



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:51 PM GMT

PDB ID : 1Q86
Title : Crystal structure of CCA-Phe-cap-biotin bound simultaneously at half occupancy to both the A-site and P-site of the the 50S ribosomal Subunit.
Authors : Hansen, J.L.; Schmeing, T.M.; Moore, P.B.; Steitz, T.A.
Deposited on : 2003-08-20
Resolution : 3.00 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:

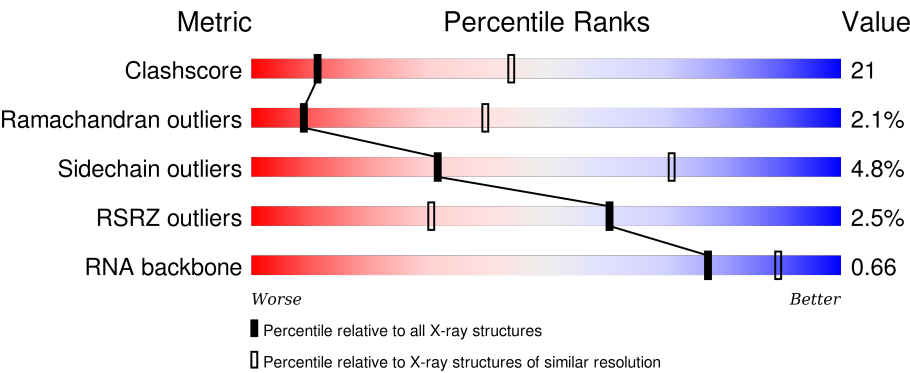
MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.




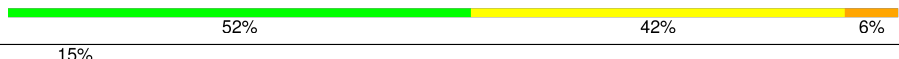
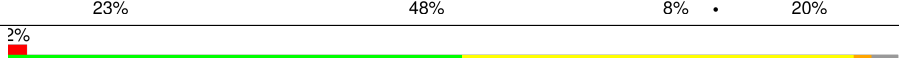


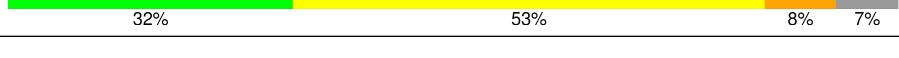
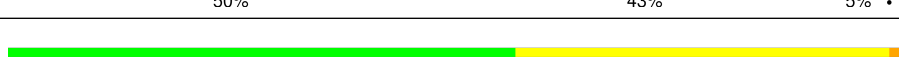

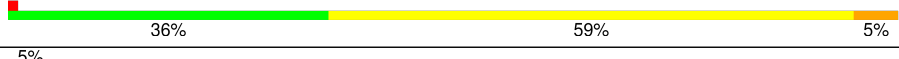

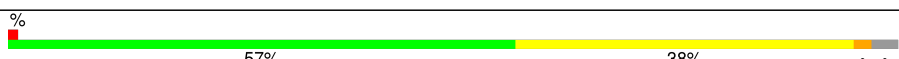



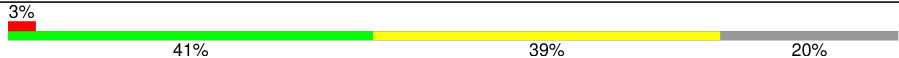

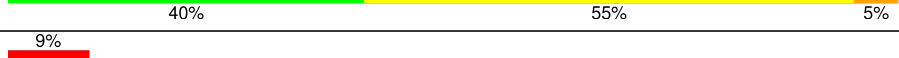
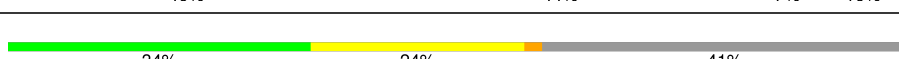





| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Clashscore | 102246 | 1912 (3.00-3.00) |
| Ramachandran outliers | 100387 | 1853 (3.00-3.00) |
| Sidechain outliers | 100360 | 1856 (3.00-3.00) |
| RSRZ outliers | 91569 | 1592 (3.00-3.00) |
| RNA backbone | 2183 | 1036 (3.40-2.60) |

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 | A | 2922 | <div><div>2%</div><div><div></div><div>53%</div><div>35%</div><div>5%</div><div>6%</div></div></div> |
| 2 | B | 122 | <div><div>5%</div><div><div></div><div>48%</div><div>39%</div><div>11%</div><div></div></div></div> |
| 3 | 5 | 3 | <div><div>33%</div><div><div></div><div>33%</div><div>33%</div><div>33%</div></div></div> |
| 3 | 6 | 3 | <div><div>100%</div><div><div></div><div>100%</div></div></div> |
| 4 | C | 239 | <div><div>3%</div><div><div></div><div>57%</div><div>36%</div><div>6%</div><div></div></div></div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 5 | D | 337 |  |
| 6 | E | 246 |  |
| 7 | F | 176 |  |
| 8 | G | 177 |  |
| 9 | H | 119 |  |
| 10 | I | 348 |  |
| 11 | J | 167 |  |
| 12 | K | 145 |  |
| 13 | L | 132 |  |
| 14 | M | 164 |  |
| 15 | N | 194 |  |
| 16 | O | 186 |  |
| 17 | P | 115 |  |
| 18 | Q | 148 |  |
| 19 | R | 95 |  |
| 20 | S | 154 |  |
| 21 | T | 84 |  |
| 22 | U | 119 |  |
| 23 | V | 66 |  |
| 24 | W | 70 |  |
| 25 | X | 154 |  |
| 26 | Y | 91 |  |
| 27 | Z | 240 |  |
| 28 | 1 | 73 | |
| 29 | 2 | 56 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 30 | 3 | 48 | |
| 31 | 4 | 92 | |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 32 | MG | 6 | 8118 | - | - | - | X |
| 32 | MG | A | 8049 | - | - | - | X |
| 32 | MG | A | 8112 | - | - | - | X |
| 33 | K | A | 8201 | - | - | - | X |
| 34 | NA | A | 8305 | - | - | - | X |
| 34 | NA | A | 8320 | - | - | - | X |
| 34 | NA | A | 8321 | - | - | - | X |
| 34 | NA | A | 8323 | - | - | - | X |
| 34 | NA | A | 8325 | - | - | - | X |
| 34 | NA | A | 8326 | - | - | - | X |
| 34 | NA | A | 8332 | - | - | - | X |
| 34 | NA | A | 8339 | - | - | - | X |
| 34 | NA | A | 8340 | - | - | - | X |
| 34 | NA | A | 8350 | - | - | - | X |
| 34 | NA | A | 8356 | - | - | - | X |
| 34 | NA | A | 8359 | - | - | - | X |
| 34 | NA | A | 8361 | - | - | - | X |
| 34 | NA | A | 8362 | - | - | - | X |
| 34 | NA | A | 8366 | - | - | - | X |
| 34 | NA | A | 8367 | - | - | - | X |
| 34 | NA | A | 8371 | - | - | - | X |
| 34 | NA | A | 8372 | - | - | - | X |
| 34 | NA | A | 8373 | - | - | - | X |
| 34 | NA | A | 8374 | - | - | - | X |
| 34 | NA | A | 8376 | - | - | - | X |
| 34 | NA | A | 8377 | - | - | - | X |
| 34 | NA | A | 8378 | - | - | - | X |
| 34 | NA | A | 8382 | - | - | - | X |
| 34 | NA | B | 8383 | - | - | - | X |
| 34 | NA | K | 8346 | - | - | - | X |
| 34 | NA | M | 8380 | - | - | - | X |
| 34 | NA | N | 8365 | - | - | - | X |
| 34 | NA | S | 8386 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 35 | CL | A | 8515 | - | - | - | X |
| 35 | CL | D | 8519 | - | - | - | X |
| 36 | PHA | 5 | 77 | - | - | - | X |

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 98659 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 23S ribosomal rna.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 1 | A | 2754 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 59017 | 26346 | 10878 | 19048 | 2745 | | | |

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 2 | B | 122 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2600 | 1160 | 472 | 847 | 121 | | | |

- Molecule 3 is a RNA chain called CCA-phenylalanine-carboxylic-acid-biotin.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 3 | 5 | 3 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 59 | 28 | 11 | 18 | 2 | | | |
| 3 | 6 | 3 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 59 | 28 | 11 | 18 | 2 | | | |

- Molecule 4 is a protein called 50S ribosomal protein L2P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4 | C | 237 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1754 | 1072 | 352 | 325 | 5 | | | |

- Molecule 5 is a protein called 50S ribosomal protein L3P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5 | D | 337 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2624 | 1616 | 493 | 510 | 5 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| D | ? | - | PRO | DELETION | UNP P20279 |
| D | 310 | ARG | PHE | CONFLICT | UNP P20279 |

- Molecule 6 is a protein called 50S ribosomal protein L4E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 6 | E | 246 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1858 | 1131 | 344 | 382 | 1 | | | |

- Molecule 7 is a protein called 50S ribosomal protein L5P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | F | 140 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1094 | 685 | 195 | 210 | 4 | | | |

- Molecule 8 is a protein called 50S ribosomal protein L6P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | G | 172 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1357 | 840 | 224 | 289 | 4 | | | |

- Molecule 9 is a protein called 50S ribosomal protein L7Ae.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9 | H | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 885 | 552 | 141 | 191 | 1 | | | |

- Molecule 10 is a protein called Acidic ribosomal protein P0 homolog.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 10 | I | 29 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 240 | 149 | 39 | 51 | 1 | | | |

- Molecule 11 is a protein called L10 Ribosomal Protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | J | 156 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1215 | 766 | 233 | 212 | 4 | | | |

- Molecule 12 is a protein called 50S ribosomal protein L13P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | K | 142 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1119 | 696 | 199 | 221 | 3 | | | |

- Molecule 13 is a protein called 50S ribosomal protein L14P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | L | 132 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 993 | 609 | 189 | 191 | 4 | | | |

- Molecule 14 is a protein called 50S ribosomal protein L15P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14 | M | 145 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1114 | 668 | 222 | 224 | | | | |

- Molecule 15 is a protein called L15 Ribosomal Protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15 | N | 194 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1605 | 988 | 346 | 266 | 5 | | | |

- Molecule 16 is a protein called 50S ribosomal protein L18P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | O | 186 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1444 | 895 | 262 | 285 | 2 | | | |

- Molecule 17 is a protein called 50S ribosomal protein L18e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17 | P | 115 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 864 | 529 | 161 | 174 | | | | |

- Molecule 18 is a protein called 50S ribosomal protein L19E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 18 | Q | 143 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1133 | 680 | 230 | 223 | | | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| Q | 71 | LYS | TYR | CONFLICT | UNP P14119 |

- Molecule 19 is a protein called 50S ribosomal protein L21e.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 19 | R | 95 | Total | C | N | O | 0 | 0 | 0 |
| | | | 734 | 450 | 141 | 143 | | | |

- Molecule 20 is a protein called 50S ribosomal protein L22P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | S | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1149 | 713 | 209 | 223 | 4 | | | |

- Molecule 21 is a protein called 50S ribosomal protein L23P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 21 | T | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 641 | 389 | 111 | 138 | 3 | | | |

- Molecule 22 is a protein called 50S ribosomal protein L24P.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 22 | U | 119 | Total | C | N | O | 0 | 0 | 0 |
| | | | 949 | 568 | 180 | 201 | | | |

- Molecule 23 is a protein called 50S ribosomal protein L24E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 23 | V | 53 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 410 | 244 | 75 | 86 | 5 | | | |

- Molecule 24 is a protein called 50S ribosomal protein L29P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|---------|-------|
| 24 | W | 65 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 499 | 304 | 94 | 100 | 1 | | | |

- Molecule 25 is a protein called 50S ribosomal protein L30P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 25 | X | 154 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1195 | 737 | 209 | 243 | 6 | | | |

- Molecule 26 is a protein called 50S ribosomal protein L31e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26 | Y | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 654 | 402 | 129 | 122 | 1 | | | |

- Molecule 27 is a protein called 50S ribosomal protein L32E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 27 | Z | 142 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1130 | 686 | 228 | 216 | | | | |

- Molecule 28 is a protein called L37Ae 50S ribosomal protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 28 | 1 | 73 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 563 | 359 | 111 | 86 | 7 | | | |

- Molecule 29 is a protein called 50S ribosomal protein L37e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 29 | 2 | 56 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 430 | 258 | 86 | 82 | 4 | | | |

- Molecule 30 is a protein called 50S ribosomal protein L39e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 30 | 3 | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 393 | 238 | 86 | 68 | 1 | | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| 3 | ? | - | ARG | DELETION | UNP P22452 |

- Molecule 31 is a protein called 50S ribosomal protein L44E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31 | 4 | 92 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 755 | 458 | 153 | 137 | 7 | | | |

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 32 | 1 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | D | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 32 | B | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | C | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | 6 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | Z | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | A | 108 | Total | Mg | 0 | 0 |
| | | | 108 | 108 | | |
| 32 | 4 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | U | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | L | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 33 | A | 2 | Total | K | 0 | 0 |
| | | | 2 | 2 | | |

- Molecule 34 is SODIUM ION (three-letter code: NA) (formula: Na).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 34 | J | 2 | Total | Na | 0 | 0 |
| | | | 2 | 2 | | |
| 34 | K | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 34 | E | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|----------|---------|---------|
| 34 | B | 2 | Total 2 | Na 2 | 0 | 0 |
| 34 | C | 1 | Total 1 | Na 1 | 0 | 0 |
| 34 | A | 70 | Total 70 | Na 70 | 0 | 0 |
| 34 | T | 1 | Total 1 | Na 1 | 0 | 0 |
| 34 | N | 2 | Total 2 | Na 2 | 0 | 0 |
| 34 | U | 1 | Total 1 | Na 1 | 0 | 0 |
| 34 | R | 1 | Total 1 | Na 1 | 0 | 0 |
| 34 | S | 3 | Total 3 | Na 3 | 0 | 0 |
| 34 | M | 1 | Total 1 | Na 1 | 0 | 0 |

- Molecule 35 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

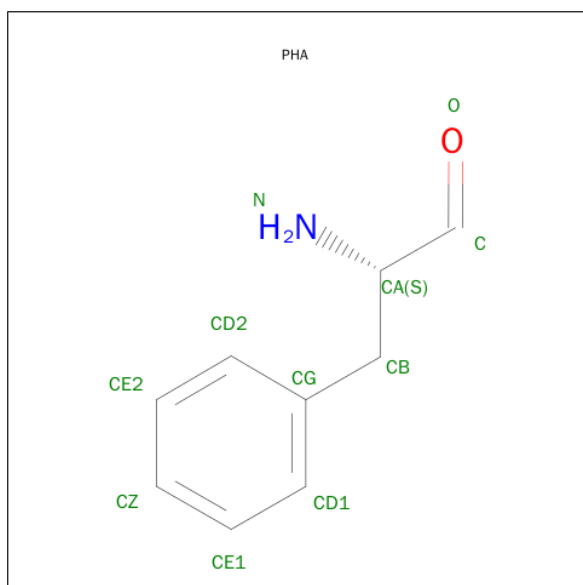
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 35 | P | 1 | Total 1 | Cl 1 | 0 | 0 |
| 35 | D | 1 | Total 1 | Cl 1 | 0 | 0 |
| 35 | K | 3 | Total 3 | Cl 3 | 0 | 0 |
| 35 | C | 1 | Total 1 | Cl 1 | 0 | 0 |
| 35 | Z | 1 | Total 1 | Cl 1 | 0 | 0 |
| 35 | A | 9 | Total 9 | Cl 9 | 0 | 0 |
| 35 | 4 | 1 | Total 1 | Cl 1 | 0 | 0 |
| 35 | N | 1 | Total 1 | Cl 1 | 0 | 0 |
| 35 | O | 1 | Total 1 | Cl 1 | 0 | 0 |
| 35 | L | 1 | Total 1 | Cl 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 35 | S | 1 | Total Cl 1 1 | 0 | 0 |
| 35 | M | 1 | Total Cl 1 1 | 0 | 0 |

- Molecule 36 is PHENYLALANINAL (three-letter code: PHA) (formula: C₉H₁₁NO).



| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-------------------------|---------|---------|
| 36 | 5 | 1 | Total C N O 11 9 1 1 | 0 | 0 |
| 36 | 6 | 1 | Total C O 10 9 1 | 0 | 0 |

- Molecule 37 is CADMIUM ION (three-letter code: CD) (formula: Cd).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 37 | P | 1 | Total Cd 1 1 | 0 | 0 |
| 37 | 2 | 1 | Total Cd 1 1 | 0 | 0 |
| 37 | 1 | 1 | Total Cd 1 1 | 0 | 0 |
| 37 | 4 | 1 | Total Cd 1 1 | 0 | 0 |
| 37 | V | 1 | Total Cd 1 1 | 0 | 0 |

- Molecule 38 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|---------------|-----------|---------|---------|
| 38 | A | 5892 | Total 5892 | O 5892 | 0 | 0 |
| 38 | B | 139 | Total 139 | O 139 | 0 | 0 |
| 38 | C | 116 | Total 116 | O 116 | 0 | 0 |
| 38 | D | 149 | Total 149 | O 149 | 0 | 0 |
| 38 | E | 173 | Total 173 | O 173 | 0 | 0 |
| 38 | F | 52 | Total 52 | O 52 | 0 | 0 |
| 38 | G | 43 | Total 43 | O 43 | 0 | 0 |
| 38 | H | 27 | Total 27 | O 27 | 0 | 0 |
| 38 | I | 21 | Total 21 | O 21 | 0 | 0 |
| 38 | J | 77 | Total 77 | O 77 | 0 | 0 |
| 38 | K | 54 | Total 54 | O 54 | 0 | 0 |
| 38 | L | 62 | Total 62 | O 62 | 0 | 0 |
| 38 | M | 82 | Total 82 | O 82 | 0 | 0 |
| 38 | N | 139 | Total 139 | O 139 | 0 | 0 |
| 38 | O | 70 | Total 70 | O 70 | 0 | 0 |
| 38 | P | 43 | Total 43 | O 43 | 0 | 0 |
| 38 | Q | 67 | Total 67 | O 67 | 0 | 0 |
| 38 | R | 54 | Total 54 | O 54 | 0 | 0 |
| 38 | S | 84 | Total 84 | O 84 | 0 | 0 |
| 38 | T | 37 | Total 37 | O 37 | 0 | 0 |
| 38 | U | 44 | Total 44 | O 44 | 0 | 0 |

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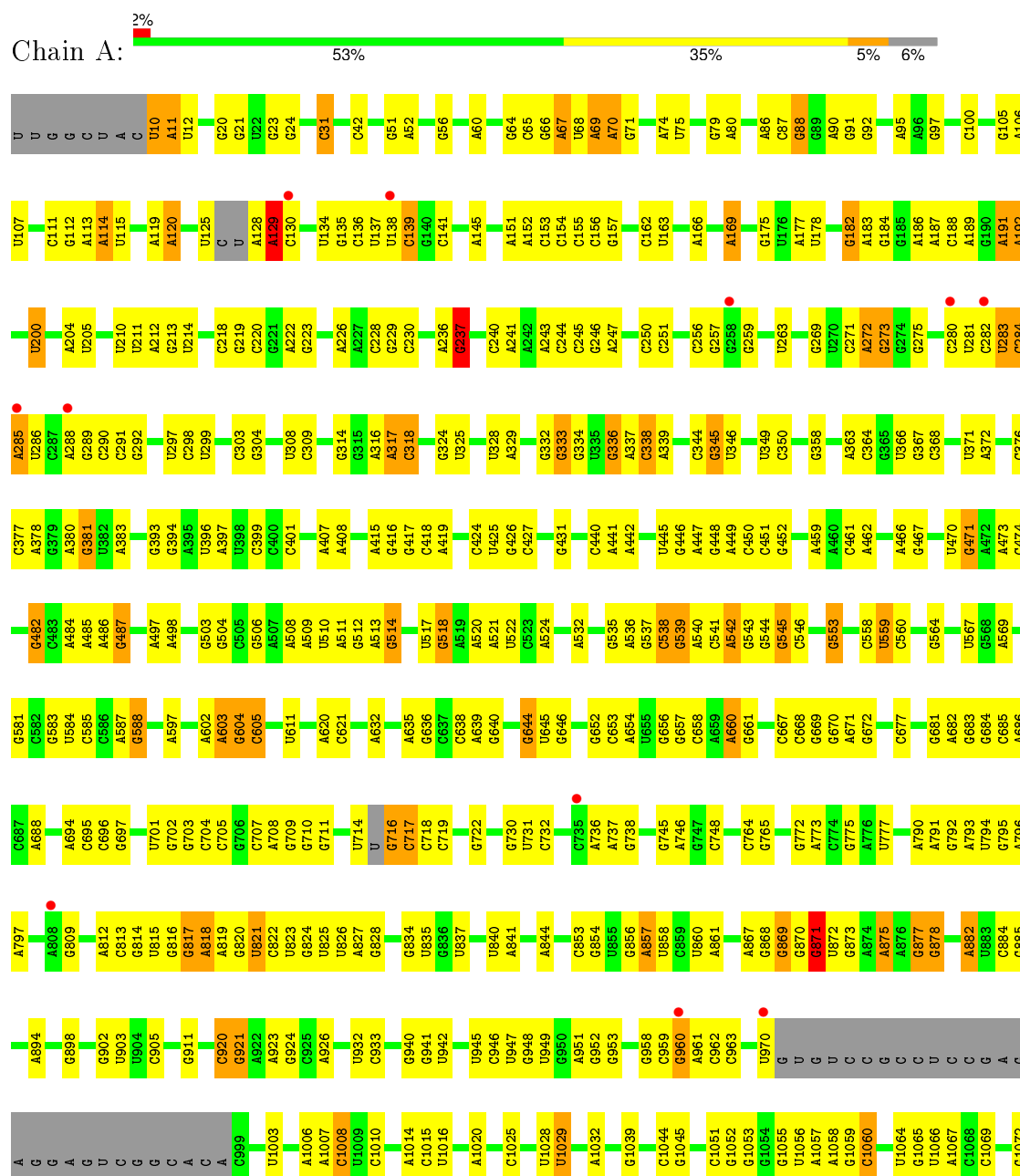
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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 38 | V | 24 | Total 24 | O 24 | 0 | 0 |
| 38 | W | 14 | Total 14 | O 14 | 0 | 0 |
| 38 | X | 71 | Total 71 | O 71 | 0 | 0 |
| 38 | Y | 31 | Total 31 | O 31 | 0 | 0 |
| 38 | Z | 93 | Total 93 | O 93 | 0 | 0 |
| 38 | 1 | 37 | Total 37 | O 37 | 0 | 0 |
| 38 | 2 | 63 | Total 63 | O 63 | 0 | 0 |
| 38 | 3 | 41 | Total 41 | O 41 | 0 | 0 |
| 38 | 4 | 70 | Total 70 | O 70 | 0 | 0 |

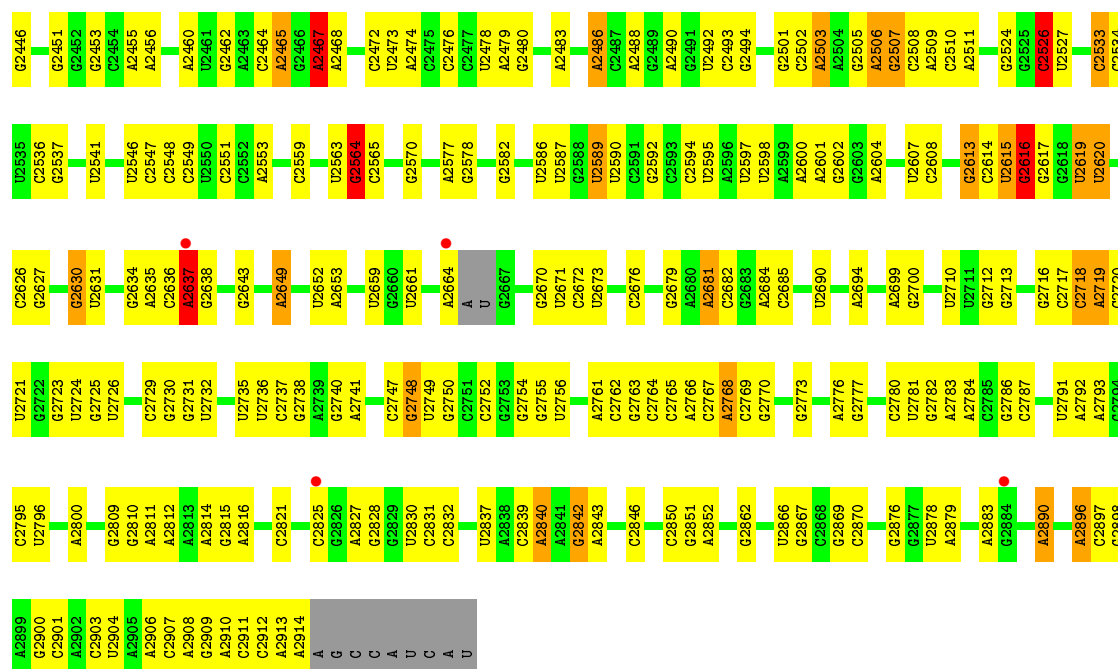
3 Residue-property plots

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.

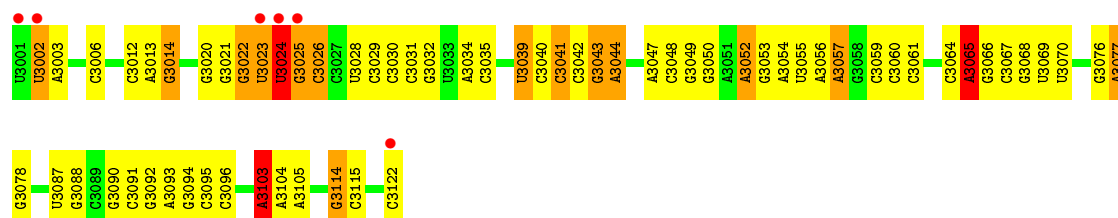
- Molecule 1: 23S ribosomal rna



| | | | | | | | | | | | | |
|-------|-------|---|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| U2358 | G2270 | A | U1940 | U1835 | A1746 | A1656 | U1581 | C1462 | C1360 | U1244 | G1172 | A1078 |
| G2359 | G2271 | G | A1941 | A1840 | A1747 | A1657 | C1562 | A1463 | C1365 | C1245 | A1173 | A1079 |
| G2360 | G2272 | C | A1942 | C1841 | G1751 | C1666 | G1563 | A1468 | C1366 | A1246 | G1174 | C1080 |
| A2361 | G2273 | A | C1943 | G1752 | G1752 | C1667 | C1564 | G1469 | C1367 | U1249 | G1175 | C1176 |
| G2362 | G2274 | A | G1944 | A1845 | A1755 | U1668 | C1565 | A1470 | A1372 | C1250 | A1177 | A1081 |
| G2363 | G2275 | C | G1945 | U1846 | G1756 | A1669 | G1568 | A1471 | C1377 | C1251 | U1180 | A1086 |
| A2364 | U2276 | A | G1946 | G1847 | G1757 | G1670 | U1569 | A1472 | C1378 | A1252 | A1181 | A1088 |
| G2365 | U2277 | U | G1947 | G1848 | U1761 | C1675 | A1573 | A1473 | U1380 | C1262 | G1182 | A1097 |
| A2366 | C2281 | G | G1951 | U1850 | C1762 | C1676 | A1574 | A1474 | C1381 | U1266 | U1185 | A1098 |
| U2377 | U2282 | U | U | G1851 | C1763 | C1677 | A1580 | C1477 | C1382 | U1267 | C1186 | G1099 |
| U2378 | G2289 | A | A | A1852 | U1766 | C1678 | A1581 | U1478 | C1383 | U1268 | U1187 | U1109 |
| G2379 | U2290 | A | C | C1853 | A1767 | G1681 | G1589 | A1482 | C1384 | C1269 | A1188 | G1110 |
| A2380 | G2291 | U | U | G1854 | C1768 | A1682 | G1590 | C1483 | C1385 | U1270 | A1189 | U1114 |
| G2381 | U2069 | A | A | C1855 | C1769 | G1683 | G1591 | C1484 | U1388 | U1271 | A1190 | U1115 |
| G2382 | G2070 | U | U | G1856 | U1770 | A1684 | G1592 | C1485 | C1389 | A1271 | A1191 | U1116 |
| G2383 | C2071 | A | G | A1857 | U1771 | A1685 | C1594 | G1486 | A1390 | C1272 | A1192 | A1117 |
| U2384 | G2072 | C | A | C1858 | C1772 | C1686 | G1595 | U1488 | C1391 | C1273 | A1193 | G1118 |
| G2385 | G2073 | C | C | C1859 | G1773 | C1687 | U1596 | A1489 | C1392 | U1278 | U1197 | U1120 |
| A2386 | U2078 | U | U1964 | G1861 | A1778 | C1688 | A1597 | A1490 | C1393 | A1279 | U1198 | A1123 |
| U2387 | G2079 | G | C1965 | C1862 | A1779 | C1689 | U1598 | A1491 | C1394 | U1285 | A1200 | C1127 |
| C2388 | G2080 | A | U1966 | G1863 | U1780 | C1690 | A1599 | A1492 | U1286 | U1287 | C1201 | U1206 |
| A2389 | A2081 | G | U1967 | G1864 | A1781 | C1691 | U1603 | C1493 | C1400 | U1288 | C1202 | C1128 |
| C2390 | G2310 | C | U1968 | G1865 | U1782 | C1692 | G1604 | A1494 | A1407 | U1289 | C1203 | G1129 |
| G2391 | G2311 | G | G1971 | G1866 | U1783 | C1693 | A1605 | A1495 | C1408 | G1290 | U1204 | U1130 |
| C2392 | G2312 | U | U1972 | G1867 | U1784 | C1694 | A1606 | C1496 | U1417 | U1291 | U1205 | G1131 |
| G2393 | G2313 | C | G1973 | G1868 | U1785 | C1695 | A1607 | C1497 | U1418 | U1292 | U1206 | G1132 |
| A2394 | G2314 | A | G1974 | G1869 | U1786 | C1696 | A1608 | C1498 | U1419 | U1293 | A1207 | A1133 |
| C2395 | G2315 | A | G1975 | G1870 | U1787 | C1697 | A1609 | C1499 | U1420 | U1294 | G1210 | G1134 |
| G2396 | G2316 | C | G1976 | G1871 | U1788 | C1698 | A1610 | U1500 | C1421 | U1304 | G1211 | G1135 |
| C2397 | G2317 | U | G1977 | G1872 | U1789 | C1699 | A1611 | A1501 | C1422 | C1305 | G1212 | U1136 |
| U2398 | G2318 | C | U1978 | G1873 | U1790 | C1700 | A1612 | U1502 | A1423 | U1306 | G1213 | G1137 |
| G2399 | G2319 | G | U1979 | G1874 | C1791 | C1701 | A1613 | U1503 | C1424 | U1307 | G1214 | U1138 |
| A2400 | G2320 | A | U1980 | G1875 | U1792 | C1702 | A1614 | A1504 | U1425 | G1311 | A1215 | G1139 |
| C2401 | G2321 | C | U1981 | G1876 | U1793 | C1703 | A1615 | U1505 | C1426 | G1312 | G1216 | C1140 |
| G2402 | G2322 | U | G1982 | G1877 | U1794 | C1704 | A1616 | U1506 | A1427 | G1313 | G1217 | G1151 |
| U2403 | G2323 | C | G1983 | G1878 | U1795 | C1705 | A1617 | C1513 | C1438 | G1314 | C1224 | A1154 |
| A2404 | G2324 | A | U1984 | G1879 | U1796 | C1706 | A1618 | C1514 | C1439 | G1315 | C1225 | G1155 |
| G2405 | G2325 | C | U1985 | G1880 | U1797 | C1707 | A1619 | U1517 | U1440 | G1316 | C1226 | G1156 |
| U2406 | G2326 | U | G1986 | G1881 | U1798 | C1708 | A1620 | C1518 | C1441 | G1317 | C1227 | G1157 |
| C2407 | G2327 | C | U1987 | G1882 | U1799 | C1709 | A1621 | U1519 | C1442 | G1318 | C1228 | G1158 |
| U2408 | G2328 | A | U1988 | G1883 | U1800 | C1710 | A1622 | C1520 | C1443 | G1319 | C1229 | G1159 |
| G2409 | G2329 | C | U1989 | G1884 | U1801 | C1711 | A1623 | U1521 | C1444 | G1320 | A1230 | G1160 |
| A2410 | G2330 | U | U1990 | G1885 | U1802 | C1712 | A1624 | C1522 | C1445 | G1321 | A1231 | A1161 |
| C2411 | G2331 | C | U1991 | G1886 | U1803 | C1713 | A1625 | U1523 | C1446 | G1322 | G1232 | G1162 |
| U2412 | G2332 | A | U1992 | G1887 | U1804 | C1714 | A1626 | C1524 | C1447 | G1323 | U1233 | G1163 |
| G2413 | G2333 | C | U1993 | G1888 | U1805 | C1715 | A1627 | U1525 | C1448 | G1324 | A1234 | U1164 |
| A2414 | G2334 | U | U1994 | G1889 | U1806 | C1716 | A1628 | C1526 | C1449 | G1325 | G1235 | G1165 |
| G2415 | G2335 | C | U1995 | G1890 | U1807 | C1717 | A1629 | U1527 | C1450 | G1326 | U1236 | G1166 |
| U2416 | G2336 | A | U1996 | G1891 | U1808 | C1718 | A1630 | C1528 | C1451 | G1327 | C1237 | G1167 |
| C2417 | G2337 | C | U1997 | G1892 | U1809 | C1719 | A1631 | U1529 | C1452 | G1328 | C1238 | C1168 |
| U2418 | G2338 | U | U1998 | G1893 | U1810 | C1720 | A1632 | C1530 | C1453 | G1329 | G1239 | U1169 |
| G2419 | G2339 | C | U1999 | G1894 | U1811 | C1721 | A1633 | U1531 | C1454 | G1330 | A1242 | U1170 |
| U2420 | G2340 | A | U2000 | G1895 | U1812 | C1722 | A1634 | C1532 | C1455 | G1331 | C1243 | A1171 |
| C2421 | G2341 | C | U2001 | G1896 | U1813 | C1723 | A1635 | U1533 | C1456 | G1332 | | |
| U2422 | G2342 | U | U2002 | G1897 | U1814 | C1724 | A1636 | C1534 | C1457 | G1333 | | |
| G2423 | G2343 | C | U2003 | G1898 | U1815 | C1725 | A1637 | U1535 | C1458 | G1334 | | |
| A2424 | G2344 | A | U2004 | G1899 | U1816 | C1726 | A1638 | C1536 | C1459 | G1335 | | |
| C2425 | G2345 | C | U2005 | G1900 | U1817 | C1727 | A1639 | U1537 | C1460 | G1336 | | |
| U2426 | G2346 | U | U2006 | G1901 | U1818 | C1728 | A1640 | C1538 | C1461 | G1337 | | |
| C2427 | G2347 | C | U2007 | G1902 | U1819 | C1729 | A1641 | U1539 | C1462 | G1338 | | |
| U2428 | G2348 | A | U2008 | G1903 | U1820 | C1730 | A1642 | C1540 | C1463 | G1339 | | |
| G2429 | G2349 | C | U2009 | G1904 | U1821 | C1731 | A1643 | C1541 | C1464 | G1340 | | |
| A2430 | G2350 | U | U2010 | G1905 | U1822 | C1732 | A1644 | U1542 | C1465 | G1341 | | |
| C2431 | G2351 | C | U2011 | G1906 | U1823 | C1733 | A1645 | C1543 | C1466 | G1342 | | |
| U2432 | G2352 | A | U2012 | G1907 | U1824 | C1734 | A1646 | U1544 | C1467 | G1343 | | |
| G2433 | G2353 | C | U2013 | G1908 | U1825 | C1735 | A1647 | C1545 | C1468 | G1344 | | |
| A2434 | G2354 | U | U2014 | G1909 | U1826 | C1736 | A1648 | U1546 | C1469 | G1345 | | |
| U2435 | G2355 | C | U2015 | G1910 | U1827 | C1737 | A1649 | C1547 | C1470 | G1346 | | |
| G2436 | G2356 | A | U2016 | G1911 | U1828 | C1738 | A1650 | U1548 | C1471 | G1347 | | |
| C2437 | G2357 | C | U2017 | G1912 | U1829 | C1739 | A1651 | C1549 | C1472 | G1348 | | |
| A2438 | G2358 | U | U2018 | G1913 | U1830 | C1740 | A1652 | U1550 | C1473 | G1349 | | |
| U2439 | G2359 | C | U2019 | G1914 | U1831 | C1741 | A1653 | C1551 | C1474 | G1350 | | |
| G2440 | G2360 | A | U2020 | G1915 | U1832 | C1742 | A1654 | U1552 | C1475 | G1351 | | |
| C2441 | G2361 | C | U2021 | G1916 | U1833 | C1743 | A1655 | C1553 | C1476 | G1352 | | |
| U2442 | G2362 | U | U2022 | G1917 | U1834 | C1744 | A1656 | U1554 | C1477 | G1353 | | |
| G2443 | G2363 | C | U2023 | G1918 | U1835 | C1745 | A1657 | C1555 | C1478 | G1354 | | |
| A2444 | G2364 | A | U2024 | G1919 | U1836 | C1746 | A1658 | U1556 | C1479 | G1355 | | |
| U2445 | G2365 | C | U2025 | G1920 | U1837 | C1747 | A1659 | C1557 | C1480 | G1356 | | |
| G2446 | G2366 | U | U2026 | G1921 | U1838 | C1748 | A1660 | U1558 | C1481 | G1357 | | |
| C2447 | G2367 | C | U2027 | G1922 | U1839 | C1749 | A1661 | C1559 | C1482 | G1358 | | |
| A2448 | G2368 | A | U2028 | G1923 | U1840 | C1750 | A1662 | U1560 | C1483 | G1359 | | |
| U2449 | G2369 | C | U2029 | G1924 | U1841 | C1751 | A1663 | C1561 | C1484 | G1360 | | |
| G2450 | G2370 | U | U2030 | G1925 | U1842 | C1752 | A1664 | U1562 | C1485 | G1361 | | |
| C2451 | G2371 | C | U2031 | G1926 | U1843 | C1753 | A1665 | C1563 | C1486 | G1362 | | |
| U2452 | G2372 | A | U2032 | G1927 | U1844 | C1754 | A1666 | U1564 | C1487 | G1363 | | |
| G2453 | G2373 | C | U2033 | G1928 | U1845 | C1755 | A1667 | C1565 | C1488 | G1364 | | |
| A2454 | G2374 | U | U2034 | G1929 | U1846 | C1756 | A1668 | U1566 | C1489 | G1365 | | |
| U2455 | G2375 | C | U2035 | G1930 | U1847 | C1757 | A1669 | C1567 | C1490 | G1366 | | |
| C2456 | G2376 | A | U2036 | G1931 | U1848 | C1758 | A1670 | U1568 | C1491 | G1367 | | |
| G2457 | G2377 | C | U2037 | G1932 | U1849 | C1759 | A1671 | C1569 | C1492 | G1368 | | |
| A2458 | G2378 | U | U2038 | G1933 | U1850 | C1760 | A1672 | U1570 | C1493 | G1369 | | |
| U2459 | G2379 | C | U2039 | G1934 | U1851 | C1761 | A1673 | C1571 | C1494 | G1370 | | |
| C2460 | G2380 | A | U2040 | G1935 | U1852 | C1762 | A1674 | U1572 | C1495 | G1371 | | |
| G2461 | G2381 | C | U2041 | G1936 | U1853 | C1763 | A1675 | C1573 | C1496 | G1372 | | |
| A2462 | G2382 | U | U2042 | G1937 | U1854 | C1764 | A1676 | U1574 | C1497 | G1373 | | |
| U2463 | G2383 | C | U2043 | G1938 | U1855 | C1765 | A1677 | C1575 | C1498 | G1374 | | |
| G2464 | G2384 | A | U2044 | G1939 | U1856 | C1766 | A1678 | U1576 | C1499 | G1375 | | |
| C2465 | G2385 | C | U2045 | G1940 | U1857 | C1767 | A1679 | C1577 | C1500 | G1376 | | |
| U2466 | G2386 | U | U2046 | G1941 | U1858 | C1768 | A1680 | U1578 | C1501 | G1377 | | |
| G2467 | G2387 | C | U2047 | G1942 | U1859 | C1769 | A1681 | C1579 | C1502 | G1378 | | |
| A2468 | G2388 | A | U2048 | G1943 | U1860 | C1770 | A1682 | U1580 | C1503 | G1379 | | |
| C2469 | G2389 | C | U2049 | G1944 | U1861 | C1771 | A1683 | C1581 | C1504 | G1380 | | |
| U2470 | G2390 | U | U2050 | G1945 | U1862 | C1772 | A1684 | U1582 | C1505 | G1381 | | |
| G2471 | G2391 | C | U2051 | G1946 | U1863 | C1773 | A1685 | C1583 | C1506 | G1382 | | |
| A2472 | G2392 | A | U2052 | G1947 | U1864 | C1774 | A1686 | U1584 | C1507 | G1383 | | |
| U2473 | G2393 | C | U2053 | G1948 | U1865 | C1775 | A1687 | C1585 | C1508 | G1384 | | |
| C2474 | G2394 | U | U2054 | G1949 | U1866 | C1776 | A1688 | U1586 | C1509 | | | |



- Molecule 2: 5S ribosomal RNA



- Molecule 3: CCA-phenylalanine-carboxylic-acid-biotin

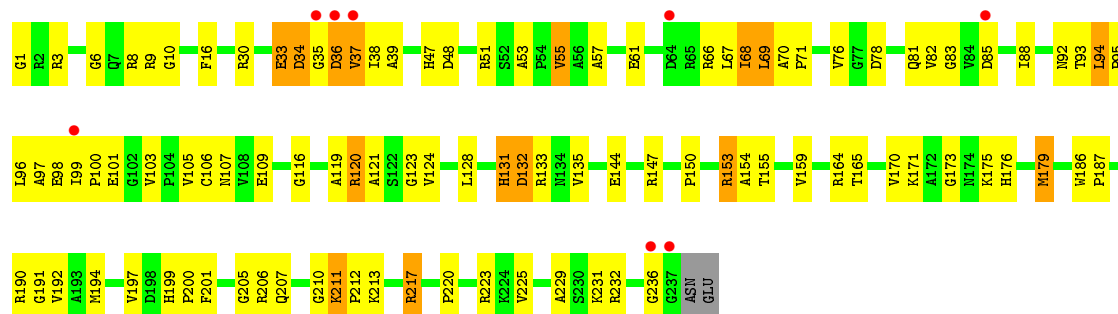


- Molecule 3: CCA-phenylalanine-carboxylic-acid-biotin

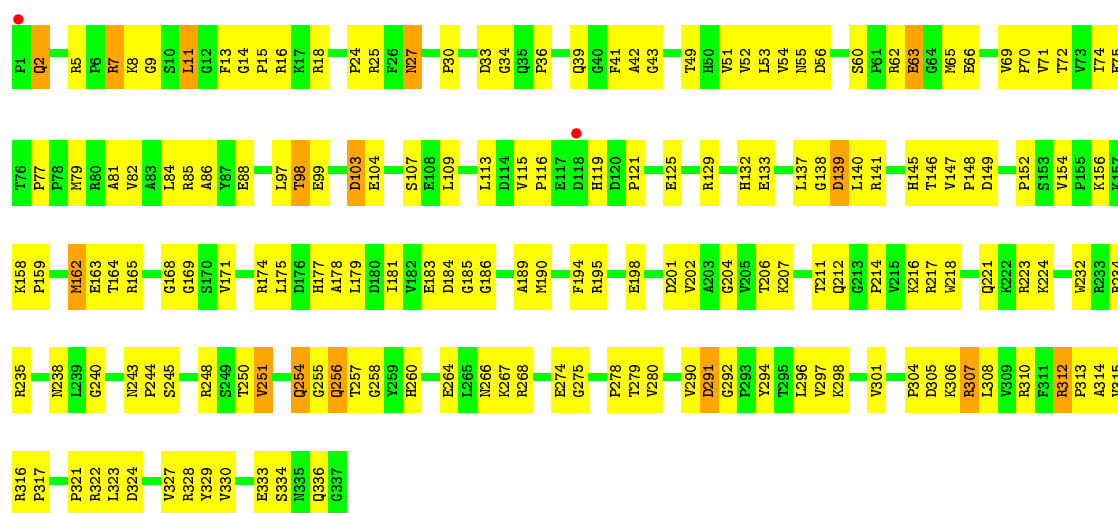


- Molecule 4: 50S ribosomal protein L2P

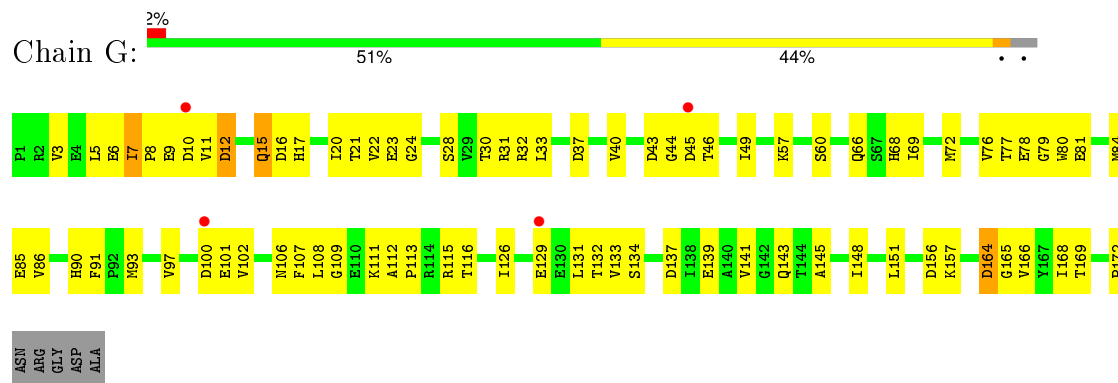




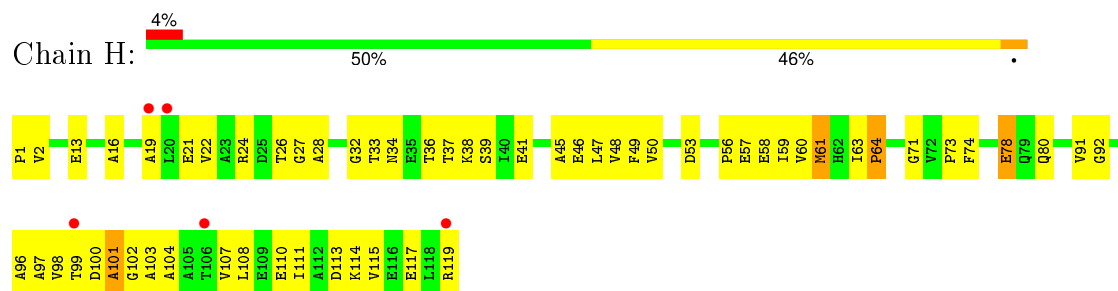
• Molecule 5: 50S ribosomal protein L3P



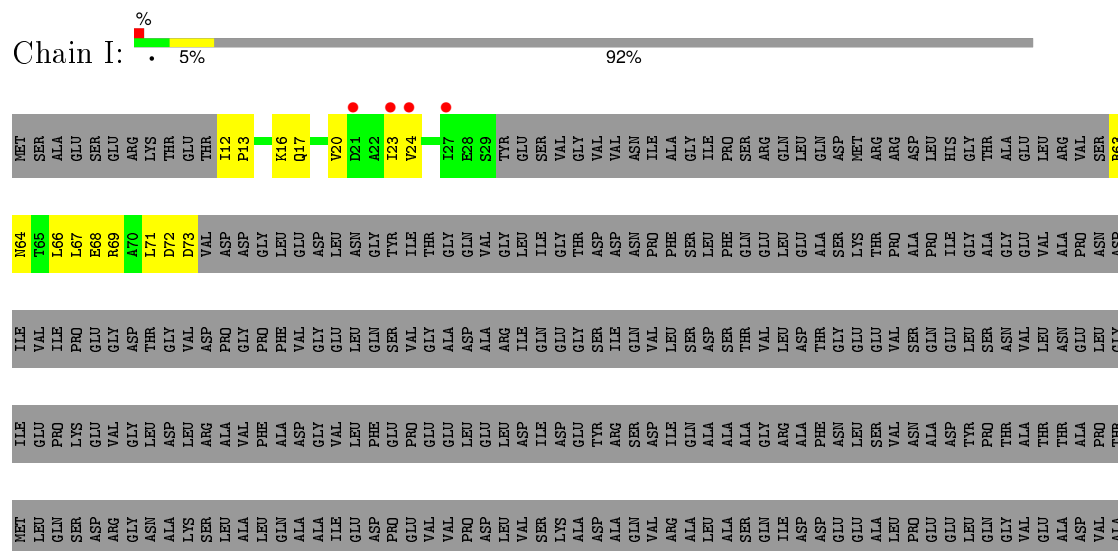
- Molecule 8: 50S ribosomal protein L6P



- Molecule 9: 50S ribosomal protein L7Ae

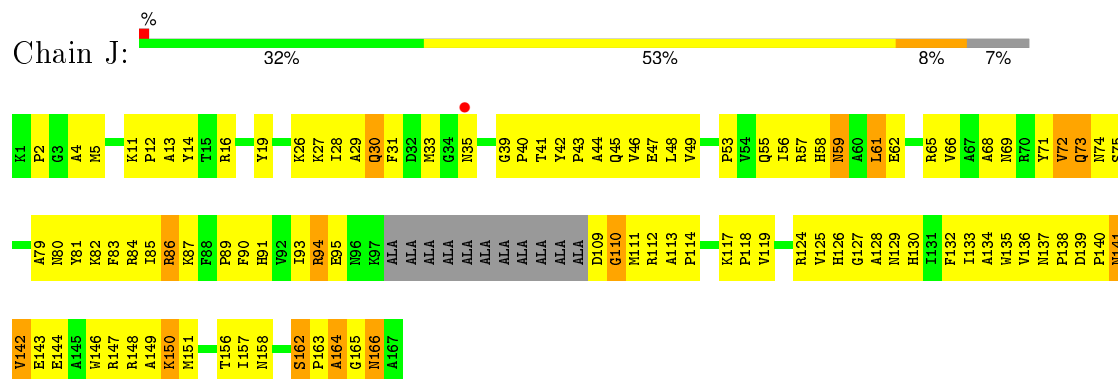


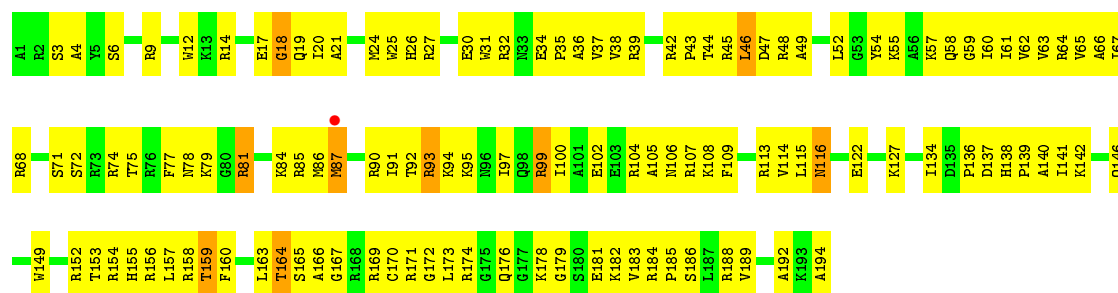
- Molecule 10: Acidic ribosomal protein P0 homolog



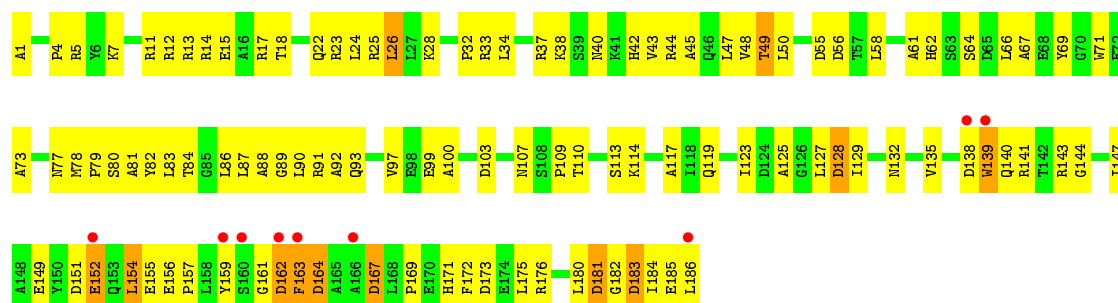
| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| THR | GLU | GLU | PRO | THR | ASP | ASP | GLN | ASP | ASP | THR | ALA | SER | GLU | ASP | ASP | ALA | ALA | ASP | ALA | ALA | GLU | GLU | ALA | ASP | ASP | ASP | ASP | ASP | GLU | GLU | ALA | GLY | ASP | ALA | LEU | GLY | ALA | MET | PHE |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

• Molecule 11: L10 Ribosomal Protein

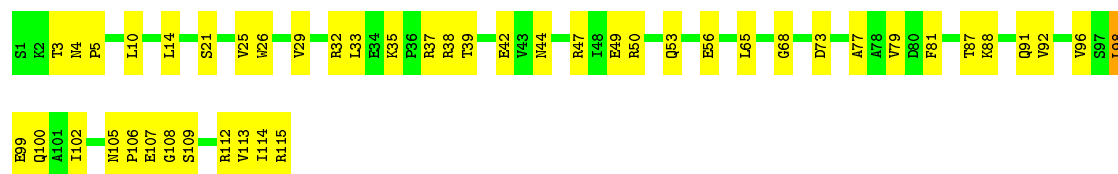




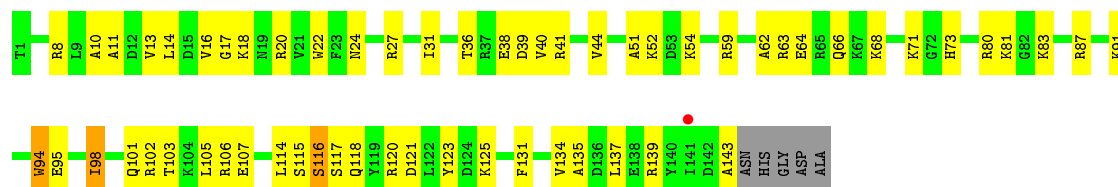
• Molecule 16: 50S ribosomal protein L18P



• Molecule 17: 50S ribosomal protein L18e



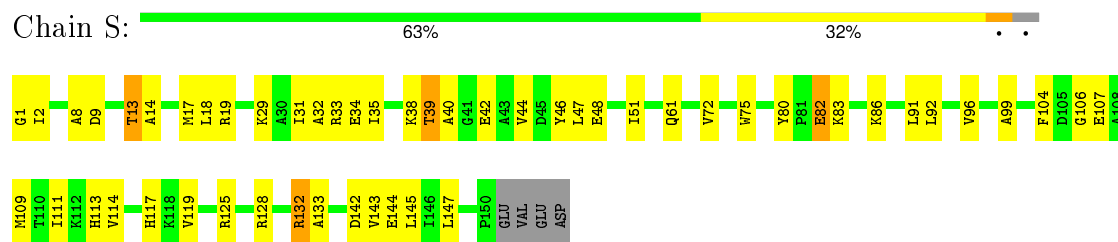
• Molecule 18: 50S ribosomal protein L19E



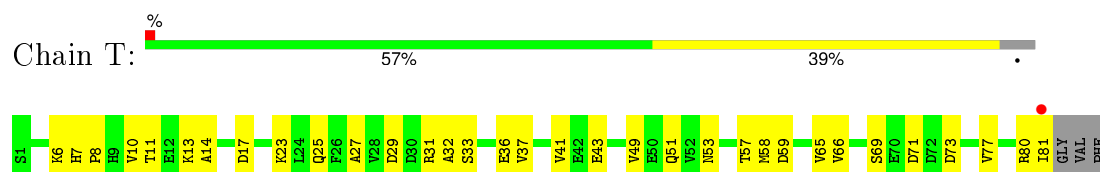
• Molecule 19: 50S ribosomal protein L21e



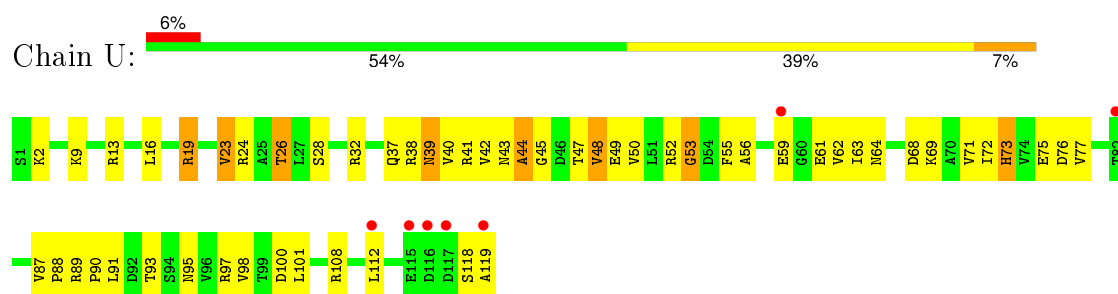
• Molecule 20: 50S ribosomal protein L22P



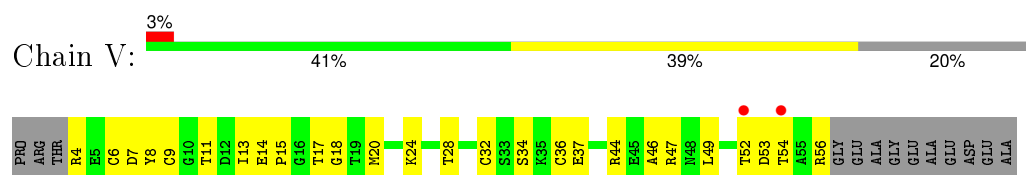
- Molecule 21: 50S ribosomal protein L23P



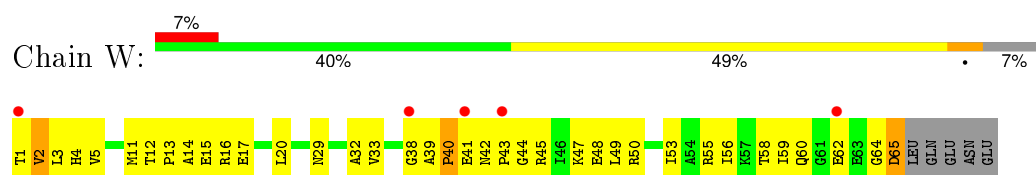
- Molecule 22: 50S ribosomal protein L24P



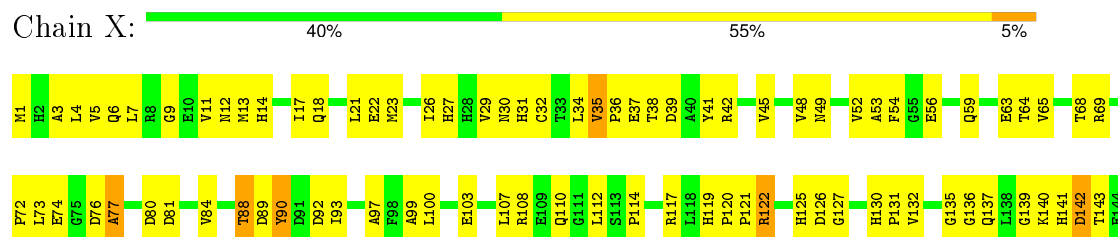
- Molecule 23: 50S ribosomal protein L24E



