 |
| 54 | MG | AA | 1745 | 1/1 | 0.64 | 0.27 | - | 97,97,97,97 | 0 |
| 54 | MG | BA | 3177 | 1/1 | 0.90 | 0.23 | - | 93,93,93,93 | 0 |
| 54 | MG | BA | 3047 | 1/1 | 0.92 | 0.39 | - | 65,65,65,65 | 0 |
| 54 | MG | BA | 3067 | 1/1 | 0.91 | 0.08 | - | 86,86,86,86 | 0 |
| 54 | MG | DA | 3319 | 1/1 | 0.91 | 0.63 | - | 83,83,83,83 | 0 |
| 54 | MG | DA | 2960 | 1/1 | 0.91 | 0.29 | - | 42,42,42,42 | 0 |
| 54 | MG | DA | 2972 | 1/1 | 0.69 | 0.48 | - | 47,47,47,47 | 0 |
| 54 | MG | AA | 1747 | 1/1 | 0.72 | 0.81 | - | 75,75,75,75 | 0 |
| 54 | MG | DA | 2962 | 1/1 | 0.98 | 0.38 | - | 37,37,37,37 | 0 |
| 54 | MG | CA | 1660 | 1/1 | 0.96 | 0.16 | - | 100,100,100,100 | 0 |
| 54 | MG | DA | 2948 | 1/1 | 0.92 | 0.33 | - | 52,52,52,52 | 0 |
| 54 | MG | DA | 3121 | 1/1 | 0.87 | 0.21 | - | 69,69,69,69 | 0 |
| 54 | MG | BA | 3059 | 1/1 | 0.94 | 0.21 | - | 60,60,60,60 | 0 |
| 54 | MG | DA | 3280 | 1/1 | 0.92 | 0.30 | - | 84,84,84,84 | 0 |
| 54 | MG | DA | 3187 | 1/1 | 0.86 | 0.22 | - | 90,90,90,90 | 0 |
| 54 | MG | DA | 3137 | 1/1 | 0.89 | 0.18 | - | 68,68,68,68 | 0 |
| 54 | MG | BA | 3305 | 1/1 | 0.40 | 0.58 | - | 103,103,103,103 | 0 |
| 54 | MG | BA | 3198 | 1/1 | 0.98 | 0.21 | - | 81,81,81,81 | 0 |
| 54 | MG | BA | 2977 | 1/1 | 0.98 | 0.28 | - | 52,52,52,52 | 0 |
| 54 | MG | BA | 2926 | 1/1 | 0.95 | 0.55 | - | 31,31,31,31 | 0 |
| 54 | MG | DA | 3119 | 1/1 | 0.66 | 0.65 | - | 88,88,88,88 | 0 |
| 54 | MG | DA | 3220 | 1/1 | 0.84 | 0.27 | - | 70,70,70,70 | 0 |
| 54 | MG | BA | 3212 | 1/1 | 0.79 | 0.40 | - | 69,69,69,69 | 0 |
| 54 | MG | BB | 203 | 1/1 | 0.91 | 0.14 | - | 83,83,83,83 | 0 |
| 54 | MG | DA | 3256 | 1/1 | 0.85 | 0.21 | - | 82,82,82,82 | 0 |
| 54 | MG | BA | 3211 | 1/1 | 0.98 | 0.37 | - | 59,59,59,59 | 0 |
| 54 | MG | DA | 2920 | 1/1 | 0.91 | 0.44 | - | 30,30,30,30 | 0 |
| 54 | MG | AA | 1757 | 1/1 | 0.54 | 0.53 | - | 89,89,89,89 | 0 |
| 54 | MG | DA | 3253 | 1/1 | 0.92 | 0.17 | - | 92,92,92,92 | 0 |
| 54 | MG | DA | 3010 | 1/1 | 0.84 | 0.65 | - | 51,51,51,51 | 0 |
| 54 | MG | DA | 2925 | 1/1 | 0.93 | 0.45 | - | 24,24,24,24 | 0 |
| 54 | MG | DA | 3008 | 1/1 | 0.90 | 0.47 | - | 59,59,59,59 | 0 |
| 54 | MG | AA | 1737 | 1/1 | 0.83 | 0.25 | - | 86,86,86,86 | 0 |
| 54 | MG | DA | 3295 | 1/1 | 0.82 | 0.26 | - | 63,63,63,63 | 0 |
| 54 | MG | AA | 1689 | 1/1 | 0.76 | 0.26 | - | 68,68,68,68 | 0 |
| 54 | MG | DB | 214 | 1/1 | 0.87 | 0.20 | - | 90,90,90,90 | 0 |
| 54 | MG | BA | 2981 | 1/1 | 0.96 | 0.15 | - | 48,48,48,48 | 0 |
| 54 | MG | BA | 3048 | 1/1 | 0.87 | 0.33 | - | 67,67,67,67 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | BA | 3035 | 1/1 | 0.90 | 0.38 | - | 44,44,44,44 | 0 |
| 54 | MG | BA | 3101 | 1/1 | 0.81 | 0.45 | - | 75,75,75,75 | 0 |
| 54 | MG | CA | 1722 | 1/1 | 0.94 | 0.38 | - | 108,108,108,108 | 0 |
| 54 | MG | DA | 2922 | 1/1 | 0.95 | 0.31 | - | 7,7,7,7 | 0 |
| 54 | MG | BA | 2937 | 1/1 | 0.95 | 0.33 | - | 36,36,36,36 | 0 |
| 54 | MG | CA | 1642 | 1/1 | 0.94 | 0.17 | - | 71,71,71,71 | 0 |
| 54 | MG | BA | 3122 | 1/1 | 0.92 | 0.30 | - | 101,101,101,101 | 0 |
| 54 | MG | AA | 1638 | 1/1 | 0.94 | 0.48 | - | 63,63,63,63 | 0 |
| 54 | MG | DA | 3240 | 1/1 | 0.92 | 0.38 | - | 60,60,60,60 | 0 |
| 54 | MG | BA | 3239 | 1/1 | 0.92 | 0.57 | - | 82,82,82,82 | 0 |
| 54 | MG | DA | 2981 | 1/1 | 0.90 | 0.30 | - | 55,55,55,55 | 0 |
| 54 | MG | DA | 2929 | 1/1 | 0.96 | 0.35 | - | 39,39,39,39 | 0 |
| 54 | MG | BA | 2974 | 1/1 | 0.98 | 0.20 | - | 45,45,45,45 | 0 |
| 54 | MG | D4 | 101 | 1/1 | 0.79 | 0.55 | - | 55,55,55,55 | 0 |
| 54 | MG | DA | 3167 | 1/1 | 0.99 | 0.17 | - | 68,68,68,68 | 0 |
| 54 | MG | CA | 1708 | 1/1 | 0.84 | 0.14 | - | 143,143,143,143 | 0 |
| 54 | MG | DA | 3184 | 1/1 | 0.88 | 0.28 | - | 117,117,117,117 | 0 |
