



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:05 AM GMT

PDB ID : 3CMA
Title : The structure of CCA and CCA-Phe-Cap-Bio bound to the large ribosomal subunit of *Haloarcula marismortui*
Authors : Simonovic, M.; Steitz, T.A.
Deposited on : 2008-03-21
Resolution : 2.80 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

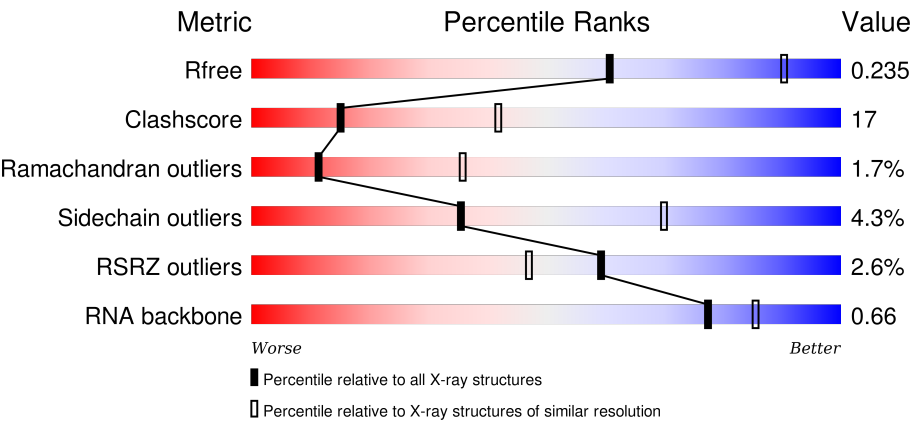
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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








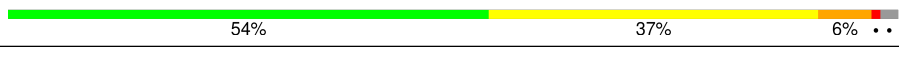




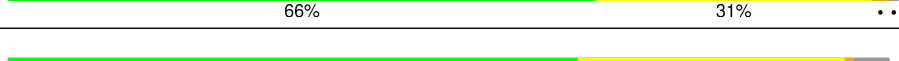
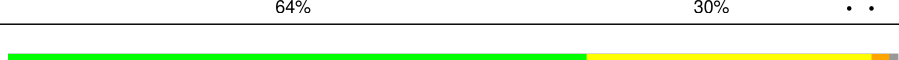
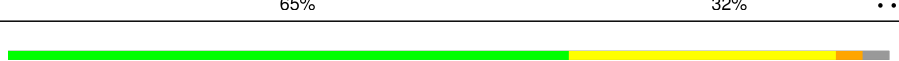

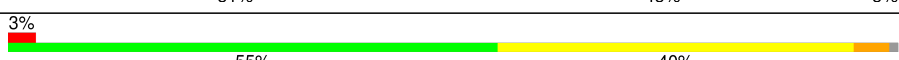
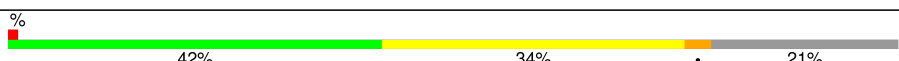
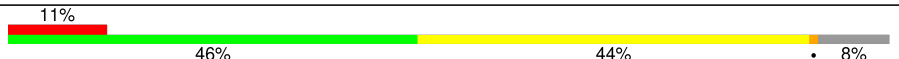
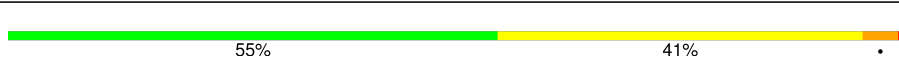

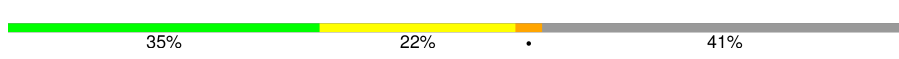
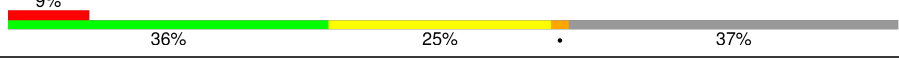
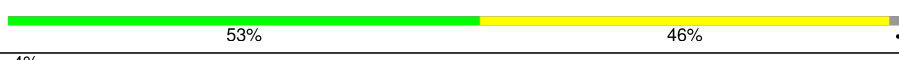

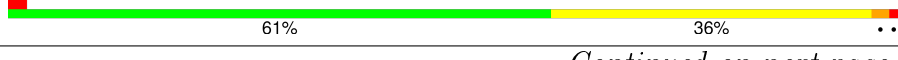

| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 91344 | 2393 (2.80-2.80) |
| Clashscore | 102246 | 2827 (2.80-2.80) |
| Ramachandran outliers | 100387 | 2782 (2.80-2.80) |
| Sidechain outliers | 100360 | 2784 (2.80-2.80) |
| RSRZ outliers | 91569 | 2404 (2.80-2.80) |
| RNA backbone | 2183 | 1091 (3.20-2.40) |

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 | 240 | <div><div>3%</div><div>54%</div><div>41%</div><div>..</div></div> |
| 2 | B | 338 | <div><div>46%</div><div>51%</div><div>.</div></div> |
| 3 | C | 246 | <div><div>62%</div><div>33%</div><div>5%</div></div> |
| 4 | D | 177 | <div><div>13%</div><div>28%</div><div>46%</div><div>..</div><div>21%</div></div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 5 | E | 178 |  |
| 6 | F | 120 |  |
| 7 | G | 348 |  |
| 8 | H | 177 |  |
| 9 | I | 162 |  |
| 10 | J | 145 |  |
| 11 | K | 132 |  |
| 12 | L | 165 |  |
| 13 | M | 196 |  |
| 14 | N | 187 |  |
| 15 | O | 116 |  |
| 16 | P | 149 |  |
| 17 | Q | 96 |  |
| 18 | R | 155 |  |
| 19 | S | 85 |  |
| 20 | T | 120 |  |
| 21 | U | 67 |  |
| 22 | V | 71 |  |
| 23 | W | 154 |  |
| 24 | X | 92 |  |
| 25 | Y | 240 |  |
| 26 | Z | 116 |  |
| 27 | 1 | 57 |  |
| 28 | 2 | 50 |  |
| 29 | 3 | 92 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 30 | 0 | 2923 | |
| 31 | 9 | 122 | |
| 32 | 5 | 3 | |
| 33 | 6 | 3 | |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 34 | PHE | 6 | 77 | - | - | - | X |
| 35 | MG | 0 | 8001 | - | - | - | X |
| 35 | MG | 0 | 8002 | - | - | - | X |
| 35 | MG | 0 | 8004 | - | - | - | X |
| 35 | MG | 0 | 8006 | - | - | - | X |
| 35 | MG | 0 | 8009 | - | - | - | X |
| 35 | MG | 0 | 8010 | - | - | - | X |
| 35 | MG | 0 | 8011 | - | - | - | X |
| 35 | MG | 0 | 8014 | - | - | - | X |
| 35 | MG | 0 | 8028 | - | - | - | X |
| 35 | MG | 0 | 8040 | - | - | - | X |
| 35 | MG | 0 | 8041 | - | - | - | X |
| 35 | MG | 0 | 8043 | - | - | - | X |
| 35 | MG | 0 | 8047 | - | - | - | X |
| 35 | MG | 0 | 8062 | - | - | - | X |
| 35 | MG | 0 | 8071 | - | - | - | X |
| 35 | MG | 0 | 8076 | - | - | - | X |
| 35 | MG | 0 | 8088 | - | - | - | X |
| 35 | MG | A | 8051 | - | - | - | X |
| 35 | MG | C | 8012 | - | - | - | X |
| 35 | MG | Y | 8086 | - | - | - | X |
| 36 | NA | 0 | 8504 | - | - | - | X |
| 36 | NA | 0 | 8512 | - | - | - | X |
| 36 | NA | 0 | 8517 | - | - | - | X |
| 36 | NA | 0 | 8519 | - | - | - | X |
| 36 | NA | 0 | 8521 | - | - | - | X |
| 36 | NA | 0 | 8522 | - | - | - | X |
| 36 | NA | 0 | 8523 | - | - | - | X |
| 36 | NA | 0 | 8527 | - | - | - | X |
| 36 | NA | 0 | 8530 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 36 | NA | 0 | 8534 | - | - | - | X |
| 36 | NA | 0 | 8542 | - | - | - | X |
| 36 | NA | 0 | 8546 | - | - | - | X |
| 36 | NA | 0 | 8547 | - | - | - | X |
| 36 | NA | 0 | 8553 | - | - | - | X |
| 36 | NA | 0 | 8558 | - | - | - | X |
| 36 | NA | 0 | 8559 | - | - | - | X |
| 36 | NA | 0 | 8560 | - | - | - | X |
| 36 | NA | 0 | 8563 | - | - | - | X |
| 36 | NA | 0 | 8565 | - | - | - | X |
| 36 | NA | 0 | 8567 | - | - | - | X |
| 37 | SR | 0 | 8902 | - | - | - | X |
| 37 | SR | 0 | 8943 | - | - | - | X |
| 37 | SR | 0 | 8947 | - | - | - | X |
| 37 | SR | 0 | 8948 | - | - | - | X |
| 37 | SR | 0 | 8969 | - | - | - | X |
| 37 | SR | B | 8987 | - | - | - | X |
| 38 | CL | B | 8819 | - | - | - | X |
| 39 | K | 0 | 8401 | - | - | - | X |
| 39 | K | 0 | 8402 | - | - | - | X |

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 99205 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 protein called 50S ribosomal protein L2P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1 | A | 237 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1752 | 1072 | 351 | 324 | 5 | | | |

- Molecule 2 is a protein called 50S ribosomal protein L3P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2 | B | 337 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2624 | 1616 | 492 | 511 | 5 | | | |

- Molecule 3 is a protein called 50S ribosomal protein L4P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | C | 246 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1859 | 1130 | 344 | 384 | 1 | | | |

- Molecule 4 is a protein called 50S ribosomal protein L5P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4 | D | 140 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1093 | 685 | 194 | 210 | 4 | | | |

- Molecule 5 is a protein called 50S ribosomal protein L6P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | E | 172 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1356 | 840 | 223 | 289 | 4 | | | |

- Molecule 6 is a protein called 50S ribosomal protein L7Ae.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | F | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 889 | 551 | 140 | 197 | 1 | | | |

- Molecule 7 is a protein called 50S ribosomal protein L10E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 7 | G | 29 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 240 | 149 | 39 | 51 | 1 | | | |

- Molecule 8 is a protein called 50S ribosomal protein L10e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | H | 160 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1281 | 798 | 239 | 238 | 6 | | | |

- Molecule 9 is a protein called 50S ribosomal protein L11P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|---------|-------|
| 9 | I | 70 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 518 | 323 | 80 | 114 | 1 | | | |

- Molecule 10 is a protein called 50S ribosomal protein L13P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | J | 142 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1119 | 696 | 198 | 222 | 3 | | | |

- Molecule 11 is a protein called 50S ribosomal protein L14P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | K | 132 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 993 | 609 | 188 | 192 | 4 | | | |

- Molecule 12 is a protein called 50S ribosomal protein L15P.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 12 | L | 145 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1117 | 670 | 221 | 226 | | | |

- Molecule 13 is a protein called 50S ribosomal protein L15e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | M | 194 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1557 | 943 | 332 | 281 | 1 | | | |

- Molecule 14 is a protein called 50S ribosomal protein L18P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14 | N | 186 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1444 | 895 | 261 | 286 | 2 | | | |

- Molecule 15 is a protein called 50S ribosomal protein L18e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 15 | O | 115 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 864 | 529 | 160 | 175 | | | | |

- Molecule 16 is a protein called 50S ribosomal protein L19e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 16 | P | 143 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 1135 | 683 | 228 | 224 | | | | |

- Molecule 17 is a protein called 50S ribosomal protein L21e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 17 | Q | 95 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 734 | 450 | 140 | 144 | | | | |

- Molecule 18 is a protein called 50S ribosomal protein L22P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 18 | R | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1148 | 713 | 208 | 223 | 4 | | | |

- Molecule 19 is a protein called 50S ribosomal protein L23P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | S | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 640 | 389 | 110 | 138 | 3 | | | |

- Molecule 20 is a protein called 50S ribosomal protein L24P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 20 | T | 119 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 949 | 568 | 179 | 202 | | | | |

- Molecule 21 is a protein called 50S ribosomal protein L24e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 21 | U | 53 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 410 | 244 | 75 | 86 | 5 | | | |

- Molecule 22 is a protein called 50S ribosomal protein L29P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|---------|-------|
| 22 | V | 65 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 499 | 304 | 94 | 100 | 1 | | | |

- Molecule 23 is a protein called 50S ribosomal protein L30P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 23 | W | 154 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1195 | 737 | 208 | 244 | 6 | | | |

- Molecule 24 is a protein called 50S ribosomal protein L31e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 24 | X | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 653 | 402 | 128 | 122 | 1 | | | |

- Molecule 25 is a protein called 50S ribosomal protein L32e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 25 | Y | 142 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 1130 | 686 | 228 | 216 | | | | |

- Molecule 26 is a protein called 50S ribosomal protein L37Ae.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26 | Z | 73 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 572 | 343 | 112 | 112 | 5 | | | |

- Molecule 27 is a protein called 50S ribosomal protein L37e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 27 | 1 | 56 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 431 | 258 | 86 | 83 | 4 | | | |

- Molecule 28 is a protein called 50S ribosomal protein L39e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 28 | 2 | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 396 | 239 | 89 | 67 | 1 | | | |

- Molecule 29 is a protein called 50S ribosomal protein L44E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 29 | 3 | 92 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 754 | 458 | 152 | 137 | 7 | | | |

- Molecule 30 is a RNA chain called 23S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 30 | 0 | 2754 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 59018 | 26346 | 10873 | 19054 | 2745 | | | |

- Molecule 31 is a RNA chain called 5S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 31 | 9 | 122 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2596 | 1157 | 471 | 847 | 121 | | | |

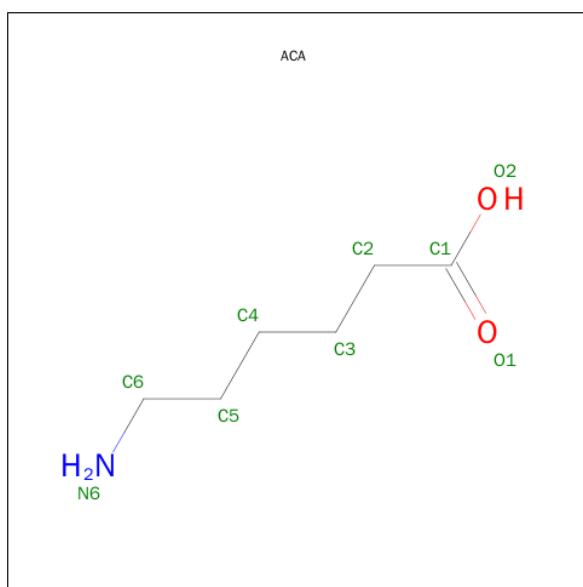
- Molecule 32 is a RNA chain called RNA (5'-R(*CP*CP*A)-3').

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 32 | 5 | 3 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 59 | 28 | 11 | 18 | 2 | | | |

- Molecule 33 is a RNA chain called RNA (5'-R(*CP*CP*(8AN))-3').

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 33 | 6 | 3 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 59 | 28 | 12 | 17 | 2 | | | |

- Molecule 34 is PHENYLALANINE (three-letter code: ACA, PHE) (formula: C₆H₁₃NO₂, C₉H₁₁NO₂).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 34 | 6 | 2 | Total | C | N | O | 0 | 0 |
| | | | 19 | 15 | 2 | 2 | | |

- Molecule 35 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 35 | 0 | 84 | Total | Mg | 0 | 0 |
| | | | 84 | 84 | | |
| 35 | Y | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 35 | K | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 35 | B | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 35 | C | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 35 | A | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 35 | T | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 35 | 2 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 35 | 9 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 36 is SODIUM ION (three-letter code: NA) (formula: Na).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|----------|---------|---------|
| 36 | 0 | 64 | Total 64 | Na 64 | 0 | 0 |
| 36 | J | 1 | Total 1 | Na 1 | 0 | 0 |
| 36 | Q | 1 | Total 1 | Na 1 | 0 | 0 |
| 36 | D | 1 | Total 1 | Na 1 | 0 | 0 |
| 36 | B | 1 | Total 1 | Na 1 | 0 | 0 |
| 36 | C | 1 | Total 1 | Na 1 | 0 | 0 |
| 36 | R | 2 | Total 2 | Na 2 | 0 | 0 |
| 36 | 9 | 1 | Total 1 | Na 1 | 0 | 0 |
| 36 | L | 1 | Total 1 | Na 1 | 0 | 0 |
| 36 | S | 1 | Total 1 | Na 1 | 0 | 0 |
| 36 | M | 1 | Total 1 | Na 1 | 0 | 0 |

- Molecule 37 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|----------|---------|---------|
| 37 | 0 | 86 | Total 86 | Sr 86 | 0 | 0 |
| 37 | 9 | 3 | Total 3 | Sr 3 | 0 | 0 |
| 37 | H | 2 | Total 2 | Sr 2 | 0 | 0 |
| 37 | B | 2 | Total 2 | Sr 2 | 0 | 0 |
| 37 | 3 | 3 | Total 3 | Sr 3 | 0 | 0 |
| 37 | A | 3 | Total 3 | Sr 3 | 0 | 0 |
| 37 | T | 2 | Total 2 | Sr 2 | 0 | 0 |
| 37 | 1 | 2 | Total 2 | Sr 2 | 0 | 0 |
| 37 | R | 1 | Total 1 | Sr 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 37 | Y | 1 | Total 1 | Sr 1 | 0 | 0 |
| 37 | S | 1 | Total 1 | Sr 1 | 0 | 0 |
| 37 | F | 1 | Total 1 | Sr 1 | 0 | 0 |

- Molecule 38 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 38 | 0 | 6 | Total 6 | Cl 6 | 0 | 0 |
| 38 | J | 3 | Total 3 | Cl 3 | 0 | 0 |
| 38 | Q | 1 | Total 1 | Cl 1 | 0 | 0 |
| 38 | K | 1 | Total 1 | Cl 1 | 0 | 0 |
| 38 | B | 1 | Total 1 | Cl 1 | 0 | 0 |
| 38 | 3 | 1 | Total 1 | Cl 1 | 0 | 0 |
| 38 | A | 1 | Total 1 | Cl 1 | 0 | 0 |
| 38 | N | 1 | Total 1 | Cl 1 | 0 | 0 |
| 38 | O | 1 | Total 1 | Cl 1 | 0 | 0 |
| 38 | 2 | 1 | Total 1 | Cl 1 | 0 | 0 |
| 38 | Y | 1 | Total 1 | Cl 1 | 0 | 0 |
| 38 | L | 2 | Total 2 | Cl 2 | 0 | 0 |
| 38 | R | 1 | Total 1 | Cl 1 | 0 | 0 |
| 38 | M | 1 | Total 1 | Cl 1 | 0 | 0 |

- Molecule 39 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 39 | 0 | 2 | Total K 2 2 | 0 | 0 |

- Molecule 40 is CADMIUM ION (three-letter code: CD) (formula: Cd).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 40 | O | 1 | Total Cd 1 1 | 0 | 0 |
| 40 | Z | 1 | Total Cd 1 1 | 0 | 0 |
| 40 | 1 | 1 | Total Cd 1 1 | 0 | 0 |
| 40 | 3 | 1 | Total Cd 1 1 | 0 | 0 |
| 40 | U | 1 | Total Cd 1 1 | 0 | 0 |

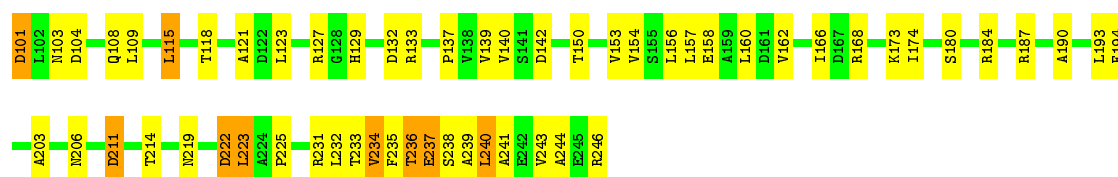
- Molecule 41 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 41 | 9 | 148 | Total O 148 148 | 0 | 0 |
| 41 | 5 | 4 | Total O 4 4 | 0 | 0 |
| 41 | 6 | 3 | Total O 3 3 | 0 | 0 |
| 41 | A | 128 | Total O 128 128 | 0 | 0 |
| 41 | B | 165 | Total O 165 165 | 0 | 0 |
| 41 | C | 170 | Total O 170 170 | 0 | 0 |
| 41 | D | 49 | Total O 49 49 | 0 | 0 |
| 41 | E | 48 | Total O 48 48 | 0 | 0 |
| 41 | F | 31 | Total O 31 31 | 0 | 0 |
| 41 | G | 19 | Total O 19 19 | 0 | 0 |
| 41 | H | 77 | Total O 77 77 | 0 | 0 |
| 41 | I | 11 | Total O 11 11 | 0 | 0 |

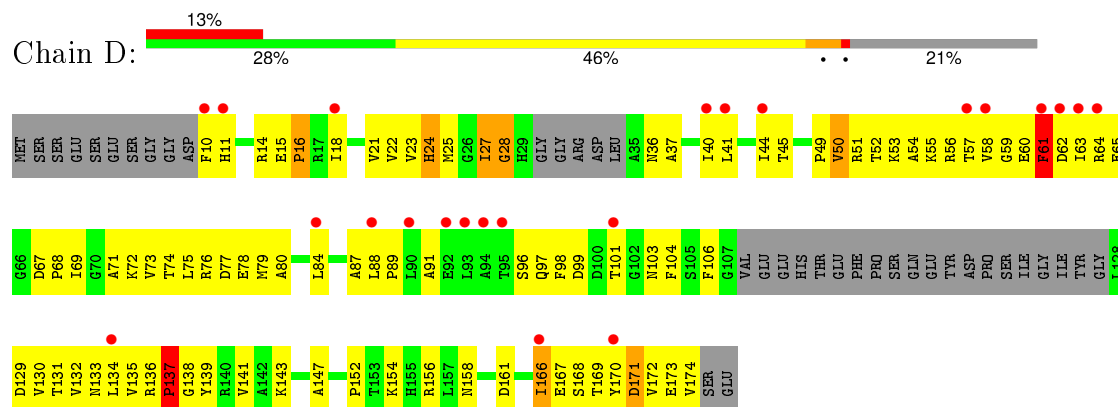
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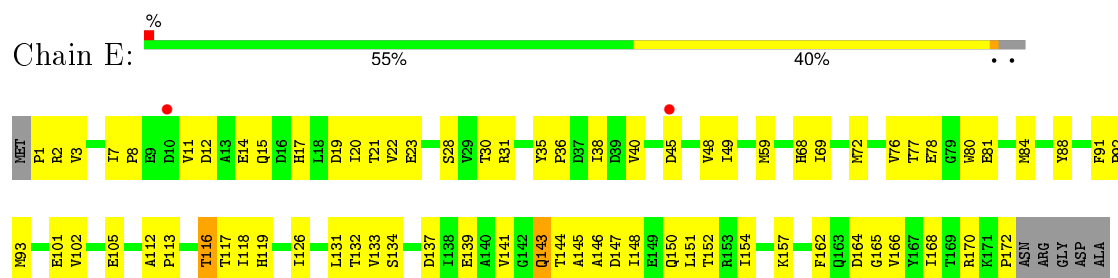
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|---------------|-----------|---------|---------|
| 41 | J | 63 | Total 63 | O 63 | 0 | 0 |
| 41 | K | 54 | Total 54 | O 54 | 0 | 0 |
| 41 | L | 92 | Total 92 | O 92 | 0 | 0 |
| 41 | M | 136 | Total 136 | O 136 | 0 | 0 |
| 41 | N | 64 | Total 64 | O 64 | 0 | 0 |
| 41 | O | 43 | Total 43 | O 43 | 0 | 0 |
| 41 | P | 69 | Total 69 | O 69 | 0 | 0 |
| 41 | Q | 51 | Total 51 | O 51 | 0 | 0 |
| 41 | R | 87 | Total 87 | O 87 | 0 | 0 |
| 41 | S | 33 | Total 33 | O 33 | 0 | 0 |
| 41 | T | 40 | Total 40 | O 40 | 0 | 0 |
| 41 | U | 30 | Total 30 | O 30 | 0 | 0 |
| 41 | V | 16 | Total 16 | O 16 | 0 | 0 |
| 41 | 0 | 5771 | Total 5771 | O 5771 | 0 | 0 |
| 41 | W | 72 | Total 72 | O 72 | 0 | 0 |
| 41 | X | 25 | Total 25 | O 25 | 0 | 0 |
| 41 | Y | 108 | Total 108 | O 108 | 0 | 0 |
| 41 | Z | 30 | Total 30 | O 30 | 0 | 0 |
| 41 | 1 | 53 | Total 53 | O 53 | 0 | 0 |
| 41 | 2 | 42 | Total 42 | O 42 | 0 | 0 |
| 41 | 3 | 66 | Total 66 | O 66 | 0 | 0 |



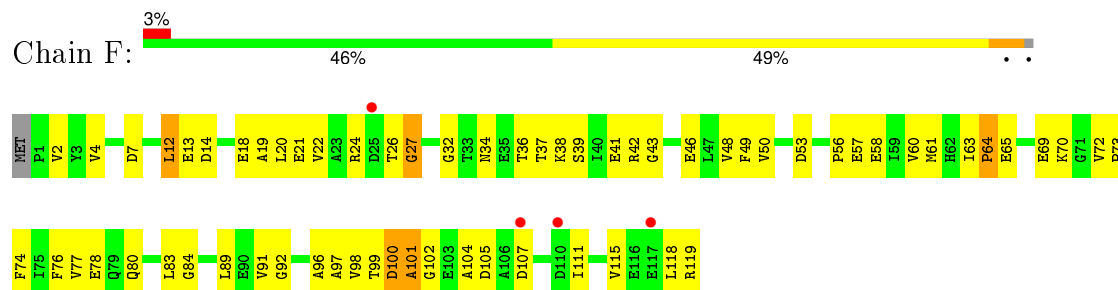
• Molecule 4: 50S ribosomal protein L5P



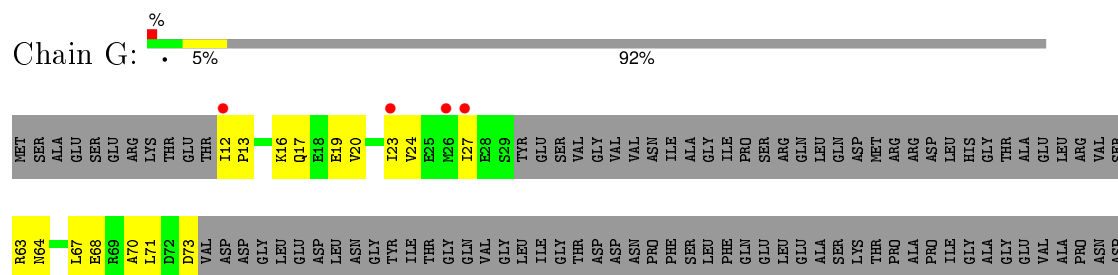
• Molecule 5: 50S ribosomal protein L6P



• Molecule 6: 50S ribosomal protein L7Ae

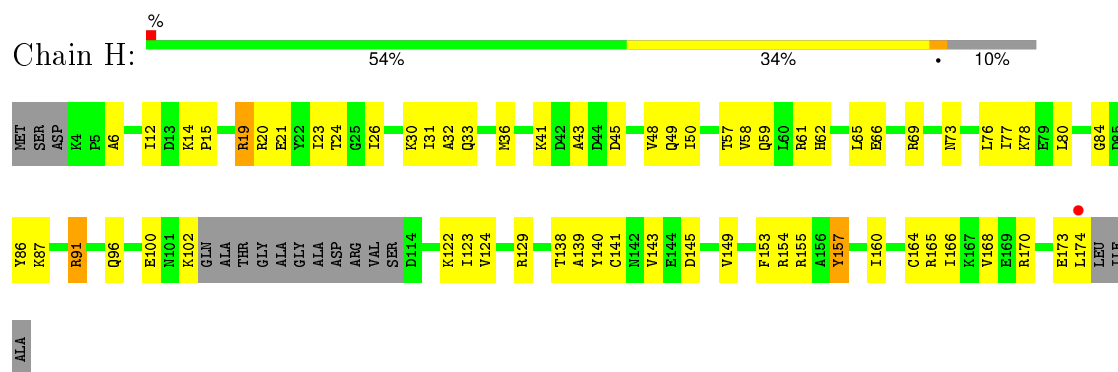


• Molecule 7: 50S ribosomal protein L10E

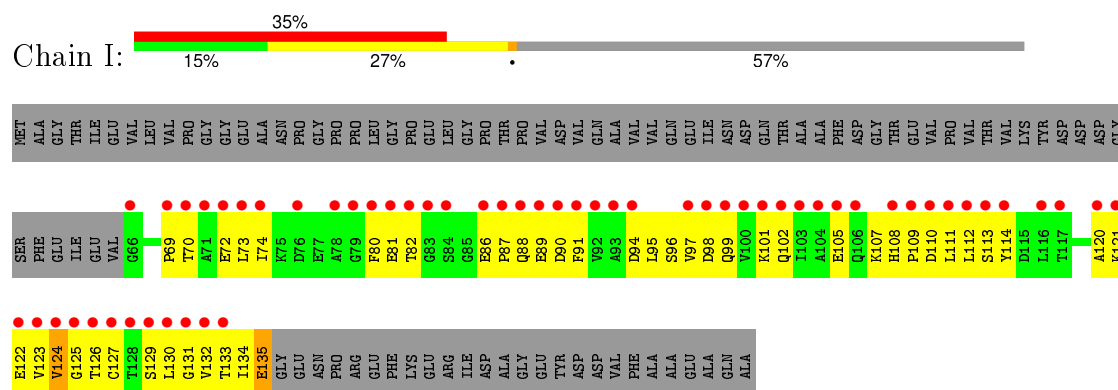


[illegible]

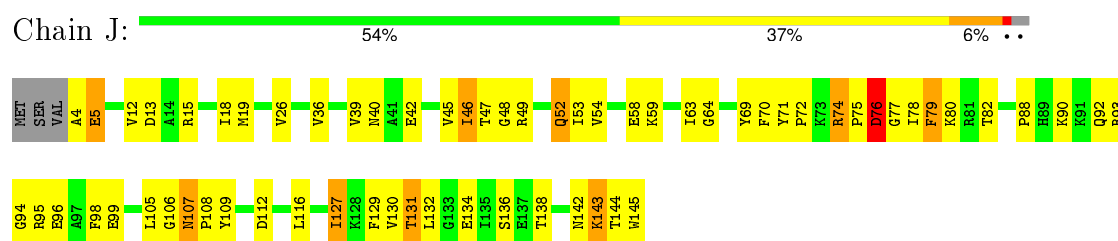
- Molecule 8: 50S ribosomal protein L10e



- Molecule 9: 50S ribosomal protein L11P

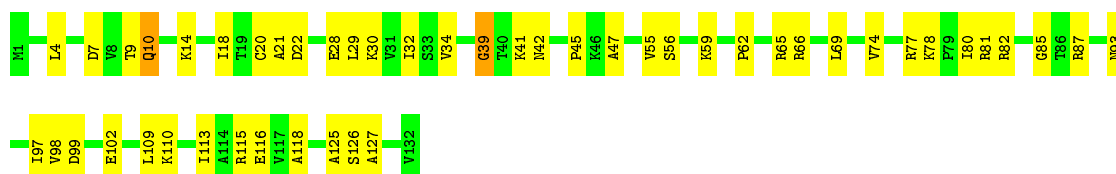


- Molecule 10: 50S ribosomal protein L13P

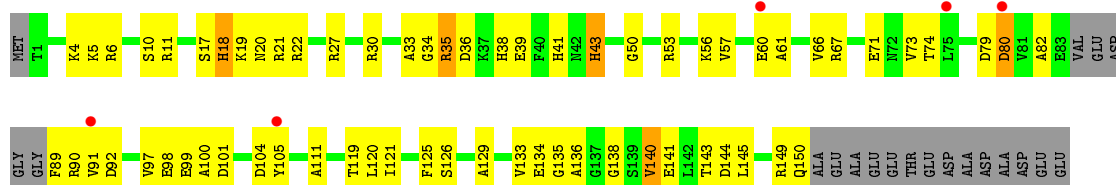


- Molecule 11: 50S ribosomal protein L14P

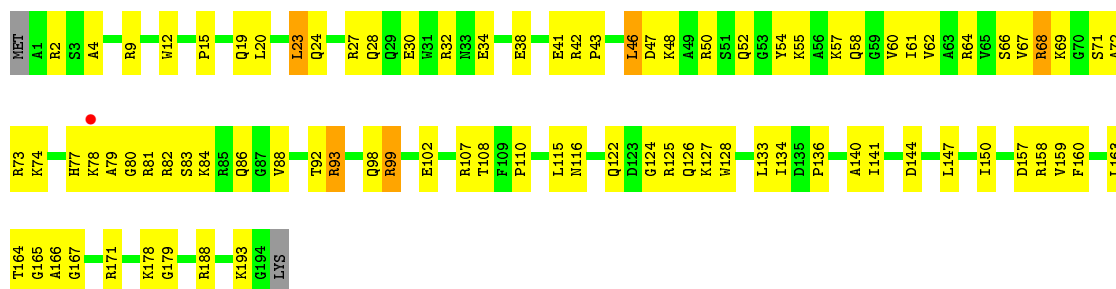




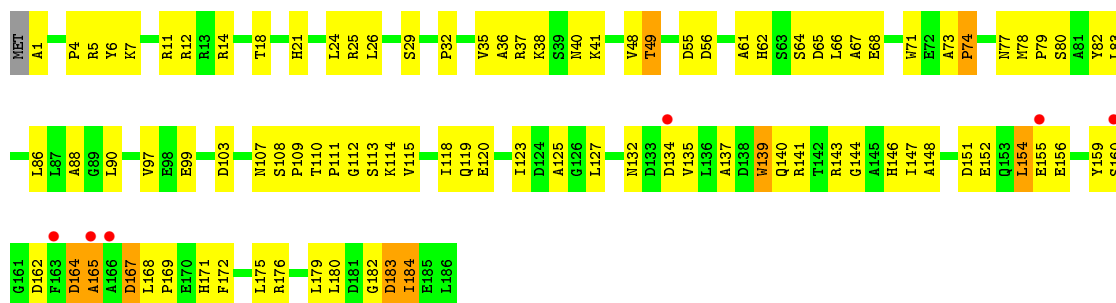
- Molecule 12: 50S ribosomal protein L15P



- Molecule 13: 50S ribosomal protein L15e



- Molecule 14: 50S ribosomal protein L18P



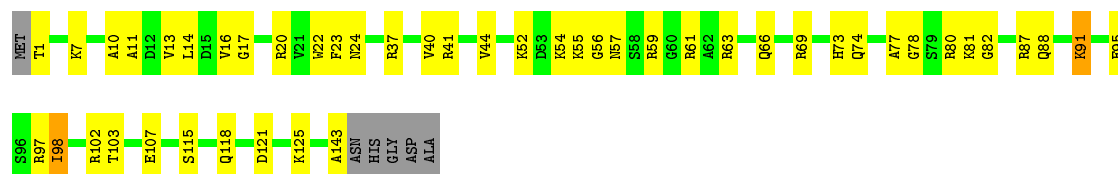
- Molecule 15: 50S ribosomal protein L18e





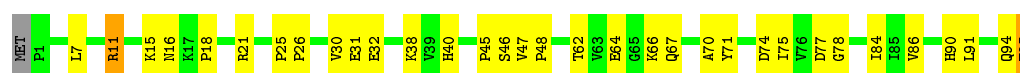
- Molecule 16: 50S ribosomal protein L19e

Chain P: 64% 30% . .



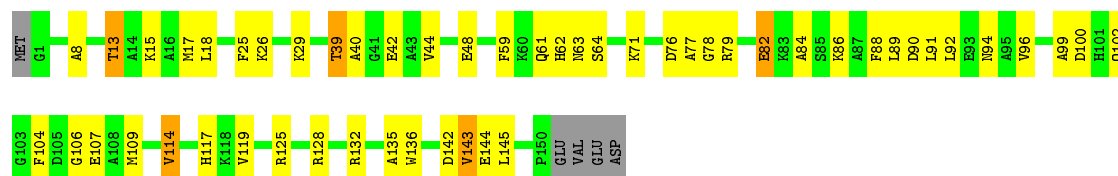
- Molecule 17: 50S ribosomal protein L21e

Chain Q: 65% 32% . .



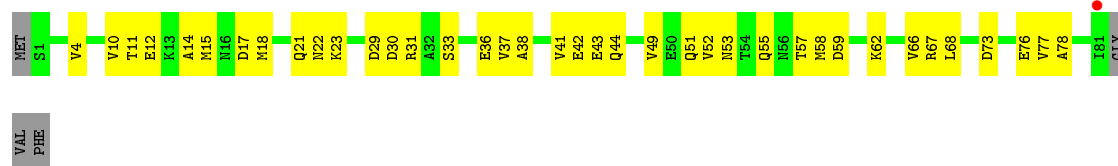
- Molecule 18: 50S ribosomal protein L22P

Chain R: 63% 30% . .



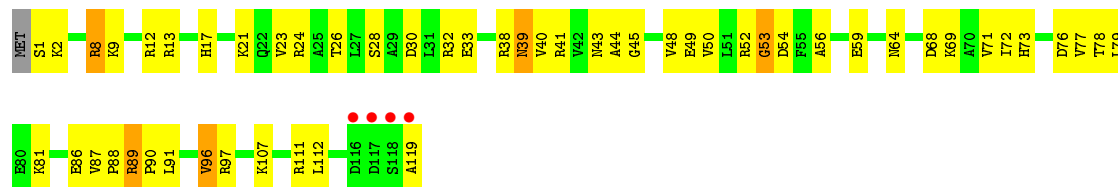
- Molecule 19: 50S ribosomal protein L23P

Chain S: % 51% 45% 5% . .

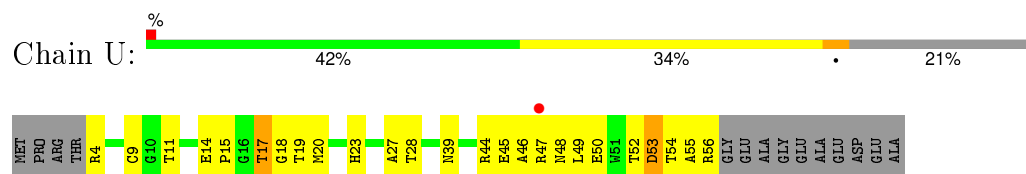


- Molecule 20: 50S ribosomal protein L24P

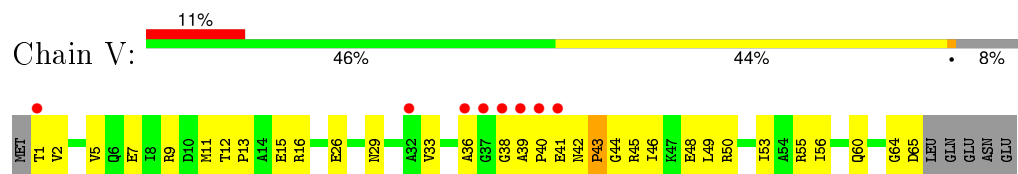
Chain T: 3% 55% 40% . .



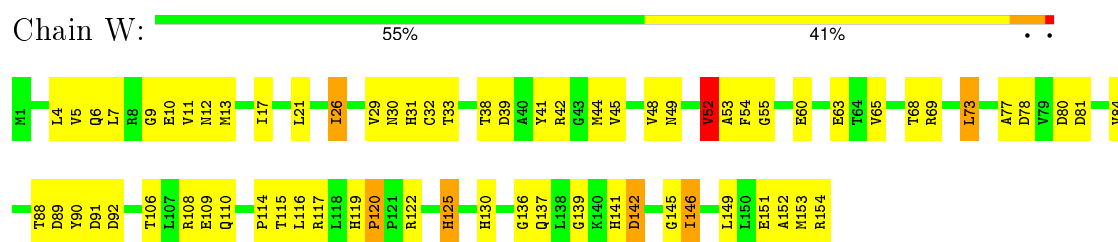
- Molecule 21: 50S ribosomal protein L24e



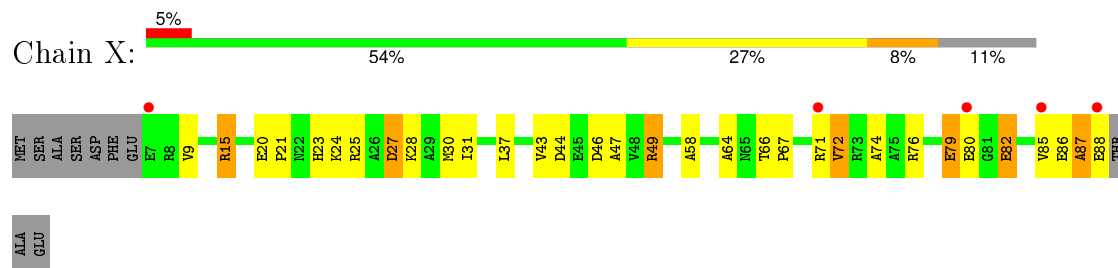
- Molecule 22: 50S ribosomal protein L29P



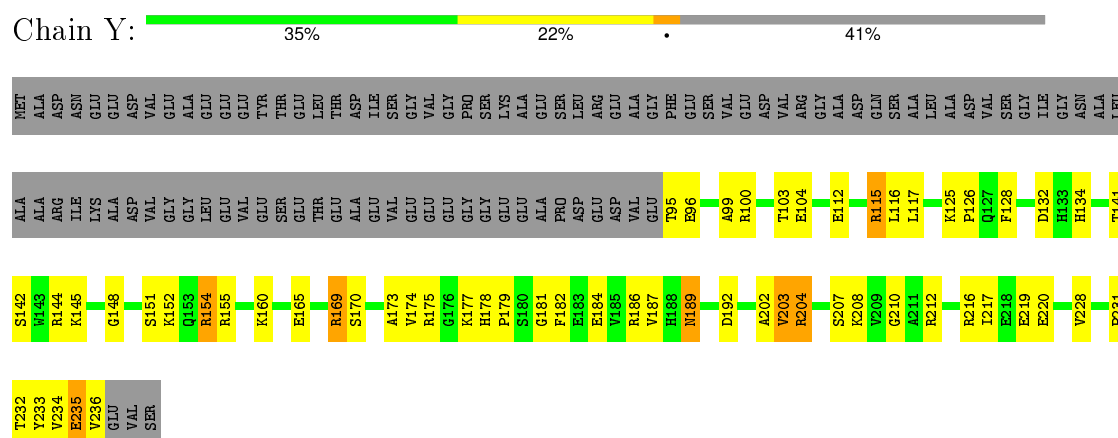
- Molecule 23: 50S ribosomal protein L30P



- Molecule 24: 50S ribosomal protein L31e

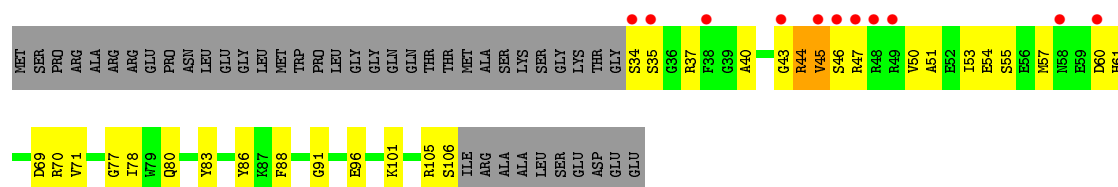


- Molecule 25: 50S ribosomal protein L32e



- Molecule 26: 50S ribosomal protein L37Ae





• Molecule 27: 50S ribosomal protein L37e

Chain 1: 53% 46%



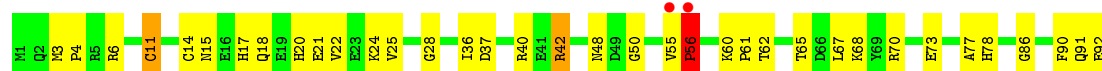
• Molecule 28: 50S ribosomal protein L39e

Chain 2: 44% 48% 8%



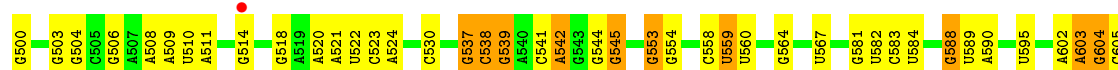
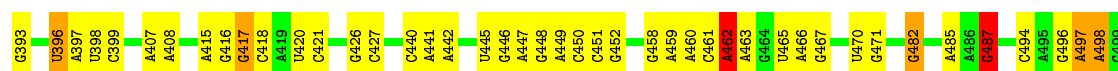
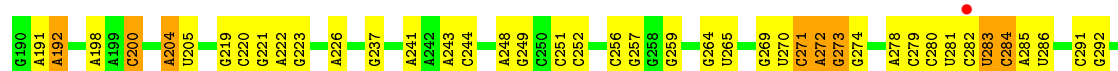
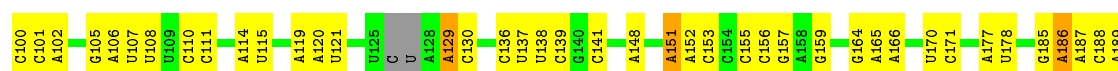
• Molecule 29: 50S ribosomal protein L44E

Chain 3: 61% 36%

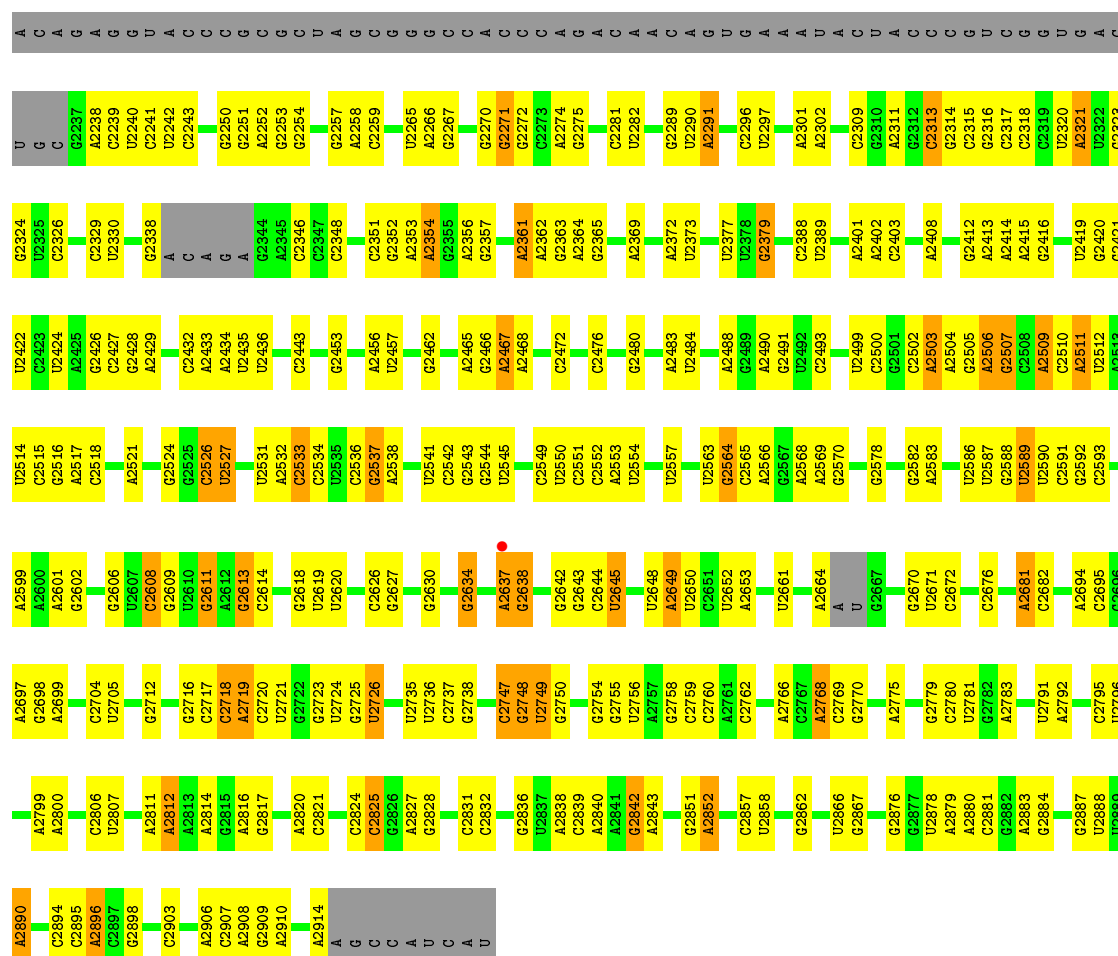


• Molecule 30: 23S RIBOSOMAL RNA

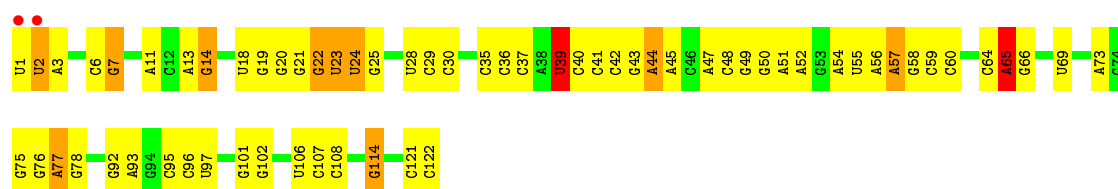
Chain 0: 55% 33% 5% 6%







• Molecule 31: 5S RIBOSOMAL RNA



• Molecule 32: RNA (5'-R(*CP*CP*A)-3')



• Molecule 33: RNA (5'-R(*CP*CP*(8AN))-3')





4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | C 2 2 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 211.32Å 297.90Å 573.14Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 49.79 – 2.80 85.22 – 2.39 | Depositor EDS |
| % Data completeness (in resolution range) | 91.2 (49.79-2.80) 90.7 (85.22-2.39) | Depositor EDS |
| R_{merge} | 0.18 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 0.00 (at 2.40Å) | Xtriage |
| Refinement program | CNS 1.0 | Depositor |
| R, R_{free} | 0.194 , 0.245 0.187 , 0.235 | Depositor DCC |
| R_{free} test set | 4312 reflections (1.09%) | DCC |
| Wilson B-factor (Å ²) | 41.8 | Xtriage |
| Anisotropy | 0.125 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.31 , 71.5 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$ | Xtriage |
| Outliers | 0 of 667161 reflections | Xtriage |
| F_o, F_c correlation | 0.93 | EDS |
| Total number of atoms | 99205 | wwPDB-VP |
| Average B, all atoms (Å ²) | 50.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.53% 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: ACA, OMG, 8AN, CL, SR, NA, K, MG, CD, OMU, UR3, 1MA, PSU

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 | 0.33 | 0/1784 | 0.64 | 0/2403 |
| 2 | B | 0.35 | 0/2687 | 0.66 | 0/3644 |
| 3 | C | 0.37 | 0/1883 | 0.62 | 0/2547 |
| 4 | D | 0.31 | 0/1109 | 0.56 | 0/1493 |
| 5 | E | 0.33 | 0/1380 | 0.61 | 0/1875 |
| 6 | F | 0.32 | 0/899 | 0.56 | 0/1219 |
| 7 | G | 0.29 | 0/241 | 0.47 | 0/324 |
| 8 | H | 0.34 | 0/1300 | 0.64 | 0/1738 |
| 9 | I | 0.27 | 0/524 | 0.50 | 0/711 |
| 10 | J | 0.36 | 0/1134 | 0.60 | 0/1525 |
| 11 | K | 0.36 | 0/1002 | 0.68 | 0/1346 |
| 12 | L | 0.33 | 0/1128 | 0.63 | 0/1504 |
| 13 | M | 0.36 | 0/1580 | 0.60 | 0/2111 |
| 14 | N | 0.29 | 0/1472 | 0.61 | 0/1994 |
| 15 | O | 0.33 | 0/872 | 0.60 | 0/1176 |
| 16 | P | 0.35 | 0/1145 | 0.54 | 0/1524 |
| 17 | Q | 0.35 | 0/747 | 0.67 | 0/1001 |
| 18 | R | 0.37 | 0/1170 | 0.63 | 0/1574 |
| 19 | S | 0.33 | 0/646 | 0.56 | 0/870 |
| 20 | T | 0.33 | 0/956 | 0.62 | 0/1284 |
| 21 | U | 0.34 | 0/417 | 0.60 | 0/562 |
| 22 | V | 0.28 | 0/502 | 0.53 | 0/675 |
| 23 | W | 0.54 | 1/1217 (0.1%) | 1.06 | 2/1650 (0.1%) |
| 24 | X | 0.33 | 0/662 | 0.59 | 0/890 |
| 25 | Y | 0.36 | 0/1146 | 0.65 | 0/1536 |
| 26 | Z | 0.34 | 0/582 | 0.59 | 0/776 |
| 27 | 1 | 0.40 | 0/438 | 0.63 | 0/578 |
| 28 | 2 | 0.34 | 0/401 | 0.55 | 0/529 |
| 29 | 3 | 0.38 | 0/769 | 0.58 | 0/1019 |
| 30 | 0 | 0.39 | 0/65951 | 0.69 | 20/102855 (0.0%) |
| 31 | 9 | 0.35 | 0/2897 | 0.71 | 1/4512 (0.0%) |
| 32 | 5 | 0.64 | 0/65 | 1.28 | 2/99 (2.0%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 33 | 6 | 0.38 | 0/40 | 0.60 | 0/60 |
| All | All | 0.38 | 1/98746 (0.0%) | 0.68 | 25/147604 (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 |
|-----|-------|---------------------|---------------------|
| 30 | 0 | 0 | 47 |
| 31 | 9 | 0 | 2 |
| 32 | 5 | 0 | 1 |
| All | All | 0 | 50 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 23 | W | 52 | VAL | CB-CG2 | -14.55 | 1.22 | 1.52 |

All (25) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 23 | W | 52 | VAL | CG1-CB-CG2 | 30.26 | 159.32 | 110.90 |
| 23 | W | 52 | VAL | CA-CB-CG2 | -16.79 | 85.72 | 110.90 |
| 30 | 0 | 1979 | G | C2'-C3'-O3' | 7.10 | 125.13 | 109.50 |
| 30 | 0 | 1942 | A | C5'-C4'-C3' | 7.05 | 127.28 | 116.00 |
| 30 | 0 | 2313 | C | C5'-C4'-O4' | 7.00 | 117.50 | 109.10 |
| 30 | 0 | 871 | G | C5'-C4'-O4' | -6.96 | 100.75 | 109.10 |
| 30 | 0 | 1942 | A | C5'-C4'-O4' | 6.65 | 117.08 | 109.10 |
| 31 | 9 | 39 | U | N1-C1'-C2' | 6.45 | 122.39 | 114.00 |
| 30 | 0 | 2726 | U | N1-C1'-C2' | 6.38 | 122.30 | 114.00 |
| 30 | 0 | 1592 | G | N9-C1'-C2' | 6.06 | 121.88 | 114.00 |
| 30 | 0 | 2313 | C | C5'-C4'-C3' | 6.02 | 125.63 | 116.00 |
| 30 | 0 | 1504 | A | N9-C1'-C2' | 5.97 | 121.76 | 114.00 |
| 30 | 0 | 2291 | A | N9-C1'-C2' | 5.94 | 121.72 | 114.00 |
| 30 | 0 | 129 | A | C2'-C3'-O3' | 5.80 | 122.99 | 113.70 |
| 30 | 0 | 1819 | G | C5'-C4'-C3' | 5.68 | 125.09 | 116.00 |
| 30 | 0 | 2467 | A | C1'-O4'-C4' | -5.63 | 105.39 | 109.90 |
| 32 | 5 | 76 | A | C5'-C4'-C3' | -5.57 | 107.08 | 116.00 |
| 30 | 0 | 2301 | A | N9-C1'-C2' | 5.48 | 121.12 | 114.00 |
| 30 | 0 | 1504 | A | C1'-O4'-C4' | -5.29 | 105.66 | 109.90 |
| 30 | 0 | 1942 | A | C1'-O4'-C4' | -5.28 | 105.68 | 109.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 30 | 0 | 2313 | C | C1'-O4'-C4' | -5.14 | 105.78 | 109.90 |
| 30 | 0 | 1701 | A | C5'-C4'-C3' | 5.08 | 124.14 | 116.00 |
| 30 | 0 | 462 | A | N9-C1'-C2' | 5.07 | 120.58 | 114.00 |
| 32 | 5 | 76 | A | C5'-C4'-O4' | -5.06 | 103.03 | 109.10 |
| 30 | 0 | 883 | U | N1-C1'-C2' | 5.05 | 120.56 | 114.00 |

There are no chirality outliers.