- Molecule 24: 50S ribosomal protein L29P

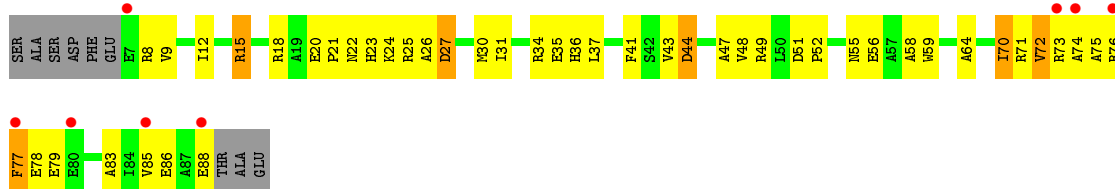


- Molecule 25: 50S ribosomal protein L30P

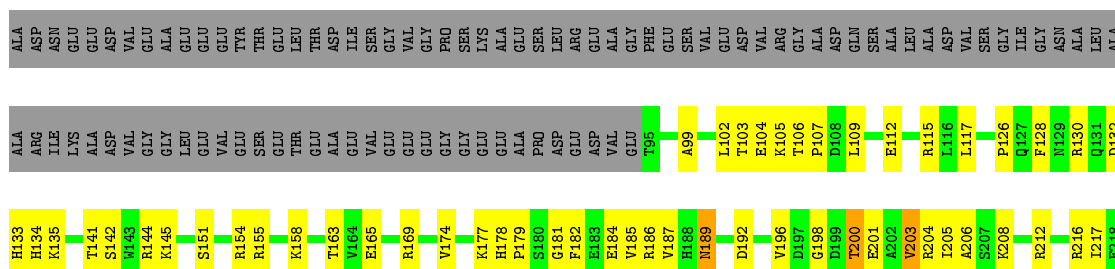
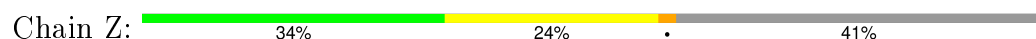




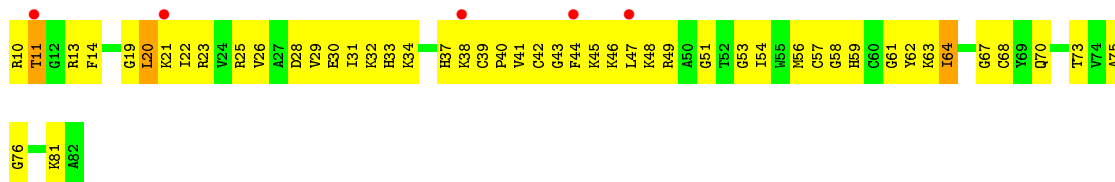
• Molecule 26: 50S ribosomal protein L31e



• Molecule 27: 50S ribosomal protein L32E



• Molecule 28: L37Ae 50S ribosomal protein

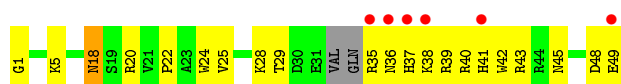


• Molecule 29: 50S ribosomal protein L37e

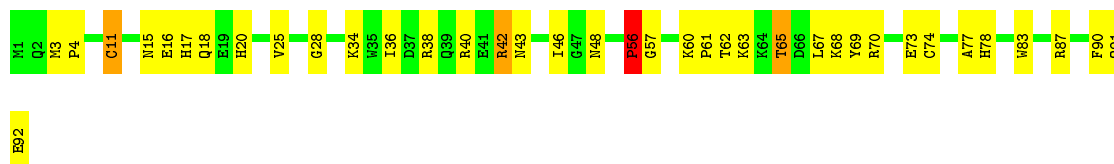


• Molecule 30: 50S ribosomal protein L39e





- Molecule 31: 50S ribosomal protein L44E



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | C 2 2 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 213.16Å 301.29Å 575.40Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 20.00 – 3.00 49.62 – 2.80 | Depositor EDS |
| % Data completeness (in resolution range) | 95.6 (20.00-3.00) 92.8 (49.62-2.80) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.01 (at 2.81Å) | Xtriage |
| Refinement program | CNS 1.0 | Depositor |
| R, R_{free} | 0.234 , 0.264 0.235 , (Not available) | Depositor DCC |
| R_{free} test set | No test flags present. | DCC |
| Wilson B-factor (Å ²) | 47.1 | Xtriage |
| Anisotropy | 0.292 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.32 , 70.2 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$ | Xtriage |
| Outliers | 0 of 447539 reflections | Xtriage |
| F_o, F_c correlation | 0.89 | EDS |
| Total number of atoms | 98659 | wwPDB-VP |
| Average B, all atoms (Å ²) | 53.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% 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: MG, CL, NA, PHA, CD, K

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 | A | 0.41 | 1/66076 (0.0%) | 0.70 | 24/103052 (0.0%) |
| 2 | B | 0.37 | 0/2905 | 0.75 | 4/4528 (0.1%) |
| 3 | 5 | 0.67 | 0/65 | 0.86 | 0/99 |
| 3 | 6 | 1.66 | 2/65 (3.1%) | 1.27 | 0/99 |
| 4 | C | 0.32 | 0/1787 | 0.65 | 0/2409 |
| 5 | D | 0.34 | 0/2689 | 0.64 | 0/3652 |
| 6 | E | 0.38 | 0/1883 | 0.65 | 0/2551 |
| 7 | F | 0.32 | 0/1111 | 0.59 | 0/1498 |
| 8 | G | 0.33 | 0/1382 | 0.59 | 0/1880 |
| 9 | H | 0.31 | 0/896 | 0.58 | 0/1219 |
| 10 | I | 0.29 | 0/241 | 0.50 | 0/324 |
| 11 | J | 0.40 | 0/1246 | 0.77 | 4/1686 (0.2%) |
| 12 | K | 0.38 | 0/1135 | 0.63 | 0/1530 |
| 13 | L | 0.35 | 0/1003 | 0.68 | 0/1351 |
| 14 | M | 0.32 | 0/1126 | 0.65 | 0/1504 |
| 15 | N | 0.38 | 0/1633 | 0.68 | 0/2180 |
| 16 | O | 0.29 | 0/1473 | 0.64 | 0/1999 |
| 17 | P | 0.34 | 0/873 | 0.61 | 0/1181 |
| 18 | Q | 0.34 | 0/1143 | 0.54 | 0/1521 |
| 19 | R | 0.37 | 0/748 | 0.69 | 1/1005 (0.1%) |
| 20 | S | 0.36 | 0/1172 | 0.67 | 0/1578 |
| 21 | T | 0.33 | 0/648 | 0.58 | 0/875 |
| 22 | U | 0.31 | 0/957 | 0.62 | 0/1289 |
| 23 | V | 0.33 | 0/417 | 0.59 | 0/562 |
| 24 | W | 0.29 | 0/502 | 0.56 | 0/675 |
| 25 | X | 0.35 | 0/1218 | 0.64 | 0/1655 |
| 26 | Y | 0.35 | 0/664 | 0.60 | 0/895 |
| 27 | Z | 0.36 | 0/1146 | 0.65 | 0/1536 |
| 28 | 1 | 0.37 | 0/575 | 0.69 | 0/763 |
| 29 | 2 | 0.37 | 0/437 | 0.63 | 0/578 |
| 30 | 3 | 0.30 | 0/398 | 0.52 | 0/527 |
| 31 | 4 | 0.41 | 0/771 | 0.62 | 0/1024 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| All | All | 0.39 | 3/98385 (0.0%) | 0.68 | 33/147225 (0.0%) |

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 |
|-----|-------|---------------------|---------------------|
| 1 | A | 2 | 50 |
| 2 | B | 1 | 3 |
| 3 | 6 | 0 | 1 |
| 25 | X | 0 | 1 |
| All | All | 3 | 55 |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 3 | 6 | 75 | C | O5'-C5' | 5.83 | 1.53 | 1.44 |
| 1 | A | 2620 | U | N1-C6 | 5.47 | 1.42 | 1.38 |
| 3 | 6 | 74 | C | C2'-O2' | 5.05 | 1.48 | 1.41 |

All (33) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 1563 | G | C2'-C3'-O3' | 9.42 | 130.23 | 109.50 |
| 2 | B | 3024 | U | C2'-C3'-O3' | 9.17 | 129.68 | 109.50 |
| 1 | A | 2637 | A | C4'-C3'-O3' | -7.22 | 94.24 | 109.40 |
| 2 | B | 3103 | A | C5'-C4'-O4' | 7.11 | 117.63 | 109.10 |
| 11 | J | 74 | ASN | N-CA-C | -6.83 | 92.57 | 111.00 |
| 1 | A | 1942 | A | C5'-C4'-C3' | 6.56 | 126.50 | 116.00 |
| 2 | B | 3039 | U | N1-C1'-C2' | 6.47 | 122.42 | 114.00 |
| 1 | A | 1504 | A | C1'-O4'-C4' | -6.41 | 104.77 | 109.90 |
| 1 | A | 871 | G | C5'-C4'-O4' | -5.97 | 101.93 | 109.10 |
| 1 | A | 2616 | G | C2'-C3'-O3' | 5.94 | 123.21 | 113.70 |
| 1 | A | 2467 | A | C1'-O4'-C4' | -5.92 | 105.17 | 109.90 |
| 1 | A | 2636 | C | OP2-P-O3' | 5.76 | 117.88 | 105.20 |
| 1 | A | 1979 | G | C2'-C3'-O3' | 5.74 | 122.89 | 113.70 |
| 1 | A | 1165 | G | O5'-P-OP2 | 5.64 | 117.46 | 110.70 |
| 1 | A | 2313 | C | C5'-C4'-O4' | 5.61 | 115.83 | 109.10 |
| 11 | J | 110 | GLY | N-CA-C | -5.50 | 99.36 | 113.10 |
| 1 | A | 2637 | A | C1'-O4'-C4' | -5.49 | 105.51 | 109.90 |
| 1 | A | 1819 | G | C5'-C4'-C3' | 5.35 | 124.56 | 116.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 2316 | G | C5'-C4'-C3' | -5.33 | 107.48 | 116.00 |
| 1 | A | 2291 | A | N9-C1'-C2' | 5.30 | 120.89 | 114.00 |
| 11 | J | 156 | THR | N-CA-C | -5.29 | 96.72 | 111.00 |
| 1 | A | 2616 | G | N9-C1'-C2' | 5.27 | 120.86 | 114.00 |
| 1 | A | 2637 | A | OP1-P-O3' | -5.25 | 93.66 | 105.20 |
| 1 | A | 1165 | G | N9-C1'-C2' | 5.20 | 120.76 | 114.00 |
| 19 | R | 68 | GLY | N-CA-C | -5.15 | 100.23 | 113.10 |
| 1 | A | 1829 | A | N9-C1'-C2' | -5.11 | 106.38 | 112.00 |
| 1 | A | 1504 | A | N9-C1'-C2' | 5.10 | 120.63 | 114.00 |
| 1 | A | 1120 | U | C5'-C4'-C3' | -5.10 | 107.84 | 116.00 |
| 1 | A | 237 | G | N9-C1'-C2' | -5.07 | 106.42 | 112.00 |
| 1 | A | 129 | A | C2'-C3'-O3' | 5.03 | 121.75 | 113.70 |
| 2 | B | 3103 | A | C1'-O4'-C4' | -5.02 | 105.88 | 109.90 |
| 11 | J | 141 | ASN | N-CA-C | -5.00 | 97.49 | 111.00 |
| 1 | A | 535 | G | N9-C1'-C2' | 5.00 | 120.50 | 114.00 |

All (3) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 1 | A | 1563 | G | C3' |
| 1 | A | 2616 | G | C3' |
| 2 | B | 3024 | U | C3' |

All (55) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 3 | 6 | 76 | A | Sidechain |
| 1 | A | 1039 | G | Sidechain |
| 1 | A | 1078 | A | Sidechain |
| 1 | A | 1226 | G | Sidechain |
| 1 | A | 1293 | U | Sidechain |
| 1 | A | 1342 | C | Sidechain |
| 1 | A | 1351 | G | Sidechain |
| 1 | A | 1417 | G | Sidechain |
| 1 | A | 1458 | A | Sidechain |
| 1 | A | 1599 | U | Sidechain |
| 1 | A | 1809 | G | Sidechain |
| 1 | A | 182 | G | Sidechain |
| 1 | A | 1829 | A | Sidechain |
| 1 | A | 1835 | U | Sidechain |
| 1 | A | 1861 | C | Sidechain |
| 1 | A | 1863 | G | Sidechain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 1 | A | 1877 | G | Sidechain |
| 1 | A | 1878 | G | Sidechain |
| 1 | A | 1972 | U | Sidechain |
| 1 | A | 2313 | C | Sidechain |
| 1 | A | 2465 | A | Sidechain |
| 1 | A | 2486 | A | Sidechain |
| 1 | A | 2492 | U | Sidechain |
| 1 | A | 2493 | C | Sidechain |
| 1 | A | 2503 | A | Sidechain |
| 1 | A | 2506 | A | Sidechain |
| 1 | A | 2526 | C | Sidechain |
| 1 | A | 2551 | C | Sidechain |
| 1 | A | 2564 | G | Sidechain |
| 1 | A | 2607 | U | Sidechain |
| 1 | A | 2615 | U | Sidechain |
| 1 | A | 2619 | U | Sidechain |
| 1 | A | 2630 | G | Sidechain |
| 1 | A | 2631 | U | Sidechain |
| 1 | A | 2637 | A | Sidechain |
| 1 | A | 2643 | G | Sidechain |
| 1 | A | 2673 | U | Sidechain |
| 1 | A | 2793 | A | Sidechain |
| 1 | A | 2840 | A | Sidechain |
| 1 | A | 2842 | G | Sidechain |
| 1 | A | 333 | G | Sidechain |
| 1 | A | 471 | G | Sidechain |
| 1 | A | 482 | G | Sidechain |
| 1 | A | 518 | G | Sidechain |
| 1 | A | 722 | G | Sidechain |
| 1 | A | 792 | G | Sidechain |
| 1 | A | 815 | U | Sidechain |
| 1 | A | 817 | G | Sidechain |
| 1 | A | 818 | A | Sidechain |
| 1 | A | 867 | A | Sidechain |
| 1 | A | 882 | A | Sidechain |
| 2 | B | 3065 | A | Sidechain |
| 2 | B | 3087 | U | Sidechain |
| 2 | B | 3090 | G | Sidechain |
| 25 | X | 90 | TYR | Sidechain |

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 | A | 59017 | 0 | 29805 | 1077 | 0 |
| 2 | B | 2600 | 0 | 1326 | 84 | 0 |
| 3 | 5 | 59 | 0 | 34 | 4 | 0 |
| 3 | 6 | 59 | 0 | 34 | 0 | 0 |
| 4 | C | 1754 | 0 | 1763 | 112 | 0 |
| 5 | D | 2624 | 0 | 2533 | 183 | 0 |
| 6 | E | 1858 | 0 | 1816 | 135 | 0 |
| 7 | F | 1094 | 0 | 1085 | 146 | 0 |
| 8 | G | 1357 | 0 | 1266 | 77 | 0 |
| 9 | H | 885 | 0 | 854 | 71 | 0 |
| 10 | I | 240 | 0 | 231 | 23 | 0 |
| 11 | J | 1215 | 0 | 1215 | 170 | 0 |
| 12 | K | 1119 | 0 | 1098 | 77 | 0 |
| 13 | L | 993 | 0 | 1027 | 72 | 0 |
| 14 | M | 1114 | 0 | 1072 | 66 | 0 |
| 15 | N | 1605 | 0 | 1676 | 182 | 0 |
| 16 | O | 1444 | 0 | 1401 | 129 | 0 |
| 17 | P | 864 | 0 | 873 | 53 | 0 |
| 18 | Q | 1133 | 0 | 1127 | 62 | 0 |
| 19 | R | 734 | 0 | 729 | 26 | 0 |
| 20 | S | 1149 | 0 | 1122 | 67 | 0 |
| 21 | T | 641 | 0 | 605 | 31 | 0 |
| 22 | U | 949 | 0 | 923 | 62 | 0 |
| 23 | V | 410 | 0 | 364 | 35 | 0 |
| 24 | W | 499 | 0 | 511 | 33 | 0 |
| 25 | X | 1195 | 0 | 1137 | 118 | 0 |
| 26 | Y | 654 | 0 | 653 | 51 | 0 |
| 27 | Z | 1130 | 0 | 1133 | 71 | 0 |
| 28 | 1 | 563 | 0 | 597 | 66 | 0 |
| 29 | 2 | 430 | 0 | 426 | 28 | 0 |
| 30 | 3 | 393 | 0 | 406 | 32 | 0 |
| 31 | 4 | 755 | 0 | 728 | 40 | 0 |
| 32 | 1 | 1 | 0 | 0 | 0 | 0 |
| 32 | 4 | 1 | 0 | 0 | 0 | 0 |
| 32 | 6 | 1 | 0 | 0 | 0 | 0 |
| 32 | A | 108 | 0 | 0 | 0 | 0 |
| 32 | B | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 32 | C | 1 | 0 | 0 | 0 | 0 |
| 32 | D | 2 | 0 | 0 | 0 | 0 |
| 32 | L | 1 | 0 | 0 | 0 | 0 |
| 32 | U | 1 | 0 | 0 | 0 | 0 |
| 32 | Z | 1 | 0 | 0 | 0 | 0 |
| 33 | A | 2 | 0 | 0 | 0 | 0 |
| 34 | A | 70 | 0 | 0 | 0 | 0 |
| 34 | B | 2 | 0 | 0 | 0 | 0 |
| 34 | C | 1 | 0 | 0 | 0 | 0 |
| 34 | E | 1 | 0 | 0 | 0 | 0 |
| 34 | J | 2 | 0 | 0 | 0 | 0 |
| 34 | K | 1 | 0 | 0 | 0 | 0 |
| 34 | M | 1 | 0 | 0 | 0 | 0 |
| 34 | N | 2 | 0 | 0 | 0 | 0 |
| 34 | R | 1 | 0 | 0 | 0 | 0 |
| 34 | S | 3 | 0 | 0 | 0 | 0 |
| 34 | T | 1 | 0 | 0 | 0 | 0 |
| 34 | U | 1 | 0 | 0 | 0 | 0 |
| 35 | 4 | 1 | 0 | 0 | 0 | 0 |
| 35 | A | 9 | 0 | 0 | 0 | 0 |
| 35 | C | 1 | 0 | 0 | 0 | 0 |
| 35 | D | 1 | 0 | 0 | 0 | 0 |
| 35 | K | 3 | 0 | 0 | 1 | 0 |
| 35 | L | 1 | 0 | 0 | 1 | 0 |
| 35 | M | 1 | 0 | 0 | 0 | 0 |
| 35 | N | 1 | 0 | 0 | 1 | 0 |
| 35 | O | 1 | 0 | 0 | 0 | 0 |
| 35 | P | 1 | 0 | 0 | 0 | 0 |
| 35 | S | 1 | 0 | 0 | 0 | 0 |
| 35 | Z | 1 | 0 | 0 | 0 | 0 |
| 36 | 5 | 11 | 0 | 10 | 5 | 0 |
| 36 | 6 | 10 | 0 | 7 | 4 | 0 |
| 37 | 1 | 1 | 0 | 0 | 0 | 0 |
| 37 | 2 | 1 | 0 | 0 | 0 | 0 |
| 37 | 4 | 1 | 0 | 0 | 0 | 0 |
| 37 | P | 1 | 0 | 0 | 0 | 0 |
| 37 | V | 1 | 0 | 0 | 0 | 0 |
| 38 | 1 | 37 | 0 | 0 | 14 | 0 |
| 38 | 2 | 63 | 0 | 0 | 4 | 0 |
| 38 | 3 | 41 | 0 | 0 | 3 | 0 |
| 38 | 4 | 70 | 0 | 0 | 10 | 0 |
| 38 | A | 5892 | 0 | 0 | 227 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 38 | B | 139 | 0 | 0 | 14 | 0 |
| 38 | C | 116 | 0 | 0 | 12 | 0 |
| 38 | D | 149 | 0 | 0 | 30 | 0 |
| 38 | E | 173 | 0 | 0 | 37 | 0 |
| 38 | F | 52 | 0 | 0 | 22 | 0 |
| 38 | G | 43 | 0 | 0 | 12 | 0 |
| 38 | H | 27 | 0 | 0 | 11 | 0 |
| 38 | I | 21 | 0 | 0 | 6 | 0 |
| 38 | J | 77 | 0 | 0 | 23 | 0 |
| 38 | K | 54 | 0 | 0 | 5 | 0 |
| 38 | L | 62 | 0 | 0 | 11 | 0 |
| 38 | M | 82 | 0 | 0 | 18 | 0 |
| 38 | N | 139 | 0 | 0 | 23 | 0 |
| 38 | O | 70 | 0 | 0 | 17 | 0 |
| 38 | P | 43 | 0 | 0 | 13 | 0 |
| 38 | Q | 67 | 0 | 0 | 5 | 0 |
| 38 | R | 54 | 0 | 0 | 5 | 0 |
| 38 | S | 84 | 0 | 0 | 7 | 0 |
| 38 | T | 37 | 0 | 0 | 6 | 0 |
| 38 | U | 44 | 0 | 0 | 7 | 0 |
| 38 | V | 24 | 0 | 0 | 5 | 0 |
| 38 | W | 14 | 0 | 0 | 3 | 0 |
| 38 | X | 71 | 0 | 0 | 14 | 0 |
| 38 | Y | 31 | 0 | 0 | 5 | 0 |
| 38 | Z | 93 | 0 | 0 | 14 | 0 |
| All | All | 98659 | 0 | 59587 | 3106 | 0 |

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 21.