| 54 | MG | DA | 3269 | 1/1 | 0.84 | 0.51 | - | 91,91,91,91 | 0 |
| 54 | MG | BA | 3075 | 1/1 | 0.72 | 0.21 | - | 67,67,67,67 | 0 |
| 54 | MG | BA | 3005 | 1/1 | 0.85 | 0.52 | - | 69,69,69,69 | 0 |
| 54 | MG | AA | 1641 | 1/1 | 0.75 | 0.35 | - | 85,85,85,85 | 0 |
| 54 | MG | CA | 1689 | 1/1 | 0.91 | 0.29 | - | 83,83,83,83 | 0 |
| 54 | MG | DA | 3093 | 1/1 | 0.91 | 0.39 | - | 69,69,69,69 | 0 |
| 54 | MG | BB | 209 | 1/1 | 0.88 | 0.24 | - | 83,83,83,83 | 0 |
| 54 | MG | DA | 3125 | 1/1 | 0.92 | 0.28 | - | 81,81,81,81 | 0 |
| 54 | MG | AA | 1727 | 1/1 | 0.93 | 0.13 | - | 100,100,100,100 | 0 |
| 54 | MG | BA | 3250 | 1/1 | 0.92 | 0.13 | - | 95,95,95,95 | 0 |
| 54 | MG | DA | 3049 | 1/1 | 0.78 | 0.21 | - | 56,56,56,56 | 0 |
| 54 | MG | CA | 1733 | 1/1 | 0.84 | 0.12 | - | 72,72,72,72 | 0 |
| 54 | MG | AA | 1673 | 1/1 | 0.62 | 0.53 | - | 61,61,61,61 | 0 |
| 54 | MG | DB | 207 | 1/1 | 0.88 | 0.28 | - | 72,72,72,72 | 0 |
| 54 | MG | AV | 6303 | 1/1 | 0.86 | 0.13 | - | 67,67,67,67 | 0 |
| 54 | MG | BA | 3149 | 1/1 | 0.68 | 0.73 | - | 82,82,82,82 | 0 |
| 54 | MG | BA | 2932 | 1/1 | 0.98 | 0.26 | - | 41,41,41,41 | 0 |
| 54 | MG | DA | 2954 | 1/1 | 0.95 | 0.31 | - | 28,28,28,28 | 0 |
| 54 | MG | DA | 3207 | 1/1 | 0.74 | 0.37 | - | 42,42,42,42 | 0 |
| 54 | MG | AA | 1642 | 1/1 | 0.69 | 0.50 | - | 97,97,97,97 | 0 |
| 54 | MG | DA | 3042 | 1/1 | 0.96 | 0.56 | - | 79,79,79,79 | 0 |
| 54 | MG | DA | 3097 | 1/1 | 0.80 | 0.29 | - | 94,94,94,94 | 0 |
| 54 | MG | CA | 1726 | 1/1 | 0.92 | 0.34 | - | 87,87,87,87 | 0 |
| 54 | MG | DA | 3061 | 1/1 | 0.77 | 0.27 | - | 75,75,75,75 | 0 |
| 54 | MG | AA | 1659 | 1/1 | 0.96 | 0.42 | - | 51,51,51,51 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | BA | 3194 | 1/1 | 0.93 | 0.53 | - | 45,45,45,45 | 0 |
| 54 | MG | BA | 2944 | 1/1 | 0.92 | 0.15 | - | 17,17,17,17 | 0 |
| 54 | MG | DA | 3027 | 1/1 | 0.86 | 0.50 | - | 53,53,53,53 | 0 |
| 54 | MG | CA | 1682 | 1/1 | 0.94 | 0.21 | - | 97,97,97,97 | 0 |
| 54 | MG | DA | 3115 | 1/1 | 0.56 | 0.49 | - | 65,65,65,65 | 0 |
| 54 | MG | DA | 3261 | 1/1 | 0.93 | 0.27 | - | 73,73,73,73 | 0 |
| 54 | MG | BA | 3195 | 1/1 | 0.97 | 0.16 | - | 53,53,53,53 | 0 |
| 54 | MG | CA | 1737 | 1/1 | 0.93 | 0.20 | - | 70,70,70,70 | 0 |
| 54 | MG | BA | 3217 | 1/1 | 0.47 | 0.34 | - | 111,111,111,111 | 0 |
| 54 | MG | BA | 2948 | 1/1 | 0.86 | 0.72 | - | 39,39,39,39 | 0 |
| 54 | MG | CA | 1616 | 1/1 | 0.78 | 0.47 | - | 75,75,75,75 | 0 |
| 54 | MG | DA | 3102 | 1/1 | 0.98 | 0.20 | - | 68,68,68,68 | 0 |
| 54 | MG | AV | 6304 | 1/1 | 0.33 | 0.43 | - | 118,118,118,118 | 0 |
| 54 | MG | AA | 1729 | 1/1 | 0.28 | 0.13 | - | 75,75,75,75 | 0 |
| 54 | MG | BA | 2989 | 1/1 | 0.95 | 0.35 | - | 53,53,53,53 | 0 |
| 54 | MG | AA | 1665 | 1/1 | 0.88 | 0.26 | - | 82,82,82,82 | 0 |
| 54 | MG | BA | 3224 | 1/1 | 0.98 | 0.22 | - | 45,45,45,45 | 0 |
| 54 | MG | AA | 1722 | 1/1 | 0.70 | 0.28 | - | 83,83,83,83 | 0 |
| 54 | MG | DA | 3307 | 1/1 | 0.78 | 0.38 | - | 73,73,73,73 | 0 |
| 54 | MG | BA | 3283 | 1/1 | 0.71 | 0.16 | - | 76,76,76,76 | 0 |
| 54 | MG | DA | 3244 | 1/1 | 0.75 | 0.27 | - | 87,87,87,87 | 0 |
| 54 | MG | BA | 3107 | 1/1 | 0.94 | 0.26 | - | 87,87,87,87 | 0 |
| 54 | MG | BA | 2907 | 1/1 | 0.96 | 0.26 | - | 7,7,7,7 | 0 |
| 54 | MG | DA | 3239 | 1/1 | 0.95 | 0.23 | - | 42,42,42,42 | 0 |
| 54 | MG | BA | 2936 | 1/1 | 0.98 | 0.18 | - | 43,43,43,43 | 0 |
| 54 | MG | CA | 1736 | 1/1 | 0.82 | 1.13 | - | 115,115,115,115 | 0 |
| 54 | MG | BA | 2978 | 1/1 | 0.93 | 0.35 | - | 59,59,59,59 | 0 |
| 54 | MG | BA | 2939 | 1/1 | 0.95 | 0.46 | - | 26,26,26,26 | 0 |
| 54 | MG | AA | 1761 | 1/1 | 0.82 | 0.20 | - | 104,104,104,104 | 0 |
| 54 | MG | BA | 3286 | 1/1 | 0.97 | 0.38 | - | 67,67,67,67 | 0 |
| 54 | MG | BA | 2985 | 1/1 | 0.83 | 0.52 | - | 54,54,54,54 | 0 |
