



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:56 AM GMT

PDB ID : 3CCQ
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation A2488U
Authors : Blaha, G.; Gurel, G.
Deposited on : 2008-02-26
Resolution : 2.90 Å(reported)

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

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

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

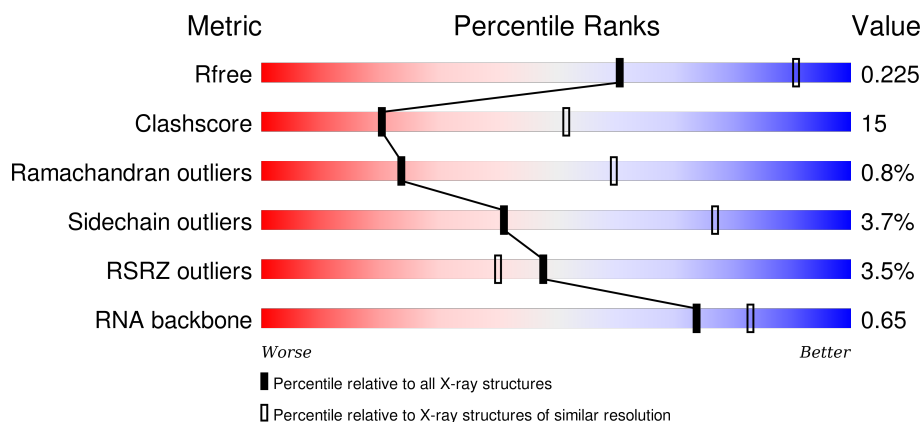
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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 | 1451 (2.90-2.90) |
| Clashscore | 102246 | 1668 (2.90-2.90) |
| Ramachandran outliers | 100387 | 1630 (2.90-2.90) |
| Sidechain outliers | 100360 | 1632 (2.90-2.90) |
| RSRZ outliers | 91569 | 1456 (2.90-2.90) |
| RNA backbone | 2183 | 1093 (3.30-2.50) |

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> <div></div> <div>71%</div> <div>25%</div> <div>••</div> </div> </div> |
| 2 | B | 338 | <div> <div>%</div> <div> <div></div> <div>68%</div> <div>29%</div> <div>•</div> </div> </div> |
| 3 | C | 246 | <div> <div>2%</div> <div> <div></div> <div>72%</div> <div>26%</div> <div>•</div> </div> </div> |
| 4 | D | 177 | <div> <div>29%</div> <div> <div></div> <div>40%</div> <div>37%</div> <div>•</div> <div>21%</div> </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 | 241 | |
| 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 | |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 32 | MG | 0 | 8009 | - | - | - | X |
| 32 | MG | 0 | 8014 | - | - | - | X |
| 32 | MG | 0 | 8028 | - | - | - | X |
| 32 | MG | 0 | 8041 | - | - | - | X |
| 32 | MG | 0 | 8047 | - | - | - | X |
| 32 | MG | 0 | 8084 | - | - | - | X |
| 32 | MG | 0 | 8085 | - | - | - | X |
| 32 | MG | A | 8051 | - | - | - | X |
| 33 | K | 0 | 8401 | - | - | - | X |
| 33 | K | 0 | 8402 | - | - | - | X |
| 34 | NA | 0 | 8521 | - | - | - | X |
| 34 | NA | 0 | 8527 | - | - | - | X |
| 34 | NA | 0 | 8528 | - | - | - | X |
| 34 | NA | 0 | 8530 | - | - | - | X |
| 34 | NA | 0 | 8542 | - | - | - | X |
| 34 | NA | 0 | 8546 | - | - | - | X |
| 34 | NA | 0 | 8547 | - | - | - | X |
| 34 | NA | 0 | 8553 | - | - | - | X |
| 34 | NA | 0 | 8555 | - | - | - | X |
| 34 | NA | 0 | 8556 | - | - | - | X |
| 34 | NA | 0 | 8559 | - | - | - | X |
| 34 | NA | 0 | 8560 | - | - | - | X |
| 34 | NA | 0 | 8562 | - | - | - | X |
| 34 | NA | 0 | 8563 | - | - | - | X |
| 34 | NA | 0 | 8564 | - | - | - | X |
| 34 | NA | 0 | 8565 | - | - | - | X |
| 34 | NA | 0 | 8567 | - | - | - | X |
| 34 | NA | 9 | 8572 | - | - | - | X |
| 34 | NA | R | 8575 | - | - | - | X |
| 36 | SR | 0 | 8903 | - | - | - | X |
| 36 | SR | 0 | 8904 | - | - | - | X |
| 36 | SR | 0 | 8949 | - | - | - | X |
| 36 | SR | B | 8987 | - | - | - | X |

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99120 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 |
| | | | 1753 | 1072 | 352 | 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 |
| | | | 2625 | 1616 | 493 | 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 |
| | | | 1860 | 1130 | 345 | 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 |
| | | | 1094 | 685 | 195 | 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 |
| | | | 1357 | 840 | 224 | 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 |
| | | | 890 | 551 | 141 | 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 |
| | | | 1282 | 798 | 240 | 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 |
| | | | 519 | 323 | 81 | 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 |
| | | | 1120 | 696 | 199 | 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 |
| | | | 994 | 609 | 189 | 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 |
| | | | 1118 | 670 | 222 | 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 |
| | | | 1558 | 943 | 333 | 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 |
| | | | 1445 | 895 | 262 | 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 |
| | | | 865 | 529 | 161 | 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 |
| | | | 1136 | 683 | 229 | 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 |
| | | | 735 | 450 | 141 | 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 |
| | | | 1149 | 713 | 209 | 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 |
| | | | 641 | 389 | 111 | 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 |
| | | | 950 | 568 | 180 | 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 |
| | | | 1196 | 737 | 209 | 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 |
| | | | 654 | 402 | 129 | 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 |
| | | | 573 | 343 | 113 | 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 |
| | | | 755 | 458 | 153 | 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 | 26348 | 10870 | 19055 | 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 |
| | | | 2599 | 1160 | 471 | 847 | 121 | | | |

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

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 32 | 0 | 87 | Total | Mg | 0 | 0 |
| | | | 87 | 87 | | |
| 32 | Y | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | K | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | B | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | A | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | T | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 32 | 9 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

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

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

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

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-------------------|---------|---------|
| 34 | 0 | 65 | Total Na 65 65 | 0 | 0 |
| 34 | J | 1 | Total Na 1 1 | 0 | 0 |
| 34 | Q | 1 | Total Na 1 1 | 0 | 0 |
| 34 | B | 1 | Total Na 1 1 | 0 | 0 |
| 34 | C | 1 | Total Na 1 1 | 0 | 0 |
| 34 | R | 2 | Total Na 2 2 | 0 | 0 |
| 34 | 9 | 2 | Total Na 2 2 | 0 | 0 |
| 34 | S | 1 | Total Na 1 1 | 0 | 0 |
| 34 | M | 1 | Total Na 1 1 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 35 | 0 | 9 | Total Cl 9 9 | 0 | 0 |
| 35 | J | 3 | Total Cl 3 3 | 0 | 0 |
| 35 | Q | 1 | Total Cl 1 1 | 0 | 0 |
| 35 | B | 1 | Total Cl 1 1 | 0 | 0 |
| 35 | A | 1 | Total Cl 1 1 | 0 | 0 |
| 35 | N | 1 | Total Cl 1 1 | 0 | 0 |
| 35 | O | 1 | Total Cl 1 1 | 0 | 0 |
| 35 | R | 1 | Total Cl 1 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 35 | Y | 1 | Total 1 | Cl 1 | 0 | 0 |
| 35 | L | 1 | Total 1 | Cl 1 | 0 | 0 |
| 35 | 3 | 1 | Total 1 | Cl 1 | 0 | 0 |
| 35 | M | 1 | Total 1 | Cl 1 | 0 | 0 |