All (3106) 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) |
|------------------|-------------------|--------------------------|-------------------|
| 6:E:236:THR:HG22 | 6:E:239:ALA:H | 1.05 | 1.18 |
| 11:J:45:GLN:HB3 | 11:J:163:PRO:HD2 | 1.31 | 1.12 |
| 11:J:86:ARG:NH1 | 11:J:133:ILE:HG13 | 1.64 | 1.11 |
| 1:A:1119:G:H2' | 12:K:52:GLN:HE22 | 1.10 | 1.10 |
| 1:A:156:C:H5'' | 15:N:171:ARG:HD3 | 1.29 | 1.09 |
| 24:W:12:THR:HG22 | 24:W:15:GLU:HG3 | 1.39 | 1.05 |
| 2:B:3023:U:H3' | 2:B:3024:U:H5'' | 1.36 | 1.04 |
| 1:A:1242:A:H5' | 12:K:82:THR:HG23 | 1.38 | 1.03 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:J:86:ARG:HH11 | 11:J:133:ILE:HG13 | 0.91 | 1.02 |
| 22:U:71:VAL:HG11 | 22:U:90:PRO:HB3 | 1.40 | 1.02 |
| 1:A:960:G:H4' | 38:A:6921:HOH:O | 1.58 | 1.02 |
| 11:J:29:ALA:HB3 | 11:J:65:ARG:HH12 | 1.23 | 1.00 |
| 5:D:201:ASP:HB2 | 5:D:312:ARG:HD2 | 1.43 | 1.00 |
| 1:A:856:G:H2' | 38:A:4918:HOH:O | 1.60 | 1.00 |
| 1:A:1119:G:H2' | 12:K:52:GLN:NE2 | 1.77 | 1.00 |
| 1:A:2717:C:H2' | 1:A:2718:C:H5'' | 1.45 | 0.98 |
| 13:L:10:GLN:NE2 | 13:L:10:GLN:H | 1.61 | 0.98 |
| 6:E:127:ARG:NH2 | 6:E:225:PRO:HG2 | 1.79 | 0.98 |
| 3:5:74:C:H2' | 3:5:75:C:H5' | 1.44 | 0.98 |
| 7:F:134:LEU:HD11 | 7:F:166:ILE:HD11 | 1.44 | 0.97 |
| 11:J:162:SER:HB2 | 11:J:163:PRO:HD3 | 1.44 | 0.97 |
| 2:B:3006:C:H5'' | 16:O:37:ARG:NH1 | 1.77 | 0.97 |
| 2:B:3076:G:H3' | 2:B:3077:A:H5'' | 1.46 | 0.97 |
| 15:N:52:LEU:HD11 | 38:N:8623:HOH:O | 1.64 | 0.96 |
| 1:A:1160:G:H5' | 1:A:1161:A:H5' | 1.45 | 0.96 |
| 5:D:140:LEU:HA | 38:D:8583:HOH:O | 1.64 | 0.96 |
| 1:A:1134:G:H4' | 11:J:151:MET:HE1 | 1.45 | 0.96 |
| 16:O:47:LEU:HD11 | 16:O:127:LEU:HD21 | 1.46 | 0.95 |
| 11:J:86:ARG:HH11 | 11:J:133:ILE:CG1 | 1.77 | 0.95 |
| 12:K:76:ASP:HA | 38:K:5907:HOH:O | 1.63 | 0.95 |
| 8:G:20:ILE:HD11 | 8:G:40:VAL:HG11 | 1.48 | 0.95 |
| 7:F:105:SER:HB2 | 7:F:131:THR:HG23 | 1.48 | 0.94 |
| 25:X:88:THR:HB | 38:X:6679:HOH:O | 1.66 | 0.94 |
| 22:U:9:LYS:HE3 | 22:U:13:ARG:NH1 | 1.82 | 0.94 |
| 7:F:154:LYS:H | 7:F:154:LYS:HD2 | 1.32 | 0.94 |
| 7:F:25:MET:HE2 | 7:F:41:LEU:HG | 1.50 | 0.93 |
| 2:B:3056:A:H2' | 2:B:3057:A:H5'' | 1.50 | 0.93 |
| 20:S:99:ALA:HB1 | 20:S:109:MET:HE1 | 1.50 | 0.93 |
| 5:D:238:ASN:HD22 | 5:D:240:GLY:H | 0.97 | 0.93 |
| 13:L:10:GLN:HE21 | 13:L:10:GLN:H | 1.04 | 0.92 |
| 13:L:29:LEU:HB3 | 13:L:55:VAL:HG11 | 1.50 | 0.92 |
| 38:A:4711:HOH:O | 13:L:39:GLY:HA2 | 1.68 | 0.92 |
| 11:J:165:GLY:HA3 | 38:J:8398:HOH:O | 1.70 | 0.92 |
| 2:B:3103:A:H4' | 38:B:8445:HOH:O | 1.69 | 0.92 |
| 15:N:164:THR:HG22 | 15:N:167:GLY:H | 1.33 | 0.92 |
| 26:Y:37:LEU:HD13 | 26:Y:85:VAL:HG21 | 1.52 | 0.91 |
| 28:1:10:ARG:HA | 38:1:8415:HOH:O | 1.68 | 0.91 |
| 1:A:1751:G:H2' | 1:A:1752:G:H5'' | 1.51 | 0.91 |
| 1:A:1667:A:H8 | 1:A:1667:A:H5' | 1.35 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:D:86:ALA:HA | 38:D:8583:HOH:O | 1.69 | 0.91 |
| 1:A:541:C:H2' | 1:A:542:A:H5'' | 1.51 | 0.90 |
| 13:L:81:ARG:HB2 | 13:L:87:ARG:HH11 | 1.31 | 0.90 |
| 16:O:7:LYS:HE3 | 19:R:21:ARG:O | 1.71 | 0.90 |
| 28:1:58:GLY:HA3 | 38:1:8438:HOH:O | 1.70 | 0.90 |
| 1:A:871:G:H8 | 1:A:871:G:H5' | 1.37 | 0.90 |
| 38:B:8474:HOH:O | 16:O:23:ARG:HD3 | 1.72 | 0.90 |
| 2:B:3023:U:H3' | 2:B:3024:U:C5' | 2.01 | 0.89 |
| 1:A:871:G:C8 | 1:A:871:G:H5' | 2.07 | 0.89 |
| 14:M:79:ASP:HB3 | 38:M:8560:HOH:O | 1.71 | 0.89 |
| 4:C:211:LYS:HB3 | 4:C:212:PRO:HD2 | 1.55 | 0.88 |
| 11:J:75:SER:O | 11:J:79:ALA:HB2 | 1.73 | 0.88 |
| 18:Q:115:SER:H | 18:Q:118:GLN:NE2 | 1.71 | 0.88 |
| 15:N:106:ASN:HD22 | 15:N:114:VAL:HG23 | 1.36 | 0.88 |
| 14:M:67:ARG:O | 14:M:71:GLU:HG3 | 1.74 | 0.88 |
| 7:F:27:ILE:HG22 | 7:F:28:GLY:H | 1.38 | 0.88 |
| 1:A:1164:U:H4' | 1:A:1165:G:OP1 | 1.73 | 0.88 |
| 28:1:38:LYS:HE2 | 28:1:45:LYS:HE2 | 1.56 | 0.88 |
| 11:J:59:ASN:H | 11:J:59:ASN:HD22 | 1.14 | 0.88 |
| 1:A:1116:U:HO2' | 1:A:1118:A:H2 | 0.89 | 0.87 |
| 1:A:545:G:H8 | 1:A:545:G:H5' | 1.39 | 0.87 |
| 6:E:236:THR:HG22 | 6:E:239:ALA:N | 1.88 | 0.87 |
| 1:A:1474:C:H5' | 1:A:1474:C:H6 | 1.39 | 0.87 |
| 8:G:97:VAL:HG12 | 38:G:4191:HOH:O | 1.73 | 0.87 |
| 1:A:1701:A:H5' | 38:A:5779:HOH:O | 1.74 | 0.87 |
| 5:D:321:PRO:HA | 38:D:8659:HOH:O | 1.75 | 0.87 |
| 12:K:52:GLN:HG3 | 12:K:53:ILE:N | 1.88 | 0.87 |
| 1:A:1679:C:H5' | 38:A:8839:HOH:O | 1.74 | 0.87 |
| 15:N:35:PRO:HG2 | 15:N:38:VAL:HG23 | 1.55 | 0.87 |
| 15:N:102:GLU:OE1 | 15:N:164:THR:HG21 | 1.73 | 0.86 |
| 4:C:223:ARG:HG3 | 38:C:8597:HOH:O | 1.73 | 0.86 |
| 15:N:106:ASN:ND2 | 35:N:8518:CL:CL | 2.45 | 0.86 |
| 13:L:81:ARG:HB2 | 13:L:87:ARG:NH1 | 1.89 | 0.86 |
| 18:Q:115:SER:N | 18:Q:118:GLN:HE21 | 1.71 | 0.86 |
| 11:J:41:THR:HA | 38:J:8395:HOH:O | 1.73 | 0.86 |
| 15:N:87:MET:HB3 | 31:4:46:ILE:HD13 | 1.57 | 0.86 |
| 1:A:1116:U:H3 | 1:A:1246:A:H62 | 1.22 | 0.86 |
| 13:L:10:GLN:N | 13:L:10:GLN:HE21 | 1.73 | 0.86 |
| 30:3:41:HIS:H | 30:3:45:ASN:HD22 | 1.23 | 0.86 |
| 1:A:711:G:H1' | 38:A:6586:HOH:O | 1.74 | 0.86 |
| 1:A:381:G:H5'' | 38:A:3825:HOH:O | 1.73 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:L:74:VAL:HG11 | 13:L:113:ILE:HG12 | 1.57 | 0.86 |
| 1:A:2586:U:H3 | 1:A:2592:G:H22 | 1.24 | 0.86 |
| 13:L:14:LYS:HB2 | 13:L:45:PRO:HG2 | 1.56 | 0.85 |
| 1:A:1184:C:H1' | 38:A:6959:HOH:O | 1.75 | 0.85 |
| 1:A:2004:U:H4' | 38:A:4800:HOH:O | 1.76 | 0.85 |
| 11:J:26:LYS:HD2 | 11:J:28:ILE:HD12 | 1.59 | 0.85 |
| 1:A:542:A:H8 | 1:A:542:A:H5' | 1.40 | 0.84 |
| 25:X:72:PRO:HG2 | 25:X:77:ALA:HB3 | 1.57 | 0.84 |
| 1:A:21:G:H5' | 20:S:2:ILE:HA | 1.59 | 0.84 |
| 38:A:3295:HOH:O | 15:N:189:VAL:HG21 | 1.77 | 0.84 |
| 6:E:132:ASP:HB3 | 38:E:8365:HOH:O | 1.77 | 0.84 |
| 12:K:52:GLN:HG3 | 12:K:53:ILE:H | 1.43 | 0.84 |
| 25:X:4:LEU:HD22 | 25:X:52:VAL:HG21 | 1.60 | 0.84 |
| 11:J:139:ASP:N | 11:J:140:PRO:HD3 | 1.93 | 0.84 |
| 7:F:20:LYS:HA | 7:F:75:LEU:O | 1.78 | 0.83 |
| 12:K:74:ARG:HH11 | 12:K:74:ARG:HB3 | 1.43 | 0.83 |
| 4:C:192:VAL:HB | 38:C:8590:HOH:O | 1.76 | 0.83 |
| 20:S:106:GLY:HA2 | 20:S:109:MET:HE3 | 1.59 | 0.83 |
| 1:A:2717:C:C2' | 1:A:2718:C:H5'' | 2.09 | 0.83 |
| 16:O:49:THR:HG22 | 16:O:56:ASP:HB2 | 1.59 | 0.83 |
| 26:Y:78:GLU:HG2 | 26:Y:79:GLU:H | 1.41 | 0.83 |
| 23:V:9:CYS:HA | 23:V:52:THR:HG23 | 1.58 | 0.83 |
| 1:A:2812:A:H2 | 1:A:2814:A:H62 | 1.24 | 0.83 |
| 11:J:137:ASN:O | 11:J:139:ASP:N | 2.11 | 0.83 |
| 7:F:146:LYS:NZ | 16:O:107:ASN:HD21 | 1.77 | 0.83 |
| 1:A:1835:U:H5 | 1:A:1840:A:N7 | 1.76 | 0.83 |
| 1:A:1166:A:H1' | 1:A:1192:A:C2 | 2.14 | 0.82 |
| 1:A:2506:A:HO2' | 1:A:2507:G:H8 | 0.86 | 0.82 |
| 1:A:282:C:H1' | 1:A:368:C:N4 | 1.94 | 0.82 |
| 1:A:541:C:C2' | 1:A:542:A:H5'' | 2.09 | 0.82 |
| 11:J:4:ALA:HB3 | 38:J:8366:HOH:O | 1.78 | 0.82 |
| 9:H:96:ALA:HA | 38:H:3111:HOH:O | 1.77 | 0.82 |
| 16:O:144:GLY:O | 16:O:147:ILE:HG22 | 1.79 | 0.82 |
| 14:M:133:VAL:HA | 38:M:8575:HOH:O | 1.79 | 0.82 |
| 20:S:8:ALA:HB1 | 20:S:13:THR:HG21 | 1.61 | 0.82 |
| 38:A:5791:HOH:O | 7:F:99:ASP:HA | 1.79 | 0.82 |
| 2:B:3024:U:O2' | 2:B:3025:G:H4' | 1.79 | 0.82 |
| 15:N:87:MET:HB2 | 15:N:91:ILE:HD11 | 1.61 | 0.82 |
| 11:J:5:MET:HG3 | 38:J:8366:HOH:O | 1.80 | 0.82 |
| 11:J:27:LYS:H | 11:J:58:HIS:HD2 | 1.26 | 0.81 |
| 27:Z:187:VAL:HG23 | 27:Z:192:ASP:HB2 | 1.60 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 15:N:35:PRO:CG | 15:N:38:VAL:HG23 | 2.09 | 0.81 |
| 11:J:55:GLN:HE21 | 11:J:124:ARG:HE | 1.24 | 0.81 |
| 5:D:62:ARG:HA | 5:D:65:MET:CE | 2.10 | 0.81 |
| 1:A:182:G:H4' | 15:N:157:LEU:HD13 | 1.61 | 0.81 |
| 5:D:162:MET:HE3 | 5:D:308:LEU:HD21 | 1.59 | 0.81 |
| 1:A:962:C:H1' | 16:O:5:ARG:NH1 | 1.96 | 0.81 |
| 4:C:109:GLU:HG2 | 4:C:116:GLY:H | 1.46 | 0.81 |
| 1:A:2506:A:O2' | 1:A:2507:G:H8 | 1.63 | 0.81 |
| 31:4:60:LYS:HG3 | 31:4:61:PRO:HD2 | 1.63 | 0.81 |
| 1:A:2533:C:H6 | 1:A:2533:C:H5' | 1.45 | 0.81 |
| 1:A:236:A:H4' | 1:A:237:G:H5' | 1.62 | 0.81 |
| 1:A:870:G:H2' | 1:A:871:G:H5'' | 1.61 | 0.80 |
| 38:A:6363:HOH:O | 15:N:178:LYS:HB2 | 1.79 | 0.80 |
| 9:H:63:ILE:HB | 9:H:64:PRO:HD3 | 1.64 | 0.80 |
| 9:H:91:VAL:HG12 | 9:H:92:GLY:N | 1.96 | 0.80 |
| 22:U:52:ARG:HB2 | 22:U:95:ASN:HB3 | 1.63 | 0.80 |
| 11:J:162:SER:HB2 | 11:J:163:PRO:CD | 2.10 | 0.80 |
| 9:H:91:VAL:HG12 | 9:H:92:GLY:H | 1.43 | 0.80 |
| 6:E:242:GLU:HG3 | 38:E:8385:HOH:O | 1.81 | 0.80 |
| 28:1:61:GLY:HA3 | 38:1:8425:HOH:O | 1.82 | 0.80 |
| 38:A:5284:HOH:O | 15:N:170:CYS:SG | 2.40 | 0.80 |
| 11:J:47:GLU:HB3 | 11:J:133:ILE:HD13 | 1.64 | 0.80 |
| 11:J:49:VAL:O | 11:J:157:ILE:HG23 | 1.81 | 0.80 |
| 1:A:1603:A:H5' | 1:A:1605:G:O4' | 1.81 | 0.80 |
| 20:S:99:ALA:HB1 | 20:S:109:MET:CE | 2.11 | 0.80 |
| 11:J:14:TYR:H | 11:J:91:HIS:CE1 | 2.00 | 0.80 |
| 6:E:115:LEU:HD13 | 6:E:223:LEU:HD21 | 1.62 | 0.80 |
| 4:C:69:LEU:HD21 | 4:C:120:ARG:HB3 | 1.61 | 0.80 |
| 31:4:25:VAL:HG22 | 31:4:68:LYS:HG3 | 1.62 | 0.80 |
| 5:D:62:ARG:HA | 5:D:65:MET:HE2 | 1.62 | 0.79 |
| 1:A:657:G:OP1 | 6:E:27:ARG:NH2 | 2.15 | 0.79 |
| 38:A:4357:HOH:O | 15:N:14:ARG:HG2 | 1.79 | 0.79 |
| 5:D:238:ASN:ND2 | 5:D:240:GLY:H | 1.78 | 0.79 |
| 1:A:111:C:O2' | 29:2:20:ARG:HG2 | 1.82 | 0.79 |
| 15:N:52:LEU:HD13 | 15:N:116:ASN:HB3 | 1.64 | 0.79 |
| 11:J:139:ASP:HA | 38:J:8372:HOH:O | 1.83 | 0.79 |
| 4:C:192:VAL:HG12 | 4:C:207:GLN:HB3 | 1.65 | 0.79 |
| 27:Z:220:GLU:HG2 | 38:Z:8545:HOH:O | 1.80 | 0.79 |
| 16:O:83:LEU:HD13 | 16:O:175:LEU:HD23 | 1.65 | 0.79 |
| 1:A:1118:A:C8 | 1:A:1118:A:H3' | 2.18 | 0.79 |
| 38:A:3234:HOH:O | 15:N:157:LEU:HD11 | 1.83 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:F:64:ARG:HG2 | 7:F:67:ASP:HB3 | 1.64 | 0.78 |
| 2:B:3023:U:H6 | 2:B:3023:U:H5'' | 1.46 | 0.78 |
| 1:A:282:C:H1' | 1:A:368:C:H42 | 1.49 | 0.78 |
| 1:A:1625:U:H4' | 38:A:4165:HOH:O | 1.84 | 0.78 |
| 6:E:5:ILE:HD11 | 6:E:16:VAL:HG23 | 1.65 | 0.78 |
| 2:B:3025:G:H3' | 2:B:3026:C:H5' | 1.64 | 0.78 |
| 6:E:115:LEU:HD21 | 6:E:243:VAL:HG13 | 1.64 | 0.78 |
| 8:G:81:GLU:HG2 | 8:G:134:SER:HB3 | 1.64 | 0.78 |
| 27:Z:186:ARG:HH11 | 27:Z:186:ARG:HG2 | 1.48 | 0.78 |
| 10:I:12:ILE:HA | 38:I:4499:HOH:O | 1.83 | 0.78 |
| 2:B:3006:C:H5'' | 16:O:37:ARG:HH12 | 1.48 | 0.78 |
| 6:E:1:MET:HG2 | 6:E:2:GLN:H | 1.48 | 0.78 |
| 1:A:1118:A:H3' | 1:A:1118:A:H8 | 1.47 | 0.77 |
| 1:A:1160:G:C5' | 1:A:1161:A:H5' | 2.13 | 0.77 |
| 6:E:236:THR:HG21 | 38:E:8376:HOH:O | 1.83 | 0.77 |
| 2:B:3025:G:H3' | 2:B:3026:C:C5' | 2.14 | 0.77 |
| 1:A:871:G:C5' | 1:A:871:G:H8 | 1.98 | 0.77 |
| 1:A:182:G:H5' | 38:A:4644:HOH:O | 1.83 | 0.77 |
| 5:D:179:LEU:O | 5:D:183:GLU:HG2 | 1.84 | 0.77 |
| 3:5:74:C:H2' | 3:5:75:C:C5' | 2.13 | 0.77 |
| 16:O:113:SER:HB2 | 38:O:8560:HOH:O | 1.84 | 0.77 |
| 5:D:238:ASN:HD22 | 5:D:240:GLY:N | 1.80 | 0.77 |
| 1:A:2526:C:O2' | 1:A:2527:U:H5' | 1.85 | 0.77 |
| 13:L:74:VAL:CG1 | 13:L:113:ILE:HG12 | 2.13 | 0.76 |
| 28:1:40:PRO:HD3 | 28:1:47:LEU:HD11 | 1.65 | 0.76 |
| 11:J:2:PRO:HB2 | 38:J:8366:HOH:O | 1.85 | 0.76 |
| 1:A:1450:C:H4' | 1:A:1451:C:OP2 | 1.86 | 0.76 |
| 12:K:19:MET:HE3 | 12:K:132:LEU:HD11 | 1.66 | 0.76 |
| 1:A:1834:C:H2' | 1:A:1840:A:N6 | 1.99 | 0.76 |
| 38:A:3191:HOH:O | 15:N:79:LYS:HD3 | 1.84 | 0.76 |
| 3:5:74:C:C2' | 3:5:75:C:H5' | 2.14 | 0.76 |
| 14:M:143:THR:HG21 | 38:M:8541:HOH:O | 1.86 | 0.76 |
| 16:O:87:LEU:HD12 | 16:O:186:LEU:HD21 | 1.67 | 0.76 |
| 1:A:2716:G:H5'' | 5:D:206:THR:HG21 | 1.67 | 0.76 |
| 7:F:25:MET:HE1 | 7:F:37:ALA:HB1 | 1.67 | 0.76 |
| 15:N:172:GLY:O | 15:N:183:VAL:HG11 | 1.84 | 0.76 |
| 1:A:1684:A:H1' | 30:3:43:ARG:HH22 | 1.48 | 0.76 |
| 1:A:2783:A:H3' | 38:A:4722:HOH:O | 1.86 | 0.76 |
| 15:N:139:PRO:O | 15:N:140:ALA:HB3 | 1.85 | 0.76 |
| 1:A:877:G:H5' | 1:A:878:G:OP1 | 1.85 | 0.76 |
| 1:A:2908:A:H2' | 1:A:2909:G:O4' | 1.87 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:Q:115:SER:OG | 18:Q:118:GLN:HG3 | 1.86 | 0.75 |
| 5:D:162:MET:CE | 5:D:308:LEU:HD21 | 2.16 | 0.75 |
| 14:M:148:GLU:HA | 38:M:8574:HOH:O | 1.85 | 0.75 |
| 5:D:168:GLY:N | 5:D:174:ARG:HD3 | 2.01 | 0.75 |
| 12:K:93:ARG:HH11 | 12:K:93:ARG:HB3 | 1.48 | 0.75 |
| 4:C:35:GLY:O | 4:C:36:ASP:HB3 | 1.85 | 0.75 |
| 26:Y:72:VAL:HG22 | 26:Y:85:VAL:HG12 | 1.68 | 0.75 |
| 16:O:48:VAL:CG1 | 16:O:55:ASP:HB3 | 2.15 | 0.75 |
| 8:G:166:VAL:HG12 | 38:G:3134:HOH:O | 1.86 | 0.75 |
| 7:F:55:LYS:HA | 38:F:6752:HOH:O | 1.86 | 0.75 |
| 38:A:5021:HOH:O | 15:N:58:GLN:HG3 | 1.87 | 0.75 |
| 1:A:1878:G:H1' | 38:A:5614:HOH:O | 1.84 | 0.75 |
| 1:A:2676:C:H4' | 12:K:70:PHE:CE1 | 2.21 | 0.75 |
| 20:S:18:LEU:HD12 | 20:S:143:VAL:HG11 | 1.66 | 0.75 |
| 24:W:1:THR:HG23 | 24:W:2:VAL:H | 1.49 | 0.75 |
| 23:V:14:GLU:O | 23:V:17:THR:HB | 1.87 | 0.75 |
| 15:N:164:THR:HG23 | 15:N:165:SER:N | 2.01 | 0.75 |
| 14:M:133:VAL:HB | 38:M:8559:HOH:O | 1.86 | 0.75 |
| 5:D:190:MET:HE2 | 5:D:194:PHE:CD1 | 2.21 | 0.75 |
| 25:X:21:LEU:HD21 | 25:X:48:VAL:CG1 | 2.17 | 0.75 |
| 1:A:383:A:H4' | 38:A:4821:HOH:O | 1.86 | 0.75 |
| 25:X:6:GLN:HB2 | 25:X:26:ILE:HD12 | 1.69 | 0.74 |
| 24:W:39:ALA:N | 24:W:40:PRO:HD2 | 2.02 | 0.74 |
| 15:N:64:ARG:HD2 | 38:N:8590:HOH:O | 1.87 | 0.74 |
| 15:N:94:LYS:HE3 | 38:N:8587:HOH:O | 1.87 | 0.74 |
| 1:A:214:U:H5' | 38:A:5633:HOH:O | 1.87 | 0.74 |
| 4:C:199:HIS:HD2 | 4:C:201:PHE:HB2 | 1.53 | 0.74 |
| 13:L:22:ASP:HB2 | 38:L:5264:HOH:O | 1.87 | 0.74 |
| 1:A:450:C:OP1 | 6:E:184:ARG:NH2 | 2.19 | 0.74 |
| 5:D:41:PHE:HA | 5:D:79:MET:HE2 | 1.69 | 0.74 |
| 5:D:168:GLY:H | 5:D:174:ARG:HD3 | 1.51 | 0.74 |
| 25:X:21:LEU:HD21 | 25:X:48:VAL:HG11 | 1.67 | 0.74 |
| 5:D:217:ARG:HG3 | 5:D:257:THR:HG22 | 1.69 | 0.74 |
| 1:A:289:G:H22 | 1:A:363:A:H2 | 1.35 | 0.74 |
| 15:N:164:THR:HG22 | 15:N:167:GLY:N | 2.02 | 0.74 |
| 1:A:1666:C:O2' | 1:A:1667:A:H5'' | 1.88 | 0.74 |
| 1:A:1372:A:H3' | 38:A:6680:HOH:O | 1.88 | 0.74 |
| 5:D:212:GLN:HB2 | 5:D:257:THR:HG21 | 1.70 | 0.74 |
| 13:L:62:PRO:HG3 | 13:L:65:ARG:HH21 | 1.51 | 0.74 |
| 1:A:21:G:C5' | 20:S:2:ILE:HA | 2.17 | 0.74 |
| 11:J:140:PRO:HB3 | 38:J:8381:HOH:O | 1.88 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:396:U:H1' | 38:A:7119:HOH:O | 1.86 | 0.74 |
| 1:A:338:C:H4' | 6:E:174:ILE:CD1 | 2.18 | 0.74 |
| 29:2:1:THR:HB | 38:2:8461:HOH:O | 1.87 | 0.74 |
| 6:E:162:VAL:HG13 | 6:E:232:LEU:HD21 | 1.70 | 0.73 |
| 1:A:1328:A:OP1 | 27:Z:169:ARG:HD2 | 1.87 | 0.73 |
| 1:A:1474:C:H5' | 1:A:1474:C:C6 | 2.21 | 0.73 |
| 27:Z:185:VAL:HG12 | 38:Z:8567:HOH:O | 1.88 | 0.73 |
| 1:A:2414:A:H2' | 1:A:2415:A:C8 | 2.23 | 0.73 |
| 1:A:1187:U:HO2' | 1:A:1189:A:H2 | 1.35 | 0.73 |
| 17:P:32:ARG:O | 17:P:32:ARG:HD3 | 1.88 | 0.73 |
| 6:E:233:THR:HG22 | 6:E:234:VAL:H | 1.53 | 0.73 |
| 12:K:107:ASN:ND2 | 12:K:109:TYR:H | 1.85 | 0.73 |
| 11:J:162:SER:CB | 11:J:163:PRO:HD3 | 2.17 | 0.73 |
| 28:1:37:HIS:HB2 | 28:1:47:LEU:HB2 | 1.70 | 0.73 |
| 20:S:14:ALA:HB3 | 20:S:147:LEU:HB2 | 1.69 | 0.73 |
| 6:E:236:THR:HA | 38:E:8454:HOH:O | 1.88 | 0.73 |
| 11:J:47:GLU:HB3 | 11:J:133:ILE:CD1 | 2.19 | 0.73 |
| 8:G:20:ILE:CD1 | 8:G:40:VAL:HG11 | 2.19 | 0.73 |
| 25:X:22:GLU:HG2 | 25:X:27:HIS:CD2 | 2.23 | 0.73 |
| 7:F:88:LEU:HB2 | 7:F:89:PRO:HD3 | 1.71 | 0.73 |
| 4:C:37:VAL:HG22 | 38:C:8592:HOH:O | 1.88 | 0.73 |
| 1:A:506:G:H22 | 1:A:509:A:C5' | 2.00 | 0.73 |
| 25:X:4:LEU:HD22 | 25:X:52:VAL:CG2 | 2.18 | 0.73 |
| 1:A:1116:U:O2' | 1:A:1118:A:H2 | 1.69 | 0.73 |
| 1:A:1191:A:H3' | 1:A:1192:A:H5'' | 1.69 | 0.73 |
| 1:A:1164:U:H3 | 1:A:1192:A:H2 | 1.37 | 0.72 |
| 27:Z:216:ARG:HD3 | 38:Z:8566:HOH:O | 1.89 | 0.72 |
| 17:P:47:ARG:HH11 | 17:P:47:ARG:HG3 | 1.53 | 0.72 |
| 7:F:135:VAL:HG21 | 7:F:139:TYR:CD1 | 2.24 | 0.72 |
| 26:Y:15:ARG:HH11 | 26:Y:15:ARG:HB3 | 1.53 | 0.72 |
| 6:E:2:GLN:HB3 | 38:E:8335:HOH:O | 1.89 | 0.72 |
| 1:A:272:A:H3' | 38:A:7022:HOH:O | 1.90 | 0.72 |
| 1:A:2851:G:O2' | 1:A:2852:A:H5' | 1.89 | 0.72 |
| 2:B:3048:C:H4' | 16:O:141:ARG:HH21 | 1.54 | 0.72 |
| 25:X:122:ARG:HG2 | 25:X:122:ARG:HH11 | 1.54 | 0.72 |
| 1:A:541:C:H2' | 1:A:542:A:C5' | 2.18 | 0.72 |
| 23:V:46:ALA:HB1 | 23:V:52:THR:HG21 | 1.72 | 0.72 |
| 16:O:159:TYR:HB3 | 16:O:162:ASP:HB2 | 1.72 | 0.72 |
| 12:K:19:MET:CE | 12:K:132:LEU:HD11 | 2.20 | 0.72 |
| 1:A:56:G:H5'' | 24:W:50:ARG:HH12 | 1.55 | 0.72 |
| 19:R:11:ARG:HD3 | 38:R:5620:HOH:O | 1.90 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:E:236:THR:CG2 | 6:E:239:ALA:H | 1.94 | 0.72 |
| 22:U:63:ILE:HD11 | 22:U:75:GLU:HB2 | 1.70 | 0.72 |
| 7:F:57:THR:HG23 | 7:F:63:ILE:HG22 | 1.72 | 0.72 |
| 1:A:2420:G:O2' | 1:A:2421:G:H5' | 1.90 | 0.72 |
| 12:K:131:THR:HG22 | 12:K:134:GLU:H | 1.53 | 0.72 |
| 1:A:1667:A:C8 | 1:A:1667:A:H5' | 2.23 | 0.72 |
| 14:M:77:ALA:HB3 | 38:M:8531:HOH:O | 1.90 | 0.72 |
| 4:C:153:ARG:HB2 | 4:C:153:ARG:HH11 | 1.55 | 0.72 |
| 1:A:962:C:H1' | 16:O:5:ARG:HH12 | 1.55 | 0.71 |
| 28:1:46:LYS:HD3 | 28:1:59:HIS:HB2 | 1.70 | 0.71 |
| 1:A:1641:A:H2' | 1:A:1642:A:H5' | 1.72 | 0.71 |
| 25:X:4:LEU:HD23 | 25:X:54:PHE:HB3 | 1.69 | 0.71 |
| 1:A:284:C:H4' | 1:A:285:A:O5' | 1.88 | 0.71 |
| 7:F:64:ARG:CG | 7:F:67:ASP:HB3 | 2.21 | 0.71 |
| 16:O:4:PRO:HD2 | 38:O:8558:HOH:O | 1.90 | 0.71 |
| 1:A:2502:C:C2' | 1:A:2503:A:H5' | 2.20 | 0.71 |
| 1:A:2578:G:H8 | 1:A:2578:G:H5' | 1.54 | 0.71 |
| 9:H:58:GLU:HA | 9:H:61:MET:HE2 | 1.71 | 0.71 |
| 6:E:237:GLU:HB2 | 38:E:8435:HOH:O | 1.89 | 0.71 |
| 1:A:1160:G:H5' | 1:A:1161:A:C5' | 2.20 | 0.71 |
| 1:A:2502:C:H4' | 11:J:151:MET:HG2 | 1.72 | 0.71 |
| 2:B:3056:A:C2' | 2:B:3057:A:H5" | 2.20 | 0.71 |
| 25:X:13:MET:HE3 | 25:X:17:ILE:HG22 | 1.72 | 0.71 |
| 24:W:42:ASN:HB3 | 38:W:7247:HOH:O | 1.90 | 0.71 |
| 9:H:99:THR:HA | 38:H:3461:HOH:O | 1.91 | 0.71 |
| 12:K:99:GLU:HA | 38:K:7377:HOH:O | 1.88 | 0.71 |
| 1:A:1701:A:H4' | 1:A:1702:U:H5" | 1.71 | 0.71 |
| 38:A:3063:HOH:O | 15:N:152:ARG:HG3 | 1.89 | 0.71 |
| 5:D:195:ARG:HG2 | 5:D:323:LEU:HD22 | 1.71 | 0.71 |
| 25:X:88:THR:HG22 | 25:X:89:ASP:H | 1.54 | 0.71 |
| 4:C:191:GLY:HA2 | 4:C:194:MET:CE | 2.21 | 0.71 |
| 1:A:2359:G:H3' | 38:A:5184:HOH:O | 1.89 | 0.71 |
| 30:3:39:ARG:HG2 | 38:3:3143:HOH:O | 1.89 | 0.71 |
| 1:A:281:U:H3' | 38:A:6697:HOH:O | 1.90 | 0.71 |
| 11:J:150:LYS:HB2 | 11:J:157:ILE:HD12 | 1.73 | 0.70 |
| 38:A:6516:HOH:O | 4:C:211:LYS:HG2 | 1.90 | 0.70 |
| 1:A:544:G:H2' | 1:A:545:G:H5" | 1.73 | 0.70 |
| 1:A:603:A:H5" | 1:A:604:G:OP1 | 1.91 | 0.70 |
| 11:J:142:VAL:HG13 | 38:J:8381:HOH:O | 1.90 | 0.70 |
| 1:A:1182:C:H1' | 1:A:1192:A:H8 | 1.57 | 0.70 |
| 7:F:136:ARG:HD2 | 7:F:155:HIS:O | 1.90 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:J:59:ASN:N | 11:J:59:ASN:HD22 | 1.87 | 0.70 |
| 1:A:31:C:H2' | 38:A:7178:HOH:O | 1.91 | 0.70 |
| 1:A:2890:A:H1' | 23:V:56:ARG:NH2 | 2.06 | 0.70 |
| 9:H:53:ASP:OD1 | 9:H:80:GLN:HB2 | 1.90 | 0.70 |
| 1:A:2827:A:H2' | 1:A:2828:G:O4' | 1.90 | 0.70 |
| 11:J:45:GLN:HE21 | 11:J:135:TRP:HE1 | 1.39 | 0.70 |
| 20:S:9:ASP:O | 20:S:13:THR:HB | 1.91 | 0.70 |
| 7:F:41:LEU:HA | 7:F:44:ILE:HG22 | 1.74 | 0.70 |
| 31:4:70:ARG:HD3 | 38:4:8538:HOH:O | 1.90 | 0.70 |
| 8:G:107:PHE:CE2 | 8:G:108:LEU:HD13 | 2.27 | 0.70 |
| 4:C:170:VAL:HG22 | 28:1:22:ILE:HG23 | 1.72 | 0.70 |
| 11:J:46:VAL:HG12 | 11:J:146:TRP:HZ3 | 1.57 | 0.70 |
| 1:A:1185:U:H2' | 1:A:1186:C:C6 | 2.27 | 0.70 |
| 1:A:1835:U:C5 | 1:A:1840:A:N7 | 2.60 | 0.70 |
| 22:U:61:GLU:HG3 | 38:U:3851:HOH:O | 1.91 | 0.70 |
| 10:I:23:ILE:HD13 | 10:I:67:LEU:HD23 | 1.74 | 0.69 |
| 4:C:131:HIS:O | 4:C:132:ASP:HB2 | 1.91 | 0.69 |
| 1:A:188:C:H5'' | 15:N:163:LEU:HD21 | 1.74 | 0.69 |
| 1:A:2862:G:H4' | 5:D:336:GLN:O | 1.91 | 0.69 |
| 1:A:2031:C:O3' | 38:A:4015:HOH:O | 2.10 | 0.69 |
| 7:F:27:ILE:HG22 | 7:F:28:GLY:N | 2.07 | 0.69 |
| 4:C:191:GLY:HA2 | 4:C:194:MET:HE3 | 1.72 | 0.69 |
| 26:Y:71:ARG:HB3 | 26:Y:88:GLU:OE1 | 1.92 | 0.69 |
| 38:A:7070:HOH:O | 28:1:31:ILE:HG13 | 1.92 | 0.69 |
| 15:N:139:PRO:O | 15:N:140:ALA:CB | 2.40 | 0.69 |
| 4:C:94:LEU:HG | 4:C:99:ILE:HD11 | 1.73 | 0.69 |
| 15:N:87:MET:HB3 | 31:4:46:ILE:HG21 | 1.73 | 0.69 |
| 11:J:55:GLN:NE2 | 11:J:124:ARG:HE | 1.90 | 0.69 |
| 1:A:1165:G:H4' | 1:A:1174:A:O2' | 1.93 | 0.69 |
| 22:U:9:LYS:HE3 | 22:U:13:ARG:HH11 | 1.58 | 0.69 |
| 1:A:1206:U:H5' | 1:A:1206:U:H6 | 1.56 | 0.69 |
| 1:A:1505:U:H6 | 1:A:1505:U:H5' | 1.56 | 0.69 |
| 4:C:105:VAL:HG11 | 4:C:154:ALA:HB1 | 1.74 | 0.69 |
| 6:E:236:THR:H | 6:E:239:ALA:HB3 | 1.58 | 0.69 |
| 2:B:3049:G:H5'' | 38:B:8465:HOH:O | 1.92 | 0.69 |
| 20:S:18:LEU:HB2 | 20:S:143:VAL:HG12 | 1.75 | 0.69 |
| 1:A:338:C:H5'' | 38:E:8426:HOH:O | 1.93 | 0.69 |
| 4:C:100:PRO:HG2 | 4:C:103:VAL:HG21 | 1.73 | 0.69 |
| 22:U:41:ARG:HG2 | 22:U:41:ARG:HH11 | 1.56 | 0.69 |
| 6:E:47:GLY:HA2 | 6:E:92:PRO:HB2 | 1.74 | 0.69 |
| 22:U:101:LEU:HD13 | 22:U:112:LEU:HD11 | 1.75 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:Z:99:ALA:HB2 | 27:Z:233:TYR:CZ | 2.28 | 0.69 |
| 1:A:553:G:P | 27:Z:204:ARG:HH22 | 2.16 | 0.69 |
| 1:A:1751:G:C2' | 1:A:1752:G:H5'' | 2.22 | 0.69 |
| 16:O:71:TRP:CE3 | 16:O:175:LEU:HD22 | 2.28 | 0.69 |
| 15:N:57:LYS:HE2 | 15:N:140:ALA:O | 1.93 | 0.69 |
| 1:A:1118:A:H62 | 1:A:1244:U:H3 | 1.39 | 0.69 |
| 1:A:871:G:C5' | 1:A:871:G:C8 | 2.75 | 0.69 |
| 1:A:545:G:H5' | 1:A:545:G:C8 | 2.26 | 0.69 |
| 5:D:145:HIS:HD2 | 5:D:146:THR:O | 1.76 | 0.69 |
| 25:X:88:THR:HG23 | 25:X:110:GLN:HE21 | 1.57 | 0.68 |
| 4:C:109:GLU:HG2 | 4:C:116:GLY:N | 2.08 | 0.68 |
| 2:B:3014:G:H8 | 2:B:3014:G:H5' | 1.56 | 0.68 |
| 24:W:12:THR:HG22 | 24:W:15:GLU:CG | 2.22 | 0.68 |
| 1:A:56:G:H5'' | 24:W:50:ARG:NH1 | 2.09 | 0.68 |
| 12:K:45:VAL:HG23 | 12:K:130:VAL:O | 1.92 | 0.68 |
| 1:A:2587:U:H2' | 1:A:2589:U:H5'' | 1.74 | 0.68 |
| 30:3:41:HIS:N | 30:3:45:ASN:HD22 | 1.91 | 0.68 |
| 1:A:2897:C:H2' | 1:A:2898:G:H8 | 1.58 | 0.68 |
| 12:K:103:VAL:HG12 | 38:K:5907:HOH:O | 1.92 | 0.68 |
| 1:A:2426:G:H1' | 38:A:5585:HOH:O | 1.93 | 0.68 |
| 20:S:18:LEU:HB2 | 20:S:143:VAL:CG1 | 2.24 | 0.68 |
| 1:A:2054:A:N3 | 20:S:128:ARG:NH2 | 2.41 | 0.68 |
| 5:D:304:PRO:HD2 | 5:D:307:ARG:HD2 | 1.76 | 0.68 |
| 1:A:2502:C:H2' | 1:A:2503:A:H5' | 1.76 | 0.68 |
| 16:O:183:ASP:OD2 | 16:O:186:LEU:HD12 | 1.93 | 0.68 |
| 16:O:48:VAL:HG11 | 16:O:55:ASP:HB3 | 1.76 | 0.68 |
| 26:Y:76:ARG:HH11 | 26:Y:76:ARG:HG3 | 1.58 | 0.68 |
| 11:J:35:ASN:ND2 | 11:J:80:ASN:HA | 2.10 | 0.67 |
| 1:A:281:U:H2' | 1:A:282:C:O4' | 1.94 | 0.67 |
| 25:X:21:LEU:HD22 | 25:X:26:ILE:HD11 | 1.75 | 0.67 |
| 1:A:2638:G:H1' | 38:A:7249:HOH:O | 1.93 | 0.67 |
| 1:A:2310:G:OP2 | 11:J:114:PRO:HD2 | 1.95 | 0.67 |
| 1:A:681:G:N3 | 1:A:681:G:H5' | 2.10 | 0.67 |
| 11:J:141:ASN:HA | 38:J:8368:HOH:O | 1.95 | 0.67 |
| 7:F:105:SER:CB | 7:F:131:THR:HG23 | 2.22 | 0.67 |
| 1:A:183:A:H5' | 15:N:157:LEU:HD12 | 1.77 | 0.67 |
| 27:Z:107:PRO:HB3 | 27:Z:182:PHE:CD2 | 2.29 | 0.67 |
| 10:I:64:ASN:O | 10:I:68:GLU:HG3 | 1.94 | 0.67 |
| 27:Z:235:GLU:CD | 27:Z:235:GLU:H | 1.97 | 0.67 |
| 5:D:314:ALA:HB3 | 5:D:317:PRO:HG3 | 1.76 | 0.67 |
| 6:E:140:VAL:HB | 38:E:8454:HOH:O | 1.93 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 14:M:136:ALA:HB3 | 38:M:8575:HOH:O | 1.94 | 0.67 |
| 4:C:88:ILE:HD13 | 4:C:100:PRO:HD3 | 1.76 | 0.67 |
| 1:A:2878:U:H2' | 1:A:2879:A:O4' | 1.95 | 0.67 |
| 1:A:2533:C:C6 | 1:A:2533:C:H5' | 2.28 | 0.67 |
| 1:A:1120:U:H6 | 1:A:1120:U:H5'' | 1.59 | 0.67 |
| 1:A:1080:C:H4' | 1:A:1081:A:OP1 | 1.94 | 0.67 |
| 26:Y:30:MET:HE1 | 26:Y:55:ASN:HA | 1.76 | 0.67 |
| 5:D:175:LEU:HD23 | 5:D:175:LEU:C | 2.14 | 0.67 |
| 5:D:18:ARG:HG3 | 5:D:256:GLN:HG3 | 1.76 | 0.67 |
| 1:A:2748:G:H5' | 38:A:7033:HOH:O | 1.95 | 0.67 |
| 18:Q:143:ALA:HA | 38:Q:168:HOH:O | 1.95 | 0.67 |
| 31:4:70:ARG:HG2 | 31:4:77:ALA:HB2 | 1.76 | 0.67 |
| 25:X:137:GLN:HE21 | 25:X:141:HIS:HE1 | 1.41 | 0.67 |
| 1:A:694:A:H2' | 1:A:695:C:H5' | 1.75 | 0.67 |
| 5:D:264:GLU:HG2 | 5:D:267:LYS:HE2 | 1.76 | 0.67 |
| 25:X:65:VAL:HA | 25:X:68:THR:HG22 | 1.76 | 0.67 |
| 10:I:12:ILE:N | 10:I:13:PRO:HD3 | 2.09 | 0.67 |
| 1:A:282:C:O2' | 1:A:283:U:H5' | 1.94 | 0.67 |
| 1:A:2301:A:H5'' | 1:A:2302:A:H5' | 1.76 | 0.67 |
| 1:A:1119:G:N2 | 1:A:1246:A:C2 | 2.62 | 0.67 |
| 4:C:33:GLU:O | 4:C:34:ASP:HB2 | 1.94 | 0.67 |
| 16:O:169:PRO:O | 16:O:172:PHE:HB3 | 1.95 | 0.67 |
| 1:A:1596:U:H2' | 1:A:1598:A:OP2 | 1.94 | 0.66 |
| 8:G:11:VAL:HG12 | 8:G:12:ASP:N | 2.11 | 0.66 |
| 18:Q:59:ARG:NH2 | 18:Q:66:GLN:HE22 | 1.92 | 0.66 |
| 21:T:23:LYS:HE2 | 38:T:8330:HOH:O | 1.95 | 0.66 |
| 1:A:1771:U:H4' | 28:1:20:LEU:HD21 | 1.75 | 0.66 |
| 11:J:59:ASN:H | 11:J:59:ASN:ND2 | 1.91 | 0.66 |
| 1:A:2676:C:H4' | 12:K:70:PHE:HE1 | 1.60 | 0.66 |
| 25:X:21:LEU:HD13 | 25:X:26:ILE:HD11 | 1.76 | 0.66 |
| 21:T:51:GLN:HE21 | 21:T:53:ASN:HD21 | 1.41 | 0.66 |
| 38:L:408:HOH:O | 23:V:37:GLU:HB3 | 1.94 | 0.66 |
| 6:E:76:ARG:HD3 | 38:E:8369:HOH:O | 1.95 | 0.66 |
| 15:N:37:VAL:HG21 | 15:N:108:LYS:HG3 | 1.76 | 0.66 |
| 15:N:138:HIS:ND1 | 15:N:139:PRO:O | 2.23 | 0.66 |
| 7:F:65:GLU:HG3 | 38:F:6752:HOH:O | 1.94 | 0.66 |
| 1:A:2256:G:H2' | 1:A:2257:G:H5' | 1.78 | 0.66 |
| 27:Z:141:THR:HG23 | 38:Z:8586:HOH:O | 1.95 | 0.66 |
| 15:N:65:VAL:HG21 | 15:N:105:ALA:HB2 | 1.77 | 0.66 |
| 15:N:169:ARG:HD2 | 38:N:8596:HOH:O | 1.94 | 0.66 |
| 17:P:87:THR:O | 17:P:91:GLN:HG3 | 1.96 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 14:M:54:PRO:HG2 | 14:M:57:VAL:HG21 | 1.78 | 0.66 |
| 1:A:558:C:H2' | 1:A:559:U:H5' | 1.75 | 0.66 |
| 11:J:56:ILE:HG22 | 11:J:61:LEU:HD22 | 1.77 | 0.66 |
| 6:E:162:VAL:HG12 | 6:E:192:ILE:HD11 | 1.78 | 0.66 |
| 4:C:105:VAL:CG1 | 4:C:154:ALA:HB1 | 2.25 | 0.66 |
| 1:A:2840:A:OP1 | 5:D:211:THR:HG23 | 1.94 | 0.66 |
| 16:O:164:ASP:CG | 16:O:167:ASP:HA | 2.16 | 0.66 |
| 1:A:1741:U:H5' | 1:A:1742:A:OP1 | 1.96 | 0.66 |
| 1:A:470:U:O2' | 29:2:16:HIS:HD2 | 1.77 | 0.66 |
| 1:A:1120:U:H5'' | 1:A:1120:U:C6 | 2.31 | 0.66 |
| 5:D:71:VAL:HG11 | 5:D:296:LEU:HB3 | 1.75 | 0.66 |
| 9:H:46:GLU:O | 9:H:73:PRO:HD2 | 1.95 | 0.66 |
| 29:2:25:LYS:HG2 | 29:2:25:LYS:O | 1.94 | 0.66 |
| 27:Z:151:SER:HB3 | 27:Z:154:ARG:HB3 | 1.77 | 0.66 |
| 1:A:1666:C:H2' | 1:A:1667:A:H5' | 1.76 | 0.66 |
| 7:F:19:GLU:O | 7:F:20:LYS:HG2 | 1.96 | 0.66 |
| 38:A:4461:HOH:O | 11:J:57:ARG:HG3 | 1.93 | 0.66 |
| 24:W:4:HIS:HB3 | 38:W:6622:HOH:O | 1.95 | 0.66 |
| 11:J:31:PHE:CD2 | 11:J:85:ILE:HG23 | 2.31 | 0.66 |
| 14:M:143:THR:HG22 | 14:M:144:ASP:N | 2.11 | 0.66 |
| 12:K:39:VAL:HG12 | 12:K:40:ASN:ND2 | 2.11 | 0.66 |
| 28:1:28:ASP:O | 28:1:31:ILE:HG22 | 1.95 | 0.66 |
| 18:Q:64:GLU:HG2 | 38:Q:169:HOH:O | 1.95 | 0.66 |
| 7:F:140:ARG:O | 7:F:144:ARG:HG2 | 1.96 | 0.66 |
| 6:E:214:THR:HG21 | 38:E:8408:HOH:O | 1.94 | 0.66 |
| 14:M:68:GLU:HA | 38:M:8545:HOH:O | 1.95 | 0.66 |
| 1:A:1130:U:H5' | 38:A:7161:HOH:O | 1.96 | 0.65 |
| 11:J:44:ALA:HA | 11:J:163:PRO:O | 1.96 | 0.65 |
| 9:H:50:VAL:HG21 | 9:H:63:ILE:HG21 | 1.77 | 0.65 |
| 25:X:90:TYR:CE2 | 25:X:99:ALA:HB2 | 2.31 | 0.65 |
| 6:E:142:ASP:OD1 | 6:E:237:GLU:HB3 | 1.95 | 0.65 |
| 18:Q:115:SER:O | 18:Q:117:SER:N | 2.30 | 0.65 |
| 4:C:95:PRO:HG2 | 4:C:98:GLU:HG2 | 1.78 | 0.65 |
| 22:U:32:ARG:NH1 | 22:U:38:ARG:HH12 | 1.93 | 0.65 |
| 1:A:1377:C:H5' | 1:A:1377:C:H6 | 1.61 | 0.65 |
| 20:S:132:ARG:HG2 | 20:S:133:ALA:N | 2.12 | 0.65 |
| 11:J:84:ARG:NH2 | 11:J:135:TRP:HH2 | 1.95 | 0.65 |
| 15:N:52:LEU:HD21 | 38:N:8623:HOH:O | 1.95 | 0.65 |
| 25:X:88:THR:HG23 | 25:X:110:GLN:HB3 | 1.78 | 0.65 |
| 7:F:64:ARG:CD | 7:F:67:ASP:HB3 | 2.25 | 0.65 |
| 28:1:49:ARG:HD2 | 38:1:8427:HOH:O | 1.97 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2508:C:H2' | 38:A:6243:HOH:O | 1.95 | 0.65 |
| 20:S:33:ARG:NH1 | 38:S:8544:HOH:O | 2.29 | 0.65 |
| 1:A:656:G:OP2 | 17:P:37:ARG:HD2 | 1.96 | 0.65 |
| 1:A:1593:C:H5' | 18:Q:116:SER:O | 1.96 | 0.65 |
| 1:A:1589:G:N2 | 1:A:1605:G:H1' | 2.11 | 0.65 |
| 16:O:143:ARG:HA | 16:O:172:PHE:CD2 | 2.32 | 0.65 |
| 1:A:1919:A:H4' | 38:A:4344:HOH:O | 1.96 | 0.65 |
| 7:F:146:LYS:HZ1 | 16:O:107:ASN:HD21 | 1.45 | 0.65 |
| 27:Z:187:VAL:HG23 | 27:Z:192:ASP:CB | 2.25 | 0.65 |
| 6:E:5:ILE:HD11 | 6:E:16:VAL:CG2 | 2.26 | 0.65 |
| 11:J:46:VAL:O | 11:J:146:TRP:HH2 | 1.80 | 0.65 |
| 25:X:81:ASP:OD1 | 25:X:92:ASP:HB2 | 1.96 | 0.65 |
| 1:A:42:C:H1' | 38:A:4174:HOH:O | 1.95 | 0.65 |
| 27:Z:189:ASN:HD22 | 27:Z:189:ASN:C | 2.00 | 0.65 |
| 28:1:25:ARG:O | 28:1:29:VAL:HG23 | 1.97 | 0.65 |
| 21:T:57:THR:HG22 | 21:T:59:ASP:H | 1.61 | 0.65 |
| 1:A:2780:C:H1' | 8:G:143:GLN:HE21 | 1.60 | 0.65 |
| 1:A:1118:A:H8 | 1:A:1119:G:H5'' | 1.61 | 0.65 |
| 1:A:1209:C:H4' | 38:A:4773:HOH:O | 1.95 | 0.65 |
| 18:Q:103:THR:HA | 18:Q:106:ARG:NH1 | 2.12 | 0.65 |
| 5:D:297:VAL:HB | 38:D:8607:HOH:O | 1.97 | 0.65 |
| 26:Y:43:VAL:HG12 | 26:Y:44:ASP:N | 2.11 | 0.65 |
| 15:N:174:ARG:HG3 | 38:N:8521:HOH:O | 1.96 | 0.65 |
| 15:N:30:GLU:O | 15:N:34:GLU:HG3 | 1.97 | 0.65 |
| 7:F:135:VAL:HG22 | 7:F:136:ARG:H | 1.61 | 0.65 |
| 6:E:104:ASP:HA | 6:E:107:ARG:HH12 | 1.61 | 0.65 |
| 11:J:130:HIS:CD2 | 11:J:133:ILE:HD11 | 2.32 | 0.64 |
| 15:N:34:GLU:HB3 | 15:N:35:PRO:HD2 | 1.79 | 0.64 |
| 38:A:3171:HOH:O | 15:N:79:LYS:HD2 | 1.96 | 0.64 |
| 1:A:1028:U:H1' | 38:A:3156:HOH:O | 1.96 | 0.64 |
| 8:G:132:THR:HB | 38:G:2227:HOH:O | 1.96 | 0.64 |
| 5:D:55:ASN:HB3 | 5:D:63:GLU:HA | 1.79 | 0.64 |
| 6:E:139:VAL:HG13 | 38:E:8451:HOH:O | 1.97 | 0.64 |
| 7:F:69:ILE:O | 7:F:69:ILE:HG22 | 1.96 | 0.64 |
| 11:J:33:MET:HB2 | 11:J:83:PHE:HB3 | 1.80 | 0.64 |
| 25:X:68:THR:HG23 | 25:X:69:ARG:HG2 | 1.77 | 0.64 |
| 16:O:154:LEU:O | 16:O:155:GLU:HB3 | 1.98 | 0.64 |
| 1:A:2768:A:H2' | 1:A:2769:C:O4' | 1.96 | 0.64 |
| 12:K:133:GLY:O | 12:K:137:GLU:HG3 | 1.97 | 0.64 |
| 5:D:140:LEU:HD23 | 38:D:8583:HOH:O | 1.98 | 0.64 |
| 17:P:42:GLU:HB2 | 38:P:2176:HOH:O | 1.96 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:2748:G:H2' | 38:A:7033:HOH:O | 1.97 | 0.64 |
| 6:E:78:ARG:HH11 | 6:E:78:ARG:HG3 | 1.61 | 0.64 |
| 17:P:44:ASN:OD1 | 17:P:65:LEU:HB2 | 1.96 | 0.64 |
| 4:C:81:GLN:HB2 | 4:C:92:ASN:ND2 | 2.11 | 0.64 |
| 27:Z:212:ARG:HD2 | 38:Z:8598:HOH:O | 1.97 | 0.64 |
| 7:F:54:ALA:CB | 7:F:69:ILE:HD12 | 2.28 | 0.64 |
| 7:F:67:ASP:O | 7:F:69:ILE:HG13 | 1.98 | 0.64 |
| 16:O:164:ASP:OD2 | 16:O:167:ASP:HA | 1.98 | 0.64 |
| 31:4:73:GLU:HB3 | 38:4:8558:HOH:O | 1.96 | 0.64 |
| 20:S:39:THR:HG23 | 20:S:107:GLU:O | 1.98 | 0.64 |
| 1:A:2472:C:O2' | 1:A:2634:G:H4' | 1.97 | 0.64 |
| 7:F:99:ASP:HB3 | 7:F:103:ASN:H | 1.62 | 0.64 |
| 1:A:1266:U:H4' | 27:Z:115:ARG:HH21 | 1.62 | 0.64 |
| 1:A:272:A:H5' | 1:A:273:G:OP2 | 1.98 | 0.64 |
| 1:A:559:U:H2' | 1:A:560:C:O4' | 1.98 | 0.64 |
| 2:B:3023:U:C3' | 2:B:3024:U:H5'' | 2.21 | 0.64 |
| 12:K:74:ARG:CB | 12:K:74:ARG:HH11 | 2.11 | 0.64 |
| 7:F:23:VAL:HG23 | 7:F:23:VAL:O | 1.97 | 0.64 |
| 7:F:38:GLU:OE2 | 7:F:51:ARG:CZ | 2.45 | 0.64 |
| 16:O:71:TRP:HE3 | 16:O:175:LEU:HD22 | 1.63 | 0.64 |
| 5:D:36:PRO:HA | 5:D:168:GLY:CA | 2.28 | 0.64 |
| 23:V:14:GLU:OE1 | 23:V:15:PRO:HD2 | 1.98 | 0.64 |
| 1:A:2346:C:O2' | 7:F:52:THR:HG21 | 1.97 | 0.64 |
| 17:P:96:VAL:HA | 38:P:4258:HOH:O | 1.98 | 0.64 |
| 1:A:506:G:H22 | 1:A:509:A:H5'' | 1.63 | 0.63 |
| 18:Q:103:THR:HB | 38:Q:180:HOH:O | 1.98 | 0.63 |
| 13:L:49:LEU:HD21 | 13:L:74:VAL:O | 1.99 | 0.63 |
| 1:A:1285:U:H4' | 25:X:74:GLU:OE1 | 1.98 | 0.63 |
| 17:P:32:ARG:HG2 | 38:P:2336:HOH:O | 1.97 | 0.63 |
| 8:G:7:ILE:HD11 | 8:G:11:VAL:C | 2.18 | 0.63 |
| 1:A:506:G:H22 | 1:A:509:A:H5' | 1.62 | 0.63 |
| 1:A:2435:U:H1' | 38:A:4921:HOH:O | 1.97 | 0.63 |
| 2:B:3092:G:H2' | 2:B:3093:A:C8 | 2.33 | 0.63 |
| 28:1:53:GLY:HA2 | 28:1:67:GLY:O | 1.98 | 0.63 |
| 11:J:26:LYS:HD2 | 11:J:28:ILE:HB | 1.78 | 0.63 |
| 15:N:38:VAL:C | 15:N:63:VAL:HG13 | 2.19 | 0.63 |
| 16:O:86:LEU:HD12 | 16:O:125:ALA:HB2 | 1.79 | 0.63 |
| 25:X:21:LEU:HD22 | 25:X:26:ILE:CD1 | 2.29 | 0.63 |
| 7:F:36:ASN:HA | 38:F:7500:HOH:O | 1.98 | 0.63 |
| 9:H:91:VAL:CG1 | 9:H:92:GLY:H | 2.11 | 0.63 |
| 38:A:3734:HOH:O | 30:3:38:LYS:HE3 | 1.99 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:G:15:GLN:HG3 | 8:G:20:ILE:HG12 | 1.81 | 0.63 |
| 1:A:2064:U:H4' | 1:A:2653:A:OP1 | 1.98 | 0.63 |
| 5:D:305:ASP:O | 5:D:306:LYS:HB2 | 1.98 | 0.63 |
| 14:M:145:LEU:O | 14:M:148:GLU:HG3 | 1.98 | 0.63 |
| 38:A:8913:HOH:O | 15:N:94:LYS:HE2 | 1.98 | 0.63 |
| 8:G:31:ARG:HH12 | 8:G:68:HIS:CD2 | 2.17 | 0.63 |
| 11:J:48:LEU:HG | 11:J:157:ILE:HG21 | 1.79 | 0.63 |
| 2:B:3023:U:H5'' | 2:B:3023:U:C6 | 2.31 | 0.63 |
| 1:A:157:G:H4' | 15:N:95:LYS:HE3 | 1.80 | 0.63 |
| 27:Z:189:ASN:ND2 | 27:Z:192:ASP:H | 1.97 | 0.63 |
| 15:N:149:TRP:O | 15:N:152:ARG:HG2 | 1.99 | 0.63 |
| 1:A:2320:U:H4' | 1:A:2321:A:O4' | 1.98 | 0.63 |
| 21:T:37:VAL:O | 21:T:41:VAL:HG23 | 1.98 | 0.63 |
| 11:J:27:LYS:N | 11:J:58:HIS:HD2 | 1.95 | 0.63 |
| 15:N:157:LEU:HB3 | 15:N:160:PHE:HD1 | 1.64 | 0.63 |
| 25:X:122:ARG:HH22 | 25:X:154:ARG:C | 2.02 | 0.63 |
| 6:E:20:ASP:O | 6:E:23:GLU:HB2 | 1.99 | 0.63 |
| 11:J:127:GLY:O | 11:J:128:ALA:HB3 | 1.98 | 0.63 |
| 5:D:275:GLY:O | 5:D:291:ASP:HA | 1.99 | 0.63 |
| 1:A:280:C:H2' | 1:A:281:U:O4' | 1.99 | 0.62 |
| 1:A:560:C:H42 | 1:A:597:A:H61 | 1.45 | 0.62 |
| 21:T:57:THR:HG22 | 21:T:59:ASP:N | 2.13 | 0.62 |
| 38:A:4043:HOH:O | 11:J:151:MET:HE2 | 1.98 | 0.62 |
| 10:I:63:ARG:N | 38:I:2569:HOH:O | 2.30 | 0.62 |
| 1:A:585:C:H5'' | 38:A:4365:HOH:O | 1.97 | 0.62 |
| 1:A:1333:U:H2' | 1:A:1334:C:C6 | 2.35 | 0.62 |
| 20:S:17:MET:HE1 | 20:S:19:ARG:NH2 | 2.13 | 0.62 |
| 20:S:40:ALA:O | 20:S:44:VAL:HG23 | 1.99 | 0.62 |
| 1:A:1559:A:H1' | 38:A:5357:HOH:O | 1.99 | 0.62 |
| 38:B:8465:HOH:O | 16:O:147:ILE:HD12 | 1.98 | 0.62 |
| 18:Q:10:ALA:HA | 18:Q:13:VAL:HG12 | 1.81 | 0.62 |
| 2:B:3029:C:H2' | 2:B:3030:C:H5' | 1.81 | 0.62 |
| 7:F:51:ARG:HD3 | 38:F:7636:HOH:O | 1.99 | 0.62 |
| 22:U:47:THR:HB | 22:U:100:ASP:HB3 | 1.81 | 0.62 |
| 1:A:2265:U:H2' | 1:A:2266:A:C8 | 2.35 | 0.62 |
| 38:A:5703:HOH:O | 5:D:2:GLN:HA | 1.99 | 0.62 |
| 26:Y:25:ARG:HD2 | 38:Y:3861:HOH:O | 1.99 | 0.62 |
| 5:D:66:GLU:OE1 | 5:D:328:ARG:HD2 | 1.99 | 0.62 |
| 11:J:47:GLU:CB | 11:J:133:ILE:HD13 | 2.29 | 0.62 |
| 11:J:28:ILE:HA | 11:J:62:GLU:OE1 | 2.00 | 0.62 |
| 4:C:53:ALA:HB3 | 38:C:8602:HOH:O | 1.98 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:F:86:THR:C | 7:F:89:PRO:HD2 | 2.19 | 0.62 |
| 28:1:29:VAL:O | 28:1:33:HIS:HB2 | 1.99 | 0.62 |
| 8:G:77:THR:OG1 | 8:G:78:GLU:N | 2.33 | 0.62 |
| 4:C:8:ARG:HG2 | 38:C:8550:HOH:O | 2.00 | 0.62 |
| 7:F:97:GLN:O | 7:F:97:GLN:HG2 | 1.98 | 0.62 |
| 11:J:45:GLN:HG3 | 11:J:135:TRP:NE1 | 2.15 | 0.62 |
| 7:F:37:ALA:O | 7:F:40:ILE:HG12 | 1.99 | 0.62 |
| 11:J:166:ASN:N | 11:J:166:ASN:HD22 | 1.96 | 0.62 |
| 9:H:2:VAL:HG22 | 9:H:57:GLU:OE1 | 2.00 | 0.62 |
| 8:G:137:ASP:O | 8:G:141:VAL:HG23 | 2.00 | 0.62 |
| 27:Z:200:THR:HG22 | 27:Z:201:GLU:CG | 2.29 | 0.62 |
| 4:C:210:GLY:HA3 | 38:C:8583:HOH:O | 1.98 | 0.62 |
| 1:A:714:U:H3' | 38:A:6432:HOH:O | 2.00 | 0.62 |
| 6:E:12:THR:HB | 38:E:8445:HOH:O | 1.99 | 0.62 |
| 16:O:163:PHE:HE1 | 16:O:171:HIS:HD1 | 1.47 | 0.62 |
| 1:A:2346:C:H6 | 1:A:2346:C:O5' | 1.83 | 0.62 |
| 18:Q:71:LYS:HG3 | 18:Q:71:LYS:O | 1.99 | 0.62 |
| 5:D:54:VAL:HB | 38:D:8614:HOH:O | 1.98 | 0.62 |
| 11:J:26:LYS:HG2 | 11:J:28:ILE:H | 1.63 | 0.62 |
| 1:A:2364:A:H5'' | 19:R:15:LYS:HD3 | 1.82 | 0.62 |
| 15:N:134:ILE:HG23 | 15:N:141:ILE:HD13 | 1.81 | 0.62 |
| 2:B:3035:C:H5'' | 38:B:8453:HOH:O | 1.99 | 0.62 |
| 2:B:3006:C:C5' | 16:O:37:ARG:NH1 | 2.60 | 0.62 |
| 7:F:35:ALA:N | 38:F:5576:HOH:O | 2.33 | 0.62 |
| 1:A:797:A:C4' | 28:1:10:ARG:N | 2.63 | 0.62 |
| 4:C:190:ARG:NH2 | 4:C:207:GLN:OE1 | 2.33 | 0.62 |
| 2:B:3028:U:H2' | 2:B:3029:C:C6 | 2.35 | 0.62 |
| 20:S:39:THR:HG22 | 20:S:42:GLU:H | 1.63 | 0.62 |
| 5:D:221:GLN:HE22 | 13:L:42:ASN:HD22 | 1.48 | 0.62 |
| 22:U:50:VAL:HG12 | 22:U:56:ALA:HA | 1.81 | 0.62 |
| 1:A:1187:U:O2' | 1:A:1189:A:H2 | 1.83 | 0.61 |
| 28:1:26:VAL:O | 28:1:30:GLU:HG3 | 1.99 | 0.61 |
| 25:X:38:THR:HG22 | 25:X:39:ASP:H | 1.65 | 0.61 |
| 14:M:30:ARG:NH2 | 38:M:8520:HOH:O | 2.32 | 0.61 |
| 17:P:14:LEU:HD23 | 17:P:102:ILE:HD11 | 1.80 | 0.61 |
| 11:J:29:ALA:HB3 | 11:J:65:ARG:NH1 | 2.07 | 0.61 |
| 8:G:15:GLN:NE2 | 8:G:40:VAL:O | 2.33 | 0.61 |
| 25:X:4:LEU:O | 25:X:32:CYS:HA | 2.00 | 0.61 |
| 26:Y:78:GLU:HG2 | 26:Y:79:GLU:N | 2.15 | 0.61 |
| 23:V:9:CYS:CA | 23:V:52:THR:HG23 | 2.27 | 0.61 |
| 7:F:146:LYS:NZ | 16:O:107:ASN:ND2 | 2.47 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 10:I:64:ASN:HD22 | 10:I:64:ASN:N | 1.97 | 0.61 |
| 8:G:5:LEU:HD21 | 8:G:66:GLN:HG3 | 1.81 | 0.61 |
| 15:N:104:ARG:O | 15:N:108:LYS:HE2 | 2.00 | 0.61 |
| 5:D:30:PRO:HB2 | 5:D:39:GLN:NE2 | 2.14 | 0.61 |
| 38:E:8358:HOH:O | 17:P:3:THR:HG21 | 2.01 | 0.61 |
| 13:L:115:ARG:HG3 | 13:L:116:GLU:N | 2.13 | 0.61 |
| 16:O:33:ARG:NH1 | 16:O:103:ASP:OD2 | 2.32 | 0.61 |
| 20:S:82:GLU:O | 20:S:86:LYS:HG3 | 2.00 | 0.61 |
| 1:A:1654:U:H2' | 4:C:47:HIS:HD2 | 1.65 | 0.61 |
| 1:A:2256:G:C2' | 1:A:2257:G:H5' | 2.30 | 0.61 |
| 14:M:148:GLU:HB2 | 38:M:8589:HOH:O | 1.99 | 0.61 |
| 1:A:559:U:H6 | 1:A:559:U:H5' | 1.65 | 0.61 |
| 1:A:2241:C:O2' | 1:A:2242:U:H5' | 2.01 | 0.61 |
| 1:A:1299:G:O6 | 14:M:6:ARG:HD3 | 2.00 | 0.61 |
| 31:4:62:THR:HB | 38:4:8548:HOH:O | 1.99 | 0.61 |
| 25:X:90:TYR:CD1 | 25:X:90:TYR:N | 2.67 | 0.61 |
| 36:5:77:PHA:N | 36:6:77:PHA:C | 2.64 | 0.61 |
| 15:N:60:ILE:C | 15:N:61:ILE:HD12 | 2.21 | 0.61 |
| 31:4:3:MET:O | 31:4:90:PHE:HA | 1.99 | 0.61 |
| 6:E:214:THR:HB | 38:E:8323:HOH:O | 2.01 | 0.61 |
| 17:P:14:LEU:CD2 | 17:P:102:ILE:HD11 | 2.30 | 0.61 |
| 29:2:21:ARG:HD2 | 29:2:39:PHE:HB2 | 1.81 | 0.61 |
| 8:G:100:ASP:HB2 | 38:G:2789:HOH:O | 2.01 | 0.61 |
| 1:A:820:G:O2' | 1:A:856:G:H4' | 2.01 | 0.61 |
| 25:X:88:THR:HG23 | 25:X:110:GLN:NE2 | 2.16 | 0.61 |
| 1:A:1058:A:H2' | 1:A:1060:C:H5'' | 1.81 | 0.61 |
| 24:W:64:GLY:O | 24:W:65:ASP:HB2 | 2.01 | 0.61 |
| 5:D:98:THR:HG22 | 5:D:99:GLU:H | 1.65 | 0.61 |
| 11:J:83:PHE:HZ | 11:J:146:TRP:HE1 | 1.45 | 0.60 |
| 4:C:94:LEU:HD23 | 4:C:94:LEU:N | 2.16 | 0.60 |
| 1:A:80:A:H3' | 22:U:43:ASN:OD1 | 2.01 | 0.60 |
| 1:A:1441:G:O2' | 1:A:1442:A:H5' | 2.00 | 0.60 |
| 10:I:16:LYS:O | 10:I:20:VAL:HG23 | 2.01 | 0.60 |
| 13:L:81:ARG:HD3 | 13:L:87:ARG:NH1 | 2.16 | 0.60 |
| 1:A:1878:G:C1' | 38:A:5614:HOH:O | 2.47 | 0.60 |
| 1:A:338:C:H4' | 6:E:174:ILE:HD11 | 1.83 | 0.60 |
| 6:E:233:THR:HG22 | 6:E:234:VAL:N | 2.15 | 0.60 |
| 5:D:82:VAL:O | 5:D:82:VAL:HG12 | 2.00 | 0.60 |
| 15:N:81:ARG:O | 15:N:86:MET:HE2 | 2.01 | 0.60 |
| 1:A:1187:U:H2' | 38:A:6385:HOH:O | 2.02 | 0.60 |
| 1:A:285:A:H2' | 1:A:286:U:O4' | 2.01 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:F:54:ALA:HB2 | 7:F:69:ILE:HD12 | 1.84 | 0.60 |
| 6:E:129:HIS:CE1 | 6:E:231:ARG:HA | 2.37 | 0.60 |
| 15:N:74:ARG:HH11 | 15:N:74:ARG:HG3 | 1.65 | 0.60 |
| 6:E:27:ARG:HG3 | 6:E:29:ASP:OD1 | 2.01 | 0.60 |
| 20:S:18:LEU:HD12 | 20:S:143:VAL:CG1 | 2.32 | 0.60 |
| 1:A:1118:A:C8 | 1:A:1119:G:H5'' | 2.37 | 0.60 |
| 11:J:55:GLN:HE22 | 11:J:91:HIS:CD2 | 2.20 | 0.60 |
| 1:A:2756:U:H3 | 1:A:2896:A:H2 | 1.47 | 0.60 |
| 1:A:88:G:H8 | 1:A:88:G:H5' | 1.66 | 0.60 |
| 17:P:79:VAL:HA | 38:P:6810:HOH:O | 2.02 | 0.60 |
| 2:B:3040:C:N4 | 7:F:51:ARG:HB2 | 2.16 | 0.60 |
| 20:S:104:PHE:HB2 | 20:S:109:MET:HE1 | 1.82 | 0.60 |
| 5:D:7:ARG:HG2 | 5:D:7:ARG:HH11 | 1.67 | 0.60 |
| 25:X:151:GLU:O | 25:X:154:ARG:HB3 | 2.02 | 0.60 |
| 5:D:177:HIS:O | 5:D:181:ILE:HG13 | 2.02 | 0.60 |
| 1:A:2548:C:OP2 | 5:D:5:ARG:NH2 | 2.33 | 0.60 |
| 1:A:1118:A:C8 | 1:A:1118:A:C3' | 2.82 | 0.60 |
| 1:A:2769:C:H2' | 1:A:2770:G:O4' | 2.02 | 0.60 |
| 15:N:186:SER:O | 15:N:189:VAL:HG12 | 2.02 | 0.60 |
| 5:D:279:THR:OG1 | 5:D:290:VAL:HB | 2.02 | 0.60 |
| 27:Z:133:HIS:HD2 | 38:Z:8579:HOH:O | 1.85 | 0.60 |
| 24:W:56:ILE:O | 24:W:60:GLN:HG3 | 2.02 | 0.60 |
| 2:B:3024:U:H3' | 2:B:3025:G:C5' | 2.30 | 0.60 |
| 1:A:870:G:C2' | 1:A:871:G:H5'' | 2.29 | 0.60 |
| 7:F:86:THR:O | 7:F:90:LEU:HG | 2.02 | 0.60 |
| 2:B:3013:A:O2' | 2:B:3014:G:H5'' | 2.02 | 0.60 |
| 1:A:1130:U:H2' | 1:A:1131:G:O4' | 2.02 | 0.60 |
| 1:A:542:A:C8 | 1:A:542:A:H5' | 2.30 | 0.59 |
| 9:H:91:VAL:CG1 | 9:H:92:GLY:N | 2.65 | 0.59 |
| 16:O:110:THR:HB | 16:O:113:SER:OG | 2.02 | 0.59 |
| 1:A:1768:C:H2' | 1:A:1769:C:O4' | 2.02 | 0.59 |
| 5:D:56:ASP:OD1 | 5:D:322:ARG:HB3 | 2.00 | 0.59 |
| 4:C:36:ASP:HA | 4:C:83:GLY:HA3 | 1.84 | 0.59 |
| 1:A:2256:G:H2' | 1:A:2257:G:C5' | 2.32 | 0.59 |
| 15:N:61:ILE:HG13 | 38:N:8632:HOH:O | 2.02 | 0.59 |
| 5:D:103:ASP:HB2 | 38:D:8594:HOH:O | 2.02 | 0.59 |
| 1:A:2912:C:OP2 | 38:A:5044:HOH:O | 2.17 | 0.59 |
| 1:A:2719:A:C2 | 5:D:70:PRO:HG3 | 2.37 | 0.59 |
| 1:A:449:A:N7 | 6:E:43:LYS:HG2 | 2.18 | 0.59 |
| 13:L:74:VAL:HG13 | 13:L:113:ILE:HG23 | 1.85 | 0.59 |
| 16:O:90:LEU:HB2 | 16:O:186:LEU:HD22 | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 14:M:143:THR:HG22 | 14:M:145:LEU:H | 1.66 | 0.59 |
| 25:X:13:MET:HE1 | 25:X:18:GLN:HA | 1.84 | 0.59 |
| 4:C:94:LEU:HG | 4:C:99:ILE:CD1 | 2.32 | 0.59 |
| 8:G:137:ASP:OD1 | 8:G:139:GLU:HB2 | 2.02 | 0.59 |
| 1:A:138:U:H5'' | 1:A:139:C:OP2 | 2.03 | 0.59 |
| 1:A:2453:G:H3' | 38:A:5413:HOH:O | 2.00 | 0.59 |
| 8:G:20:ILE:HD11 | 8:G:40:VAL:CG1 | 2.28 | 0.59 |
| 12:K:26:VAL:HG13 | 12:K:36:VAL:HG11 | 1.83 | 0.59 |
| 25:X:80:ASP:O | 25:X:84:VAL:HG23 | 2.01 | 0.59 |
| 9:H:58:GLU:HG3 | 9:H:61:MET:HE1 | 1.83 | 0.59 |
| 1:A:1329:A:H2 | 38:A:4181:HOH:O | 1.84 | 0.59 |
| 30:3:22:PRO:HG2 | 30:3:25:VAL:HG23 | 1.85 | 0.59 |
| 1:A:1234:U:N3 | 5:D:244:PRO:HB3 | 2.18 | 0.59 |
| 1:A:1244:U:OP1 | 12:K:18:ILE:HD13 | 2.03 | 0.59 |
| 23:V:52:THR:CG2 | 23:V:54:THR:HB | 2.33 | 0.59 |
| 1:A:1589:G:H22 | 1:A:1605:G:H1' | 1.68 | 0.59 |
| 11:J:57:ARG:HG3 | 11:J:57:ARG:HH11 | 1.68 | 0.59 |
| 38:A:5011:HOH:O | 5:D:298:LYS:HD3 | 2.02 | 0.59 |
| 11:J:150:LYS:HE2 | 38:J:8383:HOH:O | 2.03 | 0.59 |
| 2:B:3054:A:O2' | 2:B:3055:U:H5' | 2.02 | 0.59 |
| 6:E:118:THR:O | 6:E:136:VAL:HG13 | 2.02 | 0.59 |
| 1:A:2910:A:H5'' | 38:A:3639:HOH:O | 2.01 | 0.59 |
| 1:A:2081:A:H4' | 12:K:69:TYR:CE1 | 2.37 | 0.59 |
| 1:A:902:G:N7 | 14:M:18:HIS:HD2 | 2.01 | 0.59 |
| 1:A:2755:G:H1' | 38:A:4180:HOH:O | 2.02 | 0.59 |
| 31:4:40:ARG:HD2 | 38:4:8546:HOH:O | 2.02 | 0.59 |
| 1:A:1834:C:H2' | 1:A:1840:A:H62 | 1.67 | 0.59 |
| 9:H:61:MET:HB3 | 15:N:19:GLN:OE1 | 2.03 | 0.59 |
| 9:H:47:LEU:HB2 | 9:H:108:LEU:HD11 | 1.85 | 0.59 |
| 10:I:67:LEU:O | 10:I:71:LEU:HG | 2.03 | 0.59 |
| 18:Q:38:GLU:HA | 18:Q:41:ARG:NH1 | 2.18 | 0.59 |
| 1:A:1535:G:H2' | 1:A:1536:C:C6 | 2.37 | 0.59 |
| 7:F:44:ILE:HG12 | 7:F:83:PHE:HE1 | 1.66 | 0.59 |
| 1:A:2270:G:H4' | 4:C:223:ARG:HH12 | 1.68 | 0.59 |
| 1:A:677:C:H4' | 6:E:246:ARG:NH2 | 2.18 | 0.59 |
| 21:T:33:SER:O | 21:T:37:VAL:HG23 | 2.02 | 0.59 |
| 18:Q:11:ALA:HB2 | 18:Q:18:LYS:HA | 1.85 | 0.59 |
| 7:F:163:VAL:HA | 38:F:6326:HOH:O | 2.01 | 0.58 |
| 15:N:164:THR:CG2 | 15:N:165:SER:N | 2.66 | 0.58 |
| 13:L:74:VAL:HG12 | 13:L:75:ARG:HG3 | 1.84 | 0.58 |
| 1:A:1733:A:H4' | 5:D:212:GLN:HA | 1.84 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:O:143:ARG:NH1 | 16:O:173:ASP:OD2 | 2.33 | 0.58 |
| 1:A:1333:U:H2' | 1:A:1334:C:H6 | 1.68 | 0.58 |
| 25:X:38:THR:HG22 | 25:X:39:ASP:N | 2.17 | 0.58 |
| 1:A:2795:C:O2' | 1:A:2796:U:H5' | 2.03 | 0.58 |
| 1:A:2604:A:H5' | 38:A:5282:HOH:O | 2.02 | 0.58 |
| 23:V:13:ILE:HG12 | 23:V:32:CYS:HB3 | 1.83 | 0.58 |
| 1:A:1527:A:H1' | 1:A:1528:A:C8 | 2.38 | 0.58 |
| 1:A:288:A:H61 | 1:A:364:C:H42 | 1.50 | 0.58 |
| 26:Y:71:ARG:HD3 | 38:Y:2171:HOH:O | 2.03 | 0.58 |
| 6:E:246:ARG:NH1 | 6:E:246:ARG:HB3 | 2.17 | 0.58 |
| 22:U:44:ALA:HA | 22:U:62:VAL:HG12 | 1.84 | 0.58 |
| 26:Y:12:ILE:HD12 | 26:Y:36:HIS:ND1 | 2.18 | 0.58 |
| 13:L:62:PRO:HG3 | 13:L:65:ARG:NH2 | 2.18 | 0.58 |
| 38:A:3201:HOH:O | 8:G:143:GLN:HG2 | 2.02 | 0.58 |
| 1:A:2830:U:H3' | 38:A:4718:HOH:O | 2.03 | 0.58 |
| 1:A:1634:G:H3' | 38:A:3405:HOH:O | 2.03 | 0.58 |
| 18:Q:105:LEU:HD21 | 18:Q:137:LEU:HD21 | 1.85 | 0.58 |
| 12:K:74:ARG:O | 12:K:78:ILE:HG12 | 2.03 | 0.58 |
| 7:F:25:MET:CE | 7:F:37:ALA:HB1 | 2.31 | 0.58 |
| 5:D:314:ALA:CB | 5:D:317:PRO:HG3 | 2.34 | 0.58 |
| 16:O:151:ASP:O | 16:O:154:LEU:HB2 | 2.03 | 0.58 |
| 16:O:24:LEU:HD13 | 19:R:26:PRO:HB3 | 1.83 | 0.58 |
| 1:A:1008:C:H5'' | 11:J:16:ARG:HH12 | 1.67 | 0.58 |
| 6:E:133:ARG:HD2 | 38:E:8415:HOH:O | 2.03 | 0.58 |
| 21:T:43:GLU:HB3 | 38:T:8345:HOH:O | 2.03 | 0.58 |
| 25:X:130:HIS:O | 25:X:136:GLY:HA3 | 2.03 | 0.58 |
| 1:A:2501:G:H1' | 38:A:4043:HOH:O | 2.03 | 0.58 |
| 1:A:1701:A:H4' | 1:A:1702:U:C5' | 2.33 | 0.58 |
| 18:Q:13:VAL:HG21 | 18:Q:41:ARG:HG2 | 1.84 | 0.58 |
| 25:X:39:ASP:HB2 | 38:X:3580:HOH:O | 2.02 | 0.58 |
| 1:A:2672:C:H1' | 38:D:8635:HOH:O | 2.04 | 0.58 |
| 1:A:1197:G:N2 | 38:A:5728:HOH:O | 2.36 | 0.58 |
| 16:O:89:GLY:O | 16:O:92:ALA:HB3 | 2.04 | 0.58 |
| 22:U:9:LYS:HB2 | 38:U:7242:HOH:O | 2.04 | 0.58 |
| 1:A:544:G:C2' | 1:A:545:G:H5'' | 2.32 | 0.58 |
| 8:G:31:ARG:NH1 | 8:G:68:HIS:CG | 2.72 | 0.58 |
| 8:G:79:GLY:HA3 | 38:G:7046:HOH:O | 2.04 | 0.58 |
| 5:D:202:VAL:HG11 | 5:D:301:VAL:HG13 | 1.86 | 0.58 |
| 9:H:110:GLU:HG2 | 38:H:6926:HOH:O | 2.04 | 0.58 |
| 2:B:3006:C:OP1 | 16:O:37:ARG:NH1 | 2.36 | 0.58 |
| 23:V:52:THR:HG22 | 23:V:54:THR:H | 1.69 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 27:Z:186:ARG:NH1 | 27:Z:186:ARG:HG2 | 2.18 | 0.58 |
| 27:Z:155:ARG:NH1 | 38:Z:8555:HOH:O | 2.36 | 0.58 |
| 13:L:82:ARG:NH2 | 13:L:115:ARG:HG2 | 2.19 | 0.58 |
| 31:4:42:ARG:HG3 | 31:4:42:ARG:HH11 | 1.68 | 0.58 |
| 22:U:53:GLY:HA3 | 38:U:6384:HOH:O | 2.04 | 0.58 |
| 11:J:26:LYS:HD2 | 11:J:28:ILE:CD1 | 2.32 | 0.58 |
| 38:A:3267:HOH:O | 22:U:9:LYS:HD2 | 2.03 | 0.58 |
| 1:A:797:A:H4' | 28:1:10:ARG:N | 2.19 | 0.58 |
| 1:A:21:G:H4' | 20:S:2:ILE:HG22 | 1.86 | 0.58 |
| 11:J:139:ASP:H | 11:J:140:PRO:HD3 | 1.69 | 0.58 |
| 28:1:62:TYR:CE2 | 28:1:64:ILE:HG23 | 2.39 | 0.58 |
| 1:A:1206:U:H5' | 1:A:1206:U:C6 | 2.38 | 0.58 |
| 6:E:111:VAL:HB | 38:E:8320:HOH:O | 2.03 | 0.58 |
| 23:V:52:THR:HG22 | 23:V:54:THR:N | 2.19 | 0.58 |
| 26:Y:15:ARG:HH11 | 26:Y:15:ARG:CB | 2.16 | 0.58 |
| 1:A:1819:G:H2' | 1:A:1820:G:H4' | 1.84 | 0.58 |
| 8:G:6:GLU:HA | 8:G:46:THR:HG22 | 1.85 | 0.58 |
| 1:A:1189:A:H1' | 1:A:1209:C:Cl' | 2.34 | 0.58 |
| 4:C:88:ILE:O | 4:C:88:ILE:HG22 | 2.02 | 0.58 |
| 38:A:6948:HOH:O | 5:D:211:THR:HG21 | 2.04 | 0.58 |
| 8:G:31:ARG:HH12 | 8:G:68:HIS:CG | 2.21 | 0.58 |
| 7:F:95:THR:C | 7:F:97:GLN:H | 2.07 | 0.58 |
| 6:E:200:PRO:HB3 | 6:E:212:VAL:HG23 | 1.86 | 0.58 |
| 25:X:125:HIS:HE1 | 38:X:3071:HOH:O | 1.86 | 0.58 |
| 1:A:2524:G:H21 | 1:A:2526:C:N4 | 2.02 | 0.57 |
| 29:2:28:HIS:HD2 | 29:2:30:LYS:H | 1.51 | 0.57 |
| 5:D:51:VAL:HG13 | 5:D:53:LEU:HD13 | 1.85 | 0.57 |
| 1:A:2679:G:H2' | 1:A:2681:A:OP2 | 2.04 | 0.57 |
| 22:U:71:VAL:HG11 | 22:U:90:PRO:CB | 2.27 | 0.57 |
| 11:J:139:ASP:N | 11:J:140:PRO:CD | 2.66 | 0.57 |
| 4:C:192:VAL:O | 4:C:192:VAL:HG12 | 2.04 | 0.57 |
| 2:B:3014:G:H5' | 2:B:3014:G:C8 | 2.39 | 0.57 |
| 6:E:104:ASP:HA | 6:E:107:ARG:NH1 | 2.19 | 0.57 |
| 16:O:24:LEU:O | 16:O:28:LYS:HG2 | 2.04 | 0.57 |
| 16:O:61:ALA:HB3 | 16:O:88:ALA:HB2 | 1.85 | 0.57 |
| 30:3:20:ARG:HB3 | 38:3:5444:HOH:O | 2.03 | 0.57 |
| 1:A:2365:G:H4' | 19:R:45:PRO:O | 2.04 | 0.57 |
| 17:P:113:VAL:O | 17:P:114:ILE:HD13 | 2.04 | 0.57 |
| 1:A:1624:A:H5' | 1:A:1626:A:O4' | 2.04 | 0.57 |
| 1:A:1942:A:O2' | 1:A:1943:C:H5' | 2.05 | 0.57 |
| 13:L:34:VAL:HB | 38:L:7169:HOH:O | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 24:W:39:ALA:N | 24:W:40:PRO:CD | 2.67 | 0.57 |
| 16:O:152:GLU:C | 16:O:154:LEU:H | 2.06 | 0.57 |
| 4:C:232:ARG:NH2 | 4:C:236:GLY:O | 2.34 | 0.57 |
| 1:A:2502:C:C4' | 11:J:151:MET:HG2 | 2.33 | 0.57 |
| 18:Q:115:SER:C | 18:Q:117:SER:H | 2.08 | 0.57 |
| 15:N:38:VAL:O | 15:N:63:VAL:HG13 | 2.04 | 0.57 |
| 14:M:114:VAL:HG11 | 38:M:8575:HOH:O | 2.04 | 0.57 |
| 5:D:294:TYR:HE2 | 38:D:8652:HOH:O | 1.87 | 0.57 |
| 9:H:110:GLU:O | 9:H:114:LYS:HG3 | 2.03 | 0.57 |
| 1:A:536:A:H3' | 38:A:4538:HOH:O | 2.04 | 0.57 |
| 11:J:117:LYS:HB2 | 38:J:8339:HOH:O | 2.05 | 0.57 |
| 11:J:26:LYS:CD | 11:J:28:ILE:HB | 2.35 | 0.57 |
| 11:J:27:LYS:H | 11:J:58:HIS:CD2 | 2.15 | 0.57 |
| 12:K:93:ARG:HB3 | 12:K:93:ARG:NH1 | 2.18 | 0.57 |
| 7:F:135:VAL:HG22 | 7:F:136:ARG:N | 2.19 | 0.57 |
| 6:E:72:LYS:HG2 | 6:E:77:ALA:HA | 1.86 | 0.57 |
| 14:M:54:PRO:HG2 | 14:M:57:VAL:CG2 | 2.34 | 0.57 |
| 29:2:25:LYS:HD2 | 30:3:48:ASP:HA | 1.86 | 0.57 |
| 1:A:1636:G:O2' | 1:A:1637:A:H5' | 2.03 | 0.57 |
| 5:D:141:ARG:HB3 | 5:D:164:THR:O | 2.05 | 0.57 |
| 4:C:55:VAL:HG22 | 4:C:68:ILE:O | 2.04 | 0.57 |
| 27:Z:130:ARG:HB2 | 27:Z:142:SER:O | 2.04 | 0.57 |
| 6:E:145:GLU:HG3 | 38:E:8376:HOH:O | 2.05 | 0.57 |
| 10:I:12:ILE:HD12 | 38:I:692:HOH:O | 2.03 | 0.57 |
| 17:P:47:ARG:NH1 | 17:P:47:ARG:HG3 | 2.20 | 0.57 |
| 1:A:1205:U:H2' | 1:A:1206:U:H5'' | 1.86 | 0.57 |
| 8:G:12:ASP:HA | 38:G:1750:HOH:O | 2.03 | 0.57 |
| 31:4:3:MET:HG3 | 31:4:4:PRO:HD2 | 1.86 | 0.57 |
| 18:Q:27:ARG:O | 18:Q:31:ILE:HG13 | 2.05 | 0.57 |
| 29:2:10:LYS:HG3 | 38:2:8434:HOH:O | 2.05 | 0.57 |
| 1:A:328:U:O4' | 6:E:202:THR:HG22 | 2.03 | 0.57 |
| 16:O:34:LEU:HA | 16:O:47:LEU:HD23 | 1.86 | 0.57 |
| 2:B:3055:U:H4' | 2:B:3056:A:C8 | 2.39 | 0.57 |
| 5:D:307:ARG:HH11 | 5:D:307:ARG:HB2 | 1.69 | 0.57 |
| 1:A:952:G:OP1 | 19:R:42:LYS:HE2 | 2.03 | 0.57 |
| 7:F:174:VAL:HG13 | 38:F:6555:HOH:O | 2.04 | 0.57 |
| 29:2:21:ARG:HD2 | 29:2:37:CYS:SG | 2.43 | 0.57 |
| 22:U:37:GLN:OE1 | 22:U:118:SER:HA | 2.05 | 0.57 |
| 15:N:63:VAL:HG21 | 15:N:109:PHE:CE1 | 2.40 | 0.57 |
| 5:D:329:TYR:CE2 | 23:V:15:PRO:HG2 | 2.39 | 0.57 |
| 1:A:20:G:H21 | 20:S:117:HIS:HD2 | 1.53 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 12:K:104:TYR:HA | 38:K:2238:HOH:O | 2.04 | 0.57 |
| 2:B:3041:C:O4' | 7:F:50:VAL:HG23 | 2.04 | 0.57 |
| 1:A:175:G:H2' | 15:N:192:ALA:HB3 | 1.85 | 0.57 |
| 4:C:192:VAL:CG1 | 4:C:207:GLN:HB3 | 2.33 | 0.57 |
| 10:I:12:ILE:HG22 | 10:I:17:GLN:NE2 | 2.20 | 0.57 |
| 5:D:274:GLU:HA | 5:D:292:GLY:O | 2.05 | 0.57 |
| 16:O:12:ARG:HD3 | 16:O:18:THR:OG1 | 2.05 | 0.57 |
| 8:G:86:VAL:CG1 | 8:G:129:GLU:HA | 2.34 | 0.57 |
| 16:O:47:LEU:HD11 | 16:O:127:LEU:CD2 | 2.30 | 0.57 |
| 2:B:3078:G:N2 | 2:B:3103:A:OP2 | 2.36 | 0.57 |
| 15:N:55:LYS:HB2 | 15:N:60:ILE:CD1 | 2.35 | 0.57 |
| 1:A:1097:A:H5" | 25:X:125:HIS:NE2 | 2.20 | 0.57 |
| 16:O:80:SER:HB2 | 38:O:8537:HOH:O | 2.03 | 0.57 |
| 1:A:2846:C:OP1 | 5:D:158:LYS:HD3 | 2.05 | 0.57 |
| 2:B:3024:U:H3' | 2:B:3025:G:H5' | 1.87 | 0.56 |
| 1:A:1450:C:O2' | 1:A:1494:A:H5' | 2.05 | 0.56 |
| 24:W:39:ALA:C | 24:W:41:GLU:H | 2.08 | 0.56 |
| 1:A:2421:G:H3' | 1:A:2422:U:H5" | 1.87 | 0.56 |
| 1:A:2769:C:C2' | 1:A:2770:G:H5' | 2.35 | 0.56 |
| 1:A:1778:A:H2' | 1:A:1779:A:H5' | 1.86 | 0.56 |
| 28:1:11:THR:HG23 | 28:1:23:ARG:HD2 | 1.87 | 0.56 |
| 28:1:11:THR:OG1 | 28:1:23:ARG:HB2 | 2.04 | 0.56 |
| 1:A:2690:U:O2' | 8:G:111:LYS:HE3 | 2.05 | 0.56 |
| 1:A:1015:C:H2' | 1:A:1016:U:H6 | 1.70 | 0.56 |
| 26:Y:78:GLU:CG | 26:Y:79:GLU:H | 2.17 | 0.56 |
| 1:A:1151:G:OP1 | 10:I:63:ARG:NH1 | 2.38 | 0.56 |
| 1:A:775:G:OP1 | 29:2:16:HIS:HE1 | 1.88 | 0.56 |
| 1:A:2266:A:OP2 | 15:N:90:ARG:NH2 | 2.38 | 0.56 |
| 5:D:85:ARG:NH1 | 38:D:8635:HOH:O | 2.38 | 0.56 |
| 20:S:119:VAL:HG12 | 20:S:119:VAL:O | 2.04 | 0.56 |
| 1:A:485:A:N3 | 1:A:487:G:H5" | 2.20 | 0.56 |
| 1:A:169:A:H1' | 31:4:48:ASN:ND2 | 2.20 | 0.56 |
| 1:A:31:C:H4' | 38:U:7242:HOH:O | 2.03 | 0.56 |
| 20:S:106:GLY:HA2 | 20:S:109:MET:CE | 2.32 | 0.56 |
| 4:C:211:LYS:HB3 | 4:C:212:PRO:CD | 2.33 | 0.56 |
| 15:N:74:ARG:HD3 | 15:N:91:ILE:HD12 | 1.87 | 0.56 |
| 8:G:81:GLU:HG2 | 8:G:134:SER:CB | 2.34 | 0.56 |
| 10:I:12:ILE:HB | 38:I:4714:HOH:O | 2.05 | 0.56 |
| 1:A:1209:C:H2' | 1:A:1210:G:H8 | 1.69 | 0.56 |
| 21:T:51:GLN:NE2 | 21:T:53:ASN:HD21 | 2.02 | 0.56 |
| 21:T:77:VAL:O | 21:T:80:ARG:HG2 | 2.04 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:O:132:ASN:O | 16:O:135:VAL:HG12 | 2.05 | 0.56 |
| 1:A:2694:A:H4' | 8:G:91:PHE:CE1 | 2.40 | 0.56 |
| 26:Y:18:ARG:NH1 | 38:Y:4132:HOH:O | 2.35 | 0.56 |
| 1:A:346:U:H4' | 38:A:6332:HOH:O | 2.03 | 0.56 |
| 1:A:2291:A:C8 | 1:A:2309:C:H5' | 2.40 | 0.56 |
| 5:D:175:LEU:O | 5:D:175:LEU:HD23 | 2.05 | 0.56 |
| 15:N:74:ARG:HG3 | 15:N:74:ARG:NH1 | 2.21 | 0.56 |
| 1:A:136:C:H2' | 1:A:137:U:O4' | 2.04 | 0.56 |
| 4:C:199:HIS:CD2 | 4:C:201:PHE:HB2 | 2.37 | 0.56 |
| 30:3:48:ASP:O | 30:3:49:GLU:HB2 | 2.05 | 0.56 |
| 1:A:2780:C:H2' | 1:A:2781:U:C6 | 2.40 | 0.56 |
| 2:B:3088:G:OP1 | 25:X:130:HIS:NE2 | 2.38 | 0.56 |
| 15:N:9:ARG:HG3 | 38:N:8548:HOH:O | 2.03 | 0.56 |
| 7:F:10:PHE:CG | 7:F:11:HIS:N | 2.73 | 0.56 |
| 4:C:121:ALA:O | 4:C:124:VAL:HG22 | 2.06 | 0.56 |
| 1:A:1615:A:H4' | 38:A:5377:HOH:O | 2.05 | 0.56 |
| 1:A:256:C:H2' | 1:A:257:G:O4' | 2.05 | 0.56 |
| 20:S:34:GLU:HG2 | 20:S:46:TYR:OH | 2.05 | 0.56 |
| 6:E:1:MET:HG2 | 6:E:2:GLN:N | 2.20 | 0.56 |
| 12:K:107:ASN:HD22 | 12:K:107:ASN:C | 2.09 | 0.56 |
| 25:X:122:ARG:NH2 | 25:X:154:ARG:HD2 | 2.20 | 0.56 |
| 1:A:558:C:O2' | 1:A:559:U:H5'' | 2.06 | 0.56 |
| 11:J:53:PRO:HA | 11:J:125:VAL:O | 2.05 | 0.56 |
| 1:A:2274:A:H1' | 15:N:86:MET:SD | 2.46 | 0.56 |
| 19:R:25:PRO:HB2 | 38:R:4350:HOH:O | 2.05 | 0.56 |
| 1:A:2434:A:O3' | 31:4:28:GLY:HA3 | 2.05 | 0.56 |
| 21:T:29:ASP:OD1 | 21:T:31:ARG:NH1 | 2.39 | 0.56 |
| 7:F:99:ASP:HB2 | 7:F:103:ASN:HB2 | 1.85 | 0.56 |
| 4:C:36:ASP:OD2 | 4:C:85:ASP:HB2 | 2.05 | 0.56 |
| 1:A:794:U:H3 | 1:A:819:A:H61 | 1.53 | 0.56 |
| 1:A:154:C:H2' | 1:A:155:C:H6 | 1.70 | 0.56 |
| 1:A:2281:C:C2' | 1:A:2282:U:H5' | 2.36 | 0.56 |
| 16:O:43:VAL:HG11 | 16:O:81:ALA:HA | 1.87 | 0.56 |
| 8:G:37:ASP:OD1 | 12:K:125:SER:HB3 | 2.06 | 0.56 |
| 25:X:119:HIS:HD2 | 25:X:120:PRO:O | 1.88 | 0.56 |
| 2:B:3023:U:C3' | 2:B:3024:U:C5' | 2.81 | 0.56 |
| 11:J:166:ASN:ND2 | 11:J:166:ASN:N | 2.54 | 0.56 |
| 28:1:30:GLU:HA | 28:1:33:HIS:HB3 | 1.86 | 0.56 |
| 1:A:2070:G:H5'' | 38:A:3292:HOH:O | 2.06 | 0.56 |
| 1:A:184:G:H5'' | 15:N:153:THR:HG22 | 1.87 | 0.56 |
| 7:F:102:GLY:O | 7:F:134:LEU:HD12 | 2.06 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 38:A:9674:HOH:O | 15:N:87:MET:HE3 | 2.06 | 0.56 |
| 5:D:62:ARG:HG2 | 5:D:65:MET:HE3 | 1.87 | 0.56 |
| 9:H:50:VAL:HG13 | 9:H:60:VAL:HG11 | 1.87 | 0.56 |
| 1:A:1205:U:C2' | 1:A:1206:U:H5' | 2.36 | 0.56 |
| 27:Z:200:THR:HG22 | 27:Z:201:GLU:HG2 | 1.88 | 0.56 |
| 16:O:77:ASN:OD1 | 16:O:80:SER:HB2 | 2.06 | 0.56 |
| 1:A:2630:G:O6 | 4:C:206:ARG:NH2 | 2.39 | 0.56 |
| 29:2:8:GLN:HE22 | 29:2:11:LYS:NZ | 2.03 | 0.56 |
| 16:O:37:ARG:NE | 38:O:8534:HOH:O | 2.39 | 0.56 |
| 7:F:41:LEU:HA | 7:F:44:ILE:CG2 | 2.35 | 0.56 |
| 26:Y:73:ARG:O | 26:Y:85:VAL:HG13 | 2.06 | 0.56 |
| 1:A:281:U:O2' | 1:A:282:C:H5' | 2.06 | 0.56 |
| 4:C:51:ARG:NH1 | 4:C:120:ARG:O | 2.38 | 0.56 |
| 1:A:1020:A:O3' | 38:A:3536:HOH:O | 2.18 | 0.56 |
| 1:A:247:A:H2' | 38:A:3434:HOH:O | 2.05 | 0.56 |
| 2:B:3025:G:C3' | 2:B:3026:C:H5' | 2.33 | 0.56 |
| 15:N:67:ILE:CD1 | 15:N:104:ARG:HD2 | 2.36 | 0.56 |
| 15:N:104:ARG:O | 15:N:108:LYS:HG2 | 2.05 | 0.56 |
| 23:V:52:THR:HG22 | 23:V:54:THR:HB | 1.88 | 0.56 |
| 4:C:170:VAL:HG22 | 28:1:22:ILE:CG2 | 2.36 | 0.56 |
| 1:A:2768:A:O2' | 1:A:2769:C:H5' | 2.06 | 0.56 |
| 1:A:1972:U:H2' | 1:A:1973:A:H5' | 1.87 | 0.56 |
| 27:Z:185:VAL:HA | 38:Z:8561:HOH:O | 2.05 | 0.55 |
| 25:X:122:ARG:NE | 38:X:5817:HOH:O | 2.39 | 0.55 |
| 9:H:46:GLU:OE1 | 9:H:100:ASP:HA | 2.06 | 0.55 |
| 1:A:1377:C:C6 | 1:A:1377:C:H5' | 2.41 | 0.55 |
| 1:A:669:G:O2' | 1:A:670:G:H5' | 2.05 | 0.55 |
| 1:A:200:U:H2' | 38:A:9953:HOH:O | 2.06 | 0.55 |
| 21:T:81:ILE:HG23 | 38:T:8337:HOH:O | 2.06 | 0.55 |
| 1:A:960:G:N3 | 1:A:960:G:H2' | 2.21 | 0.55 |
| 1:A:2503:A:OP1 | 11:J:147:ARG:NH2 | 2.35 | 0.55 |
| 9:H:57:GLU:O | 9:H:61:MET:HG3 | 2.05 | 0.55 |
| 1:A:2064:U:H5' | 1:A:2652:U:O3' | 2.07 | 0.55 |
| 26:Y:75:ALA:O | 26:Y:83:ALA:HA | 2.06 | 0.55 |
| 11:J:144:GLU:OE1 | 11:J:144:GLU:HA | 2.06 | 0.55 |
| 26:Y:72:VAL:HG22 | 26:Y:85:VAL:CG1 | 2.34 | 0.55 |
| 1:A:2505:G:O2' | 1:A:2506:A:H5' | 2.06 | 0.55 |
| 5:D:62:ARG:HA | 5:D:65:MET:HE3 | 1.85 | 0.55 |
| 24:W:39:ALA:O | 24:W:41:GLU:N | 2.39 | 0.55 |
| 27:Z:106:THR:HG23 | 27:Z:107:PRO:HD2 | 1.88 | 0.55 |
| 6:E:78:ARG:NH1 | 6:E:78:ARG:HG3 | 2.21 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:E:104:ASP:O | 6:E:108:GLN:HG3 | 2.05 | 0.55 |
| 16:O:100:ALA:O | 16:O:129:ILE:HG23 | 2.06 | 0.55 |
| 1:A:1213:C:O2' | 1:A:1214:G:H5' | 2.07 | 0.55 |
| 22:U:48:VAL:HG22 | 22:U:98:VAL:HA | 1.87 | 0.55 |
| 15:N:46:LEU:HG | 38:N:8630:HOH:O | 2.05 | 0.55 |
| 1:A:1116:U:O2' | 1:A:1118:A:C2 | 2.52 | 0.55 |
| 7:F:99:ASP:CB | 7:F:103:ASN:H | 2.19 | 0.55 |
| 38:A:9211:HOH:O | 5:D:254:GLN:HG3 | 2.05 | 0.55 |
| 27:Z:200:THR:HG22 | 27:Z:201:GLU:HG3 | 1.89 | 0.55 |
| 25:X:149:LEU:HG | 25:X:153:MET:CE | 2.36 | 0.55 |
| 1:A:1864:C:OP1 | 15:N:75:THR:HG23 | 2.07 | 0.55 |
| 24:W:12:THR:HG23 | 24:W:14:ALA:H | 1.70 | 0.55 |
| 2:B:3023:U:H6 | 2:B:3023:U:C5' | 2.18 | 0.55 |
| 15:N:52:LEU:HD13 | 15:N:116:ASN:CB | 2.36 | 0.55 |
| 6:E:107:ARG:NE | 38:E:8461:HOH:O | 2.17 | 0.55 |
| 18:Q:131:PHE:CD1 | 18:Q:137:LEU:HD13 | 2.40 | 0.55 |
| 31:4:65:THR:HG23 | 31:4:67:LEU:HG | 1.88 | 0.55 |
| 38:A:3572:HOH:O | 5:D:27:ASN:HB2 | 2.05 | 0.55 |
| 16:O:47:LEU:HD13 | 16:O:97:VAL:HG11 | 1.87 | 0.55 |
| 26:Y:74:ALA:CB | 26:Y:85:VAL:HG22 | 2.37 | 0.55 |
| 6:E:115:LEU:O | 6:E:118:THR:HB | 2.06 | 0.55 |
| 31:4:17:HIS:O | 31:4:18:GLN:HG3 | 2.07 | 0.55 |
| 1:A:2468:A:H61 | 31:4:48:ASN:HD21 | 1.53 | 0.55 |
| 1:A:263:U:O4' | 9:H:59:ILE:HD13 | 2.06 | 0.55 |
| 1:A:1132:A:N6 | 1:A:1229:C:H2' | 2.22 | 0.55 |
| 7:F:91:ALA:HB1 | 38:F:5198:HOH:O | 2.06 | 0.55 |
| 1:A:1123:A:C6 | 1:A:1238:C:H5' | 2.41 | 0.55 |
| 1:A:2276:U:H2' | 1:A:2277:U:C6 | 2.41 | 0.55 |
| 5:D:204:GLY:HA3 | 38:D:8655:HOH:O | 2.06 | 0.55 |
| 5:D:152:PRO:HD2 | 38:D:8632:HOH:O | 2.06 | 0.55 |
| 15:N:37:VAL:HG21 | 15:N:108:LYS:CG | 2.36 | 0.55 |
| 30:3:40:ARG:HG3 | 30:3:45:ASN:CB | 2.37 | 0.55 |
| 30:3:41:HIS:H | 30:3:45:ASN:ND2 | 1.98 | 0.55 |
| 23:V:9:CYS:HA | 23:V:52:THR:CG2 | 2.34 | 0.55 |
| 23:V:17:THR:HG22 | 23:V:18:GLY:N | 2.22 | 0.55 |
| 1:A:588:G:O6 | 25:X:154:ARG:NH1 | 2.39 | 0.55 |
| 22:U:38:ARG:NH1 | 38:U:6217:HOH:O | 2.38 | 0.55 |
| 7:F:95:THR:O | 7:F:97:GLN:N | 2.33 | 0.55 |
| 14:M:72:ASN:HB2 | 38:M:8584:HOH:O | 2.07 | 0.55 |
| 26:Y:31:ILE:O | 26:Y:35:GLU:HG3 | 2.06 | 0.55 |
| 1:A:371:U:H2' | 1:A:372:A:H8 | 1.71 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:431:G:P | 15:N:48:ARG:HH12 | 2.30 | 0.55 |
| 1:A:21:G:H5' | 20:S:1:GLY:O | 2.07 | 0.55 |
| 26:Y:15:ARG:NH1 | 26:Y:15:ARG:HB3 | 2.22 | 0.55 |
| 28:1:57:CYS:SG | 28:1:59:HIS:HB3 | 2.47 | 0.55 |
| 25:X:13:MET:CE | 25:X:17:ILE:HG22 | 2.36 | 0.55 |
| 22:U:28:SER:O | 22:U:32:ARG:HG3 | 2.07 | 0.55 |
| 8:G:126:ILE:HB | 8:G:131:LEU:CD2 | 2.37 | 0.55 |
| 16:O:78:MET:HB2 | 16:O:79:PRO:HD3 | 1.89 | 0.55 |
| 38:A:3966:HOH:O | 15:N:146:GLN:HG2 | 2.06 | 0.55 |
| 7:F:146:LYS:HZ3 | 16:O:107:ASN:HD21 | 1.53 | 0.55 |
| 1:A:1189:A:H1' | 1:A:1209:C:O4' | 2.07 | 0.55 |
| 4:C:101:GLU:OE2 | 4:C:131:HIS:HB2 | 2.07 | 0.55 |
| 6:E:246:ARG:NE | 38:E:8429:HOH:O | 2.39 | 0.55 |
| 31:4:74:CYS:N | 38:4:8558:HOH:O | 2.39 | 0.55 |
| 19:R:23:THR:HA | 38:R:4792:HOH:O | 2.07 | 0.55 |
| 18:Q:80:ARG:HG2 | 18:Q:87:ARG:CZ | 2.37 | 0.55 |
| 26:Y:51:ASP:OD2 | 26:Y:52:PRO:HD2 | 2.07 | 0.55 |
| 19:R:64:GLU:HG3 | 19:R:74:ASP:OD2 | 2.06 | 0.55 |
| 12:K:107:ASN:HD21 | 12:K:109:TYR:HB2 | 1.72 | 0.55 |
| 6:E:214:THR:HG23 | 38:E:8440:HOH:O | 2.07 | 0.55 |
| 5:D:72:THR:O | 38:D:8607:HOH:O | 2.18 | 0.55 |
| 1:A:2769:C:O2' | 1:A:2770:G:H5' | 2.06 | 0.55 |
| 1:A:814:G:H8 | 38:A:6700:HOH:O | 1.90 | 0.55 |
| 1:A:1164:U:C4' | 1:A:1165:G:OP1 | 2.53 | 0.54 |
| 5:D:36:PRO:HA | 5:D:168:GLY:HA3 | 1.89 | 0.54 |
| 1:A:1189:A:H1' | 1:A:1209:C:H1' | 1.90 | 0.54 |
| 26:Y:41:PHE:O | 26:Y:43:VAL:HG23 | 2.07 | 0.54 |
| 1:A:1014:A:H2' | 1:A:1015:C:H5' | 1.90 | 0.54 |
| 1:A:2281:C:H2' | 1:A:2282:U:H5' | 1.90 | 0.54 |
| 21:T:6:LYS:HD3 | 38:T:8324:HOH:O | 2.07 | 0.54 |
| 27:Z:109:LEU:HA | 38:Z:8568:HOH:O | 2.07 | 0.54 |
| 1:A:1787:C:H4' | 1:A:2883:A:O4' | 2.07 | 0.54 |
| 6:E:35:VAL:HG21 | 6:E:227:GLY:HA2 | 1.90 | 0.54 |
| 4:C:217:ARG:HG2 | 4:C:229:ALA:HB2 | 1.88 | 0.54 |
| 24:W:5:VAL:HG23 | 38:W:2271:HOH:O | 2.07 | 0.54 |
| 1:A:2577:A:H5' | 38:A:7241:HOH:O | 2.07 | 0.54 |
| 18:Q:115:SER:H | 18:Q:118:GLN:HE21 | 0.85 | 0.54 |
| 15:N:39:ARG:HA | 15:N:63:VAL:HG22 | 1.89 | 0.54 |
| 12:K:19:MET:HE2 | 12:K:79:PHE:HA | 1.87 | 0.54 |
| 27:Z:112:GLU:CD | 27:Z:115:ARG:NH1 | 2.60 | 0.54 |
| 5:D:51:VAL:CG2 | 5:D:327:VAL:HG13 | 2.38 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:945:U:H2' | 1:A:946:C:C6 | 2.43 | 0.54 |
| 1:A:1003:U:O2' | 11:J:90:PHE:HE1 | 1.90 | 0.54 |
| 14:M:104:ASP:O | 14:M:105:TYR:HB3 | 2.06 | 0.54 |
| 6:E:107:ARG:HB3 | 6:E:107:ARG:NH1 | 2.23 | 0.54 |
| 15:N:12:TRP:CE2 | 15:N:20:ILE:HD11 | 2.43 | 0.54 |
| 16:O:86:LEU:O | 16:O:90:LEU:HG | 2.07 | 0.54 |
| 1:A:2241:C:H2' | 1:A:2242:U:C6 | 2.42 | 0.54 |
| 11:J:68:ALA:HB2 | 11:J:149:ALA:HB2 | 1.88 | 0.54 |
| 1:A:1242:A:H5' | 12:K:82:THR:CG2 | 2.24 | 0.54 |
| 1:A:657:G:H2' | 1:A:658:C:H6 | 1.72 | 0.54 |
| 16:O:171:HIS:CE1 | 38:O:8567:HOH:O | 2.61 | 0.54 |
| 1:A:289:G:N2 | 1:A:363:A:H2 | 2.02 | 0.54 |
| 16:O:141:ARG:N | 38:O:8570:HOH:O | 2.39 | 0.54 |
| 25:X:122:ARG:NH2 | 38:X:4276:HOH:O | 2.40 | 0.54 |
| 14:M:138:GLY:HA3 | 38:M:8555:HOH:O | 2.05 | 0.54 |
| 31:4:69:TYR:HB2 | 31:4:78:HIS:CE1 | 2.42 | 0.54 |
| 1:A:2411:C:H4' | 38:A:4443:HOH:O | 2.07 | 0.54 |
| 1:A:67:A:H5'' | 1:A:69:A:C8 | 2.43 | 0.54 |
| 1:A:1687:C:O2 | 29:2:9:GLY:HA2 | 2.06 | 0.54 |
| 16:O:11:ARG:HG3 | 16:O:14:ARG:NH1 | 2.22 | 0.54 |
| 7:F:22:VAL:HG22 | 7:F:74:THR:HG22 | 1.90 | 0.54 |
| 15:N:87:MET:CB | 31:4:46:ILE:HG21 | 2.37 | 0.54 |
| 1:A:1185:U:H5' | 38:A:6959:HOH:O | 2.07 | 0.54 |
| 1:A:682:A:H2' | 1:A:683:G:O4' | 2.07 | 0.54 |
| 27:Z:107:PRO:HB3 | 27:Z:182:PHE:CE2 | 2.42 | 0.54 |
| 6:E:246:ARG:NH2 | 38:E:8429:HOH:O | 2.40 | 0.54 |
| 1:A:2634:G:O2' | 1:A:2635:A:H5' | 2.08 | 0.54 |
| 1:A:2252:A:C5 | 1:A:2253:G:H1' | 2.42 | 0.54 |
| 24:W:58:THR:O | 24:W:62:GLU:HG3 | 2.08 | 0.54 |
| 17:P:73:ASP:HA | 17:P:92:VAL:O | 2.08 | 0.54 |
| 7:F:44:ILE:HG23 | 7:F:45:THR:HG23 | 1.90 | 0.54 |
| 15:N:172:GLY:C | 15:N:183:VAL:HG11 | 2.27 | 0.54 |
| 16:O:91:ARG:HG3 | 16:O:186:LEU:HD23 | 1.89 | 0.54 |
| 21:T:33:SER:OG | 21:T:36:GLU:HG3 | 2.08 | 0.54 |
| 2:B:3041:C:C6 | 7:F:50:VAL:HG21 | 2.43 | 0.54 |
| 5:D:119:HIS:O | 5:D:121:PRO:HD3 | 2.08 | 0.54 |
| 12:K:75:PRO:HG2 | 12:K:105:LEU:CD2 | 2.37 | 0.54 |
| 1:A:926:A:O2' | 14:M:41:HIS:HD2 | 1.90 | 0.54 |
| 5:D:329:TYR:HE2 | 23:V:15:PRO:HG2 | 1.73 | 0.54 |
| 25:X:122:ARG:HH21 | 25:X:154:ARG:HD2 | 1.72 | 0.54 |
| 4:C:153:ARG:CB | 4:C:153:ARG:HH11 | 2.20 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:E:246:ARG:CZ | 38:E:8429:HOH:O | 2.55 | 0.54 |
| 1:A:538:C:OP2 | 27:Z:134:HIS:HE1 | 1.90 | 0.54 |
| 31:4:56:PRO:HA | 38:4:8547:HOH:O | 2.08 | 0.54 |
| 2:B:3044:A:O4' | 7:F:76:ARG:NE | 2.41 | 0.54 |
| 1:A:2638:G:H1' | 38:A:4083:HOH:O | 2.07 | 0.54 |
| 27:Z:112:GLU:OE1 | 27:Z:112:GLU:HA | 2.08 | 0.54 |
| 1:A:1495:C:H1' | 1:A:1573:A:H1' | 1.90 | 0.54 |
| 22:U:49:GLU:HB3 | 22:U:59:GLU:HG3 | 1.89 | 0.54 |
| 1:A:2563:U:H2' | 1:A:2565:C:O5' | 2.08 | 0.54 |
| 1:A:447:A:OP1 | 22:U:2:LYS:HG2 | 2.08 | 0.54 |
| 1:A:1086:A:N6 | 25:X:11:VAL:HG11 | 2.22 | 0.54 |
| 1:A:100:C:H4' | 22:U:16:LEU:HB2 | 1.90 | 0.54 |
| 1:A:667:C:H2' | 1:A:668:C:H6 | 1.72 | 0.54 |
| 1:A:1182:C:H1' | 1:A:1192:A:C8 | 2.42 | 0.54 |
| 15:N:84:LYS:HE2 | 38:N:8580:HOH:O | 2.06 | 0.54 |
| 5:D:41:PHE:HB3 | 5:D:190:MET:HE1 | 1.89 | 0.54 |
| 5:D:7:ARG:HD3 | 5:D:9:GLY:O | 2.08 | 0.54 |
| 9:H:104:ALA:HA | 38:H:6617:HOH:O | 2.08 | 0.54 |
| 17:P:77:ALA:HB1 | 17:P:98:LEU:HD12 | 1.89 | 0.54 |
| 18:Q:105:LEU:CD2 | 18:Q:137:LEU:HD21 | 2.38 | 0.54 |
| 38:A:5780:HOH:O | 27:Z:158:LYS:HD3 | 2.08 | 0.54 |
| 16:O:47:LEU:HD12 | 16:O:92:ALA:HB1 | 1.89 | 0.53 |
| 7:F:25:MET:CE | 7:F:41:LEU:HG | 2.32 | 0.53 |
| 1:A:1181:A:H2' | 1:A:1182:C:O4' | 2.08 | 0.53 |
| 15:N:37:VAL:HG13 | 15:N:63:VAL:HG11 | 1.90 | 0.53 |
| 6:E:1:MET:HG2 | 6:E:2:GLN:NE2 | 2.24 | 0.53 |
| 29:2:37:CYS:SG | 29:2:39:PHE:HB2 | 2.48 | 0.53 |
| 1:A:1497:G:H4' | 1:A:1627:G:O2' | 2.08 | 0.53 |
| 16:O:139:TRP:HA | 16:O:139:TRP:CE3 | 2.43 | 0.53 |
| 38:A:9179:HOH:O | 17:P:112:ARG:HD2 | 2.08 | 0.53 |
| 1:A:1176:C:H1' | 38:A:3441:HOH:O | 2.07 | 0.53 |
| 25:X:63:GLU:HG2 | 25:X:93:ILE:HG22 | 1.89 | 0.53 |
| 11:J:157:ILE:HG22 | 11:J:158:ASN:N | 2.23 | 0.53 |
| 25:X:84:VAL:HG12 | 38:X:6679:HOH:O | 2.07 | 0.53 |
| 11:J:58:HIS:HA | 11:J:61:LEU:HD23 | 1.90 | 0.53 |
| 6:E:235:PHE:HE2 | 6:E:243:VAL:HG21 | 1.72 | 0.53 |
| 5:D:36:PRO:HA | 5:D:168:GLY:HA2 | 1.90 | 0.53 |
| 25:X:6:GLN:HB2 | 25:X:26:ILE:CD1 | 2.37 | 0.53 |
| 1:A:240:C:H4' | 15:N:146:GLN:NE2 | 2.22 | 0.53 |
| 1:A:1790:C:H2' | 1:A:1791:U:H6 | 1.72 | 0.53 |
| 1:A:660:A:H4' | 1:A:661:G:O5' | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:E:95:GLU:HG3 | 38:E:8476:HOH:O | 2.08 | 0.53 |
| 4:C:175:LYS:HE2 | 38:C:8572:HOH:O | 2.08 | 0.53 |
| 1:A:2787:C:H5 | 38:A:4131:HOH:O | 1.90 | 0.53 |
| 7:F:41:LEU:CA | 7:F:44:ILE:HG22 | 2.37 | 0.53 |
| 1:A:2506:A:O2' | 1:A:2507:G:O5' | 2.26 | 0.53 |
| 1:A:2419:U:H5'' | 1:A:2420:G:H5' | 1.90 | 0.53 |
| 24:W:64:GLY:O | 24:W:65:ASP:CB | 2.57 | 0.53 |
| 1:A:1717:A:H5'' | 18:Q:54:LYS:HB2 | 1.91 | 0.53 |
| 1:A:241:A:C2 | 1:A:378:A:H4' | 2.42 | 0.53 |
| 1:A:1730:G:H5' | 1:A:1731:C:C5 | 2.43 | 0.53 |
| 5:D:148:PRO:HD2 | 38:D:8584:HOH:O | 2.08 | 0.53 |
| 1:A:1119:G:H22 | 1:A:1246:A:H2 | 1.53 | 0.53 |
| 1:A:558:C:H2' | 1:A:559:U:C5' | 2.39 | 0.53 |
| 2:B:3030:C:OP1 | 7:F:137:PRO:O | 2.27 | 0.53 |
| 16:O:155:GLU:O | 16:O:156:GLU:HG3 | 2.08 | 0.53 |
| 20:S:17:MET:CE | 20:S:19:ARG:NH2 | 2.72 | 0.53 |
| 7:F:170:TYR:O | 7:F:171:ASP:HB3 | 2.08 | 0.53 |
| 13:L:82:ARG:HH21 | 13:L:115:ARG:HG2 | 1.73 | 0.53 |
| 2:B:3064:C:H2' | 2:B:3065:A:H5' | 1.91 | 0.53 |
| 24:W:49:LEU:O | 24:W:53:ILE:HG13 | 2.08 | 0.53 |
| 1:A:1268:C:H2' | 1:A:1269:G:H8 | 1.74 | 0.53 |
| 25:X:88:THR:HG22 | 25:X:89:ASP:N | 2.23 | 0.53 |
| 1:A:1667:A:H2' | 1:A:1668:U:C6 | 2.43 | 0.53 |
| 11:J:14:TYR:N | 11:J:91:HIS:CE1 | 2.75 | 0.53 |
| 5:D:217:ARG:HG3 | 5:D:257:THR:CG2 | 2.37 | 0.53 |
| 22:U:75:GLU:O | 22:U:76:ASP:HB2 | 2.07 | 0.53 |
| 21:T:51:GLN:HE21 | 21:T:53:ASN:ND2 | 2.07 | 0.53 |
| 7:F:94:ALA:O | 7:F:95:THR:O | 2.27 | 0.53 |
| 29:2:28:HIS:CD2 | 29:2:31:LYS:HG3 | 2.43 | 0.53 |
| 22:U:48:VAL:CG2 | 22:U:98:VAL:HA | 2.38 | 0.53 |
| 15:N:45:ARG:CZ | 15:N:48:ARG:HG3 | 2.38 | 0.53 |
| 23:V:6:CYS:C | 23:V:8:TYR:H | 2.12 | 0.53 |
| 1:A:1304:U:H2' | 1:A:1305:C:C6 | 2.44 | 0.53 |
| 11:J:150:LYS:HG2 | 38:J:8383:HOH:O | 2.07 | 0.53 |
| 15:N:81:ARG:HG3 | 15:N:85:ARG:HB2 | 1.90 | 0.53 |
| 28:1:42:CYS:SG | 28:1:44:PHE:HB2 | 2.48 | 0.53 |
| 1:A:1711:A:O2' | 1:A:1712:A:H5' | 2.08 | 0.53 |
| 17:P:38:ARG:NH1 | 38:P:7674:HOH:O | 2.41 | 0.53 |
| 2:B:3076:G:C3' | 2:B:3077:A:H5'' | 2.30 | 0.53 |
| 25:X:110:GLN:HA | 25:X:110:GLN:NE2 | 2.24 | 0.53 |
| 7:F:94:ALA:HB3 | 7:F:174:VAL:HA | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:D:221:GLN:HE22 | 13:L:42:ASN:ND2 | 2.05 | 0.53 |
| 25:X:38:THR:O | 25:X:42:ARG:HB2 | 2.09 | 0.53 |
| 1:A:154:C:H2' | 1:A:155:C:C6 | 2.44 | 0.53 |
| 1:A:1787:C:OP1 | 18:Q:68:LYS:HE2 | 2.09 | 0.53 |
| 22:U:73:HIS:CD2 | 22:U:88:PRO:HG3 | 2.43 | 0.53 |
| 1:A:1525:G:H5' | 1:A:1526:A:OP2 | 2.08 | 0.53 |
| 1:A:524:A:H5' | 20:S:29:LYS:HE2 | 1.91 | 0.53 |
| 11:J:86:ARG:NH1 | 11:J:130:HIS:CD2 | 2.77 | 0.53 |
| 12:K:130:VAL:HG12 | 12:K:131:THR:N | 2.23 | 0.53 |
| 12:K:45:VAL:HG22 | 12:K:46:ILE:N | 2.23 | 0.53 |
| 7:F:154:LYS:H | 7:F:154:LYS:CD | 2.09 | 0.53 |
| 15:N:37:VAL:CG1 | 15:N:63:VAL:HG11 | 2.37 | 0.53 |
| 9:H:50:VAL:CG2 | 9:H:63:ILE:HG21 | 2.37 | 0.53 |
| 10:I:71:LEU:C | 10:I:73:ASP:H | 2.12 | 0.53 |
| 10:I:64:ASN:N | 10:I:64:ASN:ND2 | 2.55 | 0.53 |
| 1:A:1766:U:O2 | 1:A:1778:A:H5' | 2.08 | 0.53 |
| 14:M:73:VAL:HG23 | 14:M:74:THR:N | 2.24 | 0.53 |
| 5:D:223:ARG:HG3 | 5:D:232:TRP:O | 2.08 | 0.53 |
| 1:A:818:A:O2' | 28:1:13:ARG:HD3 | 2.07 | 0.53 |
| 28:1:38:LYS:HG2 | 28:1:45:LYS:HG2 | 1.90 | 0.53 |
| 1:A:259:G:H21 | 15:N:58:GLN:NE2 | 2.06 | 0.53 |
| 1:A:1159:G:H21 | 1:A:1189:A:H8 | 1.55 | 0.53 |
| 20:S:39:THR:CG2 | 20:S:42:GLU:HG3 | 2.38 | 0.53 |
| 8:G:49:ILE:HD11 | 8:G:69:ILE:HD12 | 1.91 | 0.53 |
| 29:2:28:HIS:CD2 | 29:2:30:LYS:HB2 | 2.44 | 0.53 |
| 22:U:49:GLU:OE2 | 22:U:97:ARG:HD2 | 2.09 | 0.53 |
| 1:A:120:A:H2' | 1:A:120:A:N3 | 2.23 | 0.53 |
| 1:A:684:G:H2' | 1:A:685:C:C6 | 2.44 | 0.53 |
| 2:B:3055:U:H4' | 2:B:3056:A:H8 | 1.73 | 0.53 |
| 28:1:46:LYS:O | 28:1:57:CYS:HA | 2.09 | 0.53 |
| 5:D:315:VAL:HG23 | 5:D:316:ARG:HG2 | 1.91 | 0.53 |
| 1:A:69:A:H5' | 1:A:69:A:C8 | 2.43 | 0.53 |
| 17:P:56:GLU:HB2 | 38:P:6111:HOH:O | 2.09 | 0.53 |
| 1:A:1342:C:C2' | 1:A:1343:C:H5' | 2.39 | 0.53 |
| 4:C:220:PRO:HD2 | 4:C:223:ARG:HD3 | 1.90 | 0.52 |
| 6:E:16:VAL:HG12 | 6:E:17:ASP:N | 2.24 | 0.52 |
| 1:A:2415:A:C2 | 16:O:25:ARG:HB3 | 2.44 | 0.52 |
| 27:Z:154:ARG:NH1 | 27:Z:155:ARG:HG3 | 2.24 | 0.52 |
| 1:A:1528:A:H2' | 1:A:1529:G:O4' | 2.09 | 0.52 |
| 1:A:2439:C:H5' | 38:A:4977:HOH:O | 2.07 | 0.52 |
| 1:A:970:U:H2' | 38:A:5822:HOH:O | 2.08 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:3:35:ARG:HB2 | 38:3:2691:HOH:O | 2.07 | 0.52 |
| 11:J:71:TYR:C | 11:J:73:GLN:H | 2.12 | 0.52 |
| 2:B:3002:U:OP2 | 2:B:3003:A:H5' | 2.08 | 0.52 |
| 27:Z:117:LEU:HD12 | 27:Z:174:VAL:CG1 | 2.39 | 0.52 |
| 1:A:2721:U:H4' | 13:L:87:ARG:HG3 | 1.91 | 0.52 |
| 2:B:3048:C:H4' | 16:O:141:ARG:NH2 | 2.24 | 0.52 |
| 1:A:2781:U:H1' | 8:G:139:GLU:OE2 | 2.08 | 0.52 |
| 20:S:39:THR:HB | 20:S:42:GLU:CD | 2.30 | 0.52 |
| 11:J:53:PRO:HG3 | 11:J:127:GLY:H | 1.72 | 0.52 |
| 5:D:51:VAL:HG23 | 5:D:330:VAL:HG22 | 1.91 | 0.52 |
| 28:1:11:THR:CG2 | 28:1:23:ARG:HB2 | 2.39 | 0.52 |
| 24:W:11:MET:HB3 | 24:W:15:GLU:HB2 | 1.91 | 0.52 |
| 11:J:136:VAL:HG22 | 11:J:137:ASN:O | 2.08 | 0.52 |
| 38:B:8465:HOH:O | 16:O:147:ILE:HB | 2.09 | 0.52 |
| 1:A:869:G:OP1 | 15:N:79:LYS:HE2 | 2.10 | 0.52 |
| 1:A:2851:G:C2' | 1:A:2852:A:H5' | 2.39 | 0.52 |
| 1:A:1334:C:H2' | 1:A:1335:C:H6 | 1.73 | 0.52 |
| 24:W:20:LEU:HD22 | 24:W:60:GLN:HE22 | 1.74 | 0.52 |
| 5:D:27:ASN:HD22 | 5:D:27:ASN:H | 1.57 | 0.52 |
| 1:A:1789:G:O6 | 18:Q:73:HIS:HE1 | 1.93 | 0.52 |
| 1:A:1351:G:OP1 | 6:E:96:LYS:NZ | 2.33 | 0.52 |
| 13:L:49:LEU:HA | 13:L:73:VAL:HG12 | 1.91 | 0.52 |
| 15:N:173:LEU:HD23 | 15:N:183:VAL:HG12 | 1.90 | 0.52 |
| 15:N:185:PRO:HG2 | 15:N:189:VAL:HG11 | 1.90 | 0.52 |
| 14:M:72:ASN:O | 14:M:76:LEU:HG | 2.09 | 0.52 |
| 8:G:126:ILE:HB | 8:G:131:LEU:HD23 | 1.91 | 0.52 |
| 1:A:602:A:O2' | 1:A:605:C:H4' | 2.08 | 0.52 |
| 9:H:36:THR:HG23 | 9:H:97:ALA:HB2 | 1.91 | 0.52 |
| 9:H:48:VAL:HG12 | 9:H:97:ALA:CB | 2.39 | 0.52 |
| 6:E:7:ASP:O | 6:E:9:ASP:N | 2.43 | 0.52 |
| 1:A:1353:C:P | 38:A:4177:HOH:O | 2.68 | 0.52 |
| 7:F:149:ARG:NH1 | 38:F:3066:HOH:O | 2.29 | 0.52 |
| 7:F:58:VAL:HG12 | 7:F:59:GLY:N | 2.24 | 0.52 |
| 1:A:894:A:C2 | 6:E:87:ARG:NH2 | 2.77 | 0.52 |
| 1:A:2815:G:OP2 | 12:K:99:GLU:HG2 | 2.09 | 0.52 |
| 30:3:40:ARG:HA | 30:3:45:ASN:ND2 | 2.24 | 0.52 |
| 25:X:5:VAL:HG22 | 25:X:32:CYS:HB2 | 1.91 | 0.52 |
| 25:X:137:GLN:HE21 | 25:X:141:HIS:CE1 | 2.26 | 0.52 |
| 21:T:57:THR:CG2 | 21:T:58:MET:N | 2.71 | 0.52 |
| 20:S:39:THR:HB | 20:S:42:GLU:HG3 | 1.91 | 0.52 |
| 8:G:69:ILE:HA | 8:G:72:MET:CE | 2.40 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:N:134:ILE:O | 15:N:136:PRO:HD3 | 2.09 | 0.52 |
| 20:S:119:VAL:HG21 | 20:S:142:ASP:CG | 2.29 | 0.52 |
| 1:A:380:A:OP2 | 15:N:9:ARG:HD2 | 2.10 | 0.52 |
| 7:F:11:HIS:O | 7:F:12:GLU:HB3 | 2.09 | 0.52 |
| 18:Q:16:VAL:HG12 | 18:Q:17:GLY:N | 2.24 | 0.52 |
| 27:Z:117:LEU:HD12 | 27:Z:174:VAL:HG11 | 1.90 | 0.52 |
| 31:4:11:CYS:HB2 | 31:4:20:HIS:CE1 | 2.43 | 0.52 |
| 1:A:1098:A:H2' | 1:A:1099:G:O4' | 2.10 | 0.52 |
| 1:A:920:C:H5'' | 1:A:921:G:O5' | 2.10 | 0.52 |
| 11:J:45:GLN:HB3 | 11:J:163:PRO:CD | 2.22 | 0.52 |
| 1:A:2269:C:C2' | 1:A:2270:G:H5' | 2.40 | 0.52 |
| 36:5:77:PHA:H | 36:6:77:PHA:C | 2.21 | 0.52 |
| 11:J:95:GLU:HB3 | 11:J:119:VAL:HG11 | 1.91 | 0.52 |
| 1:A:1015:C:H2' | 1:A:1016:U:C6 | 2.45 | 0.52 |
| 1:A:2324:G:H4' | 1:A:2418:G:O2' | 2.10 | 0.52 |
| 26:Y:70:ILE:HG23 | 26:Y:70:ILE:O | 2.09 | 0.52 |
| 1:A:1166:A:H61 | 1:A:1180:U:H3 | 1.57 | 0.52 |
| 1:A:2073:G:OP2 | 1:A:2490:A:H5' | 2.09 | 0.52 |
| 9:H:58:GLU:HG3 | 9:H:61:MET:CE | 2.40 | 0.52 |
| 27:Z:112:GLU:OE1 | 27:Z:115:ARG:NH1 | 2.42 | 0.52 |
| 38:A:3366:HOH:O | 11:J:90:PHE:HD2 | 1.92 | 0.52 |
| 2:B:3114:G:O6 | 16:O:11:ARG:HD3 | 2.10 | 0.52 |
| 18:Q:16:VAL:CG1 | 18:Q:20:ARG:HB2 | 2.40 | 0.52 |
| 23:V:47:ARG:HG3 | 38:V:4381:HOH:O | 2.10 | 0.52 |
| 1:A:1139:U:H2' | 1:A:1140:C:C6 | 2.45 | 0.52 |
| 1:A:459:A:H4' | 38:A:8966:HOH:O | 2.10 | 0.52 |
| 1:A:1471:A:H2' | 1:A:1472:C:C6 | 2.43 | 0.52 |
| 20:S:111:ILE:HG23 | 20:S:145:LEU:HD11 | 1.91 | 0.52 |
| 13:L:9:THR:O | 13:L:10:GLN:C | 2.47 | 0.52 |
| 1:A:795:G:H1' | 1:A:817:G:N2 | 2.24 | 0.52 |
| 31:4:16:GLU:HG3 | 31:4:18:GLN:HE21 | 1.75 | 0.52 |
| 31:4:38:ARG:O | 31:4:42:ARG:HB2 | 2.10 | 0.52 |
| 15:N:72:SER:HB2 | 15:N:93:ARG:HG2 | 1.92 | 0.52 |
| 1:A:2684:A:H2' | 1:A:2685:C:C6 | 2.44 | 0.52 |
| 22:U:69:LYS:O | 22:U:71:VAL:HG23 | 2.10 | 0.52 |
| 16:O:37:ARG:NH2 | 38:O:8534:HOH:O | 2.43 | 0.52 |
| 1:A:2815:G:N7 | 12:K:80:LYS:NZ | 2.58 | 0.52 |
| 2:B:3039:U:H1' | 2:B:3044:A:H61 | 1.73 | 0.52 |
| 7:F:35:ALA:O | 7:F:37:ALA:N | 2.43 | 0.52 |
| 16:O:163:PHE:HA | 38:O:8519:HOH:O | 2.10 | 0.52 |
| 20:S:18:LEU:HG | 20:S:91:LEU:HD13 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:2578:G:C8 | 1:A:2578:G:H5' | 2.42 | 0.52 |
| 25:X:13:MET:HE2 | 25:X:18:GLN:N | 2.24 | 0.52 |
| 22:U:40:VAL:HG23 | 22:U:119:ALA:C | 2.30 | 0.52 |
| 22:U:41:ARG:HG2 | 22:U:41:ARG:NH1 | 2.24 | 0.52 |
| 16:O:154:LEU:O | 16:O:155:GLU:CB | 2.58 | 0.52 |
| 5:D:49:THR:HG21 | 5:D:280:VAL:HG23 | 1.91 | 0.52 |
| 1:A:113:A:OP2 | 1:A:114:A:H2' | 2.09 | 0.52 |
| 14:M:22:ARG:HG2 | 38:M:8523:HOH:O | 2.10 | 0.52 |
| 15:N:35:PRO:HD2 | 15:N:38:VAL:CG2 | 2.40 | 0.52 |
| 1:A:2780:C:H2' | 1:A:2781:U:H6 | 1.75 | 0.52 |
| 27:Z:115:ARG:NE | 38:Z:8553:HOH:O | 2.42 | 0.52 |
| 7:F:50:VAL:O | 7:F:71:ALA:HA | 2.10 | 0.52 |
| 1:A:69:A:H5' | 1:A:69:A:H8 | 1.75 | 0.52 |
| 5:D:81:ALA:O | 5:D:186:GLY:HA3 | 2.10 | 0.52 |
| 4:C:57:ALA:HA | 4:C:67:LEU:HD23 | 1.92 | 0.52 |
| 17:P:35:LYS:HD3 | 38:P:3360:HOH:O | 2.09 | 0.52 |
| 15:N:113:ARG:NH2 | 15:N:156:ARG:HG2 | 2.25 | 0.52 |
| 1:A:157:G:H4' | 15:N:95:LYS:CE | 2.40 | 0.51 |
| 15:N:87:MET:CB | 31:4:46:ILE:HD13 | 2.35 | 0.51 |
| 27:Z:187:VAL:CG2 | 27:Z:192:ASP:HB2 | 2.36 | 0.51 |
| 10:I:12:ILE:N | 10:I:13:PRO:CD | 2.72 | 0.51 |
| 1:A:2421:G:H3' | 1:A:2422:U:C5' | 2.40 | 0.51 |
| 25:X:38:THR:HG22 | 38:X:3580:HOH:O | 2.10 | 0.51 |
| 1:A:2564:G:OP2 | 1:A:2565:C:H5'' | 2.10 | 0.51 |
| 38:A:7115:HOH:O | 15:N:156:ARG:HD3 | 2.09 | 0.51 |
| 14:M:65:ASP:CG | 14:M:111:ALA:HB3 | 2.30 | 0.51 |
| 1:A:1025:C:H5' | 25:X:23:MET:O | 2.10 | 0.51 |
| 1:A:1669:A:H2' | 1:A:1670:G:C8 | 2.45 | 0.51 |
| 11:J:69:ASN:O | 11:J:72:VAL:HG12 | 2.10 | 0.51 |
| 1:A:1477:C:H5' | 1:A:1868:G:C5' | 2.40 | 0.51 |
| 1:A:156:C:H5'' | 15:N:171:ARG:CD | 2.20 | 0.51 |
| 9:H:56:PRO:CG | 15:N:44:THR:HA | 2.39 | 0.51 |
| 16:O:180:LEU:O | 16:O:181:ASP:HB3 | 2.10 | 0.51 |
| 1:A:1060:C:H6 | 1:A:1060:C:H5' | 1.74 | 0.51 |
| 1:A:2906:A:H5' | 1:A:2907:C:O4' | 2.10 | 0.51 |
| 1:A:1134:G:C4' | 11:J:151:MET:HE1 | 2.31 | 0.51 |
| 1:A:1192:A:H3' | 1:A:1193:A:H5' | 1.92 | 0.51 |
| 1:A:135:G:OP1 | 15:N:39:ARG:NH1 | 2.41 | 0.51 |
| 11:J:139:ASP:OD2 | 38:J:8392:HOH:O | 2.19 | 0.51 |
| 5:D:16:ARG:NH1 | 38:D:8618:HOH:O | 2.43 | 0.51 |
| 1:A:2300:A:H4' | 1:A:2301:A:O5' | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 23:V:34:SER:HA | 23:V:37:GLU:OE1 | 2.10 | 0.51 |
| 21:T:57:THR:HG22 | 21:T:58:MET:N | 2.24 | 0.51 |
| 20:S:44:VAL:O | 20:S:48:GLU:HG3 | 2.11 | 0.51 |
| 28:1:19:GLY:O | 28:1:23:ARG:HG2 | 2.09 | 0.51 |
| 1:A:2251:G:H2' | 1:A:2252:A:C8 | 2.45 | 0.51 |
| 7:F:158:ASN:HB2 | 7:F:161:ASP:OD2 | 2.11 | 0.51 |
| 25:X:1:MET:HB2 | 25:X:103:GLU:HG2 | 1.93 | 0.51 |
| 25:X:41:TYR:O | 25:X:45:VAL:HG13 | 2.10 | 0.51 |
| 4:C:200:PRO:HG2 | 4:C:225:VAL:HG21 | 1.91 | 0.51 |
| 2:B:3020:G:O2' | 2:B:3021:G:H5' | 2.11 | 0.51 |
| 1:A:394:G:H1 | 15:N:181:GLU:CD | 2.14 | 0.51 |
| 6:E:84:VAL:O | 6:E:85:LYS:HB2 | 2.10 | 0.51 |
| 4:C:173:GLY:O | 4:C:176:HIS:HB3 | 2.11 | 0.51 |
| 11:J:163:PRO:HG2 | 38:J:8338:HOH:O | 2.10 | 0.51 |
| 7:F:166:ILE:HD12 | 38:F:6326:HOH:O | 2.11 | 0.51 |
| 22:U:9:LYS:CE | 22:U:13:ARG:NH1 | 2.66 | 0.51 |
| 1:A:2720:C:O2 | 13:L:87:ARG:NH2 | 2.43 | 0.51 |
| 4:C:36:ASP:O | 4:C:38:ILE:N | 2.44 | 0.51 |
| 5:D:207:LYS:HG2 | 5:D:304:PRO:HB3 | 1.90 | 0.51 |
| 1:A:1500:U:P | 18:Q:41:ARG:HH22 | 2.33 | 0.51 |
| 38:A:9579:HOH:O | 20:S:83:LYS:HB3 | 2.10 | 0.51 |
| 5:D:141:ARG:HD2 | 5:D:163:GLU:OE2 | 2.10 | 0.51 |
| 5:D:248:ARG:O | 5:D:251:VAL:HG13 | 2.09 | 0.51 |
| 15:N:77:PHE:HD2 | 38:N:8527:HOH:O | 1.92 | 0.51 |
| 11:J:47:GLU:HG2 | 11:J:133:ILE:HD12 | 1.92 | 0.51 |
| 6:E:235:PHE:CE2 | 6:E:243:VAL:HG21 | 2.45 | 0.51 |
| 25:X:65:VAL:HA | 25:X:68:THR:CG2 | 2.40 | 0.51 |
| 8:G:7:ILE:HD11 | 8:G:11:VAL:O | 2.11 | 0.51 |
| 1:A:2265:U:H2' | 1:A:2266:A:H8 | 1.75 | 0.51 |
| 15:N:20:ILE:O | 15:N:24:MET:HG2 | 2.11 | 0.51 |
| 20:S:113:HIS:HE1 | 20:S:144:GLU:CD | 2.14 | 0.51 |
| 1:A:229:G:O2' | 1:A:230:C:H5' | 2.10 | 0.51 |
| 17:P:10:LEU:HD13 | 17:P:99:GLU:HG3 | 1.93 | 0.51 |
| 1:A:2115:U:H2' | 1:A:2116:U:C6 | 2.45 | 0.51 |
| 18:Q:98:ILE:HD12 | 18:Q:102:ARG:NE | 2.26 | 0.51 |
| 18:Q:94:TRP:CZ2 | 18:Q:98:ILE:HG13 | 2.45 | 0.51 |
| 1:A:821:U:H2' | 1:A:822:C:H6 | 1.75 | 0.51 |
| 14:M:143:THR:CG2 | 14:M:144:ASP:N | 2.73 | 0.51 |
| 13:L:22:ASP:O | 13:L:110:LYS:HE3 | 2.11 | 0.51 |
| 28:1:34:LYS:HE2 | 38:1:8424:HOH:O | 2.09 | 0.51 |
| 11:J:31:PHE:HE2 | 11:J:87:LYS:O | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1973:A:H2' | 1:A:1974:G:O5' | 2.10 | 0.51 |
| 28:1:42:CYS:SG | 28:1:43:GLY:N | 2.84 | 0.51 |
| 1:A:440:C:O2' | 1:A:441:A:H5' | 2.11 | 0.51 |
| 38:A:3033:HOH:O | 21:T:13:LYS:HE2 | 2.11 | 0.51 |
| 1:A:653:C:H2' | 1:A:654:A:C8 | 2.45 | 0.51 |
| 11:J:86:ARG:HD3 | 11:J:130:HIS:HD2 | 1.76 | 0.51 |
| 1:A:542:A:H2' | 1:A:543:G:O4' | 2.10 | 0.51 |
| 11:J:13:ALA:HA | 11:J:91:HIS:CE1 | 2.46 | 0.51 |
| 8:G:80:TRP:O | 8:G:134:SER:HA | 2.10 | 0.51 |
| 16:O:157:PRO:HA | 38:O:8526:HOH:O | 2.10 | 0.51 |
| 6:E:21:VAL:C | 6:E:23:GLU:H | 2.14 | 0.51 |
| 12:K:22:VAL:O | 12:K:26:VAL:HG23 | 2.10 | 0.51 |
| 18:Q:134:VAL:O | 18:Q:137:LEU:HB3 | 2.10 | 0.51 |
| 38:A:9068:HOH:O | 25:X:119:HIS:HE1 | 1.94 | 0.51 |
| 14:M:73:VAL:HG11 | 14:M:118:LEU:HD21 | 1.92 | 0.51 |
| 13:L:89:LYS:HA | 38:L:7064:HOH:O | 2.09 | 0.51 |
| 1:A:709:G:O2' | 17:P:25:VAL:HG12 | 2.11 | 0.51 |
| 1:A:419:A:H1' | 1:A:1921:A:C2 | 2.45 | 0.51 |
| 6:E:142:ASP:OD2 | 6:E:238:SER:OG | 2.27 | 0.51 |
| 11:J:35:ASN:HD21 | 11:J:80:ASN:HA | 1.75 | 0.51 |
| 1:A:1701:A:H5'' | 1:A:1702:U:H3' | 1.93 | 0.51 |
| 1:A:2269:C:H2' | 1:A:2270:G:H5' | 1.91 | 0.51 |
| 15:N:87:MET:HB2 | 15:N:91:ILE:CD1 | 2.36 | 0.51 |
| 1:A:1299:G:N7 | 14:M:6:ARG:NH1 | 2.59 | 0.51 |
| 16:O:119:GLN:O | 16:O:123:ILE:HG13 | 2.11 | 0.51 |
| 38:A:6195:HOH:O | 27:Z:165:GLU:HB3 | 2.10 | 0.51 |
| 8:G:24:GLY:HA3 | 8:G:76:VAL:HB | 1.93 | 0.51 |
| 1:A:1909:A:H2' | 1:A:1910:A:C8 | 2.46 | 0.51 |
| 1:A:1825:U:O2' | 1:A:1826:C:H5' | 2.11 | 0.51 |
| 1:A:1829:A:H2' | 1:A:1830:C:H5' | 1.93 | 0.51 |
| 2:B:3039:U:H1' | 2:B:3044:A:N6 | 2.26 | 0.51 |
| 11:J:13:ALA:HA | 11:J:91:HIS:HE1 | 1.75 | 0.51 |
| 1:A:657:G:H2' | 1:A:658:C:C6 | 2.46 | 0.51 |
| 5:D:41:PHE:CE1 | 5:D:79:MET:HG3 | 2.46 | 0.51 |
| 1:A:2363:G:O2' | 19:R:11:ARG:HG3 | 2.10 | 0.51 |
| 9:H:99:THR:O | 9:H:99:THR:HG23 | 2.10 | 0.51 |
| 1:A:2781:U:C2' | 1:A:2782:G:H5' | 2.41 | 0.51 |
| 7:F:59:GLY:C | 7:F:61:PHE:H | 2.15 | 0.51 |
| 11:J:81:TYR:CD1 | 11:J:81:TYR:C | 2.84 | 0.51 |
| 1:A:244:C:O5' | 1:A:244:C:H6 | 1.94 | 0.51 |
| 1:A:2710:U:H1' | 38:A:7111:HOH:O | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:95:A:H5'' | 1:A:97:G:O4' | 2.11 | 0.51 |
| 1:A:2821:C:H4' | 5:D:116:PRO:HB3 | 1.93 | 0.51 |
| 25:X:108:ARG:HE | 25:X:114:PRO:HG3 | 1.76 | 0.51 |
| 25:X:107:LEU:O | 25:X:112:LEU:HB2 | 2.11 | 0.51 |
| 1:A:1116:U:H3 | 1:A:1246:A:N6 | 2.02 | 0.50 |
| 11:J:26:LYS:HG2 | 11:J:28:ILE:N | 2.26 | 0.50 |
| 27:Z:189:ASN:HA | 27:Z:217:ILE:HD11 | 1.93 | 0.50 |
| 25:X:21:LEU:CD2 | 25:X:48:VAL:HG11 | 2.39 | 0.50 |
| 25:X:154:ARG:C | 38:X:4276:HOH:O | 2.49 | 0.50 |
| 7:F:57:THR:HG23 | 7:F:63:ILE:CG2 | 2.40 | 0.50 |
| 1:A:2837:U:H2' | 38:A:6328:HOH:O | 2.09 | 0.50 |
| 26:Y:26:ALA:HB1 | 26:Y:59:TRP:CE2 | 2.46 | 0.50 |
| 1:A:1819:G:H5' | 38:A:4207:HOH:O | 2.11 | 0.50 |
| 1:A:1342:C:O2' | 1:A:1343:C:H5' | 2.11 | 0.50 |
| 1:A:702:G:O2' | 1:A:703:G:H5' | 2.11 | 0.50 |
| 5:D:60:SER:C | 5:D:62:ARG:H | 2.15 | 0.50 |
| 38:A:8873:HOH:O | 29:2:1:THR:HA | 2.12 | 0.50 |
| 28:1:30:GLU:HA | 28:1:33:HIS:CB | 2.42 | 0.50 |
| 1:A:816:G:C6 | 1:A:817:G:N1 | 2.79 | 0.50 |
| 8:G:68:HIS:O | 8:G:72:MET:HG3 | 2.11 | 0.50 |
| 1:A:524:A:C5' | 20:S:29:LYS:HE2 | 2.41 | 0.50 |
| 1:A:1114:A:O2' | 1:A:1115:U:H5' | 2.11 | 0.50 |
| 19:R:93:ARG:HH11 | 19:R:93:ARG:HG3 | 1.77 | 0.50 |
| 1:A:1555:G:O2' | 1:A:1556:G:H5' | 2.11 | 0.50 |
| 12:K:80:LYS:HE2 | 12:K:98:PHE:CZ | 2.47 | 0.50 |
| 1:A:567:U:H5'' | 38:X:5817:HOH:O | 2.12 | 0.50 |
| 9:H:111:ILE:O | 9:H:115:VAL:HG23 | 2.11 | 0.50 |
| 7:F:91:ALA:HB2 | 7:F:106:PHE:CD2 | 2.47 | 0.50 |
| 15:N:72:SER:OG | 15:N:93:ARG:CZ | 2.59 | 0.50 |
| 1:A:2613:G:O2' | 1:A:2614:C:H5' | 2.12 | 0.50 |
| 18:Q:120:ARG:NH2 | 18:Q:123:TYR:CD2 | 2.80 | 0.50 |
| 11:J:75:SER:HB3 | 11:J:79:ALA:CB | 2.41 | 0.50 |
| 25:X:21:LEU:HD21 | 25:X:48:VAL:HG13 | 1.93 | 0.50 |
| 1:A:1189:A:O2' | 1:A:1208:C:H2' | 2.11 | 0.50 |
| 1:A:951:A:C2' | 1:A:952:G:H5' | 2.41 | 0.50 |
| 14:M:53:ARG:NH2 | 14:M:57:VAL:HG12 | 2.26 | 0.50 |
| 18:Q:38:GLU:HA | 18:Q:41:ARG:HH11 | 1.75 | 0.50 |
| 7:F:94:ALA:HB3 | 7:F:174:VAL:CA | 2.41 | 0.50 |
| 19:R:26:PRO:O | 19:R:30:VAL:HG23 | 2.12 | 0.50 |
| 22:U:64:ASN:HA | 38:U:5927:HOH:O | 2.10 | 0.50 |
| 1:A:2445:U:H2' | 1:A:2446:G:C8 | 2.46 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2478:U:O2' | 1:A:2479:A:H5' | 2.11 | 0.50 |
| 13:L:32:ILE:HD11 | 13:L:56:SER:HB3 | 1.93 | 0.50 |
| 13:L:34:VAL:HG22 | 13:L:47:ALA:HB2 | 1.93 | 0.50 |
| 11:J:139:ASP:HB2 | 38:J:8347:HOH:O | 2.12 | 0.50 |
| 7:F:64:ARG:HB3 | 7:F:67:ASP:OD2 | 2.12 | 0.50 |
| 23:V:17:THR:CG2 | 23:V:18:GLY:N | 2.73 | 0.50 |
| 6:E:160:LEU:O | 6:E:162:VAL:HG23 | 2.11 | 0.50 |
| 16:O:61:ALA:CB | 16:O:88:ALA:HB2 | 2.42 | 0.50 |
| 21:T:80:ARG:NH1 | 38:T:8347:HOH:O | 2.44 | 0.50 |
| 1:A:1847:A:OP1 | 4:C:175:LYS:HG3 | 2.11 | 0.50 |
| 6:E:150:THR:HA | 6:E:203:ALA:O | 2.11 | 0.50 |
| 38:A:4120:HOH:O | 4:C:6:GLY:HA3 | 2.12 | 0.50 |
| 1:A:134:U:C2 | 1:A:145:A:C2 | 3.00 | 0.50 |
| 1:A:513:A:N3 | 38:A:3169:HOH:O | 2.35 | 0.50 |
| 1:A:736:A:H2' | 1:A:737:A:O4' | 2.11 | 0.50 |
| 1:A:2773:G:H5' | 38:A:6690:HOH:O | 2.11 | 0.50 |
| 8:G:106:ASN:ND2 | 8:G:109:GLY:HA2 | 2.26 | 0.50 |