| 54 | MG | CA | 1611 | 1/1 | 0.88 | 0.19 | - | 76,76,76,76 | 0 |
| 54 | MG | BA | 3130 | 1/1 | 0.94 | 0.17 | - | 78,78,78,78 | 0 |
| 54 | MG | DA | 3258 | 1/1 | 0.74 | 0.48 | - | 72,72,72,72 | 0 |
| 54 | MG | BA | 3115 | 1/1 | 0.74 | 0.32 | - | 91,91,91,91 | 0 |
| 54 | MG | AA | 1656 | 1/1 | 0.97 | 0.31 | - | 72,72,72,72 | 0 |
| 54 | MG | CA | 1707 | 1/1 | 0.95 | 0.08 | - | 104,104,104,104 | 0 |
| 54 | MG | CA | 1640 | 1/1 | 0.95 | 0.38 | - | 69,69,69,69 | 0 |
| 54 | MG | BA | 3176 | 1/1 | 0.38 | 0.33 | - | 99,99,99,99 | 0 |
| 54 | MG | CA | 1704 | 1/1 | 0.41 | 0.52 | - | 108,108,108,108 | 0 |
| 54 | MG | CA | 1739 | 1/1 | 0.90 | 0.10 | - | 99,99,99,99 | 0 |
| 54 | MG | DA | 3152 | 1/1 | 0.88 | 0.21 | - | 77,77,77,77 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | DA | 3068 | 1/1 | 0.87 | 0.41 | - | 72,72,72,72 | 0 |
| 54 | MG | AA | 1651 | 1/1 | 0.83 | 0.51 | - | 97,97,97,97 | 0 |
| 54 | MG | DA | 3120 | 1/1 | 0.83 | 0.64 | - | 66,66,66,66 | 0 |
| 54 | MG | DA | 3334 | 1/1 | 0.82 | 0.25 | - | 72,72,72,72 | 0 |
| 54 | MG | DA | 3225 | 1/1 | 0.96 | 0.08 | - | 80,80,80,80 | 0 |
| 54 | MG | DA | 3246 | 1/1 | 0.70 | 0.60 | - | 67,67,67,67 | 0 |
| 54 | MG | CA | 1628 | 1/1 | 0.87 | 0.20 | - | 100,100,100,100 | 0 |
| 54 | MG | DA | 2924 | 1/1 | 0.98 | 0.48 | - | 41,41,41,41 | 0 |
| 54 | MG | DA | 3017 | 1/1 | 0.41 | 0.22 | - | 93,93,93,93 | 0 |
| 54 | MG | BA | 3056 | 1/1 | 0.89 | 0.49 | - | 62,62,62,62 | 0 |
| 54 | MG | DA | 3287 | 1/1 | 0.88 | 0.51 | - | 69,69,69,69 | 0 |
| 54 | MG | CA | 1601 | 1/1 | 0.83 | 0.45 | - | 53,53,53,53 | 0 |
| 54 | MG | CA | 1618 | 1/1 | 0.87 | 0.72 | - | 63,63,63,63 | 0 |
| 54 | MG | DA | 3175 | 1/1 | 0.83 | 0.18 | - | 81,81,81,81 | 0 |
| 54 | MG | BA | 3158 | 1/1 | 0.78 | 0.20 | - | 105,105,105,105 | 0 |
| 54 | MG | CA | 1693 | 1/1 | 0.92 | 0.34 | - | 65,65,65,65 | 0 |
| 54 | MG | BA | 3002 | 1/1 | 0.93 | 0.38 | - | 45,45,45,45 | 0 |
| 54 | MG | CA | 1602 | 1/1 | 0.99 | 0.09 | - | 64,64,64,64 | 0 |
| 54 | MG | DA | 3164 | 1/1 | 0.96 | 0.05 | - | 88,88,88,88 | 0 |
| 54 | MG | DA | 3103 | 1/1 | 0.84 | 0.41 | - | 79,79,79,79 | 0 |
| 54 | MG | DA | 3237 | 1/1 | 0.98 | 0.23 | - | 87,87,87,87 | 0 |
| 54 | MG | BA | 3215 | 1/1 | 0.97 | 0.36 | - | 68,68,68,68 | 0 |
| 54 | MG | DA | 3194 | 1/1 | 0.98 | 0.36 | - | 10,10,10,10 | 0 |
| 54 | MG | BA | 3274 | 1/1 | 0.97 | 0.06 | - | 78,78,78,78 | 0 |
| 54 | MG | AA | 1614 | 1/1 | 0.84 | 0.52 | - | 85,85,85,85 | 0 |
| 54 | MG | DA | 2956 | 1/1 | 0.95 | 0.28 | - | 45,45,45,45 | 0 |
| 54 | MG | BA | 3295 | 1/1 | 0.83 | 0.60 | - | 70,70,70,70 | 0 |
| 54 | MG | CA | 1653 | 1/1 | 0.97 | 0.20 | - | 84,84,84,84 | 0 |
| 54 | MG | DA | 3267 | 1/1 | 0.79 | 0.25 | - | 76,76,76,76 | 0 |
| 54 | MG | BA | 2927 | 1/1 | 0.94 | 0.29 | - | 37,37,37,37 | 0 |
| 54 | MG | BA | 3279 | 1/1 | 0.95 | 0.27 | - | 77,77,77,77 | 0 |
| 54 | MG | BA | 3134 | 1/1 | 0.98 | 0.17 | - | 64,64,64,64 | 0 |
| 54 | MG | DA | 3016 | 1/1 | 0.96 | 0.21 | - | 74,74,74,74 | 0 |
| 54 | MG | BA | 3112 | 1/1 | 0.82 | 0.34 | - | 68,68,68,68 | 0 |
| 54 | MG | DA | 3181 | 1/1 | 0.61 | 0.18 | - | 106,106,106,106 | 0 |
| 54 | MG | BA | 2912 | 1/1 | 0.94 | 0.66 | - | 36,36,36,36 | 0 |
| 54 | MG | BA | 3160 | 1/1 | 0.89 | 0.54 | - | 106,106,106,106 | 0 |
| 54 | MG | BA | 2990 | 1/1 | 0.95 | 0.19 | - | 54,54,54,54 | 0 |
| 54 | MG | CA | 1631 | 1/1 | 0.91 | 0.13 | - | 68,68,68,68 | 0 |
| 54 | MG | AA | 1699 | 1/1 | 0.87 | 0.26 | - | 91,91,91,91 | 0 |
| 54 | MG | DA | 3335 | 1/1 | 0.92 | 0.29 | - | 90,90,90,90 | 0 |
| 54 | MG | BA | 3133 | 1/1 | 0.88 | 0.26 | - | 67,67,67,67 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | BA | 3074 | 1/1 | 0.89 | 0.34 | - | 61,61,61,61 | 0 |
| 54 | MG | DA | 3309 | 1/1 | 0.78 | 0.38 | - | 30,30,30,30 | 0 |