- Molecule 36 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|----------|---------|---------|
| 36 | 0 | 93 | Total 93 | Sr 93 | 0 | 0 |
| 36 | 1 | 2 | Total 2 | Sr 2 | 0 | 0 |
| 36 | B | 2 | Total 2 | Sr 2 | 0 | 0 |
| 36 | 3 | 2 | Total 2 | Sr 2 | 0 | 0 |
| 36 | A | 3 | Total 3 | Sr 3 | 0 | 0 |
| 36 | R | 1 | Total 1 | Sr 1 | 0 | 0 |
| 36 | 9 | 3 | Total 3 | Sr 3 | 0 | 0 |
| 36 | S | 1 | Total 1 | Sr 1 | 0 | 0 |
| 36 | F | 1 | Total 1 | Sr 1 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 37 | O | 1 | Total 1 | Cd 1 | 0 | 0 |
| 37 | Z | 1 | Total 1 | Cd 1 | 0 | 0 |
| 37 | 1 | 1 | Total 1 | Cd 1 | 0 | 0 |
| 37 | 3 | 1 | Total 1 | Cd 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 37 | U | 1 | Total | Cd | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 38 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|------|---------|---------|
| 38 | 0 | 5950 | Total | O | 0 | 0 |
| | | | 5950 | 5950 | | |
| 38 | 9 | 148 | Total | O | 0 | 0 |
| | | | 148 | 148 | | |
| 38 | A | 112 | Total | O | 0 | 0 |
| | | | 112 | 112 | | |
| 38 | B | 142 | Total | O | 0 | 0 |
| | | | 142 | 142 | | |
| 38 | C | 168 | Total | O | 0 | 0 |
| | | | 168 | 168 | | |
| 38 | D | 45 | Total | O | 0 | 0 |
| | | | 45 | 45 | | |
| 38 | E | 42 | Total | O | 0 | 0 |
| | | | 42 | 42 | | |
| 38 | F | 26 | Total | O | 0 | 0 |
| | | | 26 | 26 | | |
| 38 | G | 17 | Total | O | 0 | 0 |
| | | | 17 | 17 | | |
| 38 | H | 65 | Total | O | 0 | 0 |
| | | | 65 | 65 | | |
| 38 | I | 5 | Total | O | 0 | 0 |
| | | | 5 | 5 | | |
| 38 | J | 56 | Total | O | 0 | 0 |
| | | | 56 | 56 | | |
| 38 | K | 60 | Total | O | 0 | 0 |
| | | | 60 | 60 | | |
| 38 | L | 82 | Total | O | 0 | 0 |
| | | | 82 | 82 | | |
| 38 | M | 123 | Total | O | 0 | 0 |
| | | | 123 | 123 | | |
| 38 | N | 59 | Total | O | 0 | 0 |
| | | | 59 | 59 | | |
| 38 | O | 47 | Total | O | 0 | 0 |
| | | | 47 | 47 | | |
| 38 | P | 59 | Total | O | 0 | 0 |
| | | | 59 | 59 | | |

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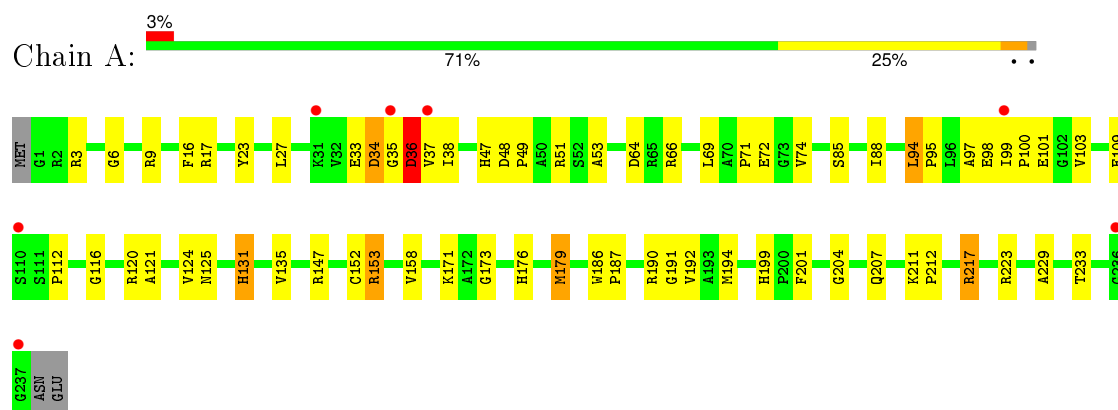
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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 38 | Q | 47 | Total 47 | O 47 | 0 | 0 |
| 38 | R | 76 | Total 76 | O 76 | 0 | 0 |
| 38 | S | 33 | Total 33 | O 33 | 0 | 0 |
| 38 | T | 36 | Total 36 | O 36 | 0 | 0 |
| 38 | U | 26 | Total 26 | O 26 | 0 | 0 |
| 38 | V | 12 | Total 12 | O 12 | 0 | 0 |
| 38 | W | 66 | Total 66 | O 66 | 0 | 0 |
| 38 | X | 28 | Total 28 | O 28 | 0 | 0 |
| 38 | Y | 97 | Total 97 | O 97 | 0 | 0 |
| 38 | Z | 31 | Total 31 | O 31 | 0 | 0 |
| 38 | 1 | 54 | Total 54 | O 54 | 0 | 0 |
| 38 | 2 | 43 | Total 43 | O 43 | 0 | 0 |
| 38 | 3 | 68 | Total 68 | O 68 | 0 | 0 |

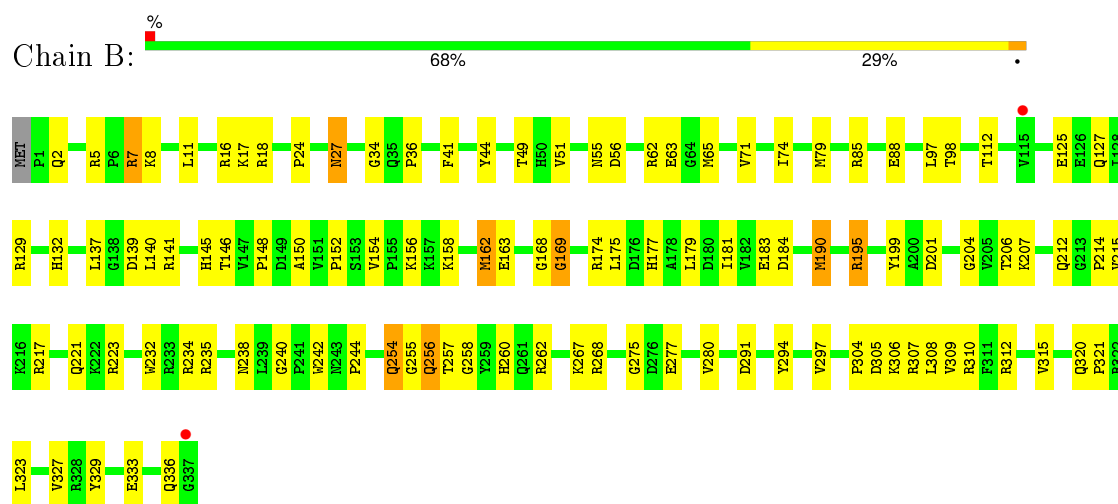
3 Residue-property plots [i](#)