| 9:H:49:PHE:HE1 | 9:H:98:VAL:HG23 | 1.77 | 0.50 |
| 15:N:67:ILE:HD11 | 15:N:104:ARG:HD2 | 1.92 | 0.50 |
| 25:X:26:ILE:HB | 38:X:5420:HOH:O | 2.11 | 0.50 |
| 20:S:119:VAL:HG11 | 38:S:8584:HOH:O | 2.11 | 0.50 |
| 14:M:104:ASP:HB3 | 38:M:8565:HOH:O | 2.11 | 0.50 |
| 28:1:13:ARG:NH1 | 28:1:14:PHE:CE2 | 2.79 | 0.50 |
| 1:A:2460:A:OP1 | 31:4:63:LYS:NZ | 2.37 | 0.50 |
| 1:A:1252:A:H2' | 1:A:1253:C:O4' | 2.12 | 0.50 |
| 1:A:344:C:H2' | 1:A:345:G:O4' | 2.11 | 0.50 |
| 1:A:1468:G:H5'' | 38:A:6508:HOH:O | 2.12 | 0.50 |
| 12:K:52:GLN:CG | 12:K:53:ILE:N | 2.67 | 0.50 |
| 8:G:81:GLU:HA | 8:G:133:VAL:O | 2.12 | 0.50 |
| 1:A:2896:A:OP1 | 26:Y:15:ARG:NH1 | 2.44 | 0.50 |
| 25:X:141:HIS:HB2 | 25:X:146:ILE:HG12 | 1.94 | 0.50 |
| 17:P:25:VAL:O | 17:P:29:VAL:HG23 | 2.12 | 0.50 |
| 1:A:1594:C:OP2 | 18:Q:120:ARG:HD2 | 2.11 | 0.50 |
| 28:1:75:ALA:HB3 | 38:1:8436:HOH:O | 2.10 | 0.50 |
| 1:A:125:U:H2' | 38:A:3277:HOH:O | 2.11 | 0.50 |
| 1:A:793:A:H5'' | 18:Q:83:LYS:HG2 | 1.94 | 0.50 |
| 6:E:236:THR:O | 6:E:237:GLU:C | 2.49 | 0.50 |
| 1:A:283:U:H5'' | 1:A:284:C:P | 2.51 | 0.50 |
| 26:Y:9:VAL:HG22 | 26:Y:88:GLU:OE2 | 2.11 | 0.50 |
| 1:A:694:A:C2' | 1:A:695:C:H5' | 2.41 | 0.50 |
| 26:Y:43:VAL:CG1 | 26:Y:44:ASP:N | 2.73 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:746:A:C6 | 17:P:65:LEU:HD13 | 2.47 | 0.50 |
| 2:B:3034:A:H2' | 2:B:3035:C:O4' | 2.11 | 0.50 |
| 23:V:47:ARG:CG | 38:V:4381:HOH:O | 2.60 | 0.50 |
| 5:D:248:ARG:O | 5:D:251:VAL:CG1 | 2.60 | 0.50 |
| 1:A:2323:G:H5' | 38:A:6510:HOH:O | 2.11 | 0.50 |
| 4:C:179:MET:HG2 | 4:C:186:TRP:CG | 2.47 | 0.50 |
| 1:A:497:A:H5'' | 38:A:3106:HOH:O | 2.10 | 0.50 |
| 1:A:1249:U:H2' | 1:A:1250:C:C6 | 2.46 | 0.50 |
| 15:N:155:HIS:CE1 | 15:N:158:ARG:HE | 2.29 | 0.50 |
| 4:C:1:GLY:HA2 | 4:C:197:VAL:HG23 | 1.94 | 0.50 |
| 1:A:1735:C:O2' | 1:A:1736:A:H5' | 2.12 | 0.50 |
| 16:O:44:ARG:HG3 | 16:O:45:ALA:N | 2.27 | 0.50 |
| 1:A:1743:G:H1' | 38:A:4383:HOH:O | 2.10 | 0.50 |
| 11:J:163:PRO:O | 11:J:164:ALA:HB2 | 2.12 | 0.50 |
| 15:N:87:MET:HG2 | 31:4:46:ILE:HG21 | 1.94 | 0.50 |
| 24:W:44:GLY:O | 24:W:48:GLU:HG2 | 2.12 | 0.50 |
| 9:H:19:ALA:O | 9:H:22:VAL:HG22 | 2.12 | 0.50 |
| 1:A:2781:U:H2' | 1:A:2782:G:H5' | 1.93 | 0.50 |
| 1:A:581:G:H5' | 38:A:7172:HOH:O | 2.10 | 0.50 |
| 6:E:196:THR:HG23 | 38:E:8405:HOH:O | 2.12 | 0.50 |
| 38:A:9458:HOH:O | 26:Y:23:HIS:HD2 | 1.94 | 0.50 |
| 1:A:2385:G:H2' | 1:A:2386:U:C6 | 2.46 | 0.50 |
| 14:M:90:ARG:NH1 | 14:M:119:THR:HG21 | 2.27 | 0.50 |
| 8:G:21:THR:HG23 | 8:G:30:THR:OG1 | 2.12 | 0.50 |
| 9:H:21:GLU:O | 9:H:24:ARG:HG3 | 2.11 | 0.50 |
| 4:C:164:ARG:HB2 | 28:1:68:CYS:SG | 2.52 | 0.50 |
| 1:A:1930:A:H2' | 1:A:1931:A:C8 | 2.47 | 0.50 |
| 1:A:1483:C:O2' | 1:A:1484:G:H5' | 2.12 | 0.50 |
| 11:J:26:LYS:CG | 11:J:28:ILE:H | 2.25 | 0.49 |
| 25:X:88:THR:CG2 | 25:X:110:GLN:NE2 | 2.75 | 0.49 |
| 15:N:164:THR:HB | 38:N:8519:HOH:O | 2.12 | 0.49 |
| 25:X:6:GLN:HG2 | 25:X:29:VAL:HA | 1.94 | 0.49 |
| 5:D:254:GLN:HG2 | 5:D:255:GLY:N | 2.26 | 0.49 |
| 1:A:553:G:H5' | 38:A:3008:HOH:O | 2.12 | 0.49 |
| 6:E:246:ARG:HH11 | 6:E:246:ARG:HB3 | 1.75 | 0.49 |
| 6:E:129:HIS:HE1 | 6:E:231:ARG:HA | 1.77 | 0.49 |
| 9:H:113:ASP:O | 9:H:117:GLU:HG3 | 2.12 | 0.49 |
| 1:A:1003:U:O2 | 11:J:90:PHE:CZ | 2.65 | 0.49 |
| 12:K:75:PRO:HG2 | 12:K:105:LEU:HD21 | 1.93 | 0.49 |
| 1:A:1086:A:C6 | 25:X:11:VAL:HG11 | 2.47 | 0.49 |
| 1:A:1853:C:OP1 | 4:C:231:LYS:HG3 | 2.11 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:C:66:ARG:HB2 | 4:C:66:ARG:HH11 | 1.76 | 0.49 |
| 1:A:2078:U:O2' | 1:A:2079:G:H5' | 2.11 | 0.49 |
| 5:D:25:ARG:HA | 5:D:310:ARG:HH21 | 1.76 | 0.49 |
| 8:G:116:THR:HG22 | 8:G:151:LEU:HD22 | 1.93 | 0.49 |
| 1:A:1613:C:H2' | 1:A:1614:G:O4' | 2.12 | 0.49 |
| 1:A:2392:C:H4' | 38:A:3775:HOH:O | 2.11 | 0.49 |
| 6:E:22:PHE:HA | 6:E:116:ALA:HA | 1.94 | 0.49 |
| 1:A:317:A:H5'' | 22:U:52:ARG:HD2 | 1.94 | 0.49 |
| 1:A:1010:C:H4' | 16:O:4:PRO:HB2 | 1.92 | 0.49 |
| 30:3:36:ASN:HB3 | 30:3:39:ARG:NE | 2.28 | 0.49 |
| 2:B:3091:C:H2' | 2:B:3092:G:O4' | 2.12 | 0.49 |
| 18:Q:13:VAL:HG11 | 18:Q:40:VAL:CG1 | 2.41 | 0.49 |
| 4:C:186:TRP:CG | 4:C:187:PRO:HA | 2.48 | 0.49 |
| 2:B:3067:C:H2' | 2:B:3068:G:H8 | 1.77 | 0.49 |
| 1:A:2243:C:H5'' | 38:A:3261:HOH:O | 2.12 | 0.49 |
| 11:J:162:SER:CB | 11:J:163:PRO:CD | 2.82 | 0.49 |
| 38:A:9404:HOH:O | 12:K:46:ILE:HA | 2.13 | 0.49 |
| 17:P:32:ARG:HB2 | 38:P:4656:HOH:O | 2.11 | 0.49 |
| 27:Z:99:ALA:HB2 | 27:Z:233:TYR:CE2 | 2.47 | 0.49 |
| 20:S:111:ILE:HG23 | 20:S:145:LEU:CD1 | 2.42 | 0.49 |
| 16:O:182:GLY:O | 16:O:183:ASP:O | 2.31 | 0.49 |
| 9:H:28:ALA:CB | 9:H:99:THR:HG23 | 2.41 | 0.49 |
| 4:C:132:ASP:OD1 | 4:C:133:ARG:N | 2.44 | 0.49 |
| 1:A:2326:U:H4' | 1:A:2412:G:H4' | 1.94 | 0.49 |
| 6:E:25:PRO:HG2 | 38:E:8321:HOH:O | 2.10 | 0.49 |
| 8:G:23:GLU:HG2 | 8:G:28:SER:HB3 | 1.94 | 0.49 |
| 1:A:1940:C:H4' | 38:A:6838:HOH:O | 2.13 | 0.49 |
| 13:L:14:LYS:NZ | 35:L:8512:CL:CL | 2.80 | 0.49 |
| 1:A:2072:G:C6 | 1:A:2533:C:H1' | 2.48 | 0.49 |
| 6:E:136:VAL:HA | 6:E:137:PRO:C | 2.32 | 0.49 |
| 1:A:2676:C:H4' | 12:K:70:PHE:CD1 | 2.47 | 0.49 |
| 1:A:212:A:O4' | 1:A:214:U:C6 | 2.66 | 0.49 |
| 4:C:191:GLY:HA2 | 4:C:194:MET:HE2 | 1.94 | 0.49 |
| 8:G:7:ILE:HG22 | 8:G:45:ASP:O | 2.12 | 0.49 |
| 1:A:814:G:H4' | 38:A:9641:HOH:O | 2.12 | 0.49 |
| 19:R:32:GLU:HA | 19:R:71:TYR:OH | 2.12 | 0.49 |
| 14:M:149:ARG:O | 14:M:150:GLN:HB2 | 2.12 | 0.49 |
| 1:A:415:A:O2' | 1:A:416:G:H5' | 2.13 | 0.49 |
| 1:A:1236:A:O2' | 1:A:1237:U:H5' | 2.12 | 0.49 |
| 1:A:128:A:O2' | 1:A:129:A:H5' | 2.12 | 0.49 |
| 1:A:638:C:H2' | 1:A:639:A:C8 | 2.48 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1756:G:H1' | 38:A:5760:HOH:O | 2.11 | 0.49 |
| 2:B:3057:A:O2' | 7:F:152:PRO:HD2 | 2.12 | 0.49 |
| 20:S:96:VAL:HG13 | 20:S:106:GLY:HA3 | 1.93 | 0.49 |
| 1:A:797:A:O4' | 28:1:10:ARG:N | 2.46 | 0.49 |
| 1:A:1666:C:C2' | 1:A:1667:A:C5' | 2.91 | 0.49 |
| 14:M:146:GLY:C | 14:M:148:GLU:H | 2.16 | 0.49 |
| 1:A:187:A:H3' | 1:A:188:C:H6 | 1.78 | 0.49 |
| 1:A:2064:U:H5' | 1:A:2652:U:H4' | 1.94 | 0.49 |
| 9:H:110:GLU:HA | 9:H:113:ASP:OD2 | 2.12 | 0.49 |
| 1:A:512:G:O3' | 1:A:513:A:H8 | 1.95 | 0.49 |
| 14:M:125:PHE:CZ | 14:M:140:VAL:HG13 | 2.46 | 0.49 |
| 16:O:64:SER:C | 16:O:66:LEU:H | 2.16 | 0.49 |
| 1:A:2010:A:H5'' | 38:A:3678:HOH:O | 2.12 | 0.49 |
| 5:D:125:GLU:O | 5:D:129:ARG:HG3 | 2.12 | 0.49 |
| 6:E:219:ASN:O | 6:E:222:ASP:OD1 | 2.31 | 0.49 |
| 6:E:237:GLU:N | 38:E:8451:HOH:O | 2.46 | 0.49 |
| 7:F:35:ALA:C | 7:F:37:ALA:H | 2.15 | 0.49 |
| 1:A:1840:A:H4' | 1:A:1841:C:O5' | 2.13 | 0.49 |
| 4:C:51:ARG:HB2 | 38:C:8602:HOH:O | 2.11 | 0.49 |
| 1:A:470:U:O2' | 29:2:16:HIS:CD2 | 2.63 | 0.49 |
| 26:Y:43:VAL:CG1 | 26:Y:47:ALA:HB3 | 2.42 | 0.49 |
| 8:G:31:ARG:NH1 | 38:G:5919:HOH:O | 2.44 | 0.49 |
| 11:J:109:ASP:HB2 | 38:J:8346:HOH:O | 2.12 | 0.49 |
| 22:U:23:VAL:CA | 22:U:93:THR:HG21 | 2.43 | 0.49 |
| 1:A:958:G:H2' | 1:A:959:C:C6 | 2.47 | 0.49 |
| 38:A:9964:HOH:O | 15:N:36:ALA:HB1 | 2.13 | 0.49 |
| 38:A:5815:HOH:O | 7:F:55:LYS:HB2 | 2.12 | 0.49 |
| 29:2:25:LYS:HE2 | 38:2:8463:HOH:O | 2.12 | 0.49 |
| 11:J:85:ILE:HB | 11:J:132:PHE:CE2 | 2.48 | 0.49 |
| 28:1:11:THR:CG2 | 28:1:23:ARG:HD2 | 2.43 | 0.49 |
| 1:A:2694:A:H4' | 8:G:91:PHE:HE1 | 1.78 | 0.49 |
| 17:P:39:THR:HB | 38:P:3360:HOH:O | 2.12 | 0.49 |
| 1:A:703:G:O2' | 1:A:704:C:H5' | 2.13 | 0.49 |
| 6:E:13:ASP:O | 6:E:13:ASP:OD1 | 2.30 | 0.49 |
| 1:A:1135:G:H5' | 38:A:5420:HOH:O | 2.11 | 0.49 |
| 1:A:2730:G:O2' | 1:A:2731:G:H5' | 2.13 | 0.49 |
| 1:A:521:A:H2' | 1:A:522:U:H5' | 1.95 | 0.49 |
| 1:A:1029:U:O2' | 1:A:1273:C:OP1 | 2.26 | 0.49 |
| 18:Q:135:ALA:HB1 | 18:Q:139:ARG:HH12 | 1.76 | 0.49 |
| 2:B:3023:U:H2' | 38:B:8479:HOH:O | 2.10 | 0.49 |
| 27:Z:187:VAL:HB | 38:Z:8567:HOH:O | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:251:C:H1' | 15:N:58:GLN:HE22 | 1.78 | 0.49 |
| 24:W:38:GLY:C | 24:W:40:PRO:HD2 | 2.32 | 0.49 |
| 1:A:1741:U:O2' | 1:A:2723:G:H4' | 2.13 | 0.49 |
| 29:2:28:HIS:CE1 | 29:2:31:LYS:HE2 | 2.47 | 0.49 |
| 1:A:818:A:H5'' | 38:A:6078:HOH:O | 2.13 | 0.49 |
| 1:A:1470:A:OP1 | 15:N:93:ARG:HD2 | 2.13 | 0.49 |
| 1:A:2044:G:OP1 | 26:Y:23:HIS:HE1 | 1.96 | 0.49 |
| 1:A:128:A:H3' | 1:A:128:A:C8 | 2.47 | 0.49 |
| 1:A:1896:G:H1' | 38:A:3765:HOH:O | 2.12 | 0.49 |
| 1:A:1163:G:N2 | 38:A:5539:HOH:O | 2.46 | 0.49 |
| 1:A:1418:U:OP1 | 30:3:42:TRP:HB3 | 2.13 | 0.49 |
| 1:A:645:U:OP2 | 14:M:4:LYS:HE2 | 2.13 | 0.49 |
| 25:X:13:MET:HE3 | 25:X:17:ILE:CG2 | 2.41 | 0.49 |
| 27:Z:184:GLU:OE1 | 27:Z:204:ARG:NH1 | 2.46 | 0.49 |
| 1:A:1398:G:H2' | 1:A:1399:A:C8 | 2.48 | 0.49 |
| 1:A:349:U:O2' | 1:A:350:C:H5' | 2.13 | 0.49 |
| 7:F:101:THR:HG22 | 38:F:7400:HOH:O | 2.13 | 0.49 |
| 7:F:35:ALA:C | 7:F:37:ALA:N | 2.66 | 0.48 |
| 1:A:2661:U:H3 | 1:A:2812:A:H62 | 1.59 | 0.48 |
| 25:X:14:HIS:HB2 | 25:X:17:ILE:HG13 | 1.94 | 0.48 |
| 25:X:65:VAL:CA | 25:X:68:THR:HG22 | 2.42 | 0.48 |
| 16:O:139:TRP:HA | 16:O:139:TRP:HE3 | 1.78 | 0.48 |
| 28:1:13:ARG:NH1 | 28:1:14:PHE:CZ | 2.81 | 0.48 |
| 6:E:7:ASP:C | 6:E:9:ASP:H | 2.17 | 0.48 |
| 25:X:1:MET:N | 25:X:103:GLU:OE2 | 2.43 | 0.48 |
| 22:U:55:PHE:CD2 | 22:U:77:VAL:HG13 | 2.48 | 0.48 |
| 1:A:23:G:H1' | 1:A:520:A:N6 | 2.28 | 0.48 |
| 23:V:11:THR:HG22 | 23:V:53:ASP:OD2 | 2.13 | 0.48 |
| 11:J:75:SER:C | 11:J:79:ALA:HB2 | 2.32 | 0.48 |
| 30:3:18:ASN:HD21 | 30:3:40:ARG:H | 1.61 | 0.48 |
| 22:U:32:ARG:NH1 | 22:U:38:ARG:NH1 | 2.60 | 0.48 |
| 2:B:3064:C:C2' | 2:B:3065:A:H5' | 2.43 | 0.48 |
| 1:A:1477:C:O2' | 1:A:1478:U:H5' | 2.12 | 0.48 |
| 9:H:13:GLU:OE2 | 9:H:78:GLU:HG2 | 2.13 | 0.48 |
| 1:A:2619:U:H2' | 1:A:2620:U:C6 | 2.48 | 0.48 |
| 1:A:1170:U:O2' | 1:A:1172:G:N7 | 2.33 | 0.48 |
| 13:L:125:ALA:C | 13:L:127:ALA:H | 2.16 | 0.48 |
| 28:1:56:MET:CE | 28:1:63:LYS:HE3 | 2.44 | 0.48 |
| 25:X:21:LEU:HB3 | 25:X:26:ILE:HG12 | 1.96 | 0.48 |
| 1:A:1772:C:H5' | 1:A:1773:G:C5 | 2.48 | 0.48 |
| 9:H:117:GLU:C | 9:H:119:ARG:H | 2.15 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 11:J:117:LYS:O | 11:J:119:VAL:HG13 | 2.12 | 0.48 |
| 1:A:440:C:H2' | 1:A:441:A:C8 | 2.48 | 0.48 |
| 1:A:941:G:O2' | 1:A:942:U:H5' | 2.12 | 0.48 |
| 15:N:107:ARG:NH1 | 38:N:8582:HOH:O | 2.46 | 0.48 |
| 16:O:58:LEU:N | 16:O:58:LEU:HD12 | 2.28 | 0.48 |
| 38:A:9528:HOH:O | 29:2:46:ARG:HA | 2.13 | 0.48 |
| 1:A:517:U:H2' | 1:A:518:G:H5' | 1.94 | 0.48 |
| 8:G:43:ASP:HA | 38:G:5864:HOH:O | 2.14 | 0.48 |
| 1:A:1656:A:H2' | 1:A:1657:A:O4' | 2.13 | 0.48 |
| 1:A:299:U:H5' | 38:A:6828:HOH:O | 2.13 | 0.48 |
| 1:A:2314:G:C2' | 1:A:2315:C:H5' | 2.44 | 0.48 |
| 2:B:3025:G:N2 | 38:B:8506:HOH:O | 2.46 | 0.48 |
| 28:1:56:MET:HA | 28:1:62:TYR:O | 2.13 | 0.48 |
| 4:C:105:VAL:HG12 | 4:C:106:CYS:N | 2.28 | 0.48 |
| 5:D:146:THR:O | 5:D:159:PRO:HB3 | 2.12 | 0.48 |
| 7:F:141:VAL:HG13 | 7:F:144:ARG:HH21 | 1.79 | 0.48 |
| 11:J:127:GLY:O | 11:J:128:ALA:CB | 2.62 | 0.48 |
| 31:4:65:THR:HB | 31:4:83:TRP:H | 1.79 | 0.48 |
| 1:A:1762:C:H2' | 1:A:1763:C:H6 | 1.78 | 0.48 |
| 1:A:2488:A:H61 | 1:A:2534:C:H42 | 1.61 | 0.48 |
| 1:A:2724:U:H2' | 1:A:2725:G:O4' | 2.12 | 0.48 |
| 1:A:1545:C:H2' | 1:A:1546:G:O4' | 2.13 | 0.48 |
| 38:A:9404:HOH:O | 12:K:18:ILE:HG23 | 2.13 | 0.48 |
| 7:F:23:VAL:HG21 | 7:F:45:THR:CG2 | 2.44 | 0.48 |
| 5:D:162:MET:HG2 | 5:D:162:MET:O | 2.13 | 0.48 |
| 5:D:16:ARG:NE | 38:D:8555:HOH:O | 2.36 | 0.48 |
| 5:D:255:GLY:O | 5:D:257:THR:HG23 | 2.13 | 0.48 |
| 26:Y:9:VAL:HG13 | 26:Y:88:GLU:OE2 | 2.12 | 0.48 |
| 2:B:3014:G:O2' | 16:O:1:ALA:HB2 | 2.14 | 0.48 |
| 1:A:86:A:C2 | 30:3:25:VAL:HG13 | 2.48 | 0.48 |
| 22:U:49:GLU:OE2 | 22:U:97:ARG:NH1 | 2.42 | 0.48 |
| 1:A:2377:U:O5' | 1:A:2377:U:H6 | 1.96 | 0.48 |
| 1:A:1783:A:O2' | 1:A:1784:U:H5' | 2.13 | 0.48 |
| 1:A:2670:G:O2' | 1:A:2671:U:H5' | 2.13 | 0.48 |
| 1:A:1827:G:H2' | 1:A:1828:G:C8 | 2.47 | 0.48 |
| 14:M:101:ASP:C | 14:M:103:ALA:H | 2.16 | 0.48 |
| 1:A:1666:C:H2' | 1:A:1667:A:C5' | 2.43 | 0.48 |
| 4:C:199:HIS:CD2 | 4:C:201:PHE:H | 2.32 | 0.48 |
| 9:H:22:VAL:HG21 | 9:H:104:ALA:HB2 | 1.96 | 0.48 |
| 26:Y:76:ARG:HG3 | 26:Y:76:ARG:NH1 | 2.25 | 0.48 |
| 8:G:11:VAL:CG1 | 8:G:12:ASP:N | 2.75 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:G:31:ARG:CZ | 38:G:5919:HOH:O | 2.61 | 0.48 |
| 22:U:43:ASN:HD22 | 22:U:108:ARG:CZ | 2.27 | 0.48 |
| 21:T:81:ILE:HG12 | 38:T:8337:HOH:O | 2.13 | 0.48 |
| 1:A:539:G:H2' | 1:A:540:A:C8 | 2.48 | 0.48 |
| 14:M:117:GLU:HB3 | 14:M:137:GLY:O | 2.13 | 0.48 |
| 1:A:2615:U:H2' | 1:A:2616:G:O4' | 2.14 | 0.48 |
| 1:A:324:G:O2' | 1:A:325:U:H5' | 2.13 | 0.48 |
| 17:P:21:SER:OG | 17:P:106:PRO:HB2 | 2.12 | 0.48 |
| 1:A:1423:C:O2' | 1:A:1424:A:H5' | 2.14 | 0.48 |
| 15:N:97:ILE:HA | 15:N:100:ILE:HD12 | 1.95 | 0.48 |
| 1:A:2387:U:H2' | 1:A:2388:C:C6 | 2.48 | 0.48 |
| 1:A:1473:U:C1' | 29:2:42:SER:HB2 | 2.43 | 0.48 |
| 31:4:91:GLN:O | 31:4:92:GLU:HB2 | 2.13 | 0.48 |
| 11:J:157:ILE:CG2 | 11:J:158:ASN:N | 2.77 | 0.48 |
| 13:L:87:ARG:NE | 38:L:4854:HOH:O | 2.47 | 0.48 |
| 16:O:159:TYR:HE2 | 16:O:163:PHE:HE2 | 1.61 | 0.48 |
| 4:C:76:VAL:HG23 | 28:1:63:LYS:HB3 | 1.94 | 0.48 |
| 1:A:2547:C:OP2 | 5:D:5:ARG:NH1 | 2.46 | 0.48 |
| 7:F:59:GLY:O | 7:F:61:PHE:N | 2.38 | 0.48 |
| 1:A:1172:G:H1' | 38:A:4463:HOH:O | 2.13 | 0.48 |
| 1:A:1352:A:N1 | 6:E:48:SER:HB3 | 2.29 | 0.48 |
| 11:J:65:ARG:NH2 | 11:J:66:VAL:HG22 | 2.28 | 0.48 |
| 7:F:19:GLU:HG3 | 38:F:6165:HOH:O | 2.13 | 0.48 |
| 17:P:47:ARG:HA | 17:P:50:ARG:NH1 | 2.29 | 0.48 |
| 9:H:107:VAL:HG23 | 38:H:6617:HOH:O | 2.14 | 0.48 |
| 4:C:105:VAL:HG11 | 4:C:154:ALA:CB | 2.43 | 0.48 |
| 1:A:1615:A:H5' | 38:A:3690:HOH:O | 2.12 | 0.48 |
| 5:D:24:PRO:CG | 5:D:204:GLY:HA2 | 2.44 | 0.48 |
| 23:V:49:LEU:CD1 | 38:V:3805:HOH:O | 2.61 | 0.48 |
| 10:I:69:ARG:NH1 | 38:I:3513:HOH:O | 2.46 | 0.48 |
| 26:Y:21:PRO:HG2 | 26:Y:24:LYS:HD3 | 1.95 | 0.48 |
| 1:A:1127:C:H2' | 1:A:1128:U:H5' | 1.96 | 0.48 |
| 18:Q:121:ASP:OD1 | 18:Q:125:LYS:HE3 | 2.13 | 0.48 |
| 5:D:260:HIS:HA | 38:D:8628:HOH:O | 2.13 | 0.48 |
| 4:C:107:ASN:OD1 | 4:C:120:ARG:HD2 | 2.14 | 0.48 |
| 1:A:2852:A:H5'' | 38:A:4724:HOH:O | 2.14 | 0.48 |
| 2:B:3047:A:C2 | 2:B:3048:C:C2 | 3.02 | 0.48 |
| 15:N:27:ARG:NH2 | 15:N:44:THR:HG23 | 2.29 | 0.48 |
| 25:X:146:ILE:HG22 | 25:X:147:ASP:N | 2.29 | 0.48 |
| 5:D:279:THR:CG2 | 5:D:280:VAL:N | 2.76 | 0.48 |
| 15:N:12:TRP:HB2 | 38:N:8607:HOH:O | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:1617:C:C4 | 1:A:1643:C:H4' | 2.49 | 0.48 |
| 1:A:474:C:O3' | 6:E:73:LEU:HD21 | 2.13 | 0.48 |
| 1:A:820:G:C6 | 4:C:171:LYS:HB2 | 2.48 | 0.48 |
| 1:A:820:G:H5' | 1:A:821:U:H5' | 1.95 | 0.48 |
| 1:A:1174:A:C5 | 1:A:1201:C:H4' | 2.48 | 0.48 |
| 25:X:52:VAL:HG22 | 25:X:53:ALA:H | 1.79 | 0.48 |
| 1:A:191:A:H2' | 1:A:237:G:O6 | 2.14 | 0.48 |
| 1:A:2896:A:H5'' | 38:A:5592:HOH:O | 2.14 | 0.48 |
| 25:X:122:ARG:HG2 | 25:X:152:ALA:O | 2.13 | 0.48 |
| 6:E:39:GLN:O | 6:E:43:LYS:HD3 | 2.14 | 0.48 |
| 1:A:945:U:H2' | 1:A:946:C:H6 | 1.78 | 0.48 |
| 28:1:41:VAL:HG12 | 28:1:42:CYS:N | 2.28 | 0.48 |
| 17:P:26:TRP:N | 38:P:3062:HOH:O | 2.46 | 0.48 |
| 1:A:1079:A:H4' | 1:A:2078:U:H5' | 1.96 | 0.48 |
| 13:L:55:VAL:HG12 | 13:L:56:SER:N | 2.29 | 0.47 |
| 15:N:66:ALA:O | 15:N:67:ILE:HD13 | 2.14 | 0.47 |
| 10:I:12:ILE:HG13 | 38:I:6833:HOH:O | 2.14 | 0.47 |
| 11:J:46:VAL:O | 11:J:146:TRP:CH2 | 2.64 | 0.47 |
| 26:Y:30:MET:CE | 26:Y:58:ALA:HB3 | 2.43 | 0.47 |
| 5:D:154:VAL:HG12 | 5:D:156:LYS:HG2 | 1.96 | 0.47 |
| 15:N:47:ASP:CG | 15:N:48:ARG:H | 2.16 | 0.47 |
| 1:A:399:C:H5' | 15:N:179:GLY:O | 2.15 | 0.47 |
| 1:A:812:A:H2' | 1:A:813:C:C6 | 2.49 | 0.47 |
| 9:H:26:THR:HG21 | 9:H:103:ALA:HB2 | 1.95 | 0.47 |
| 1:A:2904:U:H4' | 26:Y:8:ARG:NH1 | 2.29 | 0.47 |
| 22:U:71:VAL:CG1 | 22:U:90:PRO:HB3 | 2.29 | 0.47 |
| 13:L:29:LEU:HB3 | 13:L:55:VAL:CG1 | 2.33 | 0.47 |
| 1:A:877:G:H3' | 38:A:9621:HOH:O | 2.13 | 0.47 |
| 12:K:93:ARG:HH11 | 12:K:93:ARG:CB | 2.21 | 0.47 |
| 6:E:138:VAL:O | 6:E:234:VAL:HA | 2.14 | 0.47 |
| 1:A:656:G:H5' | 17:P:3:THR:HB | 1.95 | 0.47 |
| 8:G:69:ILE:HA | 8:G:72:MET:HE3 | 1.96 | 0.47 |
| 6:E:133:ARG:NH2 | 38:E:8431:HOH:O | 2.46 | 0.47 |
| 1:A:24:G:N2 | 1:A:518:G:H1' | 2.29 | 0.47 |
| 1:A:2441:U:HO2' | 14:M:51:PHE:HE1 | 1.61 | 0.47 |
| 17:P:105:ASN:HD21 | 17:P:109:SER:H | 1.62 | 0.47 |
| 11:J:111:MET:O | 11:J:114:PRO:HD3 | 2.14 | 0.47 |
| 1:A:812:A:H2' | 1:A:813:C:O4' | 2.14 | 0.47 |
| 1:A:1503:U:H2' | 1:A:1504:A:O4' | 2.15 | 0.47 |
| 1:A:1504:A:H5' | 38:A:3918:HOH:O | 2.13 | 0.47 |
| 1:A:245:C:H2' | 1:A:246:G:H5' | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:765:G:O3' | 6:E:69:HIS:HB3 | 2.14 | 0.47 |
| 1:A:1568:G:O2' | 1:A:1569:U:H5' | 2.13 | 0.47 |
| 1:A:1849:G:H1' | 1:A:2011:A:N1 | 2.29 | 0.47 |
| 11:J:26:LYS:HD3 | 11:J:89:PRO:HG3 | 1.96 | 0.47 |
| 11:J:65:ARG:CZ | 38:J:8385:HOH:O | 2.61 | 0.47 |
| 15:N:87:MET:HG3 | 15:N:87:MET:H | 1.30 | 0.47 |
| 5:D:16:ARG:NH2 | 38:D:8555:HOH:O | 2.44 | 0.47 |
| 1:A:1994:A:P | 13:L:66:ARG:HH22 | 2.38 | 0.47 |
| 12:K:39:VAL:HG13 | 12:K:106:GLY:O | 2.14 | 0.47 |
| 1:A:903:U:O4 | 14:M:18:HIS:HB2 | 2.14 | 0.47 |
| 8:G:84:MET:HE1 | 8:G:148:ILE:HD12 | 1.97 | 0.47 |
| 1:A:661:G:C5 | 1:A:686:A:C2 | 3.02 | 0.47 |
| 22:U:23:VAL:C | 22:U:93:THR:HG21 | 2.34 | 0.47 |
| 23:V:20:MET:CG | 23:V:28:THR:HG23 | 2.45 | 0.47 |
| 1:A:1947:G:N2 | 1:A:1966:U:C2 | 2.82 | 0.47 |
| 28:1:51:GLY:HA3 | 38:1:8416:HOH:O | 2.13 | 0.47 |
| 1:A:1154:A:H2' | 1:A:1155:G:C8 | 2.50 | 0.47 |
| 16:O:138:ASP:O | 16:O:140:GLN:N | 2.40 | 0.47 |
| 15:N:154:ARG:HG3 | 38:N:8620:HOH:O | 2.14 | 0.47 |
| 16:O:32:PRO:HD2 | 16:O:99:GLU:O | 2.15 | 0.47 |
| 20:S:47:LEU:O | 20:S:51:ILE:HG13 | 2.14 | 0.47 |
| 9:H:39:SER:HB3 | 9:H:45:ALA:HB2 | 1.95 | 0.47 |
| 1:A:932:U:H2' | 1:A:933:C:C6 | 2.49 | 0.47 |
| 1:A:1439:C:H5'' | 30:3:41:HIS:CE1 | 2.50 | 0.47 |
| 16:O:67:ALA:HA | 16:O:71:TRP:H | 1.79 | 0.47 |
| 6:E:16:VAL:HG12 | 6:E:17:ASP:H | 1.80 | 0.47 |
| 1:A:2748:G:H1' | 38:A:7391:HOH:O | 2.14 | 0.47 |
| 1:A:2256:G:O2' | 1:A:2257:G:H5' | 2.13 | 0.47 |
| 26:Y:25:ARG:NH1 | 38:Y:3861:HOH:O | 2.47 | 0.47 |
| 25:X:131:PRO:O | 25:X:136:GLY:N | 2.47 | 0.47 |
| 15:N:48:ARG:NH2 | 38:N:8564:HOH:O | 2.48 | 0.47 |
| 5:D:149:ASP:HB2 | 38:D:8584:HOH:O | 2.13 | 0.47 |
| 8:G:145:ALA:HB1 | 8:G:168:ILE:CD1 | 2.44 | 0.47 |
| 20:S:35:ILE:O | 20:S:38:LYS:HB2 | 2.14 | 0.47 |
| 6:E:61:PHE:HB3 | 38:E:8448:HOH:O | 2.14 | 0.47 |
| 1:A:1287:A:O4' | 25:X:117:ARG:HD3 | 2.15 | 0.47 |
| 7:F:128:LEU:HB2 | 38:F:6007:HOH:O | 2.14 | 0.47 |
| 1:A:2718:C:H6 | 1:A:2718:C:H5' | 1.80 | 0.47 |
| 5:D:140:LEU:HD13 | 5:D:175:LEU:HA | 1.97 | 0.47 |
| 13:L:109:LEU:HD13 | 13:L:113:ILE:HD11 | 1.95 | 0.47 |
| 5:D:43:GLY:O | 5:D:308:LEU:HD12 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 25:X:29:VAL:O | 25:X:30:ASN:HB2 | 2.14 | 0.47 |
| 7:F:84:LEU:C | 7:F:86:THR:H | 2.17 | 0.47 |
| 15:N:42:ARG:HA | 15:N:43:PRO:HD3 | 1.79 | 0.47 |
| 14:M:53:ARG:HH22 | 14:M:57:VAL:HG12 | 1.79 | 0.47 |
| 16:O:43:VAL:O | 16:O:43:VAL:HG12 | 2.13 | 0.47 |
| 14:M:134:GLU:HA | 14:M:138:GLY:O | 2.14 | 0.47 |
| 6:E:95:GLU:H | 6:E:95:GLU:CD | 2.18 | 0.47 |
| 7:F:142:ALA:HA | 7:F:149:ARG:O | 2.15 | 0.47 |
| 1:A:1139:U:H2' | 1:A:1140:C:H6 | 1.80 | 0.47 |
| 18:Q:22:TRP:CH2 | 18:Q:24:ASN:HA | 2.50 | 0.47 |
| 1:A:2464:C:H5'' | 1:A:2465:A:OP1 | 2.14 | 0.47 |
| 5:D:132:HIS:HB2 | 5:D:137:LEU:HD22 | 1.96 | 0.47 |
| 15:N:32:ARG:NH2 | 38:N:8604:HOH:O | 2.47 | 0.47 |
| 1:A:2405:C:H5' | 38:A:6086:HOH:O | 2.13 | 0.47 |
| 7:F:41:LEU:O | 7:F:44:ILE:HG22 | 2.15 | 0.47 |
| 26:Y:85:VAL:HG12 | 26:Y:86:GLU:N | 2.28 | 0.47 |
| 1:A:2270:G:H4' | 4:C:223:ARG:NH1 | 2.29 | 0.47 |
| 30:3:40:ARG:HG3 | 30:3:45:ASN:HB2 | 1.97 | 0.47 |
| 25:X:76:ASP:O | 25:X:77:ALA:C | 2.53 | 0.47 |
| 25:X:7:LEU:HD12 | 25:X:53:ALA:HB2 | 1.97 | 0.47 |
| 2:B:3049:G:O2' | 2:B:3050:G:H5' | 2.14 | 0.47 |
| 25:X:122:ARG:CG | 25:X:122:ARG:HH11 | 2.23 | 0.47 |
| 11:J:83:PHE:HE1 | 11:J:146:TRP:CZ2 | 2.32 | 0.47 |
| 1:A:1505:U:C6 | 1:A:1505:U:H5' | 2.44 | 0.47 |
| 1:A:695:C:H2' | 1:A:696:C:C6 | 2.50 | 0.47 |
| 15:N:166:ALA:HA | 15:N:169:ARG:NH1 | 2.30 | 0.47 |
| 15:N:55:LYS:O | 15:N:60:ILE:HD12 | 2.15 | 0.47 |
| 38:A:5956:HOH:O | 5:D:27:ASN:HB3 | 2.14 | 0.47 |
| 22:U:19:ARG:NH1 | 22:U:68:ASP:O | 2.48 | 0.47 |
| 20:S:29:LYS:HD3 | 38:S:8531:HOH:O | 2.14 | 0.47 |
| 1:A:1909:A:N1 | 1:A:2128:G:H1' | 2.29 | 0.47 |
| 9:H:21:GLU:O | 9:H:24:ARG:CG | 2.63 | 0.47 |
| 31:4:15:ASN:ND2 | 38:4:8545:HOH:O | 2.47 | 0.47 |
| 8:G:10:ASP:HA | 38:G:3707:HOH:O | 2.14 | 0.47 |
| 4:C:135:VAL:HG11 | 4:C:147:ARG:NH2 | 2.30 | 0.47 |
| 1:A:377:C:H5 | 38:A:9815:HOH:O | 1.98 | 0.47 |
| 19:R:66:LYS:HB2 | 19:R:70:ALA:O | 2.14 | 0.47 |
| 13:L:28:GLU:HG2 | 13:L:58:THR:HB | 1.96 | 0.47 |
| 2:B:3059:C:H2' | 2:B:3060:C:C6 | 2.50 | 0.47 |
| 16:O:37:ARG:CZ | 38:O:8534:HOH:O | 2.62 | 0.47 |
| 1:A:2506:A:H1' | 38:A:3257:HOH:O | 2.13 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:N:78:ASN:C | 15:N:79:LYS:HG2 | 2.36 | 0.47 |
| 5:D:41:PHE:CD1 | 5:D:79:MET:HE2 | 2.50 | 0.47 |
| 4:C:194:MET:CE | 4:C:199:HIS:HB2 | 2.45 | 0.47 |
| 28:1:31:ILE:HG23 | 28:1:32:LYS:N | 2.30 | 0.47 |
| 5:D:279:THR:HG22 | 5:D:280:VAL:N | 2.29 | 0.47 |
| 30:3:22:PRO:HG2 | 30:3:25:VAL:CG2 | 2.43 | 0.47 |
| 20:S:92:LEU:HD23 | 20:S:145:LEU:HD21 | 1.97 | 0.47 |
| 1:A:1172:G:H5'' | 38:A:6752:HOH:O | 2.13 | 0.47 |
| 1:A:1393:A:H2' | 1:A:1394:C:C6 | 2.50 | 0.47 |
| 1:A:949:U:O2' | 19:R:40:HIS:HE1 | 1.98 | 0.47 |
| 16:O:97:VAL:HG12 | 16:O:127:LEU:HD11 | 1.97 | 0.47 |
| 1:A:1180:U:H2' | 1:A:1181:A:O4' | 2.15 | 0.47 |
| 15:N:38:VAL:O | 15:N:38:VAL:HG12 | 2.14 | 0.47 |
| 13:L:75:ARG:CZ | 38:L:4172:HOH:O | 2.62 | 0.47 |
| 7:F:19:GLU:O | 7:F:133:ASN:HB3 | 2.14 | 0.47 |
| 10:I:12:ILE:HG22 | 10:I:12:ILE:O | 2.14 | 0.47 |
| 7:F:65:GLU:HA | 38:F:6752:HOH:O | 2.14 | 0.47 |
| 1:A:1641:A:C2' | 1:A:1642:A:H5' | 2.43 | 0.47 |
| 9:H:28:ALA:HB3 | 9:H:99:THR:O | 2.15 | 0.47 |
| 38:A:5744:HOH:O | 23:V:56:ARG:HD3 | 2.14 | 0.47 |
| 26:Y:76:ARG:O | 26:Y:77:PHE:HB3 | 2.15 | 0.47 |
| 38:A:9077:HOH:O | 5:D:267:LYS:HD3 | 2.14 | 0.47 |
| 7:F:167:GLU:OE2 | 7:F:173:GLU:HG2 | 2.14 | 0.47 |
| 19:R:30:VAL:O | 19:R:30:VAL:HG12 | 2.15 | 0.47 |
| 1:A:2251:G:H4' | 38:A:6900:HOH:O | 2.14 | 0.47 |
| 1:A:1269:G:H2' | 1:A:1270:U:C6 | 2.49 | 0.47 |
| 1:A:522:U:O2' | 1:A:1366:C:H5' | 2.14 | 0.47 |
| 38:A:7169:HOH:O | 15:N:154:ARG:HB2 | 2.14 | 0.47 |
| 16:O:184:ILE:HG22 | 16:O:185:GLU:HG3 | 1.97 | 0.47 |
| 17:P:49:GLU:HG2 | 38:P:5191:HOH:O | 2.15 | 0.47 |
| 1:A:825:U:H5'' | 1:A:826:U:OP1 | 2.15 | 0.47 |
| 11:J:45:GLN:CB | 11:J:163:PRO:HD2 | 2.23 | 0.47 |
| 7:F:23:VAL:HG22 | 7:F:73:VAL:HB | 1.97 | 0.47 |
| 13:L:113:ILE:HG22 | 13:L:114:ALA:O | 2.14 | 0.47 |
| 16:O:161:GLY:O | 16:O:162:ASP:C | 2.53 | 0.47 |
| 1:A:1268:C:H2' | 1:A:1269:G:C8 | 2.50 | 0.47 |
| 14:M:90:ARG:NH2 | 14:M:121:ILE:HD11 | 2.30 | 0.47 |
| 8:G:23:GLU:HG2 | 8:G:28:SER:CB | 2.44 | 0.47 |
| 1:A:1434:A:H2' | 1:A:1436:C:C5 | 2.49 | 0.47 |
| 1:A:1805:G:H2' | 1:A:1806:G:H8 | 1.79 | 0.47 |
| 1:A:772:G:H2' | 1:A:773:A:O4' | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:C:9:ARG:HG2 | 4:C:16:PHE:CD2 | 2.49 | 0.47 |
| 1:A:1380:U:H5' | 38:A:8733:HOH:O | 2.14 | 0.47 |
| 22:U:71:VAL:HG12 | 22:U:72:ILE:N | 2.29 | 0.46 |
| 5:D:175:LEU:C | 5:D:175:LEU:CD2 | 2.82 | 0.46 |
| 12:K:74:ARG:NH1 | 12:K:76:ASP:HB2 | 2.29 | 0.46 |
| 1:A:1191:A:C3' | 1:A:1192:A:H5'' | 2.40 | 0.46 |
| 1:A:251:C:H4' | 15:N:140:ALA:HB2 | 1.98 | 0.46 |
| 9:H:47:LEU:HD22 | 9:H:108:LEU:CD1 | 2.45 | 0.46 |
| 15:N:59:GLY:HA3 | 15:N:141:ILE:HD12 | 1.96 | 0.46 |
| 1:A:2694:A:H5'' | 8:G:90:HIS:CE1 | 2.50 | 0.46 |
| 19:R:93:ARG:NH1 | 19:R:93:ARG:HG3 | 2.29 | 0.46 |
| 1:A:1427:A:H61 | 1:A:1440:U:H1' | 1.81 | 0.46 |
| 8:G:172:PRO:HB3 | 38:G:6931:HOH:O | 2.14 | 0.46 |
| 38:A:4570:HOH:O | 5:D:216:LYS:HA | 2.14 | 0.46 |
| 1:A:2101:A:H5'' | 6:E:63:SER:HB3 | 1.96 | 0.46 |
| 13:L:101:ASN:HB2 | 13:L:103:ASP:OD2 | 2.16 | 0.46 |
| 6:E:154:VAL:O | 6:E:158:GLU:HG3 | 2.14 | 0.46 |
| 12:K:131:THR:HG22 | 12:K:133:GLY:N | 2.30 | 0.46 |
| 7:F:23:VAL:CG2 | 7:F:23:VAL:O | 2.63 | 0.46 |
| 1:A:1181:A:O2' | 1:A:1182:C:H5' | 2.16 | 0.46 |
| 1:A:182:G:O3' | 15:N:157:LEU:CD1 | 2.62 | 0.46 |
| 1:A:338:C:H4' | 6:E:174:ILE:HD12 | 1.96 | 0.46 |
| 28:1:32:LYS:NZ | 28:1:70:GLN:NE2 | 2.63 | 0.46 |
| 1:A:558:C:H5' | 38:A:4750:HOH:O | 2.14 | 0.46 |
| 29:2:25:LYS:HG3 | 30:3:49:GLU:H | 1.79 | 0.46 |
| 15:N:47:ASP:CG | 15:N:48:ARG:N | 2.69 | 0.46 |
| 1:A:474:C:O3' | 6:E:73:LEU:CD2 | 2.63 | 0.46 |
| 27:Z:196:VAL:CG1 | 27:Z:226:ILE:HD13 | 2.45 | 0.46 |
| 5:D:198:GLU:HB3 | 38:D:8597:HOH:O | 2.14 | 0.46 |
| 13:L:98:VAL:HG13 | 13:L:102:GLU:HA | 1.98 | 0.46 |
| 18:Q:8:ARG:HG3 | 38:Q:193:HOH:O | 2.13 | 0.46 |
| 16:O:93:GLN:HG2 | 38:O:8557:HOH:O | 2.15 | 0.46 |
| 1:A:652:G:H8 | 38:A:9520:HOH:O | 1.97 | 0.46 |
| 1:A:2403:C:H3' | 38:A:4701:HOH:O | 2.13 | 0.46 |
| 11:J:75:SER:HB3 | 11:J:79:ALA:HB1 | 1.96 | 0.46 |
| 1:A:2507:G:H5' | 38:A:3257:HOH:O | 2.15 | 0.46 |
| 1:A:250:C:O2' | 1:A:251:C:H5' | 2.15 | 0.46 |
| 7:F:52:THR:HB | 7:F:70:GLY:O | 2.15 | 0.46 |
| 5:D:24:PRO:HG2 | 5:D:204:GLY:HA2 | 1.96 | 0.46 |
| 1:A:1154:A:H2' | 1:A:1155:G:H8 | 1.81 | 0.46 |
| 5:D:189:ALA:HB1 | 38:D:8568:HOH:O | 2.14 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:333:G:O2' | 1:A:334:G:H5' | 2.16 | 0.46 |
| 1:A:1523:G:H2' | 1:A:1524:U:C6 | 2.50 | 0.46 |
| 2:B:3042:C:H2' | 38:B:8500:HOH:O | 2.15 | 0.46 |
| 1:A:2866:U:H4' | 1:A:2867:G:H5' | 1.97 | 0.46 |
| 9:H:37:THR:O | 9:H:41:GLU:HG3 | 2.15 | 0.46 |
| 1:A:106:A:H2' | 1:A:107:U:O4' | 2.16 | 0.46 |
| 7:F:49:PRO:HA | 7:F:73:VAL:HG22 | 1.98 | 0.46 |
| 11:J:59:ASN:N | 11:J:59:ASN:ND2 | 2.54 | 0.46 |
| 1:A:1589:G:H4' | 38:A:6347:HOH:O | 2.14 | 0.46 |
| 12:K:19:MET:HE1 | 12:K:132:LEU:HD21 | 1.98 | 0.46 |
| 1:A:289:G:O2' | 1:A:290:C:H5' | 2.15 | 0.46 |
| 2:B:3069:U:OP1 | 16:O:4:PRO:HG3 | 2.15 | 0.46 |
| 27:Z:234:VAL:HG12 | 27:Z:235:GLU:N | 2.31 | 0.46 |
| 1:A:558:C:C2' | 1:A:559:U:C5' | 2.93 | 0.46 |
| 15:N:59:GLY:HA3 | 15:N:141:ILE:CD1 | 2.45 | 0.46 |
| 1:A:1299:G:N2 | 38:A:4181:HOH:O | 2.48 | 0.46 |
| 7:F:11:HIS:C | 7:F:13:MET:H | 2.18 | 0.46 |
| 1:A:1236:A:H2' | 1:A:1237:U:O4' | 2.15 | 0.46 |
| 4:C:39:ALA:HB3 | 4:C:61:GLU:OE2 | 2.15 | 0.46 |
| 6:E:180:SER:HB2 | 38:E:8449:HOH:O | 2.15 | 0.46 |
| 11:J:134:ALA:HB3 | 11:J:142:VAL:HG21 | 1.96 | 0.46 |
| 20:S:8:ALA:CB | 20:S:13:THR:HG21 | 2.41 | 0.46 |
| 9:H:56:PRO:HG2 | 15:N:43:PRO:O | 2.16 | 0.46 |
| 1:A:1819:G:H2' | 1:A:1820:G:C5' | 2.46 | 0.46 |
| 14:M:80:ASP:HB2 | 14:M:90:ARG:O | 2.14 | 0.46 |
| 1:A:1053:G:OP1 | 11:J:12:PRO:HG3 | 2.15 | 0.46 |
| 1:A:1699:C:H4' | 38:A:5932:HOH:O | 2.14 | 0.46 |
| 1:A:329:A:OP1 | 6:E:205:ARG:NE | 2.45 | 0.46 |
| 2:B:3012:C:H5' | 2:B:3070:U:O4' | 2.15 | 0.46 |
| 1:A:1746:A:O4' | 1:A:1747:A:C2 | 2.68 | 0.46 |
| 38:A:9665:HOH:O | 8:G:57:LYS:HE2 | 2.16 | 0.46 |
| 11:J:39:GLY:O | 11:J:41:THR:N | 2.49 | 0.46 |
| 25:X:4:LEU:CD2 | 25:X:54:PHE:HB3 | 2.43 | 0.46 |
| 1:A:1874:U:OP1 | 4:C:51:ARG:HD2 | 2.16 | 0.46 |
| 7:F:54:ALA:HB3 | 7:F:69:ILE:HD12 | 1.95 | 0.46 |
| 5:D:195:ARG:HD2 | 5:D:324:ASP:OD1 | 2.15 | 0.46 |
| 18:Q:103:THR:O | 18:Q:107:GLU:HG3 | 2.15 | 0.46 |
| 20:S:39:THR:HB | 20:S:42:GLU:CG | 2.45 | 0.46 |
| 8:G:31:ARG:HH12 | 8:G:68:HIS:CE1 | 2.32 | 0.46 |
| 27:Z:126:PRO:HG2 | 27:Z:128:PHE:CE1 | 2.50 | 0.46 |
| 1:A:407:A:H5' | 38:A:5517:HOH:O | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:O:114:LYS:O | 16:O:117:ALA:HB3 | 2.16 | 0.46 |
| 13:L:53:ILE:HG13 | 13:L:55:VAL:CG2 | 2.45 | 0.46 |
| 15:N:35:PRO:CD | 15:N:38:VAL:HG23 | 2.46 | 0.46 |
| 1:A:711:G:N2 | 1:A:718:C:C2 | 2.83 | 0.46 |
| 12:K:107:ASN:HD22 | 12:K:109:TYR:H | 1.63 | 0.46 |
| 1:A:484:A:N1 | 1:A:506:G:H4' | 2.31 | 0.46 |
| 11:J:83:PHE:CZ | 11:J:146:TRP:NE1 | 2.81 | 0.46 |
| 1:A:1819:G:H2' | 1:A:1820:G:C4' | 2.46 | 0.46 |
| 9:H:48:VAL:HG23 | 9:H:74:PHE:CB | 2.46 | 0.46 |
| 2:B:3020:G:H3' | 38:B:8432:HOH:O | 2.15 | 0.46 |
| 9:H:78:GLU:HG3 | 38:H:5966:HOH:O | 2.16 | 0.46 |
| 38:A:3355:HOH:O | 11:J:11:LYS:HE2 | 2.16 | 0.46 |
| 1:A:65:C:O2' | 1:A:66:G:H5' | 2.15 | 0.46 |
| 1:A:2549:C:H4' | 38:A:7012:HOH:O | 2.14 | 0.46 |
| 11:J:47:GLU:HG2 | 11:J:133:ILE:CD1 | 2.46 | 0.46 |
| 7:F:23:VAL:HG23 | 7:F:41:LEU:HD22 | 1.98 | 0.46 |
| 1:A:796:A:HO2' | 28:1:10:ARG:N | 2.13 | 0.46 |
| 13:L:14:LYS:CB | 13:L:45:PRO:HG2 | 2.37 | 0.46 |
| 11:J:143:GLU:N | 38:J:8381:HOH:O | 2.47 | 0.46 |
| 16:O:69:TYR:HE2 | 16:O:183:ASP:OD2 | 1.99 | 0.46 |
| 6:E:234:VAL:O | 6:E:234:VAL:HG22 | 2.16 | 0.46 |
| 12:K:107:ASN:HD22 | 12:K:108:PRO:N | 2.14 | 0.46 |
| 9:H:101:ALA:HB2 | 9:H:108:LEU:CD2 | 2.46 | 0.46 |
| 9:H:46:GLU:N | 38:H:3461:HOH:O | 2.49 | 0.46 |
| 1:A:2890:A:H1' | 23:V:56:ARG:HH21 | 1.77 | 0.46 |
| 1:A:816:G:H5' | 1:A:1598:A:H4' | 1.97 | 0.46 |
| 16:O:151:ASP:HB3 | 38:O:8528:HOH:O | 2.15 | 0.46 |
| 7:F:92:GLU:O | 7:F:93:LEU:O | 2.33 | 0.46 |
| 1:A:671:A:O2' | 1:A:672:G:H2' | 2.16 | 0.46 |
| 18:Q:36:THR:O | 18:Q:39:ASP:HB2 | 2.15 | 0.46 |
| 15:N:114:VAL:HG21 | 15:N:159:THR:HG21 | 1.97 | 0.46 |
| 15:N:99:ARG:HD2 | 15:N:167:GLY:HA2 | 1.97 | 0.46 |
| 13:L:109:LEU:CD1 | 13:L:113:ILE:HD11 | 2.46 | 0.46 |
| 6:E:27:ARG:HD2 | 17:P:5:PRO:HD2 | 1.97 | 0.46 |
| 1:A:681:G:H1' | 1:A:683:G:O6 | 2.16 | 0.46 |
| 27:Z:106:THR:HG22 | 27:Z:107:PRO:O | 2.16 | 0.46 |
| 2:B:3029:C:C2' | 2:B:3030:C:H5' | 2.46 | 0.46 |
| 1:A:585:C:H6 | 38:A:5588:HOH:O | 1.97 | 0.46 |
| 11:J:118:PRO:HD2 | 38:J:8339:HOH:O | 2.14 | 0.46 |
| 25:X:149:LEU:HG | 25:X:153:MET:HE2 | 1.97 | 0.46 |
| 14:M:73:VAL:HG23 | 14:M:74:THR:H | 1.81 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 31:4:11:CYS:HB2 | 31:4:20:HIS:NE2 | 2.30 | 0.46 |
| 1:A:705:C:O2 | 1:A:705:C:H2' | 2.16 | 0.46 |
| 1:A:621:C:H5' | 27:Z:132:ASP:OD2 | 2.16 | 0.46 |
| 1:A:2559:C:H4' | 38:A:6749:HOH:O | 2.14 | 0.46 |
| 8:G:93:MET:HE1 | 8:G:165:GLY:N | 2.30 | 0.46 |
| 1:A:2316:G:H4' | 38:A:5585:HOH:O | 2.15 | 0.46 |
| 20:S:132:ARG:CZ | 38:S:8583:HOH:O | 2.64 | 0.46 |
| 18:Q:103:THR:O | 18:Q:106:ARG:HB3 | 2.16 | 0.46 |
| 16:O:154:LEU:HG | 16:O:155:GLU:H | 1.80 | 0.46 |
| 1:A:1654:U:H2' | 4:C:47:HIS:CD2 | 2.48 | 0.46 |
| 25:X:149:LEU:HG | 25:X:153:MET:HE1 | 1.98 | 0.46 |
| 1:A:240:C:O2 | 1:A:240:C:H2' | 2.15 | 0.46 |
| 1:A:719:C:O2' | 17:P:112:ARG:NH2 | 2.48 | 0.46 |
| 1:A:2445:U:H2' | 1:A:2446:G:H8 | 1.80 | 0.46 |
| 1:A:2325:C:H2' | 1:A:2326:U:C6 | 2.51 | 0.46 |
| 1:A:790:A:H2' | 1:A:791:A:O4' | 2.16 | 0.46 |
| 1:A:1056:U:H2' | 1:A:1057:A:O4' | 2.16 | 0.46 |
| 17:P:107:GLU:O | 17:P:108:GLY:C | 2.54 | 0.46 |
| 27:Z:144:ARG:CZ | 38:Z:8608:HOH:O | 2.64 | 0.46 |
| 1:A:514:G:N2 | 38:A:3588:HOH:O | 2.48 | 0.46 |
| 6:E:102:LEU:HD12 | 38:E:8315:HOH:O | 2.16 | 0.46 |
| 25:X:126:ASP:HB3 | 25:X:135:GLY:O | 2.16 | 0.46 |
| 15:N:35:PRO:HD2 | 15:N:38:VAL:HG21 | 1.98 | 0.45 |
| 25:X:122:ARG:CZ | 38:X:5817:HOH:O | 2.62 | 0.45 |
| 11:J:46:VAL:CG1 | 11:J:146:TRP:HZ3 | 2.28 | 0.45 |
| 7:F:95:THR:C | 7:F:97:GLN:N | 2.69 | 0.45 |
| 5:D:104:GLU:HG3 | 38:D:8594:HOH:O | 2.15 | 0.45 |
| 1:A:371:U:H2' | 1:A:372:A:C8 | 2.50 | 0.45 |
| 6:E:57:PRO:HD2 | 6:E:73:LEU:HD22 | 1.98 | 0.45 |
| 1:A:2413:A:N7 | 16:O:109:PRO:HB3 | 2.31 | 0.45 |
| 1:A:2090:G:H2' | 1:A:2091:G:C8 | 2.51 | 0.45 |
| 1:A:1162:G:H2' | 38:A:6073:HOH:O | 2.15 | 0.45 |
| 1:A:297:U:H1' | 38:A:3447:HOH:O | 2.15 | 0.45 |
| 2:B:3039:U:H3' | 2:B:3040:C:H5'' | 1.98 | 0.45 |
| 15:N:65:VAL:CG2 | 15:N:105:ALA:HB2 | 2.46 | 0.45 |
| 17:P:77:ALA:HA | 17:P:96:VAL:O | 2.16 | 0.45 |
| 17:P:14:LEU:HG | 17:P:102:ILE:HD11 | 1.98 | 0.45 |
| 12:K:36:VAL:HG12 | 12:K:37:ALA:N | 2.31 | 0.45 |
| 18:Q:131:PHE:CE1 | 18:Q:137:LEU:HD13 | 2.51 | 0.45 |
| 5:D:141:ARG:HG2 | 5:D:165:ARG:HA | 1.99 | 0.45 |
| 2:B:3114:G:H2' | 2:B:3115:C:C6 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:1594:C:O2' | 1:A:1607:A:H4' | 2.16 | 0.45 |
| 1:A:737:A:H2' | 1:A:738:G:O4' | 2.16 | 0.45 |
| 14:M:90:ARG:HG3 | 14:M:119:THR:CG2 | 2.46 | 0.45 |
| 1:A:1890:U:H4' | 1:A:2010:A:C6 | 2.52 | 0.45 |
| 1:A:1804:A:H2' | 1:A:1805:G:C8 | 2.50 | 0.45 |
| 1:A:1883:U:O2' | 1:A:1884:G:H5' | 2.16 | 0.45 |
| 1:A:707:C:C2 | 1:A:708:A:C8 | 3.04 | 0.45 |
| 1:A:1167:G:O2' | 1:A:1168:C:H5' | 2.15 | 0.45 |
| 1:A:2473:U:O3' | 1:A:2474:A:H3' | 2.16 | 0.45 |
| 25:X:54:PHE:CZ | 25:X:140:LYS:HB2 | 2.50 | 0.45 |
| 1:A:2361:A:H5' | 1:A:2361:A:H8 | 1.82 | 0.45 |
| 1:A:92:G:H4' | 24:W:44:GLY:HA3 | 1.98 | 0.45 |
| 5:D:195:ARG:NH1 | 5:D:324:ASP:OD1 | 2.43 | 0.45 |
| 21:T:25:GLN:HG2 | 21:T:65:VAL:HG22 | 1.97 | 0.45 |
| 1:A:88:G:N3 | 30:3:24:TRP:HB2 | 2.31 | 0.45 |
| 1:A:1269:G:H2' | 1:A:1270:U:H6 | 1.81 | 0.45 |
| 15:N:181:GLU:N | 15:N:181:GLU:OE1 | 2.41 | 0.45 |
| 16:O:184:ILE:HG22 | 16:O:185:GLU:N | 2.31 | 0.45 |
| 1:A:1855:G:H8 | 4:C:144:GLU:OE2 | 2.00 | 0.45 |
| 1:A:1064:U:H2' | 1:A:1065:G:C8 | 2.52 | 0.45 |
| 1:A:820:G:C5 | 4:C:171:LYS:HB2 | 2.52 | 0.45 |
| 16:O:47:LEU:HD12 | 16:O:92:ALA:CB | 2.47 | 0.45 |
| 1:A:2507:G:H2' | 1:A:2510:C:H42 | 1.82 | 0.45 |
| 1:A:2783:A:H2' | 1:A:2784:A:C8 | 2.52 | 0.45 |
| 12:K:107:ASN:C | 12:K:107:ASN:ND2 | 2.69 | 0.45 |
| 11:J:46:VAL:HG12 | 11:J:146:TRP:CZ3 | 2.43 | 0.45 |
| 8:G:84:MET:HB2 | 8:G:131:LEU:HB2 | 1.98 | 0.45 |
| 1:A:947:U:H2' | 1:A:948:G:C8 | 2.51 | 0.45 |
| 22:U:16:LEU:HA | 22:U:19:ARG:HG3 | 1.98 | 0.45 |
| 1:A:2731:G:H2' | 1:A:2732:U:O4' | 2.17 | 0.45 |
| 1:A:2735:U:H2' | 1:A:2736:U:C6 | 2.51 | 0.45 |
| 1:A:2382:A:O2' | 1:A:2383:G:H5' | 2.15 | 0.45 |
| 13:L:30:LYS:O | 13:L:55:VAL:HG13 | 2.17 | 0.45 |
| 16:O:73:ALA:N | 38:O:8567:HOH:O | 2.49 | 0.45 |
| 7:F:64:ARG:O | 7:F:67:ASP:OD2 | 2.34 | 0.45 |
| 1:A:2839:C:H2' | 1:A:2840:A:H5'' | 1.98 | 0.45 |
| 20:S:39:THR:HB | 20:S:42:GLU:OE1 | 2.17 | 0.45 |
| 31:4:42:ARG:HH11 | 31:4:42:ARG:CG | 2.29 | 0.45 |
| 1:A:485:A:O2' | 1:A:487:G:H5' | 2.16 | 0.45 |
| 21:T:6:LYS:O | 21:T:7:HIS:HB3 | 2.16 | 0.45 |
| 25:X:108:ARG:HE | 25:X:114:PRO:CG | 2.28 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 15:N:122:GLU:OE2 | 15:N:127:LYS:HE2 | 2.16 | 0.45 |
| 1:A:2831:C:H2' | 1:A:2832:C:H5' | 1.98 | 0.45 |
| 1:A:1278:A:H4' | 1:A:1279:U:C4 | 2.52 | 0.45 |
| 5:D:138:GLY:O | 5:D:139:ASP:O | 2.34 | 0.45 |
| 1:A:1685:A:H4' | 1:A:1686:C:OP2 | 2.16 | 0.45 |
| 12:K:6:PHE:O | 12:K:8:ALA:N | 2.49 | 0.45 |
| 4:C:95:PRO:HA | 4:C:153:ARG:HA | 1.98 | 0.45 |
| 9:H:107:VAL:O | 9:H:111:ILE:HG13 | 2.16 | 0.45 |
| 20:S:17:MET:HE3 | 20:S:19:ARG:CZ | 2.46 | 0.45 |
| 1:A:2911:C:H2' | 1:A:2912:C:C6 | 2.52 | 0.45 |
| 1:A:1250:C:O2' | 1:A:1251:C:H5' | 2.16 | 0.45 |
| 15:N:159:THR:HA | 38:N:8519:HOH:O | 2.16 | 0.45 |
| 7:F:27:ILE:CG2 | 7:F:28:GLY:H | 2.20 | 0.45 |
| 11:J:136:VAL:HG23 | 38:J:8343:HOH:O | 2.17 | 0.45 |
| 1:A:283:U:H5 | 1:A:284:C:N4 | 2.14 | 0.45 |
| 1:A:290:C:O2' | 1:A:291:C:H5' | 2.16 | 0.45 |
| 25:X:13:MET:CE | 25:X:18:GLN:HA | 2.47 | 0.45 |
| 8:G:107:PHE:CZ | 8:G:108:LEU:HD13 | 2.51 | 0.45 |
| 5:D:316:ARG:N | 5:D:317:PRO:HD3 | 2.32 | 0.45 |
| 18:Q:10:ALA:HA | 18:Q:13:VAL:CG1 | 2.45 | 0.45 |
| 1:A:1634:G:H2' | 1:A:1635:U:C6 | 2.51 | 0.45 |
| 11:J:72:VAL:HG13 | 11:J:72:VAL:O | 2.16 | 0.45 |
| 1:A:645:U:H2' | 1:A:646:G:C8 | 2.52 | 0.45 |
| 1:A:2467:A:H2' | 38:A:4948:HOH:O | 2.16 | 0.45 |
| 11:J:26:LYS:HD2 | 11:J:28:ILE:CG1 | 2.47 | 0.45 |
| 12:K:77:GLY:O | 12:K:78:ILE:C | 2.55 | 0.45 |
| 1:A:1450:C:C4' | 1:A:1451:C:OP2 | 2.59 | 0.45 |
| 27:Z:154:ARG:O | 27:Z:154:ARG:HG2 | 2.16 | 0.45 |
| 5:D:275:GLY:C | 38:D:8652:HOH:O | 2.55 | 0.45 |
| 29:2:8:GLN:HE22 | 29:2:11:LYS:HZ2 | 1.64 | 0.45 |
| 1:A:1973:A:C2' | 1:A:1974:G:O5' | 2.65 | 0.45 |
| 1:A:241:A:N1 | 1:A:378:A:H4' | 2.32 | 0.45 |
| 17:P:25:VAL:HG23 | 17:P:26:TRP:N | 2.31 | 0.45 |
| 1:A:64:G:H2' | 1:A:65:C:O4' | 2.17 | 0.45 |
| 5:D:147:VAL:O | 5:D:147:VAL:HG12 | 2.17 | 0.45 |
| 29:2:26:SER:HB3 | 29:2:35:SER:OG | 2.17 | 0.45 |
| 38:A:9859:HOH:O | 19:R:16:ASN:HB2 | 2.16 | 0.45 |
| 38:A:3805:HOH:O | 27:Z:208:LYS:HD2 | 2.16 | 0.45 |
| 1:A:2900:G:H2' | 1:A:2901:C:O4' | 2.17 | 0.45 |
| 28:1:73:THR:O | 28:1:76:GLY:N | 2.50 | 0.45 |
| 21:T:11:THR:H | 21:T:14:ALA:HB3 | 1.80 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:C:96:LEU:HD22 | 4:C:128:LEU:HD13 | 1.99 | 0.45 |
| 19:R:75:ILE:CD1 | 19:R:84:ILE:HD11 | 2.47 | 0.45 |
| 6:E:139:VAL:CG1 | 38:E:8451:HOH:O | 2.62 | 0.45 |
| 1:A:290:C:H2' | 1:A:291:C:O4' | 2.17 | 0.45 |
| 28:1:33:HIS:HE1 | 28:1:49:ARG:NE | 2.15 | 0.45 |
| 4:C:170:VAL:HG13 | 28:1:22:ILE:HG21 | 1.99 | 0.45 |
| 22:U:38:ARG:HG3 | 22:U:38:ARG:HH11 | 1.81 | 0.45 |
| 5:D:280:VAL:HG13 | 5:D:334:SER:HA | 1.98 | 0.45 |
| 1:A:2754:G:H2' | 1:A:2755:G:O4' | 2.17 | 0.45 |
| 19:R:25:PRO:HA | 19:R:26:PRO:HD3 | 1.79 | 0.45 |
| 2:B:3041:C:H4' | 7:F:48:MET:HB2 | 1.99 | 0.45 |
| 1:A:2326:U:H4' | 1:A:2412:G:C4' | 2.47 | 0.45 |
| 27:Z:145:LYS:NZ | 38:Z:8565:HOH:O | 2.46 | 0.45 |
| 1:A:2455:A:H2' | 1:A:2456:A:O4' | 2.17 | 0.45 |
| 1:A:1444:G:O2' | 1:A:1445:G:H5' | 2.16 | 0.45 |
| 8:G:32:ARG:O | 8:G:33:LEU:HD23 | 2.17 | 0.45 |
| 1:A:2594:C:O2' | 1:A:2595:U:H5' | 2.16 | 0.45 |
| 15:N:164:THR:CG2 | 15:N:167:GLY:H | 2.18 | 0.45 |
| 16:O:162:ASP:HB3 | 16:O:163:PHE:H | 1.58 | 0.45 |
| 1:A:2909:G:O2' | 1:A:2910:A:H5' | 2.17 | 0.45 |
| 18:Q:13:VAL:HG11 | 18:Q:40:VAL:HG11 | 1.98 | 0.45 |
| 1:A:447:A:O2' | 1:A:448:G:H5' | 2.17 | 0.45 |
| 18:Q:16:VAL:HG12 | 18:Q:20:ARG:HB2 | 1.98 | 0.45 |
| 1:A:920:C:H5' | 1:A:921:G:C4 | 2.52 | 0.45 |
| 1:A:1805:G:O2' | 1:A:1806:G:H5' | 2.17 | 0.45 |
| 1:A:314:G:N2 | 1:A:316:A:H3' | 2.31 | 0.45 |
| 1:A:318:C:H5' | 1:A:339:A:C2 | 2.51 | 0.45 |
| 1:A:1681:G:H5'' | 1:A:1682:A:H5' | 1.98 | 0.45 |
| 1:A:162:C:H2' | 1:A:163:U:H5' | 1.99 | 0.45 |
| 1:A:716:G:C2' | 1:A:717:C:O5' | 2.65 | 0.45 |
| 1:A:177:A:H2' | 1:A:178:U:O4' | 2.17 | 0.45 |
| 1:A:462:A:C2 | 30:3:37:HIS:HB3 | 2.52 | 0.45 |
| 12:K:92:GLN:HB3 | 38:K:1405:HOH:O | 2.16 | 0.45 |
| 11:J:47:GLU:CB | 11:J:133:ILE:CD1 | 2.90 | 0.44 |
| 1:A:2716:G:O2' | 1:A:2717:C:H5' | 2.17 | 0.44 |
| 24:W:1:THR:O | 24:W:3:LEU:N | 2.49 | 0.44 |
| 1:A:1189:A:H3' | 38:A:7170:HOH:O | 2.16 | 0.44 |
| 1:A:553:G:O4' | 1:A:1325:G:H5' | 2.17 | 0.44 |
| 5:D:304:PRO:HD2 | 5:D:307:ARG:NH1 | 2.32 | 0.44 |
| 1:A:584:U:H3' | 38:A:5588:HOH:O | 2.16 | 0.44 |
| 36:5:77:PHA:N | 36:6:77:PHA:CA | 2.80 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:538:C:H5' | 1:A:539:G:C8 | 2.52 | 0.44 |
| 17:P:26:TRP:HB2 | 38:P:3062:HOH:O | 2.16 | 0.44 |
| 1:A:1803:C:H2' | 1:A:1804:A:C8 | 2.52 | 0.44 |
| 1:A:2831:C:H2' | 1:A:2832:C:C5' | 2.47 | 0.44 |
| 27:Z:103:THR:HG22 | 27:Z:104:GLU:OE2 | 2.17 | 0.44 |
| 1:A:218:C:C5 | 1:A:220:C:C4 | 3.05 | 0.44 |
| 11:J:84:ARG:CZ | 11:J:135:TRP:CH2 | 3.00 | 0.44 |
| 11:J:29:ALA:C | 11:J:30:GLN:HG3 | 2.37 | 0.44 |
| 5:D:42:ALA:HB1 | 5:D:308:LEU:HD11 | 1.97 | 0.44 |
| 16:O:67:ALA:HA | 16:O:71:TRP:HB3 | 1.99 | 0.44 |
| 8:G:11:VAL:HG11 | 8:G:22:VAL:HG13 | 1.99 | 0.44 |
| 1:A:2329:C:O2' | 1:A:2330:U:H5' | 2.18 | 0.44 |
| 5:D:75:GLU:C | 5:D:77:PRO:HD3 | 2.38 | 0.44 |
| 1:A:2761:A:C4 | 1:A:2763:G:C8 | 3.06 | 0.44 |
| 6:E:126:ASP:C | 6:E:128:GLY:N | 2.70 | 0.44 |
| 1:A:745:G:O6 | 17:P:68:GLY:HA3 | 2.17 | 0.44 |
| 15:N:182:LYS:HB2 | 15:N:194:ALA:HB2 | 2.00 | 0.44 |
| 1:A:1119:G:N2 | 1:A:1246:A:H2 | 2.14 | 0.44 |
| 12:K:52:GLN:O | 12:K:53:ILE:C | 2.56 | 0.44 |
| 7:F:25:MET:SD | 7:F:40:ILE:HD11 | 2.57 | 0.44 |
| 1:A:1943:C:O4' | 4:C:212:PRO:HA | 2.16 | 0.44 |
| 9:H:58:GLU:OE1 | 15:N:27:ARG:NH2 | 2.38 | 0.44 |
| 9:H:100:ASP:HB3 | 38:H:5691:HOH:O | 2.17 | 0.44 |
| 8:G:108:LEU:HD11 | 8:G:164:ASP:HB2 | 1.99 | 0.44 |
| 1:A:553:G:P | 27:Z:204:ARG:NH2 | 2.89 | 0.44 |
| 5:D:304:PRO:CG | 5:D:307:ARG:NH1 | 2.80 | 0.44 |
| 11:J:112:ARG:O | 11:J:113:ALA:C | 2.55 | 0.44 |
| 38:A:8976:HOH:O | 20:S:83:LYS:HD3 | 2.18 | 0.44 |
| 1:A:710:G:N2 | 1:A:719:C:C2 | 2.85 | 0.44 |
| 20:S:125:ARG:HG2 | 38:S:8542:HOH:O | 2.16 | 0.44 |
| 5:D:268:ARG:NE | 38:D:8609:HOH:O | 2.50 | 0.44 |
| 18:Q:101:GLN:HG3 | 38:Q:163:HOH:O | 2.18 | 0.44 |
| 8:G:85:GLU:HG3 | 8:G:169:THR:OG1 | 2.17 | 0.44 |
| 12:K:46:ILE:HD11 | 12:K:53:ILE:HG23 | 1.98 | 0.44 |
| 1:A:2590:U:O2 | 3:5:74:C:C2 | 2.71 | 0.44 |
| 1:A:2502:C:H2' | 1:A:2503:A:C5' | 2.45 | 0.44 |
| 13:L:34:VAL:CG2 | 13:L:47:ALA:HB2 | 2.48 | 0.44 |
| 4:C:36:ASP:HB2 | 4:C:85:ASP:H | 1.82 | 0.44 |
| 7:F:55:LYS:O | 7:F:56:ARG:HB2 | 2.18 | 0.44 |
| 1:A:396:U:O2' | 1:A:418:C:H4' | 2.17 | 0.44 |
| 26:Y:30:MET:CE | 26:Y:55:ASN:HA | 2.45 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:E:77:ALA:O | 6:E:78:ARG:HG3 | 2.17 | 0.44 |
| 14:M:57:VAL:HG12 | 14:M:57:VAL:O | 2.17 | 0.44 |
| 1:A:441:A:H1' | 1:A:442:A:N7 | 2.33 | 0.44 |
| 1:A:517:U:C2' | 1:A:518:G:H5' | 2.47 | 0.44 |
| 23:V:49:LEU:HD11 | 38:V:3805:HOH:O | 2.18 | 0.44 |
| 9:H:26:THR:HG21 | 9:H:103:ALA:CB | 2.47 | 0.44 |
| 13:L:98:VAL:HG13 | 13:L:99:ASP:N | 2.31 | 0.44 |
| 21:T:8:PRO:HD2 | 24:W:32:ALA:HA | 1.98 | 0.44 |
| 13:L:72:VAL:O | 13:L:95:ALA:HA | 2.17 | 0.44 |
| 1:A:2815:G:H4' | 1:A:2816:A:OP2 | 2.18 | 0.44 |
| 1:A:1439:C:H5'' | 30:3:41:HIS:HE1 | 1.82 | 0.44 |
| 1:A:2909:G:H2' | 1:A:2910:A:H8 | 1.83 | 0.44 |
| 1:A:1209:C:H2' | 1:A:1210:G:C8 | 2.52 | 0.44 |
| 9:H:99:THR:O | 9:H:100:ASP:HB2 | 2.17 | 0.44 |
| 4:C:105:VAL:HG13 | 4:C:155:THR:O | 2.18 | 0.44 |
| 6:E:76:ARG:HD2 | 38:E:8438:HOH:O | 2.17 | 0.44 |
| 16:O:154:LEU:HG | 16:O:155:GLU:N | 2.32 | 0.44 |
| 1:A:2266:A:H2' | 1:A:2267:G:C8 | 2.53 | 0.44 |
| 1:A:1762:C:H2' | 1:A:1763:C:C6 | 2.53 | 0.44 |
| 1:A:911:G:H5' | 1:A:932:U:OP1 | 2.17 | 0.44 |
| 27:Z:102:LEU:O | 27:Z:227:ARG:HG3 | 2.17 | 0.44 |
| 16:O:42:HIS:CG | 16:O:62:HIS:HE1 | 2.35 | 0.44 |
| 1:A:1365:C:H4' | 38:A:4109:HOH:O | 2.17 | 0.44 |
| 1:A:2776:A:H2' | 1:A:2777:G:O4' | 2.17 | 0.44 |
| 11:J:84:ARG:CZ | 11:J:135:TRP:HH2 | 2.30 | 0.44 |
| 7:F:35:ALA:HB2 | 38:F:5858:HOH:O | 2.18 | 0.44 |
| 2:B:3056:A:H1' | 7:F:14:ARG:HG2 | 1.99 | 0.44 |
| 9:H:60:VAL:HG13 | 9:H:63:ILE:HG13 | 2.00 | 0.44 |
| 7:F:18:ILE:HD13 | 7:F:84:LEU:CD1 | 2.48 | 0.44 |
| 1:A:1641:A:H2' | 1:A:1642:A:C5' | 2.43 | 0.44 |
| 7:F:170:TYR:N | 7:F:170:TYR:CD1 | 2.86 | 0.44 |
| 5:D:49:THR:CG2 | 5:D:280:VAL:CG2 | 2.96 | 0.44 |
| 1:A:68:U:O2' | 1:A:69:A:H5'' | 2.18 | 0.44 |
| 1:A:2729:C:O2' | 1:A:2730:G:H5' | 2.18 | 0.44 |
| 1:A:1496:G:H5' | 1:A:1572:A:H1' | 2.00 | 0.44 |
| 24:W:55:ARG:O | 24:W:59:ILE:HG12 | 2.18 | 0.44 |
| 1:A:2107:U:O2' | 1:A:2108:A:H5' | 2.18 | 0.44 |
| 8:G:9:GLU:HA | 38:G:5240:HOH:O | 2.17 | 0.44 |
| 7:F:23:VAL:HG12 | 7:F:130:VAL:HG22 | 1.99 | 0.44 |
| 11:J:35:ASN:ND2 | 11:J:79:ALA:O | 2.51 | 0.44 |
| 15:N:37:VAL:CG2 | 15:N:108:LYS:HG3 | 2.46 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 6:E:162:VAL:O | 6:E:162:VAL:HG12 | 2.18 | 0.44 |
| 1:A:677:C:P | 38:E:8461:HOH:O | 2.76 | 0.44 |
| 1:A:155:C:OP2 | 15:N:188:ARG:HD3 | 2.18 | 0.44 |
| 20:S:61:GLN:CD | 38:S:8540:HOH:O | 2.55 | 0.44 |
| 1:A:119:A:H2' | 1:A:120:A:H5'' | 1.98 | 0.44 |
| 1:A:639:A:H2' | 1:A:640:G:C8 | 2.52 | 0.44 |
| 1:A:1007:A:H2' | 11:J:19:TYR:CZ | 2.53 | 0.44 |
| 1:A:1453:G:N2 | 1:A:1675:C:C2 | 2.85 | 0.44 |
| 1:A:611:U:O5' | 1:A:611:U:H6 | 2.01 | 0.44 |
| 27:Z:205:ILE:O | 27:Z:206:ALA:C | 2.55 | 0.44 |
| 1:A:2000:G:O2' | 1:A:2001:G:H5' | 2.18 | 0.44 |
| 15:N:25:TRP:HE3 | 15:N:26:HIS:HD2 | 1.64 | 0.44 |
| 16:O:22:GLN:HG2 | 16:O:26:LEU:HD22 | 2.00 | 0.44 |
| 1:A:189:A:OP1 | 15:N:171:ARG:NH2 | 2.51 | 0.44 |
| 1:A:960:G:N3 | 1:A:960:G:C2' | 2.80 | 0.44 |
| 15:N:115:LEU:HD13 | 15:N:116:ASN:HB2 | 2.00 | 0.44 |
| 16:O:7:LYS:HE2 | 38:O:8514:HOH:O | 2.17 | 0.44 |
| 15:N:84:LYS:O | 15:N:87:MET:HG2 | 2.17 | 0.44 |
| 4:C:192:VAL:CG1 | 4:C:192:VAL:O | 2.65 | 0.44 |
| 9:H:32:GLY:N | 38:H:3111:HOH:O | 2.50 | 0.44 |
| 1:A:1603:A:H5'' | 1:A:1605:G:H5' | 1.99 | 0.44 |
| 7:F:57:THR:HG23 | 7:F:63:ILE:CB | 2.48 | 0.44 |
| 23:V:36:CYS:O | 23:V:37:GLU:C | 2.57 | 0.44 |
| 1:A:1635:U:O2' | 1:A:1636:G:H5' | 2.17 | 0.44 |
| 29:2:10:LYS:N | 38:2:8434:HOH:O | 2.31 | 0.44 |
| 1:A:240:C:C5' | 15:N:146:GLN:NE2 | 2.81 | 0.44 |
| 21:T:6:LYS:HB2 | 21:T:27:ALA:O | 2.17 | 0.44 |
| 1:A:2348:C:C5' | 7:F:22:VAL:HG21 | 2.48 | 0.44 |
| 1:A:1236:A:C2' | 1:A:1237:U:H5' | 2.48 | 0.44 |
| 28:1:54:ILE:HD12 | 38:1:8416:HOH:O | 2.18 | 0.44 |
| 6:E:154:VAL:HG13 | 6:E:163:HIS:CE1 | 2.52 | 0.44 |
| 1:A:514:G:O5' | 1:A:514:G:H8 | 2.00 | 0.44 |
| 4:C:128:LEU:HG | 38:C:8569:HOH:O | 2.18 | 0.44 |
| 5:D:84:LEU:HD23 | 5:D:178:ALA:HB1 | 1.99 | 0.44 |
| 25:X:35:VAL:HA | 25:X:36:PRO:HD3 | 1.76 | 0.44 |
| 38:A:8593:HOH:O | 5:D:214:PRO:HD2 | 2.17 | 0.44 |
| 15:N:18:GLY:O | 15:N:21:ALA:HB3 | 2.17 | 0.44 |
| 25:X:3:ALA:O | 25:X:54:PHE:HA | 2.18 | 0.44 |
| 7:F:139:TYR:N | 38:F:3723:HOH:O | 2.47 | 0.44 |
| 11:J:85:ILE:O | 11:J:85:ILE:HG23 | 2.18 | 0.44 |
| 5:D:278:PRO:HD3 | 5:D:294:TYR:CZ | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 31:4:69:TYR:CB | 31:4:78:HIS:CE1 | 3.01 | 0.44 |
| 5:D:248:ARG:NH2 | 38:D:8527:HOH:O | 2.51 | 0.44 |
| 1:A:2385:G:H2' | 1:A:2386:U:H6 | 1.83 | 0.44 |
| 26:Y:20:GLU:CD | 26:Y:21:PRO:HD2 | 2.38 | 0.44 |
| 28:1:48:LYS:NZ | 38:1:8435:HOH:O | 2.51 | 0.44 |
| 1:A:2626:C:H2' | 1:A:2627:G:C8 | 2.53 | 0.44 |
| 6:E:49:ASP:HB3 | 6:E:52:ALA:HB2 | 2.00 | 0.44 |
| 1:A:1811:A:C2 | 1:A:2752:C:H1' | 2.52 | 0.44 |
| 2:B:3031:C:H2' | 2:B:3032:G:O4' | 2.18 | 0.44 |
| 11:J:165:GLY:C | 11:J:166:ASN:HD22 | 2.21 | 0.43 |
| 30:3:18:ASN:ND2 | 30:3:40:ARG:H | 2.15 | 0.43 |
| 1:A:2812:A:N7 | 38:A:7009:HOH:O | 2.36 | 0.43 |
| 1:A:2506:A:C1' | 38:A:5548:HOH:O | 2.66 | 0.43 |
| 16:O:67:ALA:C | 16:O:69:TYR:N | 2.71 | 0.43 |
| 10:I:63:ARG:HB2 | 10:I:66:LEU:HG | 1.99 | 0.43 |
| 1:A:841:A:OP2 | 20:S:128:ARG:HD2 | 2.18 | 0.43 |
| 14:M:61:ALA:HA | 38:M:8565:HOH:O | 2.17 | 0.43 |
| 1:A:2684:A:H2' | 1:A:2685:C:H6 | 1.80 | 0.43 |
| 13:L:28:GLU:OE2 | 13:L:58:THR:HG21 | 2.17 | 0.43 |
| 1:A:2050:G:H5'' | 20:S:80:TYR:O | 2.18 | 0.43 |
| 1:A:90:A:H2' | 1:A:91:G:O4' | 2.17 | 0.43 |
| 6:E:127:ARG:NH1 | 6:E:127:ARG:HG2 | 2.34 | 0.43 |
| 11:J:151:MET:HA | 11:J:151:MET:HE3 | 2.00 | 0.43 |
| 13:L:75:ARG:HE | 13:L:94:ALA:HB3 | 1.83 | 0.43 |
| 16:O:67:ALA:C | 16:O:69:TYR:H | 2.21 | 0.43 |
| 1:A:1595:G:O2' | 1:A:1596:U:H5' | 2.18 | 0.43 |
| 5:D:74:ILE:HG13 | 38:D:8607:HOH:O | 2.18 | 0.43 |
| 2:B:3093:A:H8 | 2:B:3093:A:O5' | 2.02 | 0.43 |
| 7:F:173:GLU:O | 7:F:174:VAL:C | 2.55 | 0.43 |
| 24:W:16:ARG:NH1 | 24:W:65:ASP:O | 2.50 | 0.43 |
| 13:L:78:LYS:HA | 13:L:79:PRO:HD3 | 1.87 | 0.43 |
| 1:A:1422:U:H2' | 1:A:1423:C:C6 | 2.52 | 0.43 |
| 5:D:132:HIS:CE1 | 5:D:171:VAL:HG21 | 2.53 | 0.43 |
| 15:N:18:GLY:HA3 | 38:N:8588:HOH:O | 2.17 | 0.43 |
| 14:M:93:VAL:HG12 | 14:M:97:VAL:HG23 | 2.01 | 0.43 |
| 1:A:74:A:H2' | 1:A:75:U:C6 | 2.52 | 0.43 |
| 20:S:31:ILE:O | 20:S:32:ALA:C | 2.54 | 0.43 |
| 6:E:168:ARG:NH2 | 6:E:190:ALA:O | 2.51 | 0.43 |
| 7:F:25:MET:HE1 | 7:F:37:ALA:O | 2.19 | 0.43 |
| 7:F:38:GLU:HB3 | 7:F:49:PRO:HG2 | 2.00 | 0.43 |
| 7:F:27:ILE:CG2 | 7:F:28:GLY:N | 2.79 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:H:100:ASP:O | 9:H:101:ALA:O | 2.37 | 0.43 |
| 28:1:32:LYS:HB3 | 28:1:32:LYS:HE2 | 1.83 | 0.43 |
| 11:J:57:ARG:HG3 | 11:J:57:ARG:NH1 | 2.33 | 0.43 |
| 25:X:38:THR:HG21 | 38:X:5390:HOH:O | 2.18 | 0.43 |
| 38:A:3614:HOH:O | 5:D:158:LYS:HB2 | 2.18 | 0.43 |
| 7:F:10:PHE:CD1 | 7:F:11:HIS:N | 2.86 | 0.43 |
| 25:X:11:VAL:O | 25:X:12:ASN:HB2 | 2.18 | 0.43 |
| 14:M:121:ILE:HG12 | 14:M:141:GLU:HB2 | 1.99 | 0.43 |
| 14:M:122:ALA:HB3 | 14:M:125:PHE:CZ | 2.54 | 0.43 |
| 13:L:118:ALA:HA | 13:L:125:ALA:HB2 | 1.98 | 0.43 |
| 13:L:118:ALA:O | 13:L:120:ARG:N | 2.51 | 0.43 |
| 1:A:407:A:H8 | 38:A:3961:HOH:O | 2.01 | 0.43 |
| 1:A:1168:C:H5 | 38:A:6989:HOH:O | 2.01 | 0.43 |
| 38:A:5852:HOH:O | 4:C:205:GLY:HA3 | 2.18 | 0.43 |
| 1:A:2740:G:H2' | 1:A:2741:A:O4' | 2.18 | 0.43 |
| 1:A:2067:A:H2' | 1:A:2068:G:O4' | 2.18 | 0.43 |
| 1:A:1653:A:N6 | 38:A:3770:HOH:O | 2.51 | 0.43 |
| 21:T:49:VAL:HG13 | 21:T:66:VAL:HG13 | 2.00 | 0.43 |
| 1:A:2045:G:H2' | 1:A:2046:G:O4' | 2.19 | 0.43 |
| 1:A:844:A:C6 | 1:A:882:A:C5 | 3.06 | 0.43 |
| 11:J:45:GLN:NE2 | 11:J:135:TRP:HE1 | 2.11 | 0.43 |
| 5:D:240:GLY:HA3 | 38:D:8530:HOH:O | 2.19 | 0.43 |
| 18:Q:115:SER:C | 18:Q:117:SER:N | 2.70 | 0.43 |
| 1:A:2428:G:N7 | 31:4:60:LYS:NZ | 2.64 | 0.43 |
| 38:A:3171:HOH:O | 15:N:79:LYS:CD | 2.59 | 0.43 |
| 4:C:105:VAL:CG1 | 4:C:106:CYS:N | 2.81 | 0.43 |
| 11:J:31:PHE:HD2 | 11:J:85:ILE:O | 2.01 | 0.43 |
| 1:A:2769:C:H2' | 1:A:2770:G:C5' | 2.48 | 0.43 |
| 20:S:39:THR:HG22 | 20:S:42:GLU:HG3 | 2.00 | 0.43 |
| 6:E:21:VAL:C | 6:E:23:GLU:N | 2.71 | 0.43 |
| 17:P:14:LEU:CG | 17:P:102:ILE:HD11 | 2.48 | 0.43 |
| 36:5:77:PHA:H2 | 36:6:77:PHA:CA | 2.31 | 0.43 |
| 15:N:61:ILE:N | 15:N:61:ILE:HD12 | 2.33 | 0.43 |
| 6:E:200:PRO:HB3 | 6:E:212:VAL:CG2 | 2.48 | 0.43 |
| 1:A:175:G:C2' | 15:N:192:ALA:HB3 | 2.47 | 0.43 |
| 22:U:73:HIS:CD2 | 22:U:88:PRO:CG | 3.01 | 0.43 |
| 5:D:258:GLY:H | 5:D:260:HIS:CE1 | 2.36 | 0.43 |
| 11:J:29:ALA:N | 11:J:62:GLU:OE1 | 2.40 | 0.43 |
| 4:C:48:ASP:HB3 | 38:C:8602:HOH:O | 2.18 | 0.43 |
| 1:A:875:A:C2 | 4:C:194:MET:SD | 3.12 | 0.43 |
| 6:E:107:ARG:NH2 | 38:E:8461:HOH:O | 2.48 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:138:U:OP2 | 1:A:139:C:H5 | 2.01 | 0.43 |
| 1:A:1973:A:H5' | 1:A:1973:A:H8 | 1.84 | 0.43 |
| 9:H:48:VAL:HG12 | 9:H:97:ALA:HB2 | 2.00 | 0.43 |
| 5:D:129:ARG:O | 5:D:133:GLU:HG3 | 2.18 | 0.43 |
| 1:A:790:A:H1' | 1:A:1710:A:H2' | 2.00 | 0.43 |
| 11:J:129:ASN:HD22 | 11:J:129:ASN:N | 2.17 | 0.43 |
| 1:A:2353:A:H4' | 1:A:2354:A:O5' | 2.17 | 0.43 |
| 6:E:65:ARG:HG3 | 6:E:67:GLN:HB2 | 2.01 | 0.43 |
| 19:R:3:SER:HB3 | 38:R:5998:HOH:O | 2.17 | 0.43 |
| 1:A:1289:C:O2' | 1:A:1290:G:H5' | 2.18 | 0.43 |
| 2:B:3024:U:C3' | 2:B:3025:G:H5' | 2.48 | 0.43 |
| 7:F:23:VAL:HG21 | 7:F:45:THR:HG21 | 2.00 | 0.43 |
| 28:1:58:GLY:CA | 38:1:8438:HOH:O | 2.47 | 0.43 |
| 7:F:99:ASP:CB | 7:F:103:ASN:HB2 | 2.48 | 0.43 |
| 28:1:30:GLU:O | 28:1:33:HIS:HB3 | 2.18 | 0.43 |
| 22:U:40:VAL:HG22 | 22:U:41:ARG:N | 2.33 | 0.43 |
| 25:X:64:THR:O | 25:X:68:THR:HG22 | 2.18 | 0.43 |
| 1:A:1500:U:OP2 | 18:Q:41:ARG:NH2 | 2.51 | 0.43 |
| 6:E:40:ALA:O | 6:E:43:LYS:HB2 | 2.19 | 0.43 |
| 11:J:93:ILE:O | 11:J:119:VAL:HG22 | 2.17 | 0.43 |
| 1:A:79:G:H22 | 1:A:97:G:H1' | 1.84 | 0.43 |
| 1:A:738:G:H3' | 38:A:6538:HOH:O | 2.19 | 0.43 |
| 2:B:3060:C:O2' | 2:B:3061:C:H5' | 2.19 | 0.43 |
| 1:A:407:A:H2' | 1:A:408:A:C8 | 2.54 | 0.43 |
| 1:A:716:G:H2' | 1:A:717:C:O5' | 2.19 | 0.43 |
| 1:A:1506:U:H5' | 1:A:1506:U:H6 | 1.83 | 0.43 |
| 1:A:1044:C:H5'' | 38:A:8544:HOH:O | 2.18 | 0.43 |
| 1:A:1235:G:C1' | 12:K:63:ILE:HG23 | 2.48 | 0.43 |
| 1:A:1513:C:O2' | 1:A:1514:C:H5' | 2.18 | 0.43 |
| 1:A:2104:C:O2 | 1:A:2486:A:C2 | 2.72 | 0.43 |
| 26:Y:34:ARG:NH1 | 26:Y:48:VAL:O | 2.49 | 0.43 |
| 1:A:192:A:C4' | 15:N:176:GLN:HE22 | 2.32 | 0.43 |
| 1:A:2766:A:O2' | 1:A:2767:C:H5' | 2.18 | 0.43 |
| 1:A:644:G:H1' | 38:A:5897:HOH:O | 2.17 | 0.43 |
| 38:A:3263:HOH:O | 15:N:108:LYS:HD2 | 2.18 | 0.43 |
| 24:W:1:THR:C | 24:W:3:LEU:N | 2.71 | 0.43 |
| 1:A:450:C:H4' | 6:E:46:TYR:CE1 | 2.53 | 0.43 |
| 12:K:6:PHE:HB3 | 12:K:109:TYR:OH | 2.18 | 0.43 |
| 1:A:2032:U:P | 38:A:4015:HOH:O | 2.76 | 0.43 |
| 28:1:32:LYS:HZ2 | 28:1:70:GLN:NE2 | 2.17 | 0.43 |
| 21:T:23:LYS:HD3 | 21:T:65:VAL:HG12 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:E:76:ARG:HG2 | 6:E:78:ARG:NH1 | 2.34 | 0.43 |
| 29:2:25:LYS:HD2 | 30:3:48:ASP:CA | 2.49 | 0.43 |
| 1:A:1654:U:C6 | 4:C:47:HIS:CD2 | 3.07 | 0.43 |
| 6:E:133:ARG:NE | 6:E:135:GLU:O | 2.52 | 0.43 |
| 1:A:2451:G:O2' | 31:4:38:ARG:NH2 | 2.52 | 0.43 |
| 1:A:941:G:C5 | 1:A:942:U:C4 | 3.07 | 0.43 |
| 8:G:145:ALA:HB1 | 8:G:168:ILE:HD11 | 1.99 | 0.43 |
| 1:A:1051:C:H2' | 1:A:1052:G:O4' | 2.18 | 0.43 |
| 1:A:860:U:H2' | 1:A:861:A:C8 | 2.53 | 0.43 |
| 27:Z:177:LYS:HD3 | 27:Z:181:GLY:O | 2.19 | 0.43 |
| 1:A:1597:A:O4' | 18:Q:95:GLU:HG2 | 2.19 | 0.43 |
| 6:E:139:VAL:CG2 | 6:E:240:LEU:HD12 | 2.49 | 0.43 |
| 12:K:131:THR:HB | 12:K:134:GLU:OE1 | 2.18 | 0.43 |
| 1:A:1878:G:C4' | 38:A:5614:HOH:O | 2.66 | 0.43 |
| 1:A:290:C:H1' | 38:A:5597:HOH:O | 2.18 | 0.43 |
| 22:U:40:VAL:HA | 22:U:119:ALA:O | 2.19 | 0.43 |
| 21:T:17:ASP:HB3 | 21:T:23:LYS:HB2 | 2.00 | 0.43 |
| 2:B:3029:C:H5'' | 7:F:140:ARG:HB3 | 2.00 | 0.43 |
| 5:D:88:GLU:O | 5:D:88:GLU:HG3 | 2.18 | 0.43 |
| 22:U:24:ARG:HH11 | 22:U:24:ARG:HG2 | 1.83 | 0.43 |
| 1:A:152:A:O2' | 1:A:153:C:H5' | 2.19 | 0.43 |
| 28:1:40:PRO:HG2 | 28:1:64:ILE:HD13 | 2.00 | 0.43 |
| 1:A:2362:A:H2' | 1:A:2363:G:C8 | 2.53 | 0.43 |
| 11:J:31:PHE:HA | 11:J:85:ILE:CG2 | 2.49 | 0.43 |
| 1:A:2781:U:H2' | 1:A:2782:G:C5' | 2.49 | 0.43 |
| 7:F:93:LEU:HB3 | 7:F:97:GLN:OE1 | 2.19 | 0.43 |
| 15:N:61:ILE:CG2 | 15:N:62:VAL:N | 2.82 | 0.43 |
| 17:P:29:VAL:O | 17:P:33:LEU:HG | 2.19 | 0.43 |
| 1:A:764:C:H2' | 1:A:765:G:O4' | 2.18 | 0.43 |
| 38:L:6493:HOH:O | 23:V:24:LYS:HG3 | 2.18 | 0.43 |
| 7:F:159:PRO:O | 7:F:162:ALA:HB3 | 2.18 | 0.43 |
| 1:A:1862:C:H1' | 38:A:6710:HOH:O | 2.19 | 0.43 |
| 12:K:90:LYS:HB2 | 35:K:8502:CL:CL | 2.56 | 0.43 |
| 12:K:84:ARG:HB2 | 12:K:98:PHE:CE1 | 2.54 | 0.43 |
| 15:N:31:TRP:HA | 15:N:34:GLU:HG3 | 2.01 | 0.43 |
| 13:L:14:LYS:HD2 | 13:L:45:PRO:HG3 | 2.00 | 0.43 |
| 23:V:52:THR:HG21 | 23:V:54:THR:HB | 2.00 | 0.43 |
| 1:A:2812:A:C2 | 1:A:2814:A:N6 | 2.80 | 0.43 |
| 38:B:8517:HOH:O | 16:O:107:ASN:HB3 | 2.18 | 0.43 |
| 28:1:39:CYS:HA | 28:1:47:LEU:HD11 | 2.01 | 0.43 |
| 15:N:78:ASN:O | 15:N:79:LYS:HG2 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:F:84:LEU:HA | 7:F:87:ALA:HB3 | 2.01 | 0.43 |
| 28:1:22:ILE:O | 28:1:26:VAL:HG23 | 2.18 | 0.43 |
| 8:G:11:VAL:HG12 | 8:G:12:ASP:H | 1.84 | 0.43 |
| 7:F:95:THR:HG21 | 7:F:174:VAL:HG22 | 2.00 | 0.43 |
| 21:T:73:ASP:O | 21:T:77:VAL:HG23 | 2.18 | 0.43 |
| 2:B:3002:U:H4' | 2:B:3002:U:OP2 | 2.18 | 0.43 |
| 11:J:72:VAL:HG11 | 11:J:81:TYR:CZ | 2.54 | 0.43 |
| 22:U:23:VAL:HA | 22:U:93:THR:HG21 | 2.01 | 0.43 |
| 18:Q:14:LEU:HD13 | 18:Q:51:ALA:HB2 | 2.00 | 0.43 |
| 1:A:731:U:H2' | 1:A:732:C:C6 | 2.54 | 0.43 |
| 1:A:827:A:H2' | 1:A:828:G:O4' | 2.18 | 0.43 |
| 1:A:2598:U:O2 | 1:A:2600:A:H8 | 2.01 | 0.43 |
| 1:A:1388:U:H2' | 1:A:1389:G:O4' | 2.19 | 0.43 |
| 6:E:236:THR:O | 6:E:239:ALA:N | 2.52 | 0.42 |
| 11:J:65:ARG:HD3 | 38:J:8385:HOH:O | 2.18 | 0.42 |
| 12:K:77:GLY:O | 12:K:80:LYS:N | 2.51 | 0.42 |
| 38:A:9304:HOH:O | 13:L:39:GLY:HA3 | 2.19 | 0.42 |
| 15:N:95:LYS:HG2 | 15:N:99:ARG:HB3 | 2.01 | 0.42 |
| 1:A:1165:G:H1' | 1:A:1174:A:H1' | 2.01 | 0.42 |
| 11:J:58:HIS:ND1 | 11:J:59:ASN:ND2 | 2.67 | 0.42 |
| 13:L:74:VAL:HG21 | 13:L:96:VAL:HG23 | 2.01 | 0.42 |
| 4:C:192:VAL:HG13 | 38:C:8554:HOH:O | 2.19 | 0.42 |
| 14:M:120:LEU:HD12 | 14:M:133:VAL:HG21 | 2.00 | 0.42 |
| 25:X:31:HIS:HB3 | 38:X:5420:HOH:O | 2.19 | 0.42 |
| 13:L:106:GLY:HA3 | 38:L:5264:HOH:O | 2.18 | 0.42 |
| 6:E:46:TYR:CE2 | 6:E:98:ARG:NH1 | 2.87 | 0.42 |
| 5:D:217:ARG:CG | 5:D:257:THR:HG22 | 2.45 | 0.42 |
| 25:X:122:ARG:NH1 | 25:X:152:ALA:O | 2.51 | 0.42 |
| 4:C:95:PRO:HG2 | 4:C:98:GLU:CG | 2.47 | 0.42 |
| 1:A:1384:C:H5' | 26:Y:30:MET:HG2 | 2.00 | 0.42 |
| 22:U:38:ARG:NH1 | 22:U:38:ARG:HG3 | 2.33 | 0.42 |
| 5:D:63:GLU:HG3 | 5:D:63:GLU:O | 2.19 | 0.42 |
| 1:A:1559:A:C1' | 38:A:5357:HOH:O | 2.62 | 0.42 |
| 17:P:39:THR:O | 17:P:115:ARG:NH2 | 2.52 | 0.42 |
| 27:Z:105:LYS:HE2 | 27:Z:198:GLY:O | 2.19 | 0.42 |
| 5:D:224:LYS:HD3 | 5:D:224:LYS:HA | 1.79 | 0.42 |
| 23:V:4:ARG:N | 38:V:5334:HOH:O | 2.51 | 0.42 |
| 1:A:2379:G:N7 | 1:A:2408:A:N1 | 2.67 | 0.42 |
| 1:A:1761:U:H5' | 18:Q:81:LYS:O | 2.19 | 0.42 |
| 16:O:15:GLU:OE1 | 16:O:17:ARG:HD2 | 2.19 | 0.42 |
| 1:A:1745:G:H5' | 38:A:3836:HOH:O | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:1165:G:O2' | 1:A:1174:A:H4' | 2.19 | 0.42 |
| 13:L:37:TYR:HD2 | 38:L:7169:HOH:O | 2.01 | 0.42 |
| 13:L:37:TYR:HE2 | 13:L:45:PRO:HA | 1.84 | 0.42 |
| 1:A:2004:U:O2 | 1:A:2004:U:H2' | 2.19 | 0.42 |
| 1:A:1878:G:O2' | 1:A:1879:U:P | 2.77 | 0.42 |
| 5:D:217:ARG:HD3 | 5:D:218:TRP:NE1 | 2.34 | 0.42 |
| 1:A:2756:U:N3 | 1:A:2896:A:H2 | 2.16 | 0.42 |
| 25:X:139:GLY:O | 25:X:141:HIS:CD2 | 2.72 | 0.42 |
| 1:A:795:G:N3 | 1:A:817:G:C2 | 2.87 | 0.42 |
| 14:M:6:ARG:NH2 | 38:M:8550:HOH:O | 2.51 | 0.42 |
| 20:S:29:LYS:NZ | 38:S:8540:HOH:O | 2.51 | 0.42 |
| 1:A:228:C:H2' | 1:A:229:G:H5' | 1.99 | 0.42 |
| 22:U:55:PHE:CG | 22:U:77:VAL:HG13 | 2.53 | 0.42 |
| 27:Z:126:PRO:HG2 | 27:Z:128:PHE:CZ | 2.54 | 0.42 |
| 1:A:1682:A:O2' | 1:A:1683:G:H5'' | 2.19 | 0.42 |
| 15:N:17:GLU:O | 15:N:21:ALA:HB2 | 2.19 | 0.42 |
| 1:A:2597:U:H2' | 1:A:2598:U:H5' | 2.02 | 0.42 |
| 1:A:853:C:H2' | 1:A:854:G:O4' | 2.19 | 0.42 |
| 1:A:2437:A:H2' | 1:A:2438:G:C8 | 2.54 | 0.42 |
| 1:A:222:A:H2' | 1:A:223:G:O4' | 2.18 | 0.42 |
| 1:A:1988:C:O2' | 1:A:1989:G:H5' | 2.19 | 0.42 |
| 1:A:1055:G:OP2 | 11:J:94:ARG:NH1 | 2.52 | 0.42 |
| 6:E:80:VAL:HA | 6:E:81:PRO:HD3 | 1.85 | 0.42 |
| 16:O:37:ARG:HA | 16:O:37:ARG:HD3 | 1.82 | 0.42 |
| 1:A:213:G:O2' | 1:A:214:U:OP2 | 2.37 | 0.42 |
| 5:D:7:ARG:CD | 5:D:9:GLY:O | 2.68 | 0.42 |
| 1:A:288:A:H2' | 1:A:289:G:C8 | 2.54 | 0.42 |
| 30:3:36:ASN:HB3 | 30:3:39:ARG:HE | 1.84 | 0.42 |
| 10:I:71:LEU:C | 10:I:73:ASP:N | 2.72 | 0.42 |
| 26:Y:25:ARG:O | 26:Y:26:ALA:C | 2.57 | 0.42 |
| 7:F:167:GLU:C | 7:F:169:THR:H | 2.23 | 0.42 |
| 1:A:1820:G:C6 | 1:A:2030:A:C2 | 3.07 | 0.42 |
| 1:A:2821:C:H4' | 5:D:116:PRO:CB | 2.49 | 0.42 |
| 29:2:36:SER:O | 29:2:46:ARG:HD3 | 2.19 | 0.42 |
| 13:L:103:ASP:O | 13:L:104:PRO:C | 2.56 | 0.42 |
| 6:E:109:LEU:HD12 | 6:E:109:LEU:O | 2.19 | 0.42 |
| 1:A:210:U:O2' | 1:A:211:U:H5' | 2.19 | 0.42 |
| 12:K:14:ALA:HB1 | 12:K:44:ALA:HB2 | 2.00 | 0.42 |
| 15:N:49:ALA:C | 15:N:54:TYR:HB3 | 2.39 | 0.42 |
| 11:J:56:ILE:HG22 | 11:J:61:LEU:CD2 | 2.48 | 0.42 |
| 15:N:157:LEU:HD23 | 38:N:8637:HOH:O | 2.18 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:482:G:H4' | 1:A:508:A:N1 | 2.34 | 0.42 |
| 1:A:2897:C:H2' | 1:A:2898:G:C8 | 2.46 | 0.42 |
| 15:N:169:ARG:NH2 | 38:N:8553:HOH:O | 2.50 | 0.42 |
| 16:O:149:GLU:O | 16:O:152:GLU:HB2 | 2.20 | 0.42 |
| 10:I:20:VAL:O | 10:I:24:VAL:HG23 | 2.19 | 0.42 |
| 5:D:243:ASN:HA | 5:D:244:PRO:C | 2.39 | 0.42 |
| 18:Q:20:ARG:NH1 | 18:Q:54:LYS:HD3 | 2.34 | 0.42 |
| 17:P:53:GLN:HG2 | 17:P:56:GLU:OE1 | 2.20 | 0.42 |
| 26:Y:22:ASN:C | 26:Y:24:LYS:H | 2.23 | 0.42 |
| 1:A:1855:G:H4' | 1:A:1856:C:O5' | 2.19 | 0.42 |
| 26:Y:27:ASP:N | 26:Y:27:ASP:OD2 | 2.50 | 0.42 |
| 1:A:1400:C:H4' | 26:Y:56:GLU:HG2 | 2.01 | 0.42 |
| 8:G:156:ASP:OD2 | 8:G:157:LYS:NZ | 2.41 | 0.42 |
| 1:A:2737:C:H2' | 38:A:5635:HOH:O | 2.19 | 0.42 |
| 11:J:49:VAL:HG22 | 11:J:130:HIS:HB3 | 2.02 | 0.42 |
| 12:K:45:VAL:HG21 | 12:K:129:PHE:CD1 | 2.54 | 0.42 |
| 38:B:8474:HOH:O | 16:O:23:ARG:NH1 | 2.52 | 0.42 |
| 11:J:58:HIS:CE1 | 11:J:59:ASN:ND2 | 2.88 | 0.42 |
| 1:A:545:G:H2' | 1:A:546:C:O4' | 2.20 | 0.42 |
| 25:X:4:LEU:HD23 | 25:X:4:LEU:HA | 1.79 | 0.42 |
| 7:F:86:THR:HG23 | 38:F:7477:HOH:O | 2.19 | 0.42 |
| 9:H:28:ALA:HB3 | 9:H:99:THR:HG23 | 2.00 | 0.42 |
| 1:A:1315:G:C4 | 27:Z:212:ARG:HB2 | 2.54 | 0.42 |
| 1:A:297:U:H2' | 1:A:298:C:H6 | 1.85 | 0.42 |
| 1:A:2379:G:H4' | 1:A:2380:A:H5'' | 2.01 | 0.42 |
| 1:A:1887:U:OP1 | 28:I:21:LYS:HE3 | 2.20 | 0.42 |
| 20:S:72:VAL:HG11 | 20:S:75:TRP:HB3 | 2.02 | 0.42 |
| 25:X:142:ASP:HB3 | 25:X:145:GLY:H | 1.84 | 0.42 |
| 1:A:2245:C:O5' | 1:A:2245:C:H6 | 2.02 | 0.42 |
| 22:U:89:ARG:C | 22:U:89:ARG:HD2 | 2.39 | 0.42 |
| 31:4:34:LYS:N | 31:4:34:LYS:HD2 | 2.34 | 0.42 |
| 16:O:13:ARG:NH1 | 16:O:13:ARG:O | 2.51 | 0.42 |
| 11:J:42:TYR:HA | 11:J:43:PRO:HD3 | 1.87 | 0.42 |
| 24:W:13:PRO:O | 24:W:17:GLU:HG3 | 2.20 | 0.42 |
| 1:A:366:U:H2' | 1:A:367:G:O4' | 2.19 | 0.42 |
| 7:F:154:LYS:HD3 | 38:F:1796:HOH:O | 2.19 | 0.42 |
| 7:F:49:PRO:HG3 | 38:F:5828:HOH:O | 2.18 | 0.42 |
| 25:X:7:LEU:CD1 | 25:X:53:ALA:HB2 | 2.50 | 0.42 |
| 11:J:31:PHE:HD2 | 11:J:85:ILE:HG23 | 1.84 | 0.42 |
| 25:X:125:HIS:CD2 | 25:X:127:GLY:H | 2.37 | 0.42 |
| 16:O:80:SER:CB | 38:O:8537:HOH:O | 2.65 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:69:A:H2' | 1:A:70:A:OP2 | 2.19 | 0.42 |
| 1:A:1669:A:H2 | 38:A:3214:HOH:O | 2.02 | 0.42 |
| 16:O:176:ARG:O | 16:O:180:LEU:HG | 2.20 | 0.42 |
| 17:P:26:TRP:HA | 17:P:26:TRP:CE3 | 2.55 | 0.42 |
| 1:A:1052:G:N3 | 1:A:1052:G:H2' | 2.34 | 0.42 |
| 5:D:13:PHE:CD1 | 5:D:13:PHE:N | 2.87 | 0.42 |
| 1:A:2842:G:H2' | 1:A:2843:A:H5' | 2.00 | 0.42 |
| 1:A:635:A:H2' | 1:A:636:G:H5'' | 2.01 | 0.42 |
| 12:K:88:PRO:O | 12:K:94:GLY:HA3 | 2.19 | 0.42 |
| 11:J:26:LYS:HD3 | 11:J:89:PRO:CG | 2.50 | 0.42 |
| 15:N:99:ARG:CD | 15:N:167:GLY:HA2 | 2.50 | 0.42 |
| 1:A:1942:A:H3' | 38:A:6838:HOH:O | 2.19 | 0.42 |
| 28:1:45:LYS:HG3 | 38:1:8410:HOH:O | 2.18 | 0.42 |
| 9:H:108:LEU:O | 9:H:111:ILE:N | 2.50 | 0.42 |
| 14:M:24:ALA:HB2 | 14:M:30:ARG:HD2 | 2.01 | 0.42 |
| 1:A:1790:C:H2' | 1:A:1791:U:C6 | 2.54 | 0.42 |
| 15:N:49:ALA:HB1 | 15:N:54:TYR:CB | 2.50 | 0.42 |
| 9:H:1:PRO:HB2 | 38:H:5897:HOH:O | 2.20 | 0.42 |
| 31:4:36:ILE:HA | 31:4:36:ILE:HD12 | 1.95 | 0.42 |
| 24:W:45:ARG:C | 24:W:47:LYS:N | 2.73 | 0.42 |
| 13:L:27:ARG:HD2 | 38:L:4747:HOH:O | 2.19 | 0.42 |
| 1:A:1902:G:H2' | 1:A:1903:U:O4' | 2.20 | 0.42 |
| 1:A:2570:G:H5'' | 38:A:4406:HOH:O | 2.19 | 0.42 |
| 1:A:451:C:O2' | 1:A:452:G:H5' | 2.19 | 0.42 |
| 38:A:4412:HOH:O | 15:N:14:ARG:HB3 | 2.19 | 0.42 |
| 12:K:70:PHE:O | 12:K:70:PHE:CD2 | 2.72 | 0.42 |
| 10:I:63:ARG:O | 10:I:67:LEU:HG | 2.19 | 0.42 |
| 27:Z:235:GLU:CD | 27:Z:235:GLU:N | 2.70 | 0.42 |
| 5:D:30:PRO:HG2 | 5:D:313:PRO:HD2 | 2.01 | 0.42 |
| 1:A:952:G:N3 | 1:A:2302:A:H2' | 2.35 | 0.42 |
| 1:A:2769:C:H2' | 1:A:2770:G:H5' | 2.02 | 0.42 |
| 1:A:1329:A:C2 | 38:A:4181:HOH:O | 2.56 | 0.42 |
| 5:D:69:VAL:HA | 5:D:70:PRO:HD3 | 1.91 | 0.42 |
| 1:A:1972:U:H2' | 1:A:1973:A:C5' | 2.50 | 0.42 |
| 1:A:926:A:O2' | 14:M:41:HIS:CD2 | 2.70 | 0.42 |
| 1:A:1730:G:C5' | 1:A:1731:C:C6 | 3.02 | 0.42 |
| 1:A:1669:A:H2' | 1:A:1670:G:H8 | 1.85 | 0.42 |
| 1:A:521:A:C2' | 1:A:522:U:H5' | 2.50 | 0.42 |
| 9:H:26:THR:HB | 9:H:102:GLY:HA3 | 2.02 | 0.42 |
| 1:A:503:G:H2' | 1:A:504:G:H8 | 1.85 | 0.42 |
| 4:C:123:GLY:HA2 | 4:C:159:VAL:O | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:4:87:ARG:NH1 | 38:4:8524:HOH:O | 2.53 | 0.42 |
| 1:A:1810:C:OP1 | 23:V:44:ARG:NE | 2.38 | 0.42 |
| 14:M:34:GLY:HA3 | 14:M:38:HIS:CE1 | 2.55 | 0.42 |
| 1:A:823:U:H2' | 1:A:824:G:O4' | 2.19 | 0.42 |
| 1:A:51:G:O2' | 1:A:52:A:H5' | 2.20 | 0.42 |
| 12:K:42:GLU:O | 12:K:131:THR:HG23 | 2.20 | 0.42 |
| 1:A:2712:G:H5' | 38:A:4711:HOH:O | 2.20 | 0.42 |
| 1:A:283:U:H5'' | 1:A:284:C:OP2 | 2.20 | 0.42 |
| 27:Z:189:ASN:ND2 | 27:Z:189:ASN:C | 2.71 | 0.42 |
| 14:M:144:ASP:HA | 14:M:147:GLU:HG3 | 2.01 | 0.42 |
| 4:C:35:GLY:O | 4:C:36:ASP:CB | 2.60 | 0.42 |
| 25:X:21:LEU:HB3 | 25:X:26:ILE:CG1 | 2.50 | 0.42 |
| 13:L:22:ASP:HA | 13:L:108:GLU:O | 2.20 | 0.42 |
| 25:X:132:VAL:HG21 | 25:X:141:HIS:CD2 | 2.55 | 0.42 |
| 21:T:57:THR:C | 21:T:59:ASP:H | 2.22 | 0.42 |
| 1:A:583:G:H2' | 1:A:584:U:H6 | 1.84 | 0.42 |
| 20:S:119:VAL:CG1 | 20:S:119:VAL:O | 2.67 | 0.42 |
| 1:A:921:G:H4' | 1:A:924:G:C6 | 2.55 | 0.42 |
| 19:R:32:GLU:O | 19:R:93:ARG:NH2 | 2.53 | 0.42 |
| 1:A:128:A:H8 | 1:A:128:A:H3' | 1.85 | 0.42 |
| 25:X:73:LEU:HA | 25:X:73:LEU:HD12 | 1.73 | 0.42 |
| 4:C:165:THR:O | 4:C:165:THR:HG22 | 2.19 | 0.42 |
| 19:R:41:LEU:HB3 | 19:R:52:PHE:CZ | 2.55 | 0.42 |
| 1:A:2297:U:H1' | 38:A:4665:HOH:O | 2.20 | 0.42 |
| 1:A:1565:C:O4' | 1:A:2738:G:H1' | 2.20 | 0.42 |
| 12:K:142:ASN:O | 12:K:144:THR:N | 2.53 | 0.42 |
| 22:U:9:LYS:HD2 | 38:U:7242:HOH:O | 2.20 | 0.42 |
| 2:B:3056:A:C3' | 2:B:3057:A:H5'' | 2.49 | 0.42 |
| 1:A:2269:C:H2' | 1:A:2270:G:C5' | 2.50 | 0.42 |
| 30:3:40:ARG:HG2 | 30:3:40:ARG:HH11 | 1.85 | 0.42 |
| 9:H:50:VAL:CG1 | 9:H:60:VAL:HG11 | 2.49 | 0.42 |
| 16:O:71:TRP:CE2 | 16:O:73:ALA:HB3 | 2.55 | 0.42 |
| 5:D:36:PRO:HG3 | 5:D:168:GLY:HA3 | 2.02 | 0.42 |
| 1:A:873:G:H2' | 1:A:875:A:N7 | 2.35 | 0.42 |
| 7:F:144:ARG:NH2 | 38:F:3839:HOH:O | 2.48 | 0.42 |
| 2:B:3093:A:C5 | 2:B:3094:G:H1' | 2.54 | 0.42 |
| 22:U:43:ASN:C | 22:U:45:GLY:H | 2.23 | 0.42 |
| 5:D:49:THR:HG21 | 5:D:280:VAL:CG2 | 2.50 | 0.42 |
| 1:A:2846:C:H4' | 5:D:156:LYS:HB3 | 2.01 | 0.42 |
| 1:A:1755:A:H2' | 1:A:1756:G:O4' | 2.20 | 0.42 |
| 17:P:81:PHE:N | 17:P:81:PHE:CD1 | 2.87 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 38:A:9721:HOH:O | 27:Z:135:LYS:HE3 | 2.20 | 0.42 |
| 7:F:15:GLU:HA | 7:F:16:PRO:HD3 | 1.88 | 0.42 |
| 1:A:424:C:H2' | 1:A:425:U:C6 | 2.55 | 0.42 |
| 6:E:37:ALA:O | 6:E:41:ASN:ND2 | 2.53 | 0.42 |
| 1:A:303:C:H2' | 1:A:304:G:O4' | 2.20 | 0.42 |
| 27:Z:178:HIS:CG | 27:Z:179:PRO:HD2 | 2.55 | 0.42 |
| 1:A:2699:A:H2' | 1:A:2700:G:O4' | 2.20 | 0.42 |
| 1:A:2589:U:H2' | 1:A:2590:U:C6 | 2.55 | 0.41 |
| 1:A:1666:C:C2' | 1:A:1667:A:H5'' | 2.49 | 0.41 |
| 15:N:184:ARG:CG | 15:N:185:PRO:HA | 2.50 | 0.41 |
| 5:D:60:SER:C | 5:D:62:ARG:N | 2.72 | 0.41 |
| 27:Z:186:ARG:CG | 27:Z:186:ARG:NH1 | 2.80 | 0.41 |
| 14:M:143:THR:HG22 | 14:M:144:ASP:H | 1.85 | 0.41 |
| 5:D:16:ARG:HB3 | 5:D:217:ARG:NH2 | 2.35 | 0.41 |
| 12:K:40:ASN:OD1 | 12:K:106:GLY:HA2 | 2.19 | 0.41 |
| 1:A:2032:U:O2' | 1:A:2033:G:H5'' | 2.19 | 0.41 |
| 31:4:18:GLN:OE1 | 31:4:73:GLU:HB3 | 2.19 | 0.41 |
| 1:A:1787:C:O2' | 1:A:1788:U:H5' | 2.20 | 0.41 |
| 9:H:49:PHE:CD1 | 9:H:49:PHE:N | 2.88 | 0.41 |
| 1:A:486:A:H1' | 38:A:6265:HOH:O | 2.19 | 0.41 |
| 1:A:1230:A:H4' | 1:A:1231:A:O5' | 2.20 | 0.41 |
| 1:A:2094:G:H4' | 5:D:245:SER:HB3 | 2.03 | 0.41 |
| 1:A:1066:U:H2' | 1:A:1067:A:C8 | 2.55 | 0.41 |
| 19:R:46:SER:O | 19:R:48:PRO:HD3 | 2.20 | 0.41 |
| 38:A:5766:HOH:O | 18:Q:63:ARG:NH2 | 2.53 | 0.41 |
| 1:A:1926:G:H2' | 1:A:1927:A:C8 | 2.55 | 0.41 |
| 11:J:26:LYS:HD2 | 11:J:28:ILE:CB | 2.45 | 0.41 |
| 7:F:40:ILE:HG23 | 38:F:5583:HOH:O | 2.20 | 0.41 |
| 19:R:18:PRO:O | 19:R:21:ARG:HB2 | 2.20 | 0.41 |
| 1:A:2005:G:OP2 | 1:A:2005:G:H3' | 2.20 | 0.41 |
| 15:N:184:ARG:HG3 | 15:N:185:PRO:HA | 2.02 | 0.41 |
| 11:J:136:VAL:HG22 | 11:J:137:ASN:N | 2.35 | 0.41 |
| 1:A:2897:C:O2' | 1:A:2898:G:H5' | 2.21 | 0.41 |
| 8:G:7:ILE:HA | 8:G:8:PRO:HD3 | 1.93 | 0.41 |
| 11:J:126:HIS:O | 11:J:127:GLY:C | 2.59 | 0.41 |
| 7:F:169:THR:C | 7:F:170:TYR:HD1 | 2.23 | 0.41 |
| 5:D:154:VAL:CG1 | 5:D:156:LYS:HG2 | 2.50 | 0.41 |
| 2:B:3003:A:N6 | 2:B:3022:G:H1' | 2.35 | 0.41 |
| 1:A:1484:G:H2' | 38:A:8620:HOH:O | 2.19 | 0.41 |
| 2:B:3042:C:H5' | 2:B:3043:G:OP2 | 2.19 | 0.41 |
| 19:R:16:ASN:HA | 19:R:16:ASN:HD22 | 1.62 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1811:A:H2' | 1:A:1812:G:H5' | 2.02 | 0.41 |
| 1:A:1391:G:H2' | 1:A:1392:A:H5' | 2.02 | 0.41 |
| 25:X:59:GLN:NE2 | 25:X:97:ALA:HB3 | 2.35 | 0.41 |
| 1:A:1850:U:H2' | 1:A:1851:G:H8 | 1.85 | 0.41 |
| 1:A:1311:G:C2 | 1:A:1312:G:C8 | 3.08 | 0.41 |
| 1:A:1224:G:H2' | 1:A:1225:C:C6 | 2.54 | 0.41 |
| 6:E:188:ARG:NH2 | 38:E:8322:HOH:O | 2.50 | 0.41 |
| 1:A:1996:U:O2' | 1:A:1997:A:H5' | 2.19 | 0.41 |
| 1:A:1456:C:H2' | 1:A:1457:U:C6 | 2.55 | 0.41 |
| 1:A:2111:G:H1' | 38:A:8566:HOH:O | 2.19 | 0.41 |
| 1:A:1462:C:H2' | 1:A:1463:A:C8 | 2.55 | 0.41 |
| 8:G:101:GLU:OE2 | 8:G:115:ARG:NH1 | 2.52 | 0.41 |
| 13:L:87:ARG:CZ | 38:L:4854:HOH:O | 2.68 | 0.41 |
| 4:C:211:LYS:HD3 | 38:C:8607:HOH:O | 2.19 | 0.41 |
| 4:C:211:LYS:CB | 4:C:212:PRO:CD | 2.98 | 0.41 |
| 1:A:711:G:C2 | 1:A:718:C:C2 | 3.08 | 0.41 |
| 4:C:100:PRO:HG2 | 4:C:103:VAL:CG2 | 2.45 | 0.41 |
| 5:D:304:PRO:CD | 5:D:307:ARG:NH1 | 2.84 | 0.41 |
| 25:X:137:GLN:HG3 | 25:X:137:GLN:O | 2.20 | 0.41 |
| 1:A:816:G:C5 | 1:A:817:G:C6 | 3.08 | 0.41 |
| 1:A:2781:U:O2' | 1:A:2782:G:H5' | 2.20 | 0.41 |
| 1:A:1332:C:O2' | 1:A:1333:U:H5' | 2.20 | 0.41 |
| 36:5:77:PHA:HD2 | 36:5:77:PHA:HA | 1.82 | 0.41 |
| 1:A:902:G:N7 | 14:M:18:HIS:CD2 | 2.85 | 0.41 |
| 22:U:87:VAL:HB | 22:U:88:PRO:HD2 | 2.02 | 0.41 |
| 7:F:59:GLY:C | 7:F:61:PHE:N | 2.74 | 0.41 |
| 17:P:26:TRP:HA | 17:P:26:TRP:HE3 | 1.85 | 0.41 |
| 1:A:2079:G:H2' | 1:A:2080:G:O4' | 2.20 | 0.41 |
| 2:B:3059:C:H5' | 38:B:8476:HOH:O | 2.19 | 0.41 |
| 8:G:112:ALA:HA | 8:G:113:PRO:HD3 | 1.84 | 0.41 |
| 9:H:34:ASN:HA | 15:N:4:ALA:HB2 | 2.02 | 0.41 |
| 1:A:11:A:H5' | 1:A:12:U:OP2 | 2.20 | 0.41 |
| 25:X:34:LEU:CD1 | 25:X:100:LEU:HD13 | 2.51 | 0.41 |
| 16:O:34:LEU:HD13 | 16:O:47:LEU:HD21 | 2.03 | 0.41 |
| 38:A:3267:HOH:O | 22:U:9:LYS:CD | 2.66 | 0.41 |
| 1:A:236:A:H4' | 1:A:237:G:OP1 | 2.19 | 0.41 |
| 2:B:3028:U:H5'' | 16:O:40:ASN:ND2 | 2.35 | 0.41 |
| 26:Y:25:ARG:HD3 | 26:Y:64:ALA:O | 2.20 | 0.41 |
| 15:N:61:ILE:HA | 38:N:8632:HOH:O | 2.20 | 0.41 |
| 5:D:82:VAL:CG1 | 5:D:82:VAL:O | 2.68 | 0.41 |
| 1:A:1003:U:O2 | 11:J:90:PHE:HZ | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2252:A:C6 | 1:A:2253:G:H1' | 2.54 | 0.41 |
| 1:A:1470:A:O4' | 15:N:93:ARG:HD3 | 2.21 | 0.41 |
| 22:U:26:THR:HA | 22:U:39:ASN:HB3 | 2.01 | 0.41 |
| 9:H:38:LYS:NZ | 15:N:3:SER:HA | 2.35 | 0.41 |
| 16:O:82:TYR:C | 16:O:82:TYR:CD2 | 2.94 | 0.41 |
| 2:B:3095:C:O2' | 2:B:3096:C:H5' | 2.21 | 0.41 |
| 14:M:17:SER:C | 14:M:19:LYS:H | 2.24 | 0.41 |
| 1:A:2659:U:H5'' | 38:A:3635:HOH:O | 2.20 | 0.41 |
| 1:A:1271:A:H2' | 1:A:1272:C:O4' | 2.21 | 0.41 |
| 4:C:97:ALA:HB2 | 4:C:150:PRO:HB2 | 2.02 | 0.41 |
| 1:A:1739:G:O2' | 1:A:1740:U:H5' | 2.20 | 0.41 |
| 38:A:7197:HOH:O | 6:E:94:THR:HG21 | 2.21 | 0.41 |
| 11:J:65:ARG:HH21 | 11:J:66:VAL:HG22 | 1.85 | 0.41 |
| 1:A:111:C:H2' | 1:A:112:G:O4' | 2.20 | 0.41 |
| 7:F:17:ARG:NH2 | 38:F:3723:HOH:O | 2.54 | 0.41 |
| 10:I:71:LEU:O | 10:I:73:ASP:N | 2.53 | 0.41 |
| 1:A:2032:U:H5' | 38:A:4015:HOH:O | 2.19 | 0.41 |
| 1:A:1384:C:H2' | 1:A:1385:G:O4' | 2.20 | 0.41 |
| 26:Y:30:MET:HE1 | 26:Y:58:ALA:HB3 | 2.02 | 0.41 |
| 18:Q:59:ARG:HH22 | 18:Q:66:GLN:HE22 | 1.65 | 0.41 |
| 18:Q:41:ARG:O | 18:Q:44:VAL:HB | 2.19 | 0.41 |
| 27:Z:117:LEU:HA | 27:Z:174:VAL:HG11 | 2.02 | 0.41 |
| 20:S:113:HIS:O | 20:S:145:LEU:HD12 | 2.21 | 0.41 |
| 16:O:38:LYS:HB2 | 16:O:38:LYS:HE3 | 1.76 | 0.41 |
| 25:X:56:GLU:O | 25:X:143:THR:HG23 | 2.20 | 0.41 |
| 1:A:569:A:H5'' | 1:A:587:A:N1 | 2.34 | 0.41 |
| 24:W:29:ASN:O | 24:W:33:VAL:HG23 | 2.20 | 0.41 |
| 4:C:30:ARG:HB3 | 4:C:30:ARG:HE | 1.62 | 0.41 |
| 1:A:1619:G:H2' | 1:A:1620:C:O4' | 2.20 | 0.41 |
| 6:E:140:VAL:HG12 | 6:E:141:SER:N | 2.34 | 0.41 |
| 1:A:1593:C:OP1 | 18:Q:117:SER:HB3 | 2.21 | 0.41 |
| 18:Q:114:LEU:HD22 | 18:Q:118:GLN:HB2 | 2.02 | 0.41 |
| 15:N:63:VAL:HG21 | 15:N:109:PHE:CZ | 2.55 | 0.41 |
| 1:A:2506:A:O2' | 1:A:2507:G:P | 2.78 | 0.41 |
| 5:D:62:ARG:HH11 | 5:D:62:ARG:HG2 | 1.86 | 0.41 |
| 5:D:7:ARG:NH1 | 5:D:11:LEU:HD22 | 2.35 | 0.41 |
| 13:L:65:ARG:O | 13:L:66:ARG:HB2 | 2.21 | 0.41 |
| 11:J:113:ALA:N | 11:J:114:PRO:HD3 | 2.36 | 0.41 |
| 17:P:96:VAL:CG1 | 17:P:100:GLN:HB2 | 2.51 | 0.41 |
| 1:A:1482:A:O2' | 1:A:1483:C:H5' | 2.21 | 0.41 |
| 1:A:1398:G:O2' | 1:A:1399:A:H5' | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 13:L:99:ASP:OD1 | 13:L:99:ASP:C | 2.58 | 0.41 |
| 1:A:1162:G:H2' | 1:A:1162:G:N3 | 2.35 | 0.41 |
| 6:E:165:ASP:O | 6:E:168:ARG:HB3 | 2.20 | 0.41 |
| 1:A:1857:A:N6 | 1:A:2247:C:H1' | 2.36 | 0.41 |
| 1:A:1245:C:O5' | 1:A:1245:C:H6 | 2.04 | 0.41 |
| 1:A:1562:C:H2' | 1:A:1562:C:O2 | 2.20 | 0.41 |
| 4:C:82:VAL:HG13 | 4:C:93:THR:HB | 2.02 | 0.41 |
| 1:A:1714:C:O2' | 1:A:1715:C:H5' | 2.21 | 0.41 |
| 1:A:2582:G:O3' | 13:L:41:LYS:HA | 2.20 | 0.41 |
| 1:A:275:G:C2 | 1:A:376:C:N3 | 2.89 | 0.41 |
| 22:U:71:VAL:HG13 | 22:U:91:LEU:O | 2.20 | 0.41 |
| 1:A:2505:G:H8 | 38:A:5130:HOH:O | 2.03 | 0.41 |
| 27:Z:189:ASN:ND2 | 27:Z:192:ASP:N | 2.65 | 0.41 |
| 1:A:137:U:OP1 | 1:A:259:G:O2' | 2.38 | 0.41 |
| 12:K:39:VAL:CG1 | 12:K:107:ASN:HB2 | 2.51 | 0.41 |
| 1:A:506:G:N2 | 1:A:508:A:H3' | 2.35 | 0.41 |
| 1:A:951:A:O2' | 1:A:952:G:H5' | 2.21 | 0.41 |
| 30:3:25:VAL:O | 30:3:29:THR:HG23 | 2.21 | 0.41 |
| 22:U:44:ALA:HA | 22:U:62:VAL:CG1 | 2.50 | 0.41 |
| 1:A:669:G:H2' | 1:A:670:G:H8 | 1.86 | 0.41 |
| 25:X:1:MET:N | 25:X:37:GLU:HG3 | 2.35 | 0.41 |
| 1:A:857:A:H4' | 4:C:176:HIS:CD2 | 2.56 | 0.41 |
| 9:H:49:PHE:HE1 | 9:H:98:VAL:CG2 | 2.33 | 0.41 |
| 27:Z:144:ARG:NE | 38:Z:8608:HOH:O | 2.53 | 0.41 |
| 14:M:97:VAL:HG12 | 14:M:98:GLU:O | 2.21 | 0.41 |
| 1:A:2546:U:H4' | 38:D:8587:HOH:O | 2.20 | 0.41 |
| 1:A:1707:G:N2 | 1:A:1709:G:H3' | 2.36 | 0.41 |
| 2:B:3104:A:O2' | 2:B:3105:A:H5' | 2.21 | 0.41 |
| 1:A:243:A:H61 | 1:A:269:G:H1' | 1.86 | 0.41 |
| 9:H:27:GLY:HA3 | 38:H:5413:HOH:O | 2.19 | 0.41 |
| 11:J:148:ARG:NE | 38:J:8345:HOH:O | 2.45 | 0.41 |
| 1:A:837:U:H4' | 38:A:9903:HOH:O | 2.20 | 0.41 |
| 1:A:564:G:N2 | 38:A:3904:HOH:O | 2.43 | 0.41 |
| 12:K:130:VAL:CG1 | 12:K:131:THR:N | 2.84 | 0.41 |
| 22:U:71:VAL:CG1 | 22:U:72:ILE:N | 2.83 | 0.41 |
| 1:A:1878:G:O2' | 1:A:1879:U:C6 | 2.70 | 0.41 |
| 24:W:42:ASN:O | 24:W:44:GLY:N | 2.54 | 0.41 |
| 1:A:1151:G:H2' | 38:A:4506:HOH:O | 2.21 | 0.41 |
| 26:Y:9:VAL:HG13 | 26:Y:88:GLU:OE1 | 2.20 | 0.41 |
| 16:O:154:LEU:HD11 | 16:O:157:PRO:HA | 2.02 | 0.41 |
| 1:A:2346:C:O3' | 7:F:52:THR:HG23 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1058:A:H2' | 1:A:1060:C:C5' | 2.49 | 0.41 |
| 1:A:88:G:C8 | 30:3:28:LYS:HB2 | 2.55 | 0.41 |
| 1:A:2289:G:H21 | 1:A:2291:A:H2 | 1.63 | 0.41 |
| 1:A:946:C:H2' | 1:A:947:U:C6 | 2.55 | 0.41 |
| 18:Q:16:VAL:CG1 | 18:Q:17:GLY:N | 2.83 | 0.41 |
| 1:A:1517:U:C2 | 1:A:1670:G:N2 | 2.89 | 0.41 |
| 1:A:1477:C:H5' | 1:A:1868:G:H5'' | 2.03 | 0.41 |
| 16:O:181:ASP:HA | 38:O:8571:HOH:O | 2.20 | 0.41 |
| 1:A:2478:U:H2' | 1:A:2479:A:C8 | 2.56 | 0.41 |
| 1:A:1743:G:O4' | 13:L:78:LYS:HD3 | 2.20 | 0.41 |
| 1:A:1436:C:O2' | 1:A:1437:A:H5' | 2.21 | 0.41 |
| 1:A:1675:C:H3' | 38:A:7301:HOH:O | 2.19 | 0.41 |
| 1:A:2001:G:O2' | 1:A:2002:C:H5' | 2.21 | 0.41 |
| 1:A:2296:C:H5 | 38:R:5998:HOH:O | 2.03 | 0.41 |
| 1:A:424:C:H2' | 1:A:425:U:H6 | 1.85 | 0.41 |
| 5:D:109:LEU:HG | 5:D:113:LEU:HD12 | 2.02 | 0.41 |
| 8:G:16:ASP:O | 8:G:17:HIS:HB2 | 2.20 | 0.41 |
| 6:E:14:GLY:O | 6:E:15:GLU:HB3 | 2.21 | 0.41 |
| 1:A:2869:G:H2' | 1:A:2870:C:C6 | 2.55 | 0.41 |
| 11:J:49:VAL:C | 11:J:157:ILE:HG23 | 2.39 | 0.41 |
| 11:J:47:GLU:OE2 | 11:J:162:SER:OG | 2.38 | 0.41 |
| 24:W:12:THR:CG2 | 24:W:15:GLU:HG3 | 2.28 | 0.41 |
| 15:N:114:VAL:HG21 | 15:N:159:THR:CG2 | 2.50 | 0.41 |
| 1:A:1942:A:HO2' | 1:A:1943:C:H5' | 1.85 | 0.41 |
| 28:1:38:LYS:HG3 | 38:1:8428:HOH:O | 2.21 | 0.41 |
| 27:Z:189:ASN:HD22 | 27:Z:192:ASP:H | 1.67 | 0.41 |
| 1:A:2072:G:H3' | 1:A:2073:G:C5' | 2.51 | 0.41 |
| 6:E:223:LEU:HD12 | 6:E:223:LEU:HA | 1.82 | 0.41 |
| 17:P:4:ASN:HA | 17:P:5:PRO:HD3 | 1.90 | 0.41 |
| 16:O:175:LEU:HA | 16:O:175:LEU:HD12 | 1.86 | 0.41 |
| 23:V:14:GLU:HA | 23:V:15:PRO:HD2 | 1.87 | 0.41 |
| 9:H:16:ALA:HA | 9:H:111:ILE:HD13 | 2.03 | 0.41 |
| 22:U:41:ARG:NH1 | 22:U:42:VAL:O | 2.54 | 0.41 |
| 1:A:2837:U:H1' | 5:D:307:ARG:HH12 | 1.85 | 0.41 |
| 5:D:313:PRO:O | 5:D:314:ALA:C | 2.59 | 0.41 |
| 21:T:32:ALA:HA | 21:T:36:GLU:OE1 | 2.21 | 0.41 |
| 1:A:1262:C:O2' | 25:X:120:PRO:HD3 | 2.21 | 0.41 |
| 1:A:69:A:C2' | 1:A:70:A:OP2 | 2.69 | 0.41 |
| 1:A:685:C:O2 | 1:A:748:C:H4' | 2.20 | 0.41 |
| 20:S:114:VAL:HA | 20:S:144:GLU:O | 2.20 | 0.41 |
| 1:A:1477:C:C5' | 1:A:1868:G:H5'' | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1845:A:O3' | 4:C:187:PRO:HB2 | 2.21 | 0.41 |
| 1:A:128:A:C8 | 1:A:128:A:C3' | 3.02 | 0.41 |
| 13:L:98:VAL:CG1 | 13:L:102:GLU:HA | 2.51 | 0.41 |
| 25:X:142:ASP:HB2 | 38:X:2729:HOH:O | 2.20 | 0.41 |
| 27:Z:203:VAL:HG12 | 27:Z:228:VAL:HG22 | 2.03 | 0.41 |
| 1:A:2809:G:H2' | 1:A:2810:G:O4' | 2.21 | 0.41 |
| 1:A:1631:A:H2' | 1:A:1632:A:C8 | 2.55 | 0.41 |
| 1:A:1200:A:H4' | 38:A:6832:HOH:O | 2.20 | 0.41 |
| 1:A:426:G:H2' | 1:A:427:C:O4' | 2.21 | 0.41 |
| 12:K:51:GLU:O | 12:K:55:GLU:HG3 | 2.21 | 0.41 |
| 1:A:2069:U:H5' | 38:A:4259:HOH:O | 2.20 | 0.41 |
| 1:A:1815:A:H2' | 1:A:1816:C:O4' | 2.21 | 0.41 |
| 1:A:2133:U:H4' | 1:A:2134:G:H5' | 2.02 | 0.41 |
| 25:X:72:PRO:HB2 | 25:X:74:GLU:O | 2.21 | 0.41 |
| 1:A:2494:G:H4' | 11:J:5:MET:SD | 2.60 | 0.41 |
| 1:A:250:C:H2' | 1:A:251:C:C6 | 2.56 | 0.41 |
| 4:C:36:ASP:CB | 4:C:85:ASP:H | 2.34 | 0.41 |
| 7:F:57:THR:HA | 7:F:63:ILE:HA | 2.02 | 0.41 |
| 28:1:30:GLU:HB3 | 28:1:34:LYS:HE3 | 2.03 | 0.41 |
| 1:A:1069:C:H4' | 1:A:1081:A:O2' | 2.20 | 0.41 |
| 1:A:1771:U:O2' | 1:A:1773:G:N7 | 2.47 | 0.41 |
| 7:F:173:GLU:HG3 | 7:F:174:VAL:N | 2.36 | 0.41 |
| 20:S:82:GLU:HG3 | 20:S:83:LYS:N | 2.35 | 0.41 |
| 1:A:154:C:P | 15:N:188:ARG:HH12 | 2.44 | 0.41 |
| 23:V:6:CYS:C | 23:V:8:TYR:N | 2.74 | 0.41 |
| 1:A:1829:A:C2' | 1:A:1830:C:H5' | 2.50 | 0.41 |
| 1:A:704:C:H2' | 1:A:705:C:H6 | 1.86 | 0.41 |
| 1:A:1783:A:C2' | 1:A:1784:U:H5' | 2.51 | 0.41 |
| 1:A:245:C:C2' | 1:A:246:G:H5' | 2.51 | 0.41 |
| 1:A:105:G:O2' | 1:A:106:A:H5' | 2.21 | 0.41 |
| 16:O:38:LYS:HD2 | 16:O:114:LYS:HE3 | 2.03 | 0.41 |
| 5:D:14:GLY:HA2 | 5:D:15:PRO:C | 2.40 | 0.41 |
| 29:2:15:THR:O | 29:2:29:THR:HG22 | 2.20 | 0.41 |
| 1:A:2443:C:O3' | 14:M:56:LYS:HE3 | 2.20 | 0.41 |
| 1:A:1425:G:O2' | 1:A:1426:C:H5' | 2.21 | 0.41 |
| 38:A:6000:HOH:O | 30:3:1:GLY:HA3 | 2.20 | 0.41 |
| 2:B:3052:A:H2' | 2:B:3053:G:O4' | 2.21 | 0.41 |
| 16:O:73:ALA:HB2 | 16:O:163:PHE:CZ | 2.56 | 0.40 |
| 1:A:1450:C:O2' | 1:A:1493:A:H2' | 2.20 | 0.40 |
| 12:K:19:MET:HE1 | 12:K:132:LEU:HD11 | 2.02 | 0.40 |
| 23:V:14:GLU:OE1 | 23:V:15:PRO:CD | 2.65 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:P:47:ARG:HA | 17:P:50:ARG:HH12 | 1.85 | 0.40 |
| 28:1:46:LYS:NZ | 38:1:8440:HOH:O | 2.53 | 0.40 |
| 1:A:696:C:H4' | 38:A:6771:HOH:O | 2.20 | 0.40 |
| 7:F:140:ARG:HG3 | 7:F:140:ARG:HH11 | 1.85 | 0.40 |
| 8:G:3:VAL:HG22 | 8:G:49:ILE:HB | 2.03 | 0.40 |
| 1:A:2912:C:H2' | 1:A:2913:A:O4' | 2.21 | 0.40 |
| 28:1:11:THR:HG23 | 28:1:11:THR:O | 2.21 | 0.40 |
| 1:A:1114:A:H2' | 1:A:1115:U:C6 | 2.56 | 0.40 |
| 1:A:1735:C:H2' | 1:A:1736:A:C8 | 2.55 | 0.40 |
| 1:A:1675:C:H5'' | 30:3:5:LYS:HD2 | 2.03 | 0.40 |
| 1:A:2134:G:C6 | 1:A:2258:A:C8 | 3.10 | 0.40 |
| 1:A:204:A:C2' | 1:A:205:U:H5' | 2.51 | 0.40 |
| 16:O:50:LEU:HD12 | 16:O:50:LEU:HA | 1.94 | 0.40 |
| 1:A:963:C:H6 | 1:A:963:C:O5' | 2.04 | 0.40 |
| 1:A:1873:G:H3' | 38:A:4700:HOH:O | 2.21 | 0.40 |
| 5:D:235:ARG:HA | 38:D:8604:HOH:O | 2.20 | 0.40 |
| 6:E:141:SER:HA | 38:E:8383:HOH:O | 2.21 | 0.40 |
| 1:A:1942:A:O3' | 4:C:213:LYS:HE2 | 2.21 | 0.40 |
| 13:L:74:VAL:HG13 | 13:L:113:ILE:HG12 | 2.01 | 0.40 |
| 1:A:2004:U:H2' | 1:A:2005:G:OP1 | 2.21 | 0.40 |
| 15:N:183:VAL:HG12 | 15:N:184:ARG:N | 2.36 | 0.40 |
| 6:E:118:THR:CG2 | 6:E:137:PRO:HB3 | 2.51 | 0.40 |
| 7:F:64:ARG:NE | 7:F:67:ASP:HB3 | 2.36 | 0.40 |
| 5:D:52:VAL:N | 5:D:329:TYR:O | 2.46 | 0.40 |
| 5:D:7:ARG:NH1 | 5:D:7:ARG:HG2 | 2.35 | 0.40 |
| 5:D:7:ARG:NH2 | 5:D:250:THR:O | 2.54 | 0.40 |
| 1:A:291:C:H2' | 1:A:292:G:O4' | 2.21 | 0.40 |
| 1:A:470:U:H2' | 1:A:471:G:O4' | 2.21 | 0.40 |
| 20:S:17:MET:CE | 20:S:19:ARG:CZ | 3.00 | 0.40 |
| 16:O:43:VAL:O | 16:O:84:THR:HG21 | 2.20 | 0.40 |
| 4:C:186:TRP:CD1 | 4:C:187:PRO:HA | 2.56 | 0.40 |
| 4:C:66:ARG:CB | 4:C:66:ARG:HH11 | 2.34 | 0.40 |
| 1:A:1127:C:C5 | 1:A:1128:U:C4 | 3.09 | 0.40 |
| 17:P:105:ASN:O | 17:P:105:ASN:CG | 2.59 | 0.40 |
| 21:T:69:SER:C | 21:T:71:ASP:N | 2.75 | 0.40 |
| 1:A:10:U:O4 | 1:A:532:A:OP2 | 2.38 | 0.40 |
| 1:A:445:U:H2' | 1:A:446:G:H8 | 1.85 | 0.40 |
| 1:A:2764:C:H2' | 1:A:2765:C:H6 | 1.85 | 0.40 |
| 12:K:15:ARG:NH1 | 12:K:43:ARG:NH1 | 2.69 | 0.40 |
| 1:A:466:A:H2' | 1:A:467:G:O4' | 2.21 | 0.40 |
| 1:A:2712:G:O2' | 1:A:2713:G:H5' | 2.22 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:2526:C:C2' | 1:A:2527:U:H5' | 2.50 | 0.40 |
| 1:A:2784:A:H1' | 8:G:60:SER:OG | 2.22 | 0.40 |
| 1:A:363:A:H8 | 1:A:363:A:O5' | 2.04 | 0.40 |
| 15:N:152:ARG:HB3 | 38:N:8649:HOH:O | 2.21 | 0.40 |
| 26:Y:71:ARG:CD | 38:Y:2171:HOH:O | 2.66 | 0.40 |
| 5:D:266:ASN:OD1 | 5:D:317:PRO:HA | 2.20 | 0.40 |
| 1:A:559:U:C6 | 1:A:559:U:H5' | 2.50 | 0.40 |
| 1:A:1741:U:H3' | 38:A:9274:HOH:O | 2.20 | 0.40 |
| 8:G:132:THR:HG23 | 8:G:132:THR:O | 2.20 | 0.40 |
| 5:D:280:VAL:HG13 | 5:D:333:GLU:O | 2.20 | 0.40 |
| 14:M:20:ASN:O | 14:M:22:ARG:N | 2.52 | 0.40 |
| 38:A:4899:HOH:O | 4:C:164:ARG:NE | 2.53 | 0.40 |
| 14:M:62:ALA:HB2 | 14:M:103:ALA:CB | 2.51 | 0.40 |
| 7:F:128:LEU:HD23 | 7:F:128:LEU:C | 2.42 | 0.40 |
| 1:A:332:G:O2' | 1:A:333:G:H5' | 2.22 | 0.40 |
| 1:A:644:G:H5' | 1:A:644:G:N3 | 2.36 | 0.40 |
| 20:S:72:VAL:CG1 | 20:S:75:TRP:HB3 | 2.51 | 0.40 |
| 1:A:226:A:H1' | 1:A:393:G:C5 | 2.56 | 0.40 |
| 12:K:24:SER:HA | 12:K:86:MET:SD | 2.61 | 0.40 |
| 1:A:697:G:H4' | 1:A:730:G:O3' | 2.21 | 0.40 |
| 1:A:401:C:O2' | 15:N:92:THR:HB | 2.21 | 0.40 |
| 4:C:70:ALA:HA | 4:C:71:PRO:HD3 | 1.78 | 0.40 |
| 31:4:43:ASN:ND2 | 38:4:8506:HOH:O | 2.50 | 0.40 |
| 6:E:236:THR:C | 38:E:8451:HOH:O | 2.59 | 0.40 |
| 2:B:3023:U:H3' | 38:B:8479:HOH:O | 2.21 | 0.40 |
| 13:L:30:LYS:C | 13:L:55:VAL:HG13 | 2.42 | 0.40 |
| 14:M:148:GLU:HG3 | 38:M:8553:HOH:O | 2.22 | 0.40 |
| 12:K:39:VAL:HG11 | 12:K:107:ASN:HB2 | 2.02 | 0.40 |
| 27:Z:216:ARG:O | 27:Z:219:GLU:HG2 | 2.21 | 0.40 |
| 1:A:2361:A:H2' | 1:A:2362:A:C8 | 2.56 | 0.40 |
| 18:Q:59:ARG:O | 18:Q:62:ALA:HB3 | 2.21 | 0.40 |
| 1:A:2241:C:H2' | 1:A:2242:U:H6 | 1.85 | 0.40 |
| 1:A:1298:U:H2' | 1:A:1299:G:C8 | 2.56 | 0.40 |
| 25:X:121:PRO:CA | 25:X:153:MET:HG2 | 2.51 | 0.40 |
| 9:H:33:THR:HG21 | 9:H:59:ILE:O | 2.22 | 0.40 |
| 1:A:316:A:N3 | 1:A:336:G:O2' | 2.48 | 0.40 |
| 38:A:9052:HOH:O | 18:Q:81:LYS:HG2 | 2.21 | 0.40 |
| 1:A:2443:C:H3' | 38:A:9982:HOH:O | 2.21 | 0.40 |
| 1:A:204:A:H2' | 1:A:205:U:H5' | 2.02 | 0.40 |
| 1:A:1498:G:O2' | 1:A:1499:U:H5' | 2.21 | 0.40 |
| 1:A:2649:A:H8 | 1:A:2649:A:H5' | 1.86 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:E:156:LEU:HD12 | 6:E:156:LEU:O | 2.21 | 0.40 |
| 1:A:1886:A:H4' | 38:1:8405:HOH:O | 2.20 | 0.40 |
| 15:N:137:ASP:O | 15:N:142:LYS:HE3 | 2.20 | 0.40 |
| 17:P:88:LYS:HB3 | 38:P:7061:HOH:O | 2.20 | 0.40 |
| 11:J:158:ASN:ND2 | 38:J:8388:HOH:O | 2.54 | 0.40 |
| 5:D:183:GLU:OE1 | 5:D:183:GLU:HA | 2.21 | 0.40 |
| 5:D:11:LEU:HA | 38:D:8618:HOH:O | 2.22 | 0.40 |
| 28:1:31:ILE:CG2 | 28:1:32:LYS:N | 2.84 | 0.40 |
| 5:D:30:PRO:HB2 | 5:D:39:GLN:HE21 | 1.83 | 0.40 |
| 38:A:6557:HOH:O | 20:S:33:ARG:HD3 | 2.20 | 0.40 |
| 1:A:656:G:H3' | 17:P:37:ARG:HH12 | 1.86 | 0.40 |
| 5:D:5:ARG:HD2 | 5:D:8:LYS:NZ | 2.36 | 0.40 |
| 5:D:115:VAL:HA | 5:D:116:PRO:HD3 | 1.88 | 0.40 |
| 1:A:1114:A:H2' | 1:A:1115:U:H6 | 1.85 | 0.40 |
| 1:A:1656:A:H5' | 38:A:3906:HOH:O | 2.22 | 0.40 |
| 1:A:473:A:O2' | 1:A:474:C:H5' | 2.22 | 0.40 |
| 1:A:2382:A:H5' | 38:4:8533:HOH:O | 2.22 | 0.40 |
| 1:A:1501:A:H4' | 38:A:5090:HOH:O | 2.21 | 0.40 |
| 1:A:2356:A:H2' | 1:A:2357:G:O4' | 2.21 | 0.40 |
| 16:O:128:ASP:HA | 38:O:8562:HOH:O | 2.21 | 0.40 |
| 1:A:1216:G:O2' | 1:A:1217:G:H5' | 2.22 | 0.40 |
| 1:A:940:G:O2' | 1:A:1032:A:N1 | 2.51 | 0.40 |
| 38:A:8843:HOH:O | 25:X:9:GLY:HA3 | 2.20 | 0.40 |