All (50) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 30 | 0 | 1039 | G | Sidechain |
| 30 | 0 | 1067 | A | Sidechain |
| 30 | 0 | 1078 | A | Sidechain |
| 30 | 0 | 1237 | U | Sidechain |
| 30 | 0 | 1293 | U | Sidechain |
| 30 | 0 | 1309 | U | Sidechain |
| 30 | 0 | 1327 | G | Sidechain |
| 30 | 0 | 1342 | C | Sidechain |
| 30 | 0 | 1380 | U | Sidechain |
| 30 | 0 | 1458 | A | Sidechain |
| 30 | 0 | 148 | A | Sidechain |
| 30 | 0 | 1488 | U | Sidechain |
| 30 | 0 | 1681 | G | Sidechain |
| 30 | 0 | 1741 | U | Sidechain |
| 30 | 0 | 1819 | G | Sidechain |
| 30 | 0 | 1829 | A | Sidechain |
| 30 | 0 | 1863 | G | Sidechain |
| 30 | 0 | 1877 | G | Sidechain |
| 30 | 0 | 1878 | G | Sidechain |
| 30 | 0 | 1993 | C | Sidechain |
| 30 | 0 | 2119 | C | Sidechain |
| 30 | 0 | 2316 | G | Sidechain |
| 30 | 0 | 2465 | A | Sidechain |
| 30 | 0 | 2466 | G | Sidechain |
| 30 | 0 | 2493 | C | Sidechain |
| 30 | 0 | 2503 | A | Sidechain |
| 30 | 0 | 2506 | A | Sidechain |
| 30 | 0 | 2524 | G | Sidechain |
| 30 | 0 | 2599 | A | Sidechain |
| 30 | 0 | 26 | U | Sidechain |
| 30 | 0 | 2630 | G | Sidechain |
| 30 | 0 | 2681 | A | Sidechain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 30 | 0 | 270 | U | Sidechain |
| 30 | 0 | 2842 | G | Sidechain |
| 30 | 0 | 396 | U | Sidechain |
| 30 | 0 | 458 | G | Sidechain |
| 30 | 0 | 460 | A | Sidechain |
| 30 | 0 | 462 | A | Sidechain |
| 30 | 0 | 471 | G | Sidechain |
| 30 | 0 | 482 | G | Sidechain |
| 30 | 0 | 487 | G | Sidechain |
| 30 | 0 | 518 | G | Sidechain |
| 30 | 0 | 722 | G | Sidechain |
| 30 | 0 | 764 | C | Sidechain |
| 30 | 0 | 779 | U | Sidechain |
| 30 | 0 | 795 | G | Sidechain |
| 30 | 0 | 868 | G | Sidechain |
| 32 | 5 | 76 | A | Sidechain |
| 31 | 9 | 39 | U | Sidechain |
| 31 | 9 | 65 | A | 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 | 1752 | 0 | 1764 | 129 | 0 |
| 2 | B | 2624 | 0 | 2530 | 190 | 0 |
| 3 | C | 1859 | 0 | 1811 | 97 | 0 |
| 4 | D | 1093 | 0 | 1083 | 96 | 0 |
| 5 | E | 1356 | 0 | 1264 | 77 | 0 |
| 6 | F | 889 | 0 | 841 | 63 | 0 |
| 7 | G | 240 | 0 | 231 | 17 | 0 |
| 8 | H | 1281 | 0 | 1290 | 63 | 0 |
| 9 | I | 518 | 0 | 495 | 49 | 0 |
| 10 | J | 1119 | 0 | 1096 | 74 | 0 |
| 11 | K | 993 | 0 | 1025 | 57 | 0 |
| 12 | L | 1117 | 0 | 1071 | 69 | 0 |
| 13 | M | 1557 | 0 | 1571 | 86 | 0 |
| 14 | N | 1444 | 0 | 1399 | 101 | 0 |
| 15 | O | 864 | 0 | 868 | 51 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 16 | P | 1135 | 0 | 1120 | 46 | 0 |
| 17 | Q | 734 | 0 | 726 | 29 | 0 |
| 18 | R | 1148 | 0 | 1119 | 51 | 0 |
| 19 | S | 640 | 0 | 600 | 30 | 0 |
| 20 | T | 949 | 0 | 922 | 54 | 0 |
| 21 | U | 410 | 0 | 364 | 32 | 0 |
| 22 | V | 499 | 0 | 511 | 41 | 0 |
| 23 | W | 1195 | 0 | 1135 | 89 | 0 |
| 24 | X | 653 | 0 | 651 | 34 | 0 |
| 25 | Y | 1130 | 0 | 1133 | 63 | 0 |
| 26 | Z | 572 | 0 | 529 | 25 | 0 |
| 27 | 1 | 431 | 0 | 426 | 35 | 0 |
| 28 | 2 | 396 | 0 | 413 | 27 | 0 |
| 29 | 3 | 754 | 0 | 727 | 33 | 0 |
| 30 | 0 | 59018 | 0 | 29811 | 1006 | 0 |
| 31 | 9 | 2596 | 0 | 1324 | 76 | 0 |
| 32 | 5 | 59 | 0 | 35 | 10 | 0 |
| 33 | 6 | 59 | 0 | 35 | 1 | 0 |
| 34 | 6 | 19 | 0 | 20 | 0 | 0 |
| 35 | 0 | 84 | 0 | 0 | 0 | 0 |
| 35 | 2 | 1 | 0 | 0 | 0 | 0 |
| 35 | 9 | 1 | 0 | 0 | 0 | 0 |
| 35 | A | 2 | 0 | 0 | 0 | 0 |
| 35 | B | 1 | 0 | 0 | 0 | 0 |
| 35 | C | 1 | 0 | 0 | 0 | 0 |
| 35 | K | 1 | 0 | 0 | 0 | 0 |
| 35 | T | 1 | 0 | 0 | 0 | 0 |
| 35 | Y | 1 | 0 | 0 | 0 | 0 |
| 36 | 0 | 64 | 0 | 0 | 0 | 0 |
| 36 | 9 | 1 | 0 | 0 | 0 | 0 |
| 36 | B | 1 | 0 | 0 | 0 | 0 |
| 36 | C | 1 | 0 | 0 | 0 | 0 |
| 36 | D | 1 | 0 | 0 | 0 | 0 |
| 36 | J | 1 | 0 | 0 | 0 | 0 |
| 36 | L | 1 | 0 | 0 | 0 | 0 |
| 36 | M | 1 | 0 | 0 | 0 | 0 |
| 36 | Q | 1 | 0 | 0 | 0 | 0 |
| 36 | R | 2 | 0 | 0 | 0 | 0 |
| 36 | S | 1 | 0 | 0 | 0 | 0 |
| 37 | 0 | 86 | 0 | 0 | 0 | 0 |
| 37 | 1 | 2 | 0 | 0 | 0 | 0 |
| 37 | 3 | 3 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 37 | 9 | 3 | 0 | 0 | 0 | 0 |
| 37 | A | 3 | 0 | 0 | 0 | 0 |
| 37 | B | 2 | 0 | 0 | 0 | 0 |
| 37 | F | 1 | 0 | 0 | 0 | 0 |
| 37 | H | 2 | 0 | 0 | 0 | 0 |
| 37 | R | 1 | 0 | 0 | 0 | 0 |
| 37 | S | 1 | 0 | 0 | 0 | 0 |
| 37 | T | 2 | 0 | 0 | 0 | 0 |
| 37 | Y | 1 | 0 | 0 | 0 | 0 |
| 38 | 0 | 6 | 0 | 0 | 0 | 0 |
| 38 | 2 | 1 | 0 | 0 | 0 | 0 |
| 38 | 3 | 1 | 0 | 0 | 0 | 0 |
| 38 | A | 1 | 0 | 0 | 0 | 0 |
| 38 | B | 1 | 0 | 0 | 0 | 0 |
| 38 | J | 3 | 0 | 0 | 2 | 0 |
| 38 | K | 1 | 0 | 0 | 1 | 0 |
| 38 | L | 2 | 0 | 0 | 0 | 0 |
| 38 | M | 1 | 0 | 0 | 1 | 0 |
| 38 | N | 1 | 0 | 0 | 0 | 0 |
| 38 | O | 1 | 0 | 0 | 0 | 0 |
| 38 | Q | 1 | 0 | 0 | 0 | 0 |
| 38 | R | 1 | 0 | 0 | 0 | 0 |
| 38 | Y | 1 | 0 | 0 | 0 | 0 |
| 39 | 0 | 2 | 0 | 0 | 0 | 0 |
| 40 | 1 | 1 | 0 | 0 | 0 | 0 |
| 40 | 3 | 1 | 0 | 0 | 0 | 0 |
| 40 | O | 1 | 0 | 0 | 0 | 0 |
| 40 | U | 1 | 0 | 0 | 0 | 0 |
| 40 | Z | 1 | 0 | 0 | 0 | 0 |
| 41 | 0 | 5771 | 0 | 0 | 145 | 0 |
| 41 | 1 | 53 | 0 | 0 | 6 | 0 |
| 41 | 2 | 42 | 0 | 0 | 1 | 0 |
| 41 | 3 | 66 | 0 | 0 | 6 | 0 |
| 41 | 5 | 4 | 0 | 0 | 2 | 0 |
| 41 | 6 | 3 | 0 | 0 | 0 | 0 |
| 41 | 9 | 148 | 0 | 0 | 10 | 0 |
| 41 | A | 128 | 0 | 0 | 21 | 0 |
| 41 | B | 165 | 0 | 0 | 19 | 0 |
| 41 | C | 170 | 0 | 0 | 14 | 0 |
| 41 | D | 49 | 0 | 0 | 7 | 0 |
| 41 | E | 48 | 0 | 0 | 3 | 0 |
| 41 | F | 31 | 0 | 0 | 4 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 41 | G | 19 | 0 | 0 | 0 | 0 |
| 41 | H | 77 | 0 | 0 | 10 | 0 |
| 41 | I | 11 | 0 | 0 | 1 | 0 |
| 41 | J | 63 | 0 | 0 | 1 | 0 |
| 41 | K | 54 | 0 | 0 | 4 | 0 |
| 41 | L | 92 | 0 | 0 | 10 | 0 |
| 41 | M | 136 | 0 | 0 | 5 | 0 |
| 41 | N | 64 | 0 | 0 | 8 | 0 |
| 41 | O | 43 | 0 | 0 | 5 | 0 |
| 41 | P | 69 | 0 | 0 | 2 | 0 |
| 41 | Q | 51 | 0 | 0 | 0 | 0 |
| 41 | R | 87 | 0 | 0 | 5 | 0 |
| 41 | S | 33 | 0 | 0 | 4 | 0 |
| 41 | T | 40 | 0 | 0 | 3 | 0 |
| 41 | U | 30 | 0 | 0 | 2 | 0 |
| 41 | V | 16 | 0 | 0 | 4 | 0 |
| 41 | W | 72 | 0 | 0 | 8 | 0 |
| 41 | X | 25 | 0 | 0 | 4 | 0 |
| 41 | Y | 108 | 0 | 0 | 6 | 0 |
| 41 | Z | 30 | 0 | 0 | 4 | 0 |
| All | All | 99205 | 0 | 59940 | 2631 | 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 17.