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

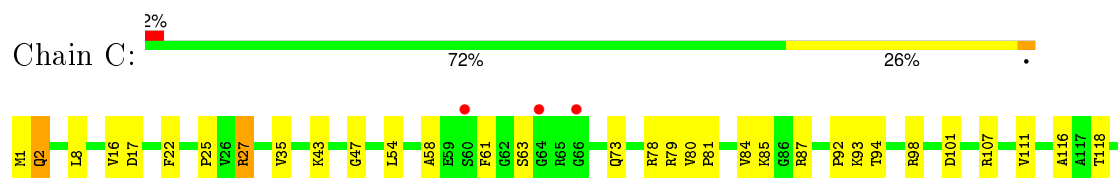
- Molecule 1: 50S ribosomal protein L2P

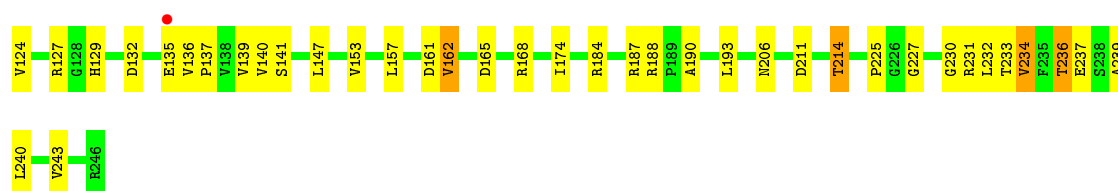


- Molecule 2: 50S ribosomal protein L3P

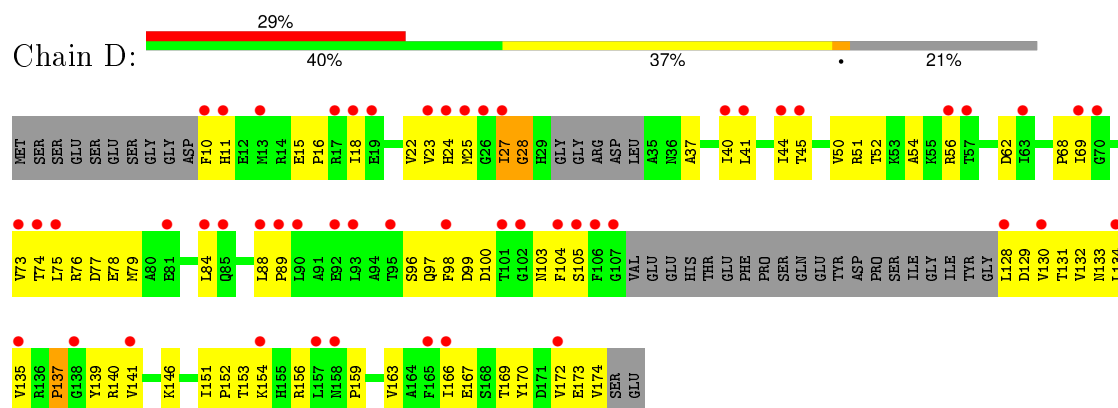


- Molecule 3: 50S ribosomal protein L4P

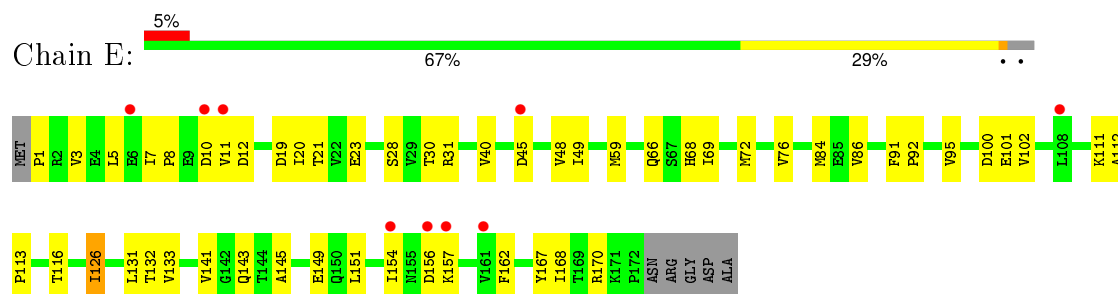




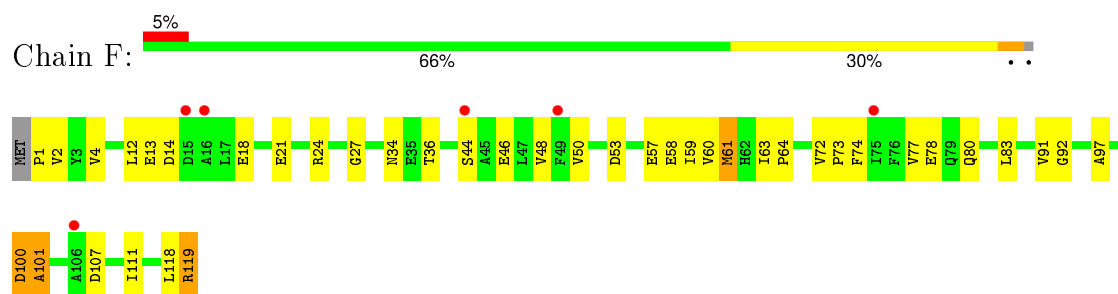
• Molecule 4: 50S ribosomal protein L5P



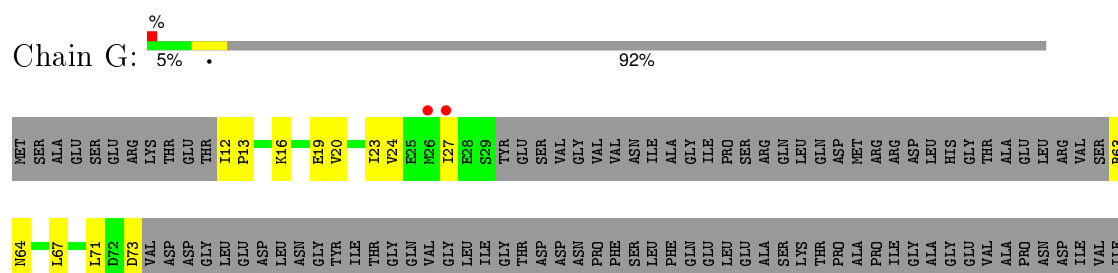
• Molecule 5: 50S ribosomal protein L6P



• Molecule 6: 50S ribosomal protein L7Ae



• Molecule 7: 50S ribosomal protein L10E



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| PRO | GLU | GLY | ASP | THR | GLY | VAL | ASP | PRO | GLY | PRO | GLY | PHE | VAL | GLY | GLU | LEU | GLN | SER | VAL | GLY | ALA | ASP | ALA | ARG | ILE | GLN | GLU | GLY | SER | ILE | GLN | VAL | LEU | SER | GLN | ASP | SER | THR | THR | VAL | LEU | ASP | THR | GLY | GLU | VAL | SER | ASN | VAL | LEU | ASN | GLY | LEU | ILE | GLY | PRO | |
| LYS | GLU | VAL | GLY | LEU | ASP | ASP | ARG | LEU | ALA | VAL | PHE | ALA | ASP | GLY | VAL | LEU | LEU | PHE | GLU | PRO | GLU | VAL | VAL | LEU | ASP | ILE | ASP | GLU | GLY | TYR | ASP | SER | GLN | ASP | ILE | ALA | GLY | ARG | ALA | ASP | PHE | ASN | LEU | SER | ASN | VAL | THR | ALA | THR | THR | ALA | PRO | THR | MET | ILE | GLY | GLN |
| SER | ALA | ARG | GLY | ASN | ALA | LYS | SER | LEU | ALA | LEU | VAL | GLN | ALA | ALA | ILE | ALA | ASP | ALA | PRO | GLU | VAL | VAL | GLU | ASP | VAL | SER | LYS | ASP | ASP | ALA | ASP | GLN | VAL | ARG | ALA | LEU | ALA | SER | GLN | ILE | ASP | GLU | ALA | LEU | PRO | GLU | GLY | LEU | LEU | GLY | VAL | ASP | ALA | THR | ALA | GLU | |
| PRO | THR | ASP | ASP | GLN | ASP | ASP | ASP | THR | THR | ALA | SER | GLU | ASP | ASP | ALA | ASP | ALA | ASP | ASP | ALA | ALA | VAL | GLU | ASP | ALA | ASP | ASP | ASP | ASP | ASP | ASP | ASP | GLU | ASP | ALA | GLY | LEU | GLY | ALA | ASP | GLU | ALA | LEU | LEU | GLY | GLN | VAL | THR | ALA | GLY | PRO | | | | | | |

• Molecule 8: 50S ribosomal protein L10e



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| SER | PHE | GLU | ILE | GLU | VAL | G66 | V67 | P68 | P69 | T70 | A71 | E72 | L73 | I74 | K75 | D76 | E77 | A78 | G79 | F80 | E81 | T82 | G83 | S84 | G85 | E86 | P87 | Q88 | E89 | D90 | F91 | V92 | A93 | D94 | V97 | D98 | Q99 | V100 | K101 | Q102 | I103 | A104 | E105 | Q106 | K107 | H108 | P109 | D110 | L111 | L112 | S113 | Y114 | A120 | K121 | V124 | G125 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| T126 | C127 | T128 | S129 | L130 | G131 | V132 | T133 | I134 | E135 | GLY | ASN | PRO | ARG | GLU | PHE | LYS | GLU | ARG | ILE | ASP | ALA | GLY | GLU | TYR | ASP | ASP | VAL | PHE | ALA | ALA | ALA | GLU | ALA | GLN | ALA | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |

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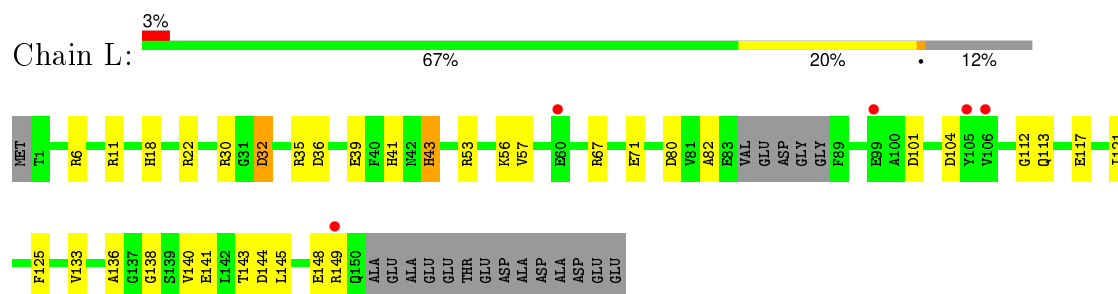
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| MET | SER | VAL | A4 | E5 | I18 | M19 | V39 | N40 | A41 | E42 | V45 | I46 | S33 | T47 | Q52 | I53 | V54 | R60 | Y69 | P70 | R74 | P75 | D76 | G77 | I78 | F79 | T82 | P88 | H89 | K90 | L105 | G106 | M107 | P108 | Y109 | L121 | I127 | V130 | T131 | L132 | S136 | E137 | T138 | W145 |
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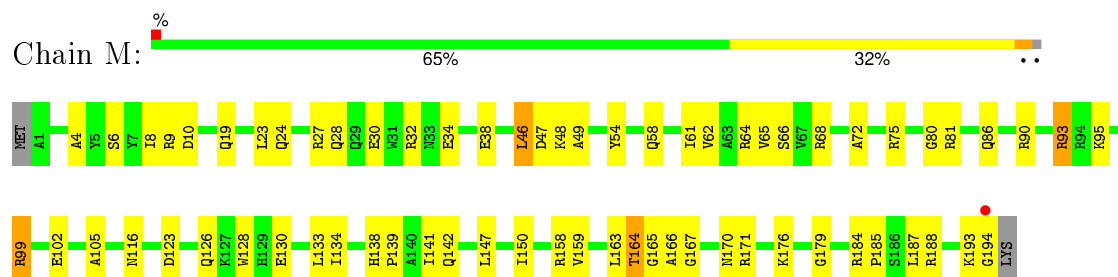