There are no symmetry-related clashes.

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 | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 4 | C | 235/239 (98%) | 202 (86%) | 27 (12%) | 6 (3%) | 7 | 33 |
| 5 | D | 335/337 (99%) | 291 (87%) | 36 (11%) | 8 (2%) | 7 | 35 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 6 | E | 244/246 (99%) | 210 (86%) | 31 (13%) | 3 (1%) | 16 | 56 |
| 7 | F | 134/176 (76%) | 95 (71%) | 28 (21%) | 11 (8%) | 1 | 5 |
| 8 | G | 170/177 (96%) | 159 (94%) | 10 (6%) | 1 (1%) | 30 | 72 |
| 9 | H | 117/119 (98%) | 100 (86%) | 13 (11%) | 4 (3%) | 5 | 25 |
| 10 | I | 25/348 (7%) | 23 (92%) | 1 (4%) | 1 (4%) | 4 | 21 |
| 11 | J | 152/167 (91%) | 129 (85%) | 18 (12%) | 5 (3%) | 5 | 26 |
| 12 | K | 140/145 (97%) | 126 (90%) | 8 (6%) | 6 (4%) | 3 | 19 |
| 13 | L | 130/132 (98%) | 115 (88%) | 13 (10%) | 2 (2%) | 13 | 50 |
| 14 | M | 141/164 (86%) | 117 (83%) | 22 (16%) | 2 (1%) | 14 | 51 |
| 15 | N | 192/194 (99%) | 164 (85%) | 25 (13%) | 3 (2%) | 12 | 48 |
| 16 | O | 184/186 (99%) | 160 (87%) | 17 (9%) | 7 (4%) | 4 | 22 |
| 17 | P | 113/115 (98%) | 105 (93%) | 8 (7%) | 0 | 100 | 100 |
| 18 | Q | 141/148 (95%) | 132 (94%) | 8 (6%) | 1 (1%) | 26 | 70 |
| 19 | R | 93/95 (98%) | 88 (95%) | 4 (4%) | 1 (1%) | 17 | 58 |
| 20 | S | 148/154 (96%) | 134 (90%) | 14 (10%) | 0 | 100 | 100 |
| 21 | T | 79/84 (94%) | 71 (90%) | 8 (10%) | 0 | 100 | 100 |
| 22 | U | 117/119 (98%) | 103 (88%) | 12 (10%) | 2 (2%) | 11 | 46 |
| 23 | V | 51/66 (77%) | 44 (86%) | 6 (12%) | 1 (2%) | 9 | 41 |
| 24 | W | 63/70 (90%) | 55 (87%) | 5 (8%) | 3 (5%) | 3 | 17 |
| 25 | X | 152/154 (99%) | 142 (93%) | 8 (5%) | 2 (1%) | 15 | 53 |
| 26 | Y | 80/91 (88%) | 70 (88%) | 8 (10%) | 2 (2%) | 7 | 34 |
| 27 | Z | 140/240 (58%) | 135 (96%) | 5 (4%) | 0 | 100 | 100 |
| 28 | 1 | 71/73 (97%) | 59 (83%) | 10 (14%) | 2 (3%) | 6 | 30 |
| 29 | 2 | 54/56 (96%) | 51 (94%) | 3 (6%) | 0 | 100 | 100 |
| 30 | 3 | 42/48 (88%) | 42 (100%) | 0 | 0 | 100 | 100 |
| 31 | 4 | 90/92 (98%) | 84 (93%) | 4 (4%) | 2 (2%) | 8 | 38 |
| All | All | 3633/4235 (86%) | 3206 (88%) | 352 (10%) | 75 (2%) | 9 | 40 |