| 54 | MG | DA | 2986 | 1/1 | 0.93 | 0.22 | - | 55,55,55,55 | 0 |
| 54 | MG | DA | 3062 | 1/1 | 0.94 | 0.12 | - | 65,65,65,65 | 0 |
| 54 | MG | DA | 3242 | 1/1 | 0.80 | 0.31 | - | 96,96,96,96 | 0 |
| 54 | MG | BA | 3148 | 1/1 | 0.88 | 0.35 | - | 68,68,68,68 | 0 |
| 54 | MG | AA | 1678 | 1/1 | 0.85 | 0.24 | - | 115,115,115,115 | 0 |
| 54 | MG | DA | 3159 | 1/1 | 0.90 | 1.09 | - | 87,87,87,87 | 0 |
| 54 | MG | DA | 3122 | 1/1 | 0.95 | 0.22 | - | 87,87,87,87 | 0 |
| 54 | MG | BA | 3154 | 1/1 | 0.95 | 0.22 | - | 89,89,89,89 | 0 |
| 54 | MG | BA | 2996 | 1/1 | 0.87 | 0.29 | - | 54,54,54,54 | 0 |
| 54 | MG | DA | 3193 | 1/1 | 0.95 | 0.57 | - | 51,51,51,51 | 0 |
| 54 | MG | BA | 3060 | 1/1 | 0.67 | 0.69 | - | 74,74,74,74 | 0 |
| 54 | MG | DA | 3021 | 1/1 | 0.81 | 0.17 | - | 67,67,67,67 | 0 |
| 54 | MG | DA | 3110 | 1/1 | 0.52 | 0.31 | - | 86,86,86,86 | 0 |
| 54 | MG | BA | 3125 | 1/1 | 0.86 | 0.26 | - | 87,87,87,87 | 0 |
| 54 | MG | DA | 3271 | 1/1 | 0.71 | 0.18 | - | 97,97,97,97 | 0 |
| 54 | MG | CA | 1721 | 1/1 | 0.95 | 0.33 | - | 101,101,101,101 | 0 |
| 54 | MG | AA | 1730 | 1/1 | 0.99 | 0.09 | - | 49,49,49,49 | 0 |
| 54 | MG | AA | 1660 | 1/1 | 0.84 | 0.30 | - | 59,59,59,59 | 0 |
| 54 | MG | DA | 3140 | 1/1 | 0.95 | 0.14 | - | 67,67,67,67 | 0 |
| 54 | MG | AA | 1687 | 1/1 | 0.90 | 0.08 | - | 73,73,73,73 | 0 |
| 54 | MG | DA | 3257 | 1/1 | 0.90 | 0.16 | - | 94,94,94,94 | 0 |
| 54 | MG | BB | 215 | 1/1 | 0.95 | 0.19 | - | 131,131,131,131 | 0 |
| 54 | MG | BA | 3156 | 1/1 | 0.96 | 0.28 | - | 80,80,80,80 | 0 |
| 54 | MG | AA | 1666 | 1/1 | 0.97 | 0.10 | - | 100,100,100,100 | 0 |
| 54 | MG | BA | 3280 | 1/1 | 0.84 | 0.40 | - | 70,70,70,70 | 0 |
| 54 | MG | DA | 3158 | 1/1 | 0.88 | 0.18 | - | 59,59,59,59 | 0 |
| 54 | MG | DA | 3218 | 1/1 | 0.91 | 0.49 | - | 48,48,48,48 | 0 |
| 54 | MG | BA | 3050 | 1/1 | 0.87 | 0.17 | - | 41,41,41,41 | 0 |
| 54 | MG | AA | 1694 | 1/1 | 0.89 | 0.23 | - | 129,129,129,129 | 0 |
| 54 | MG | DA | 3090 | 1/1 | 0.85 | 0.21 | - | 71,71,71,71 | 0 |
| 54 | MG | BA | 3045 | 1/1 | 0.90 | 0.20 | - | 80,80,80,80 | 0 |
| 54 | MG | BA | 2960 | 1/1 | 0.94 | 0.57 | - | 40,40,40,40 | 0 |
| 54 | MG | DA | 3073 | 1/1 | 0.96 | 0.10 | - | 80,80,80,80 | 0 |
| 54 | MG | BA | 3051 | 1/1 | 0.85 | 0.34 | - | 66,66,66,66 | 0 |
| 54 | MG | BA | 3071 | 1/1 | 0.93 | 0.17 | - | 72,72,72,72 | 0 |
| 54 | MG | DA | 3206 | 1/1 | 0.97 | 0.32 | - | 37,37,37,37 | 0 |
| 54 | MG | DA | 3160 | 1/1 | 0.96 | 0.16 | - | 71,71,71,71 | 0 |
| 54 | MG | BA | 3044 | 1/1 | 0.94 | 0.12 | - | 64,64,64,64 | 0 |
| 54 | MG | AA | 1680 | 1/1 | 0.64 | 0.14 | - | 90,90,90,90 | 0 |
| 54 | MG | BB | 206 | 1/1 | 0.80 | 0.23 | - | 70,70,70,70 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | BA | 3084 | 1/1 | 0.66 | 0.41 | - | 51,51,51,51 | 0 |
| 54 | MG | CA | 1668 | 1/1 | 0.72 | 1.09 | - | 116,116,116,116 | 0 |
| 54 | MG | DA | 2941 | 1/1 | 0.93 | 0.23 | - | 37,37,37,37 | 0 |
| 54 | MG | DA | 3279 | 1/1 | 0.86 | 0.09 | - | 88,88,88,88 | 0 |
| 54 | MG | CA | 1720 | 1/1 | 0.89 | 0.35 | - | 63,63,63,63 | 0 |
| 54 | MG | CA | 1667 | 1/1 | 0.94 | 0.10 | - | 67,67,67,67 | 0 |
| 54 | MG | DA | 3138 | 1/1 | 0.89 | 0.12 | - | 70,70,70,70 | 0 |
| 54 | MG | BA | 3016 | 1/1 | 0.90 | 0.31 | - | 60,60,60,60 | 0 |
| 54 | MG | BA | 3275 | 1/1 | 0.00 | 0.91 | - | 87,87,87,87 | 0 |
| 54 | MG | DA | 3143 | 1/1 | 0.70 | 0.25 | - | 77,77,77,77 | 0 |
| 54 | MG | DA | 3262 | 1/1 | 0.73 | 0.27 | - | 82,82,82,82 | 0 |
| 54 | MG | BA | 3015 | 1/1 | 0.97 | 0.42 | - | 58,58,58,58 | 0 |
| 54 | MG | CA | 1669 | 1/1 | 0.96 | 0.14 | - | 66,66,66,66 | 0 |
| 54 | MG | CA | 1690 | 1/1 | 0.99 | 0.52 | - | 61,61,61,61 | 0 |
| 54 | MG | AA | 1715 | 1/1 | 0.96 | 0.35 | - | 63,63,63,63 | 0 |