All (2631) 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) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:236:THR:HG22 | 3:C:239:ALA:H | 1.02 | 1.12 |
| 31:9:76:G:H3' | 31:9:77:A:H5'' | 1.31 | 1.12 |
| 30:0:871:G:H8 | 30:0:871:G:H5' | 1.20 | 1.06 |
| 14:N:37:ARG:NH1 | 31:9:6:C:H5'' | 1.72 | 1.03 |
| 2:B:36:PRO:HA | 2:B:168:GLY:HA3 | 1.41 | 1.03 |
| 15:O:32:ARG:HE | 15:O:35:LYS:HD2 | 1.24 | 1.02 |
| 30:0:541:C:H2' | 30:0:542:A:H5'' | 1.40 | 1.02 |
| 10:J:82:THR:HG23 | 30:0:1242:A:H5' | 1.41 | 1.02 |
| 9:I:97:VAL:HG12 | 9:I:101:LYS:HE3 | 1.43 | 1.01 |
| 30:0:871:G:C8 | 30:0:871:G:H5' | 1.96 | 1.00 |
| 5:E:81:GLU:HG2 | 5:E:134:SER:HB3 | 1.42 | 1.00 |
| 26:Z:70:ARG:HD2 | 26:Z:83:TYR:HB2 | 1.42 | 0.99 |
| 18:R:8:ALA:HB1 | 18:R:13:THR:HG21 | 1.44 | 0.99 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:0:2542:C:H1' | 41:0:7596:HOH:O | 1.58 | 0.99 |
| 30:0:870:G:H2' | 30:0:871:G:H5'' | 1.44 | 0.98 |
| 2:B:36:PRO:HG3 | 2:B:169:GLY:H | 1.29 | 0.98 |
| 10:J:52:GLN:NE2 | 30:0:1119:G:H2' | 1.79 | 0.98 |
| 30:0:1160:G:H5' | 30:0:1161:A:H5' | 1.41 | 0.98 |
| 30:0:542:A:H5' | 30:0:542:A:H8 | 1.28 | 0.98 |
| 10:J:52:GLN:HE22 | 30:0:1119:G:H2' | 1.26 | 0.97 |
| 28:2:41:HIS:H | 28:2:45:ASN:HD22 | 1.09 | 0.97 |
| 20:T:9:LYS:HE3 | 20:T:13:ARG:NH1 | 1.80 | 0.97 |
| 30:0:541:C:C2' | 30:0:542:A:H5'' | 1.94 | 0.97 |
| 14:N:144:GLY:O | 14:N:147:ILE:HG22 | 1.64 | 0.97 |
| 1:A:153:ARG:HH11 | 1:A:153:ARG:HB2 | 1.28 | 0.96 |
| 23:W:6:GLN:HB2 | 23:W:26:ILE:HD11 | 1.46 | 0.96 |
| 18:R:99:ALA:HB1 | 18:R:109:MET:HE1 | 1.48 | 0.95 |
| 3:C:127:ARG:NH2 | 3:C:225:PRO:HG2 | 1.82 | 0.95 |
| 22:V:1:THR:HG23 | 22:V:2:VAL:H | 1.27 | 0.95 |
| 3:C:236:THR:HG22 | 3:C:239:ALA:N | 1.81 | 0.95 |
| 16:P:115:SER:H | 16:P:118:GLN:HE21 | 1.06 | 0.95 |
| 11:K:29:LEU:HB3 | 11:K:55:VAL:HG11 | 1.48 | 0.94 |
| 8:H:30:LYS:H | 8:H:62:HIS:HD2 | 1.05 | 0.94 |
| 1:A:211:LYS:HB3 | 1:A:212:PRO:HD2 | 1.47 | 0.94 |
| 14:N:113:SER:HB2 | 41:N:8857:HOH:O | 1.70 | 0.92 |
| 22:V:12:THR:HG22 | 22:V:15:GLU:HG3 | 1.50 | 0.92 |
| 23:W:21:LEU:HD21 | 23:W:48:VAL:HG11 | 1.50 | 0.91 |
| 1:A:88:ILE:HD13 | 1:A:100:PRO:HD3 | 1.52 | 0.90 |
| 2:B:238:ASN:HD22 | 2:B:240:GLY:H | 1.19 | 0.90 |
| 2:B:162:MET:HE3 | 2:B:310:ARG:HD2 | 1.51 | 0.90 |
| 4:D:57:THR:HG23 | 4:D:63:ILE:HA | 1.55 | 0.89 |
| 11:K:10:GLN:H | 11:K:10:GLN:HE21 | 1.15 | 0.88 |
| 29:3:65:THR:HG22 | 29:3:67:LEU:HG | 1.56 | 0.88 |
| 2:B:179:LEU:O | 2:B:183:GLU:HG2 | 1.72 | 0.88 |
| 14:N:37:ARG:HH12 | 31:9:6:C:H5'' | 1.34 | 0.87 |
| 21:U:14:GLU:O | 21:U:17:THR:HB | 1.73 | 0.87 |
| 4:D:25:MET:HE2 | 4:D:41:LEU:HG | 1.54 | 0.87 |
| 13:M:171:ARG:HD3 | 30:0:156:C:H5'' | 1.56 | 0.87 |
| 13:M:134:ILE:HG23 | 13:M:141:ILE:HD13 | 1.56 | 0.86 |
| 5:E:3:VAL:HG22 | 5:E:49:ILE:HB | 1.57 | 0.86 |
| 6:F:91:VAL:HG12 | 6:F:92:GLY:H | 1.39 | 0.86 |
| 18:R:18:LEU:HB2 | 18:R:143:VAL:HG13 | 1.58 | 0.86 |
| 3:C:236:THR:CG2 | 3:C:239:ALA:H | 1.89 | 0.85 |
| 3:C:1:MET:HG2 | 3:C:2:GLN:H | 1.41 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:140:LEU:HA | 41:B:9054:HOH:O | 1.74 | 0.85 |
| 2:B:217:ARG:HG3 | 2:B:257:THR:HG22 | 1.58 | 0.85 |
| 30:0:545:G:H8 | 30:0:545:G:H5' | 1.40 | 0.85 |
| 25:Y:235:GLU:H | 25:Y:235:GLU:CD | 1.80 | 0.85 |
| 25:Y:189:ASN:HA | 25:Y:217:ILE:HD11 | 1.58 | 0.85 |
| 16:P:115:SER:OG | 16:P:118:GLN:HG3 | 1.76 | 0.84 |
| 2:B:275:GLY:O | 2:B:291:ASP:HA | 1.77 | 0.84 |
| 30:0:1377:C:H6 | 30:0:1377:C:H5' | 1.40 | 0.84 |
| 30:0:1118:A:H62 | 30:0:1244:U:H3 | 1.22 | 0.84 |
| 29:3:48:ASN:HD21 | 30:0:2468:A:H61 | 1.24 | 0.84 |
| 30:0:2506:A:HO2' | 30:0:2507:G:H8 | 0.85 | 0.84 |
| 24:X:37:LEU:HD13 | 24:X:85:VAL:HG21 | 1.58 | 0.84 |
| 30:0:870:G:C2' | 30:0:871:G:H5'' | 2.07 | 0.84 |
| 2:B:162:MET:HG3 | 2:B:310:ARG:NH1 | 1.92 | 0.84 |
| 4:D:99:ASP:HB3 | 4:D:103:ASN:H | 1.43 | 0.84 |
| 27:1:20:ARG:HG2 | 30:0:111:C:O2' | 1.77 | 0.84 |
| 14:N:38:LYS:HE2 | 14:N:107:ASN:HD21 | 1.40 | 0.84 |
| 11:K:74:VAL:HG11 | 11:K:113:ILE:HG12 | 1.58 | 0.83 |
| 10:J:93:ARG:HH11 | 10:J:93:ARG:HB3 | 1.41 | 0.83 |
| 5:E:116:THR:HG22 | 5:E:151:LEU:HD22 | 1.59 | 0.83 |
| 30:0:2073:G:H5'' | 41:0:4695:HOH:O | 1.75 | 0.83 |
| 30:0:1116:U:HO2' | 30:0:1118:A:H2 | 0.87 | 0.83 |
| 30:0:2506:A:O2' | 30:0:2507:G:H8 | 1.61 | 0.83 |
| 4:D:28:GLY:HA2 | 4:D:69:ILE:HG23 | 1.60 | 0.83 |
| 30:0:1451:C:H5' | 30:0:1505:U:C5 | 2.14 | 0.83 |
| 11:K:118:ALA:HA | 11:K:125:ALA:HB2 | 1.58 | 0.83 |
| 30:0:2586:U:H3 | 30:0:2592:G:H22 | 1.22 | 0.83 |
| 11:K:109:LEU:HD13 | 11:K:113:ILE:HD11 | 1.60 | 0.83 |
| 23:W:6:GLN:HB2 | 23:W:26:ILE:CD1 | 2.08 | 0.82 |
| 4:D:172:VAL:HG12 | 4:D:173:GLU:H | 1.44 | 0.82 |
| 30:0:1474:C:H6 | 30:0:1474:C:H5' | 1.44 | 0.82 |
| 24:X:21:PRO:HG2 | 24:X:24:LYS:HD3 | 1.60 | 0.82 |
| 30:0:282:C:H1' | 30:0:368:C:N4 | 1.95 | 0.82 |
| 30:0:1160:G:C5' | 30:0:1161:A:H5' | 2.10 | 0.81 |
| 31:9:56:A:H2' | 31:9:57:A:H5'' | 1.60 | 0.81 |
| 6:F:34:ASN:HA | 13:M:4:ALA:HB2 | 1.60 | 0.81 |
| 13:M:164:THR:HG22 | 13:M:166:ALA:H | 1.44 | 0.81 |
| 3:C:115:LEU:HD21 | 3:C:243:VAL:HG13 | 1.61 | 0.81 |
| 30:0:1372:A:H3' | 41:0:7983:HOH:O | 1.79 | 0.81 |
| 13:M:107:ARG:HH11 | 13:M:107:ARG:HG3 | 1.45 | 0.81 |
| 9:I:82:THR:HG23 | 30:0:1168:C:H5'' | 1.63 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:0:2534:C:H1' | 41:0:4378:HOH:O | 1.80 | 0.81 |
| 6:F:91:VAL:HG12 | 6:F:92:GLY:N | 1.96 | 0.81 |
| 3:C:233:THR:HG22 | 3:C:234:VAL:H | 1.45 | 0.81 |
| 11:K:98:VAL:CG1 | 11:K:102:GLU:HA | 2.10 | 0.81 |
| 18:R:96:VAL:HG13 | 18:R:106:GLY:HA3 | 1.61 | 0.81 |
| 5:E:23:GLU:HG2 | 5:E:28:SER:HB3 | 1.63 | 0.81 |
| 11:K:14:LYS:HB2 | 11:K:45:PRO:HG2 | 1.62 | 0.81 |
| 14:N:164:ASP:CG | 14:N:167:ASP:HA | 2.01 | 0.81 |
| 30:0:2005:G:H3' | 30:0:2005:G:OP2 | 1.81 | 0.80 |
| 2:B:86:ALA:HA | 41:B:9054:HOH:O | 1.81 | 0.80 |
| 2:B:307:ARG:HH11 | 2:B:307:ARG:HG3 | 1.44 | 0.80 |
| 30:0:2717:C:C2' | 30:0:2718:C:H5'' | 2.12 | 0.80 |
| 23:W:80:ASP:O | 23:W:84:VAL:HG23 | 1.80 | 0.80 |
| 30:0:559:U:H5' | 30:0:559:U:H6 | 1.45 | 0.80 |
| 4:D:154:LYS:HD2 | 4:D:154:LYS:H | 1.45 | 0.80 |
| 14:N:83:LEU:HD13 | 14:N:175:LEU:HD23 | 1.62 | 0.80 |
| 30:0:1835:U:H5 | 30:0:1840:A:N7 | 1.79 | 0.80 |
| 8:H:59:GLN:NE2 | 8:H:129:ARG:HE | 1.80 | 0.79 |
| 10:J:74:ARG:CB | 10:J:74:ARG:HH11 | 1.95 | 0.79 |
| 30:0:1603:A:H5' | 30:0:1605:G:O4' | 1.80 | 0.79 |
| 30:0:2908:A:H2' | 30:0:2909:G:O4' | 1.82 | 0.79 |
| 30:0:541:C:H2' | 30:0:542:A:C5' | 2.13 | 0.79 |
| 30:0:1667:A:H8 | 30:0:1667:A:H5' | 1.48 | 0.79 |
| 1:A:153:ARG:CB | 1:A:153:ARG:HH11 | 1.94 | 0.79 |
| 8:H:30:LYS:H | 8:H:62:HIS:CD2 | 1.97 | 0.79 |
| 30:0:877:G:H5' | 30:0:878:G:OP1 | 1.82 | 0.79 |
| 23:W:4:LEU:HD23 | 23:W:54:PHE:HB3 | 1.64 | 0.79 |
| 1:A:33:GLU:CD | 1:A:33:GLU:H | 1.86 | 0.79 |
| 20:T:112:LEU:HD23 | 20:T:119:ALA:HB3 | 1.63 | 0.78 |
| 4:D:54:ALA:HB2 | 4:D:69:ILE:HD12 | 1.65 | 0.78 |
| 30:0:506:G:H22 | 30:0:509:A:C5' | 1.95 | 0.78 |
| 30:0:1701:A:H4' | 30:0:1702:U:H5'' | 1.65 | 0.78 |
| 14:N:132:ASN:O | 14:N:135:VAL:HG12 | 1.84 | 0.78 |
| 30:0:2717:C:H2' | 30:0:2718:C:H5'' | 1.64 | 0.78 |
| 18:R:39:THR:HG23 | 18:R:107:GLU:O | 1.83 | 0.78 |
| 10:J:18:ILE:HD13 | 30:0:1244:U:OP1 | 1.83 | 0.77 |
| 30:0:1300:G:H1' | 41:0:5535:HOH:O | 1.82 | 0.77 |
| 30:0:2812:A:H2 | 30:0:2814:A:H62 | 1.32 | 0.77 |
| 23:W:137:GLN:HE21 | 23:W:141:HIS:HE1 | 1.32 | 0.77 |
| 2:B:162:MET:CE | 2:B:310:ARG:HD2 | 2.14 | 0.77 |
| 13:M:80:GLY:O | 13:M:81:ARG:HD2 | 1.84 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 29:3:60:LYS:HG3 | 29:3:61:PRO:HD2 | 1.66 | 0.77 |
| 11:K:32:ILE:HD11 | 11:K:56:SER:HB3 | 1.67 | 0.77 |
| 2:B:162:MET:HE3 | 2:B:310:ARG:HH11 | 1.47 | 0.77 |
| 30:0:681:G:N3 | 30:0:681:G:H5' | 1.99 | 0.77 |
| 30:0:969:G:H1 | 30:0:999:C:H42 | 1.32 | 0.77 |
| 9:I:73:LEU:HD12 | 9:I:107:LYS:NZ | 1.98 | 0.77 |
| 30:0:506:G:H22 | 30:0:509:A:H5' | 1.48 | 0.77 |
| 27:1:16:HIS:HD2 | 30:0:470:U:O2' | 1.67 | 0.77 |
| 16:P:115:SER:H | 16:P:118:GLN:NE2 | 1.82 | 0.77 |
| 4:D:36:ASN:HA | 41:D:7500:HOH:O | 1.83 | 0.77 |
| 30:0:1973:A:H5' | 30:0:1973:A:H8 | 1.50 | 0.77 |
| 30:0:2637:A:H4' | 30:0:2638:G:C5' | 2.15 | 0.76 |
| 16:P:80:ARG:HG2 | 16:P:87:ARG:CZ | 2.15 | 0.76 |
| 11:K:10:GLN:H | 11:K:10:GLN:NE2 | 1.82 | 0.76 |
| 15:O:42:GLU:HB2 | 41:O:2176:HOH:O | 1.85 | 0.76 |
| 4:D:75:LEU:HD22 | 4:D:79:MET:HB3 | 1.67 | 0.76 |
| 3:C:47:GLY:HA2 | 3:C:92:PRO:HB2 | 1.67 | 0.76 |
| 30:0:1116:U:H3 | 30:0:1246:A:H62 | 1.34 | 0.76 |
| 23:W:88:THR:HG23 | 23:W:110:GLN:HB3 | 1.66 | 0.76 |
| 11:K:74:VAL:CG1 | 11:K:113:ILE:HG12 | 2.16 | 0.76 |
| 1:A:192:VAL:HG12 | 1:A:207:GLN:HB3 | 1.68 | 0.76 |
| 4:D:22:VAL:HG22 | 4:D:74:THR:HG22 | 1.66 | 0.76 |
| 6:F:63:ILE:HB | 6:F:64:PRO:HD3 | 1.68 | 0.76 |
| 30:0:1625:U:H4' | 41:0:5518:HOH:O | 1.86 | 0.76 |
| 30:0:855:U:H3' | 41:0:4506:HOH:O | 1.85 | 0.76 |
| 10:J:77:GLY:HA2 | 10:J:80:LYS:H | 1.50 | 0.76 |
| 2:B:211:THR:HG23 | 30:0:2840:A:OP1 | 1.85 | 0.76 |
| 5:E:15:GLN:HG2 | 5:E:19:ASP:O | 1.85 | 0.76 |
| 30:0:542:A:H5' | 30:0:542:A:C8 | 2.18 | 0.75 |
| 30:0:1119:G:N2 | 30:0:1246:A:C2 | 2.54 | 0.75 |
| 30:0:1189:A:H3' | 41:0:9461:HOH:O | 1.84 | 0.75 |
| 3:C:236:THR:HG21 | 41:C:8573:HOH:O | 1.85 | 0.75 |
| 10:J:46:ILE:HD11 | 10:J:53:ILE:HG21 | 1.67 | 0.75 |
| 1:A:199:HIS:CD2 | 1:A:201:PHE:H | 2.04 | 0.75 |
| 8:H:49:GLN:HE21 | 8:H:140:TYR:HE2 | 1.35 | 0.75 |
| 30:0:1058:A:H2' | 30:0:1060:C:H5'' | 1.68 | 0.75 |
| 4:D:25:MET:HE1 | 4:D:37:ALA:HB1 | 1.68 | 0.75 |
| 30:0:1666:C:H2' | 30:0:1667:A:H5' | 1.69 | 0.75 |
| 10:J:19:MET:HE2 | 10:J:79:PHE:HA | 1.68 | 0.75 |
| 2:B:267:LYS:HD3 | 41:0:3471:HOH:O | 1.86 | 0.75 |
| 20:T:9:LYS:HE3 | 20:T:13:ARG:CZ | 2.16 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 22:V:1:THR:HB | 30:0:93:C:H5'' | 1.67 | 0.75 |
| 16:P:121:ASP:O | 16:P:125:LYS:HG3 | 1.87 | 0.75 |
| 20:T:71:VAL:HG11 | 20:T:90:PRO:HB3 | 1.69 | 0.75 |
| 23:W:88:THR:HB | 41:W:6679:HOH:O | 1.85 | 0.75 |
| 24:X:25:ARG:HD3 | 24:X:64:ALA:O | 1.87 | 0.75 |
| 6:F:58:GLU:CD | 13:M:27:ARG:HH22 | 1.89 | 0.75 |
| 22:V:12:THR:HG22 | 22:V:15:GLU:CG | 2.16 | 0.74 |
| 11:K:39:GLY:HA2 | 41:K:4183:HOH:O | 1.85 | 0.74 |
| 9:I:127:CYS:HB3 | 9:I:132:VAL:HB | 1.69 | 0.74 |
| 27:1:21:ARG:HD2 | 27:1:37:CYS:SG | 2.27 | 0.74 |
| 8:H:23:ILE:HG23 | 8:H:123:ILE:HD11 | 1.69 | 0.74 |
| 23:W:68:THR:HG23 | 23:W:69:ARG:HG2 | 1.67 | 0.74 |
| 31:9:59:C:H2' | 31:9:60:C:C6 | 2.22 | 0.74 |
| 2:B:62:ARG:HA | 2:B:65:MET:CE | 2.17 | 0.74 |
| 8:H:30:LYS:N | 8:H:62:HIS:HD2 | 1.83 | 0.74 |
| 27:1:1:THR:HA | 41:0:3266:HOH:O | 1.86 | 0.74 |
| 30:0:2291:A:C8 | 30:0:2309:C:H5' | 2.23 | 0.74 |
| 30:0:1118:A:H3' | 30:0:1118:A:C8 | 2.22 | 0.74 |
| 30:0:1118:A:H3' | 30:0:1118:A:H8 | 1.53 | 0.74 |
| 6:F:46:GLU:OE2 | 6:F:100:ASP:HA | 1.87 | 0.74 |
| 1:A:100:PRO:HG2 | 1:A:103:VAL:HG21 | 1.69 | 0.73 |
| 2:B:162:MET:HG3 | 2:B:310:ARG:HH11 | 1.53 | 0.73 |
| 2:B:88:GLU:HB3 | 2:B:97:LEU:HD12 | 1.70 | 0.73 |
| 30:0:823:U:H3' | 41:0:5309:HOH:O | 1.88 | 0.73 |
| 14:N:110:THR:HB | 14:N:113:SER:OG | 1.88 | 0.73 |
| 21:U:52:THR:HG22 | 21:U:54:THR:H | 1.52 | 0.73 |
| 30:0:1615:A:H5' | 41:0:5048:HOH:O | 1.87 | 0.73 |
| 30:0:1205:U:H2' | 30:0:1206:U:H5'' | 1.70 | 0.73 |
| 22:V:56:ILE:HG22 | 22:V:60:GLN:HE21 | 1.53 | 0.73 |
| 30:0:1160:G:H5' | 30:0:1161:A:C5' | 2.17 | 0.73 |
| 30:0:1838:U:O2' | 30:0:2644:C:H5' | 1.89 | 0.73 |
| 14:N:48:VAL:CG1 | 14:N:55:ASP:HB3 | 2.19 | 0.73 |
| 21:U:9:CYS:HA | 21:U:52:THR:HG23 | 1.71 | 0.72 |
| 30:0:2420:G:O2' | 30:0:2421:G:H5' | 1.89 | 0.72 |
| 7:G:27:ILE:HD13 | 7:G:71:LEU:HD23 | 1.71 | 0.72 |
| 21:U:46:ALA:HB1 | 21:U:52:THR:HG21 | 1.70 | 0.72 |
| 24:X:49:ARG:HG3 | 24:X:49:ARG:O | 1.88 | 0.72 |
| 3:C:5:ILE:HD11 | 3:C:16:VAL:HG22 | 1.71 | 0.72 |
| 30:0:1116:U:O2' | 30:0:1118:A:H2 | 1.68 | 0.72 |
| 13:M:134:ILE:CG2 | 13:M:141:ILE:HD13 | 2.19 | 0.72 |
| 5:E:84:MET:HE1 | 5:E:148:ILE:HD12 | 1.72 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 23:W:149:LEU:HG | 23:W:153:MET:HE2 | 1.71 | 0.72 |
| 30:0:1887:U:H5 | 41:0:7407:HOH:O | 1.72 | 0.72 |
| 14:N:49:THR:HG22 | 14:N:56:ASP:HB2 | 1.72 | 0.72 |
| 4:D:25:MET:CE | 4:D:37:ALA:HB1 | 2.21 | 0.71 |
| 2:B:51:VAL:HG23 | 2:B:330:VAL:HG22 | 1.72 | 0.71 |
| 15:O:32:ARG:HD3 | 15:O:32:ARG:O | 1.89 | 0.71 |
| 18:R:18:LEU:HG | 18:R:91:LEU:HD13 | 1.72 | 0.71 |
| 13:M:58:GLN:HG3 | 41:M:8912:HOH:O | 1.90 | 0.71 |
| 28:2:41:HIS:N | 28:2:45:ASN:HD22 | 1.84 | 0.71 |
| 18:R:18:LEU:HB2 | 18:R:143:VAL:CG1 | 2.20 | 0.71 |
| 30:0:2637:A:H4' | 30:0:2638:G:H5' | 1.72 | 0.71 |
| 31:9:29:C:H2' | 31:9:30:C:H5' | 1.71 | 0.71 |
| 18:R:99:ALA:HB1 | 18:R:109:MET:CE | 2.20 | 0.71 |
| 15:O:21:SER:OG | 15:O:106:PRO:HB2 | 1.90 | 0.71 |
| 18:R:128:ARG:NH2 | 30:0:2054:A:N3 | 2.38 | 0.71 |
| 30:0:1166:A:H1' | 30:0:1192:A:C2 | 2.26 | 0.71 |
| 31:9:75:G:H1 | 31:9:106:U:H3 | 1.39 | 0.71 |
| 2:B:212:GLN:HB2 | 2:B:257:THR:HG21 | 1.72 | 0.71 |
| 30:0:1701:A:H2' | 41:0:6861:HOH:O | 1.91 | 0.71 |
| 30:0:2748:G:H2' | 41:0:9326:HOH:O | 1.90 | 0.71 |
| 12:L:6:ARG:HD3 | 30:0:1299:G:O6 | 1.91 | 0.71 |
| 1:A:199:HIS:HD2 | 1:A:201:PHE:H | 1.37 | 0.70 |
| 15:O:32:ARG:NE | 15:O:35:LYS:HD2 | 2.05 | 0.70 |
| 30:0:1206:U:H5' | 30:0:1206:U:H6 | 1.55 | 0.70 |
| 17:Q:38:LYS:HE2 | 17:Q:62:THR:OG1 | 1.92 | 0.70 |
| 32:5:74:C:H2' | 32:5:75:C:H5' | 1.71 | 0.70 |
| 4:D:170:TYR:O | 4:D:171:ASP:HB3 | 1.91 | 0.70 |
| 3:C:104:ASP:O | 3:C:108:GLN:HG3 | 1.91 | 0.70 |
| 14:N:80:SER:HB2 | 41:N:8836:HOH:O | 1.91 | 0.70 |
| 12:L:90:ARG:HA | 12:L:119:THR:HB | 1.73 | 0.70 |
| 12:L:80:ASP:HB2 | 12:L:90:ARG:O | 1.92 | 0.70 |
| 22:V:39:ALA:N | 22:V:40:PRO:HD2 | 2.06 | 0.70 |
| 4:D:135:VAL:HG21 | 4:D:139:TYR:CD1 | 2.27 | 0.70 |
| 12:L:18:HIS:HD2 | 30:0:902:G:N7 | 1.90 | 0.70 |
| 8:H:32:ALA:HB3 | 8:H:69:ARG:HH12 | 1.56 | 0.70 |
| 13:M:164:THR:HG22 | 13:M:166:ALA:N | 2.05 | 0.70 |
| 2:B:62:ARG:HA | 2:B:65:MET:HE3 | 1.73 | 0.70 |
| 6:F:14:ASP:O | 6:F:18:GLU:HG3 | 1.92 | 0.70 |
| 11:K:34:VAL:HG22 | 11:K:47:ALA:HB2 | 1.74 | 0.69 |
| 30:0:2769:C:H2' | 30:0:2770:G:O4' | 1.92 | 0.69 |
| 14:N:38:LYS:HE2 | 14:N:107:ASN:ND2 | 2.05 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:M:72:ALA:HB2 | 13:M:93:ARG:HG2 | 1.72 | 0.69 |
| 16:P:59:ARG:NH2 | 16:P:66:GLN:HE22 | 1.90 | 0.69 |
| 12:L:53:ARG:NH2 | 12:L:57:VAL:HG12 | 2.08 | 0.69 |
| 30:0:271:C:H41 | 30:0:378:A:H2 | 1.38 | 0.69 |
| 19:S:55:GLN:NE2 | 30:0:1446:U:H2' | 2.07 | 0.69 |
| 2:B:74:ILE:HD13 | 2:B:309:VAL:HG21 | 1.74 | 0.69 |
| 41:M:8875:HOH:O | 30:0:381:G:H5'' | 1.92 | 0.69 |
| 6:F:36:THR:HG23 | 6:F:97:ALA:HB2 | 1.73 | 0.69 |
| 29:3:25:VAL:HG22 | 29:3:68:LYS:HG3 | 1.74 | 0.69 |
| 22:V:1:THR:HG23 | 22:V:2:VAL:N | 2.04 | 0.69 |
| 18:R:18:LEU:HD12 | 18:R:143:VAL:HG11 | 1.74 | 0.69 |
| 3:C:2:GLN:HB3 | 41:C:8583:HOH:O | 1.92 | 0.69 |
| 3:C:65:ARG:HG3 | 3:C:67:GLN:HB2 | 1.74 | 0.69 |
| 26:Z:61:HIS:HB2 | 26:Z:71:VAL:HB | 1.73 | 0.69 |
| 8:H:61:ARG:HG3 | 8:H:61:ARG:HH11 | 1.57 | 0.69 |
| 30:0:1206:U:H2' | 30:0:1207:A:O4' | 1.93 | 0.69 |
| 22:V:44:GLY:HA3 | 30:0:92:G:H4' | 1.74 | 0.69 |
| 3:C:103:ASN:ND2 | 30:0:663:C:H5'' | 2.08 | 0.69 |
| 30:0:1159:G:H21 | 30:0:1189:A:H8 | 1.40 | 0.69 |
| 2:B:27:ASN:HD21 | 30:0:2807:U:P | 2.16 | 0.69 |
| 2:B:36:PRO:HG3 | 2:B:169:GLY:N | 2.06 | 0.69 |
| 2:B:18:ARG:HG3 | 2:B:256:GLN:HG3 | 1.74 | 0.68 |
| 23:W:88:THR:HG22 | 23:W:90:TYR:HD1 | 1.58 | 0.68 |
| 2:B:221:GLN:HE22 | 11:K:42:ASN:HD22 | 1.41 | 0.68 |
| 30:0:2491:G:H1' | 41:0:7670:HOH:O | 1.93 | 0.68 |
| 23:W:122:ARG:HH11 | 23:W:122:ARG:HG3 | 1.57 | 0.68 |
| 8:H:59:GLN:HE21 | 8:H:129:ARG:HE | 1.41 | 0.68 |
| 30:0:1183:C:N4 | 30:0:1184:C:H41 | 1.90 | 0.68 |
| 30:0:1634:G:H3' | 41:0:4762:HOH:O | 1.92 | 0.68 |
| 20:T:50:VAL:HG12 | 20:T:56:ALA:HA | 1.75 | 0.68 |
| 30:0:871:G:H8 | 30:0:871:G:C5' | 2.03 | 0.68 |
| 30:0:2533:C:H6 | 30:0:2533:C:H5' | 1.58 | 0.68 |
| 4:D:172:VAL:HG12 | 4:D:173:GLU:N | 2.08 | 0.68 |
| 11:K:28:GLU:HB3 | 11:K:59:LYS:HB2 | 1.75 | 0.68 |
| 1:A:33:GLU:O | 1:A:34:ASP:HB2 | 1.94 | 0.68 |
| 23:W:141:HIS:HB2 | 23:W:146:ILE:HG12 | 1.76 | 0.68 |
| 26:Z:46:SER:O | 26:Z:50:VAL:HG23 | 1.93 | 0.68 |
| 30:0:1730:G:H5' | 30:0:1731:C:C5 | 2.28 | 0.68 |
| 2:B:56:ASP:OD1 | 2:B:322:ARG:HB3 | 1.94 | 0.68 |
| 23:W:106:THR:OG1 | 23:W:109:GLU:HG3 | 1.93 | 0.68 |
| 11:K:87:ARG:HB2 | 21:U:19:THR:HG23 | 1.76 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:2:20:ARG:HG2 | 41:2:5444:HOH:O | 1.93 | 0.68 |
| 10:J:46:ILE:HD11 | 10:J:53:ILE:CG2 | 2.22 | 0.68 |
| 13:M:9:ARG:HD2 | 30:0:380:A:OP2 | 1.94 | 0.68 |
| 15:O:59:VAL:HG23 | 15:O:111:VAL:HG21 | 1.75 | 0.67 |
| 8:H:102:LYS:HD3 | 8:H:122:LYS:HD3 | 1.76 | 0.67 |
| 26:Z:44:ARG:HH21 | 30:0:1771:U:H5' | 1.59 | 0.67 |
| 27:1:9:GLY:HA2 | 30:0:1687:C:O2 | 1.95 | 0.67 |
| 29:3:73:GLU:HB3 | 41:3:9053:HOH:O | 1.94 | 0.67 |
| 28:2:22:PRO:HG2 | 28:2:25:VAL:CG2 | 2.24 | 0.67 |
| 30:0:545:G:C8 | 30:0:545:G:H5' | 2.26 | 0.67 |
| 10:J:54:VAL:HG11 | 10:J:138:THR:HG21 | 1.76 | 0.67 |
| 14:N:147:ILE:HD12 | 41:9:9090:HOH:O | 1.93 | 0.67 |
| 30:0:2505:G:O2' | 30:0:2506:A:H5' | 1.95 | 0.67 |
| 41:0:7596:HOH:O | 32:5:76:A:C2 | 2.47 | 0.67 |
| 30:0:1474:C:C6 | 30:0:1474:C:H5' | 2.29 | 0.67 |
| 11:K:81:ARG:HB2 | 11:K:87:ARG:HH11 | 1.59 | 0.67 |
| 2:B:312:ARG:HD3 | 2:B:315:VAL:HG13 | 1.75 | 0.67 |
| 25:Y:212:ARG:HD2 | 41:Y:8911:HOH:O | 1.95 | 0.67 |
| 8:H:6:ALA:HA | 8:H:61:ARG:NH1 | 2.10 | 0.67 |
| 30:0:2502:C:H2' | 30:0:2503:A:H5' | 1.76 | 0.67 |
| 30:0:2851:G:O2' | 30:0:2852:A:H5' | 1.94 | 0.67 |
| 22:V:1:THR:HG23 | 22:V:2:VAL:HG23 | 1.76 | 0.67 |
| 9:I:101:LYS:O | 9:I:105:GLU:HG3 | 1.96 | 0.66 |
| 4:D:57:THR:HA | 41:D:5728:HOH:O | 1.94 | 0.66 |
| 5:E:20:ILE:HD11 | 5:E:40:VAL:HG11 | 1.75 | 0.66 |
| 10:J:131:THR:HG22 | 10:J:134:GLU:H | 1.60 | 0.66 |
| 19:S:51:GLN:HE21 | 19:S:53:ASN:HD21 | 1.43 | 0.66 |
| 30:0:2766:A:H5' | 41:0:3471:HOH:O | 1.94 | 0.66 |
| 18:R:106:GLY:HA2 | 18:R:109:MET:HE3 | 1.76 | 0.66 |
| 3:C:78:ARG:HG3 | 3:C:78:ARG:HH11 | 1.60 | 0.66 |
| 1:A:94:LEU:HD12 | 1:A:98:GLU:HB2 | 1.76 | 0.66 |
| 20:T:49:GLU:OE2 | 20:T:97:ARG:HD2 | 1.95 | 0.66 |
| 9:I:112:LEU:HD11 | 30:0:1162:G:H1' | 1.78 | 0.66 |
| 32:5:76:A:C5' | 32:5:76:A:C8 | 2.79 | 0.66 |
| 30:0:2320:U:H4' | 30:0:2321:A:O4' | 1.96 | 0.66 |
| 30:0:1878:G:HO2' | 30:0:1879:U:H6 | 1.43 | 0.66 |
| 14:N:37:ARG:NH1 | 31:9:6:C:OP1 | 2.28 | 0.66 |
| 18:R:39:THR:HB | 18:R:42:GLU:HG3 | 1.76 | 0.66 |
| 23:W:137:GLN:HE21 | 23:W:141:HIS:CE1 | 2.14 | 0.65 |
| 25:Y:169:ARG:HD2 | 30:0:1328:A:OP1 | 1.96 | 0.65 |
| 6:F:96:ALA:HA | 41:F:3111:HOH:O | 1.95 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:320:GLN:HE21 | 2:B:321:PRO:HD2 | 1.61 | 0.65 |
| 16:P:77:ALA:O | 16:P:78:GLY:CA | 2.44 | 0.65 |
| 31:9:78:G:N1 | 31:9:78:G:N7 | 2.43 | 0.65 |
| 22:V:12:THR:CG2 | 22:V:15:GLU:HG3 | 2.24 | 0.65 |
| 30:0:544:G:H2' | 30:0:545:G:H5'' | 1.78 | 0.65 |
| 27:1:16:HIS:HE1 | 30:0:775:G:OP1 | 1.79 | 0.65 |
| 31:9:14:G:H5' | 31:9:14:G:H8 | 1.61 | 0.65 |
| 30:0:1175:G:H1' | 30:0:1193:A:H2' | 1.78 | 0.65 |
| 15:O:3:THR:HB | 30:0:656:G:H5' | 1.76 | 0.65 |
| 18:R:114:VAL:HA | 18:R:144:GLU:O | 1.97 | 0.65 |
| 22:V:50:ARG:NH1 | 30:0:56:G:H5'' | 2.12 | 0.65 |
| 2:B:36:PRO:CA | 2:B:168:GLY:HA3 | 2.22 | 0.65 |
| 23:W:52:VAL:HG23 | 23:W:53:ALA:N | 1.86 | 0.65 |
| 16:P:74:GLN:HG2 | 30:0:1786:C:OP1 | 1.97 | 0.65 |
| 25:Y:187:VAL:HG23 | 25:Y:192:ASP:CB | 2.27 | 0.65 |
| 16:P:14:LEU:O | 16:P:16:VAL:HG23 | 1.96 | 0.65 |
| 31:9:76:G:C3' | 31:9:77:A:H5'' | 2.20 | 0.65 |
| 6:F:58:GLU:HA | 6:F:61:MET:HE2 | 1.78 | 0.65 |
| 10:J:39:VAL:HG13 | 10:J:106:GLY:O | 1.97 | 0.65 |
| 1:A:153:ARG:NH1 | 1:A:153:ARG:HB2 | 2.06 | 0.65 |
| 21:U:56:ARG:NH2 | 30:0:2890:A:H1' | 2.12 | 0.65 |
| 2:B:329:TYR:CE2 | 21:U:15:PRO:HG2 | 2.32 | 0.64 |
| 21:U:52:THR:HG22 | 21:U:54:THR:N | 2.12 | 0.64 |
| 25:Y:116:LEU:HD12 | 25:Y:173:ALA:HB3 | 1.77 | 0.64 |
| 2:B:150:ALA:O | 2:B:152:PRO:HD3 | 1.96 | 0.64 |
| 28:2:41:HIS:HD2 | 28:2:44:ARG:H | 1.43 | 0.64 |
| 30:0:558:C:C2' | 30:0:559:U:H5'' | 2.28 | 0.64 |
| 10:J:74:ARG:HB3 | 10:J:74:ARG:HH11 | 1.61 | 0.64 |
| 23:W:137:GLN:NE2 | 23:W:141:HIS:HE1 | 1.94 | 0.64 |
| 30:0:2578:G:H5' | 30:0:2578:G:H8 | 1.63 | 0.64 |
| 25:Y:154:ARG:HH12 | 25:Y:155:ARG:HG3 | 1.62 | 0.64 |
| 25:Y:154:ARG:NH1 | 25:Y:155:ARG:HG3 | 2.12 | 0.64 |
| 31:9:73:A:H61 | 31:9:108:C:H42 | 1.45 | 0.64 |
| 25:Y:174:VAL:HG13 | 25:Y:177:LYS:HD2 | 1.79 | 0.64 |
| 2:B:190:MET:HE2 | 2:B:194:PHE:CD1 | 2.32 | 0.64 |
| 1:A:94:LEU:HG | 1:A:99:ILE:HD11 | 1.78 | 0.64 |
| 2:B:229:ARG:NH2 | 30:0:1753:C:O2 | 2.30 | 0.64 |
| 1:A:163:GLY:HA2 | 1:A:166:ASP:OD2 | 1.96 | 0.64 |
| 30:0:256:C:H2' | 30:0:257:G:O4' | 1.98 | 0.64 |
| 2:B:185:GLY:HA2 | 41:B:9117:HOH:O | 1.97 | 0.64 |
| 5:E:7:ILE:HG22 | 5:E:45:ASP:O | 1.97 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 23:W:65:VAL:HA | 23:W:68:THR:HG22 | 1.80 | 0.64 |
| 11:K:10:GLN:N | 11:K:10:GLN:HE21 | 1.92 | 0.64 |
| 1:A:191:GLY:HA2 | 1:A:194:MET:CE | 2.28 | 0.64 |
| 11:K:34:VAL:CG2 | 11:K:47:ALA:HB2 | 2.27 | 0.64 |
| 28:2:36:ASN:HB3 | 28:2:39:ARG:HG3 | 1.79 | 0.64 |
| 10:J:95:ARG:O | 10:J:99:GLU:HG3 | 1.97 | 0.64 |
| 6:F:12:LEU:HD21 | 6:F:111:ILE:HG23 | 1.80 | 0.64 |
| 25:Y:235:GLU:CD | 25:Y:235:GLU:N | 2.48 | 0.64 |
| 11:K:74:VAL:HG13 | 11:K:113:ILE:HG23 | 1.80 | 0.64 |
| 23:W:110:GLN:NE2 | 23:W:110:GLN:HA | 2.13 | 0.64 |
| 30:0:2851:G:C2' | 30:0:2852:A:H5' | 2.28 | 0.64 |
| 3:C:184:ARG:NH2 | 30:0:450:C:OP1 | 2.30 | 0.64 |
| 30:0:2073:G:OP2 | 30:0:2490:A:H5' | 1.98 | 0.64 |
| 11:K:98:VAL:HG11 | 11:K:102:GLU:HA | 1.77 | 0.64 |
| 20:T:26:THR:HA | 20:T:39:ASN:HB3 | 1.79 | 0.64 |
| 16:P:88:GLN:HE22 | 30:0:1799:G:H21 | 1.45 | 0.64 |
| 1:A:66:ARG:HH11 | 1:A:66:ARG:HB2 | 1.62 | 0.64 |
| 30:0:1377:C:H5' | 30:0:1377:C:C6 | 2.29 | 0.64 |
| 9:I:129:SER:O | 9:I:130:LEU:HD23 | 1.97 | 0.64 |
| 31:9:13:A:O2' | 31:9:14:G:H5'' | 1.97 | 0.64 |
| 20:T:77:VAL:HG11 | 20:T:91:LEU:HD11 | 1.79 | 0.64 |
| 29:3:55:VAL:HG22 | 41:3:9004:HOH:O | 1.97 | 0.64 |
| 24:X:43:VAL:HG12 | 24:X:44:ASP:H | 1.62 | 0.64 |
| 31:9:50:G:H2' | 31:9:51:A:C8 | 2.32 | 0.64 |
| 13:M:171:ARG:CD | 30:0:156:C:H5'' | 2.26 | 0.64 |
| 13:M:24:GLN:O | 13:M:28:GLN:HG3 | 1.97 | 0.64 |
| 2:B:175:LEU:O | 2:B:175:LEU:HD23 | 1.97 | 0.64 |
| 31:9:76:G:H3' | 31:9:77:A:C5' | 2.20 | 0.63 |
| 20:T:2:LYS:HG2 | 30:0:447:A:OP1 | 1.98 | 0.63 |
| 2:B:207:LYS:HG3 | 30:0:2717:C:OP1 | 1.98 | 0.63 |
| 14:N:36:ALA:HB1 | 14:N:118:ILE:HD12 | 1.81 | 0.63 |
| 20:T:71:VAL:HG11 | 20:T:90:PRO:CB | 2.27 | 0.63 |
| 24:X:43:VAL:HG12 | 24:X:44:ASP:N | 2.13 | 0.63 |
| 20:T:54:ASP:OD2 | 30:0:316:A:H5' | 1.97 | 0.63 |
| 1:A:207:GLN:HA | 41:A:9034:HOH:O | 1.97 | 0.63 |
| 32:5:76:A:H8 | 32:5:76:A:H5' | 1.64 | 0.63 |
| 23:W:21:LEU:HD22 | 23:W:26:ILE:HD13 | 1.81 | 0.63 |
| 11:K:20:CYS:HB2 | 11:K:29:LEU:HG | 1.81 | 0.63 |
| 30:0:1701:A:H4' | 30:0:1702:U:C5' | 2.29 | 0.63 |
| 30:0:2502:C:C2' | 30:0:2503:A:H5' | 2.29 | 0.63 |
| 1:A:37:VAL:HG23 | 41:A:9070:HOH:O | 1.98 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:1:25:LYS:O | 27:1:25:LYS:HG2 | 1.99 | 0.63 |
| 31:9:24:U:H3' | 31:9:25:G:H5' | 1.80 | 0.63 |
| 7:G:20:VAL:O | 7:G:24:VAL:HG23 | 1.99 | 0.63 |
| 14:N:152:GLU:C | 14:N:154:LEU:H | 2.02 | 0.63 |
| 27:1:28:HIS:CD2 | 27:1:31:LYS:HG3 | 2.34 | 0.63 |
| 31:9:56:A:C2' | 31:9:57:A:H5'' | 2.28 | 0.63 |
| 5:E:23:GLU:HG2 | 5:E:28:SER:CB | 2.28 | 0.63 |
| 23:W:39:ASP:OD1 | 23:W:42:ARG:NH2 | 2.32 | 0.63 |
| 32:5:76:A:C8 | 32:5:76:A:H5'' | 2.34 | 0.62 |
| 10:J:131:THR:HB | 10:J:134:GLU:OE1 | 1.99 | 0.62 |
| 11:K:66:ARG:HH22 | 30:0:1994:A:P | 2.22 | 0.62 |
| 15:O:57:THR:O | 15:O:111:VAL:HG23 | 2.00 | 0.62 |
| 1:A:121:ALA:O | 1:A:124:VAL:HG22 | 2.00 | 0.62 |
| 8:H:160:ILE:HD11 | 8:H:164:CYS:SG | 2.38 | 0.62 |
| 30:0:281:U:H2' | 30:0:282:C:O4' | 1.99 | 0.62 |
| 13:M:23:LEU:HD13 | 13:M:27:ARG:NH2 | 2.14 | 0.62 |
| 13:M:57:LYS:HE2 | 13:M:140:ALA:O | 2.00 | 0.62 |
| 14:N:5:ARG:NH1 | 30:0:962:C:H1' | 2.14 | 0.62 |
| 19:S:57:THR:HG22 | 19:S:58:MET:N | 2.13 | 0.62 |
| 5:E:126:ILE:HB | 5:E:131:LEU:HD23 | 1.80 | 0.62 |
| 14:N:164:ASP:OD1 | 14:N:167:ASP:HA | 1.99 | 0.62 |
| 25:Y:165:GLU:HB3 | 41:0:7500:HOH:O | 1.99 | 0.62 |
| 9:I:73:LEU:HD12 | 9:I:107:LYS:HZ2 | 1.62 | 0.62 |
| 20:T:52:ARG:HD2 | 30:0:317:A:H5'' | 1.81 | 0.62 |
| 23:W:91:ASP:HB2 | 41:W:5425:HOH:O | 1.99 | 0.62 |
| 22:V:1:THR:CG2 | 22:V:2:VAL:H | 2.04 | 0.62 |
| 11:K:98:VAL:HG13 | 11:K:102:GLU:HA | 1.82 | 0.62 |
| 30:0:380:A:H2' | 41:0:9029:HOH:O | 1.98 | 0.62 |
| 11:K:81:ARG:HB2 | 11:K:87:ARG:NH1 | 2.14 | 0.62 |
| 1:A:88:ILE:HG22 | 1:A:88:ILE:O | 1.98 | 0.62 |
| 13:M:102:GLU:OE1 | 13:M:164:THR:HG21 | 1.99 | 0.62 |
| 30:0:2718:C:H6 | 30:0:2718:C:H5' | 1.65 | 0.62 |
| 14:N:169:PRO:O | 14:N:172:PHE:HB3 | 2.00 | 0.62 |
| 3:C:77:ALA:C | 3:C:78:ARG:CA | 2.68 | 0.62 |
| 30:0:558:C:H2' | 30:0:559:U:C5' | 2.29 | 0.62 |
| 30:0:2896:A:H5'' | 41:0:6924:HOH:O | 2.00 | 0.62 |
| 9:I:69:PRO:HA | 30:0:1164:U:OP1 | 2.00 | 0.62 |
| 13:M:24:GLN:NE2 | 13:M:27:ARG:HH11 | 1.98 | 0.62 |
| 11:K:87:ARG:HG3 | 30:0:2721:U:H4' | 1.81 | 0.62 |
| 12:L:120:LEU:HD12 | 12:L:133:VAL:HG21 | 1.82 | 0.62 |
| 23:W:26:ILE:HB | 41:W:5420:HOH:O | 1.98 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:173:GLU:O | 4:D:174:VAL:O | 2.18 | 0.61 |
| 30:0:482:G:H4' | 30:0:508:A:N1 | 2.15 | 0.61 |
| 30:0:2239:C:H2' | 30:0:2240:U:H6 | 1.66 | 0.61 |
| 8:H:168:VAL:HG13 | 41:H:9015:HOH:O | 1.99 | 0.61 |
| 1:A:107:ASN:OD1 | 1:A:120:ARG:HD2 | 2.00 | 0.61 |
| 24:X:47:ALA:HB1 | 24:X:82:GLU:HB3 | 1.83 | 0.61 |
| 5:E:3:VAL:CG2 | 5:E:49:ILE:HB | 2.31 | 0.61 |
| 3:C:115:LEU:HD13 | 3:C:223:LEU:HD21 | 1.81 | 0.61 |
| 30:0:2401:A:H2' | 30:0:2402:A:C8 | 2.36 | 0.61 |
| 30:0:2472:C:O2' | 30:0:2634:G:H4' | 1.99 | 0.61 |
| 4:D:52:THR:HG21 | 30:0:2346:C:O2' | 1.99 | 0.61 |
| 12:L:35:ARG:HH11 | 12:L:35:ARG:HB2 | 1.63 | 0.61 |
| 14:N:164:ASP:OD2 | 14:N:167:ASP:HA | 2.01 | 0.61 |
| 4:D:58:VAL:CG1 | 4:D:60:GLU:HG2 | 2.30 | 0.61 |
| 3:C:27:ARG:NH2 | 30:0:657:G:OP1 | 2.33 | 0.61 |
| 30:0:1666:C:O2' | 30:0:1667:A:H5'' | 2.01 | 0.61 |
| 24:X:43:VAL:HG11 | 24:X:82:GLU:HA | 1.81 | 0.61 |
| 17:Q:7:LEU:HD13 | 41:0:3528:HOH:O | 2.01 | 0.61 |
| 24:X:80:GLU:HB3 | 41:X:5564:HOH:O | 2.00 | 0.61 |
| 4:D:25:MET:CE | 4:D:41:LEU:HG | 2.27 | 0.61 |
| 6:F:46:GLU:O | 6:F:73:PRO:HD2 | 2.00 | 0.61 |
| 15:O:47:ARG:HG3 | 15:O:47:ARG:HH11 | 1.65 | 0.61 |
| 30:0:2795:C:O2' | 30:0:2796:U:H5' | 2.01 | 0.61 |
| 1:A:211:LYS:O | 30:0:1943:C:H4' | 2.01 | 0.61 |
| 1:A:88:ILE:HD13 | 1:A:100:PRO:CD | 2.29 | 0.61 |
| 4:D:99:ASP:HB3 | 4:D:103:ASN:N | 2.16 | 0.61 |
| 30:0:1184:C:H1' | 41:0:9254:HOH:O | 2.01 | 0.61 |
| 6:F:91:VAL:CG1 | 6:F:92:GLY:H | 2.12 | 0.61 |
| 20:T:41:ARG:HG2 | 20:T:41:ARG:HH11 | 1.64 | 0.61 |
| 9:I:110:ASP:O | 30:0:1163:G:H5' | 2.01 | 0.61 |
| 16:P:59:ARG:HH22 | 16:P:66:GLN:HE22 | 1.48 | 0.61 |
| 8:H:80:LEU:HD21 | 8:H:145:ASP:HB3 | 1.83 | 0.61 |
| 30:0:2003:U:H4' | 30:0:2004:U:H5 | 1.66 | 0.61 |
| 30:0:1080:C:H4' | 30:0:1081:A:OP1 | 1.99 | 0.61 |
| 30:0:272:A:H5' | 30:0:273:G:OP2 | 2.00 | 0.61 |
| 3:C:236:THR:H | 3:C:239:ALA:HB3 | 1.65 | 0.60 |
| 30:0:2005:G:O2' | 30:0:2008:U:OP2 | 2.18 | 0.60 |
| 5:E:7:ILE:HD11 | 5:E:11:VAL:HG12 | 1.83 | 0.60 |
| 30:0:1748:U:H4' | 41:0:9307:HOH:O | 2.00 | 0.60 |
| 6:F:50:VAL:HG13 | 6:F:60:VAL:HG11 | 1.83 | 0.60 |
| 30:0:1205:U:H2' | 30:0:1206:U:C5' | 2.31 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:H:49:GLN:NE2 | 8:H:140:TYR:HE2 | 1.97 | 0.60 |
| 21:U:11:THR:HG22 | 21:U:53:ASP:CG | 2.21 | 0.60 |
| 17:Q:32:GLU:HA | 17:Q:71:TYR:OH | 2.01 | 0.60 |
| 30:0:664:U:O4 | 30:0:681:G:H5'' | 2.01 | 0.60 |
| 10:J:107:ASN:ND2 | 10:J:109:TYR:H | 1.99 | 0.60 |
| 2:B:314:ALA:HB3 | 2:B:317:PRO:HG3 | 1.84 | 0.60 |
| 16:P:115:SER:N | 16:P:118:GLN:HE21 | 1.88 | 0.60 |
| 3:C:235:PHE:HE2 | 3:C:243:VAL:HG21 | 1.65 | 0.60 |
| 10:J:130:VAL:HG12 | 10:J:131:THR:H | 1.65 | 0.60 |
| 3:C:81:PRO:HD3 | 41:0:4391:HOH:O | 2.01 | 0.60 |
| 16:P:91:LYS:O | 16:P:95:GLU:HG3 | 2.01 | 0.60 |
| 26:Z:43:GLY:O | 26:Z:47:ARG:HG2 | 2.01 | 0.60 |
| 30:0:1165:G:H4' | 30:0:1174:A:O2' | 2.01 | 0.60 |
| 7:G:23:ILE:HD13 | 7:G:67:LEU:HD23 | 1.84 | 0.60 |
| 4:D:135:VAL:HG21 | 4:D:139:TYR:CG | 2.37 | 0.60 |
| 6:F:53:ASP:OD1 | 6:F:80:GLN:HB2 | 2.01 | 0.60 |
| 2:B:211:THR:HG21 | 41:0:9244:HOH:O | 2.01 | 0.60 |
| 4:D:58:VAL:HG12 | 4:D:60:GLU:HG2 | 1.83 | 0.60 |
| 5:E:91:PHE:CE1 | 30:0:2694:A:H4' | 2.36 | 0.60 |
| 5:E:154:ILE:HD11 | 5:E:157:LYS:HB2 | 1.82 | 0.60 |
| 28:2:41:HIS:CD2 | 28:2:44:ARG:H | 2.19 | 0.60 |
| 1:A:212:PRO:HB2 | 41:A:9038:HOH:O | 2.02 | 0.60 |
| 30:0:2896:A:N3 | 30:0:2896:A:H2' | 2.17 | 0.60 |
| 19:S:52:VAL:HG22 | 19:S:66:VAL:HG22 | 1.84 | 0.60 |
| 21:U:49:LEU:HG | 41:U:3805:HOH:O | 2.02 | 0.60 |
| 2:B:206:THR:HG21 | 30:0:2716:G:H5'' | 1.84 | 0.60 |
| 1:A:211:LYS:HB2 | 41:A:9094:HOH:O | 2.01 | 0.60 |
| 14:N:40:ASN:ND2 | 31:9:28:U:H5'' | 2.17 | 0.60 |
| 30:0:65:C:O2' | 30:0:66:G:H5' | 2.01 | 0.60 |
| 30:0:2415:A:H2' | 30:0:2416:G:H5' | 1.84 | 0.60 |
| 30:0:1679:C:H5' | 41:0:3233:HOH:O | 2.02 | 0.60 |
| 10:J:75:PRO:HG2 | 10:J:105:LEU:HD21 | 1.83 | 0.60 |
| 1:A:36:ASP:OD2 | 1:A:85:SER:HB2 | 2.01 | 0.60 |
| 13:M:41:GLU:O | 13:M:42:ARG:HD3 | 2.02 | 0.60 |
| 15:O:59:VAL:CG2 | 15:O:111:VAL:HG21 | 2.31 | 0.60 |
| 1:A:48:ASP:HB3 | 41:A:9081:HOH:O | 2.01 | 0.60 |
| 22:V:43:PRO:O | 22:V:46:ILE:HG22 | 2.01 | 0.60 |
| 30:0:544:G:C2' | 30:0:545:G:H5'' | 2.31 | 0.59 |
| 30:0:1766:U:O2 | 30:0:1778:A:H5' | 2.02 | 0.59 |
| 9:I:114:TYR:HE1 | 30:0:1186:C:H4' | 1.67 | 0.59 |
| 6:F:118:LEU:O | 6:F:119:ARG:HB3 | 2.02 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:233:THR:HG22 | 3:C:234:VAL:N | 2.16 | 0.59 |
| 30:0:1834:C:H2' | 30:0:1840:A:N6 | 2.17 | 0.59 |
| 19:S:37:VAL:O | 19:S:41:VAL:HG23 | 2.03 | 0.59 |
| 28:2:41:HIS:HB3 | 28:2:44:ARG:HB2 | 1.83 | 0.59 |
| 10:J:19:MET:CE | 10:J:132:LEU:HD11 | 2.33 | 0.59 |
| 1:A:211:LYS:HB3 | 1:A:212:PRO:CD | 2.21 | 0.59 |
| 25:Y:154:ARG:HH21 | 30:0:1293:U:H5' | 1.67 | 0.59 |
| 30:0:2429:A:H5' | 41:0:3404:HOH:O | 2.02 | 0.59 |
| 31:9:39:U:HO2' | 31:9:42:C:H5 | 1.50 | 0.59 |
| 4:D:173:GLU:HG3 | 4:D:174:VAL:HG23 | 1.84 | 0.59 |
| 30:0:1180:U:H2' | 30:0:1181:A:C8 | 2.37 | 0.59 |
| 15:O:59:VAL:HG23 | 15:O:111:VAL:CG2 | 2.32 | 0.59 |
| 2:B:336:GLN:O | 30:0:2862:G:H4' | 2.02 | 0.59 |
| 18:R:18:LEU:HD12 | 18:R:143:VAL:CG1 | 2.33 | 0.59 |
| 5:E:145:ALA:HB1 | 5:E:168:ILE:CD1 | 2.32 | 0.59 |
| 9:I:107:LYS:HB3 | 9:I:110:ASP:HB2 | 1.83 | 0.59 |
| 16:P:55:LYS:HG2 | 16:P:56:GLY:N | 2.17 | 0.59 |
| 30:0:2089:A:O2' | 30:0:2090:G:H5' | 2.02 | 0.59 |
| 12:L:4:LYS:HE2 | 30:0:645:U:OP2 | 2.02 | 0.59 |
| 2:B:177:HIS:O | 2:B:181:ILE:HG13 | 2.03 | 0.59 |
| 30:0:558:C:O2' | 30:0:559:U:H5'' | 2.03 | 0.59 |
| 28:2:22:PRO:HG2 | 28:2:25:VAL:HG21 | 1.83 | 0.59 |
| 12:L:143:THR:HG22 | 12:L:144:ASP:N | 2.17 | 0.59 |
| 30:0:2827:A:H2' | 30:0:2828:G:O4' | 2.03 | 0.59 |
| 30:0:1632:A:H2' | 30:0:1633:C:H5' | 1.85 | 0.59 |
| 2:B:36:PRO:HB3 | 2:B:174:ARG:HB3 | 1.85 | 0.59 |
| 23:W:21:LEU:O | 23:W:26:ILE:HG23 | 2.03 | 0.59 |
| 14:N:77:ASN:C | 14:N:80:SER:HB3 | 2.22 | 0.59 |
| 30:0:316:A:N3 | 30:0:336:G:O2' | 2.34 | 0.59 |
| 14:N:139:TRP:HA | 14:N:139:TRP:HE3 | 1.68 | 0.59 |
| 7:G:12:ILE:HG22 | 7:G:17:GLN:NE2 | 2.16 | 0.59 |
| 18:R:117:HIS:HD2 | 30:0:20:G:H21 | 1.48 | 0.59 |
| 30:0:459:A:H5'' | 41:0:2968:HOH:O | 2.02 | 0.59 |
| 2:B:307:ARG:NH1 | 2:B:307:ARG:HG3 | 2.15 | 0.59 |
| 10:J:19:MET:HE3 | 10:J:132:LEU:HD11 | 1.84 | 0.59 |
| 30:0:1552:G:N2 | 30:0:1634:G:H1' | 2.18 | 0.59 |
| 12:L:143:THR:HG22 | 12:L:145:LEU:H | 1.68 | 0.59 |
| 28:2:10:ARG:NH2 | 30:0:121:U:OP2 | 2.35 | 0.59 |
| 10:J:52:GLN:HG3 | 10:J:53:ILE:N | 2.17 | 0.59 |
| 1:A:105:VAL:CG1 | 1:A:154:ALA:HB1 | 2.33 | 0.59 |
| 23:W:110:GLN:HE21 | 23:W:110:GLN:HA | 1.67 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:V:56:ILE:O | 22:V:60:GLN:HG3 | 2.02 | 0.59 |
| 2:B:108:GLU:HB3 | 2:B:111:ARG:HD2 | 1.85 | 0.59 |
| 5:E:145:ALA:HB1 | 5:E:168:ILE:HD11 | 1.84 | 0.58 |
| 23:W:4:LEU:O | 23:W:32:CYS:HA | 2.03 | 0.58 |
| 22:V:49:LEU:O | 22:V:53:ILE:HG13 | 2.02 | 0.58 |
| 30:0:1681:G:H5'' | 30:0:1682:A:H5' | 1.84 | 0.58 |
| 30:0:2070:G:H5'' | 41:0:4653:HOH:O | 2.03 | 0.58 |
| 2:B:144:THR:HB | 41:B:9108:HOH:O | 2.02 | 0.58 |
| 30:0:1116:U:O2' | 30:0:1118:A:C2 | 2.49 | 0.58 |
| 1:A:201:PHE:HA | 41:A:9062:HOH:O | 2.03 | 0.58 |
| 10:J:19:MET:HE1 | 10:J:132:LEU:HD21 | 1.85 | 0.58 |
| 7:G:12:ILE:HG23 | 41:0:6294:HOH:O | 2.02 | 0.58 |
| 21:U:45:GLU:HB2 | 21:U:48:ASN:ND2 | 2.17 | 0.58 |
| 14:N:86:LEU:O | 14:N:90:LEU:HG | 2.02 | 0.58 |
| 6:F:37:THR:O | 6:F:41:GLU:HG3 | 2.03 | 0.58 |
| 25:Y:203:VAL:HG12 | 25:Y:228:VAL:HG22 | 1.84 | 0.58 |
| 15:O:14:LEU:CD2 | 15:O:102:ILE:HD11 | 2.33 | 0.58 |
| 30:0:1461:U:H2' | 30:0:1462:C:C6 | 2.39 | 0.58 |
| 22:V:39:ALA:N | 22:V:40:PRO:CD | 2.66 | 0.58 |
| 5:E:36:PRO:HD3 | 10:J:127:ILE:HD12 | 1.84 | 0.58 |
| 41:L:8846:HOH:O | 30:0:2453:G:H5'' | 2.04 | 0.58 |
| 5:E:31:ARG:NH1 | 5:E:68:HIS:CG | 2.71 | 0.58 |
| 8:H:66:GLU:HA | 41:H:9036:HOH:O | 2.03 | 0.58 |
| 14:N:154:LEU:O | 14:N:155:GLU:HB3 | 2.02 | 0.58 |
| 2:B:297:VAL:HB | 41:B:9083:HOH:O | 2.03 | 0.58 |
| 19:S:29:ASP:OD1 | 19:S:31:ARG:HG3 | 2.04 | 0.58 |
| 17:Q:66:LYS:HB2 | 17:Q:70:ALA:O | 2.04 | 0.58 |
| 18:R:71:LYS:HE2 | 30:0:2831:C:O3' | 2.03 | 0.58 |
| 20:T:53:GLY:HA3 | 41:0:7601:HOH:O | 2.03 | 0.58 |
| 30:0:119:A:H2' | 30:0:120:A:H5'' | 1.85 | 0.58 |
| 30:0:2419:U:H5'' | 30:0:2420:G:H5' | 1.86 | 0.58 |
| 12:L:35:ARG:HD3 | 12:L:35:ARG:C | 2.24 | 0.58 |
| 3:C:246:ARG:NH1 | 3:C:246:ARG:HB3 | 2.18 | 0.58 |
| 3:C:58:ALA:HA | 3:C:73:GLN:HE21 | 1.68 | 0.58 |
| 4:D:23:VAL:HG21 | 4:D:45:THR:HG21 | 1.84 | 0.58 |
| 14:N:61:ALA:HB3 | 14:N:88:ALA:HB2 | 1.86 | 0.58 |
| 30:0:2626:C:H2' | 30:0:2627:G:C8 | 2.39 | 0.58 |
| 11:K:77:ARG:C | 11:K:78:LYS:CA | 2.72 | 0.58 |
| 25:Y:184:GLU:OE1 | 25:Y:204:ARG:NH1 | 2.37 | 0.58 |
| 30:0:2588:OMG:N2 | 41:0:7596:HOH:O | 2.36 | 0.58 |
| 25:Y:234:VAL:HG12 | 25:Y:235:GLU:N | 2.18 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:53:LEU:HD21 | 2:B:270:ILE:HD12 | 1.85 | 0.58 |
| 30:0:1878:G:H1' | 41:0:6945:HOH:O | 2.03 | 0.58 |
| 14:N:139:TRP:HA | 14:N:139:TRP:CE3 | 2.37 | 0.58 |
| 25:Y:126:PRO:HG2 | 25:Y:128:PHE:CE1 | 2.38 | 0.58 |
| 17:Q:25:PRO:HB2 | 41:9:9081:HOH:O | 2.03 | 0.58 |
| 12:L:34:GLY:HA3 | 12:L:38:HIS:CE1 | 2.39 | 0.58 |
| 23:W:130:HIS:O | 23:W:136:GLY:HA3 | 2.03 | 0.58 |
| 5:E:31:ARG:HH12 | 5:E:68:HIS:CG | 2.21 | 0.58 |
| 2:B:85:ARG:HB2 | 2:B:99:GLU:HG2 | 1.86 | 0.58 |
| 1:A:35:GLY:O | 1:A:36:ASP:HB3 | 2.03 | 0.58 |
| 30:0:951:A:C2' | 30:0:952:G:H5' | 2.34 | 0.58 |
| 25:Y:186:ARG:HG2 | 25:Y:186:ARG:HH11 | 1.68 | 0.58 |
| 19:S:10:VAL:HG11 | 22:V:36:ALA:HB2 | 1.84 | 0.58 |
| 12:L:73:VAL:HG23 | 12:L:74:THR:H | 1.68 | 0.58 |
| 19:S:22:ASN:ND2 | 19:S:68:LEU:HB2 | 2.18 | 0.58 |
| 4:D:152:PRO:HD2 | 31:9:57:A:O2' | 2.04 | 0.58 |
| 23:W:5:VAL:HG11 | 23:W:153:MET:HE3 | 1.85 | 0.58 |
| 10:J:130:VAL:HG12 | 10:J:131:THR:N | 2.18 | 0.58 |
| 25:Y:187:VAL:HG23 | 25:Y:192:ASP:HB3 | 1.86 | 0.58 |
| 9:I:121:LYS:HD3 | 30:0:1185:U:OP1 | 2.04 | 0.58 |
| 17:Q:26:PRO:O | 17:Q:30:VAL:HG23 | 2.03 | 0.58 |
| 30:0:1562:C:H42 | 30:0:2738:G:H1 | 1.52 | 0.58 |
| 3:C:174:ILE:CD1 | 30:0:338:C:H4' | 2.34 | 0.58 |
| 13:M:99:ARG:HD2 | 13:M:167:GLY:HA2 | 1.84 | 0.58 |
| 23:W:88:THR:HG22 | 23:W:89:ASP:N | 2.19 | 0.58 |
| 10:J:74:ARG:CG | 10:J:74:ARG:HH11 | 2.16 | 0.58 |
| 30:0:1973:A:H5' | 30:0:1973:A:C8 | 2.37 | 0.58 |
| 2:B:320:GLN:NE2 | 2:B:321:PRO:HD2 | 2.18 | 0.58 |
| 30:0:2251:G:H2' | 30:0:2252:A:C8 | 2.38 | 0.58 |
| 9:I:86:GLU:HB2 | 9:I:90:ASP:OD2 | 2.04 | 0.58 |
| 30:0:1333:U:H2' | 30:0:1334:C:C6 | 2.39 | 0.58 |
| 29:3:70:ARG:HB3 | 41:3:9062:HOH:O | 2.03 | 0.58 |
| 30:0:1463:U:H2' | 30:0:1464:C:C6 | 2.39 | 0.58 |
| 30:0:871:G:C8 | 30:0:871:G:C5' | 2.80 | 0.57 |
| 6:F:56:PRO:HB2 | 6:F:58:GLU:OE1 | 2.03 | 0.57 |
| 2:B:97:LEU:O | 2:B:98:THR:HG23 | 2.04 | 0.57 |
| 14:N:1:ALA:HB2 | 31:9:14:G:O2' | 2.04 | 0.57 |
| 2:B:139:ASP:OD2 | 2:B:165:ARG:HD2 | 2.04 | 0.57 |
| 2:B:238:ASN:HD22 | 2:B:240:GLY:N | 1.96 | 0.57 |
| 2:B:254:GLN:HG2 | 2:B:255:GLY:N | 2.17 | 0.57 |
| 30:0:1700:C:H5'' | 30:0:1701:A:OP2 | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 27:1:25:LYS:HD2 | 28:2:49:GLU:H | 1.69 | 0.57 |
| 8:H:19:ARG:HH12 | 30:0:1008:C:H5'' | 1.69 | 0.57 |
| 9:I:88:GLN:HA | 9:I:91:PHE:HE2 | 1.69 | 0.57 |
| 26:Z:34:SER:OG | 30:0:797:A:H4' | 2.03 | 0.57 |
| 3:C:236:THR:HA | 41:C:8652:HOH:O | 2.03 | 0.57 |
| 15:O:39:THR:HG21 | 41:0:5468:HOH:O | 2.04 | 0.57 |
| 3:C:1:MET:HG2 | 3:C:2:GLN:N | 2.15 | 0.57 |
| 30:0:1182:C:H1' | 30:0:1192:A:H8 | 1.67 | 0.57 |
| 30:0:2717:C:O2' | 30:0:2718:C:H5'' | 2.04 | 0.57 |
| 8:H:23:ILE:HG23 | 8:H:123:ILE:CD1 | 2.34 | 0.57 |
| 14:N:119:GLN:O | 14:N:123:ILE:HG13 | 2.04 | 0.57 |
| 16:P:98:ILE:HD12 | 16:P:102:ARG:NE | 2.20 | 0.57 |
| 13:M:84:LYS:HG3 | 30:0:171:C:OP2 | 2.04 | 0.57 |
| 14:N:37:ARG:NE | 41:N:8833:HOH:O | 2.37 | 0.57 |
| 30:0:506:G:H22 | 30:0:509:A:H5'' | 1.69 | 0.57 |
| 10:J:54:VAL:O | 10:J:58:GLU:HG3 | 2.05 | 0.57 |
| 10:J:4:ALA:O | 10:J:5:GLU:HB2 | 2.02 | 0.57 |
| 18:R:77:ALA:O | 18:R:78:GLY:CA | 2.52 | 0.57 |
| 30:0:282:C:O2' | 30:0:283:U:H5' | 2.04 | 0.57 |
| 21:U:50:GLU:HB3 | 30:0:2866:U:C4 | 2.40 | 0.57 |
| 18:R:39:THR:HB | 18:R:42:GLU:CG | 2.34 | 0.57 |
| 6:F:50:VAL:CG2 | 6:F:63:ILE:HG21 | 2.34 | 0.57 |
| 30:0:1189:A:H1' | 30:0:1209:C:H1' | 1.87 | 0.57 |
| 22:V:42:ASN:HB3 | 41:V:7247:HOH:O | 2.05 | 0.57 |
| 30:0:946:C:H2' | 30:0:947:U:C6 | 2.40 | 0.57 |
| 30:0:2064:U:H5' | 30:0:2652:U:H4' | 1.87 | 0.57 |
| 7:G:67:LEU:O | 7:G:71:LEU:HG | 2.05 | 0.57 |
| 14:N:86:LEU:HD21 | 14:N:180:LEU:CD1 | 2.35 | 0.57 |
| 30:0:292:G:H2' | 30:0:358:G:N2 | 2.20 | 0.57 |
| 2:B:24:PRO:HG3 | 2:B:204:GLY:HA2 | 1.86 | 0.57 |
| 30:0:241:A:C2 | 30:0:378:A:H4' | 2.40 | 0.57 |
| 29:3:68:LYS:HE2 | 30:0:2436:U:H5' | 1.86 | 0.57 |
| 30:0:78:G:N3 | 30:0:78:G:N9 | 2.52 | 0.57 |
| 21:U:14:GLU:OE1 | 21:U:15:PRO:HD2 | 2.04 | 0.57 |
| 4:D:27:ILE:HD11 | 4:D:37:ALA:CB | 2.35 | 0.57 |
| 1:A:190:ARG:NH2 | 1:A:207:GLN:OE1 | 2.37 | 0.57 |
| 30:0:1298:U:H2' | 30:0:1299:G:C8 | 2.40 | 0.57 |
| 30:0:1299:G:H5' | 41:0:4943:HOH:O | 2.04 | 0.57 |
| 29:3:77:ALA:C | 29:3:78:HIS:CA | 2.73 | 0.57 |
| 30:0:1878:G:O2' | 30:0:1879:U:H6 | 1.87 | 0.57 |
| 2:B:75:GLU:C | 2:B:77:PRO:HD3 | 2.24 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 20:T:68:ASP:HB2 | 41:0:6493:HOH:O | 2.04 | 0.57 |
| 30:0:699:C:H2' | 30:0:744:G:O4' | 2.05 | 0.57 |
| 4:D:131:THR:HG21 | 30:0:2348:C:H1' | 1.87 | 0.57 |
| 14:N:11:ARG:HG3 | 14:N:14:ARG:NH1 | 2.19 | 0.57 |
| 14:N:32:PRO:HD2 | 14:N:99:GLU:O | 2.05 | 0.57 |
| 30:0:820:G:H5' | 30:0:821:U:H5' | 1.86 | 0.57 |
| 23:W:151:GLU:O | 23:W:154:ARG:HB2 | 2.05 | 0.57 |
| 26:Z:96:GLU:OE1 | 26:Z:101:LYS:HE2 | 2.03 | 0.57 |
| 3:C:72:LYS:HG2 | 3:C:77:ALA:HA | 1.85 | 0.57 |
| 2:B:8:LYS:HG3 | 2:B:220:VAL:HG12 | 1.87 | 0.57 |
| 30:0:2361:A:H8 | 30:0:2361:A:H5' | 1.70 | 0.57 |
| 13:M:188:ARG:HD3 | 30:0:155:C:OP2 | 2.05 | 0.56 |
| 19:S:33:SER:O | 19:S:37:VAL:HG23 | 2.04 | 0.56 |
| 31:9:20:G:O2' | 31:9:21:G:H5' | 2.04 | 0.56 |
| 2:B:36:PRO:CG | 2:B:169:GLY:H | 2.09 | 0.56 |
| 30:0:558:C:H2' | 30:0:559:U:H5' | 1.86 | 0.56 |
| 30:0:2090:G:H2' | 30:0:2091:G:C8 | 2.40 | 0.56 |
| 2:B:141:ARG:HG2 | 2:B:165:ARG:HA | 1.87 | 0.56 |
| 8:H:6:ALA:HB3 | 30:0:2521:A:OP2 | 2.05 | 0.56 |
| 22:V:12:THR:HG22 | 22:V:15:GLU:OE2 | 2.05 | 0.56 |
| 4:D:64:ARG:NE | 4:D:67:ASP:HB3 | 2.20 | 0.56 |
| 41:Z:8705:HOH:O | 30:0:1886:A:H4' | 2.06 | 0.56 |
| 8:H:170:ARG:HD2 | 41:H:8991:HOH:O | 2.04 | 0.56 |
| 31:9:92:G:H2' | 31:9:93:A:C8 | 2.40 | 0.56 |
| 14:N:7:LYS:HE3 | 17:Q:21:ARG:O | 2.06 | 0.56 |
| 1:A:36:ASP:O | 1:A:38:ILE:N | 2.31 | 0.56 |
| 14:N:82:TYR:OH | 14:N:176:ARG:NH1 | 2.39 | 0.56 |
| 41:0:6025:HOH:O | 32:5:76:A:H1' | 2.05 | 0.56 |
| 23:W:84:VAL:HG12 | 41:W:6679:HOH:O | 2.03 | 0.56 |
| 30:0:2004:U:H4' | 41:0:6144:HOH:O | 2.04 | 0.56 |
| 30:0:960:G:H3' | 30:0:960:G:N3 | 2.20 | 0.56 |
| 16:P:1:THR:O | 30:0:1396:C:H1' | 2.04 | 0.56 |
| 12:L:149:ARG:O | 12:L:150:GLN:HB2 | 2.05 | 0.56 |
| 1:A:26:ASP:O | 1:A:28:GLU:N | 2.38 | 0.56 |
| 12:L:56:LYS:HE3 | 30:0:2443:C:O3' | 2.06 | 0.56 |
| 1:A:192:VAL:HB | 41:A:9067:HOH:O | 2.05 | 0.56 |
| 12:L:133:VAL:HA | 41:L:8879:HOH:O | 2.05 | 0.56 |
| 30:0:2356:A:H2' | 30:0:2357:G:O4' | 2.06 | 0.56 |
| 30:0:1555:G:H4' | 30:0:1630:A:H2 | 1.70 | 0.56 |
| 1:A:51:ARG:NH1 | 1:A:120:ARG:O | 2.39 | 0.56 |
| 1:A:80:LEU:HD22 | 1:A:91:GLY:O | 2.06 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:82:VAL:HG13 | 1:A:93:THR:HB | 1.88 | 0.56 |
| 27:1:46:ARG:HA | 41:0:3910:HOH:O | 2.05 | 0.56 |
| 30:0:2426:G:H1' | 41:0:6917:HOH:O | 2.06 | 0.56 |
| 15:O:99:GLU:OE1 | 15:O:99:GLU:N | 2.39 | 0.56 |
| 2:B:16:ARG:NH1 | 41:B:9097:HOH:O | 2.38 | 0.56 |
| 24:X:66:THR:HG23 | 24:X:67:PRO:HD2 | 1.87 | 0.56 |
| 30:0:1829:A:H2' | 30:0:1830:C:H5' | 1.88 | 0.56 |
| 11:K:81:ARG:HD3 | 11:K:87:ARG:NH1 | 2.20 | 0.56 |
| 18:R:114:VAL:HB | 18:R:145:LEU:HD12 | 1.88 | 0.56 |
| 24:X:76:ARG:HG3 | 24:X:76:ARG:HH11 | 1.71 | 0.56 |
| 30:0:447:A:O2' | 30:0:448:G:H5' | 2.06 | 0.56 |
| 23:W:38:THR:HG22 | 23:W:39:ASP:N | 2.20 | 0.56 |
| 4:D:23:VAL:HG22 | 4:D:73:VAL:HB | 1.86 | 0.56 |
| 8:H:48:VAL:HA | 8:H:170:ARG:O | 2.05 | 0.56 |
| 30:0:603:A:H5'' | 30:0:604:G:OP1 | 2.06 | 0.56 |
| 1:A:223:ARG:NH1 | 30:0:2270:G:H4' | 2.21 | 0.56 |
| 4:D:18:ILE:HG12 | 4:D:134:LEU:CD2 | 2.36 | 0.56 |
| 16:P:11:ALA:HB1 | 16:P:16:VAL:O | 2.06 | 0.56 |
| 30:0:2611:G:H3' | 41:0:3252:HOH:O | 2.04 | 0.56 |
| 5:E:84:MET:HG2 | 5:E:168:ILE:HD13 | 1.88 | 0.56 |
| 23:W:88:THR:HG22 | 23:W:89:ASP:H | 1.71 | 0.56 |
| 6:F:111:ILE:O | 6:F:115:VAL:HG23 | 2.06 | 0.56 |
| 23:W:154:ARG:NH1 | 30:0:588:G:O6 | 2.38 | 0.56 |
| 13:M:77:HIS:C | 13:M:78:LYS:CA | 2.74 | 0.56 |
| 30:0:69:A:H5' | 30:0:69:A:C8 | 2.40 | 0.56 |
| 5:E:137:ASP:OD1 | 5:E:139:GLU:HB2 | 2.05 | 0.56 |
| 4:D:99:ASP:HA | 41:D:5675:HOH:O | 2.06 | 0.55 |
| 30:0:1201:C:H5'' | 41:0:7053:HOH:O | 2.05 | 0.55 |
| 25:Y:187:VAL:HG23 | 25:Y:192:ASP:HB2 | 1.88 | 0.55 |
| 20:T:2:LYS:HE2 | 41:T:2822:HOH:O | 2.06 | 0.55 |
| 29:3:3:MET:HG3 | 29:3:4:PRO:HD2 | 1.88 | 0.55 |
| 6:F:65:GLU:O | 6:F:69:GLU:HG2 | 2.07 | 0.55 |
| 30:0:101:C:H2' | 30:0:102:A:C8 | 2.41 | 0.55 |
| 10:J:76:ASP:HA | 41:J:5907:HOH:O | 2.05 | 0.55 |
| 30:0:1189:A:O2' | 30:0:1208:C:H2' | 2.05 | 0.55 |
| 30:0:1209:C:H2' | 30:0:1210:G:H8 | 1.71 | 0.55 |
| 23:W:41:TYR:HA | 23:W:44:MET:HE3 | 1.88 | 0.55 |
| 30:0:2252:A:H2' | 30:0:2253:G:O4' | 2.06 | 0.55 |
| 30:0:1314:U:H5'' | 30:0:1316:G:O4' | 2.06 | 0.55 |
| 9:I:89:GLU:OE2 | 30:0:1181:A:H5' | 2.07 | 0.55 |
| 29:3:60:LYS:NZ | 30:0:2428:G:N7 | 2.54 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:191:GLY:HA2 | 1:A:194:MET:HE2 | 1.88 | 0.55 |
| 4:D:58:VAL:HB | 4:D:62:ASP:HB3 | 1.88 | 0.55 |
| 1:A:88:ILE:CD1 | 1:A:100:PRO:HD3 | 2.29 | 0.55 |
| 30:0:2072:G:C6 | 30:0:2533:C:H1' | 2.41 | 0.55 |
| 30:0:1835:U:C5 | 30:0:1840:A:N7 | 2.69 | 0.55 |
| 10:J:77:GLY:C | 10:J:78:ILE:CA | 2.75 | 0.55 |
| 8:H:69:ARG:HD3 | 41:H:9036:HOH:O | 2.05 | 0.55 |
| 10:J:75:PRO:HG2 | 10:J:105:LEU:CD2 | 2.36 | 0.55 |
| 1:A:89:ALA:O | 1:A:92:ASN:HB2 | 2.07 | 0.55 |
| 30:0:304:G:H1' | 30:0:347:A:N6 | 2.20 | 0.55 |
| 9:I:97:VAL:O | 9:I:101:LYS:HG3 | 2.07 | 0.55 |
| 5:E:101:GLU:HB3 | 5:E:117:THR:HA | 1.89 | 0.55 |
| 30:0:280:C:H2' | 30:0:281:U:O4' | 2.06 | 0.55 |
| 23:W:122:ARG:NH1 | 23:W:152:ALA:O | 2.39 | 0.55 |
| 31:9:23:U:O2' | 31:9:24:U:H4' | 2.07 | 0.55 |
| 3:C:27:ARG:CG | 3:C:27:ARG:HH11 | 2.20 | 0.55 |
| 18:R:44:VAL:O | 18:R:48:GLU:HG3 | 2.07 | 0.55 |
| 30:0:1909:A:N1 | 30:0:2128:G:H1' | 2.22 | 0.55 |
| 2:B:51:VAL:HG13 | 2:B:53:LEU:HD13 | 1.87 | 0.55 |
| 14:N:77:ASN:OD1 | 14:N:79:PRO:HD2 | 2.06 | 0.55 |
| 3:C:78:ARG:HG3 | 3:C:78:ARG:NH1 | 2.21 | 0.55 |
| 25:Y:169:ARG:HD3 | 30:0:1328:A:C8 | 2.41 | 0.55 |
| 13:M:71:SER:O | 13:M:73:ARG:NH1 | 2.38 | 0.55 |
| 9:I:108:HIS:N | 9:I:109:PRO:HD2 | 2.22 | 0.55 |
| 2:B:139:ASP:HB2 | 2:B:165:ARG:HE | 1.70 | 0.55 |
| 14:N:74:PRO:HG2 | 14:N:159:TYR:CE1 | 2.41 | 0.55 |
| 4:D:49:PRO:HB3 | 41:D:5828:HOH:O | 2.07 | 0.55 |
| 3:C:154:VAL:O | 3:C:158:GLU:HG3 | 2.07 | 0.55 |
| 2:B:279:THR:HG22 | 2:B:280:VAL:N | 2.22 | 0.55 |
| 30:0:2362:A:H2' | 30:0:2363:G:C8 | 2.42 | 0.55 |
| 8:H:141:CYS:HB2 | 41:H:8995:HOH:O | 2.06 | 0.55 |
| 30:0:1350:U:H4' | 41:0:5964:HOH:O | 2.06 | 0.55 |
| 30:0:737:A:H2' | 30:0:738:G:O4' | 2.06 | 0.55 |
| 27:1:28:HIS:HE1 | 30:0:776:A:OP1 | 1.90 | 0.55 |
| 15:O:98:LEU:O | 15:O:102:ILE:HG13 | 2.07 | 0.55 |
| 2:B:16:ARG:HD3 | 41:B:9088:HOH:O | 2.06 | 0.55 |
| 30:0:2103:A:O2' | 30:0:2104:C:H5' | 2.06 | 0.55 |
| 26:Z:77:GLY:HA2 | 26:Z:91:GLY:O | 2.06 | 0.55 |
| 19:S:73:ASP:OD1 | 19:S:76:GLU:HG3 | 2.06 | 0.55 |
| 25:Y:189:ASN:HD22 | 25:Y:189:ASN:C | 2.09 | 0.55 |
| 1:A:192:VAL:CG1 | 1:A:207:GLN:HB3 | 2.35 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 30:0:1730:G:H5' | 30:0:1731:C:H5 | 1.72 | 0.55 |
| 2:B:102:THR:HG21 | 2:B:182:VAL:O | 2.06 | 0.55 |
| 30:0:2032:U:O2' | 30:0:2033:G:H5'' | 2.06 | 0.55 |
| 3:C:168:ARG:NH2 | 3:C:190:ALA:O | 2.40 | 0.55 |
| 30:0:1118:A:C8 | 30:0:1118:A:C3' | 2.86 | 0.54 |
| 14:N:67:ALA:HA | 14:N:71:TRP:HB3 | 1.89 | 0.54 |
| 30:0:1309:U:O2' | 30:0:1310:U:H5' | 2.07 | 0.54 |
| 30:0:2531:U:O2' | 30:0:2532:A:H5' | 2.06 | 0.54 |
| 2:B:85:ARG:NH1 | 41:B:9118:HOH:O | 2.39 | 0.54 |
| 7:G:16:LYS:O | 7:G:20:VAL:HG23 | 2.07 | 0.54 |
| 2:B:232:TRP:CD1 | 2:B:235:ARG:HD2 | 2.43 | 0.54 |
| 5:E:152:THR:HG21 | 5:E:165:GLY:HA2 | 1.89 | 0.54 |
| 1:A:165:THR:HG22 | 41:A:9093:HOH:O | 2.07 | 0.54 |
| 19:S:43:GLU:HB3 | 41:S:7106:HOH:O | 2.08 | 0.54 |
| 13:M:43:PRO:HG3 | 13:M:62:VAL:HG21 | 1.88 | 0.54 |
| 12:L:79:ASP:HB3 | 41:L:8862:HOH:O | 2.06 | 0.54 |
| 8:H:6:ALA:HA | 8:H:61:ARG:HH12 | 1.73 | 0.54 |
| 5:E:131:LEU:HD12 | 5:E:166:VAL:HG11 | 1.90 | 0.54 |
| 30:0:1205:U:C2' | 30:0:1206:U:H5'' | 2.36 | 0.54 |
| 31:9:14:G:H5' | 31:9:14:G:C8 | 2.42 | 0.54 |
| 24:X:47:ALA:HB1 | 24:X:82:GLU:CB | 2.37 | 0.54 |
| 20:T:1:SER:HB2 | 30:0:447:A:P | 2.47 | 0.54 |
| 31:9:39:U:H3' | 31:9:40:C:H5'' | 1.88 | 0.54 |
| 5:E:139:GLU:OE2 | 30:0:2781:U:H1' | 2.08 | 0.54 |
| 15:O:44:ASN:CG | 15:O:67:SER:HB2 | 2.26 | 0.54 |
| 5:E:119:HIS:HE1 | 5:E:147:ASP:OD2 | 1.90 | 0.54 |
| 15:O:25:VAL:HG12 | 30:0:709:G:O2' | 2.07 | 0.54 |
| 20:T:32:ARG:NH1 | 20:T:38:ARG:HH12 | 2.04 | 0.54 |
| 20:T:38:ARG:NH1 | 41:T:6217:HOH:O | 2.41 | 0.54 |
| 31:9:1:U:H5' | 31:9:121:C:O2 | 2.07 | 0.54 |
| 30:0:1189:A:H1' | 30:0:1209:C:C1' | 2.37 | 0.54 |
| 26:Z:51:ALA:HA | 41:Z:8712:HOH:O | 2.08 | 0.54 |
| 12:L:39:GLU:OE2 | 30:0:926:A:H5' | 2.08 | 0.54 |
| 2:B:2:GLN:NE2 | 30:0:2545:U:OP2 | 2.40 | 0.54 |
| 3:C:43:LYS:HG2 | 30:0:449:A:N7 | 2.22 | 0.54 |
| 20:T:23:VAL:HG23 | 20:T:41:ARG:HG3 | 1.90 | 0.54 |
| 6:F:2:VAL:HG22 | 6:F:57:GLU:OE1 | 2.08 | 0.54 |
| 30:0:136:C:H2' | 30:0:137:U:O4' | 2.08 | 0.54 |
| 25:Y:151:SER:HB3 | 25:Y:154:ARG:HB3 | 1.90 | 0.54 |
| 25:Y:148:GLY:O | 25:Y:154:ARG:HD3 | 2.06 | 0.54 |
| 5:E:91:PHE:HE1 | 30:0:2694:A:H4' | 1.73 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:Z:54:GLU:HB2 | 41:Z:8712:HOH:O | 2.07 | 0.54 |
| 30:0:2324:G:N2 | 30:0:2377:U:H1' | 2.22 | 0.54 |
| 30:0:1218:U:H2' | 30:0:1219:U:C6 | 2.42 | 0.54 |
| 13:M:178:LYS:HB2 | 41:0:7676:HOH:O | 2.07 | 0.54 |
| 2:B:145:HIS:HD2 | 2:B:159:PRO:HB3 | 1.72 | 0.54 |
| 30:0:602:A:O2' | 30:0:605:C:H4' | 2.06 | 0.54 |
| 30:0:151:A:H2' | 30:0:152:A:O4' | 2.08 | 0.54 |
| 18:R:29:LYS:NZ | 41:R:8945:HOH:O | 2.40 | 0.54 |
| 22:V:7:GLU:O | 22:V:11:MET:HG3 | 2.08 | 0.54 |
| 13:M:171:ARG:NH2 | 30:0:189:A:OP1 | 2.39 | 0.54 |
| 5:E:49:ILE:HD11 | 5:E:69:ILE:HD12 | 1.89 | 0.54 |
| 13:M:164:THR:CG2 | 13:M:165:GLY:N | 2.70 | 0.54 |
| 30:0:138:U:H5'' | 30:0:139:C:OP2 | 2.07 | 0.54 |
| 30:0:1730:G:C5' | 30:0:1731:C:C6 | 2.90 | 0.54 |
| 30:0:2894:C:O2' | 30:0:2895:C:H5' | 2.07 | 0.54 |
| 30:0:1592:G:H2' | 30:0:1593:C:C6 | 2.42 | 0.54 |
| 10:J:70:PHE:CE1 | 30:0:2676:C:H4' | 2.42 | 0.54 |
| 1:A:95:PRO:HG2 | 1:A:98:GLU:HG2 | 1.90 | 0.54 |
| 23:W:48:VAL:HG12 | 23:W:48:VAL:O | 2.07 | 0.54 |
| 30:0:137:U:H2' | 30:0:139:C:C5 | 2.41 | 0.54 |
| 11:K:87:ARG:NH2 | 30:0:2720:C:O2 | 2.41 | 0.54 |
| 22:V:64:GLY:O | 22:V:65:ASP:HB2 | 2.07 | 0.54 |
| 23:W:78:ASP:HB2 | 41:W:6694:HOH:O | 2.07 | 0.54 |
| 8:H:20:ARG:HD3 | 8:H:26:ILE:HD12 | 1.90 | 0.54 |
| 1:A:8:ARG:HG2 | 41:A:9029:HOH:O | 2.07 | 0.54 |
| 15:O:39:THR:O | 15:O:115:ARG:NH2 | 2.41 | 0.54 |
| 4:D:135:VAL:HG22 | 4:D:136:ARG:N | 2.23 | 0.54 |
| 27:1:25:LYS:HE2 | 41:1:7213:HOH:O | 2.07 | 0.54 |
| 2:B:141:ARG:HD2 | 2:B:163:GLU:OE2 | 2.08 | 0.54 |
| 15:O:96:VAL:CG1 | 15:O:100:GLN:HB2 | 2.38 | 0.54 |
| 7:G:64:ASN:O | 7:G:68:GLU:HG3 | 2.07 | 0.54 |
| 27:1:9:GLY:HA3 | 30:0:1695:G:H1' | 1.90 | 0.54 |
| 9:I:111:LEU:HD22 | 9:I:122:GLU:OE1 | 2.07 | 0.54 |
| 30:0:2265:U:H2' | 30:0:2266:A:C8 | 2.42 | 0.54 |
| 30:0:1342:C:C2' | 30:0:1343:C:H5' | 2.37 | 0.54 |
| 6:F:26:THR:HG21 | 6:F:102:GLY:C | 2.28 | 0.54 |
| 30:0:185:G:H4' | 30:0:186:A:H4' | 1.89 | 0.54 |
| 14:N:115:VAL:HG22 | 41:N:8857:HOH:O | 2.08 | 0.54 |
| 21:U:52:THR:CG2 | 21:U:54:THR:HB | 2.38 | 0.54 |
| 8:H:31:ILE:HA | 8:H:66:GLU:OE1 | 2.08 | 0.54 |
| 25:Y:117:LEU:HD13 | 25:Y:174:VAL:HG11 | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:L:145:LEU:HD23 | 12:L:145:LEU:O | 2.08 | 0.54 |
| 15:O:25:VAL:HG23 | 15:O:26:TRP:N | 2.22 | 0.54 |
| 30:0:1406:A:H4' | 30:0:1407:A:H5'' | 1.89 | 0.54 |
| 2:B:199:TYR:CE2 | 2:B:268:ARG:HB2 | 2.44 | 0.54 |
| 30:0:1559:A:H1' | 41:0:6694:HOH:O | 2.07 | 0.54 |
| 8:H:61:ARG:HG3 | 8:H:61:ARG:NH1 | 2.22 | 0.53 |
| 31:9:2:U:OP2 | 31:9:3:A:H5' | 2.08 | 0.53 |
| 30:0:1132:A:N6 | 30:0:1229:C:H2' | 2.23 | 0.53 |
| 30:0:612:U:H2' | 30:0:613:C:C6 | 2.44 | 0.53 |
| 3:C:157:LEU:HD13 | 3:C:166:ILE:HD11 | 1.90 | 0.53 |
| 1:A:94:LEU:HD21 | 1:A:156:ILE:HD11 | 1.90 | 0.53 |
| 4:D:167:GLU:C | 4:D:169:THR:H | 2.12 | 0.53 |
| 12:L:91:VAL:CG1 | 12:L:120:LEU:HD23 | 2.38 | 0.53 |
| 22:V:5:VAL:HG12 | 22:V:9:ARG:NH1 | 2.23 | 0.53 |
| 14:N:62:HIS:HB3 | 14:N:65:ASP:OD1 | 2.08 | 0.53 |
| 13:M:179:GLY:O | 30:0:399:C:H5' | 2.08 | 0.53 |
| 13:M:122:GLN:OE1 | 13:M:127:LYS:HE2 | 2.08 | 0.53 |
| 13:M:30:GLU:O | 13:M:34:GLU:HG3 | 2.08 | 0.53 |
| 30:0:2372:A:H2' | 30:0:2373:U:C6 | 2.43 | 0.53 |
| 5:E:77:THR:C | 5:E:78:GLU:CA | 2.77 | 0.53 |
| 31:9:57:A:H2' | 31:9:58:G:H5' | 1.89 | 0.53 |
| 1:A:191:GLY:HA2 | 1:A:194:MET:HE3 | 1.90 | 0.53 |
| 30:0:834:G:H3' | 30:0:835:U:H4' | 1.90 | 0.53 |
| 30:0:920:C:H4' | 30:0:921:G:C2 | 2.44 | 0.53 |
| 3:C:20:ASP:O | 3:C:23:GLU:HB2 | 2.08 | 0.53 |
| 3:C:140:VAL:HB | 41:C:8652:HOH:O | 2.08 | 0.53 |
| 14:N:37:ARG:NH1 | 31:9:6:C:C5' | 2.59 | 0.53 |
| 5:E:81:GLU:O | 5:E:172:PRO:HD3 | 2.09 | 0.53 |
| 4:D:18:ILE:HG12 | 4:D:134:LEU:HD23 | 1.91 | 0.53 |
| 30:0:2748:G:C5' | 41:0:9326:HOH:O | 2.57 | 0.53 |
| 29:3:73:GLU:HB2 | 41:3:9021:HOH:O | 2.09 | 0.53 |
| 5:E:8:PRO:HB2 | 5:E:11:VAL:HG23 | 1.89 | 0.53 |
| 23:W:41:TYR:O | 23:W:45:VAL:HG22 | 2.08 | 0.53 |
| 30:0:2878:U:H2' | 30:0:2879:A:O4' | 2.09 | 0.53 |
| 4:D:50:VAL:O | 4:D:71:ALA:HA | 2.07 | 0.53 |
| 30:0:2047:C:H5' | 41:0:3721:HOH:O | 2.07 | 0.53 |
| 30:0:1278:A:H4' | 30:0:1279:U:C4 | 2.43 | 0.53 |
| 30:0:1878:G:O2' | 30:0:1879:U:P | 2.67 | 0.53 |
| 29:3:3:MET:O | 29:3:90:PHE:HA | 2.07 | 0.53 |
| 30:0:204:A:C2' | 30:0:205:U:H5' | 2.37 | 0.53 |
| 30:0:1527:A:H1' | 30:0:1528:A:C8 | 2.43 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:4:ILE:HG22 | 1:A:198:ASP:O | 2.09 | 0.53 |
| 4:D:27:ILE:HD11 | 4:D:37:ALA:HB3 | 1.90 | 0.53 |
| 5:E:144:THR:O | 5:E:148:ILE:HG13 | 2.08 | 0.53 |
| 19:S:55:GLN:HE22 | 30:0:1446:U:H2' | 1.72 | 0.53 |
| 30:0:2239:C:H2' | 30:0:2240:U:C6 | 2.44 | 0.53 |
| 30:0:1528:A:H2' | 30:0:1529:G:O4' | 2.08 | 0.53 |
| 16:P:77:ALA:C | 16:P:78:GLY:CA | 2.76 | 0.53 |
| 30:0:2453:G:H5' | 41:0:5543:HOH:O | 2.08 | 0.53 |
| 9:I:124:VAL:O | 9:I:124:VAL:HG12 | 2.09 | 0.53 |
| 30:0:1042:U:O2' | 30:0:1043:C:H5' | 2.08 | 0.53 |
| 30:0:2351:C:H2' | 30:0:2352:G:O4' | 2.08 | 0.53 |
| 30:0:2824:C:O3' | 30:0:2825:C:H6 | 1.91 | 0.53 |
| 30:0:1666:C:H2' | 30:0:1667:A:C5' | 2.38 | 0.53 |
| 30:0:1730:G:H5'' | 30:0:1731:C:H6 | 1.74 | 0.53 |
| 28:2:20:ARG:HG3 | 28:2:21:VAL:N | 2.24 | 0.53 |
| 30:0:2266:A:H2' | 30:0:2267:G:C8 | 2.44 | 0.53 |
| 30:0:95:A:H5'' | 30:0:97:G:O4' | 2.09 | 0.53 |
| 9:I:94:ASP:OD1 | 9:I:133:THR:HB | 2.08 | 0.53 |
| 30:0:790:A:H1' | 30:0:1710:A:H2' | 1.91 | 0.53 |
| 30:0:1714:C:O2' | 30:0:1715:C:H5' | 2.09 | 0.53 |
| 30:0:2755:G:H1' | 41:0:5534:HOH:O | 2.09 | 0.53 |
| 30:0:2583:A:H3' | 41:0:5454:HOH:O | 2.08 | 0.53 |
| 1:A:186:TRP:CG | 1:A:187:PRO:HA | 2.43 | 0.53 |
| 23:W:5:VAL:HG11 | 23:W:153:MET:CE | 2.39 | 0.53 |
| 27:1:28:HIS:CD2 | 27:1:30:LYS:HB2 | 2.43 | 0.53 |
| 30:0:192:A:H5' | 41:0:9428:HOH:O | 2.08 | 0.53 |
| 10:J:71:TYR:CD1 | 10:J:72:PRO:HD2 | 2.44 | 0.53 |
| 30:0:2551:C:O2' | 30:0:2552:C:H5' | 2.08 | 0.53 |
| 6:F:4:VAL:HG13 | 6:F:76:PHE:CE1 | 2.44 | 0.53 |
| 26:Z:70:ARG:CD | 26:Z:83:TYR:HB2 | 2.28 | 0.53 |
| 2:B:212:GLN:HA | 30:0:1733:A:H4' | 1.90 | 0.53 |
| 30:0:969:G:H1 | 30:0:999:C:N4 | 2.03 | 0.53 |
| 12:L:90:ARG:NH2 | 12:L:121:ILE:HD11 | 2.24 | 0.53 |
| 30:0:1878:G:O2' | 30:0:1879:U:C6 | 2.57 | 0.53 |
| 2:B:175:LEU:C | 2:B:175:LEU:HD23 | 2.29 | 0.53 |
| 4:D:143:LYS:O | 31:9:45:A:H4' | 2.09 | 0.53 |
| 3:C:236:THR:HG22 | 3:C:239:ALA:CB | 2.40 | 0.52 |
| 11:K:30:LYS:O | 11:K:55:VAL:HG13 | 2.09 | 0.52 |
| 9:I:130:LEU:HD22 | 30:0:1167:G:H4' | 1.91 | 0.52 |
| 10:J:74:ARG:NH1 | 10:J:76:ASP:OD2 | 2.41 | 0.52 |
| 4:D:51:ARG:HH11 | 4:D:68:PRO:HB3 | 1.73 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:0:2314:G:C2' | 30:0:2315:C:H5' | 2.39 | 0.52 |
| 2:B:277:GLU:N | 2:B:278:PRO:HD2 | 2.23 | 0.52 |
| 19:S:67:ARG:HD3 | 41:S:3430:HOH:O | 2.08 | 0.52 |
| 4:D:53:LYS:O | 4:D:54:ALA:HB2 | 2.08 | 0.52 |
| 30:0:1972:U:H2' | 30:0:1973:A:H5' | 1.91 | 0.52 |
| 2:B:51:VAL:HG22 | 2:B:327:VAL:HG13 | 1.92 | 0.52 |
| 30:0:2769:C:C2' | 30:0:2770:G:H5' | 2.38 | 0.52 |
| 41:C:8658:HOH:O | 30:0:656:G:H1' | 2.10 | 0.52 |
| 25:Y:154:ARG:HH12 | 25:Y:155:ARG:CG | 2.22 | 0.52 |
| 21:U:45:GLU:HB2 | 21:U:48:ASN:HD22 | 1.73 | 0.52 |
| 25:Y:203:VAL:CG1 | 25:Y:228:VAL:HG22 | 2.39 | 0.52 |
| 14:N:162:ASP:HA | 41:N:8830:HOH:O | 2.08 | 0.52 |
| 30:0:1067:A:H5' | 41:0:5209:HOH:O | 2.10 | 0.52 |
| 17:Q:77:ASP:C | 17:Q:78:GLY:CA | 2.77 | 0.52 |
| 12:L:71:GLU:HG2 | 30:0:700:A:C2 | 2.45 | 0.52 |
| 9:I:98:ASP:HA | 9:I:101:LYS:HD2 | 1.92 | 0.52 |
| 14:N:160:SER:HB3 | 31:9:51:A:H5' | 1.91 | 0.52 |
| 13:M:107:ARG:NH1 | 13:M:107:ARG:HG3 | 2.17 | 0.52 |
| 30:0:558:C:H2' | 30:0:559:U:H5'' | 1.90 | 0.52 |
| 20:T:69:LYS:O | 20:T:71:VAL:HG23 | 2.09 | 0.52 |
| 13:M:9:ARG:NH2 | 30:0:378:A:OP1 | 2.42 | 0.52 |
| 22:V:50:ARG:HH12 | 30:0:56:G:H5'' | 1.72 | 0.52 |
| 14:N:151:ASP:OD1 | 14:N:154:LEU:HD13 | 2.10 | 0.52 |
| 30:0:1595:G:O2' | 30:0:1596:U:H5' | 2.08 | 0.52 |
| 30:0:564:G:H1' | 41:0:7127:HOH:O | 2.10 | 0.52 |
| 30:0:325:U:H2' | 30:0:326:G:H8 | 1.74 | 0.52 |
| 11:K:4:LEU:HD22 | 11:K:116:GLU:HB3 | 1.92 | 0.52 |
| 31:9:59:C:H2' | 31:9:60:C:H6 | 1.71 | 0.52 |
| 30:0:1778:A:H2' | 30:0:1779:A:H5' | 1.91 | 0.52 |
| 31:9:3:A:H2 | 31:9:21:G:N3 | 2.08 | 0.52 |
| 30:0:1279:U:O2 | 30:0:1279:U:H2' | 2.10 | 0.52 |
| 30:0:204:A:H2' | 30:0:205:U:H5' | 1.90 | 0.52 |
| 22:V:55:ARG:NE | 41:V:4428:HOH:O | 2.37 | 0.52 |
| 30:0:164:G:H3' | 41:0:4517:HOH:O | 2.10 | 0.52 |
| 30:0:1130:U:H2' | 30:0:1131:G:O4' | 2.08 | 0.52 |
| 30:0:2507:G:H2' | 30:0:2510:C:H42 | 1.75 | 0.52 |
| 5:E:126:ILE:HB | 5:E:131:LEU:CD2 | 2.39 | 0.52 |
| 30:0:2717:C:H2' | 30:0:2718:C:C5' | 2.36 | 0.52 |
| 30:0:2748:G:H4' | 30:0:2749:U:H5' | 1.91 | 0.52 |
| 29:3:11:CYS:HB2 | 29:3:20:HIS:CE1 | 2.44 | 0.52 |
| 15:O:77:ALA:C | 15:O:78:ALA:CA | 2.78 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 30:0:1477:C:H5' | 30:0:1868:G:C5' | 2.39 | 0.52 |
| 2:B:222:LYS:HE2 | 41:0:4152:HOH:O | 2.09 | 0.52 |
| 2:B:223:ARG:O | 2:B:228:ALA:HB2 | 2.09 | 0.52 |
| 30:0:1426:C:H3' | 41:0:9544:HOH:O | 2.09 | 0.52 |
| 8:H:15:PRO:HG3 | 30:0:1053:G:OP1 | 2.09 | 0.52 |
| 3:C:49:ASP:HB3 | 3:C:52:ALA:HB2 | 1.89 | 0.52 |
| 30:0:364:U:H2' | 30:0:365:G:O4' | 2.09 | 0.52 |
| 23:W:6:GLN:CB | 23:W:26:ILE:HD11 | 2.30 | 0.52 |
| 18:R:39:THR:HB | 18:R:42:GLU:CD | 2.30 | 0.52 |
| 20:T:71:VAL:HG12 | 20:T:72:ILE:N | 2.24 | 0.52 |
| 23:W:122:ARG:NH1 | 23:W:122:ARG:HG3 | 2.23 | 0.52 |
| 18:R:77:ALA:C | 18:R:78:GLY:CA | 2.78 | 0.52 |
| 31:9:3:A:H2' | 41:9:9045:HOH:O | 2.08 | 0.52 |
| 30:0:2353:A:H4' | 30:0:2354:A:O5' | 2.10 | 0.52 |
| 14:N:179:LEU:HA | 14:N:184:ILE:HD12 | 1.92 | 0.52 |
| 27:1:4:GLY:O | 27:1:8:GLN:HG2 | 2.10 | 0.52 |
| 25:Y:112:GLU:CD | 25:Y:115:ARG:NH1 | 2.63 | 0.52 |
| 30:0:2003:U:H4' | 30:0:2004:U:C5 | 2.45 | 0.52 |
| 15:O:14:LEU:HD23 | 15:O:102:ILE:HD11 | 1.92 | 0.52 |
| 2:B:214:PRO:HD2 | 41:0:2992:HOH:O | 2.08 | 0.52 |
| 30:0:299:U:H5' | 41:0:9133:HOH:O | 2.09 | 0.52 |
| 8:H:174:LEU:HA | 41:H:9026:HOH:O | 2.10 | 0.52 |
| 4:D:10:PHE:CE1 | 4:D:11:HIS:HB3 | 2.45 | 0.52 |
| 23:W:90:TYR:N | 23:W:90:TYR:CD1 | 2.78 | 0.52 |
| 23:W:4:LEU:HB2 | 23:W:33:THR:CG2 | 2.40 | 0.52 |
| 2:B:62:ARG:HA | 2:B:65:MET:HE2 | 1.91 | 0.52 |
| 18:R:25:PHE:CE2 | 18:R:29:LYS:HE2 | 2.45 | 0.52 |
| 2:B:280:VAL:HG12 | 2:B:334:SER:HA | 1.91 | 0.52 |
| 30:0:1700:C:P | 41:0:6861:HOH:O | 2.66 | 0.52 |
| 14:N:78:MET:HB2 | 14:N:146:HIS:CE1 | 2.45 | 0.52 |
| 27:1:36:SER:O | 27:1:46:ARG:HD3 | 2.09 | 0.52 |
| 30:0:834:G:H4' | 30:0:835:U:OP2 | 2.09 | 0.52 |
| 1:A:175:LYS:HG3 | 30:0:1847:A:OP1 | 2.10 | 0.52 |
| 30:0:1352:A:O2' | 30:0:1353:C:OP1 | 2.23 | 0.52 |
| 4:D:172:VAL:CG1 | 4:D:173:GLU:H | 2.19 | 0.52 |
| 28:2:48:ASP:O | 28:2:49:GLU:HB2 | 2.10 | 0.52 |
| 27:1:42:SER:HB2 | 41:1:354:HOH:O | 2.09 | 0.52 |
| 29:3:15:ASN:O | 30:0:2408:A:H4' | 2.10 | 0.52 |
| 2:B:30:PRO:HB2 | 2:B:39:GLN:NE2 | 2.25 | 0.52 |
| 15:O:35:LYS:HD3 | 41:0:5468:HOH:O | 2.10 | 0.51 |
| 30:0:2488:A:H61 | 30:0:2534:C:H42 | 1.58 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:48:VAL:HG12 | 6:F:97:ALA:CB | 2.40 | 0.51 |
| 20:T:76:ASP:C | 20:T:78:THR:HG23 | 2.31 | 0.51 |
| 10:J:70:PHE:CD1 | 30:0:2676:C:H4' | 2.44 | 0.51 |
| 9:I:120:ALA:O | 9:I:124:VAL:HG23 | 2.10 | 0.51 |
| 1:A:173:GLY:O | 1:A:176:HIS:HB3 | 2.10 | 0.51 |
| 1:A:47:HIS:HD2 | 30:0:1654:U:H2' | 1.74 | 0.51 |
| 18:R:64:SER:OG | 30:0:1369:A:H4' | 2.11 | 0.51 |
| 30:0:462:A:H2' | 41:0:5731:HOH:O | 2.10 | 0.51 |
| 23:W:4:LEU:HB2 | 23:W:33:THR:HG22 | 1.92 | 0.51 |
| 13:M:24:GLN:HE22 | 13:M:27:ARG:HH11 | 1.59 | 0.51 |
| 30:0:137:U:OP1 | 30:0:259:G:O2' | 2.29 | 0.51 |
| 8:H:32:ALA:O | 8:H:33:GLN:HG3 | 2.10 | 0.51 |
| 21:U:50:GLU:O | 21:U:56:ARG:HG3 | 2.10 | 0.51 |
| 30:0:2338:G:H1 | 30:0:2346:C:H42 | 1.58 | 0.51 |
| 20:T:28:SER:O | 20:T:32:ARG:HG3 | 2.11 | 0.51 |
| 1:A:217:ARG:CG | 1:A:217:ARG:HH11 | 2.23 | 0.51 |
| 14:N:21:HIS:HD2 | 41:0:5578:HOH:O | 1.91 | 0.51 |
| 30:0:2563:U:H2' | 30:0:2565:C:O5' | 2.10 | 0.51 |
| 2:B:24:PRO:CG | 2:B:204:GLY:HA2 | 2.40 | 0.51 |
| 10:J:74:ARG:NH1 | 10:J:76:ASP:HB2 | 2.24 | 0.51 |
| 30:0:1667:A:H2' | 30:0:1668:U:C6 | 2.45 | 0.51 |
| 6:F:58:GLU:HG3 | 6:F:61:MET:HE1 | 1.92 | 0.51 |
| 14:N:11:ARG:HD3 | 31:9:114:G:O6 | 2.09 | 0.51 |
| 12:L:97:VAL:HG12 | 12:L:98:GLU:O | 2.11 | 0.51 |
| 30:0:407:A:O2' | 30:0:408:A:H5' | 2.11 | 0.51 |
| 8:H:139:ALA:HB3 | 8:H:149:VAL:HG21 | 1.93 | 0.51 |
| 19:S:21:GLN:NE2 | 30:0:1508:C:H5' | 2.25 | 0.51 |
| 30:0:1790:C:H2' | 30:0:1791:U:H6 | 1.75 | 0.51 |
| 2:B:17:LYS:O | 2:B:260:HIS:CD2 | 2.64 | 0.51 |
| 27:1:20:ARG:HH21 | 30:0:120:A:H5' | 1.75 | 0.51 |
| 10:J:93:ARG:HH11 | 10:J:93:ARG:CB | 2.17 | 0.51 |
| 8:H:59:GLN:HE22 | 8:H:96:GLN:HG2 | 1.75 | 0.51 |
| 2:B:190:MET:CE | 2:B:194:PHE:CD1 | 2.94 | 0.51 |
| 30:0:2103:A:N7 | 30:0:2538:A:N6 | 2.58 | 0.51 |
| 25:Y:95:THR:N | 25:Y:236:VAL:O | 2.43 | 0.51 |
| 2:B:305:ASP:O | 2:B:306:LYS:HB2 | 2.11 | 0.51 |
| 2:B:81:ALA:HB1 | 2:B:142:LEU:HD13 | 1.92 | 0.51 |
| 16:P:73:HIS:HE1 | 30:0:1789:G:O6 | 1.94 | 0.51 |
| 3:C:241:ALA:O | 3:C:244:ALA:HB3 | 2.11 | 0.51 |
| 10:J:90:LYS:HB2 | 38:J:8802:CL:CL | 2.47 | 0.51 |
| 16:P:54:LYS:HB2 | 30:0:1717:A:H5'' | 1.90 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 30:0:1183:C:H5 | 30:0:1192:A:OP1 | 1.94 | 0.51 |
| 14:N:86:LEU:HD12 | 14:N:125:ALA:HB2 | 1.92 | 0.51 |
| 15:O:97:SER:OG | 15:O:100:GLN:HG3 | 2.09 | 0.51 |
| 25:Y:132:ASP:OD2 | 30:0:621:C:H5' | 2.10 | 0.51 |
| 21:U:23:HIS:HB2 | 21:U:27:ALA:HB3 | 1.93 | 0.51 |
| 5:E:133:VAL:HG12 | 5:E:141:VAL:HG13 | 1.93 | 0.51 |
| 3:C:129:HIS:CE1 | 3:C:231:ARG:HA | 2.46 | 0.51 |
| 21:U:17:THR:CG2 | 21:U:18:GLY:N | 2.74 | 0.51 |
| 10:J:80:LYS:HE2 | 10:J:98:PHE:CZ | 2.46 | 0.51 |
| 6:F:57:GLU:O | 6:F:61:MET:HG3 | 2.10 | 0.51 |
| 9:I:91:PHE:HA | 9:I:131:GLY:HA3 | 1.91 | 0.51 |
| 30:0:2241:C:O2' | 30:0:2242:U:H5' | 2.10 | 0.51 |
| 30:0:2456:A:H2' | 30:0:2457:U:C6 | 2.46 | 0.51 |
| 6:F:27:GLY:HA3 | 6:F:101:ALA:O | 2.10 | 0.51 |
| 30:0:625:U:H5'' | 30:0:1044:C:N4 | 2.25 | 0.51 |
| 11:K:109:LEU:CD1 | 11:K:113:ILE:HD11 | 2.37 | 0.51 |
| 2:B:18:ARG:HE | 2:B:256:GLN:NE2 | 2.08 | 0.51 |
| 16:P:55:LYS:CG | 16:P:56:GLY:N | 2.74 | 0.51 |
| 41:X:4132:HOH:O | 30:0:2895:C:H4' | 2.10 | 0.51 |
| 1:A:130:THR:HB | 1:A:137:VAL:HB | 1.91 | 0.51 |
| 6:F:21:GLU:O | 6:F:24:ARG:HG3 | 2.10 | 0.51 |
| 14:N:41:LYS:HD3 | 41:9:9064:HOH:O | 2.10 | 0.51 |
| 28:2:40:ARG:HG3 | 28:2:45:ASN:HB2 | 1.91 | 0.51 |
| 4:D:57:THR:HG23 | 4:D:63:ILE:CA | 2.35 | 0.51 |
| 24:X:72:VAL:HG22 | 24:X:85:VAL:HG12 | 1.91 | 0.51 |
| 21:U:47:ARG:HG2 | 21:U:54:THR:HG22 | 1.93 | 0.51 |
| 10:J:75:PRO:HD3 | 10:J:136:SER:OG | 2.09 | 0.51 |
| 30:0:304:G:H1' | 30:0:347:A:H61 | 1.75 | 0.51 |
| 13:M:34:GLU:HB3 | 13:M:38:GLU:HG3 | 1.93 | 0.51 |
| 30:0:441:A:H1' | 30:0:442:A:N7 | 2.25 | 0.51 |
| 30:0:1833:U:O2' | 30:0:1834:C:H5' | 2.11 | 0.51 |
| 13:M:9:ARG:HB2 | 13:M:47:ASP:OD2 | 2.11 | 0.51 |
| 14:N:25:ARG:HG2 | 30:0:2416:G:O2' | 2.10 | 0.51 |
| 30:0:1829:A:C2' | 30:0:1830:C:H5' | 2.40 | 0.51 |
| 30:0:398:U:H2' | 30:0:399:C:C6 | 2.46 | 0.51 |
| 3:C:206:ASN:HB2 | 30:0:329:A:OP2 | 2.11 | 0.51 |
| 10:J:63:ILE:HD11 | 30:0:1236:A:C8 | 2.46 | 0.51 |
| 28:2:5:LYS:O | 28:2:9:LYS:HG3 | 2.11 | 0.51 |
| 31:9:64:C:C2' | 31:9:65:A:H5' | 2.41 | 0.51 |
| 24:X:74:ALA:CB | 24:X:85:VAL:HG22 | 2.41 | 0.51 |
| 30:0:1183:C:H2' | 41:0:7062:HOH:O | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:W:88:THR:HG22 | 23:W:90:TYR:CD1 | 2.43 | 0.51 |
| 30:0:876:A:N3 | 30:0:876:A:H2' | 2.25 | 0.51 |
| 23:W:65:VAL:HG12 | 23:W:116:LEU:HD13 | 1.93 | 0.51 |
| 9:I:112:LEU:CD1 | 30:0:1162:G:H1' | 2.41 | 0.51 |
| 3:C:27:ARG:NH1 | 3:C:29:ASP:OD2 | 2.44 | 0.51 |
| 30:0:2414:A:H2' | 30:0:2415:A:C8 | 2.46 | 0.51 |
| 26:Z:77:GLY:C | 26:Z:78:ILE:CA | 2.79 | 0.51 |
| 7:G:64:ASN:N | 7:G:64:ASN:HD22 | 2.09 | 0.51 |
| 30:0:1755:A:H2' | 30:0:1756:G:O4' | 2.11 | 0.51 |
| 3:C:101:ASP:HB2 | 30:0:750:A:O3' | 2.11 | 0.51 |
| 23:W:13:MET:CE | 23:W:17:ILE:HG22 | 2.41 | 0.51 |
| 30:0:1566:C:H2' | 30:0:1567:G:H8 | 1.76 | 0.51 |
| 4:D:77:ASP:C | 4:D:78:GLU:CA | 2.79 | 0.51 |
| 23:W:137:GLN:HG3 | 23:W:137:GLN:O | 2.11 | 0.50 |
| 29:3:61:PRO:HG2 | 41:0:9341:HOH:O | 2.10 | 0.50 |
| 30:0:1159:G:H1 | 30:0:1208:C:H42 | 1.59 | 0.50 |
| 20:T:71:VAL:CG1 | 20:T:90:PRO:HB3 | 2.39 | 0.50 |
| 18:R:114:VAL:HG13 | 18:R:114:VAL:O | 2.12 | 0.50 |
| 30:0:248:A:H5' | 30:0:249:G:OP2 | 2.11 | 0.50 |
| 16:P:61:ARG:NH2 | 30:0:2737:C:OP2 | 2.41 | 0.50 |
| 30:0:1171:A:H2' | 30:0:1172:G:H5' | 1.93 | 0.50 |
| 20:T:112:LEU:CD2 | 20:T:119:ALA:HB3 | 2.38 | 0.50 |
| 1:A:179:MET:HG2 | 1:A:186:TRP:HB2 | 1.92 | 0.50 |
| 21:U:56:ARG:CD | 21:U:56:ARG:O | 2.60 | 0.50 |
| 6:F:69:GLU:O | 6:F:70:LYS:HG2 | 2.11 | 0.50 |
| 2:B:294:TYR:HE2 | 41:B:9134:HOH:O | 1.93 | 0.50 |
| 24:X:30:MET:HE1 | 24:X:58:ALA:HB3 | 1.93 | 0.50 |
| 14:N:12:ARG:HD3 | 14:N:18:THR:OG1 | 2.11 | 0.50 |
| 24:X:85:VAL:HG12 | 24:X:86:GLU:N | 2.26 | 0.50 |
| 30:0:558:C:C2' | 30:0:559:U:C5' | 2.89 | 0.50 |
| 23:W:149:LEU:HG | 23:W:153:MET:CE | 2.40 | 0.50 |
| 5:E:11:VAL:HG12 | 5:E:12:ASP:N | 2.27 | 0.50 |
| 30:0:1529:G:H5' | 41:0:9181:HOH:O | 2.09 | 0.50 |
| 1:A:103:VAL:O | 1:A:105:VAL:HG23 | 2.11 | 0.50 |
| 2:B:212:GLN:HB2 | 2:B:257:THR:CG2 | 2.39 | 0.50 |
| 25:Y:234:VAL:HG12 | 25:Y:235:GLU:H | 1.77 | 0.50 |
| 30:0:559:U:H2' | 30:0:560:U:O4' | 2.11 | 0.50 |
| 1:A:179:MET:HG2 | 1:A:186:TRP:CB | 2.41 | 0.50 |
| 6:F:41:GLU:OE2 | 13:M:2:ARG:HB2 | 2.11 | 0.50 |
| 30:0:1909:A:H2' | 30:0:1910:A:C8 | 2.47 | 0.50 |
| 30:0:530:C:H4' | 30:0:612:U:H4' | 1.92 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:C:153:VAL:O | 3:C:157:LEU:HG | 2.11 | 0.50 |
| 30:0:29:C:O2' | 30:0:30:U:H5' | 2.11 | 0.50 |
| 25:Y:96:GLU:O | 25:Y:235:GLU:HA | 2.11 | 0.50 |
| 30:0:110:C:H2' | 30:0:111:C:H6 | 1.75 | 0.50 |
| 4:D:170:TYR:O | 4:D:171:ASP:CB | 2.59 | 0.50 |
| 15:O:99:GLU:HG3 | 41:O:6044:HOH:O | 2.10 | 0.50 |
| 20:T:32:ARG:NH1 | 20:T:38:ARG:NH1 | 2.59 | 0.50 |
| 22:V:5:VAL:HG23 | 41:V:2271:HOH:O | 2.11 | 0.50 |
| 2:B:1:PRO:HG3 | 30:0:2591:C:OP1 | 2.11 | 0.50 |
| 30:0:1414:A:H2' | 30:0:1415:G:O4' | 2.11 | 0.50 |
| 30:0:1819:G:H2' | 30:0:1820:G:C5' | 2.42 | 0.50 |
| 4:D:63:ILE:HG13 | 4:D:64:ARG:N | 2.25 | 0.50 |
| 8:H:96:GLN:NE2 | 8:H:129:ARG:NH2 | 2.59 | 0.50 |
| 18:R:39:THR:HG22 | 18:R:42:GLU:H | 1.75 | 0.50 |
| 5:E:143:GLN:HE21 | 30:0:2780:C:H1' | 1.76 | 0.50 |
| 18:R:136:TRP:CE2 | 30:0:2053:G:H4' | 2.47 | 0.50 |
| 23:W:29:VAL:O | 23:W:30:ASN:HB2 | 2.10 | 0.50 |
| 10:J:47:THR:HG21 | 30:0:1244:U:H2' | 1.94 | 0.50 |
| 2:B:42:ALA:HB1 | 2:B:308:LEU:HD11 | 1.93 | 0.50 |
| 30:0:1941:A:H4' | 41:0:5079:HOH:O | 2.11 | 0.50 |
| 30:0:2115:U:H2' | 30:0:2116:U:C6 | 2.46 | 0.50 |
| 2:B:217:ARG:CG | 2:B:257:THR:HG22 | 2.35 | 0.50 |
| 30:0:1667:A:C8 | 30:0:1667:A:H5' | 2.36 | 0.50 |
| 1:A:187:PRO:HB2 | 30:0:1845:A:O3' | 2.10 | 0.50 |
| 10:J:107:ASN:HD21 | 10:J:109:TYR:HB2 | 1.77 | 0.50 |
| 1:A:36:ASP:C | 1:A:38:ILE:H | 2.13 | 0.50 |
| 30:0:2114:C:O2' | 30:0:2115:U:H5' | 2.10 | 0.50 |
| 16:P:40:VAL:O | 16:P:44:VAL:HG23 | 2.12 | 0.50 |
| 14:N:141:ARG:HH12 | 31:9:35:C:H2' | 1.77 | 0.50 |
| 5:E:80:TRP:O | 5:E:134:SER:HA | 2.12 | 0.50 |
| 30:0:1183:C:H41 | 30:0:1192:A:P | 2.35 | 0.50 |
| 6:F:50:VAL:CG1 | 6:F:60:VAL:HG11 | 2.40 | 0.50 |
| 3:C:72:LYS:CG | 3:C:77:ALA:HA | 2.42 | 0.50 |
| 25:Y:112:GLU:OE2 | 25:Y:115:ARG:NH1 | 2.43 | 0.50 |
| 2:B:314:ALA:CB | 2:B:317:PRO:HG3 | 2.41 | 0.50 |
| 31:9:39:U:H1' | 31:9:44:A:H61 | 1.77 | 0.50 |
| 30:0:945:U:H2' | 30:0:946:C:C6 | 2.47 | 0.50 |
| 2:B:215:VAL:HA | 2:B:220:VAL:HG22 | 1.93 | 0.50 |
| 17:Q:11:ARG:NH1 | 30:0:2363:G:O3' | 2.45 | 0.50 |
| 30:0:2326:C:H4' | 30:0:2412:G:H4' | 1.94 | 0.50 |
| 3:C:79:ARG:O | 3:C:87:ARG:HG2 | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 25:Y:134:HIS:HE1 | 30:0:538:C:OP2 | 1.94 | 0.50 |
| 17:Q:15:LYS:HD3 | 30:0:2364:A:H5'' | 1.93 | 0.50 |
| 26:Z:37:ARG:HD3 | 41:0:5547:HOH:O | 2.12 | 0.50 |
| 4:D:60:GLU:O | 4:D:60:GLU:HG3 | 2.12 | 0.49 |
| 30:0:285:A:H2' | 30:0:286:U:O4' | 2.11 | 0.49 |
| 22:V:29:ASN:O | 22:V:33:VAL:HG23 | 2.12 | 0.49 |
| 30:0:589:U:H2' | 30:0:590:A:H8 | 1.76 | 0.49 |
| 3:C:173:LYS:HE3 | 30:0:1311:G:O6 | 2.11 | 0.49 |
| 30:0:1783:A:O2' | 30:0:1784:U:H5' | 2.12 | 0.49 |
| 30:0:396:U:O2' | 30:0:418:C:H4' | 2.11 | 0.49 |
| 3:C:132:ASP:O | 3:C:133:ARG:HB2 | 2.11 | 0.49 |
| 17:Q:67:GLN:NE2 | 30:0:2403:C:O2 | 2.45 | 0.49 |
| 30:0:1925:G:O2' | 30:0:1926:G:H5' | 2.12 | 0.49 |
| 9:I:102:GLN:HA | 9:I:105:GLU:OE2 | 2.12 | 0.49 |
| 1:A:105:VAL:HG12 | 1:A:106:CYS:N | 2.28 | 0.49 |
| 3:C:1:MET:HG2 | 3:C:2:GLN:NE2 | 2.27 | 0.49 |
| 30:0:2505:G:C2' | 30:0:2506:A:H5' | 2.42 | 0.49 |
| 30:0:110:C:H2' | 30:0:111:C:C6 | 2.47 | 0.49 |
| 30:0:1187:U:O2' | 30:0:1189:A:H2 | 1.95 | 0.49 |
| 4:D:138:GLY:HA2 | 31:9:29:C:O3' | 2.12 | 0.49 |
| 30:0:336:G:H5'' | 41:0:4598:HOH:O | 2.11 | 0.49 |
| 4:D:76:ARG:NE | 31:9:44:A:O4' | 2.45 | 0.49 |
| 25:Y:126:PRO:HG2 | 25:Y:128:PHE:CZ | 2.48 | 0.49 |
| 30:0:1741:U:O2' | 30:0:2723:G:H4' | 2.12 | 0.49 |
| 30:0:1200:A:H3' | 41:0:6584:HOH:O | 2.10 | 0.49 |
| 30:0:812:A:H2' | 30:0:813:C:C6 | 2.47 | 0.49 |
| 2:B:265:LEU:HD21 | 2:B:316:ARG:HD3 | 1.93 | 0.49 |
| 24:X:43:VAL:HG22 | 24:X:76:ARG:NH1 | 2.27 | 0.49 |
| 14:N:29:SER:HB3 | 30:0:2415:A:O2' | 2.12 | 0.49 |
| 19:S:4:VAL:HG11 | 19:S:37:VAL:HA | 1.94 | 0.49 |
| 12:L:50:GLY:C | 30:0:2453:G:H4' | 2.32 | 0.49 |
| 12:L:56:LYS:HE3 | 30:0:2443:C:H1' | 1.93 | 0.49 |
| 11:K:82:ARG:NH2 | 11:K:115:ARG:HG2 | 2.27 | 0.49 |
| 30:0:2326:C:H4' | 30:0:2412:G:C4' | 2.42 | 0.49 |
| 1:A:109:GLU:HG2 | 1:A:116:GLY:H | 1.76 | 0.49 |
| 1:A:140:LEU:HB3 | 1:A:141:PRO:HD2 | 1.94 | 0.49 |
| 28:2:43:ARG:HH22 | 30:0:1684:A:H1' | 1.77 | 0.49 |
| 30:0:333:G:O2' | 30:0:334:G:H5' | 2.12 | 0.49 |
| 12:L:66:VAL:HG23 | 12:L:67:ARG:N | 2.27 | 0.49 |
| 8:H:61:ARG:HG3 | 41:H:9007:HOH:O | 2.13 | 0.49 |
| 13:M:164:THR:CG2 | 13:M:166:ALA:H | 2.19 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:F:58:GLU:HA | 6:F:61:MET:CE | 2.42 | 0.49 |
| 7:G:63:ARG:O | 7:G:67:LEU:HG | 2.13 | 0.49 |
| 10:J:42:GLU:O | 10:J:131:THR:HG23 | 2.12 | 0.49 |
| 6:F:107:ASP:O | 6:F:111:ILE:HG13 | 2.12 | 0.49 |
| 1:A:65:ARG:C | 1:A:66:ARG:HG3 | 2.32 | 0.49 |
| 19:S:57:THR:HG22 | 19:S:59:ASP:N | 2.26 | 0.49 |
| 12:L:136:ALA:HB3 | 41:L:8879:HOH:O | 2.12 | 0.49 |
| 3:C:43:LYS:HG2 | 30:0:449:A:C8 | 2.48 | 0.49 |
| 6:F:101:ALA:HA | 41:F:5413:HOH:O | 2.11 | 0.49 |
| 8:H:57:THR:O | 8:H:58:VAL:HG13 | 2.13 | 0.49 |
| 16:P:103:THR:O | 16:P:107:GLU:HG3 | 2.13 | 0.49 |
| 10:J:69:TYR:CE1 | 30:0:2081:A:H4' | 2.47 | 0.49 |
| 41:S:2012:HOH:O | 30:0:1507:C:H4' | 2.12 | 0.49 |
| 5:E:1:PRO:HG2 | 5:E:59:MET:SD | 2.52 | 0.49 |
| 30:0:1545:C:H2' | 30:0:1546:G:O4' | 2.12 | 0.49 |
| 30:0:1736:A:H1' | 41:0:9369:HOH:O | 2.10 | 0.49 |
| 10:J:45:VAL:HG23 | 10:J:130:VAL:O | 2.13 | 0.49 |
| 3:C:77:ALA:O | 3:C:78:ARG:CA | 2.60 | 0.49 |
| 15:O:14:LEU:HG | 15:O:102:ILE:HD11 | 1.95 | 0.49 |
| 30:0:2832:C:H5 | 41:0:9015:HOH:O | 1.96 | 0.49 |
| 13:M:84:LYS:NZ | 30:0:391:U:OP2 | 2.46 | 0.49 |
| 30:0:407:A:H5' | 41:0:6851:HOH:O | 2.12 | 0.49 |
| 2:B:14:GLY:HA2 | 2:B:15:PRO:C | 2.32 | 0.49 |
| 17:Q:64:GLU:HG3 | 17:Q:74:ASP:OD2 | 2.13 | 0.49 |
| 3:C:156:LEU:O | 3:C:160:LEU:HG | 2.10 | 0.49 |
| 20:T:43:ASN:C | 20:T:45:GLY:H | 2.16 | 0.49 |
| 30:0:2758:G:H2' | 30:0:2759:C:C6 | 2.48 | 0.49 |
| 20:T:64:ASN:HB3 | 20:T:73:HIS:HB2 | 1.95 | 0.49 |
| 10:J:47:THR:HG22 | 10:J:48:GLY:N | 2.28 | 0.49 |
| 3:C:194:PHE:HA | 3:C:234:VAL:HG13 | 1.94 | 0.49 |
| 22:V:56:ILE:HG22 | 22:V:60:GLN:NE2 | 2.24 | 0.49 |
| 12:L:92:ASP:HA | 12:L:121:ILE:HB | 1.95 | 0.49 |
| 23:W:119:HIS:HD2 | 23:W:120:PRO:O | 1.96 | 0.49 |
| 16:P:16:VAL:HG12 | 16:P:17:GLY:N | 2.28 | 0.49 |
| 10:J:107:ASN:HD22 | 10:J:107:ASN:C | 2.16 | 0.49 |
| 31:9:73:A:N6 | 31:9:108:C:H42 | 2.09 | 0.49 |
| 1:A:66:ARG:NH1 | 1:A:66:ARG:CB | 2.76 | 0.49 |
| 14:N:11:ARG:HG3 | 14:N:14:ARG:HH12 | 1.77 | 0.49 |
| 15:O:44:ASN:OD1 | 15:O:67:SER:HB2 | 2.12 | 0.49 |
| 9:I:134:ILE:HG22 | 9:I:135:GLU:N | 2.27 | 0.49 |
| 2:B:243:ASN:HA | 2:B:244:PRO:C | 2.32 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 9:I:96:SER:OG | 9:I:99:GLN:HG3 | 2.12 | 0.49 |
| 30:0:932:U:H2' | 30:0:933:C:C6 | 2.48 | 0.49 |
| 2:B:102:THR:HG23 | 2:B:182:VAL:HG12 | 1.95 | 0.49 |
| 1:A:51:ARG:HB2 | 41:A:9081:HOH:O | 2.11 | 0.49 |
| 5:E:36:PRO:HD3 | 10:J:127:ILE:CD1 | 2.42 | 0.49 |
| 4:D:23:VAL:HG21 | 4:D:45:THR:CG2 | 2.43 | 0.49 |
| 14:N:11:ARG:HA | 14:N:14:ARG:CZ | 2.43 | 0.49 |
| 14:N:82:TYR:HE1 | 14:N:120:GLU:HG2 | 1.78 | 0.49 |
| 14:N:183:ASP:O | 14:N:184:ILE:O | 2.30 | 0.49 |
| 30:0:396:U:HO2' | 30:0:418:C:H4' | 1.78 | 0.49 |
| 30:0:697:G:H4' | 30:0:730:G:O3' | 2.13 | 0.49 |
| 31:9:96:C:H2' | 31:9:97:U:C6 | 2.48 | 0.49 |
| 30:0:1166:A:H1' | 30:0:1192:A:H2 | 1.78 | 0.49 |
| 9:I:70:THR:OG1 | 9:I:107:LYS:HE2 | 2.13 | 0.49 |
| 10:J:19:MET:HE1 | 10:J:132:LEU:CD2 | 2.43 | 0.49 |
| 6:F:48:VAL:CG2 | 6:F:74:PHE:HB3 | 2.43 | 0.49 |
| 30:0:1461:U:H2' | 30:0:1462:C:H6 | 1.78 | 0.49 |
| 4:D:156:ARG:HG3 | 4:D:156:ARG:HH11 | 1.78 | 0.49 |
| 1:A:232:ARG:NH2 | 1:A:236:GLY:O | 2.45 | 0.49 |
| 30:0:1304:U:H2' | 30:0:1305:C:C6 | 2.48 | 0.49 |
| 30:0:221:G:H2' | 30:0:222:A:C8 | 2.48 | 0.49 |
| 10:J:88:PRO:HD3 | 30:0:1104:C:H4' | 1.94 | 0.49 |
| 19:S:77:VAL:C | 19:S:78:ALA:CA | 2.81 | 0.49 |
| 4:D:54:ALA:HB2 | 4:D:69:ILE:CD1 | 2.40 | 0.49 |
| 30:0:2866:U:H4' | 30:0:2867:G:H5' | 1.94 | 0.49 |
| 30:0:951:A:H2' | 30:0:952:G:H5' | 1.94 | 0.49 |
| 24:X:30:MET:HG2 | 30:0:1384:C:H5' | 1.95 | 0.49 |
| 6:F:99:THR:HG23 | 6:F:99:THR:O | 2.13 | 0.49 |
| 23:W:11:VAL:O | 23:W:12:ASN:HB2 | 2.13 | 0.49 |
| 30:0:1506:U:H6 | 30:0:1506:U:H5' | 1.78 | 0.49 |
| 10:J:92:GLN:HG2 | 10:J:96:GLU:OE2 | 2.13 | 0.49 |
| 30:0:1803:C:H2' | 30:0:1804:A:C8 | 2.48 | 0.49 |
| 25:Y:208:LYS:HB3 | 30:0:1312:G:O2' | 2.13 | 0.49 |
| 5:E:101:GLU:HB2 | 5:E:116:THR:O | 2.12 | 0.49 |
| 30:0:1730:G:C5' | 30:0:1731:C:H6 | 2.25 | 0.49 |
| 18:R:92:LEU:HD23 | 18:R:145:LEU:HD21 | 1.94 | 0.49 |
| 15:O:47:ARG:HG3 | 15:O:47:ARG:NH1 | 2.28 | 0.49 |
| 26:Z:34:SER:HB2 | 41:Z:8712:HOH:O | 2.13 | 0.49 |
| 30:0:1406:A:H4' | 30:0:1407:A:C5' | 2.43 | 0.49 |
| 30:0:284:C:H4' | 30:0:285:A:H8 | 1.78 | 0.49 |
| 28:2:8:LYS:NZ | 30:0:1677:U:OP2 | 2.46 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 30:0:1759:A:N3 | 30:0:1818:C:H2' | 2.28 | 0.49 |
| 4:D:40:ILE:HG13 | 4:D:41:LEU:N | 2.27 | 0.48 |
| 30:0:1666:C:C2' | 30:0:1667:A:C5' | 2.90 | 0.48 |
| 13:M:58:GLN:NE2 | 30:0:259:G:H21 | 2.11 | 0.48 |
| 4:D:60:GLU:O | 4:D:61:PHE:C | 2.51 | 0.48 |
| 4:D:76:ARG:NH1 | 31:9:42:C:O2 | 2.45 | 0.48 |
| 2:B:258:GLY:H | 2:B:260:HIS:CE1 | 2.31 | 0.48 |
| 25:Y:178:HIS:CG | 25:Y:179:PRO:HD2 | 2.48 | 0.48 |
| 16:P:82:GLY:O | 30:0:1761:U:H4' | 2.13 | 0.48 |
| 9:I:82:THR:CG2 | 30:0:1168:C:H5'' | 2.38 | 0.48 |
| 31:9:28:U:H2' | 31:9:29:C:C6 | 2.48 | 0.48 |
| 27:1:28:HIS:CE1 | 27:1:31:LYS:HE2 | 2.49 | 0.48 |
| 30:0:952:G:N3 | 30:0:2302:A:H2' | 2.28 | 0.48 |
| 1:A:82:VAL:HG22 | 1:A:93:THR:HB | 1.95 | 0.48 |
| 1:A:109:GLU:HG2 | 1:A:116:GLY:N | 2.28 | 0.48 |
| 25:Y:170:SER:OG | 25:Y:175:ARG:HG3 | 2.13 | 0.48 |
| 16:P:81:LYS:HG2 | 41:0:3445:HOH:O | 2.12 | 0.48 |
| 20:T:71:VAL:HG12 | 20:T:72:ILE:H | 1.78 | 0.48 |
| 21:U:52:THR:HG22 | 21:U:54:THR:HB | 1.95 | 0.48 |
| 2:B:321:PRO:HA | 41:B:9143:HOH:O | 2.12 | 0.48 |
| 22:V:64:GLY:O | 22:V:65:ASP:CB | 2.60 | 0.48 |
| 8:H:77:ILE:C | 8:H:78:LYS:CA | 2.81 | 0.48 |
| 30:0:2063:U:O4 | 30:0:2083:A:H2 | 1.95 | 0.48 |
| 23:W:108:ARG:HH21 | 23:W:114:PRO:HG2 | 1.78 | 0.48 |
| 30:0:553:G:H2' | 30:0:554:G:H5' | 1.95 | 0.48 |
| 14:N:143:ARG:HH21 | 14:N:169:PRO:HB2 | 1.78 | 0.48 |
| 14:N:78:MET:HB2 | 14:N:146:HIS:HE1 | 1.79 | 0.48 |
| 12:L:80:ASP:HB3 | 12:L:90:ARG:HB3 | 1.96 | 0.48 |
| 19:S:57:THR:HG22 | 19:S:59:ASP:H | 1.78 | 0.48 |
| 30:0:1185:U:H2' | 30:0:1186:C:C6 | 2.49 | 0.48 |
| 30:0:2443:C:H3' | 41:0:4356:HOH:O | 2.13 | 0.48 |
| 30:0:1819:G:H2' | 30:0:1820:G:H4' | 1.93 | 0.48 |
| 17:Q:95:GLU:HA | 30:0:949:U:H4' | 1.95 | 0.48 |
| 30:0:2619:UR3:H2' | 30:0:2620:U:C6 | 2.49 | 0.48 |
| 5:E:2:ARG:HH21 | 5:E:48:VAL:HG21 | 1.77 | 0.48 |
| 18:R:125:ARG:HG2 | 41:R:8947:HOH:O | 2.14 | 0.48 |
| 1:A:95:PRO:HA | 1:A:153:ARG:HA | 1.96 | 0.48 |
| 8:H:24:THR:O | 8:H:123:ILE:HD12 | 2.14 | 0.48 |
| 19:S:57:THR:CG2 | 19:S:58:MET:N | 2.76 | 0.48 |
| 30:0:1632:A:C2' | 30:0:1633:C:H5' | 2.43 | 0.48 |
| 13:M:71:SER:HB2 | 13:M:92:THR:HG22 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 30:0:2372:A:H2' | 30:0:2373:U:H6 | 1.78 | 0.48 |
| 30:0:625:U:H5' | 41:0:4074:HOH:O | 2.12 | 0.48 |
| 13:M:125:ARG:HD3 | 41:0:5827:HOH:O | 2.12 | 0.48 |
| 29:3:42:ARG:HG3 | 29:3:42:ARG:HH11 | 1.79 | 0.48 |
| 24:X:28:LYS:HD2 | 24:X:31:ILE:HD12 | 1.94 | 0.48 |
| 17:Q:45:PRO:O | 30:0:2365:G:H4' | 2.14 | 0.48 |
| 8:H:14:LYS:HE2 | 41:0:4714:HOH:O | 2.14 | 0.48 |
| 1:A:128:LEU:HG | 41:A:9050:HOH:O | 2.13 | 0.48 |
| 16:P:143:ALA:HA | 41:P:194:HOH:O | 2.12 | 0.48 |
| 30:0:1098:A:H2' | 30:0:1099:G:O4' | 2.13 | 0.48 |
| 11:K:41:LYS:HE3 | 41:0:6399:HOH:O | 2.13 | 0.48 |
| 2:B:280:VAL:HG13 | 2:B:333:GLU:O | 2.13 | 0.48 |
| 13:M:61:ILE:N | 13:M:61:ILE:HD12 | 2.29 | 0.48 |
| 30:0:1451:C:H5' | 30:0:1505:U:H5 | 1.73 | 0.48 |
| 4:D:167:GLU:OE2 | 4:D:173:GLU:HB3 | 2.12 | 0.48 |
| 3:C:77:ALA:O | 3:C:78:ARG:HG3 | 2.13 | 0.48 |
| 41:C:8558:HOH:O | 15:O:3:THR:HG21 | 2.12 | 0.48 |
| 1:A:66:ARG:NH1 | 1:A:66:ARG:HB2 | 2.27 | 0.48 |
| 30:0:2613:G:O2' | 30:0:2614:C:H5' | 2.13 | 0.48 |
| 26:Z:77:GLY:O | 26:Z:78:ILE:CA | 2.62 | 0.48 |
| 27:1:45:ARG:NH2 | 41:1:2086:HOH:O | 2.41 | 0.48 |
| 1:A:75:GLY:HA2 | 26:Z:88:PHE:HA | 1.95 | 0.48 |
| 30:0:1946:C:H2' | 30:0:1971:G:C8 | 2.49 | 0.48 |
| 2:B:125:GLU:O | 2:B:129:ARG:HG3 | 2.13 | 0.48 |
| 15:O:62:GLY:O | 15:O:79:VAL:HG23 | 2.14 | 0.48 |
| 14:N:4:PRO:HG3 | 31:9:69:U:OP1 | 2.14 | 0.48 |
| 23:W:26:ILE:O | 23:W:26:ILE:HG12 | 2.13 | 0.48 |
| 30:0:1175:G:H1' | 30:0:1193:A:C2' | 2.42 | 0.48 |
| 30:0:1198:U:H2' | 30:0:1200:A:OP2 | 2.13 | 0.48 |
| 8:H:12:ILE:HD12 | 8:H:57:THR:CG2 | 2.44 | 0.48 |
| 28:2:40:ARG:HA | 28:2:45:ASN:ND2 | 2.29 | 0.48 |
| 11:K:55:VAL:HG12 | 11:K:56:SER:N | 2.28 | 0.48 |
| 30:0:1058:A:H2' | 30:0:1060:C:C5' | 2.41 | 0.48 |
| 25:Y:112:GLU:O | 25:Y:116:LEU:HG | 2.14 | 0.48 |
| 12:L:30:ARG:HD3 | 30:0:164:G:H4' | 1.94 | 0.48 |
| 1:A:47:HIS:CD2 | 30:0:1654:U:H2' | 2.49 | 0.48 |
| 5:E:143:GLN:NE2 | 30:0:2779:G:H21 | 2.12 | 0.48 |
| 3:C:150:THR:HA | 3:C:203:ALA:O | 2.14 | 0.48 |
| 23:W:139:GLY:O | 23:W:141:HIS:HD2 | 1.96 | 0.48 |
| 5:E:14:GLU:O | 5:E:15:GLN:HB2 | 2.14 | 0.48 |
| 30:0:2748:G:H4' | 30:0:2749:U:C5' | 2.43 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 10:J:39:VAL:CG1 | 10:J:40:ASN:N | 2.76 | 0.48 |
| 12:L:143:THR:CG2 | 12:L:144:ASP:N | 2.76 | 0.48 |
| 7:G:12:ILE:HA | 41:0:6294:HOH:O | 2.13 | 0.48 |
| 2:B:72:THR:HB | 41:B:9083:HOH:O | 2.12 | 0.48 |
| 2:B:77:PRO:HA | 2:B:293:PRO:HB2 | 1.95 | 0.48 |
| 2:B:13:PHE:HB2 | 2:B:16:ARG:NH1 | 2.28 | 0.48 |
| 30:0:2032:U:H2' | 30:0:2033:G:C5' | 2.43 | 0.48 |
| 16:P:10:ALA:HA | 16:P:13:VAL:HG12 | 1.96 | 0.48 |
| 17:Q:16:ASN:HD21 | 17:Q:45:PRO:HD2 | 1.79 | 0.48 |
| 13:M:159:VAL:HG12 | 38:M:8818:CL:CL | 2.51 | 0.48 |
| 6:F:19:ALA:O | 6:F:22:VAL:HG22 | 2.13 | 0.48 |
| 10:J:26:VAL:HG13 | 10:J:36:VAL:HG11 | 1.95 | 0.48 |
| 9:I:87:PRO:HD3 | 41:0:4123:HOH:O | 2.14 | 0.48 |
| 30:0:2748:G:H5' | 41:0:9326:HOH:O | 2.13 | 0.48 |
| 6:F:32:GLY:N | 41:F:3111:HOH:O | 2.47 | 0.48 |
| 3:C:58:ALA:HA | 3:C:73:GLN:NE2 | 2.28 | 0.48 |
| 14:N:24:LEU:HD13 | 17:Q:26:PRO:HB3 | 1.96 | 0.48 |
| 30:0:603:A:H4' | 30:0:604:G:O5' | 2.13 | 0.48 |
| 22:V:26:GLU:OE2 | 22:V:45:ARG:HD3 | 2.13 | 0.48 |
| 30:0:200:C:H2' | 41:0:4329:HOH:O | 2.14 | 0.48 |
| 2:B:42:ALA:HB2 | 2:B:162:MET:CE | 2.43 | 0.47 |
| 30:0:1181:A:H2' | 30:0:1182:C:H5' | 1.96 | 0.47 |
| 1:A:186:TRP:CD1 | 1:A:187:PRO:HA | 2.49 | 0.47 |
| 22:V:39:ALA:O | 22:V:41:GLU:N | 2.42 | 0.47 |
| 2:B:104:GLU:HB2 | 41:B:9117:HOH:O | 2.14 | 0.47 |
| 1:A:204:GLY:N | 30:0:2634:G:OP2 | 2.47 | 0.47 |
| 30:0:757:C:H2' | 30:0:758:A:C8 | 2.48 | 0.47 |
| 16:P:69:ARG:HA | 16:P:73:HIS:O | 2.14 | 0.47 |
| 30:0:1171:A:N6 | 30:0:1172:G:C2 | 2.82 | 0.47 |
| 16:P:7:LYS:HD3 | 16:P:23:PHE:CZ | 2.49 | 0.47 |
| 27:1:56:GLU:OXT | 27:1:56:GLU:HG2 | 2.14 | 0.47 |
| 30:0:343:C:H2' | 30:0:344:C:H6 | 1.79 | 0.47 |
| 30:0:2499:U:H2' | 30:0:2500:C:H6 | 1.78 | 0.47 |
| 5:E:69:ILE:HA | 5:E:72:MET:CE | 2.44 | 0.47 |
| 30:0:1060:C:H6 | 30:0:1060:C:H5' | 1.79 | 0.47 |
| 4:D:138:GLY:N | 41:D:7597:HOH:O | 2.46 | 0.47 |
| 2:B:17:LYS:O | 2:B:260:HIS:HD2 | 1.96 | 0.47 |
| 3:C:51:TYR:CE2 | 27:1:53:LYS:HB3 | 2.49 | 0.47 |
| 30:0:690:G:H4' | 30:0:741:C:O2 | 2.14 | 0.47 |
| 13:M:15:PRO:HA | 13:M:20:LEU:HD23 | 1.94 | 0.47 |
| 29:3:56:PRO:HA | 41:0:6865:HOH:O | 2.12 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:58:PRO:HA | 2:B:63:GLU:CD | 2.34 | 0.47 |
| 28:2:40:ARG:HG3 | 28:2:45:ASN:CB | 2.44 | 0.47 |
| 1:A:94:LEU:HG | 1:A:99:ILE:CD1 | 2.42 | 0.47 |
| 11:K:125:ALA:C | 11:K:127:ALA:H | 2.17 | 0.47 |
| 4:D:141:VAL:HG21 | 31:9:57:A:C8 | 2.48 | 0.47 |
| 10:J:39:VAL:HG11 | 10:J:107:ASN:HB2 | 1.96 | 0.47 |
| 30:0:1940:C:H4' | 41:0:9143:HOH:O | 2.13 | 0.47 |
| 30:0:1422:U:H2' | 30:0:1423:C:C6 | 2.49 | 0.47 |
| 25:Y:103:THR:HG22 | 25:Y:104:GLU:OE2 | 2.14 | 0.47 |
| 30:0:451:C:O2' | 30:0:452:G:H5' | 2.14 | 0.47 |
| 30:0:2587:OMU:H2' | 30:0:2589:U:H5'' | 1.95 | 0.47 |
| 32:5:74:C:C2' | 32:5:75:C:H5' | 2.41 | 0.47 |
| 14:N:61:ALA:CB | 14:N:88:ALA:HB2 | 2.44 | 0.47 |
| 30:0:947:U:O2' | 30:0:948:G:H5' | 2.15 | 0.47 |
| 14:N:73:ALA:HB1 | 14:N:74:PRO:CD | 2.44 | 0.47 |
| 8:H:91:ARG:NH1 | 8:H:138:THR:OG1 | 2.47 | 0.47 |
| 2:B:132:HIS:NE2 | 2:B:171:VAL:HG23 | 2.29 | 0.47 |
| 3:C:27:ARG:HG2 | 3:C:27:ARG:NH1 | 2.29 | 0.47 |
| 30:0:292:G:H1' | 30:0:360:A:H61 | 1.80 | 0.47 |
| 30:0:1066:U:H2' | 30:0:1067:A:C8 | 2.49 | 0.47 |
| 21:U:4:ARG:NH1 | 21:U:4:ARG:HG2 | 2.30 | 0.47 |
| 30:0:2323:G:H5'' | 41:0:5629:HOH:O | 2.14 | 0.47 |
| 30:0:1416:G:C2' | 30:0:1417:G:H5' | 2.45 | 0.47 |
| 30:0:2836:G:O2' | 30:0:2838:A:N7 | 2.43 | 0.47 |
| 24:X:87:ALA:O | 24:X:88:GLU:CB | 2.63 | 0.47 |
| 2:B:282:GLY:O | 30:0:2898:G:H1' | 2.15 | 0.47 |
| 30:0:2670:G:O2' | 30:0:2671:U:H5' | 2.13 | 0.47 |
| 23:W:31:HIS:HB3 | 23:W:115:THR:HG21 | 1.95 | 0.47 |
| 30:0:1203:G:O2' | 30:0:1204:C:H5' | 2.15 | 0.47 |
| 2:B:51:VAL:HG13 | 2:B:53:LEU:CD1 | 2.45 | 0.47 |
| 23:W:122:ARG:NH2 | 41:0:6126:HOH:O | 2.47 | 0.47 |
| 31:9:24:U:H3' | 31:9:25:G:C5' | 2.43 | 0.47 |
| 12:L:35:ARG:HB2 | 12:L:35:ARG:NH1 | 2.30 | 0.47 |
| 12:L:150:GLN:HB3 | 41:L:8876:HOH:O | 2.15 | 0.47 |
| 30:0:1447:U:H3' | 30:0:1506:U:O2 | 2.15 | 0.47 |
| 30:0:666:A:H2' | 30:0:667:C:O4' | 2.15 | 0.47 |
| 1:A:76:VAL:HG12 | 1:A:77:GLY:N | 2.29 | 0.47 |
| 30:0:90:A:H2' | 30:0:91:G:O4' | 2.13 | 0.47 |
| 3:C:139:VAL:HG13 | 41:C:8649:HOH:O | 2.14 | 0.47 |
| 23:W:60:GLU:O | 23:W:63:GLU:HB2 | 2.14 | 0.47 |
| 30:0:2554:U:H1' | 41:0:6960:HOH:O | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 30:0:1902:G:H2' | 30:0:1903:U:O4' | 2.15 | 0.47 |
| 30:0:1641:A:H2' | 30:0:1642:A:H5' | 1.95 | 0.47 |
| 2:B:36:PRO:HA | 2:B:168:GLY:CA | 2.30 | 0.47 |
| 2:B:36:PRO:HB3 | 2:B:174:ARG:CB | 2.44 | 0.47 |
| 23:W:21:LEU:CD2 | 23:W:48:VAL:HG11 | 2.33 | 0.47 |
| 22:V:11:MET:HB3 | 22:V:15:GLU:HB2 | 1.96 | 0.47 |
| 2:B:42:ALA:HB2 | 2:B:162:MET:HE2 | 1.95 | 0.47 |
| 4:D:41:LEU:HA | 4:D:44:ILE:HG22 | 1.97 | 0.47 |
| 13:M:60:VAL:C | 13:M:61:ILE:HD12 | 2.35 | 0.47 |
| 30:0:2506:A:O2' | 30:0:2507:G:O5' | 2.33 | 0.47 |
| 30:0:120:A:H2' | 30:0:120:A:N3 | 2.30 | 0.47 |
| 5:E:116:THR:CG2 | 5:E:151:LEU:HD22 | 2.39 | 0.47 |
| 3:C:115:LEU:O | 3:C:118:THR:HB | 2.14 | 0.47 |
| 23:W:4:LEU:HD22 | 23:W:52:VAL:HB | 1.95 | 0.47 |
| 1:A:32:VAL:HG12 | 1:A:34:ASP:H | 1.80 | 0.47 |
| 30:0:1174:A:C5 | 30:0:1201:C:H4' | 2.50 | 0.47 |
| 10:J:45:VAL:HG21 | 10:J:129:PHE:CD1 | 2.50 | 0.47 |
| 14:N:152:GLU:C | 14:N:154:LEU:N | 2.66 | 0.47 |
| 19:S:42:GLU:HG2 | 19:S:49:VAL:HG23 | 1.96 | 0.47 |
| 30:0:2828:G:H8 | 30:0:2828:G:O5' | 1.98 | 0.47 |
| 30:0:946:C:H2' | 30:0:947:U:H6 | 1.78 | 0.47 |
| 4:D:21:VAL:HA | 4:D:131:THR:O | 2.15 | 0.47 |
| 12:L:98:GLU:O | 12:L:99:GLU:HB2 | 2.15 | 0.47 |
| 30:0:343:C:O2' | 30:0:344:C:H5' | 2.15 | 0.47 |
| 30:0:1416:G:H2' | 30:0:1417:G:H5' | 1.97 | 0.47 |
| 1:A:117:LYS:HA | 41:A:9014:HOH:O | 2.14 | 0.47 |
| 24:X:27:ASP:OD2 | 24:X:27:ASP:N | 2.48 | 0.47 |
| 30:0:1006:A:N1 | 30:0:2311:A:H1' | 2.30 | 0.47 |
| 30:0:629:A:H2' | 30:0:630:A:O4' | 2.15 | 0.47 |
| 30:0:867:A:H2 | 30:0:880:C:O2 | 1.97 | 0.47 |
| 17:Q:75:ILE:CD1 | 17:Q:84:ILE:HD11 | 2.45 | 0.47 |
| 20:T:8:ARG:NH1 | 30:0:31:C:OP2 | 2.47 | 0.47 |
| 32:5:76:A:H8 | 32:5:76:A:C5' | 2.20 | 0.47 |
| 30:0:1118:A:H8 | 30:0:1119:G:H5'' | 1.78 | 0.47 |
| 20:T:9:LYS:HD2 | 41:0:4630:HOH:O | 2.15 | 0.47 |
| 3:C:118:THR:HG22 | 3:C:137:PRO:HB3 | 1.97 | 0.47 |
| 9:I:70:THR:O | 9:I:74:ILE:HG13 | 2.15 | 0.47 |
| 5:E:7:ILE:CG1 | 5:E:11:VAL:HB | 2.45 | 0.47 |
| 25:Y:144:ARG:CZ | 41:Y:8923:HOH:O | 2.63 | 0.47 |
| 30:0:958:G:O2' | 30:0:959:C:H5' | 2.15 | 0.47 |
| 19:S:15:MET:O | 19:S:18:MET:HB3 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 30:0:2281:C:C2' | 30:0:2282:U:H5' | 2.44 | 0.47 |
| 2:B:42:ALA:CB | 2:B:162:MET:HE2 | 2.45 | 0.47 |
| 2:B:212:GLN:OE1 | 2:B:216:LYS:HD3 | 2.15 | 0.47 |
| 4:D:99:ASP:CB | 4:D:103:ASN:HB2 | 2.45 | 0.47 |
| 4:D:166:ILE:O | 4:D:169:THR:N | 2.48 | 0.47 |
| 30:0:2289:G:H21 | 30:0:2291:A:H2 | 1.61 | 0.47 |
| 14:N:155:GLU:O | 14:N:156:GLU:HG3 | 2.14 | 0.47 |
| 30:0:2756:U:N3 | 30:0:2896:A:C2 | 2.77 | 0.47 |
| 20:T:73:HIS:HD2 | 20:T:88:PRO:HG3 | 1.79 | 0.47 |
| 9:I:126:THR:HG22 | 9:I:126:THR:O | 2.15 | 0.47 |
| 30:0:861:A:H4' | 30:0:1697:G:H4' | 1.97 | 0.47 |
| 30:0:1249:U:H2' | 30:0:1250:C:C6 | 2.49 | 0.47 |
| 30:0:251:C:O2' | 30:0:252:C:H5' | 2.14 | 0.47 |
| 30:0:2072:G:N2 | 41:0:7670:HOH:O | 2.48 | 0.47 |
| 30:0:1167:G:H2' | 30:0:1168:C:O4' | 2.14 | 0.47 |
| 14:N:164:ASP:OD1 | 14:N:167:ASP:OD1 | 2.33 | 0.47 |
| 30:0:1684:A:H5' | 30:0:1692:C:OP1 | 2.15 | 0.47 |
| 30:0:1947:G:H2' | 30:0:1948:G:H8 | 1.79 | 0.47 |
| 6:F:49:PHE:HE1 | 6:F:98:VAL:HG23 | 1.79 | 0.47 |
| 30:0:1419:U:H2' | 30:0:1685:A:C2 | 2.49 | 0.47 |
| 20:T:21:LYS:HA | 20:T:24:ARG:HG3 | 1.97 | 0.47 |
| 30:0:2102:G:H2' | 41:0:9547:HOH:O | 2.14 | 0.47 |
| 30:0:2016:U:H6 | 30:0:2016:U:O5' | 1.97 | 0.47 |
| 30:0:1930:A:H2' | 30:0:1931:A:C8 | 2.50 | 0.47 |
| 2:B:24:PRO:HB2 | 2:B:310:ARG:HG3 | 1.96 | 0.46 |
| 2:B:321:PRO:HG3 | 41:B:9077:HOH:O | 2.14 | 0.46 |
| 30:0:708:A:H2' | 30:0:709:G:O4' | 2.15 | 0.46 |
| 30:0:2880:A:H2' | 30:0:2881:C:H5' | 1.97 | 0.46 |
| 30:0:1278:A:H2' | 30:0:1280:A:C8 | 2.50 | 0.46 |
| 10:J:63:ILE:HG22 | 10:J:64:GLY:N | 2.30 | 0.46 |
| 20:T:86:GLU:HB2 | 41:T:6653:HOH:O | 2.15 | 0.46 |
| 18:R:17:MET:HE2 | 41:R:8953:HOH:O | 2.15 | 0.46 |
| 30:0:420:U:H2' | 30:0:421:C:C6 | 2.50 | 0.46 |
| 30:0:1522:A:H2' | 30:0:1523:G:H5' | 1.97 | 0.46 |
| 13:M:69:LYS:HG3 | 13:M:126:GLN:CA | 2.45 | 0.46 |
| 15:O:32:ARG:HH21 | 15:O:35:LYS:NZ | 2.12 | 0.46 |
| 30:0:2618:G:N2 | 41:0:6025:HOH:O | 2.36 | 0.46 |
| 23:W:31:HIS:CE1 | 23:W:117:ARG:HG2 | 2.50 | 0.46 |
| 13:M:24:GLN:NE2 | 13:M:27:ARG:NH1 | 2.62 | 0.46 |
| 2:B:62:ARG:CA | 2:B:65:MET:HE3 | 2.43 | 0.46 |
| 30:0:2769:C:O2' | 30:0:2770:G:H5' | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 29:3:77:ALA:HB3 | 30:0:2436:U:O3' | 2.15 | 0.46 |
| 15:O:37:ARG:HD2 | 30:0:656:G:OP2 | 2.15 | 0.46 |
| 30:0:2426:G:H5'' | 30:0:2427:C:O4' | 2.15 | 0.46 |
| 30:0:1592:G:O2' | 30:0:1593:C:O4' | 2.32 | 0.46 |
| 17:Q:94:GLN:O | 17:Q:95:GLU:HB2 | 2.15 | 0.46 |
| 13:M:12:TRP:O | 13:M:15:PRO:HD3 | 2.15 | 0.46 |
| 2:B:3:PRO:HG2 | 41:0:9679:HOH:O | 2.15 | 0.46 |
| 2:B:233:ARG:NH1 | 2:B:233:ARG:HG2 | 2.29 | 0.46 |
| 29:3:36:ILE:HG23 | 29:3:37:ASP:N | 2.30 | 0.46 |
| 30:0:59:A:H5' | 41:0:5192:HOH:O | 2.14 | 0.46 |
| 20:T:30:ASP:O | 20:T:33:GLU:HB3 | 2.15 | 0.46 |
| 30:0:1787:C:H4' | 30:0:2883:A:O4' | 2.16 | 0.46 |
| 30:0:806:A:H2' | 30:0:807:A:O4' | 2.15 | 0.46 |
| 41:Y:8884:HOH:O | 30:0:1355:A:H5'' | 2.14 | 0.46 |
| 10:J:93:ARG:NH1 | 10:J:93:ARG:HB3 | 2.21 | 0.46 |
| 9:I:130:LEU:HA | 41:I:7210:HOH:O | 2.15 | 0.46 |
| 14:N:71:TRP:CE3 | 14:N:175:LEU:HD22 | 2.50 | 0.46 |
| 2:B:98:THR:HG22 | 30:0:2820:A:OP1 | 2.14 | 0.46 |
| 11:K:81:ARG:HD3 | 11:K:87:ARG:CZ | 2.46 | 0.46 |
| 5:E:93:MET:HE1 | 5:E:165:GLY:N | 2.31 | 0.46 |
| 7:G:64:ASN:N | 7:G:64:ASN:ND2 | 2.63 | 0.46 |
| 2:B:258:GLY:HA2 | 41:0:4877:HOH:O | 2.15 | 0.46 |
| 3:C:55:ARG:NH2 | 27:1:56:GLU:OE2 | 2.40 | 0.46 |
| 2:B:82:VAL:CG1 | 2:B:101:TRP:CZ3 | 2.97 | 0.46 |
| 4:D:24:HIS:HB2 | 4:D:72:LYS:HB3 | 1.96 | 0.46 |
| 30:0:12:U:H2' | 30:0:13:G:H5' | 1.95 | 0.46 |
| 18:R:82:GLU:O | 18:R:86:LYS:HG3 | 2.15 | 0.46 |
| 24:X:23:HIS:NE2 | 24:X:24:LYS:HD2 | 2.31 | 0.46 |
| 23:W:88:THR:HG23 | 23:W:110:GLN:NE2 | 2.31 | 0.46 |
| 30:0:1158:G:O2' | 30:0:1159:G:H5' | 2.15 | 0.46 |
| 17:Q:25:PRO:HA | 17:Q:26:PRO:HD3 | 1.83 | 0.46 |
| 29:3:24:LYS:HE3 | 29:3:90:PHE:HE1 | 1.81 | 0.46 |
| 30:0:1592:G:H2' | 30:0:1593:C:H6 | 1.80 | 0.46 |
| 22:V:16:ARG:NH1 | 22:V:65:ASP:O | 2.49 | 0.46 |
| 30:0:334:G:H2' | 30:0:335:U:O4' | 2.16 | 0.46 |
| 8:H:14:LYS:HB3 | 41:H:9006:HOH:O | 2.15 | 0.46 |
| 2:B:171:VAL:HG23 | 2:B:172:SER:N | 2.30 | 0.46 |
| 30:0:1931:A:H2' | 30:0:1932:G:H5' | 1.97 | 0.46 |
| 27:1:5:THR:N | 27:1:6:PRO:HD2 | 2.30 | 0.46 |
| 30:0:2274:A:O2' | 30:0:2275:G:H5' | 2.15 | 0.46 |
| 4:D:135:VAL:HG22 | 4:D:136:ARG:H | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 13:M:47:ASP:CG | 13:M:48:LYS:N | 2.69 | 0.46 |
| 25:Y:112:GLU:CD | 25:Y:115:ARG:HH12 | 2.18 | 0.46 |
| 16:P:91:LYS:HA | 41:0:3945:HOH:O | 2.15 | 0.46 |
| 29:3:70:ARG:NH1 | 29:3:70:ARG:HG2 | 2.30 | 0.46 |
| 2:B:5:ARG:HD2 | 2:B:8:LYS:NZ | 2.31 | 0.46 |
| 30:0:757:C:H4' | 41:0:5053:HOH:O | 2.15 | 0.46 |
| 30:0:407:A:H3' | 41:0:5323:HOH:O | 2.15 | 0.46 |
| 8:H:149:VAL:HG22 | 41:H:9033:HOH:O | 2.15 | 0.46 |
| 17:Q:16:ASN:HB2 | 41:0:7759:HOH:O | 2.15 | 0.46 |
| 13:M:158:ARG:HB2 | 13:M:163:LEU:HB2 | 1.96 | 0.46 |
| 1:A:167:LYS:HB2 | 26:Z:53:ILE:HD13 | 1.97 | 0.46 |
| 8:H:165:ARG:HD2 | 41:H:9038:HOH:O | 2.14 | 0.46 |
| 5:E:31:ARG:NH1 | 41:E:5919:HOH:O | 2.48 | 0.46 |
| 30:0:1603:A:H5' | 30:0:1605:G:H5' | 1.97 | 0.46 |
| 2:B:98:THR:HG21 | 2:B:127:GLN:OE1 | 2.16 | 0.46 |
| 21:U:9:CYS:O | 21:U:53:ASP:HB2 | 2.15 | 0.46 |
| 6:F:38:LYS:HE3 | 30:0:244:C:OP2 | 2.15 | 0.46 |
| 30:0:291:C:H2' | 30:0:292:G:O4' | 2.16 | 0.46 |
| 30:0:2531:U:C2' | 30:0:2532:A:H5' | 2.46 | 0.46 |
| 30:0:2265:U:H2' | 30:0:2266:A:H8 | 1.80 | 0.46 |
| 30:0:1131:G:C6 | 30:0:1230:A:C4 | 3.02 | 0.46 |
| 30:0:407:A:H2' | 30:0:408:A:C8 | 2.51 | 0.46 |
| 29:3:17:HIS:O | 29:3:18:GLN:HG3 | 2.16 | 0.46 |
| 30:0:2649:A:H5' | 30:0:2649:A:H8 | 1.81 | 0.46 |
| 30:0:1119:G:N2 | 30:0:1246:A:N1 | 2.63 | 0.46 |
| 14:N:110:THR:HB | 14:N:113:SER:HG | 1.81 | 0.46 |
| 31:9:78:G:C8 | 31:9:78:G:N3 | 2.84 | 0.46 |
| 30:0:1172:G:H1' | 41:0:5820:HOH:O | 2.14 | 0.46 |
| 20:T:12:ARG:NH2 | 30:0:31:C:OP1 | 2.49 | 0.46 |
| 3:C:193:LEU:HD22 | 3:C:222:ASP:O | 2.15 | 0.46 |
| 30:0:2105:C:H2' | 30:0:2106:C:C6 | 2.51 | 0.46 |
| 5:E:69:ILE:HA | 5:E:72:MET:HE3 | 1.96 | 0.46 |
| 4:D:22:VAL:CG2 | 4:D:74:THR:HG22 | 2.42 | 0.46 |
| 30:0:1201:C:H2' | 30:0:1202:A:H5' | 1.97 | 0.46 |
| 6:F:61:MET:HB3 | 13:M:19:GLN:OE1 | 2.15 | 0.46 |
| 30:0:2820:A:H2' | 30:0:2821:C:C6 | 2.50 | 0.46 |
| 12:L:80:ASP:CB | 12:L:90:ARG:HB3 | 2.46 | 0.46 |
| 2:B:84:LEU:O | 2:B:99:GLU:HA | 2.16 | 0.46 |
| 17:Q:7:LEU:HD12 | 30:0:2424:U:H1' | 1.97 | 0.46 |
| 6:F:38:LYS:HA | 6:F:41:GLU:OE1 | 2.15 | 0.46 |
| 30:0:2047:C:H2' | 30:0:2048:C:H6 | 1.81 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:217:ARG:HH11 | 1:A:217:ARG:HG3 | 1.79 | 0.46 |
| 1:A:131:HIS:O | 1:A:132:ASP:HB2 | 2.16 | 0.46 |
| 30:0:1393:A:H2' | 30:0:1394:C:C6 | 2.50 | 0.46 |
| 30:0:1398:G:H2' | 30:0:1399:A:C8 | 2.51 | 0.46 |
| 30:0:1021:G:O2' | 30:0:1022:A:H5' | 2.15 | 0.46 |
| 12:L:20:ASN:HA | 41:L:8872:HOH:O | 2.16 | 0.46 |
| 30:0:1985:U:C2 | 30:0:1996:U:O4' | 2.69 | 0.46 |
| 30:0:2039:A:H4' | 30:0:2760:C:O2' | 2.16 | 0.46 |
| 30:0:2588:OMG:N2 | 41:5:3737:HOH:O | 2.49 | 0.46 |
| 14:N:115:VAL:HG13 | 41:9:9109:HOH:O | 2.16 | 0.46 |
| 1:A:101:GLU:O | 1:A:103:VAL:HG23 | 2.16 | 0.46 |
| 13:M:102:GLU:CD | 13:M:164:THR:HG21 | 2.36 | 0.46 |
| 30:0:1180:U:H1' | 41:0:4123:HOH:O | 2.16 | 0.46 |
| 5:E:15:GLN:NE2 | 5:E:17:HIS:O | 2.48 | 0.46 |
| 25:Y:177:LYS:HD3 | 25:Y:181:GLY:O | 2.16 | 0.46 |
| 15:O:26:TRP:N | 41:O:3062:HOH:O | 2.49 | 0.46 |
| 30:0:694:A:H2' | 30:0:695:C:H5' | 1.97 | 0.46 |
| 6:F:20:LEU:HD13 | 6:F:98:VAL:HG22 | 1.97 | 0.46 |
| 2:B:128:ILE:O | 2:B:131:ALA:HB3 | 2.16 | 0.46 |
| 30:0:2019:A:H5' | 41:0:5396:HOH:O | 2.15 | 0.46 |
| 18:R:79:ARG:HB3 | 30:0:2050:G:OP1 | 2.15 | 0.46 |
| 12:L:89:PHE:N | 41:L:8877:HOH:O | 2.48 | 0.46 |
| 31:9:49:G:H5'' | 41:9:9090:HOH:O | 2.16 | 0.46 |
| 11:K:29:LEU:HB3 | 11:K:55:VAL:CG1 | 2.31 | 0.46 |
| 30:0:1183:C:H42 | 30:0:1184:C:H41 | 1.59 | 0.46 |
| 1:A:179:MET:HA | 1:A:179:MET:CE | 2.46 | 0.46 |
| 1:A:194:MET:SD | 30:0:875:A:C2 | 3.09 | 0.46 |
| 8:H:43:ALA:HB1 | 8:H:140:TYR:CE2 | 2.51 | 0.46 |
| 7:G:63:ARG:NH1 | 30:0:1151:G:OP1 | 2.49 | 0.46 |
| 28:2:22:PRO:HG2 | 28:2:25:VAL:HG23 | 1.98 | 0.46 |
| 19:S:33:SER:OG | 19:S:36:GLU:HG3 | 2.15 | 0.46 |
| 30:0:920:C:H5'' | 30:0:921:G:O5' | 2.16 | 0.46 |
| 2:B:305:ASP:O | 2:B:306:LYS:CB | 2.63 | 0.46 |
| 31:9:95:C:O2' | 31:9:96:C:H5' | 2.16 | 0.46 |
| 30:0:1761:U:H2' | 30:0:1762:C:C6 | 2.51 | 0.46 |
| 30:0:1971:G:N2 | 30:0:2009:G:H2' | 2.31 | 0.46 |
| 1:A:42:VAL:HG12 | 1:A:76:VAL:HA | 1.97 | 0.46 |
| 30:0:2775:A:C6 | 30:0:2799:A:C8 | 3.04 | 0.46 |
| 12:L:10:SER:O | 12:L:11:ARG:HB3 | 2.16 | 0.46 |
| 30:0:1014:A:H5'' | 31:9:101:G:O2' | 2.16 | 0.46 |
| 30:0:445:U:O2' | 30:0:446:G:H5' | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 13:M:54:TYR:CG | 13:M:55:LYS:N | 2.84 | 0.46 |
| 30:0:282:C:H1' | 30:0:368:C:H42 | 1.76 | 0.45 |
| 3:C:115:LEU:CD2 | 3:C:243:VAL:HG13 | 2.41 | 0.45 |
| 30:0:1159:G:H1 | 30:0:1208:C:N4 | 2.14 | 0.45 |
| 23:W:119:HIS:CG | 41:0:6126:HOH:O | 2.69 | 0.45 |
| 30:0:820:G:O2' | 30:0:856:G:H4' | 2.16 | 0.45 |
| 30:0:2032:U:H2' | 30:0:2033:G:H5' | 1.97 | 0.45 |
| 15:O:25:VAL:CG1 | 30:0:710:G:H5' | 2.46 | 0.45 |
| 30:0:530:C:C4' | 30:0:612:U:H4' | 2.46 | 0.45 |
| 10:J:88:PRO:O | 10:J:94:GLY:HA3 | 2.16 | 0.45 |
| 30:0:2016:U:H2' | 30:0:2017:U:O4' | 2.16 | 0.45 |
| 30:0:2649:A:H5' | 30:0:2649:A:C8 | 2.51 | 0.45 |
| 4:D:104:PHE:CZ | 4:D:132:VAL:HG21 | 2.51 | 0.45 |
| 19:S:11:THR:H | 19:S:14:ALA:HB3 | 1.81 | 0.45 |
| 30:0:226:A:H1' | 30:0:393:G:C5 | 2.51 | 0.45 |
| 2:B:245:SER:OG | 30:0:2094:G:H4' | 2.17 | 0.45 |
| 4:D:84:LEU:HA | 4:D:87:ALA:HB3 | 1.98 | 0.45 |
| 30:0:816:G:C6 | 30:0:817:G:N1 | 2.84 | 0.45 |
| 31:9:49:G:O2' | 31:9:50:G:H5' | 2.16 | 0.45 |
| 16:P:59:ARG:O | 16:P:63:ARG:HG3 | 2.16 | 0.45 |
| 30:0:1730:G:H5' | 30:0:1731:C:C6 | 2.51 | 0.45 |
| 31:9:73:A:H61 | 31:9:108:C:N4 | 2.10 | 0.45 |
| 30:0:2314:G:H2' | 30:0:2315:C:H5' | 1.98 | 0.45 |
| 17:Q:40:HIS:HE1 | 30:0:949:U:O2' | 1.98 | 0.45 |
| 17:Q:86:VAL:HG11 | 17:Q:91:LEU:HD21 | 1.97 | 0.45 |
| 30:0:1636:G:O2' | 30:0:1637:A:H5' | 2.17 | 0.45 |
| 1:A:69:LEU:HD21 | 1:A:120:ARG:HB3 | 1.99 | 0.45 |
| 31:9:39:U:H3' | 31:9:40:C:C5' | 2.47 | 0.45 |
| 12:L:30:ARG:HD2 | 41:0:2938:HOH:O | 2.15 | 0.45 |
| 3:C:54:LEU:HD23 | 3:C:79:ARG:HG3 | 1.99 | 0.45 |
| 30:0:2649:A:H2' | 41:0:6956:HOH:O | 2.15 | 0.45 |
| 14:N:109:PRO:HB3 | 30:0:2413:A:N7 | 2.31 | 0.45 |
| 12:L:22:ARG:HG2 | 41:0:3882:HOH:O | 2.16 | 0.45 |
| 3:C:214:THR:HG23 | 41:C:8637:HOH:O | 2.16 | 0.45 |
| 1:A:164:ARG:NE | 41:A:9064:HOH:O | 2.49 | 0.45 |
| 3:C:162:VAL:CG2 | 3:C:232:LEU:HD21 | 2.47 | 0.45 |
| 3:C:142:ASP:CG | 3:C:238:SER:HG | 2.20 | 0.45 |
| 11:K:80:ILE:HG23 | 41:K:7064:HOH:O | 2.16 | 0.45 |
| 30:0:303:C:H2' | 30:0:304:G:O4' | 2.16 | 0.45 |
| 30:0:612:U:H2' | 30:0:613:C:H6 | 1.82 | 0.45 |
| 31:9:64:C:O2' | 31:9:65:A:H5' | 2.15 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:X:87:ALA:O | 24:X:88:GLU:HB3 | 2.16 | 0.45 |
| 2:B:41:PHE:CD1 | 2:B:79:MET:HE2 | 2.51 | 0.45 |
| 13:M:79:ALA:HB1 | 30:0:770:C:OP1 | 2.16 | 0.45 |
| 23:W:81:ASP:OD1 | 23:W:92:ASP:HB2 | 2.16 | 0.45 |
| 30:0:824:G:N2 | 41:0:6927:HOH:O | 2.48 | 0.45 |
| 30:0:2533:C:C6 | 30:0:2533:C:H5' | 2.43 | 0.45 |
| 2:B:62:ARG:HG2 | 2:B:62:ARG:HH11 | 1.82 | 0.45 |
| 23:W:38:THR:CG2 | 23:W:39:ASP:N | 2.78 | 0.45 |
| 23:W:42:ARG:HA | 23:W:45:VAL:CG2 | 2.47 | 0.45 |
| 3:C:27:ARG:CG | 3:C:27:ARG:NH1 | 2.77 | 0.45 |
| 30:0:1230:A:OP1 | 30:0:1230:A:H8 | 2.00 | 0.45 |
| 16:P:41:ARG:O | 16:P:44:VAL:HB | 2.17 | 0.45 |
| 18:R:119:VAL:HG13 | 18:R:119:VAL:O | 2.16 | 0.45 |
| 11:K:62:PRO:HG3 | 11:K:65:ARG:NH2 | 2.31 | 0.45 |
| 30:0:1377:C:O2' | 30:0:1378:G:H5'' | 2.17 | 0.45 |
| 23:W:55:GLY:CA | 23:W:146:ILE:HG13 | 2.46 | 0.45 |
| 6:F:58:GLU:OE1 | 13:M:27:ARG:NH2 | 2.48 | 0.45 |
| 12:L:41:HIS:HD2 | 30:0:926:A:O2' | 1.99 | 0.45 |
| 1:A:217:ARG:NH2 | 30:0:1853:C:O2' | 2.49 | 0.45 |
| 30:0:1044:C:H5 | 41:0:7405:HOH:O | 2.00 | 0.45 |
| 30:0:1566:C:H2' | 30:0:1567:G:C8 | 2.52 | 0.45 |
| 30:0:2038:A:O2' | 30:0:2039:A:H5' | 2.16 | 0.45 |
| 30:0:42:C:H3' | 41:0:5033:HOH:O | 2.16 | 0.45 |
| 30:0:106:A:O2' | 30:0:107:U:H5' | 2.17 | 0.45 |
| 30:0:669:G:O2' | 30:0:670:G:H5' | 2.16 | 0.45 |
| 30:0:583:C:H2' | 30:0:584:U:H6 | 1.82 | 0.45 |
| 25:Y:142:SER:OG | 30:0:1331:G:OP2 | 2.28 | 0.45 |
| 2:B:254:GLN:HG3 | 41:B:9001:HOH:O | 2.16 | 0.45 |
| 30:0:2768:A:O2' | 30:0:2769:C:H5' | 2.17 | 0.45 |
| 21:U:39:ASN:ND2 | 21:U:44:ARG:HH11 | 2.15 | 0.45 |
| 26:Z:51:ALA:O | 26:Z:55:SER:HB2 | 2.15 | 0.45 |
| 2:B:80:ARG:HB2 | 2:B:145:HIS:CE1 | 2.51 | 0.45 |
| 31:9:18:U:H2' | 31:9:19:G:H8 | 1.82 | 0.45 |
| 4:D:91:ALA:HB2 | 4:D:106:PHE:CD2 | 2.52 | 0.45 |
| 6:F:77:VAL:C | 6:F:78:GLU:CA | 2.85 | 0.45 |
| 5:E:22:VAL:HG12 | 5:E:76:VAL:HG11 | 1.99 | 0.45 |
| 30:0:1202:A:H2' | 30:0:1203:G:O4' | 2.17 | 0.45 |
| 25:Y:112:GLU:OE1 | 25:Y:112:GLU:HA | 2.17 | 0.45 |
| 4:D:52:THR:O | 4:D:68:PRO:HA | 2.16 | 0.45 |
| 2:B:232:TRP:HD1 | 2:B:235:ARG:HD2 | 1.82 | 0.45 |
| 30:0:2831:C:H2' | 30:0:2832:C:H5' | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:D:21:VAL:HG23 | 4:D:80:ALA:HB1 | 1.99 | 0.45 |
| 14:N:7:LYS:HB3 | 30:0:2353:A:O2' | 2.17 | 0.45 |
| 2:B:268:ARG:NH2 | 2:B:325:PRO:HG3 | 2.32 | 0.45 |
| 24:X:30:MET:CE | 24:X:58:ALA:HB3 | 2.46 | 0.45 |
| 5:E:2:ARG:NH2 | 5:E:48:VAL:HG21 | 2.32 | 0.45 |
| 26:Z:60:ASP:HB3 | 26:Z:69:ASP:HB3 | 1.99 | 0.45 |
| 15:O:103:GLU:O | 15:O:106:PRO:HD3 | 2.16 | 0.45 |
| 26:Z:54:GLU:HG2 | 26:Z:57:MET:CE | 2.47 | 0.45 |
| 30:0:2047:C:H2' | 30:0:2048:C:C6 | 2.52 | 0.45 |
| 12:L:27:ARG:HD2 | 30:0:757:C:OP1 | 2.17 | 0.45 |
| 1:A:130:THR:HG22 | 1:A:131:HIS:N | 2.30 | 0.45 |
| 2:B:233:ARG:HH11 | 2:B:233:ARG:HG2 | 1.81 | 0.45 |
| 1:A:125:ASN:CB | 1:A:158:VAL:HG12 | 2.47 | 0.45 |
| 15:O:63:LYS:HG3 | 15:O:80:ASP:O | 2.16 | 0.45 |
| 28:2:2:LYS:HG3 | 30:0:1486:A:C5 | 2.52 | 0.45 |
| 8:H:143:VAL:HG21 | 8:H:173:GLU:HG2 | 1.98 | 0.45 |
| 30:0:1739:G:O2' | 30:0:1740:U:H5' | 2.17 | 0.45 |
| 9:I:108:HIS:N | 9:I:109:PRO:CD | 2.80 | 0.45 |
| 22:V:5:VAL:CG1 | 22:V:9:ARG:NH1 | 2.80 | 0.45 |
| 20:T:79:LEU:HG | 20:T:89:ARG:HB2 | 1.99 | 0.45 |
| 19:S:30:ASP:HA | 19:S:62:LYS:HE3 | 1.98 | 0.45 |
| 13:M:64:ARG:HD2 | 41:M:8887:HOH:O | 2.17 | 0.45 |
| 20:T:48:VAL:O | 20:T:59:GLU:HA | 2.17 | 0.45 |
| 13:M:102:GLU:OE2 | 13:M:164:THR:HG21 | 2.16 | 0.44 |
| 5:E:22:VAL:O | 5:E:28:SER:HA | 2.17 | 0.44 |
| 20:T:41:ARG:NH1 | 20:T:41:ARG:HG2 | 2.31 | 0.44 |
| 30:0:1165:G:O2' | 30:0:1174:A:H4' | 2.17 | 0.44 |
| 8:H:49:GLN:NE2 | 8:H:140:TYR:CE2 | 2.73 | 0.44 |
| 8:H:32:ALA:C | 8:H:33:GLN:HG3 | 2.38 | 0.44 |
| 31:9:78:G:N2 | 31:9:102:G:H2' | 2.33 | 0.44 |
| 4:D:59:GLY:O | 4:D:61:PHE:N | 2.50 | 0.44 |
| 30:0:2754:G:H2' | 30:0:2755:G:O4' | 2.17 | 0.44 |
| 5:E:170:ARG:NH2 | 41:E:4761:HOH:O | 2.50 | 0.44 |
| 30:0:2432:C:O2' | 30:0:2433:A:H5' | 2.17 | 0.44 |
| 6:F:39:SER:O | 6:F:43:GLY:N | 2.50 | 0.44 |
| 29:3:62:THR:HB | 41:3:9041:HOH:O | 2.17 | 0.44 |
| 24:X:71:ARG:HD3 | 41:X:7542:HOH:O | 2.16 | 0.44 |
| 8:H:36:MET:HB3 | 8:H:73:ASN:ND2 | 2.32 | 0.44 |
| 9:I:129:SER:HB3 | 30:0:1192:A:N6 | 2.32 | 0.44 |
| 3:C:233:THR:CG2 | 3:C:234:VAL:H | 2.24 | 0.44 |
| 30:0:559:U:H5' | 30:0:559:U:C6 | 2.37 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:F:50:VAL:HG21 | 6:F:63:ILE:HG21 | 1.99 | 0.44 |
| 41:K:4183:HOH:O | 30:0:2712:G:H5' | 2.17 | 0.44 |
| 41:B:9118:HOH:O | 30:0:2672:C:H1' | 2.17 | 0.44 |
| 21:U:44:ARG:HB3 | 41:U:3805:HOH:O | 2.17 | 0.44 |
| 13:M:82:ARG:O | 13:M:84:LYS:N | 2.50 | 0.44 |
| 1:A:58:VAL:HG21 | 1:A:80:LEU:HD12 | 1.98 | 0.44 |
| 30:0:1342:C:H2' | 30:0:1343:C:H5' | 1.99 | 0.44 |
| 30:0:2379:G:N7 | 30:0:2408:A:N1 | 2.64 | 0.44 |
| 1:A:1:GLY:HA2 | 30:0:2114:C:OP1 | 2.18 | 0.44 |
| 30:0:2589:U:H2' | 30:0:2590:U:C6 | 2.52 | 0.44 |
| 30:0:661:G:C5 | 30:0:686:A:C2 | 3.06 | 0.44 |
| 13:M:66:SER:HB3 | 13:M:128:TRP:CD1 | 2.52 | 0.44 |
| 30:0:1839:A:H5' | 30:0:2643:G:H4' | 1.99 | 0.44 |
| 41:N:8814:HOH:O | 31:9:36:C:H4' | 2.17 | 0.44 |
| 30:0:416:G:OP1 | 30:0:417:G:H5' | 2.18 | 0.44 |
| 13:M:167:GLY:O | 13:M:171:ARG:HG3 | 2.18 | 0.44 |
| 25:Y:189:ASN:CA | 25:Y:217:ILE:HD11 | 2.38 | 0.44 |
| 18:R:40:ALA:HB3 | 18:R:107:GLU:HA | 1.99 | 0.44 |
| 9:I:72:GLU:C | 9:I:74:ILE:H | 2.20 | 0.44 |
| 30:0:1204:C:H2' | 30:0:1205:U:O4' | 2.16 | 0.44 |
| 6:F:83:LEU:HD11 | 6:F:96:ALA:HB3 | 1.98 | 0.44 |
| 21:U:56:ARG:HD2 | 21:U:56:ARG:O | 2.17 | 0.44 |
| 2:B:262:ARG:HG3 | 30:0:2716:G:H5' | 1.99 | 0.44 |
| 30:0:77:G:C2' | 30:0:78:G:H5' | 2.47 | 0.44 |
| 3:C:84:VAL:O | 3:C:85:LYS:HB2 | 2.17 | 0.44 |
| 30:0:2816:A:H5'' | 30:0:2817:G:H5' | 1.98 | 0.44 |
| 20:T:17:HIS:HB3 | 30:0:100:C:O2 | 2.17 | 0.44 |
| 5:E:88:TYR:CE1 | 5:E:92:PRO:HA | 2.52 | 0.44 |
| 13:M:133:LEU:O | 13:M:134:ILE:HD13 | 2.17 | 0.44 |
| 23:W:65:VAL:HA | 23:W:68:THR:CG2 | 2.47 | 0.44 |
| 14:N:40:ASN:HD21 | 31:9:28:U:H5'' | 1.81 | 0.44 |
| 6:F:7:ASP:O | 6:F:118:LEU:HD21 | 2.18 | 0.44 |
| 15:O:14:LEU:CG | 15:O:102:ILE:HD11 | 2.48 | 0.44 |
| 2:B:77:PRO:C | 2:B:78:PRO:HG3 | 2.38 | 0.44 |
| 14:N:141:ARG:HH21 | 31:9:48:C:H4' | 1.82 | 0.44 |
| 21:U:4:ARG:HH11 | 21:U:4:ARG:HG2 | 1.82 | 0.44 |
| 25:Y:144:ARG:NE | 41:Y:8923:HOH:O | 2.51 | 0.44 |
| 30:0:1774:G:H1' | 41:0:5396:HOH:O | 2.16 | 0.44 |
| 30:0:308:U:H5' | 30:0:309:C:OP1 | 2.16 | 0.44 |
| 9:I:123:VAL:C | 9:I:125:GLY:H | 2.21 | 0.44 |
| 18:R:94:ASN:ND2 | 30:0:500:G:O2' | 2.49 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:0:2857:C:H2' | 30:0:2858:U:C6 | 2.52 | 0.44 |
| 14:N:37:ARG:HA | 14:N:37:ARG:HD3 | 1.88 | 0.44 |
| 2:B:183:GLU:O | 2:B:184:ASP:C | 2.56 | 0.44 |
| 13:M:60:VAL:HG22 | 13:M:134:ILE:HD12 | 1.99 | 0.44 |
| 11:K:14:LYS:CB | 11:K:45:PRO:HG2 | 2.42 | 0.44 |
| 30:0:380:A:O4' | 30:0:382:U:H1' | 2.18 | 0.44 |
| 10:J:39:VAL:HG11 | 10:J:107:ASN:CB | 2.48 | 0.44 |
| 13:M:57:LYS:NZ | 13:M:144:ASP:HB2 | 2.32 | 0.44 |
| 3:C:174:ILE:HD11 | 30:0:338:C:H4' | 1.98 | 0.44 |
| 2:B:145:HIS:CD2 | 2:B:159:PRO:HB3 | 2.51 | 0.44 |
| 23:W:108:ARG:NH2 | 23:W:114:PRO:HG2 | 2.32 | 0.44 |
| 30:0:629:A:C2 | 30:0:2074:A:C2 | 3.06 | 0.44 |
| 30:0:1805:G:O2' | 30:0:1806:G:H5' | 2.18 | 0.44 |
| 30:0:1427:A:H61 | 30:0:1440:U:C1' | 2.30 | 0.44 |
| 15:O:51:TYR:CD1 | 30:0:721:A:H4' | 2.52 | 0.44 |
| 3:C:180:SER:HB3 | 41:C:8647:HOH:O | 2.18 | 0.44 |
| 3:C:225:PRO:O | 30:0:1308:A:H4' | 2.17 | 0.44 |
| 13:M:134:ILE:HG23 | 13:M:141:ILE:CD1 | 2.38 | 0.44 |
| 1:A:33:GLU:CD | 1:A:33:GLU:N | 2.60 | 0.44 |
| 31:9:29:C:C2' | 31:9:30:C:H5' | 2.43 | 0.44 |
| 14:N:77:ASN:C | 14:N:78:MET:CA | 2.86 | 0.44 |
| 12:L:121:ILE:HG12 | 12:L:141:GLU:HB2 | 2.00 | 0.44 |
| 8:H:155:ARG:NH1 | 30:0:2503:A:H5'' | 2.33 | 0.44 |
| 23:W:44:MET:CE | 30:0:944:G:H21 | 2.30 | 0.44 |
| 4:D:129:ASP:OD1 | 30:0:2338:G:H2' | 2.17 | 0.44 |
| 11:K:41:LYS:HA | 30:0:2582:G:O3' | 2.17 | 0.44 |
| 3:C:85:LYS:HD3 | 41:0:3695:HOH:O | 2.17 | 0.44 |
| 5:E:162:PHE:CD1 | 5:E:162:PHE:N | 2.85 | 0.44 |
| 24:X:15:ARG:HB3 | 24:X:15:ARG:HH11 | 1.83 | 0.44 |
| 30:0:485:A:HO2' | 30:0:487:G:H8 | 1.65 | 0.44 |
| 30:0:318:U:H5' | 30:0:339:A:C2 | 2.53 | 0.44 |
| 30:0:2906:A:H5' | 30:0:2907:C:O4' | 2.18 | 0.44 |
| 30:0:157:G:H3' | 41:0:4825:HOH:O | 2.16 | 0.44 |
| 2:B:264:GLU:OE2 | 2:B:302:PRO:HD3 | 2.18 | 0.44 |
| 12:L:104:ASP:O | 12:L:105:TYR:HB3 | 2.17 | 0.44 |
| 4:D:158:ASN:HB2 | 4:D:161:ASP:OD2 | 2.17 | 0.44 |
| 18:R:84:ALA:O | 18:R:88:PHE:HD1 | 2.01 | 0.44 |
| 2:B:284:PHE:HB2 | 2:B:287:TYR:HB3 | 1.99 | 0.44 |
| 30:0:463:A:H5' | 30:0:465:U:O4' | 2.17 | 0.44 |
| 23:W:115:THR:HG23 | 41:W:5420:HOH:O | 2.18 | 0.44 |
| 2:B:238:ASN:ND2 | 2:B:240:GLY:H | 2.01 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 30:0:1603:A:H5'' | 30:0:1604:G:H3' | 2.00 | 0.44 |
| 18:R:135:ALA:O | 30:0:2054:A:H4' | 2.18 | 0.44 |
| 30:0:336:G:H2' | 41:0:4598:HOH:O | 2.16 | 0.44 |
| 2:B:266:ASN:OD1 | 2:B:317:PRO:HA | 2.17 | 0.44 |
| 30:0:1682:A:H5'' | 41:0:3364:HOH:O | 2.18 | 0.44 |
| 30:0:2253:G:O2' | 30:0:2254:G:H5' | 2.18 | 0.44 |
| 30:0:1333:U:H2' | 30:0:1334:C:H6 | 1.81 | 0.44 |
| 15:O:97:SER:H | 15:O:100:GLN:NE2 | 2.16 | 0.44 |
| 1:A:217:ARG:NH1 | 1:A:217:ARG:CG | 2.80 | 0.44 |
| 30:0:814:G:H2' | 30:0:815:U:C6 | 2.52 | 0.44 |
| 27:1:45:ARG:HB3 | 41:1:988:HOH:O | 2.18 | 0.44 |
| 26:Z:40:ALA:HA | 30:0:1773:G:C8 | 2.51 | 0.44 |
| 30:0:764:C:H2' | 30:0:765:G:O4' | 2.17 | 0.44 |
| 31:9:7:G:H5' | 41:9:9099:HOH:O | 2.18 | 0.44 |
| 30:0:2543:G:H2' | 30:0:2544:G:O4' | 2.18 | 0.44 |
| 11:K:21:ALA:HB1 | 11:K:110:LYS:O | 2.18 | 0.44 |
| 5:E:112:ALA:HA | 5:E:113:PRO:HD3 | 1.86 | 0.44 |
| 1:A:212:PRO:HA | 30:0:1943:C:O4' | 2.17 | 0.44 |
| 30:0:2718:C:H5' | 30:0:2718:C:C6 | 2.50 | 0.44 |
| 18:R:39:THR:CB | 18:R:42:GLU:HG3 | 2.47 | 0.44 |
| 30:0:1207:A:H5' | 30:0:1208:C:OP2 | 2.18 | 0.44 |
| 31:9:13:A:H3' | 31:9:14:G:H5' | 2.00 | 0.44 |
| 19:S:10:VAL:HG11 | 22:V:36:ALA:CB | 2.48 | 0.44 |
| 30:0:2032:U:C2' | 30:0:2033:G:H5'' | 2.48 | 0.44 |
| 30:0:613:C:H2' | 30:0:614:U:H6 | 1.83 | 0.44 |
| 30:0:2879:A:H2' | 30:0:2880:A:O4' | 2.17 | 0.44 |
| 14:N:182:GLY:O | 14:N:184:ILE:HG22 | 2.18 | 0.44 |
| 27:1:8:GLN:HE22 | 27:1:11:LYS:HZ2 | 1.66 | 0.44 |
| 10:J:64:GLY:HA3 | 38:J:8821:CL:CL | 2.55 | 0.44 |
| 4:D:156:ARG:HG3 | 4:D:156:ARG:NH1 | 2.32 | 0.44 |
| 2:B:132:HIS:CE1 | 2:B:171:VAL:HG21 | 2.53 | 0.44 |
| 8:H:86:TYR:C | 8:H:86:TYR:CD1 | 2.91 | 0.44 |
| 14:N:6:TYR:HB3 | 31:9:11:A:N6 | 2.32 | 0.44 |
| 25:Y:145:LYS:HE2 | 41:Y:8917:HOH:O | 2.17 | 0.44 |
| 30:0:746:A:H4' | 30:0:747:G:H5' | 1.99 | 0.44 |
| 2:B:300:SER:HB3 | 41:0:5521:HOH:O | 2.18 | 0.44 |
| 30:0:2608:C:H2' | 41:0:4450:HOH:O | 2.18 | 0.44 |
| 30:0:522:U:O2' | 30:0:1366:C:H5' | 2.17 | 0.44 |
| 14:N:112:GLY:HA2 | 14:N:137:ALA:H | 1.82 | 0.44 |
| 30:0:177:A:H2' | 30:0:178:U:O4' | 2.17 | 0.44 |
| 13:M:124:GLY:HA3 | 30:0:2132:C:H1' | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:0:1160:G:H5' | 30:0:1161:A:C4' | 2.48 | 0.44 |
| 4:D:103:ASN:ND2 | 4:D:134:LEU:H | 2.16 | 0.44 |
| 24:X:49:ARG:NH1 | 30:0:1385:G:O3' | 2.51 | 0.44 |
| 14:N:140:GLN:O | 14:N:143:ARG:HB2 | 2.18 | 0.44 |
| 6:F:48:VAL:HG23 | 6:F:74:PHE:CB | 2.47 | 0.44 |
| 7:G:13:PRO:HD2 | 7:G:16:LYS:HD2 | 1.99 | 0.44 |
| 27:1:28:HIS:O | 27:1:32:LYS:N | 2.45 | 0.44 |
| 6:F:101:ALA:HB3 | 6:F:105:ASP:OD1 | 2.18 | 0.44 |
| 13:M:159:VAL:HG13 | 13:M:160:PHE:N | 2.32 | 0.44 |
| 30:0:2323:G:H5' | 41:0:7820:HOH:O | 2.17 | 0.44 |
| 30:0:1697:G:H1' | 41:0:9075:HOH:O | 2.17 | 0.44 |
| 30:0:660:A:H4' | 30:0:661:G:O5' | 2.18 | 0.44 |
| 23:W:9:GLY:H | 30:0:1086:A:P | 2.41 | 0.44 |
| 10:J:12:VAL:HG21 | 10:J:116:LEU:HD11 | 1.99 | 0.44 |
| 30:0:1252:A:H2' | 30:0:1253:C:O4' | 2.18 | 0.44 |
| 10:J:142:ASN:O | 10:J:144:THR:N | 2.51 | 0.44 |
| 2:B:274:GLU:HA | 2:B:292:GLY:O | 2.17 | 0.44 |
| 25:Y:182:PHE:CG | 25:Y:202:ALA:HB2 | 2.53 | 0.44 |
| 12:L:134:GLU:HA | 12:L:138:GLY:O | 2.18 | 0.44 |
| 8:H:59:GLN:HG2 | 8:H:129:ARG:HG2 | 1.99 | 0.43 |
| 30:0:855:U:H5' | 41:0:9252:HOH:O | 2.18 | 0.43 |
| 6:F:48:VAL:HG12 | 6:F:97:ALA:HB2 | 2.00 | 0.43 |
| 41:C:8558:HOH:O | 30:0:656:G:H4' | 2.18 | 0.43 |
| 30:0:314:G:N2 | 30:0:316:A:H3' | 2.33 | 0.43 |
| 30:0:2346:C:O5' | 30:0:2346:C:H6 | 2.01 | 0.43 |
| 12:L:73:VAL:HG23 | 12:L:74:THR:N | 2.31 | 0.43 |
| 30:0:152:A:O2' | 30:0:153:C:H5' | 2.17 | 0.43 |
| 30:0:1790:C:H2' | 30:0:1791:U:C6 | 2.53 | 0.43 |
| 30:0:538:C:H5" | 30:0:539:G:C8 | 2.51 | 0.43 |
| 23:W:10:GLU:HG3 | 23:W:11:VAL:N | 2.32 | 0.43 |
| 25:Y:99:ALA:HB2 | 25:Y:233:TYR:CZ | 2.53 | 0.43 |
| 30:0:1855:G:H4' | 30:0:1856:C:O5' | 2.17 | 0.43 |
| 30:0:671:A:O2' | 30:0:672:G:H2' | 2.18 | 0.43 |
| 30:0:2511:A:H4' | 41:0:6305:HOH:O | 2.18 | 0.43 |
| 30:0:243:A:H61 | 30:0:269:G:H1' | 1.83 | 0.43 |
| 30:0:187:A:H3' | 30:0:188:C:H6 | 1.83 | 0.43 |
| 15:O:38:ARG:NH1 | 41:O:7674:HOH:O | 2.50 | 0.43 |
| 30:0:2510:C:H42 | 30:0:2564:G:H22 | 1.66 | 0.43 |
| 11:K:14:LYS:HD2 | 38:K:8812:CL:CL | 2.55 | 0.43 |
| 18:R:39:THR:O | 18:R:40:ALA:C | 2.56 | 0.43 |
| 11:K:28:GLU:CB | 11:K:59:LYS:HB2 | 2.44 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 30:0:1730:G:H5'' | 30:0:1731:C:C6 | 2.53 | 0.43 |
| 27:1:18:LYS:HA | 27:1:25:LYS:HA | 2.00 | 0.43 |
| 30:0:319:A:H4' | 30:0:338:C:C5 | 2.53 | 0.43 |
| 30:0:2537:G:O5' | 30:0:2538:A:H5'' | 2.18 | 0.43 |
| 30:0:1309:U:C2' | 30:0:1310:U:H5' | 2.49 | 0.43 |
| 15:O:24:ALA:HB3 | 30:0:710:G:OP1 | 2.17 | 0.43 |
| 17:Q:77:ASP:O | 17:Q:78:GLY:CA | 2.66 | 0.43 |
| 12:L:27:ARG:NH2 | 12:L:30:ARG:HG2 | 2.33 | 0.43 |
| 4:D:10:PHE:O | 4:D:14:ARG:HG3 | 2.18 | 0.43 |
| 9:I:96:SER:HB3 | 9:I:99:GLN:NE2 | 2.34 | 0.43 |
| 30:0:1659:A:H2' | 30:0:1660:G:O4' | 2.17 | 0.43 |
| 12:L:17:SER:C | 12:L:19:LYS:H | 2.21 | 0.43 |
| 30:0:1979:G:O2' | 30:0:1980:U:OP1 | 2.34 | 0.43 |
| 18:R:59:PHE:O | 18:R:63:ASN:HB3 | 2.18 | 0.43 |
| 29:3:65:THR:CG2 | 29:3:67:LEU:HG | 2.39 | 0.43 |
| 9:I:127:CYS:C | 9:I:129:SER:H | 2.22 | 0.43 |
| 14:N:165:ALA:C | 14:N:167:ASP:H | 2.21 | 0.43 |
| 30:0:2645:U:OP2 | 30:0:2645:U:H6 | 2.02 | 0.43 |
| 19:S:49:VAL:HG13 | 19:S:66:VAL:HG13 | 2.00 | 0.43 |
| 30:0:951:A:O2' | 30:0:952:G:H5' | 2.18 | 0.43 |
| 19:S:73:ASP:HB3 | 19:S:76:GLU:OE1 | 2.17 | 0.43 |
| 30:0:1477:C:H5' | 30:0:1868:G:H5' | 2.00 | 0.43 |
| 16:P:37:ARG:NH2 | 30:0:1502:A:OP1 | 2.50 | 0.43 |
| 1:A:235:ARG:HB2 | 41:A:9026:HOH:O | 2.17 | 0.43 |
| 23:W:142:ASP:HB3 | 23:W:145:GLY:H | 1.84 | 0.43 |
| 30:0:841:A:H5'' | 41:0:7715:HOH:O | 2.17 | 0.43 |
| 30:0:2507:G:H2' | 30:0:2510:C:N4 | 2.32 | 0.43 |
| 5:E:84:MET:SD | 5:E:168:ILE:HD13 | 2.58 | 0.43 |
| 3:C:115:LEU:HA | 3:C:115:LEU:HD12 | 1.80 | 0.43 |
| 23:W:65:VAL:CA | 23:W:68:THR:HG22 | 2.48 | 0.43 |
| 19:S:38:ALA:O | 19:S:42:GLU:HG3 | 2.19 | 0.43 |
| 11:K:82:ARG:O | 11:K:85:GLY:N | 2.50 | 0.43 |
| 16:P:41:ARG:HH22 | 30:0:1500:U:P | 2.41 | 0.43 |
| 30:0:1803:C:H2' | 30:0:1804:A:H8 | 1.82 | 0.43 |
| 15:O:65:LEU:HD13 | 30:0:746:A:C6 | 2.53 | 0.43 |
| 9:I:81:GLU:N | 9:I:81:GLU:OE1 | 2.51 | 0.43 |
| 30:0:1056:U:H2' | 30:0:1057:A:O4' | 2.19 | 0.43 |
| 2:B:154:VAL:HG12 | 2:B:156:LYS:HG2 | 2.00 | 0.43 |
| 18:R:106:GLY:HA2 | 18:R:109:MET:CE | 2.47 | 0.43 |
| 3:C:234:VAL:HG13 | 3:C:234:VAL:O | 2.18 | 0.43 |
| 30:0:2748:G:H8 | 41:0:9326:HOH:O | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 30:0:2768:A:H2' | 30:0:2769:C:O4' | 2.19 | 0.43 |
| 30:0:95:A:O5' | 30:0:97:G:H5' | 2.19 | 0.43 |
| 14:N:21:HIS:HB2 | 41:N:8831:HOH:O | 2.19 | 0.43 |
| 20:T:43:ASN:O | 20:T:45:GLY:N | 2.50 | 0.43 |
| 31:9:54:A:O2' | 31:9:55:U:H5' | 2.18 | 0.43 |
| 30:0:2557:U:H3' | 41:0:7487:HOH:O | 2.18 | 0.43 |
| 14:N:111:PRO:HD2 | 31:9:37:C:H4' | 2.00 | 0.43 |
| 22:V:1:THR:CB | 30:0:93:C:H5'' | 2.44 | 0.43 |
| 4:D:25:MET:CE | 4:D:40:ILE:HD11 | 2.49 | 0.43 |
| 1:A:190:ARG:NH1 | 30:0:1845:A:OP2 | 2.51 | 0.43 |
| 30:0:2769:C:H2' | 30:0:2770:G:C5' | 2.49 | 0.43 |
| 16:P:59:ARG:HH22 | 16:P:66:GLN:NE2 | 2.13 | 0.43 |
| 1:A:132:ASP:OD1 | 1:A:133:ARG:N | 2.49 | 0.43 |
| 10:J:59:LYS:O | 10:J:63:ILE:HG13 | 2.19 | 0.43 |
| 23:W:13:MET:HE3 | 23:W:17:ILE:HG22 | 2.00 | 0.43 |
| 30:0:1926:G:H2' | 30:0:1927:A:C8 | 2.53 | 0.43 |
| 22:V:45:ARG:HA | 22:V:48:GLU:HB2 | 2.00 | 0.43 |
| 11:K:62:PRO:HG3 | 11:K:65:ARG:HH22 | 1.82 | 0.43 |
| 14:N:97:VAL:HG12 | 14:N:127:LEU:HD11 | 1.99 | 0.43 |
| 11:K:69:LEU:HD12 | 11:K:97:ILE:HD13 | 2.01 | 0.43 |
| 4:D:88:LEU:HB2 | 4:D:89:PRO:HD3 | 2.00 | 0.43 |
| 30:0:706:G:N2 | 30:0:707:C:H41 | 2.16 | 0.43 |
| 30:0:23:G:H1' | 30:0:520:A:N6 | 2.34 | 0.43 |
| 4:D:15:GLU:HA | 4:D:16:PRO:HD3 | 1.84 | 0.43 |
| 41:3:9017:HOH:O | 30:0:2468:A:H4' | 2.18 | 0.43 |
| 30:0:2506:A:O2' | 30:0:2507:G:P | 2.77 | 0.43 |
| 5:E:118:ILE:HG23 | 5:E:144:THR:HG21 | 2.00 | 0.43 |
| 24:X:20:GLU:CD | 24:X:21:PRO:HD2 | 2.39 | 0.43 |
| 30:0:878:G:H4' | 30:0:1835:U:H4' | 2.01 | 0.43 |
| 20:T:40:VAL:HG23 | 20:T:119:ALA:C | 2.39 | 0.43 |
| 5:E:15:GLN:HG3 | 5:E:20:ILE:HG12 | 2.01 | 0.43 |
| 2:B:102:THR:CG2 | 2:B:182:VAL:HG12 | 2.48 | 0.43 |
| 30:0:77:G:H2' | 30:0:78:G:H5' | 2.00 | 0.43 |
| 1:A:223:ARG:NH2 | 41:A:9054:HOH:O | 2.51 | 0.43 |
| 15:O:96:VAL:HG13 | 15:O:100:GLN:CD | 2.38 | 0.43 |
| 1:A:176:HIS:CD2 | 30:0:857:A:H4' | 2.54 | 0.43 |
| 30:0:521:A:H2' | 30:0:522:U:H5' | 2.00 | 0.43 |
| 1:A:114:ASP:OD1 | 1:A:115:GLY:N | 2.52 | 0.43 |
| 17:Q:31:GLU:OE1 | 17:Q:31:GLU:HA | 2.19 | 0.43 |
| 30:0:1524:U:H5'' | 30:0:1524:U:H6 | 1.83 | 0.43 |
| 28:2:13:LYS:O | 28:2:17:GLN:HG3 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 33:6:75:C:H5'' | 33:6:76:8AN:O1P | 2.18 | 0.43 |
| 4:D:96:SER:C | 4:D:98:PHE:H | 2.22 | 0.43 |
| 30:0:264:G:H1' | 30:0:265:U:H5 | 1.84 | 0.43 |
| 13:M:99:ARG:CD | 13:M:167:GLY:HA2 | 2.48 | 0.43 |
| 25:Y:189:ASN:ND2 | 25:Y:189:ASN:C | 2.72 | 0.43 |
| 30:0:1180:U:H2' | 30:0:1181:A:H8 | 1.81 | 0.43 |
| 9:I:87:PRO:HB2 | 9:I:129:SER:HA | 2.01 | 0.43 |
| 30:0:1603:A:H5' | 30:0:1605:G:C4' | 2.48 | 0.43 |
| 6:F:48:VAL:HG23 | 6:F:74:PHE:HB3 | 1.99 | 0.43 |
| 2:B:201:ASP:HB2 | 2:B:312:ARG:HD2 | 2.01 | 0.43 |
| 30:0:317:A:H5' | 41:0:4644:HOH:O | 2.18 | 0.43 |
| 30:0:2550:U:O2' | 30:0:2551:C:H5' | 2.19 | 0.43 |
| 11:K:115:ARG:HG3 | 11:K:116:GLU:N | 2.33 | 0.43 |
| 1:A:1:GLY:HA2 | 1:A:197:VAL:HG23 | 2.00 | 0.43 |
| 1:A:42:VAL:O | 1:A:76:VAL:HG13 | 2.19 | 0.43 |
| 3:C:193:LEU:HA | 3:C:211:ASP:O | 2.19 | 0.43 |
| 17:Q:86:VAL:HG13 | 17:Q:91:LEU:HD11 | 1.99 | 0.43 |
| 5:E:146:ALA:O | 5:E:150:GLN:HG2 | 2.19 | 0.43 |
| 30:0:1120:U:C6 | 30:0:1120:U:H5'' | 2.54 | 0.43 |
| 30:0:1921:A:C6 | 30:0:1922:A:C2 | 3.07 | 0.43 |
| 30:0:497:A:H2' | 30:0:498:A:C5' | 2.49 | 0.43 |
| 8:H:153:PHE:HD1 | 8:H:166:ILE:HG23 | 1.84 | 0.43 |
| 30:0:607:G:H2' | 30:0:608:A:O4' | 2.19 | 0.43 |
| 2:B:285:VAL:O | 2:B:286:ASN:HB2 | 2.18 | 0.43 |
| 30:0:1117:A:C2 | 30:0:1244:U:C2 | 3.07 | 0.43 |
| 1:A:105:VAL:HG11 | 1:A:154:ALA:HB1 | 2.00 | 0.43 |
| 2:B:279:THR:CG2 | 2:B:280:VAL:N | 2.81 | 0.43 |
| 30:0:559:U:C5' | 30:0:559:U:H6 | 2.25 | 0.43 |
| 16:P:80:ARG:HG2 | 16:P:87:ARG:NH2 | 2.34 | 0.43 |
| 22:V:50:ARG:HD3 | 41:V:2826:HOH:O | 2.18 | 0.43 |
| 25:Y:155:ARG:NH1 | 41:Y:8864:HOH:O | 2.52 | 0.43 |
| 24:X:79:GLU:CD | 24:X:80:GLU:H | 2.22 | 0.43 |
| 9:I:91:PHE:HA | 9:I:131:GLY:CA | 2.49 | 0.43 |
| 14:N:73:ALA:HB1 | 14:N:74:PRO:HD2 | 2.00 | 0.43 |
| 1:A:217:ARG:HG2 | 1:A:229:ALA:HB2 | 2.01 | 0.43 |
| 12:L:99:GLU:C | 12:L:101:ASP:H | 2.21 | 0.43 |
| 1:A:71:PRO:HA | 1:A:158:VAL:O | 2.19 | 0.43 |
| 30:0:1698:U:H6 | 30:0:1698:U:O5' | 2.02 | 0.43 |
| 23:W:73:LEU:HA | 23:W:73:LEU:HD12 | 1.82 | 0.43 |
| 25:Y:152:LYS:HB3 | 25:Y:160:LYS:HG3 | 2.01 | 0.43 |
| 30:0:1268:C:H2' | 30:0:1269:G:H8 | 1.84 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:132:THR:HB | 41:E:2227:HOH:O | 2.19 | 0.43 |
| 27:1:10:LYS:HG3 | 41:1:2979:HOH:O | 2.18 | 0.43 |
| 30:0:2618:G:N3 | 32:5:76:A:C2 | 2.87 | 0.43 |
| 9:I:130:LEU:HB2 | 9:I:132:VAL:HG23 | 2.00 | 0.43 |
| 4:D:136:ARG:HB3 | 4:D:137:PRO:HD2 | 2.01 | 0.43 |
| 23:W:77:ALA:C | 23:W:78:ASP:CA | 2.87 | 0.43 |
| 6:F:4:VAL:HG13 | 6:F:76:PHE:CD1 | 2.54 | 0.43 |
| 30:0:2456:A:H2' | 30:0:2457:U:H6 | 1.83 | 0.43 |
| 1:A:70:ALA:HA | 1:A:71:PRO:HD3 | 1.85 | 0.43 |
| 30:0:485:A:N3 | 30:0:487:G:H5'' | 2.34 | 0.43 |
| 30:0:2697:A:H2' | 30:0:2698:G:O4' | 2.19 | 0.43 |
| 30:0:1657:A:H2' | 30:0:1658:A:C8 | 2.54 | 0.43 |
| 17:Q:46:SER:O | 17:Q:48:PRO:HD3 | 2.18 | 0.43 |
| 11:K:9:THR:HA | 41:0:4173:HOH:O | 2.19 | 0.43 |
| 30:0:523:C:H2' | 30:0:524:A:H8 | 1.84 | 0.43 |
| 3:C:19:PRO:CD | 3:C:240:LEU:HD22 | 2.49 | 0.43 |
| 23:W:125:HIS:NE2 | 30:0:1097:A:H5'' | 2.34 | 0.43 |
| 14:N:147:ILE:HG23 | 14:N:148:ALA:N | 2.34 | 0.42 |
| 13:M:98:GLN:O | 13:M:102:GLU:HG3 | 2.19 | 0.42 |
| 30:0:876:A:N3 | 30:0:876:A:C2' | 2.82 | 0.42 |
| 10:J:39:VAL:HG11 | 10:J:107:ASN:CG | 2.40 | 0.42 |
| 2:B:152:PRO:HA | 41:B:9043:HOH:O | 2.19 | 0.42 |
| 14:N:114:LYS:O | 14:N:118:ILE:HG13 | 2.19 | 0.42 |
| 12:L:35:ARG:NH1 | 12:L:43:HIS:CD2 | 2.87 | 0.42 |
| 6:F:80:GLN:HB3 | 41:F:2563:HOH:O | 2.19 | 0.42 |
| 1:A:223:ARG:HH12 | 30:0:2270:G:H4' | 1.84 | 0.42 |
| 30:0:2611:G:H5' | 30:0:2613:G:C8 | 2.53 | 0.42 |
| 15:O:97:SER:H | 15:O:100:GLN:HE21 | 1.67 | 0.42 |
| 2:B:199:TYR:HE2 | 2:B:268:ARG:HB2 | 1.83 | 0.42 |
| 8:H:76:LEU:HD21 | 8:H:149:VAL:HA | 2.01 | 0.42 |
| 20:T:81:LYS:HG3 | 20:T:87:VAL:HG13 | 2.00 | 0.42 |
| 13:M:157:ASP:HB3 | 13:M:160:PHE:HD1 | 1.84 | 0.42 |
| 30:0:1947:G:H2' | 30:0:1948:G:C8 | 2.54 | 0.42 |
| 30:0:2106:C:H1' | 30:0:2484:U:O2 | 2.19 | 0.42 |
| 32:5:74:C:N4 | 41:5:3737:HOH:O | 2.39 | 0.42 |
| 31:9:49:G:C2' | 31:9:50:G:H5' | 2.50 | 0.42 |
| 5:E:68:HIS:O | 5:E:72:MET:HG3 | 2.18 | 0.42 |
| 29:3:48:ASN:ND2 | 29:3:50:GLY:H | 2.17 | 0.42 |
| 3:C:118:THR:HG23 | 41:C:8504:HOH:O | 2.19 | 0.42 |
| 30:0:1210:G:O2' | 30:0:1211:G:H5' | 2.19 | 0.42 |
| 1:A:194:MET:CE | 1:A:199:HIS:HB2 | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 16:P:16:VAL:HG13 | 16:P:20:ARG:CZ | 2.49 | 0.42 |
| 30:0:2756:U:O2 | 30:0:2896:A:H2 | 2.02 | 0.42 |
| 12:L:50:GLY:HA2 | 30:0:2453:G:O3' | 2.19 | 0.42 |
| 30:0:2064:U:H5' | 30:0:2652:U:O3' | 2.19 | 0.42 |
| 12:L:41:HIS:CD2 | 30:0:926:A:O2' | 2.73 | 0.42 |
| 3:C:157:LEU:CD1 | 3:C:166:ILE:HD11 | 2.49 | 0.42 |
| 30:0:1574:C:O5' | 30:0:1574:C:H6 | 2.03 | 0.42 |
| 30:0:772:G:H2' | 30:0:773:A:O4' | 2.19 | 0.42 |
| 30:0:2087:C:O2' | 30:0:2088:C:H5' | 2.20 | 0.42 |
| 30:0:426:G:O2' | 30:0:427:C:H5' | 2.19 | 0.42 |
| 15:O:19:ARG:NH1 | 30:0:1276:U:H3' | 2.34 | 0.42 |
| 8:H:62:HIS:HA | 8:H:65:LEU:HD23 | 2.02 | 0.42 |
| 13:M:188:ARG:HB2 | 30:0:156:C:OP2 | 2.18 | 0.42 |
| 5:E:101:GLU:HA | 5:E:118:ILE:HG13 | 2.02 | 0.42 |
| 21:U:52:THR:HG21 | 21:U:54:THR:HB | 2.01 | 0.42 |
| 14:N:143:ARG:HB3 | 14:N:143:ARG:HE | 1.61 | 0.42 |
| 1:A:38:ILE:HD13 | 1:A:38:ILE:HA | 1.86 | 0.42 |
| 7:G:12:ILE:HG22 | 7:G:17:GLN:HE21 | 1.82 | 0.42 |
| 2:B:87:TYR:O | 2:B:138:GLY:N | 2.42 | 0.42 |
| 23:W:154:ARG:NH2 | 41:W:321:HOH:O | 2.51 | 0.42 |
| 13:M:71:SER:CB | 13:M:92:THR:HG22 | 2.49 | 0.42 |
| 2:B:119:HIS:O | 2:B:121:PRO:HD3 | 2.19 | 0.42 |
| 30:0:2129:U:H2' | 30:0:2130:C:C6 | 2.54 | 0.42 |
| 30:0:1378:G:O4' | 30:0:2747:C:N4 | 2.48 | 0.42 |
| 2:B:87:TYR:OH | 2:B:163:GLU:OE2 | 2.27 | 0.42 |
| 30:0:960:G:N3 | 30:0:960:G:C2' | 2.83 | 0.42 |
| 4:D:88:LEU:N | 4:D:89:PRO:CD | 2.82 | 0.42 |
| 30:0:523:C:H2' | 30:0:524:A:C8 | 2.54 | 0.42 |
| 30:0:2569:A:H2' | 30:0:2570:G:O5' | 2.20 | 0.42 |
| 15:O:32:ARG:O | 15:O:35:LYS:HB2 | 2.20 | 0.42 |
| 30:0:1307:A:H2' | 30:0:1308:A:C8 | 2.55 | 0.42 |
| 1:A:211:LYS:CB | 41:A:9094:HOH:O | 2.65 | 0.42 |
| 4:D:99:ASP:OD2 | 4:D:101:THR:HB | 2.18 | 0.42 |
| 27:1:28:HIS:HD2 | 27:1:31:LYS:H | 1.66 | 0.42 |
| 29:3:70:ARG:HH11 | 29:3:70:ARG:HG2 | 1.84 | 0.42 |
| 2:B:75:GLU:O | 2:B:77:PRO:HD3 | 2.19 | 0.42 |
| 5:E:137:ASP:OD1 | 5:E:139:GLU:N | 2.52 | 0.42 |
| 30:0:1819:G:H2' | 30:0:1820:G:C4' | 2.50 | 0.42 |
| 14:N:108:SER:HA | 14:N:109:PRO:HD3 | 1.75 | 0.42 |
| 30:0:858:U:H2' | 30:0:859:C:C6 | 2.54 | 0.42 |
| 4:D:55:LYS:HA | 4:D:65:GLU:HG3 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 31:9:107:C:H5 | 41:9:9060:HOH:O | 2.02 | 0.42 |
| 16:P:97:ARG:HD2 | 41:P:163:HOH:O | 2.19 | 0.42 |
| 13:M:46:LEU:HD22 | 13:M:50:ARG:CD | 2.50 | 0.42 |
| 30:0:371:U:H2' | 30:0:372:A:H8 | 1.84 | 0.42 |
| 30:0:1589:G:C2 | 30:0:1605:G:N3 | 2.87 | 0.42 |
| 12:L:18:HIS:HB2 | 30:0:903:U:O4 | 2.20 | 0.42 |
| 25:Y:115:ARG:HH21 | 30:0:1266:U:H4' | 1.84 | 0.42 |
| 11:K:66:ARG:HD2 | 30:0:1992:U:OP2 | 2.19 | 0.42 |
| 3:C:51:TYR:O | 3:C:54:LEU:HB2 | 2.20 | 0.42 |
| 30:0:696:C:O2' | 30:0:697:G:H5' | 2.20 | 0.42 |
| 30:0:595:U:H6 | 30:0:595:U:O5' | 2.03 | 0.42 |
| 30:0:2435:U:H1' | 41:0:6264:HOH:O | 2.19 | 0.42 |
| 30:0:1139:U:H2' | 30:0:1140:C:C6 | 2.54 | 0.42 |
| 15:O:1:SER:HA | 41:O:7521:HOH:O | 2.18 | 0.42 |
| 3:C:237:GLU:HB2 | 41:C:8632:HOH:O | 2.19 | 0.42 |
| 5:E:84:MET:HB2 | 5:E:131:LEU:HB2 | 2.00 | 0.42 |
| 31:9:56:A:C3' | 31:9:57:A:H5'' | 2.50 | 0.42 |
| 2:B:51:VAL:CG2 | 2:B:330:VAL:HG22 | 2.47 | 0.42 |
| 2:B:56:ASP:HB3 | 2:B:322:ARG:HH21 | 1.83 | 0.42 |
| 11:K:87:ARG:CZ | 41:K:4854:HOH:O | 2.67 | 0.42 |
| 5:E:7:ILE:HD11 | 5:E:11:VAL:CG1 | 2.48 | 0.42 |
| 12:L:140:VAL:HB | 41:L:8861:HOH:O | 2.18 | 0.42 |
| 30:0:2064:U:H4' | 30:0:2653:A:OP1 | 2.18 | 0.42 |
| 24:X:66:THR:CG2 | 24:X:67:PRO:HD2 | 2.50 | 0.42 |
| 30:0:440:C:H2' | 30:0:441:A:C8 | 2.54 | 0.42 |
| 2:B:244:PRO:HB3 | 30:0:1234:U:N3 | 2.34 | 0.42 |
| 30:0:553:G:O4' | 30:0:1325:G:H5' | 2.19 | 0.42 |
| 12:L:89:PHE:CD1 | 12:L:89:PHE:N | 2.87 | 0.42 |
| 30:0:1386:G:O2' | 30:0:1387:G:H5' | 2.20 | 0.42 |
| 1:A:188:ASN:HA | 41:A:9046:HOH:O | 2.19 | 0.42 |
| 30:0:2842:G:H2' | 30:0:2843:A:H5' | 2.01 | 0.42 |
| 30:0:2042:U:H2' | 30:0:2043:U:C6 | 2.53 | 0.42 |
| 5:E:31:ARG:HH12 | 5:E:68:HIS:CE1 | 2.37 | 0.42 |
| 30:0:2592:G:H2' | 30:0:2593:C:C6 | 2.55 | 0.42 |
| 30:0:1182:C:H1' | 30:0:1192:A:C8 | 2.52 | 0.42 |
| 9:I:127:CYS:C | 9:I:129:SER:N | 2.73 | 0.42 |
| 30:0:506:G:N1 | 30:0:509:A:OP2 | 2.51 | 0.42 |
| 30:0:1298:U:H2' | 30:0:1299:G:H8 | 1.81 | 0.42 |
| 2:B:84:LEU:HB2 | 2:B:182:VAL:HG21 | 2.01 | 0.42 |
| 12:L:41:HIS:HE1 | 41:0:3673:HOH:O | 2.03 | 0.42 |
| 30:0:1405:U:H4' | 30:0:1406:A:H5'' | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 27:1:11:LYS:HG2 | 30:0:777:U:O2' | 2.20 | 0.42 |
| 16:P:13:VAL:HG21 | 16:P:41:ARG:HG2 | 2.00 | 0.42 |
| 31:9:47:A:C2 | 31:9:48:C:C2 | 3.08 | 0.42 |
| 30:0:816:G:H5' | 30:0:1598:A:H4' | 2.02 | 0.42 |
| 4:D:106:PHE:CZ | 4:D:130:VAL:HG11 | 2.54 | 0.42 |
| 13:M:193:LYS:HB3 | 30:0:392:U:C5' | 2.50 | 0.42 |
| 8:H:41:LYS:HE2 | 8:H:45:ASP:HB3 | 2.02 | 0.42 |
| 21:U:17:THR:HG23 | 21:U:18:GLY:N | 2.35 | 0.42 |
| 5:E:84:MET:CG | 5:E:168:ILE:HD13 | 2.50 | 0.42 |
| 31:9:59:C:H6 | 31:9:59:C:O5' | 2.03 | 0.42 |
| 23:W:39:ASP:HB2 | 41:W:3580:HOH:O | 2.20 | 0.42 |
| 14:N:25:ARG:HB3 | 30:0:2415:A:C2 | 2.55 | 0.42 |
| 25:Y:125:LYS:HB2 | 25:Y:126:PRO:HD2 | 2.02 | 0.42 |
| 30:0:292:G:H1' | 30:0:360:A:N6 | 2.34 | 0.42 |
| 30:0:537:G:H4' | 30:0:538:C:O5' | 2.20 | 0.42 |
| 30:0:695:C:H2' | 30:0:696:C:C6 | 2.55 | 0.42 |
| 10:J:12:VAL:HG22 | 10:J:116:LEU:HD21 | 2.02 | 0.42 |
| 30:0:644:G:N3 | 30:0:644:G:H5' | 2.35 | 0.42 |
| 18:R:132:ARG:NH2 | 30:0:2055:A:H4' | 2.35 | 0.42 |
| 30:0:766:A:HO2' | 30:0:767:A:H8 | 1.67 | 0.42 |
| 1:A:150:PRO:HB3 | 41:A:9069:HOH:O | 2.20 | 0.42 |
| 30:0:503:G:H2' | 30:0:504:G:H8 | 1.84 | 0.42 |
| 13:M:32:ARG:NH2 | 41:M:8901:HOH:O | 2.53 | 0.42 |
| 2:B:60:SER:HA | 2:B:61:PRO:HD3 | 1.94 | 0.42 |
| 3:C:127:ARG:HD3 | 3:C:129:HIS:HE1 | 1.84 | 0.42 |
| 30:0:2506:A:H1' | 41:0:4621:HOH:O | 2.20 | 0.42 |
| 1:A:190:ARG:HD2 | 30:0:1884:G:O6 | 2.19 | 0.42 |
| 30:0:2644:C:O2' | 30:0:2645:U:H5' | 2.19 | 0.42 |
| 14:N:48:VAL:HG11 | 14:N:55:ASP:HB3 | 2.00 | 0.42 |
| 2:B:77:PRO:C | 2:B:78:PRO:CA | 2.89 | 0.42 |
| 10:J:63:ILE:CG2 | 10:J:64:GLY:N | 2.82 | 0.42 |
| 2:B:294:TYR:CD1 | 2:B:294:TYR:C | 2.93 | 0.42 |
| 30:0:1741:U:H5'' | 41:0:3670:HOH:O | 2.20 | 0.42 |
| 30:0:2568:A:H2' | 30:0:2569:A:O4' | 2.20 | 0.42 |
| 5:E:35:TYR:HB3 | 5:E:38:ILE:HD12 | 2.02 | 0.42 |
| 18:R:26:LYS:HD3 | 18:R:62:HIS:CG | 2.55 | 0.42 |
| 1:A:17:ARG:HD2 | 41:A:9018:HOH:O | 2.19 | 0.42 |
| 18:R:100:ASP:C | 18:R:102:GLN:H | 2.23 | 0.42 |
| 30:0:2388:C:O2' | 30:0:2389:U:H5' | 2.19 | 0.42 |
| 13:M:67:VAL:HA | 41:M:8841:HOH:O | 2.20 | 0.42 |
| 5:E:81:GLU:HA | 5:E:133:VAL:O | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:E:84:MET:HG2 | 5:E:168:ILE:HA | 2.02 | 0.41 |
| 30:0:1183:C:C5 | 30:0:1192:A:OP1 | 2.71 | 0.41 |
| 30:0:1209:C:O2' | 30:0:1210:G:H5' | 2.20 | 0.41 |
| 8:H:23:ILE:CG2 | 8:H:123:ILE:CD1 | 2.97 | 0.41 |
| 14:N:79:PRO:HG3 | 14:N:143:ARG:C | 2.39 | 0.41 |
| 22:V:38:GLY:C | 22:V:40:PRO:HD2 | 2.39 | 0.41 |
| 12:L:133:VAL:HB | 41:L:8861:HOH:O | 2.20 | 0.41 |
| 1:A:48:ASP:HA | 1:A:49:PRO:HD3 | 1.85 | 0.41 |
| 6:F:38:LYS:O | 6:F:42:ARG:HG3 | 2.19 | 0.41 |
| 30:0:170:U:H2' | 30:0:171:C:H5' | 2.01 | 0.41 |
| 30:0:1342:C:O2' | 30:0:1343:C:H5' | 2.19 | 0.41 |
| 8:H:50:ILE:HD12 | 8:H:149:VAL:CG1 | 2.49 | 0.41 |
| 30:0:1236:A:H2' | 30:0:1237:U:O4' | 2.20 | 0.41 |
| 20:T:43:ASN:OD1 | 30:0:80:A:H3' | 2.19 | 0.41 |
| 30:0:553:G:C2' | 30:0:554:G:H5' | 2.50 | 0.41 |
| 30:0:2499:U:O2' | 30:0:2500:C:H5' | 2.19 | 0.41 |
| 30:0:2642:G:H2' | 30:0:2643:G:O4' | 2.19 | 0.41 |
| 2:B:241:PRO:HG3 | 30:0:2606:G:N2 | 2.34 | 0.41 |
| 30:0:2512:U:H4' | 30:0:2514:U:O4 | 2.20 | 0.41 |
| 30:0:1074:G:H4' | 30:0:1260:G:C6 | 2.55 | 0.41 |
| 4:D:169:THR:C | 4:D:170:TYR:HD1 | 2.23 | 0.41 |
| 23:W:88:THR:HG23 | 23:W:110:GLN:CB | 2.43 | 0.41 |
| 7:G:19:GLU:O | 7:G:23:ILE:HG13 | 2.20 | 0.41 |
| 24:X:49:ARG:CG | 24:X:49:ARG:O | 2.65 | 0.41 |
| 16:P:98:ILE:HD12 | 16:P:102:ARG:CZ | 2.50 | 0.41 |
| 30:0:814:G:H2' | 30:0:815:U:H6 | 1.85 | 0.41 |
| 30:0:583:C:H2' | 30:0:584:U:C6 | 2.55 | 0.41 |
| 30:0:2329:C:H2' | 30:0:2330:U:C6 | 2.56 | 0.41 |
| 30:0:2257:G:H4' | 30:0:2259:C:C2 | 2.55 | 0.41 |
| 12:L:33:ALA:HB2 | 30:0:165:A:H5'' | 2.01 | 0.41 |
| 30:0:912:A:C4 | 30:0:1294:A:C2 | 3.08 | 0.41 |
| 1:A:105:VAL:HG11 | 1:A:154:ALA:CB | 2.50 | 0.41 |
| 29:3:22:VAL:HG11 | 29:3:67:LEU:HD13 | 2.02 | 0.41 |
| 8:H:59:GLN:NE2 | 8:H:96:GLN:HG2 | 2.34 | 0.41 |
| 30:0:1207:A:OP2 | 30:0:1207:A:H8 | 2.03 | 0.41 |
| 1:A:194:MET:HE1 | 1:A:199:HIS:HB2 | 2.01 | 0.41 |
| 14:N:48:VAL:HG13 | 14:N:55:ASP:HB3 | 1.99 | 0.41 |
| 2:B:316:ARG:HB2 | 30:0:2768:A:C8 | 2.55 | 0.41 |
| 3:C:67:GLN:HG2 | 41:C:8627:HOH:O | 2.19 | 0.41 |
| 28:2:29:THR:O | 28:2:30:ASP:C | 2.59 | 0.41 |
| 25:Y:117:LEU:HD13 | 25:Y:174:VAL:CG1 | 2.48 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 12:L:126:SER:O | 12:L:129:ALA:HB3 | 2.20 | 0.41 |
| 2:B:139:ASP:CB | 2:B:165:ARG:HE | 2.32 | 0.41 |
| 30:0:1910:A:H2' | 30:0:1911:C:C6 | 2.56 | 0.41 |
| 27:1:8:GLN:HE22 | 27:1:11:LYS:NZ | 2.18 | 0.41 |
| 17:Q:94:GLN:NE2 | 30:0:1019:C:O2 | 2.53 | 0.41 |
| 30:0:2281:C:H2' | 30:0:2282:U:H5' | 2.02 | 0.41 |
| 30:0:1806:G:HO2' | 30:0:2883:A:H2 | 1.65 | 0.41 |
| 30:0:1366:C:H1' | 41:0:3161:HOH:O | 2.20 | 0.41 |
| 25:Y:216:ARG:O | 25:Y:219:GLU:HG2 | 2.20 | 0.41 |
| 14:N:103:ASP:OD1 | 14:N:103:ASP:C | 2.58 | 0.41 |
| 30:0:494:C:H2' | 30:0:496:G:OP2 | 2.20 | 0.41 |
| 15:O:112:ARG:HD2 | 41:0:3574:HOH:O | 2.21 | 0.41 |
| 30:0:307:G:H3' | 30:0:342:C:OP2 | 2.20 | 0.41 |
| 24:X:9:VAL:HG12 | 41:X:6893:HOH:O | 2.21 | 0.41 |
| 10:J:143:LYS:HG3 | 10:J:145:TRP:CE2 | 2.55 | 0.41 |
| 30:0:636:G:H1' | 30:0:2058:G:C4 | 2.55 | 0.41 |
| 14:N:35:VAL:HG11 | 31:9:6:C:H4' | 2.03 | 0.41 |
| 30:0:541:C:O2' | 30:0:542:A:H5'' | 2.20 | 0.41 |
| 2:B:333:GLU:HB2 | 21:U:14:GLU:OE2 | 2.20 | 0.41 |
| 4:D:44:ILE:HG12 | 4:D:44:ILE:O | 2.21 | 0.41 |
| 2:B:255:GLY:O | 2:B:257:THR:HG23 | 2.19 | 0.41 |
| 30:0:2072:G:H3' | 30:0:2073:G:H5'' | 2.03 | 0.41 |
| 30:0:1972:U:H2' | 30:0:1973:A:C5' | 2.50 | 0.41 |
| 30:0:1973:A:H2' | 30:0:1974:G:O4' | 2.21 | 0.41 |
| 30:0:2637:A:H4' | 30:0:2638:G:O5' | 2.20 | 0.41 |
| 30:0:1211:G:H2' | 30:0:1212:C:C6 | 2.55 | 0.41 |
| 2:B:28:SER:HB3 | 30:0:2807:U:OP1 | 2.21 | 0.41 |
| 3:C:78:ARG:O | 3:C:80:VAL:N | 2.51 | 0.41 |
| 12:L:129:ALA:O | 12:L:133:VAL:HG23 | 2.20 | 0.41 |
| 30:0:1565:C:O4' | 30:0:2738:G:H1' | 2.21 | 0.41 |
| 12:L:98:GLU:O | 12:L:99:GLU:CB | 2.68 | 0.41 |
| 25:Y:99:ALA:HB2 | 25:Y:233:TYR:CE2 | 2.55 | 0.41 |
| 30:0:187:A:H3' | 30:0:188:C:C6 | 2.56 | 0.41 |
| 3:C:109:LEU:O | 3:C:109:LEU:HD12 | 2.19 | 0.41 |
| 3:C:123:LEU:HA | 3:C:123:LEU:HD23 | 1.87 | 0.41 |
| 30:0:970:U:O5' | 30:0:970:U:H6 | 2.04 | 0.41 |
| 30:0:1039:G:H2' | 30:0:1040:A:O4' | 2.20 | 0.41 |
| 2:B:70:PRO:HG3 | 30:0:2719:A:C2 | 2.55 | 0.41 |
| 30:0:2271:G:H8 | 41:0:4562:HOH:O | 2.04 | 0.41 |
| 30:0:1649:G:H1' | 41:0:6370:HOH:O | 2.20 | 0.41 |
| 8:H:6:ALA:CA | 8:H:61:ARG:HH12 | 2.32 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:61:PHE:CD2 | 3:C:65:ARG:CZ | 3.04 | 0.41 |
| 2:B:198:GLU:HA | 41:B:9143:HOH:O | 2.20 | 0.41 |
| 10:J:107:ASN:HD22 | 10:J:108:PRO:N | 2.19 | 0.41 |
| 26:Z:35:SER:HB3 | 26:Z:47:ARG:HB2 | 2.02 | 0.41 |
| 1:A:36:ASP:O | 1:A:36:ASP:CG | 2.59 | 0.41 |
| 2:B:235:ARG:HD3 | 30:0:2091:G:O3' | 2.21 | 0.41 |
| 25:Y:186:ARG:HG2 | 25:Y:186:ARG:NH1 | 2.33 | 0.41 |
| 30:0:1741:U:H3' | 41:0:3670:HOH:O | 2.20 | 0.41 |
| 12:L:67:ARG:HB2 | 12:L:111:ALA:O | 2.21 | 0.41 |
| 30:0:2081:A:H2' | 30:0:2082:G:O4' | 2.21 | 0.41 |
| 30:0:222:A:H2' | 30:0:223:G:O4' | 2.20 | 0.41 |
| 30:0:415:A:O2' | 30:0:416:G:H5' | 2.20 | 0.41 |
| 13:M:46:LEU:HD22 | 13:M:50:ARG:HD2 | 2.02 | 0.41 |
| 25:Y:100:ARG:HD2 | 25:Y:232:THR:HB | 2.02 | 0.41 |
| 12:L:36:ASP:HB2 | 41:L:8839:HOH:O | 2.20 | 0.41 |
| 30:0:1291:A:H2 | 41:0:6129:HOH:O | 2.03 | 0.41 |
| 1:A:169:PHE:O | 1:A:171:LYS:N | 2.47 | 0.41 |
| 2:B:66:GLU:OE1 | 2:B:328:ARG:HD2 | 2.20 | 0.41 |
| 12:L:57:VAL:HG12 | 12:L:57:VAL:O | 2.20 | 0.41 |
| 5:E:7:ILE:HD11 | 5:E:11:VAL:C | 2.40 | 0.41 |
| 12:L:125:PHE:CZ | 12:L:140:VAL:HG22 | 2.56 | 0.41 |
| 30:0:2831:C:C2' | 30:0:2832:C:H5' | 2.51 | 0.41 |
| 12:L:34:GLY:HA2 | 41:0:6243:HOH:O | 2.19 | 0.41 |
| 23:W:130:HIS:C | 23:W:136:GLY:HA3 | 2.39 | 0.41 |
| 18:R:61:GLN:CD | 41:R:8945:HOH:O | 2.59 | 0.41 |
| 2:B:277:GLU:N | 2:B:278:PRO:CD | 2.84 | 0.41 |
| 29:3:6:ARG:NH1 | 29:3:21:GLU:HG3 | 2.35 | 0.41 |
| 28:2:2:LYS:HG3 | 30:0:1486:A:C4 | 2.55 | 0.41 |
| 8:H:100:GLU:HB3 | 8:H:124:VAL:HG11 | 2.03 | 0.41 |
| 30:0:2704:C:H2' | 30:0:2705:U:O4' | 2.20 | 0.41 |
| 30:0:2296:C:H2' | 30:0:2297:U:H6 | 1.85 | 0.41 |
| 21:U:20:MET:CG | 21:U:28:THR:HG23 | 2.50 | 0.41 |
| 6:F:84:GLY:O | 6:F:89:LEU:HB2 | 2.21 | 0.41 |
| 4:D:27:ILE:HD11 | 4:D:37:ALA:HB2 | 2.01 | 0.41 |
| 30:0:2072:G:H3' | 30:0:2073:G:C5' | 2.51 | 0.41 |
| 20:T:96:VAL:CG1 | 20:T:97:ARG:N | 2.84 | 0.41 |
| 5:E:7:ILE:HG13 | 5:E:11:VAL:HB | 2.03 | 0.41 |
| 24:X:43:VAL:HG12 | 24:X:47:ALA:HB3 | 2.02 | 0.41 |
| 31:9:39:U:H1' | 31:9:44:A:N6 | 2.35 | 0.41 |
| 26:Z:54:GLU:HA | 26:Z:57:MET:HB3 | 2.02 | 0.41 |
| 27:1:2:GLY:O | 27:1:6:PRO:HG2 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:219:ASN:O | 3:C:222:ASP:OD1 | 2.38 | 0.41 |
| 9:I:80:PHE:N | 9:I:80:PHE:CD1 | 2.89 | 0.41 |
| 13:M:68:ARG:HD3 | 13:M:68:ARG:O | 2.20 | 0.41 |
| 30:0:1497:G:H4' | 30:0:1627:G:O2' | 2.21 | 0.41 |
| 5:E:21:THR:HG23 | 5:E:30:THR:OG1 | 2.20 | 0.41 |
| 25:Y:207:SER:HB3 | 30:0:1335:C:OP2 | 2.20 | 0.41 |
| 30:0:2135:A:O2' | 30:0:2136:G:H5' | 2.21 | 0.41 |
| 30:0:278:A:H2' | 30:0:279:C:O4' | 2.20 | 0.41 |
| 10:J:13:ASP:OD1 | 10:J:15:ARG:HB3 | 2.20 | 0.41 |
| 30:0:1375:A:H1' | 30:0:2045:G:O5' | 2.21 | 0.41 |
| 20:T:40:VAL:HG23 | 20:T:119:ALA:OXT | 2.21 | 0.41 |
| 6:F:60:VAL:O | 6:F:60:VAL:CG1 | 2.69 | 0.41 |
| 30:0:875:A:H5' | 30:0:876:A:N7 | 2.35 | 0.41 |
| 28:2:48:ASP:O | 28:2:49:GLU:CB | 2.68 | 0.41 |
| 31:9:35:C:H5'' | 41:9:9078:HOH:O | 2.21 | 0.41 |
| 2:B:112:THR:OG1 | 2:B:158:LYS:HG3 | 2.20 | 0.41 |
| 30:0:1445:G:N2 | 30:0:1678:A:H1' | 2.36 | 0.41 |
| 29:3:28:GLY:HA3 | 30:0:2434:A:O3' | 2.20 | 0.41 |
| 30:0:220:C:H1' | 41:0:6586:HOH:O | 2.21 | 0.41 |
| 30:0:2724:U:H2' | 30:0:2725:G:O4' | 2.20 | 0.41 |
| 30:0:1533:A:H4' | 30:0:1534:C:O4' | 2.20 | 0.41 |
| 30:0:1809:G:N2 | 30:0:1811:A:H3' | 2.35 | 0.41 |
| 30:0:1816:C:H2' | 30:0:1817:U:O4' | 2.21 | 0.41 |
| 29:3:91:GLN:O | 29:3:92:GLU:HB2 | 2.20 | 0.41 |
| 15:O:32:ARG:HD3 | 15:O:32:ARG:C | 2.42 | 0.41 |
| 18:R:8:ALA:HB3 | 18:R:15:LYS:HE2 | 2.02 | 0.41 |
| 9:I:95:LEU:HG | 9:I:132:VAL:CG1 | 2.51 | 0.41 |
| 4:D:154:LYS:H | 4:D:154:LYS:CD | 2.19 | 0.41 |
| 30:0:1603:A:C5' | 30:0:1605:G:H5' | 2.50 | 0.41 |
| 20:T:40:VAL:HG22 | 20:T:41:ARG:N | 2.35 | 0.41 |
| 30:0:1165:G:H1' | 30:0:1174:A:H1' | 2.02 | 0.41 |
| 27:1:1:THR:HB | 41:0:7939:HOH:O | 2.21 | 0.41 |
| 22:V:42:ASN:O | 22:V:44:GLY:N | 2.53 | 0.41 |
| 30:0:2806:C:H2' | 30:0:2807:U:C6 | 2.56 | 0.41 |
| 28:2:25:VAL:O | 28:2:29:THR:HG23 | 2.21 | 0.41 |
| 8:H:154:ARG:NH2 | 30:0:2503:A:OP1 | 2.53 | 0.41 |
| 30:0:907:A:H4' | 30:0:1328:A:C2 | 2.56 | 0.41 |
| 21:U:50:GLU:O | 21:U:56:ARG:CG | 2.69 | 0.41 |
| 20:T:77:VAL:N | 20:T:78:THR:HG23 | 2.35 | 0.41 |
| 31:9:22:G:H5' | 31:9:23:U:OP1 | 2.20 | 0.41 |
| 1:A:51:ARG:HD2 | 30:0:1874:U:OP1 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:53:ALA:HB3 | 41:A:9081:HOH:O | 2.19 | 0.41 |
| 4:D:52:THR:CG2 | 30:0:2346:C:O3' | 2.69 | 0.41 |
| 30:0:945:U:H2' | 30:0:946:C:H6 | 1.86 | 0.41 |
| 1:A:82:VAL:HA | 1:A:93:THR:O | 2.21 | 0.41 |
| 13:M:77:HIS:CE1 | 13:M:86:GLN:HG2 | 2.55 | 0.41 |
| 18:R:44:VAL:HG13 | 18:R:89:LEU:HD22 | 2.03 | 0.41 |
| 3:C:168:ARG:NH1 | 30:0:1310:U:OP2 | 2.54 | 0.41 |
| 6:F:26:THR:CG2 | 6:F:102:GLY:HA3 | 2.50 | 0.41 |
| 30:0:1343:C:H2' | 30:0:1344:G:O5' | 2.21 | 0.41 |
| 19:S:23:LYS:HE2 | 41:S:3430:HOH:O | 2.19 | 0.41 |
| 29:3:6:ARG:HA | 29:3:20:HIS:O | 2.21 | 0.41 |
| 16:P:37:ARG:HH21 | 30:0:1502:A:P | 2.44 | 0.41 |
| 30:0:813:C:H2' | 30:0:814:G:O4' | 2.21 | 0.41 |
| 30:0:1902:G:N2 | 30:0:1936:C:C2 | 2.88 | 0.41 |
| 6:F:20:LEU:HB2 | 6:F:49:PHE:CZ | 2.56 | 0.41 |
| 2:B:82:VAL:HG11 | 2:B:101:TRP:CZ3 | 2.55 | 0.41 |
| 2:B:79:MET:O | 2:B:187:GLU:HA | 2.21 | 0.41 |
| 5:E:105:GLU:HG2 | 5:E:113:PRO:HB3 | 2.02 | 0.41 |
| 30:0:1980:U:O2' | 30:0:1981:A:H5' | 2.20 | 0.41 |
| 8:H:157:TYR:CD1 | 8:H:157:TYR:C | 2.93 | 0.41 |
| 30:0:2515:C:H2' | 30:0:2516:G:O4' | 2.20 | 0.41 |
| 30:0:2517:A:C2' | 30:0:2518:C:H5' | 2.50 | 0.41 |
| 30:0:2526:C:O2' | 30:0:2527:U:H5' | 2.21 | 0.41 |
| 3:C:93:LYS:O | 3:C:98:ARG:NH2 | 2.53 | 0.41 |
| 3:C:96:LYS:NZ | 30:0:1351:G:OP1 | 2.43 | 0.41 |
| 16:P:22:TRP:CH2 | 16:P:24:ASN:HA | 2.56 | 0.41 |
| 23:W:7:LEU:HD23 | 23:W:7:LEU:HA | 1.92 | 0.41 |
| 26:Z:80:GLN:HA | 26:Z:86:TYR:O | 2.21 | 0.41 |
| 2:B:202:VAL:HG11 | 2:B:301:VAL:HG13 | 2.02 | 0.41 |
| 30:0:74:G:H2' | 30:0:75:U:C6 | 2.56 | 0.41 |
| 30:0:1409:G:C2 | 30:0:1410:G:C8 | 3.09 | 0.41 |
| 14:N:171:HIS:CE1 | 41:N:8862:HOH:O | 2.74 | 0.41 |
| 30:0:2290:U:H2' | 41:0:7931:HOH:O | 2.19 | 0.41 |
| 30:0:362:G:O2' | 30:0:363:C:H5' | 2.21 | 0.41 |
| 30:0:731:U:H2' | 30:0:732:C:C6 | 2.56 | 0.41 |
| 30:0:542:A:C5' | 30:0:542:A:C8 | 2.98 | 0.41 |
| 20:T:9:LYS:CE | 20:T:13:ARG:NH1 | 2.67 | 0.41 |
| 30:0:2509:A:H2' | 30:0:2510:C:O4' | 2.20 | 0.41 |
| 14:N:167:ASP:C | 14:N:168:LEU:HG | 2.42 | 0.41 |
| 30:0:2089:A:C2' | 30:0:2090:G:H5' | 2.50 | 0.41 |
| 1:A:26:ASP:CG | 1:A:26:ASP:O | 2.58 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 30:0:101:C:H2' | 30:0:102:A:H8 | 1.84 | 0.41 |
| 15:O:26:TRP:HA | 15:O:26:TRP:CE3 | 2.56 | 0.41 |
| 22:V:13:PRO:HA | 22:V:16:ARG:NH1 | 2.35 | 0.41 |
| 27:1:11:LYS:HA | 41:1:5026:HOH:O | 2.22 | 0.41 |
| 12:L:5:LYS:NZ | 30:0:1353:C:N3 | 2.69 | 0.41 |
| 23:W:13:MET:HE2 | 23:W:17:ILE:HG22 | 2.02 | 0.41 |
| 20:T:87:VAL:HB | 20:T:88:PRO:HD2 | 2.03 | 0.41 |
| 4:D:24:HIS:HB2 | 4:D:72:LYS:CB | 2.51 | 0.41 |
| 30:0:1588:G:H1' | 30:0:1607:A:N6 | 2.36 | 0.41 |
| 30:0:541:C:C3' | 30:0:542:A:H5'' | 2.49 | 0.40 |
| 8:H:61:ARG:O | 8:H:65:LEU:HD22 | 2.21 | 0.40 |
| 13:M:134:ILE:O | 13:M:136:PRO:HD3 | 2.21 | 0.40 |
| 30:0:1166:A:H61 | 30:0:1180:U:H3 | 1.69 | 0.40 |
| 23:W:110:GLN:HE21 | 23:W:110:GLN:CA | 2.30 | 0.40 |
| 2:B:265:LEU:CD2 | 2:B:316:ARG:HD3 | 2.52 | 0.40 |
| 13:M:93:ARG:HD2 | 30:0:1470:A:OP1 | 2.22 | 0.40 |
| 13:M:48:LYS:HE3 | 13:M:52:GLN:NE2 | 2.36 | 0.40 |
| 3:C:80:VAL:HA | 3:C:81:PRO:HD3 | 1.87 | 0.40 |
| 20:T:96:VAL:HG13 | 20:T:97:ARG:N | 2.36 | 0.40 |
| 20:T:77:VAL:C | 20:T:78:THR:CA | 2.90 | 0.40 |
| 10:J:75:PRO:HD3 | 10:J:136:SER:CB | 2.51 | 0.40 |
| 30:0:2361:A:H2' | 30:0:2362:A:O4' | 2.21 | 0.40 |
| 5:E:170:ARG:HE | 5:E:170:ARG:HB2 | 1.63 | 0.40 |
| 1:A:146:LYS:NZ | 30:0:1855:G:O3' | 2.53 | 0.40 |
| 30:0:243:A:H2 | 30:0:274:G:N3 | 2.19 | 0.40 |
| 30:0:2698:G:H2' | 30:0:2699:A:C8 | 2.56 | 0.40 |
| 30:0:567:U:O5' | 30:0:567:U:H6 | 2.04 | 0.40 |
| 25:Y:141:THR:HG23 | 41:0:7305:HOH:O | 2.21 | 0.40 |
| 11:K:18:ILE:HG22 | 11:K:93:ASN:HB2 | 2.03 | 0.40 |
| 29:3:86:GLY:HA3 | 30:0:2318:C:OP1 | 2.21 | 0.40 |
| 30:0:639:A:H2' | 30:0:640:G:C8 | 2.55 | 0.40 |
| 30:0:466:A:H2' | 30:0:467:G:O4' | 2.20 | 0.40 |
| 30:0:1117:A:H2' | 41:0:5743:HOH:O | 2.20 | 0.40 |
| 2:B:254:GLN:NE2 | 41:B:9065:HOH:O | 2.53 | 0.40 |
| 30:0:2504:A:H2' | 30:0:2505:G:O4' | 2.21 | 0.40 |
| 24:X:23:HIS:HE1 | 30:0:2044:G:OP1 | 2.04 | 0.40 |
| 2:B:205:VAL:O | 2:B:307:ARG:NE | 2.49 | 0.40 |
| 26:Z:45:VAL:CG2 | 30:0:1887:U:OP1 | 2.69 | 0.40 |
| 10:J:39:VAL:HG12 | 10:J:40:ASN:CG | 2.42 | 0.40 |
| 30:0:2250:G:H2' | 30:0:2251:G:O4' | 2.21 | 0.40 |
| 2:B:101:TRP:HB2 | 2:B:119:HIS:CD2 | 2.57 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 30:0:1014:A:H2' | 30:0:1015:C:H5' | 2.02 | 0.40 |
| 3:C:214:THR:HB | 41:C:8522:HOH:O | 2.22 | 0.40 |
| 11:K:22:ASP:OD1 | 11:K:22:ASP:C | 2.60 | 0.40 |
| 30:0:2566:A:H2 | 30:0:2695:C:O2 | 2.04 | 0.40 |
| 30:0:2887:G:H2' | 30:0:2888:U:O4' | 2.20 | 0.40 |
| 30:0:2079:G:H2' | 30:0:2080:G:O4' | 2.21 | 0.40 |
| 30:0:1889:C:H2' | 30:0:1890:U:O4' | 2.21 | 0.40 |
| 3:C:236:THR:O | 3:C:237:GLU:C | 2.59 | 0.40 |
| 15:O:32:ARG:HG2 | 15:O:32:ARG:HH11 | 1.86 | 0.40 |
| 10:J:49:ARG:NH1 | 30:0:1119:G:OP1 | 2.55 | 0.40 |
| 11:K:125:ALA:O | 11:K:127:ALA:N | 2.47 | 0.40 |
| 4:D:169:THR:HG22 | 4:D:170:TYR:HD1 | 1.86 | 0.40 |
| 13:M:107:ARG:O | 13:M:110:PRO:HD3 | 2.21 | 0.40 |
| 11:K:98:VAL:HG13 | 11:K:102:GLU:CA | 2.51 | 0.40 |
| 30:0:2661:U:H3 | 30:0:2812:A:H62 | 1.70 | 0.40 |
| 23:W:55:GLY:HA3 | 23:W:146:ILE:HG13 | 2.03 | 0.40 |
| 14:N:154:LEU:C | 14:N:156:GLU:H | 2.25 | 0.40 |
| 30:0:64:G:H2' | 30:0:65:C:O4' | 2.22 | 0.40 |
| 19:S:29:ASP:OD1 | 19:S:31:ARG:NH1 | 2.55 | 0.40 |
| 6:F:70:LYS:C | 6:F:72:VAL:H | 2.24 | 0.40 |
| 2:B:145:HIS:HD2 | 2:B:146:THR:O | 2.04 | 0.40 |
| 9:I:133:THR:HG22 | 9:I:134:ILE:N | 2.37 | 0.40 |
| 30:0:2549:C:H2' | 30:0:2550:U:O4' | 2.21 | 0.40 |
| 14:N:41:LYS:HE3 | 41:9:9021:HOH:O | 2.20 | 0.40 |
| 30:0:107:U:H2' | 30:0:108:U:H5' | 2.02 | 0.40 |
| 12:L:61:ALA:HB2 | 12:L:105:TYR:CZ | 2.55 | 0.40 |
| 30:0:1573:A:H2' | 30:0:1574:C:O4' | 2.21 | 0.40 |
| 18:R:100:ASP:C | 18:R:102:GLN:N | 2.73 | 0.40 |
| 1:A:203:GLY:HA2 | 41:A:9022:HOH:O | 2.21 | 0.40 |
| 13:M:74:LYS:HE2 | 30:0:159:G:OP1 | 2.21 | 0.40 |
| 17:Q:47:VAL:HB | 17:Q:90:HIS:CE1 | 2.57 | 0.40 |
| 14:N:64:SER:C | 14:N:66:LEU:H | 2.24 | 0.40 |
| 30:0:1190:G:H2' | 41:0:4926:HOH:O | 2.20 | 0.40 |
| 23:W:21:LEU:HD23 | 23:W:21:LEU:HA | 1.78 | 0.40 |
| 18:R:104:PHE:HB2 | 18:R:109:MET:HE1 | 2.03 | 0.40 |
| 30:0:368:C:H2' | 30:0:369:G:H5' | 2.02 | 0.40 |
| 13:M:108:THR:O | 13:M:110:PRO:HD2 | 2.20 | 0.40 |
| 2:B:304:PRO:HD2 | 2:B:307:ARG:NE | 2.37 | 0.40 |
| 30:0:2909:G:O2' | 30:0:2910:A:H5' | 2.21 | 0.40 |
| 4:D:36:ASN:HB3 | 41:D:7502:HOH:O | 2.21 | 0.40 |
| 7:G:27:ILE:HD12 | 7:G:70:ALA:HB1 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:J:107:ASN:HD22 | 10:J:109:TYR:H | 1.70 | 0.40 |
| 2:B:102:THR:HB | 41:B:9117:HOH:O | 2.21 | 0.40 |
| 11:K:66:ARG:NH2 | 30:0:1994:A:OP1 | 2.54 | 0.40 |
| 30:0:2415:A:C2' | 30:0:2416:G:H5' | 2.49 | 0.40 |
| 28:2:5:LYS:HD2 | 30:0:1675:C:H5'' | 2.03 | 0.40 |
| 16:P:37:ARG:O | 16:P:41:ARG:HG3 | 2.21 | 0.40 |
| 30:0:1423:C:O2' | 30:0:1424:A:H5' | 2.21 | 0.40 |
| 30:0:2883:A:H2' | 30:0:2884:G:O4' | 2.20 | 0.40 |
| 20:T:107:LYS:O | 20:T:111:ARG:HB2 | 2.21 | 0.40 |
| 30:0:1484:G:H2' | 41:0:3018:HOH:O | 2.21 | 0.40 |
| 13:M:147:LEU:O | 13:M:150:ILE:HG22 | 2.22 | 0.40 |
| 30:0:581:G:O2' | 30:0:582:U:H5' | 2.21 | 0.40 |
| 16:P:57:ASN:HB3 | 41:0:7671:HOH:O | 2.21 | 0.40 |
| 18:R:76:ASP:HA | 41:R:8919:HOH:O | 2.20 | 0.40 |
| 25:Y:210:GLY:N | 30:0:1313:A:H5'' | 2.36 | 0.40 |
| 25:Y:210:GLY:H | 30:0:1313:A:H5'' | 1.86 | 0.40 |
| 4:D:27:ILE:HG21 | 41:D:5858:HOH:O | 2.21 | 0.40 |
| 11:K:98:VAL:CG1 | 11:K:99:ASP:N | 2.84 | 0.40 |
| 30:0:2839:C:H2' | 30:0:2840:A:H5'' | 2.04 | 0.40 |
| 12:L:53:ARG:NH2 | 12:L:57:VAL:CG1 | 2.81 | 0.40 |
| 30:0:69:A:H5' | 30:0:69:A:H8 | 1.84 | 0.40 |
| 22:V:16:ARG:HH12 | 22:V:65:ASP:C | 2.25 | 0.40 |
| 30:0:185:G:C4' | 30:0:186:A:H4' | 2.52 | 0.40 |
| 30:0:790:A:H1' | 30:0:1710:A:C2' | 2.51 | 0.40 |
| 30:0:1948:G:H2' | 30:0:1949:G:O4' | 2.21 | 0.40 |
| 30:0:1522:A:H2' | 30:0:1523:G:C5' | 2.51 | 0.40 |
| 30:0:1773:G:N2 | 30:0:1774:G:C8 | 2.89 | 0.40 |
| 30:0:105:G:O2' | 30:0:106:A:H5' | 2.21 | 0.40 |
| 6:F:13:GLU:OE1 | 6:F:77:VAL:HG13 | 2.22 | 0.40 |
| 1:A:125:ASN:HB3 | 1:A:158:VAL:HG12 | 2.03 | 0.40 |
| 30:0:1894:C:N4 | 30:0:1939:U:H2' | 2.36 | 0.40 |
| 30:0:830:G:O2' | 30:0:831:U:H5' | 2.21 | 0.40 |
| 30:0:1764:C:H2' | 30:0:1765:G:O4' | 2.22 | 0.40 |
| 30:0:306:A:H2' | 30:0:341:C:O2' | 2.22 | 0.40 |
| 30:0:2735:U:H2' | 30:0:2736:U:C6 | 2.56 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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 | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1 | A | 233/240 (97%) | 197 (84%) | 31 (13%) | 5 (2%) | 9 | 29 |
| 2 | B | 333/338 (98%) | 300 (90%) | 29 (9%) | 4 (1%) | 16 | 47 |
| 3 | C | 242/246 (98%) | 215 (89%) | 25 (10%) | 2 (1%) | 24 | 58 |
| 4 | D | 132/177 (75%) | 98 (74%) | 23 (17%) | 11 (8%) | 1 | 2 |
| 5 | E | 168/178 (94%) | 159 (95%) | 9 (5%) | 0 | 100 | 100 |
| 6 | F | 115/120 (96%) | 97 (84%) | 13 (11%) | 5 (4%) | 3 | 10 |
| 7 | G | 25/348 (7%) | 22 (88%) | 3 (12%) | 0 | 100 | 100 |
| 8 | H | 154/177 (87%) | 131 (85%) | 21 (14%) | 2 (1%) | 15 | 44 |
| 9 | I | 66/162 (41%) | 45 (68%) | 19 (29%) | 2 (3%) | 5 | 18 |
| 10 | J | 138/145 (95%) | 126 (91%) | 9 (6%) | 3 (2%) | 8 | 28 |
| 11 | K | 128/132 (97%) | 117 (91%) | 9 (7%) | 2 (2%) | 12 | 38 |
| 12 | L | 139/165 (84%) | 115 (83%) | 19 (14%) | 5 (4%) | 4 | 14 |
| 13 | M | 190/196 (97%) | 171 (90%) | 17 (9%) | 2 (1%) | 17 | 50 |
| 14 | N | 182/187 (97%) | 156 (86%) | 18 (10%) | 8 (4%) | 3 | 10 |
| 15 | O | 111/116 (96%) | 103 (93%) | 8 (7%) | 0 | 100 | 100 |
| 16 | P | 139/149 (93%) | 133 (96%) | 6 (4%) | 0 | 100 | 100 |
| 17 | Q | 91/96 (95%) | 82 (90%) | 8 (9%) | 1 (1%) | 17 | 50 |
| 18 | R | 146/155 (94%) | 132 (90%) | 13 (9%) | 1 (1%) | 26 | 62 |
| 19 | S | 77/85 (91%) | 73 (95%) | 4 (5%) | 0 | 100 | 100 |
| 20 | T | 115/120 (96%) | 109 (95%) | 4 (4%) | 2 (2%) | 11 | 36 |
| 21 | U | 51/67 (76%) | 46 (90%) | 4 (8%) | 1 (2%) | 9 | 30 |
| 22 | V | 63/71 (89%) | 57 (90%) | 5 (8%) | 1 (2%) | 12 | 38 |
| 23 | W | 150/154 (97%) | 140 (93%) | 9 (6%) | 1 (1%) | 26 | 62 |
| 24 | X | 78/92 (85%) | 70 (90%) | 7 (9%) | 1 (1%) | 15 | 44 |
| 25 | Y | 140/240 (58%) | 135 (96%) | 5 (4%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 26 | Z | 69/116 (60%) | 60 (87%) | 6 (9%) | 3 (4%) | 3 | 10 |
| 27 | 1 | 54/57 (95%) | 48 (89%) | 6 (11%) | 0 | 100 | 100 |
| 28 | 2 | 42/50 (84%) | 36 (86%) | 6 (14%) | 0 | 100 | 100 |
| 29 | 3 | 88/92 (96%) | 83 (94%) | 4 (4%) | 1 (1%) | 17 | 50 |
| All | All | 3659/4471 (82%) | 3256 (89%) | 340 (9%) | 63 (2%) | 11 | 36 |