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| H1 | L4 | D7 | Q10 | K14 | C20 | L29 | I32 | S33 | V34 | G39 | T40 | K41 | N42 | P45 | R46 | A47 | V55 | S56 | E63 | M64 | R65 | R66 | Q67 | V74 | R75 | K78 | P79 | I80 | R81 | R87 | V88 | K89 | V98 | E102 | I113 | E116 | V117 | A118 | A125 | S126 | | |
| A127 | M130 | I131 | V132 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |

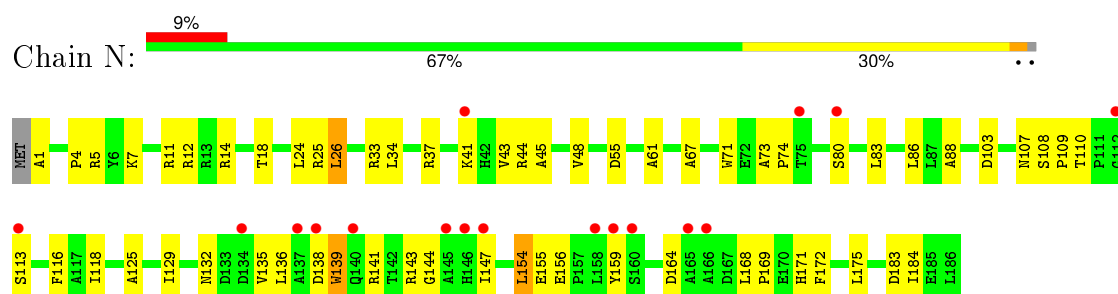
- Molecule 12: 50S ribosomal protein L15P



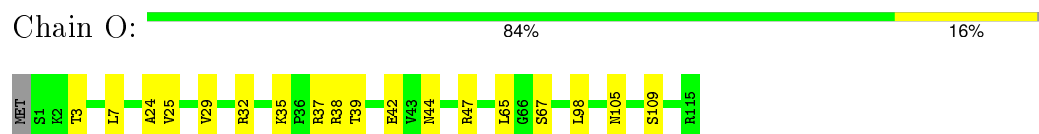
- Molecule 13: 50S ribosomal protein L15e



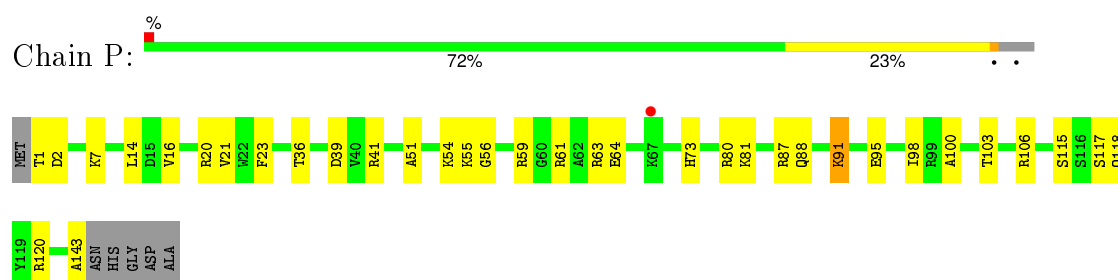
- Molecule 14: 50S ribosomal protein L18P



- Molecule 15: 50S ribosomal protein L18e

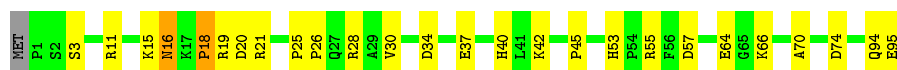


- Molecule 16: 50S ribosomal protein L19e



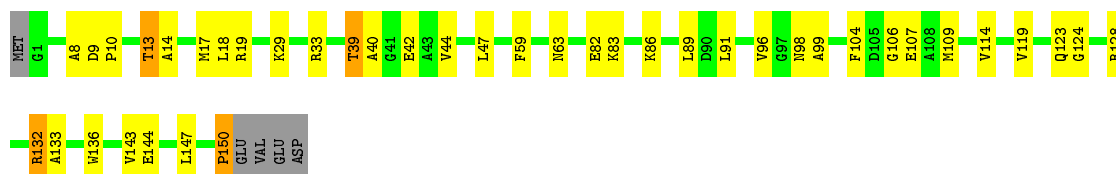
- Molecule 17: 50S ribosomal protein L21e

Chain Q:  72% 25% ..



- Molecule 18: 50S ribosomal protein L22P

Chain R:  70% 24% . .




- Molecule 19: 50S ribosomal protein L23P

Chain S:  2% 75% 20% 5%



- Molecule 20: 50S ribosomal protein L24P

Chain T:  3% 80% 18% ..



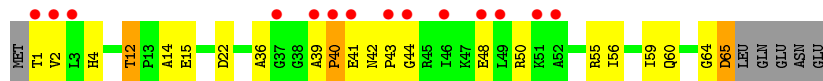
- Molecule 21: 50S ribosomal protein L24e

Chain U:  0% 51% 27% 21%



- Molecule 22: 50S ribosomal protein L29P

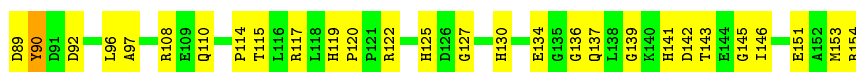
Chain V:  20% 61% 27% 8%



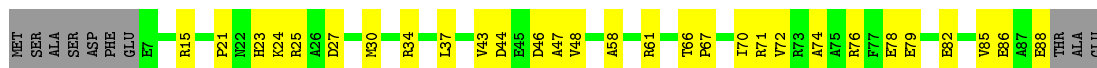
- Molecule 23: 50S ribosomal protein L30P

Chain W:  57% 42% .

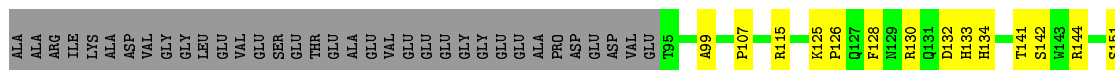
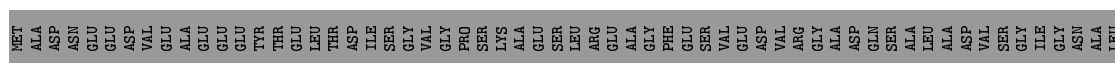




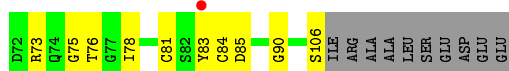
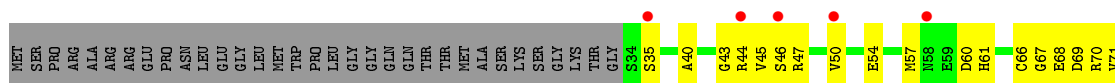
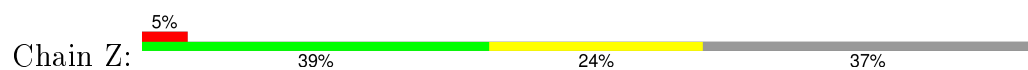
- Molecule 24: 50S ribosomal protein L31e



- Molecule 25: 50S ribosomal protein L32e



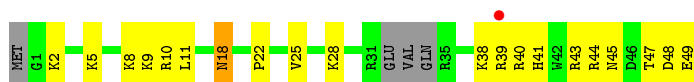
- Molecule 26: 50S ribosomal protein L37Ae



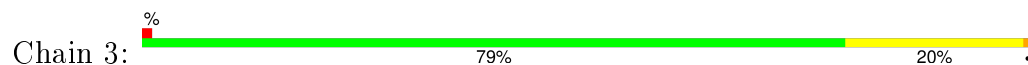
- Molecule 27: 50S ribosomal protein L37e