| 54 | MG | AA | 1648 | 1/1 | 0.96 | 0.40 | - | 76,76,76,76 | 0 |
| 54 | MG | BA | 3009 | 1/1 | 0.84 | 0.51 | - | 87,87,87,87 | 0 |
| 54 | MG | DA | 3330 | 1/1 | 0.88 | 0.39 | - | 69,69,69,69 | 0 |
| 54 | MG | BA | 3145 | 1/1 | 0.82 | 0.19 | - | 67,67,67,67 | 0 |
| 54 | MG | DA | 3296 | 1/1 | 0.79 | 0.15 | - | 104,104,104,104 | 0 |
| 54 | MG | BA | 3086 | 1/1 | 0.97 | 0.26 | - | 102,102,102,102 | 0 |
| 54 | MG | BA | 3246 | 1/1 | 0.95 | 0.24 | - | 73,73,73,73 | 0 |
| 54 | MG | DA | 3317 | 1/1 | 0.78 | 0.42 | - | 97,97,97,97 | 0 |
| 54 | MG | AA | 1608 | 1/1 | 0.94 | 0.36 | - | 47,47,47,47 | 0 |
| 54 | MG | DA | 3135 | 1/1 | 0.95 | 0.22 | - | 65,65,65,65 | 0 |
| 54 | MG | DA | 3098 | 1/1 | 0.81 | 0.37 | - | 71,71,71,71 | 0 |
| 54 | MG | DA | 3081 | 1/1 | 0.98 | 0.10 | - | 71,71,71,71 | 0 |
| 54 | MG | BA | 3066 | 1/1 | 0.84 | 0.46 | - | 56,56,56,56 | 0 |
| 54 | MG | BA | 3210 | 1/1 | 0.97 | 0.33 | - | 48,48,48,48 | 0 |
| 54 | MG | CA | 1636 | 1/1 | 0.72 | 0.33 | - | 93,93,93,93 | 0 |
| 54 | MG | BA | 3240 | 1/1 | 0.76 | 0.10 | - | 114,114,114,114 | 0 |
| 54 | MG | BA | 2935 | 1/1 | 0.94 | 0.56 | - | 34,34,34,34 | 0 |
| 54 | MG | DA | 3327 | 1/1 | 0.71 | 0.32 | - | 68,68,68,68 | 0 |
| 54 | MG | DA | 3127 | 1/1 | 0.81 | 0.37 | - | 90,90,90,90 | 0 |
| 54 | MG | DA | 3266 | 1/1 | 0.94 | 0.33 | - | 83,83,83,83 | 0 |
| 54 | MG | DA | 3243 | 1/1 | 0.60 | 0.35 | - | 72,72,72,72 | 0 |
| 54 | MG | DA | 3091 | 1/1 | 0.87 | 0.49 | - | 125,125,125,125 | 0 |
| 54 | MG | DA | 3116 | 1/1 | 0.79 | 0.25 | - | 115,115,115,115 | 0 |
| 54 | MG | DA | 3163 | 1/1 | 0.50 | 0.19 | - | 83,83,83,83 | 0 |
| 54 | MG | BA | 3029 | 1/1 | 0.92 | 0.58 | - | 63,63,63,63 | 0 |
| 54 | MG | BA | 3159 | 1/1 | 0.81 | 0.42 | - | 78,78,78,78 | 0 |
| 54 | MG | AA | 1675 | 1/1 | 0.86 | 0.15 | - | 77,77,77,77 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | AA | 1732 | 1/1 | 0.91 | 0.24 | - | 63,63,63,63 | 0 |
| 54 | MG | BA | 3165 | 1/1 | 0.84 | 0.26 | - | 71,71,71,71 | 0 |
| 54 | MG | BA | 3261 | 1/1 | 0.91 | 0.30 | - | 53,53,53,53 | 0 |
| 54 | MG | AA | 1746 | 1/1 | 0.92 | 0.27 | - | 100,100,100,100 | 0 |
| 54 | MG | DA | 3203 | 1/1 | 0.98 | 0.23 | - | 46,46,46,46 | 0 |
| 54 | MG | DA | 3032 | 1/1 | 0.88 | 0.10 | - | 49,49,49,49 | 0 |
| 54 | MG | DA | 2919 | 1/1 | 0.98 | 0.28 | - | 45,45,45,45 | 0 |
| 54 | MG | BA | 2984 | 1/1 | 0.95 | 0.22 | - | 41,41,41,41 | 0 |
| 54 | MG | AA | 1635 | 1/1 | 0.96 | 0.33 | - | 68,68,68,68 | 0 |
| 54 | MG | DA | 3196 | 1/1 | 0.73 | 1.09 | - | 39,39,39,39 | 0 |
| 54 | MG | DA | 3186 | 1/1 | 0.78 | 0.13 | - | 90,90,90,90 | 0 |
| 54 | MG | BA | 3064 | 1/1 | 0.95 | 0.31 | - | 40,40,40,40 | 0 |
| 54 | MG | AA | 1686 | 1/1 | 0.95 | 0.13 | - | 72,72,72,72 | 0 |
| 54 | MG | BA | 3076 | 1/1 | 0.96 | 0.25 | - | 68,68,68,68 | 0 |
| 54 | MG | BA | 2992 | 1/1 | 0.90 | 0.50 | - | 70,70,70,70 | 0 |
| 54 | MG | AA | 1683 | 1/1 | 0.93 | 0.17 | - | 102,102,102,102 | 0 |
| 54 | MG | CA | 1657 | 1/1 | 0.91 | 0.39 | - | 78,78,78,78 | 0 |
| 54 | MG | BA | 3062 | 1/1 | 0.76 | 0.36 | - | 76,76,76,76 | 0 |
| 54 | MG | DA | 2987 | 1/1 | 0.77 | 0.44 | - | 70,70,70,70 | 0 |
| 54 | MG | BA | 3099 | 1/1 | 0.85 | 0.15 | - | 78,78,78,78 | 0 |
| 54 | MG | DA | 3028 | 1/1 | 0.93 | 0.15 | - | 78,78,78,78 | 0 |
| 54 | MG | CA | 1727 | 1/1 | 0.82 | 0.26 | - | 75,75,75,75 | 0 |
| 54 | MG | DA | 3064 | 1/1 | 0.61 | 0.19 | - | 80,80,80,80 | 0 |
| 54 | MG | CA | 1627 | 1/1 | 0.94 | 0.18 | - | 67,67,67,67 | 0 |
| 54 | MG | BA | 3285 | 1/1 | 0.90 | 0.24 | - | 87,87,87,87 | 0 |
| 54 | MG | BB | 205 | 1/1 | 0.69 | 0.41 | - | 71,71,71,71 | 0 |
| 54 | MG | DA | 2957 | 1/1 | 0.96 | 0.09 | - | 63,63,63,63 | 0 |
| 54 | MG | DA | 3283 | 1/1 | 0.94 | 0.27 | - | 53,53,53,53 | 0 |