All (63) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 27 | LEU |
| 1 | A | 34 | ASP |
| 1 | A | 37 | VAL |
| 4 | D | 27 | ILE |
| 4 | D | 171 | ASP |
| 6 | F | 101 | ALA |
| 12 | L | 80 | ASP |
| 14 | N | 154 | LEU |
| 14 | N | 183 | ASP |
| 14 | N | 184 | ILE |
| 18 | R | 114 | VAL |
| 21 | U | 55 | ALA |
| 26 | Z | 44 | ARG |
| 26 | Z | 105 | ARG |
| 29 | 3 | 56 | PRO |
| 1 | A | 204 | GLY |
| 4 | D | 16 | PRO |
| 4 | D | 97 | GLN |
| 4 | D | 147 | ALA |
| 6 | F | 27 | GLY |
| 9 | I | 113 | SER |
| 12 | L | 82 | ALA |
| 14 | N | 165 | ALA |
| 14 | N | 167 | ASP |
| 20 | T | 44 | ALA |
| 20 | T | 53 | GLY |
| 22 | V | 43 | PRO |
| 24 | X | 87 | ALA |
| 1 | A | 119 | ALA |
| 2 | B | 184 | ASP |
| 3 | C | 121 | ALA |
| 4 | D | 61 | PHE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 4 | D | 137 | PRO |
| 6 | F | 104 | ALA |
| 8 | H | 19 | ARG |
| 10 | J | 143 | LYS |
| 11 | K | 126 | SER |
| 12 | L | 21 | ARG |
| 23 | W | 49 | ASN |
| 26 | Z | 45 | VAL |
| 2 | B | 185 | GLY |
| 4 | D | 28 | GLY |
| 4 | D | 56 | ARG |
| 4 | D | 168 | SER |
| 13 | M | 83 | SER |
| 2 | B | 2 | GLN |
| 4 | D | 166 | ILE |
| 6 | F | 100 | ASP |
| 8 | H | 84 | GLY |
| 10 | J | 5 | GLU |
| 10 | J | 76 | ASP |
| 14 | N | 68 | GLU |
| 14 | N | 164 | ASP |
| 12 | L | 100 | ALA |
| 13 | M | 88 | VAL |
| 14 | N | 74 | PRO |
| 2 | B | 169 | GLY |
| 3 | C | 234 | VAL |
| 9 | I | 124 | VAL |
| 6 | F | 64 | PRO |
| 11 | K | 39 | GLY |
| 12 | L | 135 | GLY |
| 17 | Q | 18 | PRO |