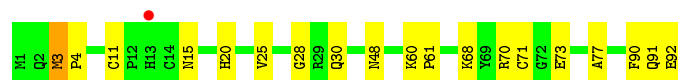


- Molecule 28: 50S ribosomal protein L39e

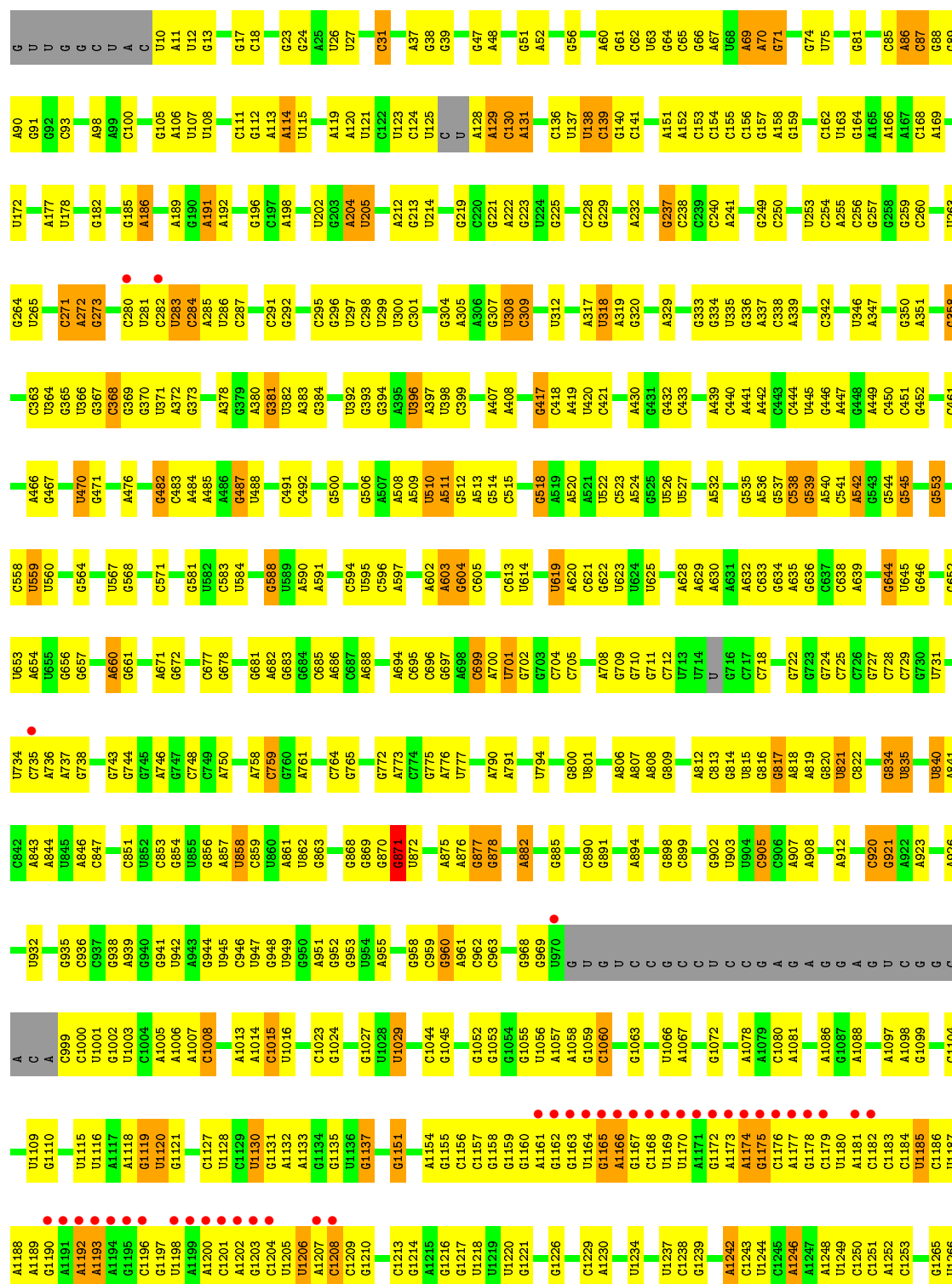


- Molecule 29: 50S ribosomal protein L44E

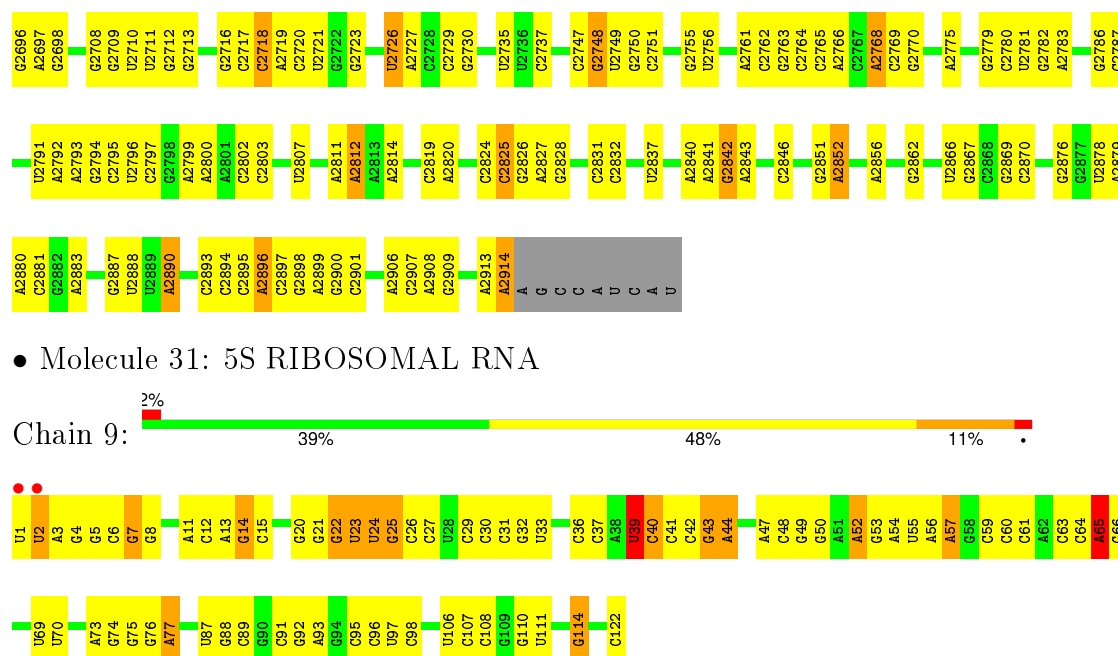




Molecule 30: 23S RIBOSOMAL RNA



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| C2593 | C2594 | C2595 | C2596 | C2597 | C2598 | C2599 | C2600 | C2601 | C2602 | C2603 | C2604 | C2605 | C2606 | C2607 | C2608 | C2609 | C2610 | C2611 | C2612 | C2613 | C2614 | C2615 | C2616 | C2617 | C2618 | C2619 | C2620 | C2621 | C2622 | C2623 | C2624 | C2625 | C2626 | C2627 | C2628 | C2629 | C2630 | C2631 | C2632 | C2633 | C2634 | C2635 | C2636 | C2637 | C2638 | C2639 | C2640 | C2641 | C2642 | C2643 | C2644 | C2645 | C2646 | C2647 | C2648 | C2649 | C2650 | C2651 | C2652 | C2653 | C2654 | C2655 | C2656 | C2657 | C2658 | C2659 | C2660 | C2661 | C2662 | C2663 | C2664 | C2665 | C2666 | C2667 | C2668 | C2669 | C2670 | C2671 | C2672 | C2673 | C2674 | C2675 | C2676 | C2677 | C2678 | C2679 | C2680 | C2681 | C2682 | C2683 | C2684 | C2685 | C2686 | C2687 | C2688 | C2689 | C2690 | C2691 | C2692 | C2693 | C2694 | C2695 | C2696 | C2697 | C2698 | C2699 | C2700 | C2701 | C2702 | C2703 | C2704 | C2705 | C2706 | C2707 | C2708 | C2709 | C2710 | C2711 | C2712 | C2713 | C2714 | C2715 | C2716 | C2717 | C2718 | C2719 | C2720 | C2721 | C2722 | C2723 | C2724 | C2725 | C2726 | C2727 | C2728 | C2729 | C2730 | C2731 | C2732 | C2733 | C2734 | C2735 | C2736 | C2737 | C2738 | C2739 | C2740 | C2741 | C2742 | C2743 | C2744 | C2745 | C2746 | C2747 | C2748 | C2749 | C2750 | C2751 | C2752 | C2753 | C2754 | C2755 | C2756 | C2757 | C2758 | C2759 | C2760 | C2761 | C2762 | C2763 | C2764 | C2765 | C2766 | C2767 | C2768 | C2769 | C2770 | C2771 | C2772 | C2773 | C2774 | C2775 | C2776 | C2777 | C2778 | C2779 | C2780 | C2781 | C2782 | C2783 | C2784 | C2785 | C2786 | C2787 | C2788 | C2789 | C2790 | C2791 | C2792 | C2793 | C2794 | C2795 | C2796 | C2797 | C2798 | C2799 | C2800 | C2801 | C2802 | C2803 | C2804 | C2805 | C2806 | C2807 | C2808 | C2809 | C2810 | C2811 | C2812 | C2813 | C2814 | C2815 | C2816 | C2817 | C2818 | C2819 | C2820 | C2821 | C2822 | C2823 | C2824 | C2825 | C2826 | C2827 | C2828 | C2829 | C2830 | C2831 | C2832 | C2833 | C2834 | C2835 | C2836 | C2837 | C2838 | C2839 | C2840 | C2841 | C2842 | C2843 | C2844 | C2845 | C2846 | C2847 | C2848 | C2849 | C2850 | C2851 | C2852 | C2853 | C2854 | C2855 | C2856 | C2857 | C2858 | C2859 | C2860 | C2861 | C2862 | C2863 | C2864 | C2865 | C2866 | C2867 | C2868 | C2869 | C2870 | C2871 | C2872 | C2873 | C2874 | C2875 | C2876 | C2877 | C2878 | C2879 | C2880 | C2881 | C2882 | C2883 | C2884 | C2885 | C2886 | C2887 | C2888 | C2889 | C2890 | C2891 | C2892 | C2893 | C2894 | C2895 | C2896 | C2897 | C2898 | C2899 | C2900 | C2901 | C2902 | C2903 | C2904 | C2905 | C2906 | C2907 | C2908 | C2909 | C2910 | C2911 | C2912 | C2913 | C2914 | C2915 | C2916 | C2917 | C2918 | C2919 | C2920 | C2921 | C2922 | C2923 | C2924 | C2925 | C2926 | C2927 | C2928 | C2929 | C2930 | C2931 | C2932 | C2933 | C2934 | C2935 | C2936 | C2937 | C2938 | C2939 | C2940 | C2941 | C2942 | C2943 | C2944 | C2945 | C2946 | C2947 | C2948 | C2949 | C2950 | C2951 | C2952 | C2953 | C2954 | C2955 | C2956 | C2957 | C2958 | C2959 | C2960 | C2961 | C2962 | C2963 | C2964 | C2965 | C2966 | C2967 | C2968 | C2969 | C2970 | C2971 | C2972 | C2973 | C2974 | C2975 | C2976 | C2977 | C2978 | C2979 | C2980 | C2981 | C2982 | C2983 | C2984 | C2985 | C2986 | C2987 | C2988 | C2989 | C2990 | C2991 | C2992 | C2993 | C2994 | C2995 | C2996 | C2997 | C2998 | C2999 | C3000 | C3001 | C3002 | C3003 | C3004 | C3005 | C3006 | C3007 | C3008 | C3009 | C3010 | C3011 | C3012 | C3013 | C3014 | C3015 | C3016 | C3017 | C3018 | C3019 | C3020 | C3021 | C3022 | C3023 | C3024 | C3025 | C3026 | C3027 | C3028 | C3029 | C3030 | C3031 | C3032 | C3033 | C3034 | C3035 | C3036 | C3037 | C3038 | C3039 | C3040 | C3041 | C3042 | C3043 | C3044 | C3045 | C3046 | C3047 | C3048 | C3049 | C3050 | C3051 | C3052 | C3053 | C3054 | C3055 | C3056 | C3057 | C3058 | C3059 | C3060 | C3061 | C3062 | C3063 | C3064 | C3065 | C3066 | C3067 | C3068 | C3069 | C3070 | C3071 | C3072 | C3073 | C3074 | C3075 | C3076 | C3077 | C3078 | C3079 | C3080 | C3081 | C3082 | C3083 | C3084 | C3085 | C3086 | C3087 | C3088 | C3089 | C3090 | C3091 | C3092 | C3093 | C3094 | C3095 | C3096 | C3097 | C3098 | C3099 | C3100 | C3101 | C3102 | C3103 | C3104 | C3105 | C3106 | C3107 | C3108 | C3109 | C3110 | C3111 | C3112 | C3113 | C3114 | C3115 | C3116 | C3117 | C3118 | C3119 | C3120 | C3121 | C3122 | C3123 | C3124 | C3125 | C3126 | C3127 | C3128 | C3129 | C3130 | C3131 | C3132 | C3133 | C3134 | C3135 | C3136 | C3137 | C3138 | C3139 | C3140 | C3141 | C3142 | C3143 | C3144 | C3145 | C3146 | C3147 | C3148 | C3149 | C3150 | C3151 | C3152 | C3153 | C3154 | C3155 | C3156 | C3157 | C3158 | C3159 | C3160 | C3161 | C3162 | C3163 | C3164 | C3165 | C3166 | C3167 | C3168 | C3169 | C3170 | C3171 | C3172 | C3173 | C3174 | C3175 | C3176 | C3177 | C3178 | C3179 | C3180 | C3181 | C3182 | C3183 | C3184 | C3185 | C3186 | C3187 | C3188 | C3189 | C3190 | C3191 | C3192 | C3193 | C3194 | C3195 | C3196 | C3197 | C3198 | C3199 | C3200 | C3201 | C3202 | C3203 | C3204 | C3205 | C3206 | C3207 | C3208 | C3209 | C3210 | C3211 | C3212 | C3213 | C3214 | C3215 | C3216 | C3217 | C3218 | C3219 | C3220 | C3221 | C3222 | C3223 | C3224 | C3225 | C3226 | C3227 | C3228 | C3229 | C3230 | C3231 | C3232 | C3233 | C3234 | C3235 | C3236 | C3237 | C3238 | C3239 | C3240 | C3241 | C3242 | C3243 | C3244 | C3245 | C3246 | C3247 | C3248 | C3249 | C3250 | C3251 | C3252 | C3253 | C3254 | C3255 | C3256 | C3257 | C3258 | C3259 | C3260 | C3261 | C3262 | C3263 | C3264 | C3265 | C3266 | C3267 | C3268 | C3269 | C3270 | C3271 | C3272 | C3273 | C3274 | C3275 | C3276 | C3277 | C3278 | C3279 | C3280 | C3281 | C3282 | C3283 | C3284 | C3285 | C3286 | C3287 | C3288 | C3289 | C3290 | C3291 | C3292 | C3293 | C3294 | C3295 | C3296 | C3297 | C3298 | C3299 | C3300 | C3301 | C3302 | C3303 | C3304 | C3305 | C3306 | C3307 | C3308 | C3309 | C3310 | C3311 | C3312 | C3313 | C3314 | C3315 | C3316 | C3317 | C3318 | C3319 | C3320 | C3321 | C3322 | C3323 | C3324 | C3325 | C3326 | C3327 | C3328 | C3329 | C3330 | C3331 | C3332 | C3333 | C3334 | C3335 | C3336 | C3337 | C3338 | C3339 | C3340 | C3341 | C3342 | C3343 | C3344 | C3345 | C3346 | C3347 | C3348 | C3349 | C3350 | C3351 | C3352 | C3353 | C3354 | C3355 | C3356 | C3357 | C3358 | C3359 | C3360 | C3361 | C3362 | C3363 | C3364 | C3365 | C3366 | C3367 | C3368 | C3369 | C3370 | C3371 | C3372 | C3373 | C3374 | C3375 | C3376 | C3377 | C3378 | C3379 | C3380 | C3381 | C3382 | C3383 | C3384 | C3385 | C3386 | C3387 | C3388 | C3389 | C3390 | C3391 | C3392 | C3393 | C3394 | C3395 | C3396 | C3397 | C3398 | C3399 | C3400 | C3401 | C3402 | C3403 | C3404 | C3405 | C3406 | C3407 | C3408 | C3409 | C3410 | C3411 | C3412 | C3413 | C3414 | C3415 | C3416 | C3417 | C3418 | C3419 | C3420 | C3421 | C3422 | C3423 | C3424 | C3425 | C3426 | C3427 | C3428 | C3429 | C3430 | C3431 | C3432 | C3433 | C3434 | C3435 | C3436 | C3437 | C3438 | C3439 | C3440 | C3441 | C3442 | C3443 | C3444 | C3445 | C3446 | C3447 | C3448 | C3449 | C3450 | C3451 | C3452 | C3453 | C3454 | C3455 | C3456 | C3457 | C3458 | C3459 | C3460 | C3461 | C3462 | C3463 | C3464 | C3465 | C3466 | C3467 | C3468 | C3469 | C3470 | C3471 | C3472 | C3473 | C3474 | C3475 | C3476 | C3477 | C3478 | C3479 | C3480 | C3481 | C3482 | C3483 | C3484 | C3485 | C3486 | C3487 | C3488 | C3489 | C3490 | C3491 | C3492 | C3493 | C3494 | C3495 | C3496 | C3497 | C3498 | C3499 | C3500 | C3501 | C3502 | C3503 | C3504 | C3505 | C3506 | C3507 | C3508 | C3509 | C3510 | C3511 | C3512 | C3513 | C3514 | C3515 | C3516 | C3517 | C3518 | C3519 | C3520 | C3521 | C3522 | C3523 | C3524 | C3525 | C3526 | C3527 | C3528 | C3529 | C3530 | C3531 | C3532 | C3533 | C3534 | C3535 | C3536 | C3537 | C3538 | C3539 | C3540 | C3541 | C3542 | C3543 | C3544 | C3545 | C3546 | C3547 | C3548 | C3549 | C3550 | C3551 | C3552 | C3553 | C3554 | C3555 | C3556 | C3557 | C3558 | C3559 | C3560 | C3561 | C3562 | C3563 | C3564 | C3565 | C3566 | C3567 | C3568 | C3569 | C3570 | C3571 | C3572 | C3573 | C3574 | C3575 | C3576 | C3577 | C3578 | C3579 | C3580 | C3581 | C3582 | C3583 | C3584 | C3585 | C3586 | C3587 | C3588 | C3589 | C3590 | C3591 | C3592 | C3593 | C3594 | C3595 | C3596 | C3597 | C3598 | C3599 | C3600 | C3601 | C3602 | C3603 | C3604 | C3605 | C3606 | C3607 | C3608 | C3609 | C3610 | C3611 | C3612 | C3613 | C3614 | C3615 | C3616 | C3617 | C3618 | C3619 | C3620 | C3621 | C3622 | C3623 | C3624 | C3625 | C3626 | C3627 | C3628 | C3629 | C3630 | C3631 | C3632 | C3633 | C3634 | C3635 | C3636 | C3637 | C3638 | C3639 | C3640 | C3641 | C3642 | C3643 | C3644 | C3645 | C3646 | C3647 | C3648 | C3649 | C3650 | C3651 | C3652 | C3653 | C3654 | C3655 | C3656 | C3657 | C3658 | C3659 | C3660 | C3661 | C3662 | C3663 | C3664 | C3665 | C3666 | C3667 | C3668 | C3669 | C3670 | C3671 | C3672 | C3673 | C3674 | C3675 | C3676 | C3677 | C3678 | C3679 | C3680 | C3681 | C3682 | C3683 | C3684 | C3685 | C3686 | C3687 | C3688 | C3689 | C3690 | C3691 | C3692 | C3693 | C3694 | C3695 | C3696 | C3697 | C3698 | C3699 | C3700 | C3701 | C3702 | C3703 | C3704 | C3705 | C3706 | C3707 | C3708 | C3709 | C3710 | C3711 | C3712 | C3713 | C3714 | C3715 | C3716 | C3717 | C3718 | C3719 | C3720 | C3721 | C3722 | C3723 | C3724 | C3725 | C3726 | C3727 | C3728 | C3729 | C3730 | C3731 | C3732 | C3733 | C3734 | C3735 | C3736 | C3737 | C3738 | C3739 | C3740 | C3741 | C3742 | C3743 | C3744 | C3745 | C3746 | C3747 | C3748 | C3749 | C3750 | C3751 | C3752 | C3753 | C3754 | C3755 | C3756 | C3757 | C3758 | C3759 | C3760 | C3761 | C3762 | C3763 | C3764 | C3765 | C3766 | C3767 | C3768 | C3769 | C3770 | C3771 | C3772 | C3773 | C3774 | C3775 | C3776 | C3777 | C3778 | C3779 | C3780 | C3781 | C3782 | C3783 | C3784 | C3785 | C3786 | C3787 | C3788 | C3789 | C3790 | C3791 | C3792 | C3793 | C3794 | C3795 | C3796 | C3797 | C3798 | C3799 | C3800 | C3801 | C3802 | C3803 | C3804 | C3805 | C3806 | C3807 | C3808 | C3809 | C3810 | C3811 | C3812 | C3813 | C3814 | C3815 | C3816 | C3817 | C3818 | C3819 | C3820 | C3821 | C3822 | C3823 | C3824 | C3825 | C3826 | C3827 | C3828 | C3829 | C3830 | C3831 | C3832 | C3833 | C3834 | C3835 | C3836 | C3837 | C3838 | C3839 | C3840 | C3841 | C3842 | C3843 | C3844 | C3845 | C3846 | C3847 | C3848 | C3849 | C3850 | C3851 | C3852 | C3853 | C3854 | C3855 | C3856 | C3857 | C3858 | C3859 | C3860 | C3861 | C3862 | C3863 | C3864 | C3865 | C3866 | C3867 | C3868 | C3869 | C3870 | C3871 | C3872 | C3873 | C3874 | C3875 | C3876 | C3877 | C3878 | C3879 | C3880 | C3881 | C3882 | C3883 | C3884 | C3885 | C3886 | C3887 | C3888 | C3889 | C3890 | C3891 | C3892 | C3893 | C3894 | C3895 | C3896 | C3897 | C3898 | C3899 | C3900 | C3901 | C3902 | C3903 | C3904 | C3905 | C3906 | C3907 | C3908 | C3909 | C3910 | C3911 | C3912 | C3913 | C3914 | C3915 | C3916 | C3917 | C3918 | C3919 | C3920 | C3921 | C3922 | C3923 | C3924 | C3925 | C3926 | C3927 | C3928 | C3929 | C3930 | C3931 | C3932 | C3933 | C3934 | C3935 | C3936 | C3937 | C3938 | C3939 | C3940 | C3941 | C3942 | C3943 | C3944 | C3945 | C3946 | C3947 | C3948 | C3949 | C3950 | C3951 | C3952 | C3953 | C3954 | C3955 | C3956 | C3957 | C3958 | C3959 | C3960 | C3961 | C3962 | C3963 | C3964 | C3965 | C3966 | C3967 | C396 |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|