| 54 | MG | BA | 3303 | 1/1 | 0.71 | 0.20 | - | 98,98,98,98 | 0 |
| 54 | MG | CA | 1697 | 1/1 | 0.50 | 0.47 | - | 74,74,74,74 | 0 |
| 54 | MG | BA | 3190 | 1/1 | 0.69 | 0.26 | - | 115,115,115,115 | 0 |
| 54 | MG | BA | 3178 | 1/1 | 0.68 | 0.50 | - | 72,72,72,72 | 0 |
| 55 | ZN | AN | 101 | 1/1 | 0.98 | 0.14 | - | 120,120,120,120 | 0 |
| 54 | MG | AA | 1602 | 1/1 | 0.91 | 0.58 | - | 49,49,49,49 | 0 |
| 54 | MG | DA | 2977 | 1/1 | 0.88 | 0.17 | - | 47,47,47,47 | 0 |
| 54 | MG | BA | 3300 | 1/1 | 0.88 | 0.45 | - | 83,83,83,83 | 0 |
| 54 | MG | CA | 1709 | 1/1 | 0.92 | 0.39 | - | 81,81,81,81 | 0 |
| 54 | MG | CA | 1724 | 1/1 | 0.68 | 0.32 | - | 74,74,74,74 | 0 |
| 54 | MG | BA | 3225 | 1/1 | 0.60 | 0.48 | - | 74,74,74,74 | 0 |
| 54 | MG | DB | 217 | 1/1 | 0.94 | 0.14 | - | 74,74,74,74 | 0 |
| 54 | MG | AA | 1709 | 1/1 | 0.71 | 0.37 | - | 83,83,83,83 | 0 |
| 54 | MG | DA | 3114 | 1/1 | 0.94 | 0.36 | - | 83,83,83,83 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | BA | 3094 | 1/1 | 0.89 | 0.68 | - | 70,70,70,70 | 0 |
| 54 | MG | AA | 1693 | 1/1 | 0.76 | 0.32 | - | 74,74,74,74 | 0 |
| 54 | MG | DA | 3170 | 1/1 | 0.88 | 0.20 | - | 80,80,80,80 | 0 |
| 54 | MG | BA | 3069 | 1/1 | 0.84 | 0.13 | - | 109,109,109,109 | 0 |
| 54 | MG | DA | 2979 | 1/1 | 0.89 | 0.23 | - | 69,69,69,69 | 0 |
| 54 | MG | DA | 3108 | 1/1 | 0.90 | 0.19 | - | 50,50,50,50 | 0 |
| 54 | MG | DA | 3291 | 1/1 | 0.74 | 0.48 | - | 78,78,78,78 | 0 |
| 54 | MG | BA | 3137 | 1/1 | 0.94 | 0.52 | - | 54,54,54,54 | 0 |
| 54 | MG | DA | 3336 | 1/1 | 0.92 | 0.07 | - | 89,89,89,89 | 0 |
| 54 | MG | DA | 3305 | 1/1 | 0.89 | 0.12 | - | 110,110,110,110 | 0 |
| 54 | MG | BA | 2946 | 1/1 | 0.97 | 0.46 | - | 33,33,33,33 | 0 |
| 54 | MG | DA | 3213 | 1/1 | 0.96 | 0.20 | - | 66,66,66,66 | 0 |
| 54 | MG | CA | 1713 | 1/1 | 0.92 | 0.17 | - | 80,80,80,80 | 0 |
| 54 | MG | AA | 1701 | 1/1 | 0.81 | 0.35 | - | 83,83,83,83 | 0 |
| 54 | MG | DA | 3166 | 1/1 | 0.84 | 0.12 | - | 87,87,87,87 | 0 |
| 54 | MG | BA | 3117 | 1/1 | 0.61 | 0.11 | - | 77,77,77,77 | 0 |
| 54 | MG | CA | 1673 | 1/1 | 0.96 | 0.15 | - | 73,73,73,73 | 0 |
| 54 | MG | BA | 3164 | 1/1 | 0.46 | 0.63 | - | 88,88,88,88 | 0 |
| 54 | MG | DA | 3086 | 1/1 | 0.91 | 0.68 | - | 92,92,92,92 | 0 |
| 54 | MG | BA | 3108 | 1/1 | 0.88 | 0.42 | - | 99,99,99,99 | 0 |
| 54 | MG | DA | 3002 | 1/1 | 0.93 | 0.43 | - | 59,59,59,59 | 0 |
| 54 | MG | BA | 2983 | 1/1 | 0.95 | 0.45 | - | 62,62,62,62 | 0 |
| 54 | MG | CA | 1718 | 1/1 | 0.93 | 0.15 | - | 78,78,78,78 | 0 |
| 54 | MG | DA | 3095 | 1/1 | 0.90 | 0.17 | - | 67,67,67,67 | 0 |
| 54 | MG | BA | 2988 | 1/1 | 0.38 | 0.33 | - | 60,60,60,60 | 0 |
| 54 | MG | BA | 3162 | 1/1 | 0.96 | 0.08 | - | 94,94,94,94 | 0 |
| 54 | MG | DA | 3113 | 1/1 | 0.82 | 0.09 | - | 71,71,71,71 | 0 |
| 54 | MG | DA | 3219 | 1/1 | 0.98 | 0.29 | - | 67,67,67,67 | 0 |
| 54 | MG | BA | 3272 | 1/1 | 0.61 | 0.45 | - | 119,119,119,119 | 0 |
| 54 | MG | BA | 3068 | 1/1 | 0.86 | 0.34 | - | 59,59,59,59 | 0 |
| 54 | MG | CA | 1714 | 1/1 | 0.94 | 0.29 | - | 74,74,74,74 | 0 |
| 54 | MG | BA | 3128 | 1/1 | 0.92 | 0.48 | - | 59,59,59,59 | 0 |
| 54 | MG | DA | 3044 | 1/1 | 0.98 | 0.08 | - | 59,59,59,59 | 0 |
| 54 | MG | BA | 3254 | 1/1 | 0.95 | 0.48 | - | 81,81,81,81 | 0 |
| 54 | MG | CA | 1654 | 1/1 | 0.93 | 0.13 | - | 111,111,111,111 | 0 |
| 54 | MG | BA | 2933 | 1/1 | 0.98 | 0.30 | - | 32,32,32,32 | 0 |
| 54 | MG | BA | 3150 | 1/1 | 0.88 | 0.38 | - | 79,79,79,79 | 0 |
| 54 | MG | AA | 1705 | 1/1 | 0.95 | 0.30 | - | 92,92,92,92 | 0 |
| 54 | MG | DA | 3117 | 1/1 | 0.94 | 0.20 | - | 87,87,87,87 | 0 |
| 54 | MG | CA | 1701 | 1/1 | 0.81 | 0.34 | - | 112,112,112,112 | 0 |
| 54 | MG | BB | 214 | 1/1 | 0.90 | 0.20 | - | 101,101,101,101 | 0 |