All (75) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | D | 139 | ASP |
| 5 | D | 184 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | E | 8 | LEU |
| 7 | F | 93 | LEU |
| 7 | F | 95 | THR |
| 7 | F | 173 | GLU |
| 9 | H | 101 | ALA |
| 11 | J | 138 | PRO |
| 11 | J | 162 | SER |
| 16 | O | 154 | LEU |
| 16 | O | 162 | ASP |
| 16 | O | 183 | ASP |
| 18 | Q | 116 | SER |
| 31 | 4 | 56 | PRO |
| 4 | C | 34 | ASP |
| 4 | C | 37 | VAL |
| 4 | C | 132 | ASP |
| 5 | D | 34 | GLY |
| 5 | D | 107 | SER |
| 5 | D | 169 | GLY |
| 7 | F | 11 | HIS |
| 7 | F | 20 | LYS |
| 7 | F | 137 | PRO |
| 7 | F | 171 | ASP |
| 11 | J | 164 | ALA |
| 12 | K | 5 | GLU |
| 14 | M | 80 | ASP |
| 15 | N | 18 | GLY |
| 16 | O | 164 | ASP |
| 24 | W | 43 | PRO |
| 25 | X | 77 | ALA |
| 28 | 1 | 20 | LEU |
| 31 | 4 | 57 | GLY |
| 6 | E | 58 | ALA |
| 7 | F | 16 | PRO |
| 7 | F | 36 | ASN |
| 7 | F | 147 | ALA |
| 10 | I | 72 | ASP |
| 12 | K | 7 | ASP |
| 12 | K | 143 | LYS |
| 13 | L | 119 | GLN |
| 13 | L | 126 | SER |
| 14 | M | 21 | ARG |
| 16 | O | 181 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19 | R | 23 | THR |
| 6 | E | 232 | LEU |
| 7 | F | 82 | GLU |
| 8 | G | 44 | GLY |
| 9 | H | 64 | PRO |
| 12 | K | 65 | ASN |
| 15 | N | 6 | SER |
| 15 | N | 71 | SER |
| 22 | U | 53 | GLY |
| 23 | V | 7 | ASP |
| 25 | X | 49 | ASN |
| 26 | Y | 70 | ILE |
| 28 | 1 | 81 | LYS |
| 4 | C | 10 | GLY |
| 4 | C | 119 | ALA |
| 5 | D | 291 | ASP |
| 9 | H | 61 | MET |
| 11 | J | 40 | PRO |
| 12 | K | 89 | HIS |
| 12 | K | 141 | ALA |
| 16 | O | 139 | TRP |
| 22 | U | 44 | ALA |
| 24 | W | 40 | PRO |
| 9 | H | 71 | GLY |
| 16 | O | 167 | ASP |
| 26 | Y | 77 | PHE |
| 11 | J | 110 | GLY |
| 4 | C | 211 | LYS |
| 5 | D | 2 | GLN |
| 5 | D | 185 | GLY |
| 24 | W | 2 | 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 | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 4 | C | 179/181 (99%) | 166 (93%) | 13 (7%) | 17 | 52 |
| 5 | D | 282/282 (100%) | 267 (95%) | 15 (5%) | 28 | 67 |
| 6 | E | 193/193 (100%) | 177 (92%) | 16 (8%) | 14 | 46 |
| 7 | F | 117/147 (80%) | 108 (92%) | 9 (8%) | 16 | 50 |
| 8 | G | 152/155 (98%) | 147 (97%) | 5 (3%) | 45 | 82 |
| 9 | H | 92/92 (100%) | 91 (99%) | 1 (1%) | 80 | 94 |
| 10 | I | 27/283 (10%) | 27 (100%) | 0 | 100 | 100 |
| 11 | J | 122/122 (100%) | 111 (91%) | 11 (9%) | 12 | 41 |
| 12 | K | 118/121 (98%) | 107 (91%) | 11 (9%) | 11 | 39 |
| 13 | L | 106/106 (100%) | 104 (98%) | 2 (2%) | 65 | 90 |
| 14 | M | 112/126 (89%) | 107 (96%) | 5 (4%) | 34 | 74 |
| 15 | N | 166/166 (100%) | 157 (95%) | 9 (5%) | 27 | 66 |
| 16 | O | 149/149 (100%) | 144 (97%) | 5 (3%) | 44 | 81 |
| 17 | P | 93/93 (100%) | 92 (99%) | 1 (1%) | 80 | 94 |
| 18 | Q | 113/116 (97%) | 109 (96%) | 4 (4%) | 43 | 80 |
| 19 | R | 79/79 (100%) | 75 (95%) | 4 (5%) | 29 | 69 |
| 20 | S | 117/121 (97%) | 113 (97%) | 4 (3%) | 44 | 81 |
| 21 | T | 71/73 (97%) | 70 (99%) | 1 (1%) | 74 | 93 |
| 22 | U | 105/105 (100%) | 99 (94%) | 6 (6%) | 25 | 64 |
| 23 | V | 44/52 (85%) | 44 (100%) | 0 | 100 | 100 |
| 24 | W | 51/56 (91%) | 50 (98%) | 1 (2%) | 63 | 89 |
| 25 | X | 130/130 (100%) | 124 (95%) | 6 (5%) | 33 | 73 |
| 26 | Y | 66/73 (90%) | 61 (92%) | 5 (8%) | 16 | 51 |
| 27 | Z | 120/195 (62%) | 115 (96%) | 5 (4%) | 36 | 76 |
| 28 | 1 | 56/56 (100%) | 54 (96%) | 2 (4%) | 42 | 79 |
| 29 | 2 | 46/46 (100%) | 46 (100%) | 0 | 100 | 100 |
| 30 | 3 | 42/44 (96%) | 41 (98%) | 1 (2%) | 57 | 87 |
| 31 | 4 | 79/79 (100%) | 75 (95%) | 4 (5%) | 29 | 69 |
| All | All | 3027/3441 (88%) | 2881 (95%) | 146 (5%) | 31 | 71 |