• Molecule 31: 5S RIBOSOMAL RNA

4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | C 2 2 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 212.33Å 299.62Å 575.24Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 30.00 – 2.90 85.65 – 2.41 | Depositor EDS |
| % Data completeness (in resolution range) | 98.1 (30.00-2.90) 98.2 (85.65-2.41) | Depositor EDS |
| R_{merge} | 0.17 | 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} | 0.186 , 0.233 0.182 , 0.225 | Depositor DCC |
| R_{free} test set | 3920 reflections (1.01%) | DCC |
| Wilson B-factor (Å ²) | 61.2 | Xtriage |
| Anisotropy | 0.153 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.32 , 82.8 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$ | Xtriage |
| Outliers | 1 of 667142 reflections (0.000%) | Xtriage |
| F_o, F_c correlation | 0.94 | EDS |
| Total number of atoms | 99120 | wwPDB-VP |
| Average B, all atoms (Å ²) | 60.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, SR, NA, K, 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 | 0/1786 | 0.64 | 0/2408 |
| 2 | B | 0.34 | 0/2690 | 0.65 | 0/3652 |
| 3 | C | 0.36 | 0/1885 | 0.62 | 0/2552 |
| 4 | D | 0.32 | 0/1111 | 0.56 | 1/1498 (0.1%) |
| 5 | E | 0.33 | 0/1382 | 0.57 | 0/1880 |
| 6 | F | 0.35 | 0/901 | 0.57 | 0/1224 |
| 7 | G | 0.33 | 0/241 | 0.51 | 0/324 |
| 8 | H | 0.33 | 0/1302 | 0.63 | 0/1743 |
| 9 | I | 0.30 | 0/526 | 0.50 | 0/716 |
| 10 | J | 0.36 | 0/1136 | 0.61 | 0/1530 |
| 11 | K | 0.34 | 0/1004 | 0.66 | 0/1351 |
| 12 | L | 0.35 | 0/1130 | 0.64 | 0/1509 |
| 13 | M | 0.36 | 0/1582 | 0.61 | 0/2116 |
| 14 | N | 0.30 | 0/1474 | 0.61 | 0/1999 |
| 15 | O | 0.35 | 0/874 | 0.59 | 0/1181 |
| 16 | P | 0.33 | 0/1147 | 0.53 | 0/1528 |
| 17 | Q | 0.34 | 0/749 | 0.65 | 0/1005 |
| 18 | R | 1.26 | 7/1172 (0.6%) | 1.09 | 6/1578 (0.4%) |
| 19 | S | 0.33 | 0/648 | 0.54 | 0/875 |
| 20 | T | 0.32 | 0/958 | 0.64 | 0/1289 |
| 21 | U | 0.32 | 0/417 | 0.57 | 0/562 |
| 22 | V | 0.32 | 0/502 | 0.54 | 0/675 |
| 23 | W | 0.36 | 0/1219 | 0.63 | 0/1655 |
| 24 | X | 0.35 | 0/664 | 0.60 | 0/895 |
| 25 | Y | 0.37 | 0/1146 | 0.62 | 0/1536 |
| 26 | Z | 0.36 | 0/584 | 0.63 | 0/781 |
| 27 | 1 | 0.39 | 0/438 | 0.62 | 0/578 |
| 28 | 2 | 0.34 | 0/401 | 0.58 | 0/529 |
| 29 | 3 | 0.37 | 0/771 | 0.57 | 0/1024 |
| 30 | 0 | 0.39 | 0/65954 | 0.68 | 9/102862 (0.0%) |
| 31 | 9 | 0.33 | 0/2904 | 0.68 | 1/4526 (0.0%) |
| All | All | 0.40 | 7/98698 (0.0%) | 0.67 | 17/147581 (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 |
|-----|-------|---------------------|---------------------|
| 18 | R | 1 | 0 |
| 23 | W | 0 | 1 |
| 30 | 0 | 0 | 32 |
| 31 | 9 | 0 | 3 |
| All | All | 1 | 36 |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 18 | R | 150 | PRO | CB-CG | 27.45 | 2.87 | 1.50 |
| 18 | R | 150 | PRO | CA-C | -18.11 | 1.16 | 1.52 |
| 18 | R | 150 | PRO | CG-CD | 13.90 | 1.96 | 1.50 |
| 18 | R | 150 | PRO | C-O | 11.92 | 1.47 | 1.23 |
| 18 | R | 150 | PRO | N-CA | 11.35 | 1.66 | 1.47 |
| 18 | R | 150 | PRO | N-CD | 10.74 | 1.62 | 1.47 |
| 18 | R | 150 | PRO | CA-CB | 7.56 | 1.68 | 1.53 |