| 54 | MG | AA | 1734 | 1/1 | 0.67 | 0.37 | - | 103,103,103,103 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | BA | 3020 | 1/1 | 0.98 | 0.30 | - | 62,62,62,62 | 0 |
| 54 | MG | BA | 3072 | 1/1 | 0.78 | 0.43 | - | 67,67,67,67 | 0 |
| 54 | MG | DA | 3162 | 1/1 | 0.79 | 0.16 | - | 143,143,143,143 | 0 |
| 54 | MG | BA | 3146 | 1/1 | 0.84 | 0.28 | - | 83,83,83,83 | 0 |
| 54 | MG | BA | 2923 | 1/1 | 0.95 | 0.33 | - | 29,29,29,29 | 0 |
| 54 | MG | AA | 1691 | 1/1 | 0.77 | 0.42 | - | 78,78,78,78 | 0 |
| 54 | MG | BA | 3171 | 1/1 | 0.87 | 0.19 | - | 68,68,68,68 | 0 |
| 54 | MG | BA | 3042 | 1/1 | 0.94 | 0.15 | - | 90,90,90,90 | 0 |
| 54 | MG | BA | 3096 | 1/1 | 0.96 | 0.24 | - | 65,65,65,65 | 0 |
| 54 | MG | DA | 3126 | 1/1 | 0.90 | 0.08 | - | 77,77,77,77 | 0 |
| 54 | MG | DA | 3329 | 1/1 | 0.90 | 0.71 | - | 69,69,69,69 | 0 |
| 54 | MG | AA | 1696 | 1/1 | 0.61 | 0.24 | - | 132,132,132,132 | 0 |
| 54 | MG | CA | 1641 | 1/1 | 0.78 | 0.13 | - | 85,85,85,85 | 0 |
| 54 | MG | BA | 3038 | 1/1 | 0.81 | 0.17 | - | 65,65,65,65 | 0 |
| 54 | MG | DA | 3173 | 1/1 | 0.87 | 0.18 | - | 97,97,97,97 | 0 |
| 54 | MG | BA | 3207 | 1/1 | 0.92 | 0.36 | - | 94,94,94,94 | 0 |
| 54 | MG | BA | 3008 | 1/1 | 0.98 | 0.18 | - | 57,57,57,57 | 0 |
| 54 | MG | DA | 3045 | 1/1 | 0.95 | 0.30 | - | 48,48,48,48 | 0 |
| 54 | MG | DA | 3065 | 1/1 | 0.81 | 0.36 | - | 56,56,56,56 | 0 |
| 54 | MG | DA | 3063 | 1/1 | 0.97 | 0.26 | - | 79,79,79,79 | 0 |
| 54 | MG | BA | 2954 | 1/1 | 0.95 | 0.19 | - | 52,52,52,52 | 0 |
| 54 | MG | BA | 3023 | 1/1 | 0.82 | 0.51 | - | 64,64,64,64 | 0 |
| 54 | MG | CA | 1649 | 1/1 | 0.96 | 0.22 | - | 80,80,80,80 | 0 |
| 54 | MG | DA | 3300 | 1/1 | 0.76 | 0.21 | - | 68,68,68,68 | 0 |
| 54 | MG | BA | 3196 | 1/1 | 0.96 | 0.23 | - | 51,51,51,51 | 0 |
| 54 | MG | DA | 3270 | 1/1 | 0.95 | 0.29 | - | 81,81,81,81 | 0 |
| 54 | MG | CA | 1679 | 1/1 | 0.92 | 0.12 | - | 93,93,93,93 | 0 |
| 54 | MG | BA | 3147 | 1/1 | 0.91 | 0.32 | - | 72,72,72,72 | 0 |
| 54 | MG | BA | 3221 | 1/1 | 0.85 | 0.34 | - | 48,48,48,48 | 0 |
| 54 | MG | DA | 3019 | 1/1 | 0.94 | 0.36 | - | 51,51,51,51 | 0 |
| 54 | MG | BA | 3031 | 1/1 | 0.82 | 0.83 | - | 87,87,87,87 | 0 |
| 54 | MG | BA | 3228 | 1/1 | 0.93 | 0.12 | - | 66,66,66,66 | 0 |
| 54 | MG | BA | 3116 | 1/1 | 0.86 | 0.39 | - | 85,85,85,85 | 0 |
| 54 | MG | CA | 1712 | 1/1 | 0.97 | 0.11 | - | 78,78,78,78 | 0 |
| 54 | MG | DA | 3265 | 1/1 | 0.65 | 0.32 | - | 120,120,120,120 | 0 |
| 54 | MG | AA | 1733 | 1/1 | 0.93 | 0.22 | - | 91,91,91,91 | 0 |
| 54 | MG | DA | 3058 | 1/1 | 0.95 | 0.11 | - | 54,54,54,54 | 0 |
| 54 | MG | DA | 2963 | 1/1 | 0.94 | 0.39 | - | 53,53,53,53 | 0 |
| 54 | MG | BA | 3025 | 1/1 | 0.57 | 0.30 | - | 65,65,65,65 | 0 |
| 54 | MG | CA | 1639 | 1/1 | 0.51 | 0.63 | - | 66,66,66,66 | 0 |
| 54 | MG | DA | 2953 | 1/1 | 0.93 | 0.45 | - | 58,58,58,58 | 0 |
| 54 | MG | DB | 201 | 1/1 | 0.96 | 0.24 | - | 63,63,63,63 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | BA | 3092 | 1/1 | 0.93 | 0.17 | - | 63,63,63,63 | 0 |
| 54 | MG | CA | 1650 | 1/1 | 0.73 | 0.31 | - | 108,108,108,108 | 0 |
| 54 | MG | AA | 1606 | 1/1 | 0.98 | 0.36 | - | 53,53,53,53 | 0 |
| 54 | MG | AA | 1633 | 1/1 | 0.95 | 0.15 | - | 73,73,73,73 | 0 |
| 54 | MG | DA | 2997 | 1/1 | 0.98 | 0.17 | - | 35,35,35,35 | 0 |
| 54 | MG | AA | 1688 | 1/1 | 0.91 | 0.14 | - | 68,68,68,68 | 0 |
| 54 | MG | DA | 3107 | 1/1 | 0.92 | 0.27 | - | 67,67,67,67 | 0 |
| 54 | MG | DA | 3333 | 1/1 | 0.94 | 0.15 | - | 126,126,126,126 | 0 |
| 54 | MG | DA | 3229 | 1/1 | 0.73 | 0.42 | - | 64,64,64,64 | 0 |
| 54 | MG | DA | 3111 | 1/1 | 0.80 | 0.39 | - | 67,67,67,67 | 0 |
| 54 | MG | CA | 1656 | 1/1 | 0.92 | 0.14 | - | 79,79,79,79 | 0 |
| 54 | MG | BA | 3258 | 1/1 | 0.85 | 0.21 | - | 104,104,104,104 | 0 |