All (146) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | C | 3 | ARG |
| 4 | C | 33 | GLU |
| 4 | C | 36 | ASP |
| 4 | C | 55 | VAL |
| 4 | C | 68 | ILE |
| 4 | C | 69 | LEU |
| 4 | C | 78 | ASP |
| 4 | C | 94 | LEU |
| 4 | C | 120 | ARG |
| 4 | C | 131 | HIS |
| 4 | C | 153 | ARG |
| 4 | C | 179 | MET |
| 4 | C | 217 | ARG |
| 5 | D | 7 | ARG |
| 5 | D | 11 | LEU |
| 5 | D | 27 | ASN |
| 5 | D | 33 | ASP |
| 5 | D | 63 | GLU |
| 5 | D | 97 | LEU |
| 5 | D | 98 | THR |
| 5 | D | 103 | ASP |
| 5 | D | 162 | MET |
| 5 | D | 234 | ARG |
| 5 | D | 251 | VAL |
| 5 | D | 254 | GLN |
| 5 | D | 256 | GLN |
| 5 | D | 307 | ARG |
| 5 | D | 312 | ARG |
| 6 | E | 2 | GLN |
| 6 | E | 27 | ARG |
| 6 | E | 67 | GLN |
| 6 | E | 76 | ARG |
| 6 | E | 91 | PRO |
| 6 | E | 94 | THR |
| 6 | E | 115 | LEU |
| 6 | E | 136 | VAL |
| 6 | E | 180 | SER |
| 6 | E | 187 | ARG |
| 6 | E | 214 | THR |
| 6 | E | 222 | ASP |
| 6 | E | 223 | LEU |
| 6 | E | 234 | VAL |
| 6 | E | 236 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | E | 240 | LEU |
| 7 | F | 24 | HIS |
| 7 | F | 61 | PHE |
| 7 | F | 99 | ASP |
| 7 | F | 100 | ASP |
| 7 | F | 131 | THR |
| 7 | F | 136 | ARG |
| 7 | F | 137 | PRO |
| 7 | F | 149 | ARG |
| 7 | F | 170 | TYR |
| 8 | G | 7 | ILE |
| 8 | G | 12 | ASP |
| 8 | G | 15 | GLN |
| 8 | G | 102 | VAL |
| 8 | G | 164 | ASP |
| 9 | H | 78 | GLU |
| 11 | J | 30 | GLN |
| 11 | J | 59 | ASN |
| 11 | J | 61 | LEU |
| 11 | J | 72 | VAL |
| 11 | J | 73 | GLN |
| 11 | J | 82 | LYS |
| 11 | J | 86 | ARG |
| 11 | J | 94 | ARG |
| 11 | J | 142 | VAL |
| 11 | J | 150 | LYS |
| 11 | J | 166 | ASN |
| 12 | K | 46 | ILE |
| 12 | K | 47 | THR |
| 12 | K | 52 | GLN |
| 12 | K | 74 | ARG |
| 12 | K | 76 | ASP |
| 12 | K | 79 | PHE |
| 12 | K | 107 | ASN |
| 12 | K | 112 | ASP |
| 12 | K | 120 | SER |
| 12 | K | 127 | ILE |
| 12 | K | 131 | THR |
| 13 | L | 10 | GLN |
| 13 | L | 98 | VAL |
| 14 | M | 30 | ARG |
| 14 | M | 35 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14 | M | 80 | ASP |
| 14 | M | 99 | GLU |
| 14 | M | 117 | GLU |
| 15 | N | 46 | LEU |
| 15 | N | 68 | ARG |
| 15 | N | 81 | ARG |
| 15 | N | 87 | MET |
| 15 | N | 93 | ARG |
| 15 | N | 99 | ARG |
| 15 | N | 116 | ASN |
| 15 | N | 159 | THR |
| 15 | N | 164 | THR |
| 16 | O | 26 | LEU |
| 16 | O | 49 | THR |
| 16 | O | 128 | ASP |
| 16 | O | 152 | GLU |
| 16 | O | 163 | PHE |
| 17 | P | 98 | LEU |
| 18 | Q | 52 | LYS |
| 18 | Q | 91 | LYS |
| 18 | Q | 94 | TRP |
| 18 | Q | 98 | ILE |
| 19 | R | 11 | ARG |
| 19 | R | 16 | ASN |
| 19 | R | 57 | ASP |
| 19 | R | 95 | GLU |
| 20 | S | 13 | THR |
| 20 | S | 39 | THR |
| 20 | S | 82 | GLU |
| 20 | S | 132 | ARG |
| 21 | T | 10 | VAL |
| 22 | U | 19 | ARG |
| 22 | U | 23 | VAL |
| 22 | U | 26 | THR |
| 22 | U | 39 | ASN |
| 22 | U | 48 | VAL |
| 22 | U | 73 | HIS |
| 24 | W | 65 | ASP |
| 25 | X | 35 | VAL |
| 25 | X | 88 | THR |
| 25 | X | 122 | ARG |
| 25 | X | 142 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | X | 146 | ILE |
| 25 | X | 154 | ARG |
| 26 | Y | 15 | ARG |
| 26 | Y | 27 | ASP |
| 26 | Y | 44 | ASP |
| 26 | Y | 49 | ARG |
| 26 | Y | 72 | VAL |
| 27 | Z | 163 | THR |
| 27 | Z | 189 | ASN |
| 27 | Z | 200 | THR |
| 27 | Z | 203 | VAL |
| 27 | Z | 235 | GLU |
| 28 | 1 | 11 | THR |
| 28 | 1 | 64 | ILE |
| 30 | 3 | 18 | ASN |
| 31 | 4 | 11 | CYS |
| 31 | 4 | 42 | ARG |
| 31 | 4 | 56 | PRO |
| 31 | 4 | 65 | THR |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | C | 29 | HIS |
| 4 | C | 47 | HIS |
| 4 | C | 92 | ASN |
| 4 | C | 125 | ASN |
| 4 | C | 127 | GLN |
| 4 | C | 176 | HIS |
| 4 | C | 199 | HIS |
| 5 | D | 27 | ASN |
| 5 | D | 145 | HIS |
| 5 | D | 221 | GLN |
| 5 | D | 238 | ASN |
| 5 | D | 260 | HIS |
| 5 | D | 320 | GLN |
| 5 | D | 332 | ASN |
| 6 | E | 2 | GLN |
| 6 | E | 39 | GLN |
| 6 | E | 129 | HIS |
| 6 | E | 163 | HIS |
| 7 | F | 47 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | F | 85 | GLN |
| 7 | F | 103 | ASN |
| 7 | F | 133 | ASN |
| 8 | G | 106 | ASN |
| 8 | G | 119 | HIS |
| 8 | G | 143 | GLN |
| 9 | H | 80 | GLN |
| 10 | I | 17 | GLN |
| 10 | I | 64 | ASN |
| 11 | J | 35 | ASN |
| 11 | J | 36 | ASN |
| 11 | J | 45 | GLN |
| 11 | J | 55 | GLN |
| 11 | J | 58 | HIS |
| 11 | J | 59 | ASN |
| 11 | J | 69 | ASN |
| 11 | J | 74 | ASN |
| 11 | J | 91 | HIS |
| 11 | J | 129 | ASN |
| 11 | J | 130 | HIS |
| 11 | J | 166 | ASN |
| 12 | K | 52 | GLN |
| 12 | K | 107 | ASN |
| 12 | K | 126 | ASN |
| 13 | L | 10 | GLN |
| 14 | M | 18 | HIS |
| 14 | M | 41 | HIS |
| 14 | M | 42 | ASN |
| 15 | N | 26 | HIS |
| 15 | N | 58 | GLN |
| 15 | N | 176 | GLN |
| 16 | O | 40 | ASN |
| 16 | O | 107 | ASN |
| 17 | P | 53 | GLN |
| 18 | Q | 50 | GLN |
| 18 | Q | 66 | GLN |
| 18 | Q | 73 | HIS |
| 18 | Q | 118 | GLN |
| 19 | R | 16 | ASN |
| 19 | R | 40 | HIS |
| 20 | S | 61 | GLN |
| 20 | S | 94 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20 | S | 98 | ASN |
| 20 | S | 113 | HIS |
| 20 | S | 117 | HIS |
| 20 | S | 122 | GLN |
| 21 | T | 53 | ASN |
| 22 | U | 39 | ASN |
| 22 | U | 73 | HIS |
| 23 | V | 39 | ASN |
| 24 | W | 60 | GLN |
| 25 | X | 2 | HIS |
| 25 | X | 12 | ASN |
| 25 | X | 27 | HIS |
| 25 | X | 28 | HIS |
| 25 | X | 59 | GLN |
| 25 | X | 87 | HIS |
| 25 | X | 110 | GLN |
| 25 | X | 119 | HIS |
| 25 | X | 125 | HIS |
| 25 | X | 141 | HIS |
| 26 | Y | 23 | HIS |
| 27 | Z | 133 | HIS |
| 27 | Z | 134 | HIS |
| 27 | Z | 149 | GLN |
| 27 | Z | 189 | ASN |
| 28 | 1 | 33 | HIS |
| 28 | 1 | 70 | GLN |
| 29 | 2 | 8 | GLN |
| 29 | 2 | 16 | HIS |
| 29 | 2 | 28 | HIS |
| 30 | 3 | 16 | ASN |
| 30 | 3 | 18 | ASN |
| 30 | 3 | 41 | HIS |
| 30 | 3 | 45 | ASN |
| 31 | 4 | 15 | ASN |
| 31 | 4 | 30 | GLN |
| 31 | 4 | 48 | ASN |