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 | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 1 | A | 178/182 (98%) | 168 (94%) | 10 (6%) | 26 | 59 |
| 2 | B | 281/283 (99%) | 271 (96%) | 10 (4%) | 42 | 76 |
| 3 | C | 192/193 (100%) | 176 (92%) | 16 (8%) | 14 | 38 |
| 4 | D | 116/148 (78%) | 111 (96%) | 5 (4%) | 35 | 70 |
| 5 | E | 151/156 (97%) | 147 (97%) | 4 (3%) | 54 | 86 |
| 6 | F | 92/94 (98%) | 91 (99%) | 1 (1%) | 80 | 95 |
| 7 | G | 27/282 (10%) | 26 (96%) | 1 (4%) | 41 | 76 |
| 8 | H | 133/145 (92%) | 129 (97%) | 4 (3%) | 48 | 82 |
| 9 | I | 58/130 (45%) | 57 (98%) | 1 (2%) | 68 | 92 |
| 10 | J | 117/121 (97%) | 108 (92%) | 9 (8%) | 16 | 41 |
| 11 | K | 105/106 (99%) | 103 (98%) | 2 (2%) | 65 | 91 |
| 12 | L | 113/127 (89%) | 108 (96%) | 5 (4%) | 35 | 69 |
| 13 | M | 157/160 (98%) | 150 (96%) | 7 (4%) | 34 | 68 |
| 14 | N | 148/150 (99%) | 144 (97%) | 4 (3%) | 52 | 85 |
| 15 | O | 93/94 (99%) | 91 (98%) | 2 (2%) | 60 | 89 |
| 16 | P | 113/117 (97%) | 110 (97%) | 3 (3%) | 52 | 85 |
| 17 | Q | 79/80 (99%) | 77 (98%) | 2 (2%) | 55 | 86 |
| 18 | R | 117/122 (96%) | 111 (95%) | 6 (5%) | 29 | 63 |
| 19 | S | 71/74 (96%) | 68 (96%) | 3 (4%) | 36 | 71 |
| 20 | T | 104/106 (98%) | 100 (96%) | 4 (4%) | 40 | 74 |
| 21 | U | 44/53 (83%) | 42 (96%) | 2 (4%) | 34 | 68 |
| 22 | V | 51/57 (90%) | 51 (100%) | 0 | 100 | 100 |
| 23 | W | 129/130 (99%) | 122 (95%) | 7 (5%) | 27 | 60 |
| 24 | X | 65/74 (88%) | 58 (89%) | 7 (11%) | 8 | 23 |
| 25 | Y | 120/195 (62%) | 111 (92%) | 9 (8%) | 17 | 43 |
| 26 | Z | 59/94 (63%) | 58 (98%) | 1 (2%) | 68 | 92 |
| 27 | 1 | 46/47 (98%) | 45 (98%) | 1 (2%) | 60 | 89 |
| 28 | 2 | 42/46 (91%) | 40 (95%) | 2 (5%) | 31 | 66 |
| 29 | 3 | 78/79 (99%) | 73 (94%) | 5 (6%) | 22 | 52 |
| All | All | 3079/3645 (84%) | 2946 (96%) | 133 (4%) | 35 | 70 |