| 54 | MG | DA | 2952 | 1/1 | 0.93 | 0.30 | - | 50,50,50,50 | 0 |
| 54 | MG | DA | 3141 | 1/1 | 0.82 | 0.14 | - | 95,95,95,95 | 0 |
| 54 | MG | AA | 1706 | 1/1 | 0.72 | 0.38 | - | 103,103,103,103 | 0 |
| 54 | MG | AA | 1646 | 1/1 | 0.68 | 0.25 | - | 99,99,99,99 | 0 |
| 54 | MG | DA | 3308 | 1/1 | 0.67 | 0.37 | - | 91,91,91,91 | 0 |
| 54 | MG | BA | 3298 | 1/1 | 0.92 | 0.10 | - | 74,74,74,74 | 0 |
| 54 | MG | BA | 2963 | 1/1 | 0.87 | 0.19 | - | 54,54,54,54 | 0 |
| 54 | MG | CA | 1740 | 1/1 | 0.54 | 0.24 | - | 117,117,117,117 | 0 |
| 54 | MG | AA | 1623 | 1/1 | 0.63 | 0.39 | - | 93,93,93,93 | 0 |
| 54 | MG | BA | 3123 | 1/1 | 0.74 | 0.36 | - | 52,52,52,52 | 0 |
| 54 | MG | BA | 3132 | 1/1 | 0.94 | 0.20 | - | 79,79,79,79 | 0 |
| 54 | MG | BA | 2955 | 1/1 | 0.92 | 0.19 | - | 50,50,50,50 | 0 |
| 54 | MG | CA | 1675 | 1/1 | 0.94 | 0.28 | - | 107,107,107,107 | 0 |
| 54 | MG | BA | 3073 | 1/1 | 0.47 | 0.28 | - | 89,89,89,89 | 0 |
| 54 | MG | BA | 3109 | 1/1 | 0.71 | 0.83 | - | 90,90,90,90 | 0 |
| 54 | MG | DA | 2937 | 1/1 | 0.98 | 0.55 | - | 25,25,25,25 | 0 |
| 54 | MG | DA | 3104 | 1/1 | 0.96 | 0.27 | - | 99,99,99,99 | 0 |
| 54 | MG | DA | 3169 | 1/1 | 0.80 | 0.12 | - | 112,112,112,112 | 0 |
| 54 | MG | BA | 3079 | 1/1 | 0.60 | 0.43 | - | 86,86,86,86 | 0 |
| 54 | MG | DA | 3326 | 1/1 | 0.94 | 0.18 | - | 85,85,85,85 | 0 |
| 54 | MG | AA | 1762 | 1/1 | 0.74 | 0.10 | - | 155,155,155,155 | 0 |
| 54 | MG | AA | 1610 | 1/1 | 0.70 | 0.28 | - | 78,78,78,78 | 0 |
| 54 | MG | BA | 2994 | 1/1 | 0.94 | 0.65 | - | 56,56,56,56 | 0 |
| 54 | MG | DA | 3177 | 1/1 | 0.84 | 0.32 | - | 62,62,62,62 | 0 |
| 54 | MG | BA | 3037 | 1/1 | 0.81 | 0.14 | - | 93,93,93,93 | 0 |
| 54 | MG | DA | 2940 | 1/1 | 0.75 | 0.71 | - | 51,51,51,51 | 0 |
| 54 | MG | DA | 3285 | 1/1 | 0.88 | 0.34 | - | 113,113,113,113 | 0 |
| 54 | MG | BA | 3141 | 1/1 | 0.43 | 0.17 | - | 78,78,78,78 | 0 |
| 54 | MG | CA | 1661 | 1/1 | 0.94 | 0.48 | - | 92,92,92,92 | 0 |
| 54 | MG | DA | 3031 | 1/1 | 0.94 | 0.07 | - | 62,62,62,62 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | CA | 1710 | 1/1 | 0.91 | 0.18 | - | 119,119,119,119 | 0 |
| 54 | MG | AA | 1712 | 1/1 | 0.84 | 0.50 | - | 75,75,75,75 | 0 |
| 54 | MG | BA | 3187 | 1/1 | 0.92 | 0.46 | - | 40,40,40,40 | 0 |
| 54 | MG | AA | 1616 | 1/1 | 0.94 | 0.19 | - | 63,63,63,63 | 0 |
| 54 | MG | DA | 3057 | 1/1 | 0.77 | 0.22 | - | 59,59,59,59 | 0 |
| 54 | MG | DB | 209 | 1/1 | 0.77 | 0.12 | - | 75,75,75,75 | 0 |
| 54 | MG | DA | 3332 | 1/1 | 0.74 | 0.45 | - | 60,60,60,60 | 0 |
| 54 | MG | AA | 1670 | 1/1 | 0.95 | 0.14 | - | 85,85,85,85 | 0 |
| 54 | MG | BA | 3121 | 1/1 | 0.93 | 0.26 | - | 77,77,77,77 | 0 |
| 54 | MG | BA | 2942 | 1/1 | 0.95 | 0.35 | - | 22,22,22,22 | 0 |
| 54 | MG | BA | 3119 | 1/1 | 0.82 | 0.28 | - | 64,64,64,64 | 0 |
| 54 | MG | CA | 1694 | 1/1 | 0.86 | 0.32 | - | 59,59,59,59 | 0 |
| 54 | MG | CA | 1678 | 1/1 | 0.94 | 0.11 | - | 107,107,107,107 | 0 |
| 54 | MG | CA | 1621 | 1/1 | 0.78 | 0.39 | - | 67,67,67,67 | 0 |
| 54 | MG | BA | 3026 | 1/1 | 0.81 | 0.39 | - | 82,82,82,82 | 0 |
| 54 | MG | DA | 3227 | 1/1 | 0.97 | 0.31 | - | 34,34,34,34 | 0 |
| 54 | MG | CA | 1729 | 1/1 | 0.97 | 0.17 | - | 98,98,98,98 | 0 |
| 54 | MG | BA | 2997 | 1/1 | 0.92 | 0.38 | - | 57,57,57,57 | 0 |
| 54 | MG | BA | 3247 | 1/1 | 0.99 | 0.15 | - | 52,52,52,52 | 0 |
| 54 | MG | BA | 3105 | 1/1 | 0.91 | 0.21 | - | 60,60,60,60 | 0 |
| 54 | MG | CA | 1665 | 1/1 | 0.94 | 0.25 | - | 89,89,89,89 | 0 |
| 54 | MG | DA | 2973 | 1/1 | 0.97 | 0.30 | - | 50,50,50,50 | 0 |
| 54 | MG | DB | 208 | 1/1 | 0.87 | 0.31 | - | 96,96,96,96 | 0 |
| 54 | MG | DA | 3080 | 1/1 | 0.72 | 0.41 | - | 69,69,69,69 | 0 |
| 54 | MG | BA | 3033 | 1/1 | 0.80 | 0.19 | - | 67,67,67,67 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.