5.3.3 RNA

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | A | 2747/2922 (94%) | 244 (8%) | 32 (1%) |

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| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 2 | B | 121/122 (99%) | 16 (13%) | 3 (2%) |
| 3 | 5 | 2/3 (66%) | 1 (50%) | 0 |
| 3 | 6 | 2/3 (66%) | 0 | 0 |
| All | All | 2872/3050 (94%) | 261 (9%) | 35 (1%) |

All (261) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 11 | A |
| 1 | A | 31 | C |
| 1 | A | 60 | A |
| 1 | A | 67 | A |
| 1 | A | 69 | A |
| 1 | A | 70 | A |
| 1 | A | 71 | G |
| 1 | A | 87 | C |
| 1 | A | 88 | G |
| 1 | A | 114 | A |
| 1 | A | 115 | U |
| 1 | A | 120 | A |
| 1 | A | 130 | C |
| 1 | A | 139 | C |
| 1 | A | 141 | C |
| 1 | A | 151 | A |
| 1 | A | 166 | A |
| 1 | A | 169 | A |
| 1 | A | 186 | A |
| 1 | A | 191 | A |
| 1 | A | 192 | A |
| 1 | A | 200 | U |
| 1 | A | 219 | G |
| 1 | A | 237 | G |
| 1 | A | 271 | C |
| 1 | A | 272 | A |
| 1 | A | 273 | G |
| 1 | A | 283 | U |
| 1 | A | 284 | C |
| 1 | A | 285 | A |
| 1 | A | 308 | U |
| 1 | A | 309 | C |
| 1 | A | 317 | A |
| 1 | A | 318 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 336 | G |
| 1 | A | 337 | A |
| 1 | A | 345 | G |
| 1 | A | 358 | G |
| 1 | A | 381 | G |
| 1 | A | 397 | A |
| 1 | A | 417 | G |
| 1 | A | 461 | C |
| 1 | A | 487 | G |
| 1 | A | 498 | A |
| 1 | A | 510 | U |
| 1 | A | 511 | A |
| 1 | A | 514 | G |
| 1 | A | 537 | G |
| 1 | A | 538 | C |
| 1 | A | 539 | G |
| 1 | A | 542 | A |
| 1 | A | 545 | G |
| 1 | A | 553 | G |
| 1 | A | 559 | U |
| 1 | A | 588 | G |
| 1 | A | 604 | G |
| 1 | A | 605 | C |
| 1 | A | 620 | A |
| 1 | A | 632 | A |
| 1 | A | 644 | G |
| 1 | A | 660 | A |
| 1 | A | 688 | A |
| 1 | A | 701 | U |
| 1 | A | 717 | C |
| 1 | A | 777 | U |
| 1 | A | 809 | G |
| 1 | A | 821 | U |
| 1 | A | 835 | U |
| 1 | A | 840 | U |
| 1 | A | 857 | A |
| 1 | A | 858 | U |
| 1 | A | 868 | G |
| 1 | A | 869 | G |
| 1 | A | 871 | G |
| 1 | A | 872 | U |
| 1 | A | 875 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 877 | G |
| 1 | A | 878 | G |
| 1 | A | 884 | C |
| 1 | A | 885 | G |
| 1 | A | 898 | G |
| 1 | A | 905 | C |
| 1 | A | 920 | C |
| 1 | A | 921 | G |
| 1 | A | 923 | A |
| 1 | A | 953 | G |
| 1 | A | 960 | G |
| 1 | A | 961 | A |
| 1 | A | 1006 | A |
| 1 | A | 1008 | C |
| 1 | A | 1029 | U |
| 1 | A | 1045 | G |
| 1 | A | 1059 | G |
| 1 | A | 1060 | C |
| 1 | A | 1072 | G |
| 1 | A | 1081 | A |
| 1 | A | 1087 | G |
| 1 | A | 1088 | A |
| 1 | A | 1109 | U |
| 1 | A | 1110 | G |
| 1 | A | 1119 | G |
| 1 | A | 1130 | U |
| 1 | A | 1137 | G |
| 1 | A | 1151 | G |
| 1 | A | 1161 | A |
| 1 | A | 1162 | G |
| 1 | A | 1164 | U |
| 1 | A | 1165 | G |
| 1 | A | 1166 | A |
| 1 | A | 1171 | A |
| 1 | A | 1174 | A |
| 1 | A | 1175 | G |
| 1 | A | 1177 | A |
| 1 | A | 1185 | U |
| 1 | A | 1192 | A |
| 1 | A | 1193 | A |
| 1 | A | 1206 | U |
| 1 | A | 1216 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1237 | U |
| 1 | A | 1238 | C |
| 1 | A | 1239 | G |
| 1 | A | 1279 | U |
| 1 | A | 1289 | C |
| 1 | A | 1342 | C |
| 1 | A | 1353 | C |
| 1 | A | 1360 | C |
| 1 | A | 1377 | C |
| 1 | A | 1407 | A |
| 1 | A | 1451 | C |
| 1 | A | 1474 | C |
| 1 | A | 1488 | U |
| 1 | A | 1505 | U |
| 1 | A | 1506 | U |
| 1 | A | 1524 | U |
| 1 | A | 1525 | G |
| 1 | A | 1526 | A |
| 1 | A | 1528 | A |
| 1 | A | 1564 | C |
| 1 | A | 1580 | A |
| 1 | A | 1592 | G |
| 1 | A | 1625 | U |
| 1 | A | 1626 | A |
| 1 | A | 1633 | C |
| 1 | A | 1634 | G |
| 1 | A | 1656 | A |
| 1 | A | 1667 | A |
| 1 | A | 1682 | A |
| 1 | A | 1684 | A |
| 1 | A | 1685 | A |
| 1 | A | 1692 | C |
| 1 | A | 1701 | A |
| 1 | A | 1722 | U |
| 1 | A | 1723 | G |
| 1 | A | 1725 | C |
| 1 | A | 1730 | G |
| 1 | A | 1731 | C |
| 1 | A | 1752 | G |
| 1 | A | 1778 | A |
| 1 | A | 1798 | C |
| 1 | A | 1819 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1820 | G |
| 1 | A | 1829 | A |
| 1 | A | 1856 | C |
| 1 | A | 1879 | U |
| 1 | A | 1904 | A |
| 1 | A | 1919 | A |
| 1 | A | 1942 | A |
| 1 | A | 1971 | G |
| 1 | A | 1973 | A |
| 1 | A | 1974 | G |
| 1 | A | 1978 | A |
| 1 | A | 1980 | U |
| 1 | A | 1996 | U |
| 1 | A | 2008 | U |
| 1 | A | 2011 | A |
| 1 | A | 2012 | U |
| 1 | A | 2013 | G |
| 1 | A | 2033 | G |
| 1 | A | 2034 | U |
| 1 | A | 2064 | U |
| 1 | A | 2072 | G |
| 1 | A | 2073 | G |
| 1 | A | 2074 | A |
| 1 | A | 2096 | A |
| 1 | A | 2101 | A |
| 1 | A | 2102 | G |
| 1 | A | 2103 | A |
| 1 | A | 2110 | G |
| 1 | A | 2238 | A |
| 1 | A | 2258 | A |
| 1 | A | 2271 | G |
| 1 | A | 2272 | G |
| 1 | A | 2317 | C |
| 1 | A | 2321 | A |
| 1 | A | 2346 | C |
| 1 | A | 2354 | A |
| 1 | A | 2361 | A |
| 1 | A | 2369 | A |
| 1 | A | 2379 | G |
| 1 | A | 2422 | U |
| 1 | A | 2462 | G |
| 1 | A | 2467 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 2476 | C |
| 1 | A | 2480 | G |
| 1 | A | 2483 | A |
| 1 | A | 2507 | G |
| 1 | A | 2509 | A |
| 1 | A | 2511 | A |
| 1 | A | 2533 | C |
| 1 | A | 2537 | G |
| 1 | A | 2541 | U |
| 1 | A | 2553 | A |
| 1 | A | 2564 | G |
| 1 | A | 2589 | U |
| 1 | A | 2601 | A |
| 1 | A | 2602 | G |
| 1 | A | 2608 | C |
| 1 | A | 2613 | G |
| 1 | A | 2616 | G |
| 1 | A | 2617 | G |
| 1 | A | 2637 | A |
| 1 | A | 2649 | A |
| 1 | A | 2664 | A |
| 1 | A | 2681 | A |
| 1 | A | 2682 | C |
| 1 | A | 2719 | A |
| 1 | A | 2726 | U |
| 1 | A | 2747 | C |
| 1 | A | 2748 | G |
| 1 | A | 2749 | U |
| 1 | A | 2750 | G |
| 1 | A | 2762 | C |
| 1 | A | 2768 | A |
| 1 | A | 2786 | G |
| 1 | A | 2792 | A |
| 1 | A | 2800 | A |
| 1 | A | 2811 | A |
| 1 | A | 2825 | C |
| 1 | A | 2850 | C |
| 1 | A | 2876 | G |
| 1 | A | 2890 | A |
| 1 | A | 2896 | A |
| 1 | A | 2903 | C |
| 1 | A | 2914 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | B | 3002 | U |
| 2 | B | 3014 | G |
| 2 | B | 3022 | G |
| 2 | B | 3023 | U |
| 2 | B | 3024 | U |
| 2 | B | 3025 | G |
| 2 | B | 3026 | C |
| 2 | B | 3041 | C |
| 2 | B | 3043 | G |
| 2 | B | 3044 | A |
| 2 | B | 3052 | A |
| 2 | B | 3057 | A |
| 2 | B | 3066 | G |
| 2 | B | 3077 | A |
| 2 | B | 3114 | G |
| 2 | B | 3122 | C |
| 3 | 5 | 75 | C |

All (35) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 10 | U |
| 1 | A | 129 | A |
| 1 | A | 284 | C |
| 1 | A | 338 | C |
| 1 | A | 603 | A |
| 1 | A | 604 | G |
| 1 | A | 716 | G |
| 1 | A | 834 | G |
| 1 | A | 857 | A |
| 1 | A | 871 | G |
| 1 | A | 877 | G |
| 1 | A | 898 | G |
| 1 | A | 1080 | C |
| 1 | A | 1232 | A |
| 1 | A | 1237 | U |
| 1 | A | 1352 | A |
| 1 | A | 1377 | C |
| 1 | A | 1450 | C |
| 1 | A | 1563 | G |
| 1 | A | 1667 | A |
| 1 | A | 1730 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1856 | C |
| 1 | A | 1979 | G |
| 1 | A | 2011 | A |
| 1 | A | 2313 | C |
| 1 | A | 2467 | A |
| 1 | A | 2526 | C |
| 1 | A | 2536 | C |
| 1 | A | 2616 | G |
| 1 | A | 2649 | A |
| 1 | A | 2718 | C |
| 1 | A | 2791 | U |
| 2 | B | 3024 | U |
| 2 | B | 3065 | A |
| 2 | B | 3103 | 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 235 ligands modelled in this entry, 233 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 36 | PHA | 5 | 77 | 3 | 10,11,11 | 0.85 | 0 | 10,13,13 | 1.01 | 0 |
| 36 | PHA | 6 | 77 | 3 | 10,10,11 | 0.71 | 0 | 10,11,13 | 0.38 | 0 |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|---------|
| 36 | PHA | 5 | 77 | 3 | - | 0/4/6/6 | 0/1/1/1 |
| 36 | PHA | 6 | 77 | 3 | - | 0/3/4/6 | 0/1/1/1 |

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.

2 monomers are involved in 5 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 36 | 5 | 77 | PHA | 5 | 0 |
| 36 | 6 | 77 | PHA | 4 | 0 |

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 | A | 2754/2922 (94%) | 0.18 | 51 (1%) 70 41 | 19, 47, 95, 154 | 0 |
| 2 | B | 122/122 (100%) | 0.16 | 6 (4%) 33 13 | 30, 62, 92, 154 | 0 |
| 3 | 5 | 3/3 (100%) | 1.71 | 1 (33%) 0 0 | 29, 29, 31, 35 | 3 (100%) |
| 3 | 6 | 3/3 (100%) | 2.49 | 3 (100%) 0 0 | 15, 15, 17, 31 | 3 (100%) |
| 4 | C | 237/239 (99%) | 0.24 | 8 (3%) 49 21 | 27, 52, 91, 115 | 0 |
| 5 | D | 337/337 (100%) | 0.06 | 2 (0%) 90 73 | 26, 55, 84, 96 | 0 |
| 6 | E | 246/246 (100%) | -0.20 | 0 100 100 | 19, 47, 71, 80 | 0 |
| 7 | F | 140/176 (79%) | 1.00 | 27 (19%) 2 1 | 53, 101, 124, 131 | 0 |
| 8 | G | 172/177 (97%) | 0.32 | 4 (2%) 64 33 | 41, 68, 91, 99 | 0 |
| 9 | H | 119/119 (100%) | 0.50 | 5 (4%) 40 16 | 53, 77, 104, 111 | 0 |
| 10 | I | 29/348 (8%) | 1.28 | 4 (13%) 4 1 | 66, 86, 97, 103 | 0 |
| 11 | J | 156/167 (93%) | -0.07 | 1 (0%) 90 73 | 30, 52, 77, 81 | 0 |
| 12 | K | 142/145 (97%) | -0.17 | 0 100 100 | 34, 47, 71, 90 | 0 |
| 13 | L | 132/132 (100%) | 0.01 | 0 100 100 | 31, 53, 78, 86 | 0 |
| 14 | M | 145/164 (88%) | 0.10 | 5 (3%) 49 21 | 21, 67, 108, 117 | 0 |
| 15 | N | 194/194 (100%) | -0.02 | 1 (0%) 91 76 | 30, 47, 68, 80 | 0 |
| 16 | O | 186/186 (100%) | 0.19 | 9 (4%) 34 14 | 35, 65, 112, 125 | 0 |
| 17 | P | 115/115 (100%) | -0.09 | 0 100 100 | 36, 54, 74, 83 | 0 |
| 18 | Q | 143/148 (96%) | 0.42 | 1 (0%) 89 70 | 36, 57, 71, 80 | 0 |
| 19 | R | 95/95 (100%) | -0.25 | 0 100 100 | 32, 42, 57, 73 | 0 |
| 20 | S | 150/154 (97%) | -0.01 | 0 100 100 | 29, 43, 64, 75 | 0 |
| 21 | T | 81/84 (96%) | 0.26 | 1 (1%) 81 55 | 41, 62, 81, 85 | 0 |
| 22 | U | 119/119 (100%) | 0.39 | 7 (5%) 26 10 | 38, 60, 86, 105 | 0 |
| 23 | V | 53/66 (80%) | 0.41 | 2 (3%) 44 18 | 42, 53, 71, 80 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|--------|
| 24 | W | 65/70 (92%) | 0.88 | 5 (7%) 16 6 | 56, 79, 120, 125 | 0 |
| 25 | X | 154/154 (100%) | -0.38 | 0 100 100 | 29, 45, 62, 74 | 0 |
| 26 | Y | 82/91 (90%) | 0.55 | 8 (9%) 10 4 | 42, 56, 79, 100 | 0 |
| 27 | Z | 142/240 (59%) | -0.10 | 1 (0%) 89 70 | 25, 45, 67, 86 | 0 |
| 28 | 1 | 73/73 (100%) | 0.34 | 5 (6%) 20 7 | 43, 61, 76, 81 | 0 |
| 29 | 2 | 56/56 (100%) | -0.26 | 0 100 100 | 24, 33, 39, 41 | 0 |
| 30 | 3 | 46/48 (95%) | 0.89 | 6 (13%) 5 2 | 35, 65, 118, 126 | 0 |
| 31 | 4 | 92/92 (100%) | 0.06 | 0 100 100 | 39, 55, 69, 78 | 0 |
| All | All | 6583/7285 (90%) | 0.16 | 163 (2%) 61 30 | 15, 52, 97, 154 | 6 (0%) |

All (163) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 24 | W | 1 | THR | 12.4 |
| 2 | B | 3001 | U | 7.8 |
| 1 | A | 2237 | G | 5.4 |
| 1 | A | 1172 | G | 5.3 |
| 7 | F | 66 | GLY | 5.3 |
| 24 | W | 43 | PRO | 4.6 |
| 1 | A | 1173 | A | 4.5 |
| 2 | B | 3025 | G | 4.5 |
| 7 | F | 57 | THR | 4.3 |
| 7 | F | 62 | ASP | 4.2 |
| 1 | A | 1177 | A | 4.1 |
| 7 | F | 63 | ILE | 4.1 |
| 21 | T | 81 | ILE | 3.8 |
| 22 | U | 119 | ALA | 3.8 |
| 26 | Y | 88 | GLU | 3.8 |
| 7 | F | 89 | PRO | 3.6 |
| 9 | H | 106 | THR | 3.6 |
| 10 | I | 21 | ASP | 3.6 |
| 5 | D | 1 | PRO | 3.6 |
| 1 | A | 1169 | U | 3.5 |
| 7 | F | 90 | LEU | 3.5 |
| 16 | O | 162 | ASP | 3.5 |
| 7 | F | 10 | PHE | 3.5 |
| 28 | 1 | 11 | THR | 3.4 |
| 2 | B | 3023 | U | 3.4 |
| 4 | C | 236 | GLY | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 735 | C | 3.3 |
| 16 | O | 186 | LEU | 3.3 |
| 1 | A | 1525 | G | 3.3 |
| 30 | 3 | 36 | ASN | 3.2 |
| 7 | F | 85 | GLN | 3.2 |
| 30 | 3 | 41 | HIS | 3.1 |
| 9 | H | 19 | ALA | 3.1 |
| 1 | A | 1171 | A | 3.1 |
| 4 | C | 36 | ASP | 3.0 |
| 7 | F | 170 | TYR | 3.0 |
| 30 | 3 | 35 | ARG | 3.0 |
| 7 | F | 55 | LYS | 3.0 |
| 10 | I | 23 | ILE | 3.0 |
| 1 | A | 1174 | A | 3.0 |
| 7 | F | 171 | ASP | 2.9 |
| 8 | G | 100 | ASP | 2.9 |
| 1 | A | 1198 | U | 2.9 |
| 3 | 6 | 76 | A | 2.9 |
| 7 | F | 69 | ILE | 2.9 |
| 1 | A | 1951 | G | 2.9 |
| 7 | F | 102 | GLY | 2.9 |
| 1 | A | 2238 | A | 2.9 |
| 16 | O | 159 | TYR | 2.9 |
| 1 | A | 285 | A | 2.8 |
| 1 | A | 2637 | A | 2.8 |
| 30 | 3 | 38 | LYS | 2.8 |
| 1 | A | 970 | U | 2.8 |
| 1 | A | 1170 | U | 2.8 |
| 4 | C | 85 | ASP | 2.8 |
| 1 | A | 960 | G | 2.8 |
| 16 | O | 166 | ALA | 2.7 |
| 2 | B | 3122 | C | 2.7 |
| 1 | A | 1190 | G | 2.7 |
| 1 | A | 1950 | G | 2.7 |
| 1 | A | 2254 | G | 2.7 |
| 1 | A | 1948 | G | 2.7 |
| 1 | A | 1181 | A | 2.7 |
| 9 | H | 20 | LEU | 2.7 |
| 22 | U | 115 | GLU | 2.7 |
| 5 | D | 118 | ASP | 2.7 |
| 7 | F | 154 | LYS | 2.7 |
| 1 | A | 2250 | G | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 22 | U | 82 | THR | 2.7 |
| 27 | Z | 235 | GLU | 2.6 |
| 7 | F | 92 | GLU | 2.6 |
| 24 | W | 38 | GLY | 2.6 |
| 1 | A | 138 | U | 2.6 |
| 26 | Y | 80 | GLU | 2.6 |
| 1 | A | 1175 | G | 2.6 |
| 1 | A | 1167 | G | 2.6 |
| 1 | A | 2825 | C | 2.6 |
| 10 | I | 24 | VAL | 2.6 |
| 1 | A | 130 | C | 2.5 |
| 2 | B | 3024 | U | 2.5 |
| 8 | G | 129 | GLU | 2.5 |
| 7 | F | 56 | ARG | 2.5 |
| 4 | C | 35 | GLY | 2.5 |
| 14 | M | 60 | GLU | 2.5 |
| 8 | G | 10 | ASP | 2.5 |
| 1 | A | 1204 | C | 2.5 |
| 1 | A | 2004 | U | 2.4 |
| 3 | 5 | 74 | C | 2.4 |
| 8 | G | 45 | ASP | 2.4 |
| 1 | A | 282 | C | 2.4 |
| 24 | W | 41 | GLU | 2.4 |
| 4 | C | 37 | VAL | 2.4 |
| 23 | V | 52 | THR | 2.4 |
| 22 | U | 116 | ASP | 2.4 |
| 4 | C | 99 | ILE | 2.4 |
| 7 | F | 165 | PHE | 2.4 |
| 7 | F | 64 | ARG | 2.4 |
| 26 | Y | 74 | ALA | 2.4 |
| 1 | A | 1182 | C | 2.4 |
| 10 | I | 27 | ILE | 2.4 |
| 28 | 1 | 47 | LEU | 2.4 |
| 9 | H | 99 | THR | 2.4 |
| 1 | A | 2664 | A | 2.4 |
| 16 | O | 139 | TRP | 2.4 |
| 1 | A | 1205 | U | 2.3 |
| 4 | C | 237 | GLY | 2.3 |
| 22 | U | 117 | ASP | 2.3 |
| 1 | A | 1947 | G | 2.3 |
| 18 | Q | 141 | ILE | 2.3 |
| 2 | B | 3002 | U | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 16 | O | 160 | SER | 2.3 |
| 7 | F | 65 | GLU | 2.3 |
| 1 | A | 280 | C | 2.3 |
| 1 | A | 2884 | G | 2.3 |
| 3 | 6 | 75 | C | 2.3 |
| 1 | A | 1561 | U | 2.3 |
| 28 | 1 | 38 | LYS | 2.3 |
| 30 | 3 | 37 | HIS | 2.3 |
| 3 | 6 | 74 | C | 2.3 |
| 24 | W | 62 | GLU | 2.3 |
| 30 | 3 | 49 | GLU | 2.3 |
| 4 | C | 64 | ASP | 2.3 |
| 7 | F | 166 | ILE | 2.3 |
| 1 | A | 1192 | A | 2.2 |
| 26 | Y | 7 | GLU | 2.2 |
| 1 | A | 258 | G | 2.2 |
| 1 | A | 1168 | C | 2.2 |
| 11 | J | 35 | ASN | 2.2 |
| 1 | A | 2344 | G | 2.2 |
| 7 | F | 53 | LYS | 2.2 |
| 26 | Y | 85 | VAL | 2.2 |
| 14 | M | 104 | ASP | 2.2 |
| 23 | V | 54 | THR | 2.2 |
| 9 | H | 119 | ARG | 2.1 |
| 14 | M | 97 | VAL | 2.1 |
| 26 | Y | 76 | ARG | 2.1 |
| 1 | A | 1199 | A | 2.1 |
| 1 | A | 1200 | A | 2.1 |
| 1 | A | 1184 | C | 2.1 |
| 14 | M | 100 | ALA | 2.1 |
| 1 | A | 1180 | U | 2.1 |
| 26 | Y | 77 | PHE | 2.1 |
| 7 | F | 67 | ASP | 2.1 |
| 15 | N | 87 | MET | 2.1 |
| 28 | 1 | 21 | LYS | 2.1 |
| 7 | F | 26 | GLY | 2.1 |
| 16 | O | 152 | GLU | 2.1 |
| 7 | F | 54 | ALA | 2.1 |
| 7 | F | 27 | ILE | 2.1 |
| 1 | A | 1527 | A | 2.1 |
| 1 | A | 288 | A | 2.1 |
| 14 | M | 80 | ASP | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 16 | O | 138 | ASP | 2.1 |
| 22 | U | 112 | LEU | 2.1 |
| 22 | U | 59 | GLU | 2.0 |
| 1 | A | 1279 | U | 2.0 |
| 16 | O | 163 | PHE | 2.0 |
| 7 | F | 50 | VAL | 2.0 |
| 26 | Y | 73 | ARG | 2.0 |
| 1 | A | 808 | A | 2.0 |
| 1 | A | 1626 | A | 2.0 |
| 28 | 1 | 44 | PHE | 2.0 |
| 7 | F | 88 | LEU | 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(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 34 | NA | A | 8356 | 1/1 | 0.90 | 0.70 | 32.93 | 44,44,44,44 | 0 |
| 34 | NA | A | 8326 | 1/1 | 0.86 | 1.04 | 30.44 | 54,54,54,54 | 0 |
| 34 | NA | A | 8371 | 1/1 | 0.90 | 0.53 | 28.08 | 62,62,62,62 | 0 |
| 34 | NA | A | 8359 | 1/1 | 0.62 | 0.74 | 26.75 | 48,48,48,48 | 0 |
| 35 | CL | A | 8515 | 1/1 | 0.82 | 0.57 | 23.73 | 85,85,85,85 | 0 |
| 34 | NA | A | 8372 | 1/1 | 0.64 | 0.56 | 19.68 | 55,55,55,55 | 0 |
| 34 | NA | A | 8350 | 1/1 | 0.77 | 0.44 | 18.00 | 36,36,36,36 | 0 |
| 34 | NA | A | 8378 | 1/1 | 0.93 | 0.59 | 14.70 | 46,46,46,46 | 0 |
| 34 | NA | A | 8377 | 1/1 | 0.74 | 0.41 | 14.05 | 76,76,76,76 | 0 |
| 34 | NA | A | 8367 | 1/1 | 0.97 | 0.36 | 13.83 | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 34 | NA | S | 8386 | 1/1 | 0.35 | 0.80 | 13.43 | 63,63,63,63 | 0 |
| 34 | NA | A | 8320 | 1/1 | 0.80 | 0.25 | 13.11 | 24,24,24,24 | 0 |
| 34 | NA | A | 8340 | 1/1 | 0.77 | 0.31 | 11.38 | 38,38,38,38 | 0 |
| 34 | NA | A | 8362 | 1/1 | 0.95 | 0.30 | 11.14 | 70,70,70,70 | 0 |
| 34 | NA | A | 8321 | 1/1 | 0.91 | 0.40 | 10.74 | 49,49,49,49 | 0 |
| 34 | NA | A | 8374 | 1/1 | 0.79 | 0.28 | 9.52 | 60,60,60,60 | 0 |
| 34 | NA | B | 8383 | 1/1 | 0.88 | 0.28 | 6.70 | 72,72,72,72 | 0 |
| 33 | K | A | 8201 | 1/1 | 0.89 | 0.32 | 6.18 | 76,76,76,76 | 0 |
| 34 | NA | A | 8332 | 1/1 | 0.93 | 0.28 | 6.04 | 35,35,35,35 | 0 |
| 34 | NA | A | 8325 | 1/1 | 0.92 | 0.25 | 5.25 | 49,49,49,49 | 0 |
| 34 | NA | N | 8365 | 1/1 | 0.87 | 0.49 | 4.90 | 46,46,46,46 | 0 |
| 34 | NA | A | 8361 | 1/1 | 0.92 | 0.27 | 4.86 | 48,48,48,48 | 0 |
| 34 | NA | A | 8323 | 1/1 | 0.91 | 0.30 | 4.71 | 34,34,34,34 | 0 |
| 34 | NA | A | 8373 | 1/1 | 0.85 | 0.40 | 4.70 | 45,45,45,45 | 0 |
| 32 | MG | A | 8112 | 1/1 | 0.87 | 0.27 | 4.21 | 43,43,43,43 | 0 |
| 34 | NA | A | 8339 | 1/1 | 0.97 | 0.22 | 4.10 | 14,14,14,14 | 0 |
| 32 | MG | 6 | 8118 | 1/1 | 0.65 | 0.68 | 3.58 | 61,61,61,61 | 0 |
| 36 | PHA | 5 | 77 | 11/11 | 0.70 | 0.51 | 3.44 | 24,25,29,29 | 11 |
| 34 | NA | M | 8380 | 1/1 | 0.94 | 0.27 | 3.36 | 61,61,61,61 | 0 |
| 35 | CL | D | 8519 | 1/1 | 0.93 | 0.27 | 2.78 | 47,47,47,47 | 0 |
| 34 | NA | A | 8305 | 1/1 | 0.86 | 0.21 | 2.78 | 27,27,27,27 | 0 |
| 34 | NA | A | 8376 | 1/1 | 0.92 | 0.21 | 2.42 | 42,42,42,42 | 0 |
| 34 | NA | A | 8366 | 1/1 | 0.45 | 0.24 | 2.41 | 51,51,51,51 | 0 |
| 32 | MG | A | 8049 | 1/1 | 0.91 | 0.24 | 2.37 | 67,67,67,67 | 0 |
| 34 | NA | K | 8346 | 1/1 | 0.85 | 0.30 | 2.24 | 33,33,33,33 | 0 |
| 34 | NA | A | 8382 | 1/1 | 0.71 | 0.25 | 2.15 | 54,54,54,54 | 0 |
| 32 | MG | A | 8067 | 1/1 | 0.91 | 0.28 | 1.79 | 55,55,55,55 | 0 |
| 34 | NA | A | 8303 | 1/1 | 0.92 | 0.22 | 1.76 | 55,55,55,55 | 0 |
| 34 | NA | A | 8327 | 1/1 | 0.74 | 0.21 | 1.59 | 34,34,34,34 | 0 |
| 32 | MG | A | 8044 | 1/1 | 0.75 | 0.20 | 1.57 | 50,50,50,50 | 0 |
| 32 | MG | A | 8064 | 1/1 | 0.92 | 0.20 | 1.52 | 29,29,29,29 | 0 |
| 34 | NA | A | 8335 | 1/1 | 0.92 | 0.21 | 1.41 | 58,58,58,58 | 0 |
| 34 | NA | A | 8368 | 1/1 | 0.80 | 0.22 | 1.10 | 69,69,69,69 | 0 |
| 34 | NA | A | 8324 | 1/1 | 0.59 | 0.31 | 1.09 | 58,58,58,58 | 0 |
| 35 | CL | P | 8508 | 1/1 | 0.72 | 0.22 | 0.86 | 72,72,72,72 | 0 |
| 32 | MG | A | 8059 | 1/1 | 0.73 | 0.20 | 0.60 | 65,65,65,65 | 0 |
| 34 | NA | S | 8338 | 1/1 | 0.85 | 0.23 | 0.38 | 48,48,48,48 | 0 |
| 35 | CL | 4 | 8504 | 1/1 | 0.90 | 0.27 | 0.26 | 56,56,56,56 | 0 |
| 34 | NA | A | 8364 | 1/1 | 0.94 | 0.19 | 0.12 | 39,39,39,39 | 0 |
| 34 | NA | A | 8314 | 1/1 | 0.91 | 0.17 | -0.26 | 21,21,21,21 | 0 |
| 35 | CL | M | 8510 | 1/1 | 0.90 | 0.19 | -0.64 | 57,57,57,57 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 32 | MG | A | 8071 | 1/1 | 0.76 | 0.19 | -0.71 | 80,80,80,80 | 0 |
| 35 | CL | K | 8521 | 1/1 | 0.90 | 0.19 | -0.80 | 51,51,51,51 | 0 |
| 34 | NA | A | 8317 | 1/1 | 0.66 | 0.19 | -0.84 | 63,63,63,63 | 0 |
| 34 | NA | A | 8381 | 1/1 | 0.83 | 0.16 | -1.07 | 54,54,54,54 | 0 |
| 34 | NA | N | 8347 | 1/1 | 0.89 | 0.16 | -1.07 | 36,36,36,36 | 0 |
| 35 | CL | A | 8505 | 1/1 | 0.87 | 0.16 | -1.20 | 60,60,60,60 | 0 |
| 34 | NA | S | 8337 | 1/1 | 0.89 | 0.18 | -1.21 | 45,45,45,45 | 0 |
| 32 | MG | A | 8096 | 1/1 | 0.75 | 0.18 | -1.27 | 46,46,46,46 | 0 |
| 34 | NA | U | 8343 | 1/1 | 0.93 | 0.18 | -1.41 | 23,23,23,23 | 0 |
| 32 | MG | U | 8073 | 1/1 | 0.68 | 0.27 | -1.50 | 52,52,52,52 | 0 |
| 34 | NA | C | 8345 | 1/1 | 0.84 | 0.18 | -1.51 | 48,48,48,48 | 0 |
| 32 | MG | 4 | 8078 | 1/1 | 0.73 | 0.12 | -1.61 | 63,63,63,63 | 0 |
| 34 | NA | E | 8304 | 1/1 | 0.92 | 0.18 | -1.84 | 39,39,39,39 | 0 |
| 34 | NA | A | 8353 | 1/1 | 0.89 | 0.13 | -1.92 | 26,26,26,26 | 0 |
| 37 | CD | 4 | 8404 | 1/1 | 0.97 | 0.08 | -2.00 | 63,63,63,63 | 0 |
| 37 | CD | 1 | 8403 | 1/1 | 0.86 | 0.09 | -2.16 | 60,60,60,60 | 0 |
| 35 | CL | L | 8512 | 1/1 | 0.82 | 0.15 | -2.26 | 47,47,47,47 | 0 |
| 32 | MG | C | 8065 | 1/1 | 0.58 | 0.16 | -2.35 | 40,40,40,40 | 0 |
| 32 | MG | A | 8107 | 1/1 | 0.96 | 0.06 | -2.41 | 39,39,39,39 | 0 |
| 34 | NA | A | 8333 | 1/1 | 0.87 | 0.11 | -2.52 | 24,24,24,24 | 0 |
| 34 | NA | J | 8309 | 1/1 | 0.96 | 0.12 | -2.55 | 31,31,31,31 | 0 |
| 37 | CD | V | 8401 | 1/1 | 0.89 | 0.07 | -2.60 | 69,69,69,69 | 0 |
| 32 | MG | A | 8058 | 1/1 | 0.84 | 0.15 | -2.67 | 33,33,33,33 | 0 |
| 35 | CL | N | 8518 | 1/1 | 0.96 | 0.12 | -2.70 | 41,41,41,41 | 0 |
| 32 | MG | D | 8056 | 1/1 | 0.92 | 0.14 | -2.87 | 44,44,44,44 | 0 |
| 32 | MG | Z | 8109 | 1/1 | 0.83 | 0.11 | -2.90 | 28,28,28,28 | 0 |
| 32 | MG | A | 8052 | 1/1 | 0.96 | 0.12 | -2.92 | 39,39,39,39 | 0 |
| 32 | MG | A | 8014 | 1/1 | 0.93 | 0.12 | -2.95 | 21,21,21,21 | 0 |
| 32 | MG | A | 8108 | 1/1 | 0.94 | 0.12 | -2.95 | 72,72,72,72 | 0 |
| 32 | MG | D | 8055 | 1/1 | 0.89 | 0.09 | -3.19 | 34,34,34,34 | 0 |
| 34 | NA | A | 8331 | 1/1 | 0.94 | 0.12 | -3.19 | 34,34,34,34 | 0 |
| 32 | MG | A | 8013 | 1/1 | 0.89 | 0.15 | -3.22 | 45,45,45,45 | 0 |
| 32 | MG | A | 8012 | 1/1 | 0.98 | 0.10 | -3.30 | 33,33,33,33 | 0 |
| 32 | MG | A | 8027 | 1/1 | 0.98 | 0.07 | -3.37 | 35,35,35,35 | 0 |
| 32 | MG | A | 8015 | 1/1 | 0.84 | 0.09 | -3.55 | 38,38,38,38 | 0 |
| 32 | MG | A | 8080 | 1/1 | 0.72 | 0.14 | -3.90 | 33,33,33,33 | 0 |
| 37 | CD | 2 | 8402 | 1/1 | 0.94 | 0.07 | -3.98 | 64,64,64,64 | 0 |
| 34 | NA | R | 8348 | 1/1 | 0.99 | 0.10 | -4.03 | 29,29,29,29 | 0 |
| 32 | MG | A | 8074 | 1/1 | 0.96 | 0.05 | -4.15 | 15,15,15,15 | 0 |
| 32 | MG | A | 8003 | 1/1 | 0.96 | 0.10 | -4.27 | 29,29,29,29 | 0 |
| 32 | MG | A | 8054 | 1/1 | 0.82 | 0.12 | -4.45 | 37,37,37,37 | 0 |
| 32 | MG | A | 8077 | 1/1 | 0.93 | 0.11 | -4.48 | 33,33,33,33 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|--------|-----------------------------|-------|
| 32 | MG | A | 8039 | 1/1 | 0.87 | 0.10 | -4.52 | 52,52,52,52 | 0 |
| 32 | MG | A | 8091 | 1/1 | 0.79 | 0.09 | -4.56 | 53,53,53,53 | 0 |
| 34 | NA | A | 8379 | 1/1 | 0.90 | 0.12 | -5.22 | 34,34,34,34 | 0 |
| 32 | MG | A | 8057 | 1/1 | 0.94 | 0.10 | -5.31 | 34,34,34,34 | 0 |
| 34 | NA | A | 8308 | 1/1 | 0.93 | 0.12 | -5.85 | 49,49,49,49 | 0 |
| 32 | MG | A | 8020 | 1/1 | 0.89 | 0.14 | -5.92 | 27,27,27,27 | 0 |
| 32 | MG | A | 8032 | 1/1 | 0.87 | 0.09 | -5.97 | 24,24,24,24 | 0 |
| 32 | MG | A | 8004 | 1/1 | 0.91 | 0.09 | -6.10 | 28,28,28,28 | 0 |
| 32 | MG | A | 8001 | 1/1 | 0.91 | 0.09 | -6.28 | 23,23,23,23 | 0 |
| 32 | MG | A | 8017 | 1/1 | 0.97 | 0.04 | -6.58 | 24,24,24,24 | 0 |
| 32 | MG | A | 8053 | 1/1 | 0.93 | 0.12 | -6.72 | 39,39,39,39 | 0 |
| 32 | MG | A | 8002 | 1/1 | 0.95 | 0.07 | -6.84 | 33,33,33,33 | 0 |
| 32 | MG | A | 8038 | 1/1 | 0.97 | 0.09 | -6.89 | 29,29,29,29 | 0 |
| 32 | MG | A | 8060 | 1/1 | 0.94 | 0.10 | -7.07 | 49,49,49,49 | 0 |
| 32 | MG | A | 8018 | 1/1 | 0.93 | 0.09 | -7.24 | 44,44,44,44 | 0 |
| 32 | MG | A | 8007 | 1/1 | 0.91 | 0.09 | -7.61 | 19,19,19,19 | 0 |
| 32 | MG | A | 8035 | 1/1 | 0.77 | 0.11 | -7.83 | 54,54,54,54 | 0 |
| 34 | NA | A | 8344 | 1/1 | 0.94 | 0.09 | -8.42 | 17,17,17,17 | 0 |
| 32 | MG | A | 8062 | 1/1 | 0.87 | 0.09 | -9.12 | 61,61,61,61 | 0 |
| 33 | K | A | 8202 | 1/1 | 0.98 | 0.08 | -9.85 | 53,53,53,53 | 0 |
| 32 | MG | A | 8006 | 1/1 | 0.86 | 0.09 | -10.67 | 34,34,34,34 | 0 |
| 32 | MG | A | 8033 | 1/1 | 0.91 | 0.06 | -12.13 | 22,22,22,22 | 0 |
| 32 | MG | A | 8019 | 1/1 | 0.82 | 0.09 | -13.03 | 15,15,15,15 | 0 |
| 32 | MG | A | 8084 | 1/1 | 0.82 | 0.14 | -13.42 | 56,56,56,56 | 0 |
| 32 | MG | A | 8010 | 1/1 | 0.89 | 0.09 | -16.64 | 26,26,26,26 | 0 |
| 32 | MG | A | 8008 | 1/1 | 0.91 | 0.07 | -17.80 | 20,20,20,20 | 0 |
| 36 | PHA | 6 | 77 | 10/11 | 0.69 | 0.42 | - | 35,38,41,41 | 10 |
| 32 | MG | A | 8037 | 1/1 | 0.87 | 0.12 | - | 46,46,46,46 | 0 |
| 34 | NA | A | 8334 | 1/1 | 0.91 | 0.11 | - | 46,46,46,46 | 0 |
| 32 | MG | A | 8100 | 1/1 | 0.92 | 0.25 | - | 53,53,53,53 | 0 |
| 32 | MG | A | 8031 | 1/1 | 0.96 | 0.11 | - | 19,19,19,19 | 0 |
| 32 | MG | A | 8115 | 1/1 | 0.74 | 0.20 | - | 36,36,36,36 | 0 |
| 32 | MG | A | 8079 | 1/1 | 0.96 | 0.07 | - | 27,27,27,27 | 0 |
| 32 | MG | A | 8113 | 1/1 | 0.70 | 0.18 | - | 43,43,43,43 | 0 |
| 34 | NA | A | 8349 | 1/1 | 0.95 | 0.20 | - | 40,40,40,40 | 0 |
| 32 | MG | A | 8117 | 1/1 | 0.81 | 0.13 | - | 26,26,26,26 | 0 |
| 34 | NA | A | 8355 | 1/1 | 0.90 | 0.65 | - | 72,72,72,72 | 0 |
| 34 | NA | A | 8369 | 1/1 | 0.60 | 0.38 | - | 59,59,59,59 | 0 |
| 35 | CL | O | 8507 | 1/1 | 0.90 | 0.34 | - | 63,63,63,63 | 0 |
| 32 | MG | A | 8021 | 1/1 | 0.85 | 0.11 | - | 22,22,22,22 | 0 |
| 34 | NA | A | 8370 | 1/1 | 0.79 | 0.30 | - | 50,50,50,50 | 0 |
| 32 | MG | A | 8034 | 1/1 | 0.97 | 0.05 | - | 24,24,24,24 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 35 | CL | A | 8516 | 1/1 | 0.87 | 0.19 | - | 51,51,51,51 | 0 |
| 34 | NA | A | 8301 | 1/1 | 0.91 | 0.14 | - | 26,26,26,26 | 0 |
| 32 | MG | A | 8081 | 1/1 | 0.76 | 0.09 | - | 51,51,51,51 | 0 |
| 32 | MG | A | 8045 | 1/1 | 0.86 | 0.19 | - | 52,52,52,52 | 0 |
| 32 | MG | A | 8005 | 1/1 | 0.95 | 0.10 | - | 32,32,32,32 | 0 |
| 32 | MG | A | 8051 | 1/1 | 0.96 | 0.22 | - | 87,87,87,87 | 0 |
| 32 | MG | A | 8063 | 1/1 | 0.85 | 0.10 | - | 54,54,54,54 | 0 |
| 32 | MG | A | 8106 | 1/1 | 0.59 | 0.17 | - | 45,45,45,45 | 0 |
| 34 | NA | A | 8329 | 1/1 | 0.74 | 0.38 | - | 65,65,65,65 | 0 |
| 34 | NA | A | 8342 | 1/1 | 0.86 | 0.21 | - | 34,34,34,34 | 0 |
| 32 | MG | A | 8082 | 1/1 | 0.90 | 0.27 | - | 51,51,51,51 | 0 |
| 32 | MG | A | 8097 | 1/1 | 0.92 | 0.12 | - | 27,27,27,27 | 0 |
| 35 | CL | S | 8506 | 1/1 | 0.92 | 0.22 | - | 41,41,41,41 | 0 |
| 32 | MG | A | 8104 | 1/1 | 0.76 | 0.29 | - | 51,51,51,51 | 0 |
| 32 | MG | B | 8095 | 1/1 | 0.91 | 0.10 | - | 69,69,69,69 | 0 |
| 34 | NA | A | 8316 | 1/1 | 0.85 | 0.23 | - | 30,30,30,30 | 0 |
| 32 | MG | A | 8028 | 1/1 | 0.89 | 0.06 | - | 30,30,30,30 | 0 |
| 32 | MG | A | 8025 | 1/1 | 0.95 | 0.09 | - | 63,63,63,63 | 0 |
| 32 | MG | A | 8042 | 1/1 | 0.93 | 0.10 | - | 35,35,35,35 | 0 |
| 32 | MG | A | 8094 | 1/1 | 0.86 | 0.15 | - | 67,67,67,67 | 0 |
| 35 | CL | A | 8503 | 1/1 | 0.90 | 0.24 | - | 47,47,47,47 | 0 |
| 32 | MG | A | 8026 | 1/1 | 0.96 | 0.10 | - | 20,20,20,20 | 0 |
| 32 | MG | A | 8102 | 1/1 | 0.90 | 0.09 | - | 53,53,53,53 | 0 |
| 35 | CL | K | 8502 | 1/1 | 0.89 | 0.14 | - | 62,62,62,62 | 0 |
| 32 | MG | A | 8030 | 1/1 | 0.88 | 0.10 | - | 23,23,23,23 | 0 |
| 32 | MG | A | 8070 | 1/1 | 0.91 | 0.28 | - | 36,36,36,36 | 0 |
| 32 | MG | L | 8069 | 1/1 | 0.91 | 0.09 | - | 56,56,56,56 | 0 |
| 34 | NA | A | 8302 | 1/1 | 0.91 | 0.34 | - | 39,39,39,39 | 0 |
| 34 | NA | A | 8306 | 1/1 | 0.88 | 0.84 | - | 42,42,42,42 | 0 |
| 34 | NA | A | 8318 | 1/1 | 0.87 | 0.61 | - | 37,37,37,37 | 0 |
| 32 | MG | A | 8092 | 1/1 | 0.78 | 0.33 | - | 92,92,92,92 | 0 |
| 35 | CL | A | 8511 | 1/1 | 0.84 | 0.19 | - | 65,65,65,65 | 0 |
| 34 | NA | B | 8351 | 1/1 | 0.69 | 0.30 | - | 85,85,85,85 | 0 |
| 32 | MG | A | 8110 | 1/1 | 0.75 | 0.14 | - | 29,29,29,29 | 0 |
| 32 | MG | A | 8036 | 1/1 | 0.94 | 0.10 | - | 27,27,27,27 | 0 |
| 34 | NA | A | 8310 | 1/1 | 0.80 | 0.38 | - | 33,33,33,33 | 0 |
| 32 | MG | A | 8083 | 1/1 | 0.95 | 0.05 | - | 43,43,43,43 | 0 |
| 32 | MG | A | 8022 | 1/1 | 0.90 | 0.06 | - | 17,17,17,17 | 0 |
| 32 | MG | A | 8043 | 1/1 | 0.91 | 0.16 | - | 38,38,38,38 | 0 |
| 35 | CL | A | 8522 | 1/1 | 0.92 | 0.31 | - | 78,78,78,78 | 0 |
| 32 | MG | A | 8016 | 1/1 | 0.75 | 0.22 | - | 38,38,38,38 | 0 |
| 32 | MG | A | 8090 | 1/1 | 0.78 | 0.35 | - | 62,62,62,62 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 35 | CL | A | 8517 | 1/1 | 0.96 | 0.10 | - | 61,61,61,61 | 0 |
| 32 | MG | A | 8024 | 1/1 | 0.65 | 0.81 | - | 95,95,95,95 | 0 |
| 32 | MG | A | 8023 | 1/1 | 0.94 | 0.08 | - | 34,34,34,34 | 0 |
| 32 | MG | A | 8093 | 1/1 | 0.96 | 0.12 | - | 48,48,48,48 | 0 |
| 34 | NA | A | 8341 | 1/1 | 0.96 | 0.11 | - | 28,28,28,28 | 0 |
| 34 | NA | A | 8385 | 1/1 | 0.62 | 0.28 | - | 43,43,43,43 | 0 |
| 34 | NA | A | 8375 | 1/1 | 0.78 | 0.73 | - | 63,63,63,63 | 0 |
| 34 | NA | J | 8322 | 1/1 | 0.77 | 0.31 | - | 68,68,68,68 | 0 |
| 32 | MG | A | 8041 | 1/1 | 0.56 | 0.21 | - | 79,79,79,79 | 0 |
| 32 | MG | A | 8088 | 1/1 | 0.86 | 0.21 | - | 23,23,23,23 | 0 |
| 32 | MG | A | 8066 | 1/1 | 0.88 | 0.11 | - | 72,72,72,72 | 0 |
| 34 | NA | A | 8357 | 1/1 | 0.81 | 0.09 | - | 53,53,53,53 | 0 |
| 32 | MG | A | 8029 | 1/1 | 0.64 | 0.15 | - | 53,53,53,53 | 0 |
| 34 | NA | A | 8384 | 1/1 | 0.23 | 0.69 | - | 101,101,101,101 | 0 |
| 32 | MG | A | 8061 | 1/1 | 0.87 | 0.11 | - | 25,25,25,25 | 0 |
| 34 | NA | A | 8319 | 1/1 | 0.77 | 0.15 | - | 33,33,33,33 | 0 |
| 32 | MG | 1 | 8105 | 1/1 | 0.67 | 0.46 | - | 30,30,30,30 | 0 |
| 32 | MG | A | 8111 | 1/1 | 0.79 | 0.15 | - | 67,67,67,67 | 0 |
| 34 | NA | A | 8328 | 1/1 | 0.76 | 0.55 | - | 54,54,54,54 | 0 |
| 34 | NA | A | 8354 | 1/1 | 0.79 | 0.54 | - | 31,31,31,31 | 0 |
| 34 | NA | A | 8311 | 1/1 | 0.92 | 0.17 | - | 52,52,52,52 | 0 |
| 34 | NA | A | 8358 | 1/1 | 0.83 | 0.45 | - | 113,113,113,113 | 0 |
| 32 | MG | A | 8103 | 1/1 | 0.94 | 0.13 | - | 73,73,73,73 | 0 |
| 35 | CL | A | 8514 | 1/1 | 0.76 | 0.29 | - | 55,55,55,55 | 0 |
| 32 | MG | A | 8116 | 1/1 | 0.79 | 0.12 | - | 67,67,67,67 | 0 |
| 32 | MG | A | 8040 | 1/1 | 0.65 | 0.17 | - | 71,71,71,71 | 0 |
| 35 | CL | A | 8513 | 1/1 | 0.94 | 0.13 | - | 50,50,50,50 | 0 |
| 34 | NA | A | 8307 | 1/1 | 0.79 | 0.24 | - | 53,53,53,53 | 0 |
| 34 | NA | A | 8330 | 1/1 | 0.81 | 0.40 | - | 42,42,42,42 | 0 |
| 32 | MG | A | 8047 | 1/1 | 0.95 | 0.17 | - | 58,58,58,58 | 0 |
| 35 | CL | Z | 8520 | 1/1 | 0.89 | 0.12 | - | 39,39,39,39 | 0 |
| 32 | MG | A | 8076 | 1/1 | 0.54 | 0.16 | - | 37,37,37,37 | 0 |
| 35 | CL | K | 8501 | 1/1 | 0.79 | 0.13 | - | 69,69,69,69 | 0 |
| 32 | MG | A | 8086 | 1/1 | 0.86 | 0.16 | - | 49,49,49,49 | 0 |
| 32 | MG | A | 8089 | 1/1 | 0.91 | 0.21 | - | 60,60,60,60 | 0 |
| 35 | CL | C | 8509 | 1/1 | 0.96 | 0.17 | - | 55,55,55,55 | 0 |
| 32 | MG | A | 8087 | 1/1 | 0.88 | 0.10 | - | 56,56,56,56 | 0 |
| 32 | MG | A | 8085 | 1/1 | 0.91 | 0.17 | - | 61,61,61,61 | 0 |
| 32 | MG | A | 8075 | 1/1 | 0.84 | 0.15 | - | 64,64,64,64 | 0 |
| 32 | MG | A | 8072 | 1/1 | 0.95 | 0.14 | - | 44,44,44,44 | 0 |
| 32 | MG | A | 8099 | 1/1 | 0.89 | 0.15 | - | 32,32,32,32 | 0 |
| 32 | MG | A | 8011 | 1/1 | 0.73 | 0.10 | - | 37,37,37,37 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 32 | MG | A | 8101 | 1/1 | 0.94 | 0.22 | - | 54,54,54,54 | 0 |
| 34 | NA | A | 8315 | 1/1 | 0.92 | 0.30 | - | 29,29,29,29 | 0 |
| 32 | MG | A | 8048 | 1/1 | 0.91 | 0.09 | - | 57,57,57,57 | 0 |
| 34 | NA | A | 8313 | 1/1 | 0.82 | 0.23 | - | 44,44,44,44 | 0 |
| 34 | NA | A | 8360 | 1/1 | 0.90 | 0.46 | - | 45,45,45,45 | 0 |
| 34 | NA | T | 8312 | 1/1 | 0.71 | 0.47 | - | 108,108,108,108 | 0 |
| 34 | NA | A | 8352 | 1/1 | 0.74 | 0.44 | - | 51,51,51,51 | 0 |
| 37 | CD | P | 8405 | 1/1 | 0.72 | 0.12 | - | 184,184,184,184 | 0 |
| 32 | MG | A | 8114 | 1/1 | 0.46 | 0.29 | - | 51,51,51,51 | 0 |
| 34 | NA | A | 8363 | 1/1 | 0.94 | 0.20 | - | 46,46,46,46 | 0 |
| 32 | MG | A | 8050 | 1/1 | 0.94 | 0.09 | - | 65,65,65,65 | 0 |
| 32 | MG | A | 8046 | 1/1 | 0.39 | 0.18 | - | 45,45,45,45 | 0 |
| 32 | MG | A | 8009 | 1/1 | 0.84 | 0.08 | - | 15,15,15,15 | 0 |
| 34 | NA | A | 8336 | 1/1 | 0.79 | 0.18 | - | 41,41,41,41 | 0 |
| 32 | MG | A | 8068 | 1/1 | 0.84 | 0.16 | - | 58,58,58,58 | 0 |
| 32 | MG | A | 8098 | 1/1 | 0.94 | 0.20 | - | 28,28,28,28 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.