All (133) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 3 | ARG |
| 1 | A | 36 | ASP |
| 1 | A | 37 | VAL |
| 1 | A | 68 | ILE |
| 1 | A | 69 | LEU |
| 1 | A | 131 | HIS |
| 1 | A | 153 | ARG |
| 1 | A | 179 | MET |
| 1 | A | 216 | SER |
| 1 | A | 217 | ARG |
| 2 | B | 7 | ARG |
| 2 | B | 11 | LEU |
| 2 | B | 27 | ASN |
| 2 | B | 71 | VAL |
| 2 | B | 90 | THR |
| 2 | B | 103 | ASP |
| 2 | B | 132 | HIS |
| 2 | B | 162 | MET |
| 2 | B | 254 | GLN |
| 2 | B | 277 | GLU |
| 3 | C | 2 | GLN |
| 3 | C | 16 | VAL |
| 3 | C | 27 | ARG |
| 3 | C | 67 | GLN |
| 3 | C | 76 | ARG |
| 3 | C | 91 | PRO |
| 3 | C | 94 | THR |
| 3 | C | 101 | ASP |
| 3 | C | 115 | LEU |
| 3 | C | 187 | ARG |
| 3 | C | 211 | ASP |
| 3 | C | 222 | ASP |
| 3 | C | 223 | LEU |
| 3 | C | 236 | THR |
| 3 | C | 237 | GLU |
| 3 | C | 240 | LEU |
| 4 | D | 24 | HIS |
| 4 | D | 50 | VAL |
| 4 | D | 61 | PHE |
| 4 | D | 133 | ASN |
| 4 | D | 137 | PRO |
| 5 | E | 102 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | E | 116 | THR |
| 5 | E | 143 | GLN |
| 5 | E | 164 | ASP |
| 6 | F | 12 | LEU |
| 7 | G | 73 | ASP |
| 8 | H | 21 | GLU |
| 8 | H | 87 | LYS |
| 8 | H | 91 | ARG |
| 8 | H | 157 | TYR |
| 9 | I | 135 | GLU |
| 10 | J | 46 | ILE |
| 10 | J | 52 | GLN |
| 10 | J | 74 | ARG |
| 10 | J | 76 | ASP |
| 10 | J | 79 | PHE |
| 10 | J | 107 | ASN |
| 10 | J | 112 | ASP |
| 10 | J | 127 | ILE |
| 10 | J | 131 | THR |
| 11 | K | 7 | ASP |
| 11 | K | 10 | GLN |
| 12 | L | 18 | HIS |
| 12 | L | 35 | ARG |
| 12 | L | 43 | HIS |
| 12 | L | 60 | GLU |
| 12 | L | 140 | VAL |
| 13 | M | 23 | LEU |
| 13 | M | 46 | LEU |
| 13 | M | 68 | ARG |
| 13 | M | 93 | ARG |
| 13 | M | 99 | ARG |
| 13 | M | 115 | LEU |
| 13 | M | 116 | ASN |
| 14 | N | 26 | LEU |
| 14 | N | 49 | THR |
| 14 | N | 134 | ASP |
| 14 | N | 139 | TRP |
| 15 | O | 98 | LEU |
| 15 | O | 115 | ARG |
| 16 | P | 52 | LYS |
| 16 | P | 91 | LYS |
| 16 | P | 98 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17 | Q | 11 | ARG |
| 17 | Q | 95 | GLU |
| 18 | R | 13 | THR |
| 18 | R | 39 | THR |
| 18 | R | 82 | GLU |
| 18 | R | 90 | ASP |
| 18 | R | 142 | ASP |
| 18 | R | 143 | VAL |
| 19 | S | 12 | GLU |
| 19 | S | 17 | ASP |
| 19 | S | 44 | GLN |
| 20 | T | 8 | ARG |
| 20 | T | 39 | ASN |
| 20 | T | 89 | ARG |
| 20 | T | 96 | VAL |
| 21 | U | 17 | THR |
| 21 | U | 53 | ASP |
| 23 | W | 26 | ILE |
| 23 | W | 52 | VAL |
| 23 | W | 73 | LEU |
| 23 | W | 120 | PRO |
| 23 | W | 125 | HIS |
| 23 | W | 142 | ASP |
| 23 | W | 146 | ILE |
| 24 | X | 15 | ARG |
| 24 | X | 27 | ASP |
| 24 | X | 46 | ASP |
| 24 | X | 49 | ARG |
| 24 | X | 72 | VAL |
| 24 | X | 79 | GLU |
| 24 | X | 82 | GLU |
| 25 | Y | 115 | ARG |
| 25 | Y | 154 | ARG |
| 25 | Y | 169 | ARG |
| 25 | Y | 189 | ASN |
| 25 | Y | 203 | VAL |
| 25 | Y | 204 | ARG |
| 25 | Y | 220 | GLU |
| 25 | Y | 231 | PRO |
| 25 | Y | 235 | GLU |
| 26 | Z | 106 | SER |
| 27 | 1 | 47 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28 | 2 | 16 | ASN |
| 28 | 2 | 18 | ASN |
| 29 | 3 | 11 | CYS |
| 29 | 3 | 14 | CYS |
| 29 | 3 | 40 | ARG |
| 29 | 3 | 42 | ARG |
| 29 | 3 | 56 | PRO |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 127 | GLN |
| 1 | A | 199 | HIS |
| 2 | B | 27 | ASN |
| 2 | B | 145 | HIS |
| 2 | B | 221 | GLN |
| 2 | B | 238 | ASN |
| 2 | B | 254 | GLN |
| 2 | B | 256 | GLN |
| 2 | B | 260 | HIS |
| 2 | B | 320 | GLN |
| 2 | B | 332 | ASN |
| 3 | C | 2 | GLN |
| 3 | C | 11 | ASN |
| 3 | C | 39 | GLN |
| 3 | C | 73 | GLN |
| 3 | C | 129 | HIS |
| 3 | C | 163 | HIS |
| 4 | D | 47 | GLN |
| 4 | D | 103 | ASN |
| 4 | D | 133 | ASN |
| 5 | E | 15 | GLN |
| 5 | E | 106 | ASN |
| 5 | E | 119 | HIS |
| 5 | E | 143 | GLN |
| 5 | E | 150 | GLN |
| 7 | G | 17 | GLN |
| 7 | G | 64 | ASN |
| 8 | H | 34 | HIS |
| 8 | H | 59 | GLN |
| 8 | H | 62 | HIS |
| 9 | I | 88 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | J | 25 | GLN |
| 10 | J | 52 | GLN |
| 10 | J | 107 | ASN |
| 10 | J | 126 | ASN |
| 11 | K | 10 | GLN |
| 11 | K | 44 | HIS |
| 12 | L | 18 | HIS |
| 12 | L | 41 | HIS |
| 12 | L | 42 | ASN |
| 12 | L | 43 | HIS |
| 12 | L | 116 | HIS |
| 13 | M | 24 | GLN |
| 13 | M | 26 | GLN |
| 13 | M | 58 | GLN |
| 13 | M | 122 | GLN |
| 13 | M | 129 | HIS |
| 13 | M | 137 | ASN |
| 13 | M | 170 | ASN |
| 14 | N | 21 | HIS |
| 14 | N | 40 | ASN |
| 14 | N | 107 | ASN |
| 14 | N | 119 | GLN |
| 15 | O | 100 | GLN |
| 16 | P | 50 | GLN |
| 16 | P | 66 | GLN |
| 16 | P | 73 | HIS |
| 16 | P | 88 | GLN |
| 16 | P | 118 | GLN |
| 17 | Q | 16 | ASN |
| 17 | Q | 40 | HIS |
| 18 | R | 61 | GLN |
| 18 | R | 94 | ASN |
| 18 | R | 98 | ASN |
| 18 | R | 113 | HIS |
| 18 | R | 117 | HIS |
| 19 | S | 44 | GLN |
| 19 | S | 51 | GLN |
| 19 | S | 55 | GLN |
| 20 | T | 7 | GLN |
| 20 | T | 37 | GLN |
| 20 | T | 39 | ASN |
| 20 | T | 64 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20 | T | 73 | HIS |
| 21 | U | 39 | ASN |
| 21 | U | 48 | ASN |
| 22 | V | 29 | ASN |
| 22 | V | 60 | GLN |
| 23 | W | 28 | HIS |
| 23 | W | 59 | GLN |
| 23 | W | 110 | GLN |
| 23 | W | 119 | HIS |
| 23 | W | 125 | HIS |
| 23 | W | 141 | HIS |
| 25 | Y | 133 | HIS |
| 25 | Y | 134 | HIS |
| 25 | Y | 149 | GLN |
| 25 | Y | 189 | ASN |
| 26 | Z | 58 | ASN |
| 27 | 1 | 8 | GLN |
| 27 | 1 | 16 | HIS |
| 27 | 1 | 28 | HIS |
| 28 | 2 | 16 | ASN |
| 28 | 2 | 18 | ASN |
| 28 | 2 | 41 | HIS |
| 28 | 2 | 45 | ASN |
| 29 | 3 | 15 | ASN |
| 29 | 3 | 30 | GLN |
| 29 | 3 | 48 | ASN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 30 | 0 | 2745/2923 (93%) | 248 (9%) | 30 (1%) |
| 31 | 9 | 121/122 (99%) | 16 (13%) | 1 (0%) |
| 32 | 5 | 2/3 (66%) | 1 (50%) | 0 |
| 33 | 6 | 1/3 (33%) | 0 | 0 |
| All | All | 2869/3051 (94%) | 265 (9%) | 31 (1%) |

All (265) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30 | 0 | 31 | C |
| 30 | 0 | 67 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30 | 0 | 69 | A |
| 30 | 0 | 70 | A |
| 30 | 0 | 71 | G |
| 30 | 0 | 86 | A |
| 30 | 0 | 87 | C |
| 30 | 0 | 88 | G |
| 30 | 0 | 114 | A |
| 30 | 0 | 115 | U |
| 30 | 0 | 130 | C |
| 30 | 0 | 141 | C |
| 30 | 0 | 151 | A |
| 30 | 0 | 166 | A |
| 30 | 0 | 186 | A |
| 30 | 0 | 191 | A |
| 30 | 0 | 192 | A |
| 30 | 0 | 198 | A |
| 30 | 0 | 200 | C |
| 30 | 0 | 204 | A |
| 30 | 0 | 219 | G |
| 30 | 0 | 237 | G |
| 30 | 0 | 271 | C |
| 30 | 0 | 272 | A |
| 30 | 0 | 273 | G |
| 30 | 0 | 283 | U |
| 30 | 0 | 284 | C |
| 30 | 0 | 308 | U |
| 30 | 0 | 309 | C |
| 30 | 0 | 318 | U |
| 30 | 0 | 336 | G |
| 30 | 0 | 337 | A |
| 30 | 0 | 358 | G |
| 30 | 0 | 381 | G |
| 30 | 0 | 397 | A |
| 30 | 0 | 417 | G |
| 30 | 0 | 461 | C |
| 30 | 0 | 487 | G |
| 30 | 0 | 497 | A |
| 30 | 0 | 498 | A |
| 30 | 0 | 510 | U |
| 30 | 0 | 511 | A |
| 30 | 0 | 514 | G |
| 30 | 0 | 537 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 30 | 0 | 538 | C |
| 30 | 0 | 539 | G |
| 30 | 0 | 542 | A |
| 30 | 0 | 545 | G |
| 30 | 0 | 553 | G |
| 30 | 0 | 559 | U |
| 30 | 0 | 588 | G |
| 30 | 0 | 604 | G |
| 30 | 0 | 620 | A |
| 30 | 0 | 632 | A |
| 30 | 0 | 644 | G |
| 30 | 0 | 660 | A |
| 30 | 0 | 688 | A |
| 30 | 0 | 701 | U |
| 30 | 0 | 702 | G |
| 30 | 0 | 735 | C |
| 30 | 0 | 746 | A |
| 30 | 0 | 759 | C |
| 30 | 0 | 777 | U |
| 30 | 0 | 809 | G |
| 30 | 0 | 821 | U |
| 30 | 0 | 835 | U |
| 30 | 0 | 840 | U |
| 30 | 0 | 857 | A |
| 30 | 0 | 858 | U |
| 30 | 0 | 868 | G |
| 30 | 0 | 869 | G |
| 30 | 0 | 871 | G |
| 30 | 0 | 872 | U |
| 30 | 0 | 875 | A |
| 30 | 0 | 877 | G |
| 30 | 0 | 878 | G |
| 30 | 0 | 882 | A |
| 30 | 0 | 905 | C |
| 30 | 0 | 920 | C |
| 30 | 0 | 921 | G |
| 30 | 0 | 923 | A |
| 30 | 0 | 953 | G |
| 30 | 0 | 960 | G |
| 30 | 0 | 961 | A |
| 30 | 0 | 1006 | A |
| 30 | 0 | 1008 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 30 | 0 | 1029 | U |
| 30 | 0 | 1045 | G |
| 30 | 0 | 1059 | G |
| 30 | 0 | 1060 | C |
| 30 | 0 | 1072 | G |
| 30 | 0 | 1081 | A |
| 30 | 0 | 1087 | G |
| 30 | 0 | 1088 | A |
| 30 | 0 | 1109 | U |
| 30 | 0 | 1110 | G |
| 30 | 0 | 1119 | G |
| 30 | 0 | 1129 | C |
| 30 | 0 | 1130 | U |
| 30 | 0 | 1151 | G |
| 30 | 0 | 1164 | U |
| 30 | 0 | 1165 | G |
| 30 | 0 | 1166 | A |
| 30 | 0 | 1174 | A |
| 30 | 0 | 1175 | G |
| 30 | 0 | 1185 | U |
| 30 | 0 | 1192 | A |
| 30 | 0 | 1193 | A |
| 30 | 0 | 1205 | U |
| 30 | 0 | 1206 | U |
| 30 | 0 | 1208 | C |
| 30 | 0 | 1216 | G |
| 30 | 0 | 1237 | U |
| 30 | 0 | 1238 | C |
| 30 | 0 | 1239 | G |
| 30 | 0 | 1279 | U |
| 30 | 0 | 1287 | A |
| 30 | 0 | 1289 | C |
| 30 | 0 | 1342 | C |
| 30 | 0 | 1353 | C |
| 30 | 0 | 1357 | A |
| 30 | 0 | 1360 | C |
| 30 | 0 | 1377 | C |
| 30 | 0 | 1378 | G |
| 30 | 0 | 1407 | A |
| 30 | 0 | 1474 | C |
| 30 | 0 | 1505 | U |
| 30 | 0 | 1506 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 30 | 0 | 1524 | U |
| 30 | 0 | 1525 | G |
| 30 | 0 | 1526 | A |
| 30 | 0 | 1528 | A |
| 30 | 0 | 1559 | A |
| 30 | 0 | 1592 | G |
| 30 | 0 | 1617 | C |
| 30 | 0 | 1625 | U |
| 30 | 0 | 1626 | A |
| 30 | 0 | 1634 | G |
| 30 | 0 | 1656 | A |
| 30 | 0 | 1667 | A |
| 30 | 0 | 1682 | A |
| 30 | 0 | 1684 | A |
| 30 | 0 | 1685 | A |
| 30 | 0 | 1692 | C |
| 30 | 0 | 1701 | A |
| 30 | 0 | 1722 | U |
| 30 | 0 | 1723 | G |
| 30 | 0 | 1725 | C |
| 30 | 0 | 1731 | C |
| 30 | 0 | 1738 | C |
| 30 | 0 | 1752 | G |
| 30 | 0 | 1778 | A |
| 30 | 0 | 1779 | A |
| 30 | 0 | 1798 | C |
| 30 | 0 | 1819 | G |
| 30 | 0 | 1820 | G |
| 30 | 0 | 1829 | A |
| 30 | 0 | 1856 | C |
| 30 | 0 | 1873 | G |
| 30 | 0 | 1879 | U |
| 30 | 0 | 1919 | A |
| 30 | 0 | 1942 | A |
| 30 | 0 | 1971 | G |
| 30 | 0 | 1973 | A |
| 30 | 0 | 1978 | A |
| 30 | 0 | 1979 | G |
| 30 | 0 | 1980 | U |
| 30 | 0 | 1996 | U |
| 30 | 0 | 2004 | U |
| 30 | 0 | 2006 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 30 | 0 | 2008 | U |
| 30 | 0 | 2011 | A |
| 30 | 0 | 2012 | U |
| 30 | 0 | 2013 | G |
| 30 | 0 | 2034 | U |
| 30 | 0 | 2064 | U |
| 30 | 0 | 2072 | G |
| 30 | 0 | 2073 | G |
| 30 | 0 | 2074 | A |
| 30 | 0 | 2096 | A |
| 30 | 0 | 2101 | A |
| 30 | 0 | 2102 | G |
| 30 | 0 | 2103 | A |
| 30 | 0 | 2104 | C |
| 30 | 0 | 2110 | G |
| 30 | 0 | 2238 | A |
| 30 | 0 | 2243 | C |
| 30 | 0 | 2258 | A |
| 30 | 0 | 2271 | G |
| 30 | 0 | 2272 | G |
| 30 | 0 | 2317 | C |
| 30 | 0 | 2321 | A |
| 30 | 0 | 2354 | A |
| 30 | 0 | 2361 | A |
| 30 | 0 | 2369 | A |
| 30 | 0 | 2379 | G |
| 30 | 0 | 2422 | U |
| 30 | 0 | 2462 | G |
| 30 | 0 | 2467 | A |
| 30 | 0 | 2476 | C |
| 30 | 0 | 2480 | G |
| 30 | 0 | 2483 | A |
| 30 | 0 | 2507 | G |
| 30 | 0 | 2509 | A |
| 30 | 0 | 2511 | A |
| 30 | 0 | 2527 | U |
| 30 | 0 | 2533 | C |
| 30 | 0 | 2537 | G |
| 30 | 0 | 2541 | U |
| 30 | 0 | 2553 | A |
| 30 | 0 | 2564 | G |
| 30 | 0 | 2589 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 30 | 0 | 2601 | A |
| 30 | 0 | 2602 | G |
| 30 | 0 | 2608 | C |
| 30 | 0 | 2609 | G |
| 30 | 0 | 2611 | G |
| 30 | 0 | 2613 | G |
| 30 | 0 | 2634 | G |
| 30 | 0 | 2637 | A |
| 30 | 0 | 2638 | G |
| 30 | 0 | 2645 | U |
| 30 | 0 | 2648 | U |
| 30 | 0 | 2649 | A |
| 30 | 0 | 2650 | U |
| 30 | 0 | 2664 | A |
| 30 | 0 | 2681 | A |
| 30 | 0 | 2682 | C |
| 30 | 0 | 2719 | A |
| 30 | 0 | 2726 | U |
| 30 | 0 | 2747 | C |
| 30 | 0 | 2748 | G |
| 30 | 0 | 2749 | U |
| 30 | 0 | 2750 | G |
| 30 | 0 | 2762 | C |
| 30 | 0 | 2768 | A |
| 30 | 0 | 2783 | A |
| 30 | 0 | 2792 | A |
| 30 | 0 | 2800 | A |
| 30 | 0 | 2811 | A |
| 30 | 0 | 2812 | A |
| 30 | 0 | 2825 | C |
| 30 | 0 | 2852 | A |
| 30 | 0 | 2876 | G |
| 30 | 0 | 2890 | A |
| 30 | 0 | 2896 | A |
| 30 | 0 | 2903 | C |
| 30 | 0 | 2914 | A |
| 31 | 9 | 2 | U |
| 31 | 9 | 7 | G |
| 31 | 9 | 14 | G |
| 31 | 9 | 22 | G |
| 31 | 9 | 23 | U |
| 31 | 9 | 24 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31 | 9 | 39 | U |
| 31 | 9 | 41 | C |
| 31 | 9 | 43 | G |
| 31 | 9 | 44 | A |
| 31 | 9 | 52 | A |
| 31 | 9 | 57 | A |
| 31 | 9 | 66 | G |
| 31 | 9 | 77 | A |
| 31 | 9 | 114 | G |
| 31 | 9 | 122 | C |
| 32 | 5 | 76 | A |

All (31) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 30 | 0 | 129 | A |
| 30 | 0 | 338 | C |
| 30 | 0 | 603 | A |
| 30 | 0 | 644 | G |
| 30 | 0 | 699 | C |
| 30 | 0 | 834 | G |
| 30 | 0 | 857 | A |
| 30 | 0 | 871 | G |
| 30 | 0 | 877 | G |
| 30 | 0 | 1080 | C |
| 30 | 0 | 1237 | U |
| 30 | 0 | 1352 | A |
| 30 | 0 | 1506 | U |
| 30 | 0 | 1684 | A |
| 30 | 0 | 1685 | A |
| 30 | 0 | 1692 | C |
| 30 | 0 | 1730 | G |
| 30 | 0 | 1942 | A |
| 30 | 0 | 1979 | G |
| 30 | 0 | 2103 | A |
| 30 | 0 | 2313 | C |
| 30 | 0 | 2467 | A |
| 30 | 0 | 2526 | C |
| 30 | 0 | 2536 | C |
| 30 | 0 | 2637 | A |
| 30 | 0 | 2649 | A |
| 30 | 0 | 2718 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 30 | 0 | 2726 | U |
| 30 | 0 | 2791 | U |
| 30 | 0 | 2852 | A |
| 31 | 9 | 65 | A |

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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$ |
| 30 | OMU | 0 | 2587 | 30 | 12,22,23 | 0.98 | 2 (16%) | 19,31,34 | 3.17 | 2 (10%) |
| 30 | OMG | 0 | 2588 | 32,30 | 17,26,27 | 1.00 | 1 (5%) | 21,38,41 | 2.55 | 3 (14%) |
| 30 | UR3 | 0 | 2619 | 30 | 12,22,23 | 0.90 | 1 (8%) | 16,32,35 | 0.86 | 0 |
| 30 | PSU | 0 | 2621 | 30 | 13,21,22 | 1.64 | 2 (15%) | 18,30,33 | 6.15 | 3 (16%) |
| 30 | 1MA | 0 | 628 | 30 | 14,25,26 | 0.98 | 1 (7%) | 15,37,40 | 1.22 | 1 (6%) |
| 33 | 8AN | 6 | 76 | 33 | 15,24,25 | 1.09 | 1 (6%) | 11,35,38 | 1.99 | 3 (27%) |

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 |
|-----|------|-------|------|-------|---------|-----------|---------|
| 30 | OMU | 0 | 2587 | 30 | - | 0/5/27/28 | 0/2/2/2 |
| 30 | OMG | 0 | 2588 | 32,30 | - | 0/5/27/28 | 0/3/3/3 |
| 30 | UR3 | 0 | 2619 | 30 | - | 0/3/25/26 | 0/2/2/2 |
| 30 | PSU | 0 | 2621 | 30 | - | 0/7/25/26 | 0/2/2/2 |
| 30 | 1MA | 0 | 628 | 30 | - | 0/3/25/26 | 0/3/3/3 |
| 33 | 8AN | 6 | 76 | 33 | - | 0/3/25/26 | 0/3/3/3 |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 30 | 0 | 2621 | PSU | C5-C1' | -4.81 | 1.48 | 1.52 |
| 33 | 6 | 76 | 8AN | C3'-N3' | -2.59 | 1.43 | 1.47 |
| 30 | 0 | 2619 | UR3 | C6-C5 | -2.04 | 1.33 | 1.38 |
| 30 | 0 | 2587 | OMU | C6-C5 | -2.00 | 1.33 | 1.38 |
| 30 | 0 | 2587 | OMU | C4-N3 | 2.22 | 1.37 | 1.33 |
| 30 | 0 | 628 | 1MA | C6-N6 | 2.45 | 1.33 | 1.29 |
| 30 | 0 | 2621 | PSU | C4-N3 | 2.84 | 1.38 | 1.33 |
| 30 | 0 | 2588 | OMG | C6-N1 | 3.05 | 1.38 | 1.33 |

All (12) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 30 | 0 | 2621 | PSU | N1-C2-N3 | -21.76 | 114.45 | 128.33 |
| 30 | 0 | 2588 | OMG | C5-C6-N1 | -8.87 | 111.46 | 123.59 |
| 30 | 0 | 628 | 1MA | C2-N3-C4 | -3.71 | 110.66 | 116.40 |
| 30 | 0 | 2587 | OMU | C5-C4-N3 | -3.33 | 114.57 | 123.12 |
| 30 | 0 | 2588 | OMG | N3-C2-N1 | -2.12 | 124.22 | 127.44 |
| 30 | 0 | 2621 | PSU | C6-N1-C2 | 2.91 | 120.15 | 115.47 |
| 33 | 6 | 76 | 8AN | C2'-C1'-N9 | 3.39 | 119.47 | 114.29 |
| 33 | 6 | 76 | 8AN | O4'-C4'-C3' | 3.40 | 109.19 | 104.09 |
| 33 | 6 | 76 | 8AN | O2'-C2'-C3' | 3.98 | 121.22 | 111.26 |
| 30 | 0 | 2588 | OMG | C6-N1-C2 | 6.60 | 125.10 | 115.94 |
| 30 | 0 | 2587 | OMU | C4-N3-C2 | 13.16 | 127.18 | 114.14 |
| 30 | 0 | 2621 | PSU | C4-N3-C2 | 13.50 | 126.92 | 115.25 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 30 | 0 | 2587 | OMU | 1 | 0 |
| 30 | 0 | 2588 | OMG | 2 | 0 |
| 30 | 0 | 2619 | UR3 | 1 | 0 |
| 33 | 6 | 76 | 8AN | 1 | 0 |

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 306 ligands modelled in this entry, 304 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 | $\# Z > 2$ |
| 34 | PHE | 6 | 77 | - | 10,11,12 | 1.89 | 3 (30%) | 10,13,15 | 0.64 | 0 |
| 34 | ACA | 6 | 78 | - | 7,7,8 | 2.09 | 2 (28%) | 5,6,8 | 0.87 | 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 |
|-----|------|-------|-----|------|---------|----------|---------|
| 34 | PHE | 6 | 77 | - | - | 0/4/6/8 | 0/1/1/1 |
| 34 | ACA | 6 | 78 | - | - | 0/4/5/6 | 0/0/0/0 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 34 | 6 | 78 | ACA | C3-C2 | -4.00 | 1.37 | 1.52 |
| 34 | 6 | 78 | ACA | C2-C1 | -2.85 | 1.41 | 1.49 |
| 34 | 6 | 77 | PHE | CB-CG | 2.08 | 1.56 | 1.51 |
| 34 | 6 | 77 | PHE | CE1-CD1 | 2.43 | 1.43 | 1.38 |
| 34 | 6 | 77 | PHE | CE2-CD2 | 3.36 | 1.45 | 1.38 |

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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 | 237/240 (98%) | -0.52 | 7 (2%) 54 41 | 22, 45, 81, 106 | 0 |
| 2 | B | 337/338 (99%) | -0.74 | 0 100 100 | 20, 45, 72, 88 | 0 |
| 3 | C | 246/246 (100%) | -0.62 | 0 100 100 | 17, 41, 65, 82 | 0 |
| 4 | D | 140/177 (79%) | 0.83 | 23 (16%) 2 1 | 54, 93, 129, 137 | 0 |
| 5 | E | 172/178 (96%) | -0.46 | 2 (1%) 81 73 | 38, 60, 81, 91 | 0 |
| 6 | F | 119/120 (99%) | 0.29 | 4 (3%) 49 36 | 41, 70, 106, 115 | 0 |
| 7 | G | 29/348 (8%) | 0.81 | 4 (13%) 4 2 | 66, 93, 107, 109 | 0 |
| 8 | H | 160/177 (90%) | -0.27 | 1 (0%) 90 86 | 34, 56, 93, 104 | 0 |
| 9 | I | 70/162 (43%) | 4.04 | 57 (81%) 0 0 | 143, 158, 174, 175 | 0 |
| 10 | J | 142/145 (97%) | -0.71 | 0 100 100 | 28, 44, 63, 81 | 0 |
| 11 | K | 132/132 (100%) | -0.83 | 0 100 100 | 25, 39, 60, 72 | 0 |
| 12 | L | 145/165 (87%) | 0.03 | 5 (3%) 49 36 | 20, 61, 109, 127 | 0 |
| 13 | M | 194/196 (98%) | -0.68 | 1 (0%) 91 88 | 24, 40, 63, 74 | 0 |
| 14 | N | 186/187 (99%) | -0.21 | 6 (3%) 51 39 | 37, 60, 119, 126 | 0 |
| 15 | O | 115/116 (99%) | -0.51 | 0 100 100 | 33, 53, 68, 74 | 0 |
| 16 | P | 143/149 (95%) | -0.74 | 0 100 100 | 30, 45, 58, 67 | 0 |
| 17 | Q | 95/96 (98%) | -0.63 | 0 100 100 | 30, 42, 60, 74 | 0 |
| 18 | R | 150/155 (96%) | -0.72 | 0 100 100 | 23, 37, 59, 70 | 0 |
| 19 | S | 81/85 (95%) | -0.27 | 1 (1%) 81 73 | 37, 53, 74, 95 | 0 |
| 20 | T | 119/120 (99%) | -0.32 | 4 (3%) 49 36 | 36, 51, 80, 121 | 0 |
| 21 | U | 53/67 (79%) | -0.44 | 1 (1%) 70 59 | 32, 47, 71, 81 | 0 |
| 22 | V | 65/71 (91%) | 1.02 | 8 (12%) 5 3 | 44, 74, 117, 125 | 0 |
| 23 | W | 154/154 (100%) | -0.70 | 0 100 100 | 30, 45, 66, 80 | 0 |
| 24 | X | 82/92 (89%) | -0.31 | 5 (6%) 25 15 | 37, 52, 83, 106 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|--|-----------------------|-------|
| 25 | Y | 142/240 (59%) | -0.72 | 0 100 100 | 18, 39, 62, 85 | 0 |
| 26 | Z | 73/116 (62%) | 0.56 | 11 (15%) 3 2 | 44, 82, 99, 108 | 0 |
| 27 | 1 | 56/57 (98%) | -0.80 | 0 100 100 | 21, 28, 36, 43 | 0 |
| 28 | 2 | 46/50 (92%) | -0.44 | 2 (4%) 39 27 | 30, 52, 68, 86 | 0 |
| 29 | 3 | 92/92 (100%) | -0.41 | 2 (2%) 65 54 | 34, 53, 71, 80 | 0 |
| 30 | 0 | 2749/2923 (94%) | -0.63 | 26 (0%) 85 79 | 17, 40, 89, 186 | 0 |
| 31 | 9 | 122/122 (100%) | -0.69 | 2 (1%) 74 66 | 33, 61, 86, 151 | 0 |
| 32 | 5 | 3/3 (100%) | 1.91 | 1 (33%) 0 0 | 81, 81, 83, 86 | 0 |
| 33 | 6 | 2/3 (66%) | 0.92 | 0 100 100 | 96, 96, 96, 104 | 0 |
| All | All | 6651/7522 (88%) | -0.45 | 173 (2%) 59 47 | 17, 46, 98, 186 | 0 |

All (173) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 22 | V | 40 | PRO | 13.7 |
| 9 | I | 66 | GLY | 11.4 |
| 9 | I | 74 | ILE | 10.0 |
| 22 | V | 1 | THR | 8.7 |
| 4 | D | 57 | THR | 8.6 |
| 9 | I | 100 | VAL | 8.4 |
| 9 | I | 70 | THR | 8.4 |
| 22 | V | 39 | ALA | 8.0 |
| 9 | I | 111 | LEU | 7.9 |
| 9 | I | 103 | ILE | 7.8 |
| 14 | N | 166 | ALA | 7.8 |
| 9 | I | 72 | GLU | 7.7 |
| 9 | I | 128 | THR | 7.1 |
| 9 | I | 80 | PHE | 7.1 |
| 4 | D | 63 | ILE | 7.1 |
| 20 | T | 119 | ALA | 6.9 |
| 26 | Z | 34 | SER | 6.9 |
| 22 | V | 38 | GLY | 6.9 |
| 9 | I | 104 | ALA | 6.8 |
| 9 | I | 71 | ALA | 6.7 |
| 26 | Z | 46 | SER | 6.5 |
| 9 | I | 99 | GLN | 6.3 |
| 9 | I | 97 | VAL | 6.2 |
| 9 | I | 98 | ASP | 6.0 |
| 9 | I | 91 | PHE | 5.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 9 | I | 132 | VAL | 5.8 |
| 9 | I | 78 | ALA | 5.6 |
| 9 | I | 76 | ASP | 5.4 |
| 20 | T | 116 | ASP | 5.3 |
| 30 | 0 | 1172 | G | 5.3 |
| 26 | Z | 35 | SER | 5.3 |
| 9 | I | 133 | THR | 5.3 |
| 9 | I | 131 | GLY | 5.3 |
| 9 | I | 82 | THR | 5.1 |
| 9 | I | 69 | PRO | 4.9 |
| 4 | D | 90 | LEU | 4.9 |
| 9 | I | 86 | GLU | 4.9 |
| 9 | I | 108 | HIS | 4.6 |
| 30 | 0 | 1199 | A | 4.6 |
| 4 | D | 95 | THR | 4.4 |
| 9 | I | 123 | VAL | 4.4 |
| 9 | I | 81 | GLU | 4.4 |
| 9 | I | 93 | ALA | 4.4 |
| 22 | V | 36 | ALA | 4.3 |
| 9 | I | 109 | PRO | 4.3 |
| 9 | I | 113 | SER | 4.2 |
| 9 | I | 94 | ASP | 4.2 |
| 19 | S | 81 | ILE | 4.2 |
| 9 | I | 88 | GLN | 4.0 |
| 7 | G | 23 | ILE | 4.0 |
| 14 | N | 155 | GLU | 4.0 |
| 4 | D | 166 | ILE | 3.9 |
| 28 | 2 | 49 | GLU | 3.9 |
| 26 | Z | 45 | VAL | 3.9 |
| 14 | N | 160 | SER | 3.8 |
| 9 | I | 127 | CYS | 3.8 |
| 9 | I | 102 | GLN | 3.8 |
| 4 | D | 170 | TYR | 3.8 |
| 26 | Z | 49 | ARG | 3.8 |
| 30 | 0 | 735 | C | 3.6 |
| 9 | I | 92 | VAL | 3.6 |
| 9 | I | 84 | SER | 3.6 |
| 30 | 0 | 1163 | G | 3.6 |
| 30 | 0 | 1177 | A | 3.5 |
| 4 | D | 92 | GLU | 3.5 |
| 9 | I | 106 | GLN | 3.5 |
| 30 | 0 | 1200 | A | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 9 | I | 101 | LYS | 3.5 |
| 30 | 0 | 1196 | C | 3.4 |
| 9 | I | 120 | ALA | 3.4 |
| 4 | D | 93 | LEU | 3.4 |
| 22 | V | 37 | GLY | 3.4 |
| 4 | D | 101 | THR | 3.4 |
| 1 | A | 237 | GLY | 3.3 |
| 4 | D | 134 | LEU | 3.3 |
| 9 | I | 90 | ASP | 3.3 |
| 26 | Z | 58 | ASN | 3.3 |
| 26 | Z | 48 | ARG | 3.2 |
| 9 | I | 129 | SER | 3.2 |
| 9 | I | 116 | LEU | 3.1 |
| 30 | 0 | 1198 | U | 3.1 |
| 9 | I | 73 | LEU | 3.1 |
| 9 | I | 79 | GLY | 3.1 |
| 30 | 0 | 1951 | G | 3.1 |
| 9 | I | 105 | GLU | 3.1 |
| 1 | A | 236 | GLY | 3.0 |
| 30 | 0 | 1965 | C | 3.0 |
| 4 | D | 88 | LEU | 3.0 |
| 1 | A | 37 | VAL | 3.0 |
| 4 | D | 84 | LEU | 2.9 |
| 9 | I | 83 | GLY | 2.9 |
| 26 | Z | 43 | GLY | 2.9 |
| 5 | E | 45 | ASP | 2.9 |
| 7 | G | 26 | MET | 2.9 |
| 30 | 0 | 1169 | U | 2.8 |
| 9 | I | 130 | LEU | 2.8 |
| 4 | D | 10 | PHE | 2.8 |
| 32 | 5 | 75 | C | 2.8 |
| 4 | D | 11 | HIS | 2.8 |
| 9 | I | 126 | THR | 2.8 |
| 31 | 9 | 1 | U | 2.8 |
| 21 | U | 47 | ARG | 2.8 |
| 9 | I | 121 | LYS | 2.8 |
| 6 | F | 110 | ASP | 2.8 |
| 6 | F | 25 | ASP | 2.7 |
| 4 | D | 18 | ILE | 2.7 |
| 14 | N | 134 | ASP | 2.7 |
| 24 | X | 88 | GLU | 2.6 |
| 30 | 0 | 1202 | A | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 9 | I | 122 | GLU | 2.6 |
| 12 | L | 75 | LEU | 2.6 |
| 20 | T | 118 | SER | 2.6 |
| 20 | T | 117 | ASP | 2.6 |
| 12 | L | 60 | GLU | 2.5 |
| 29 | 3 | 56 | PRO | 2.5 |
| 30 | 0 | 514 | G | 2.5 |
| 4 | D | 62 | ASP | 2.5 |
| 9 | I | 87 | PRO | 2.4 |
| 12 | L | 91 | VAL | 2.4 |
| 1 | A | 31 | LYS | 2.4 |
| 14 | N | 163 | PHE | 2.4 |
| 30 | 0 | 1181 | A | 2.4 |
| 30 | 0 | 1165 | G | 2.4 |
| 26 | Z | 47 | ARG | 2.4 |
| 1 | A | 35 | GLY | 2.3 |
| 12 | L | 105 | TYR | 2.3 |
| 30 | 0 | 1175 | G | 2.3 |
| 30 | 0 | 1173 | A | 2.3 |
| 4 | D | 61 | PHE | 2.3 |
| 9 | I | 110 | ASP | 2.3 |
| 30 | 0 | 1164 | U | 2.3 |
| 31 | 9 | 2 | U | 2.3 |
| 9 | I | 112 | LEU | 2.3 |
| 9 | I | 114 | TYR | 2.3 |
| 24 | X | 80 | GLU | 2.3 |
| 6 | F | 107 | ASP | 2.3 |
| 30 | 0 | 1170 | U | 2.3 |
| 8 | H | 174 | LEU | 2.3 |
| 30 | 0 | 1197 | G | 2.3 |
| 29 | 3 | 55 | VAL | 2.3 |
| 7 | G | 27 | ILE | 2.2 |
| 24 | X | 71 | ARG | 2.2 |
| 5 | E | 10 | ASP | 2.2 |
| 6 | F | 117 | GLU | 2.2 |
| 30 | 0 | 2637 | A | 2.2 |
| 26 | Z | 38 | PHE | 2.2 |
| 4 | D | 44 | ILE | 2.2 |
| 4 | D | 64 | ARG | 2.2 |
| 30 | 0 | 1168 | C | 2.2 |
| 22 | V | 41 | GLU | 2.2 |
| 4 | D | 41 | LEU | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 9 | I | 89 | GLU | 2.2 |
| 4 | D | 40 | ILE | 2.2 |
| 30 | 0 | 1195 | G | 2.2 |
| 30 | 0 | 1176 | C | 2.1 |
| 14 | N | 165 | ALA | 2.1 |
| 30 | 0 | 1171 | A | 2.1 |
| 9 | I | 117 | THR | 2.1 |
| 30 | 0 | 282 | C | 2.1 |
| 24 | X | 7 | GLU | 2.1 |
| 24 | X | 85 | VAL | 2.1 |
| 9 | I | 124 | VAL | 2.1 |
| 4 | D | 94 | ALA | 2.1 |
| 12 | L | 80 | ASP | 2.1 |
| 28 | 2 | 35 | ARG | 2.1 |
| 13 | M | 78 | LYS | 2.1 |
| 1 | A | 133 | ARG | 2.1 |
| 9 | I | 125 | GLY | 2.0 |
| 26 | Z | 60 | ASP | 2.0 |
| 7 | G | 12 | ILE | 2.0 |
| 4 | D | 58 | VAL | 2.0 |
| 22 | V | 32 | ALA | 2.0 |
| 1 | A | 36 | ASP | 2.0 |

6.2 Non-standard residues in protein, DNA, RNA chains

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 |
|-----|------|-------|------|-------|------|------|------|----------------------------|-------|
| 30 | OMU | 0 | 2587 | 21/22 | 0.98 | 0.09 | - | 24,28,32,33 | 0 |
| 30 | UR3 | 0 | 2619 | 21/22 | 0.97 | 0.13 | - | 33,35,40,41 | 0 |
| 30 | PSU | 0 | 2621 | 20/21 | 0.97 | 0.14 | - | 29,31,38,39 | 0 |
| 33 | 8AN | 6 | 76 | 22/23 | 0.87 | 0.28 | - | 84,92,94,95 | 0 |
| 30 | 1MA | 0 | 628 | 23/24 | 0.97 | 0.15 | - | 25,28,29,30 | 0 |
| 30 | OMG | 0 | 2588 | 24/25 | 0.97 | 0.11 | - | 24,29,31,33 | 0 |

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 35 | MG | 0 | 8047 | 1/1 | 0.77 | 0.89 | 43.59 | 89,89,89,89 | 0 |
| 36 | NA | 0 | 8558 | 1/1 | 0.88 | 0.65 | 42.86 | 56,56,56,56 | 0 |
| 35 | MG | 0 | 8071 | 1/1 | 0.95 | 0.49 | 39.55 | 98,98,98,98 | 0 |
| 36 | NA | 0 | 8559 | 1/1 | 0.66 | 0.36 | 32.94 | 75,75,75,75 | 0 |
| 36 | NA | 0 | 8553 | 1/1 | 0.95 | 0.53 | 32.83 | 100,100,100,100 | 0 |
| 36 | NA | 0 | 8519 | 1/1 | 0.80 | 0.54 | 30.59 | 53,53,53,53 | 0 |
| 36 | NA | 0 | 8517 | 1/1 | 0.90 | 0.41 | 27.69 | 40,40,40,40 | 0 |
| 35 | MG | 0 | 8076 | 1/1 | 0.85 | 0.52 | 26.85 | 81,81,81,81 | 0 |
| 38 | CL | B | 8819 | 1/1 | 0.99 | 0.34 | 25.71 | 56,56,56,56 | 0 |
| 35 | MG | 0 | 8062 | 1/1 | 0.86 | 0.60 | 21.29 | 76,76,76,76 | 0 |
| 36 | NA | 0 | 8521 | 1/1 | 0.88 | 0.39 | 19.33 | 61,61,61,61 | 0 |
| 35 | MG | 0 | 8041 | 1/1 | 0.96 | 0.26 | 18.77 | 31,31,31,31 | 0 |
| 36 | NA | 0 | 8567 | 1/1 | 0.52 | 0.44 | 18.36 | 75,75,75,75 | 0 |
| 36 | NA | 0 | 8547 | 1/1 | 0.48 | 0.40 | 17.70 | 66,66,66,66 | 0 |
| 35 | MG | 0 | 8002 | 1/1 | 0.91 | 0.43 | 16.55 | 62,62,62,62 | 0 |
| 36 | NA | 0 | 8560 | 1/1 | 0.33 | 0.61 | 16.12 | 107,107,107,107 | 0 |
| 36 | NA | 0 | 8534 | 1/1 | 0.97 | 0.68 | 14.99 | 78,78,78,78 | 0 |
| 37 | SR | B | 8987 | 1/1 | 0.65 | 0.43 | 14.59 | 200,200,200,200 | 0 |
| 36 | NA | 0 | 8512 | 1/1 | 0.94 | 0.43 | 13.52 | 43,43,43,43 | 0 |
| 36 | NA | 0 | 8565 | 1/1 | 0.82 | 0.32 | 13.12 | 59,59,59,59 | 0 |
| 35 | MG | 0 | 8010 | 1/1 | 0.87 | 0.35 | 11.34 | 103,103,103,103 | 0 |
| 35 | MG | 0 | 8014 | 1/1 | 0.95 | 0.21 | 9.18 | 9,9,9,9 | 0 |
| 35 | MG | 0 | 8009 | 1/1 | 0.99 | 0.30 | 8.86 | 1,1,1,1 | 0 |
| 36 | NA | 0 | 8523 | 1/1 | 0.91 | 0.19 | 8.46 | 49,49,49,49 | 0 |
| 35 | MG | 0 | 8004 | 1/1 | 0.94 | 0.21 | 8.45 | 13,13,13,13 | 0 |
| 37 | SR | 0 | 8948 | 1/1 | 0.99 | 0.16 | 8.30 | 57,57,57,57 | 0 |
| 36 | NA | 0 | 8530 | 1/1 | 0.90 | 0.23 | 8.04 | 38,38,38,38 | 0 |
| 35 | MG | 0 | 8028 | 1/1 | 0.97 | 0.27 | 8.00 | 1,1,1,1 | 0 |
| 35 | MG | C | 8012 | 1/1 | 0.97 | 0.22 | 7.59 | 13,13,13,13 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 35 | MG | A | 8051 | 1/1 | 0.86 | 0.38 | 6.96 | 58,58,58,58 | 0 |
| 35 | MG | 0 | 8040 | 1/1 | 0.84 | 0.20 | 6.56 | 75,75,75,75 | 0 |
| 34 | PHE | 6 | 77 | 11/12 | 0.62 | 0.45 | 6.32 | 72,73,77,80 | 0 |
| 35 | MG | 0 | 8001 | 1/1 | 0.89 | 0.24 | 5.95 | 22,22,22,22 | 0 |
| 36 | NA | 0 | 8527 | 1/1 | 0.94 | 0.20 | 5.70 | 40,40,40,40 | 0 |
| 36 | NA | 0 | 8504 | 1/1 | 0.85 | 0.20 | 4.71 | 20,20,20,20 | 0 |
| 36 | NA | 0 | 8563 | 1/1 | 0.96 | 0.24 | 4.70 | 55,55,55,55 | 0 |
| 37 | SR | 0 | 8969 | 1/1 | 0.64 | 0.20 | 4.70 | 154,154,154,154 | 0 |
| 36 | NA | 0 | 8542 | 1/1 | 0.83 | 0.22 | 4.55 | 38,38,38,38 | 0 |
| 37 | SR | 0 | 8947 | 1/1 | 0.97 | 0.17 | 4.48 | 84,84,84,84 | 0 |
| 35 | MG | 0 | 8011 | 1/1 | 0.98 | 0.20 | 3.94 | 17,17,17,17 | 0 |
| 36 | NA | 0 | 8522 | 1/1 | 0.70 | 0.15 | 3.85 | 64,64,64,64 | 0 |
| 35 | MG | 0 | 8088 | 1/1 | 0.98 | 0.18 | 3.70 | 37,37,37,37 | 0 |
| 39 | K | 0 | 8401 | 1/1 | 0.81 | 0.24 | 3.63 | 66,66,66,66 | 0 |
| 35 | MG | Y | 8086 | 1/1 | 0.94 | 0.19 | 3.57 | 46,46,46,46 | 0 |
| 35 | MG | 0 | 8006 | 1/1 | 0.98 | 0.15 | 2.69 | 6,6,6,6 | 0 |
| 37 | SR | 0 | 8943 | 1/1 | 0.97 | 0.13 | 2.68 | 65,65,65,65 | 0 |
| 36 | NA | 0 | 8546 | 1/1 | 0.74 | 0.24 | 2.65 | 79,79,79,79 | 0 |
| 35 | MG | 0 | 8043 | 1/1 | 0.95 | 0.15 | 2.57 | 37,37,37,37 | 0 |
| 39 | K | 0 | 8402 | 1/1 | 0.52 | 0.22 | 2.54 | 81,81,81,81 | 0 |
| 37 | SR | 0 | 8902 | 1/1 | 0.99 | 0.17 | 2.13 | 32,32,32,32 | 0 |
| 36 | NA | L | 8568 | 1/1 | 0.96 | 0.17 | 1.95 | 30,30,30,30 | 0 |
| 37 | SR | 0 | 8945 | 1/1 | 0.97 | 0.13 | 1.83 | 89,89,89,89 | 0 |
| 35 | MG | 0 | 8008 | 1/1 | 0.94 | 0.12 | 1.80 | 13,13,13,13 | 0 |
| 37 | SR | 0 | 8949 | 1/1 | 0.99 | 0.13 | 1.77 | 49,49,49,49 | 0 |
| 37 | SR | 0 | 8904 | 1/1 | 0.99 | 0.16 | 1.71 | 39,39,39,39 | 0 |
| 35 | MG | 0 | 8003 | 1/1 | 0.98 | 0.17 | 1.64 | 18,18,18,18 | 0 |
| 37 | SR | R | 8912 | 1/1 | 0.99 | 0.18 | 1.52 | 64,64,64,64 | 0 |
| 36 | NA | 0 | 8556 | 1/1 | 0.85 | 0.17 | 1.41 | 39,39,39,39 | 0 |
| 37 | SR | 0 | 8910 | 1/1 | 1.00 | 0.13 | 1.12 | 40,40,40,40 | 0 |
| 38 | CL | J | 8821 | 1/1 | 0.93 | 0.17 | 1.11 | 61,61,61,61 | 0 |
| 36 | NA | 0 | 8575 | 1/1 | 0.93 | 0.15 | 1.05 | 59,59,59,59 | 0 |
| 36 | NA | R | 8533 | 1/1 | 0.94 | 0.14 | 1.04 | 42,42,42,42 | 0 |
| 36 | NA | J | 8538 | 1/1 | 0.84 | 0.21 | 0.99 | 31,31,31,31 | 0 |
| 37 | SR | 0 | 8981 | 1/1 | 0.99 | 0.16 | 0.87 | 107,107,107,107 | 0 |
| 36 | NA | 0 | 8515 | 1/1 | 0.91 | 0.15 | 0.65 | 20,20,20,20 | 0 |
| 37 | SR | 1 | 8913 | 1/1 | 0.99 | 0.15 | 0.61 | 42,42,42,42 | 0 |
| 36 | NA | 0 | 8513 | 1/1 | 0.97 | 0.15 | 0.53 | 29,29,29,29 | 0 |
| 36 | NA | 0 | 8557 | 1/1 | 0.83 | 0.10 | 0.53 | 57,57,57,57 | 0 |
| 37 | SR | 3 | 8932 | 1/1 | 0.99 | 0.15 | 0.26 | 68,68,68,68 | 0 |
| 35 | MG | 0 | 8034 | 1/1 | 0.98 | 0.12 | -0.03 | 31,31,31,31 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|--------|-----------------------------|-------|
| 37 | SR | A | 8930 | 1/1 | 0.98 | 0.13 | -0.07 | 72,72,72,72 | 0 |
| 37 | SR | 0 | 8922 | 1/1 | 0.97 | 0.14 | -0.16 | 62,62,62,62 | 0 |
| 35 | MG | 0 | 8084 | 1/1 | 0.98 | 0.11 | -0.25 | 31,31,31,31 | 0 |
| 37 | SR | 0 | 8935 | 1/1 | 0.98 | 0.11 | -0.28 | 64,64,64,64 | 0 |
| 37 | SR | F | 9005 | 1/1 | 0.94 | 0.12 | -0.34 | 85,85,85,85 | 0 |
| 40 | CD | U | 8701 | 1/1 | 1.00 | 0.11 | -0.38 | 50,50,50,50 | 0 |
| 37 | SR | 0 | 8991 | 1/1 | 0.97 | 0.09 | -0.64 | 147,147,147,147 | 0 |
| 36 | NA | 0 | 8528 | 1/1 | 0.86 | 0.10 | -0.64 | 42,42,42,42 | 0 |
| 36 | NA | Q | 8540 | 1/1 | 0.65 | 0.10 | -0.88 | 48,48,48,48 | 0 |
| 36 | NA | 9 | 8572 | 1/1 | 0.74 | 0.08 | -0.89 | 85,85,85,85 | 0 |
| 37 | SR | H | 8972 | 1/1 | 0.92 | 0.11 | -0.92 | 119,119,119,119 | 0 |
| 35 | MG | T | 8057 | 1/1 | 0.69 | 0.13 | -0.95 | 65,65,65,65 | 0 |
| 36 | NA | M | 8539 | 1/1 | 0.83 | 0.10 | -0.95 | 33,33,33,33 | 0 |
| 38 | CL | O | 8808 | 1/1 | 0.94 | 0.10 | -1.12 | 63,63,63,63 | 0 |
| 38 | CL | 0 | 8816 | 1/1 | 0.98 | 0.11 | -1.16 | 60,60,60,60 | 0 |
| 35 | MG | 0 | 8083 | 1/1 | 0.96 | 0.09 | -1.17 | 36,36,36,36 | 0 |
| 37 | SR | 0 | 8985 | 1/1 | 0.95 | 0.07 | -1.19 | 116,116,116,116 | 0 |
| 40 | CD | 1 | 8702 | 1/1 | 0.99 | 0.09 | -1.36 | 50,50,50,50 | 0 |
| 40 | CD | Z | 8703 | 1/1 | 0.99 | 0.08 | -1.41 | 62,62,62,62 | 0 |
| 40 | CD | 3 | 8704 | 1/1 | 1.00 | 0.09 | -1.54 | 54,54,54,54 | 0 |
| 37 | SR | 0 | 8964 | 1/1 | 0.97 | 0.08 | -1.94 | 92,92,92,92 | 0 |
| 37 | SR | A | 8929 | 1/1 | 0.81 | 0.06 | -1.97 | 105,105,105,105 | 0 |
| 35 | MG | 0 | 8075 | 1/1 | 0.90 | 0.08 | -2.01 | 35,35,35,35 | 0 |
| 38 | CL | K | 8812 | 1/1 | 0.99 | 0.06 | -2.11 | 43,43,43,43 | 0 |
| 35 | MG | 0 | 8007 | 1/1 | 0.96 | 0.12 | -2.13 | 37,37,37,37 | 0 |
| 36 | NA | 0 | 8564 | 1/1 | 0.80 | 0.08 | -2.50 | 68,68,68,68 | 0 |
| 37 | SR | 0 | 8992 | 1/1 | 0.98 | 0.07 | -2.56 | 102,102,102,102 | 0 |
| 38 | CL | M | 8818 | 1/1 | 0.98 | 0.08 | -2.57 | 33,33,33,33 | 0 |
| 35 | MG | 0 | 8052 | 1/1 | 0.96 | 0.07 | -2.70 | 37,37,37,37 | 0 |
| 38 | CL | 3 | 8804 | 1/1 | 0.68 | 0.09 | -3.24 | 88,88,88,88 | 0 |
| 37 | SR | 0 | 8975 | 1/1 | 0.94 | 0.04 | -3.36 | 115,115,115,115 | 0 |
| 35 | MG | 0 | 8044 | 1/1 | 0.94 | 0.08 | -3.54 | 47,47,47,47 | 0 |
| 38 | CL | 0 | 8805 | 1/1 | 0.96 | 0.07 | -3.62 | 46,46,46,46 | 0 |
| 36 | NA | 0 | 8537 | 1/1 | 0.96 | 0.04 | -3.71 | 22,22,22,22 | 0 |
| 37 | SR | 0 | 8970 | 1/1 | 0.99 | 0.05 | -3.74 | 88,88,88,88 | 0 |
| 35 | MG | 0 | 8021 | 1/1 | 0.92 | 0.07 | -3.81 | 24,24,24,24 | 0 |
| 35 | MG | A | 8025 | 1/1 | 0.98 | 0.06 | -4.26 | 40,40,40,40 | 0 |
| 35 | MG | 0 | 8013 | 1/1 | 0.94 | 0.04 | -11.68 | 28,28,28,28 | 0 |
| 37 | SR | 0 | 8921 | 1/1 | 0.99 | 0.13 | - | 51,51,51,51 | 0 |
| 38 | CL | 0 | 8822 | 1/1 | 0.95 | 0.15 | - | 53,53,53,53 | 0 |
| 37 | SR | 0 | 8925 | 1/1 | 0.99 | 0.15 | - | 66,66,66,66 | 0 |
| 37 | SR | 0 | 8993 | 1/1 | 0.91 | 0.05 | - | 126,126,126,126 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 37 | SR | 0 | 8917 | 1/1 | 0.96 | 0.17 | - | 61,61,61,61 | 0 |
| 35 | MG | 0 | 8072 | 1/1 | 0.98 | 0.14 | - | 25,25,25,25 | 0 |
| 35 | MG | 0 | 8059 | 1/1 | 0.81 | 0.13 | - | 58,58,58,58 | 0 |
| 37 | SR | Y | 9002 | 1/1 | 0.93 | 0.10 | - | 118,118,118,118 | 0 |
| 38 | CL | 0 | 8813 | 1/1 | 0.90 | 0.08 | - | 53,53,53,53 | 0 |
| 37 | SR | 0 | 8927 | 1/1 | 0.99 | 0.17 | - | 67,67,67,67 | 0 |
| 37 | SR | 0 | 8962 | 1/1 | 0.95 | 0.09 | - | 96,96,96,96 | 0 |
| 36 | NA | 0 | 8511 | 1/1 | 0.79 | 0.19 | - | 48,48,48,48 | 0 |
| 35 | MG | 0 | 8092 | 1/1 | 0.80 | 0.12 | - | 48,48,48,48 | 0 |
| 35 | MG | 9 | 8074 | 1/1 | 0.97 | 0.24 | - | 53,53,53,53 | 0 |
| 35 | MG | 0 | 8085 | 1/1 | 0.74 | 0.33 | - | 91,91,91,91 | 0 |
| 35 | MG | 0 | 8015 | 1/1 | 0.98 | 0.18 | - | 45,45,45,45 | 0 |
| 36 | NA | 0 | 8545 | 1/1 | 0.92 | 0.15 | - | 40,40,40,40 | 0 |
| 36 | NA | 0 | 8514 | 1/1 | 0.92 | 0.39 | - | 53,53,53,53 | 0 |
| 36 | NA | 0 | 8561 | 1/1 | 0.98 | 0.33 | - | 89,89,89,89 | 0 |
| 38 | CL | N | 8807 | 1/1 | 0.95 | 0.07 | - | 62,62,62,62 | 0 |
| 36 | NA | 0 | 8529 | 1/1 | 0.96 | 0.04 | - | 20,20,20,20 | 0 |
| 35 | MG | 2 | 8060 | 1/1 | 0.98 | 0.12 | - | 42,42,42,42 | 0 |
| 37 | SR | 0 | 8903 | 1/1 | 0.98 | 0.16 | - | 44,44,44,44 | 0 |
| 37 | SR | 0 | 8924 | 1/1 | 0.99 | 0.18 | - | 65,65,65,65 | 0 |
| 37 | SR | 0 | 8973 | 1/1 | 0.98 | 0.10 | - | 91,91,91,91 | 0 |
| 37 | SR | 0 | 8940 | 1/1 | 0.99 | 0.12 | - | 53,53,53,53 | 0 |
| 36 | NA | D | 8543 | 1/1 | 0.84 | 0.07 | - | 60,60,60,60 | 0 |
| 35 | MG | 0 | 8033 | 1/1 | 0.86 | 0.09 | - | 59,59,59,59 | 0 |
| 37 | SR | 0 | 8997 | 1/1 | 0.96 | 0.05 | - | 116,116,116,116 | 0 |
| 36 | NA | 0 | 8573 | 1/1 | 0.27 | 0.98 | - | 107,107,107,107 | 0 |
| 37 | SR | 0 | 8938 | 1/1 | 0.96 | 0.07 | - | 101,101,101,101 | 0 |
| 37 | SR | 0 | 8974 | 1/1 | 0.81 | 0.19 | - | 110,110,110,110 | 0 |
| 35 | MG | 0 | 8005 | 1/1 | 0.76 | 0.33 | - | 30,30,30,30 | 0 |
| 37 | SR | 0 | 8955 | 1/1 | 0.86 | 0.09 | - | 115,115,115,115 | 0 |
| 38 | CL | R | 8806 | 1/1 | 0.99 | 0.08 | - | 36,36,36,36 | 0 |
| 37 | SR | 0 | 8965 | 1/1 | 0.97 | 0.11 | - | 88,88,88,88 | 0 |
| 35 | MG | 0 | 8078 | 1/1 | 0.71 | 0.88 | - | 104,104,104,104 | 0 |
| 37 | SR | 0 | 8946 | 1/1 | 0.98 | 0.17 | - | 86,86,86,86 | 0 |
| 36 | NA | 0 | 8566 | 1/1 | 0.84 | 0.24 | - | 39,39,39,39 | 0 |
| 35 | MG | 0 | 8027 | 1/1 | 0.91 | 0.14 | - | 44,44,44,44 | 0 |
| 37 | SR | 0 | 9004 | 1/1 | 0.93 | 0.16 | - | 107,107,107,107 | 0 |
| 37 | SR | 0 | 8914 | 1/1 | 0.98 | 0.22 | - | 75,75,75,75 | 0 |
| 36 | NA | 0 | 8516 | 1/1 | 0.81 | 0.19 | - | 42,42,42,42 | 0 |
| 35 | MG | 0 | 8089 | 1/1 | 0.84 | 0.15 | - | 35,35,35,35 | 0 |
| 36 | NA | 0 | 8555 | 1/1 | 0.83 | 0.73 | - | 64,64,64,64 | 0 |
| 36 | NA | 0 | 8569 | 1/1 | 0.83 | 0.21 | - | 44,44,44,44 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 37 | SR | 0 | 8988 | 1/1 | 0.91 | 0.06 | - | 110,110,110,110 | 0 |
| 36 | NA | 0 | 8509 | 1/1 | 0.79 | 0.40 | - | 83,83,83,83 | 0 |
| 37 | SR | 0 | 8982 | 1/1 | 0.93 | 0.12 | - | 105,105,105,105 | 0 |
| 37 | SR | 1 | 8952 | 1/1 | 0.98 | 0.15 | - | 60,60,60,60 | 0 |
| 36 | NA | 0 | 8535 | 1/1 | 0.83 | 0.40 | - | 64,64,64,64 | 0 |
| 36 | NA | 0 | 8531 | 1/1 | 0.88 | 0.21 | - | 37,37,37,37 | 0 |
| 34 | ACA | 6 | 78 | 8/9 | 0.75 | 0.37 | - | 74,74,81,82 | 0 |
| 37 | SR | 0 | 8934 | 1/1 | 0.98 | 0.18 | - | 67,67,67,67 | 0 |
| 37 | SR | 0 | 9008 | 1/1 | 0.96 | 0.14 | - | 80,80,80,80 | 0 |
| 35 | MG | 0 | 8081 | 1/1 | 0.83 | 0.52 | - | 103,103,103,103 | 0 |
| 37 | SR | 0 | 9007 | 1/1 | 0.51 | 0.72 | - | 200,200,200,200 | 0 |
| 37 | SR | 0 | 8908 | 1/1 | 0.99 | 0.13 | - | 66,66,66,66 | 0 |
| 37 | SR | 0 | 8905 | 1/1 | 0.99 | 0.22 | - | 49,49,49,49 | 0 |
| 35 | MG | 0 | 8020 | 1/1 | 0.98 | 0.20 | - | 24,24,24,24 | 0 |
| 35 | MG | 0 | 8066 | 1/1 | 0.96 | 0.24 | - | 32,32,32,32 | 0 |
| 37 | SR | 0 | 9000 | 1/1 | 0.88 | 0.18 | - | 137,137,137,137 | 0 |
| 38 | CL | J | 8802 | 1/1 | 0.96 | 0.06 | - | 66,66,66,66 | 0 |
| 36 | NA | 0 | 8544 | 1/1 | 0.94 | 0.34 | - | 67,67,67,67 | 0 |
| 37 | SR | 0 | 8996 | 1/1 | 0.48 | 0.11 | - | 148,148,148,148 | 0 |
| 37 | SR | 3 | 8953 | 1/1 | 0.99 | 0.12 | - | 103,103,103,103 | 0 |
| 37 | SR | T | 8911 | 1/1 | 1.00 | 0.10 | - | 52,52,52,52 | 0 |
| 35 | MG | 0 | 8090 | 1/1 | 0.17 | 1.00 | - | 126,126,126,126 | 0 |
| 37 | SR | 0 | 8923 | 1/1 | 0.96 | 0.17 | - | 66,66,66,66 | 0 |
| 35 | MG | 0 | 8046 | 1/1 | 0.72 | 0.83 | - | 99,99,99,99 | 0 |
| 37 | SR | A | 8977 | 1/1 | 0.96 | 0.10 | - | 95,95,95,95 | 0 |
| 35 | MG | 0 | 8070 | 1/1 | 0.98 | 0.22 | - | 62,62,62,62 | 0 |
| 35 | MG | 0 | 8056 | 1/1 | 0.83 | 0.18 | - | 69,69,69,69 | 0 |
| 36 | NA | 0 | 8508 | 1/1 | 0.85 | 0.12 | - | 31,31,31,31 | 0 |
| 36 | NA | 0 | 8548 | 1/1 | 0.98 | 0.20 | - | 27,27,27,27 | 0 |
| 37 | SR | 9 | 8980 | 1/1 | 0.89 | 0.05 | - | 155,155,155,155 | 0 |
| 35 | MG | 0 | 8018 | 1/1 | 0.98 | 0.26 | - | 9,9,9,9 | 0 |
| 36 | NA | B | 8552 | 1/1 | 0.85 | 0.45 | - | 69,69,69,69 | 0 |
| 37 | SR | 9 | 9003 | 1/1 | 0.91 | 0.06 | - | 127,127,127,127 | 0 |
| 37 | SR | 0 | 8986 | 1/1 | 0.93 | 0.12 | - | 114,114,114,114 | 0 |
| 37 | SR | 0 | 8971 | 1/1 | 0.91 | 0.07 | - | 157,157,157,157 | 0 |
| 35 | MG | 0 | 8024 | 1/1 | 0.85 | 0.25 | - | 80,80,80,80 | 0 |
| 36 | NA | 0 | 8536 | 1/1 | 0.82 | 0.15 | - | 69,69,69,69 | 0 |
| 37 | SR | 0 | 8984 | 1/1 | 0.96 | 0.10 | - | 89,89,89,89 | 0 |
| 37 | SR | B | 8950 | 1/1 | 0.95 | 0.17 | - | 89,89,89,89 | 0 |
| 36 | NA | 0 | 8551 | 1/1 | 0.88 | 0.28 | - | 53,53,53,53 | 0 |
| 35 | MG | 0 | 8017 | 1/1 | 0.93 | 0.66 | - | 80,80,80,80 | 0 |
| 35 | MG | 0 | 8029 | 1/1 | 0.93 | 0.27 | - | 87,87,87,87 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 35 | MG | 0 | 8036 | 1/1 | 0.94 | 0.15 | - | 47,47,47,47 | 0 |
| 36 | NA | 0 | 8506 | 1/1 | 0.68 | 0.20 | - | 65,65,65,65 | 0 |
| 35 | MG | 0 | 8080 | 1/1 | 0.94 | 0.16 | - | 62,62,62,62 | 0 |
| 37 | SR | 0 | 8967 | 1/1 | 0.96 | 0.11 | - | 92,92,92,92 | 0 |
| 36 | NA | 0 | 8518 | 1/1 | 0.86 | 0.21 | - | 68,68,68,68 | 0 |
| 35 | MG | 0 | 8093 | 1/1 | 0.97 | 0.12 | - | 25,25,25,25 | 0 |
| 36 | NA | 0 | 8549 | 1/1 | 0.84 | 0.34 | - | 61,61,61,61 | 0 |
| 40 | CD | O | 8705 | 1/1 | 0.97 | 0.03 | - | 103,103,103,103 | 0 |
| 37 | SR | 0 | 8959 | 1/1 | 0.61 | 0.06 | - | 131,131,131,131 | 0 |
| 37 | SR | 0 | 8928 | 1/1 | 0.95 | 0.08 | - | 87,87,87,87 | 0 |
| 37 | SR | 0 | 9001 | 1/1 | 0.77 | 0.09 | - | 155,155,155,155 | 0 |
| 35 | MG | 0 | 8031 | 1/1 | 0.96 | 0.12 | - | 48,48,48,48 | 0 |
| 35 | MG | 0 | 8016 | 1/1 | 0.48 | 0.88 | - | 98,98,98,98 | 0 |
| 37 | SR | H | 8907 | 1/1 | 1.00 | 0.15 | - | 41,41,41,41 | 0 |
| 35 | MG | 0 | 8079 | 1/1 | 0.50 | 0.34 | - | 64,64,64,64 | 0 |
| 35 | MG | 0 | 8077 | 1/1 | 0.91 | 0.09 | - | 37,37,37,37 | 0 |
| 37 | SR | 0 | 8944 | 1/1 | 0.87 | 0.14 | - | 113,113,113,113 | 0 |
| 35 | MG | 0 | 8065 | 1/1 | 0.66 | 0.41 | - | 84,84,84,84 | 0 |
| 35 | MG | 0 | 8064 | 1/1 | 0.85 | 0.17 | - | 51,51,51,51 | 0 |
| 37 | SR | 0 | 8918 | 1/1 | 0.99 | 0.14 | - | 41,41,41,41 | 0 |
| 37 | SR | 0 | 8916 | 1/1 | 0.94 | 0.13 | - | 65,65,65,65 | 0 |
| 35 | MG | 0 | 8055 | 1/1 | 0.95 | 0.29 | - | 30,30,30,30 | 0 |
| 35 | MG | 0 | 8026 | 1/1 | 0.99 | 0.14 | - | 35,35,35,35 | 0 |
| 37 | SR | 0 | 8983 | 1/1 | 0.92 | 0.23 | - | 195,195,195,195 | 0 |
| 35 | MG | 0 | 8049 | 1/1 | 0.88 | 0.54 | - | 141,141,141,141 | 0 |
| 38 | CL | 0 | 8817 | 1/1 | 0.97 | 0.06 | - | 42,42,42,42 | 0 |
| 36 | NA | C | 8503 | 1/1 | 0.98 | 0.23 | - | 22,22,22,22 | 0 |
| 36 | NA | 0 | 8541 | 1/1 | 0.74 | 0.39 | - | 80,80,80,80 | 0 |
| 35 | MG | K | 8054 | 1/1 | 0.99 | 0.17 | - | 18,18,18,18 | 0 |
| 36 | NA | 0 | 8502 | 1/1 | 0.94 | 0.21 | - | 55,55,55,55 | 0 |
| 37 | SR | 0 | 8926 | 1/1 | 1.00 | 0.16 | - | 81,81,81,81 | 0 |
| 38 | CL | A | 8809 | 1/1 | 0.95 | 0.07 | - | 57,57,57,57 | 0 |
| 37 | SR | 0 | 8941 | 1/1 | 0.95 | 0.14 | - | 71,71,71,71 | 0 |
| 37 | SR | 0 | 8954 | 1/1 | 0.97 | 0.12 | - | 67,67,67,67 | 0 |
| 37 | SR | 0 | 8995 | 1/1 | 0.92 | 0.15 | - | 86,86,86,86 | 0 |
| 37 | SR | 0 | 8936 | 1/1 | 0.95 | 0.16 | - | 59,59,59,59 | 0 |
| 35 | MG | 0 | 8035 | 1/1 | 0.94 | 0.18 | - | 94,94,94,94 | 0 |
| 36 | NA | 0 | 8571 | 1/1 | 0.48 | 0.70 | - | 131,131,131,131 | 0 |
| 35 | MG | B | 8042 | 1/1 | 0.85 | 0.11 | - | 92,92,92,92 | 0 |
| 38 | CL | J | 8801 | 1/1 | 0.95 | 0.10 | - | 58,58,58,58 | 0 |
| 35 | MG | 0 | 8032 | 1/1 | 0.92 | 0.07 | - | 44,44,44,44 | 0 |
| 35 | MG | 0 | 8022 | 1/1 | 0.99 | 0.19 | - | 12,12,12,12 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|-------|------|------|-----------------------------|-------|
| 35 | MG | 0 | 8038 | 1/1 | 0.08 | 2.39 | - | 112,112,112,112 | 0 |
| 37 | SR | T | 8939 | 1/1 | 0.99 | 0.09 | - | 70,70,70,70 | 0 |
| 36 | NA | 0 | 8524 | 1/1 | 0.95 | 0.09 | - | 37,37,37,37 | 0 |
| 37 | SR | 0 | 8998 | 1/1 | 0.73 | 0.20 | - | 159,159,159,159 | 0 |
| 35 | MG | 0 | 8039 | 1/1 | 0.91 | 0.22 | - | 32,32,32,32 | 0 |
| 37 | SR | 0 | 9006 | 1/1 | 0.55 | 0.59 | - | 199,199,199,199 | 0 |
| 37 | SR | 3 | 8999 | 1/1 | 0.99 | 0.12 | - | 70,70,70,70 | 0 |
| 37 | SR | 9 | 8968 | 1/1 | 0.89 | 0.09 | - | 105,105,105,105 | 0 |
| 36 | NA | 0 | 8520 | 1/1 | 0.92 | 0.17 | - | 43,43,43,43 | 0 |
| 37 | SR | 0 | 8915 | 1/1 | 0.99 | 0.10 | - | 73,73,73,73 | 0 |
| 37 | SR | 0 | 8957 | 1/1 | 0.93 | 0.12 | - | 122,122,122,122 | 0 |
| 35 | MG | 0 | 8068 | 1/1 | 0.95 | 0.24 | - | 74,74,74,74 | 0 |
| 35 | MG | 0 | 8087 | 1/1 | 0.28 | 1.16 | - | 106,106,106,106 | 0 |
| 37 | SR | 0 | 8963 | 1/1 | 0.98 | 0.16 | - | 70,70,70,70 | 0 |
| 37 | SR | 0 | 8919 | 1/1 | 0.92 | 0.12 | - | 82,82,82,82 | 0 |
| 35 | MG | 0 | 8058 | 1/1 | 0.99 | 0.20 | - | 1,1,1,1 | 0 |
| 37 | SR | 0 | 8958 | 1/1 | 0.97 | 0.10 | - | 68,68,68,68 | 0 |
| 36 | NA | 0 | 8562 | 1/1 | 0.94 | 0.46 | - | 61,61,61,61 | 0 |
| 35 | MG | 0 | 8048 | 1/1 | 0.82 | 0.16 | - | 43,43,43,43 | 0 |
| 37 | SR | 0 | 8951 | 1/1 | 0.86 | 0.09 | - | 107,107,107,107 | 0 |
| 37 | SR | 0 | 8966 | 1/1 | 0.94 | 0.13 | - | 86,86,86,86 | 0 |
| 36 | NA | 0 | 8501 | 1/1 | 0.92 | 0.32 | - | 100,100,100,100 | 0 |
| 36 | NA | 0 | 8505 | 1/1 | 0.91 | 0.40 | - | 29,29,29,29 | 0 |
| 37 | SR | 0 | 8937 | 1/1 | 0.99 | 0.19 | - | 59,59,59,59 | 0 |
| 37 | SR | 0 | 8931 | 1/1 | 0.98 | 0.12 | - | 74,74,74,74 | 0 |
| 36 | NA | 0 | 8554 | 1/1 | 0.94 | 0.46 | - | 53,53,53,53 | 0 |
| 37 | SR | 0 | 8906 | 1/1 | 0.97 | 0.17 | - | 49,49,49,49 | 0 |
| 37 | SR | 0 | 8978 | 1/1 | 0.98 | 0.16 | - | 60,60,60,60 | 0 |
| 37 | SR | S | 8961 | 1/1 | 0.81 | 0.08 | - | 189,189,189,189 | 0 |
| 35 | MG | 0 | 8082 | 1/1 | 0.85 | 0.31 | - | 64,64,64,64 | 0 |
| 35 | MG | 0 | 8050 | 1/1 | 0.76 | 0.58 | - | 162,162,162,162 | 0 |
| 35 | MG | 0 | 8023 | 1/1 | 0.88 | 0.14 | - | 21,21,21,21 | 0 |
| 38 | CL | 2 | 8803 | 1/1 | 0.97 | 0.07 | - | 51,51,51,51 | 0 |
| 36 | NA | 0 | 8550 | 1/1 | 0.94 | 0.19 | - | 43,43,43,43 | 0 |
| 37 | SR | 0 | 8976 | 1/1 | 0.73 | 0.22 | - | 124,124,124,124 | 0 |
| 37 | SR | 0 | 8901 | 1/1 | 0.99 | 0.13 | - | 44,44,44,44 | 0 |
| 38 | CL | L | 8814 | 1/1 | 0.96 | 0.07 | - | 49,49,49,49 | 0 |
| 38 | CL | L | 8810 | 1/1 | 0.98 | 0.05 | - | 52,52,52,52 | 0 |
| 37 | SR | 0 | 8942 | 1/1 | -0.18 | 0.22 | - | 186,186,186,186 | 0 |
| 35 | MG | 0 | 8019 | 1/1 | 0.98 | 0.19 | - | 9,9,9,9 | 0 |
| 36 | NA | S | 8510 | 1/1 | 0.90 | 0.14 | - | 58,58,58,58 | 0 |
| 35 | MG | 0 | 8061 | 1/1 | 0.99 | 0.20 | - | 17,17,17,17 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|-------|------|------|-----------------------------|-------|
| 35 | MG | 0 | 8073 | 1/1 | 0.93 | 0.09 | - | 62,62,62,62 | 0 |
| 35 | MG | 0 | 8069 | 1/1 | 0.83 | 0.25 | - | 88,88,88,88 | 0 |
| 38 | CL | 0 | 8815 | 1/1 | 1.00 | 0.06 | - | 61,61,61,61 | 0 |
| 36 | NA | R | 8532 | 1/1 | 0.97 | 0.09 | - | 29,29,29,29 | 0 |
| 37 | SR | 0 | 8933 | 1/1 | 0.01 | 0.41 | - | 168,168,168,168 | 0 |
| 37 | SR | 0 | 8909 | 1/1 | 1.00 | 0.17 | - | 59,59,59,59 | 0 |
| 35 | MG | 0 | 8067 | 1/1 | 0.93 | 0.29 | - | 48,48,48,48 | 0 |
| 35 | MG | 0 | 8037 | 1/1 | 0.80 | 0.14 | - | 70,70,70,70 | 0 |
| 38 | CL | Q | 8811 | 1/1 | 0.95 | 0.06 | - | 68,68,68,68 | 0 |
| 36 | NA | 0 | 8507 | 1/1 | 0.77 | 0.37 | - | 88,88,88,88 | 0 |
| 35 | MG | 0 | 8045 | 1/1 | 0.98 | 0.58 | - | 147,147,147,147 | 0 |
| 38 | CL | Y | 8820 | 1/1 | 0.96 | 0.05 | - | 35,35,35,35 | 0 |
| 36 | NA | 0 | 8574 | 1/1 | 0.97 | 0.44 | - | 48,48,48,48 | 0 |
| 37 | SR | 0 | 8920 | 1/1 | 0.52 | 0.69 | - | 200,200,200,200 | 0 |
| 37 | SR | 0 | 8956 | 1/1 | 0.93 | 0.12 | - | 105,105,105,105 | 0 |
| 35 | MG | 0 | 8030 | 1/1 | 0.69 | 0.14 | - | 188,188,188,188 | 0 |
| 36 | NA | 0 | 8526 | 1/1 | 0.97 | 0.13 | - | 47,47,47,47 | 0 |
| 37 | SR | 0 | 8989 | 1/1 | 0.99 | 0.11 | - | 71,71,71,71 | 0 |
| 35 | MG | 0 | 8053 | 1/1 | 0.80 | 0.11 | - | 54,54,54,54 | 0 |
| 37 | SR | 0 | 8960 | 1/1 | 0.96 | 0.08 | - | 98,98,98,98 | 0 |
| 36 | NA | 0 | 8525 | 1/1 | 0.64 | 0.32 | - | 63,63,63,63 | 0 |
| 37 | SR | 0 | 8994 | 1/1 | 0.86 | 0.53 | - | 200,200,200,200 | 0 |
| 37 | SR | 0 | 8990 | 1/1 | 0.99 | 0.17 | - | 39,39,39,39 | 0 |
| 35 | MG | 0 | 8063 | 1/1 | -0.06 | 0.42 | - | 87,87,87,87 | 0 |
| 36 | NA | 0 | 8570 | 1/1 | 0.91 | 0.14 | - | 53,53,53,53 | 0 |
| 35 | MG | 0 | 8091 | 1/1 | 0.85 | 0.10 | - | 59,59,59,59 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.