All (17) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 18 | R | 150 | PRO | CB-CA-C | -22.47 | 55.81 | 112.00 |
| 18 | R | 150 | PRO | N-CA-C | -19.38 | 61.71 | 112.10 |
| 18 | R | 150 | PRO | CA-N-CD | 12.28 | 128.89 | 111.70 |
| 18 | R | 150 | PRO | N-CA-CB | 10.98 | 116.47 | 103.30 |
| 18 | R | 150 | PRO | CA-C-O | -8.52 | 99.75 | 120.20 |
| 31 | 9 | 39 | U | N1-C1'-C2' | 6.32 | 122.22 | 114.00 |
| 18 | R | 150 | PRO | CA-CB-CG | -6.13 | 92.34 | 104.00 |
| 30 | 0 | 1592 | G | N9-C1'-C2' | 6.12 | 121.95 | 114.00 |
| 30 | 0 | 1504 | A | C1'-O4'-C4' | -5.86 | 105.21 | 109.90 |
| 30 | 0 | 1504 | A | N9-C1'-C2' | 5.70 | 121.41 | 114.00 |
| 30 | 0 | 871 | G | C5'-C4'-O4' | -5.36 | 102.67 | 109.10 |
| 30 | 0 | 1120 | U | C5'-C4'-C3' | -5.35 | 107.45 | 116.00 |
| 30 | 0 | 841 | A | C1'-O4'-C4' | -5.30 | 105.66 | 109.90 |
| 30 | 0 | 2726 | U | N1-C1'-C2' | 5.24 | 120.81 | 114.00 |
| 30 | 0 | 1819 | G | C5'-C4'-C3' | 5.05 | 124.07 | 116.00 |
| 30 | 0 | 2301 | A | N9-C1'-C2' | 5.01 | 120.52 | 114.00 |
| 4 | D | 170 | TYR | N-CA-C | 5.01 | 124.53 | 111.00 |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 18 | R | 150 | PRO | CA |

All (36) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 30 | 0 | 1078 | A | Sidechain |
| 30 | 0 | 1080 | C | Sidechain |
| 30 | 0 | 1309 | U | Sidechain |
| 30 | 0 | 1327 | G | Sidechain |
| 30 | 0 | 1417 | G | Sidechain |
| 30 | 0 | 1592 | G | Sidechain |
| 30 | 0 | 1684 | A | Sidechain |
| 30 | 0 | 1829 | A | Sidechain |
| 30 | 0 | 1863 | G | Sidechain |
| 30 | 0 | 1877 | G | Sidechain |
| 30 | 0 | 1878 | G | Sidechain |
| 30 | 0 | 1979 | G | Sidechain |
| 30 | 0 | 202 | U | Sidechain |
| 30 | 0 | 205 | U | Sidechain |
| 30 | 0 | 221 | G | Sidechain |
| 30 | 0 | 2492 | U | Sidechain |
| 30 | 0 | 2493 | C | Sidechain |
| 30 | 0 | 2503 | A | Sidechain |
| 30 | 0 | 2506 | A | Sidechain |
| 30 | 0 | 2543 | G | Sidechain |
| 30 | 0 | 2607 | U | Sidechain |
| 30 | 0 | 2632 | G | Sidechain |
| 30 | 0 | 2673 | U | Sidechain |
| 30 | 0 | 2842 | G | Sidechain |
| 30 | 0 | 396 | U | Sidechain |
| 30 | 0 | 470 | U | Sidechain |
| 30 | 0 | 48 | A | Sidechain |
| 30 | 0 | 482 | G | Sidechain |
| 30 | 0 | 518 | G | Sidechain |
| 30 | 0 | 619 | U | Sidechain |
| 30 | 0 | 817 | G | Sidechain |
| 30 | 0 | 818 | A | Sidechain |
| 31 | 9 | 39 | U | Sidechain |
| 31 | 9 | 65 | A | Sidechain |
| 31 | 9 | 87 | U | Sidechain |
| 23 | W | 90 | TYR | Sidechain |

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 1753 | 0 | 1766 | 66 | 0 |
| 2 | B | 2625 | 0 | 2533 | 94 | 0 |
| 3 | C | 1860 | 0 | 1813 | 53 | 0 |
| 4 | D | 1094 | 0 | 1085 | 52 | 0 |
| 5 | E | 1357 | 0 | 1266 | 36 | 0 |
| 6 | F | 890 | 0 | 843 | 30 | 0 |
| 7 | G | 240 | 0 | 231 | 11 | 0 |
| 8 | H | 1282 | 0 | 1292 | 41 | 0 |
| 9 | I | 519 | 0 | 500 | 21 | 0 |
| 10 | J | 1120 | 0 | 1098 | 38 | 0 |
| 11 | K | 994 | 0 | 1027 | 39 | 0 |
| 12 | L | 1118 | 0 | 1076 | 33 | 0 |
| 13 | M | 1558 | 0 | 1573 | 59 | 0 |
| 14 | N | 1445 | 0 | 1401 | 54 | 0 |
| 15 | O | 865 | 0 | 873 | 18 | 0 |
| 16 | P | 1136 | 0 | 1123 | 30 | 0 |
| 17 | Q | 735 | 0 | 729 | 26 | 0 |
| 18 | R | 1149 | 0 | 1122 | 32 | 0 |
| 19 | S | 641 | 0 | 605 | 10 | 0 |
| 20 | T | 950 | 0 | 924 | 22 | 0 |
| 21 | U | 410 | 0 | 364 | 17 | 0 |
| 22 | V | 499 | 0 | 511 | 17 | 0 |
| 23 | W | 1196 | 0 | 1137 | 66 | 0 |
| 24 | X | 654 | 0 | 653 | 22 | 0 |
| 25 | Y | 1130 | 0 | 1133 | 33 | 0 |
| 26 | Z | 573 | 0 | 531 | 21 | 0 |
| 27 | 1 | 431 | 0 | 426 | 21 | 0 |
| 28 | 2 | 396 | 0 | 413 | 21 | 0 |
| 29 | 3 | 755 | 0 | 728 | 17 | 0 |
| 30 | 0 | 59018 | 0 | 29809 | 1329 | 0 |
| 31 | 9 | 2599 | 0 | 1325 | 97 | 0 |
| 32 | 0 | 87 | 0 | 0 | 0 | 0 |
| 32 | 9 | 1 | 0 | 0 | 0 | 0 |
| 32 | A | 1 | 0 | 0 | 0 | 0 |
| 32 | B | 1 | 0 | 0 | 0 | 0 |
| 32 | K | 1 | 0 | 0 | 0 | 0 |
| 32 | T | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 32 | Y | 1 | 0 | 0 | 0 | 0 |
| 33 | 0 | 2 | 0 | 0 | 0 | 0 |
| 34 | 0 | 65 | 0 | 0 | 0 | 0 |
| 34 | 9 | 2 | 0 | 0 | 0 | 0 |
| 34 | B | 1 | 0 | 0 | 0 | 0 |
| 34 | C | 1 | 0 | 0 | 0 | 0 |
| 34 | J | 1 | 0 | 0 | 0 | 0 |
| 34 | M | 1 | 0 | 0 | 0 | 0 |
| 34 | Q | 1 | 0 | 0 | 0 | 0 |
| 34 | R | 2 | 0 | 0 | 0 | 0 |
| 34 | S | 1 | 0 | 0 | 0 | 0 |
| 35 | 0 | 9 | 0 | 0 | 3 | 0 |
| 35 | 3 | 1 | 0 | 0 | 0 | 0 |
| 35 | A | 1 | 0 | 0 | 0 | 0 |
| 35 | B | 1 | 0 | 0 | 0 | 0 |
| 35 | J | 3 | 0 | 0 | 2 | 0 |
| 35 | L | 1 | 0 | 0 | 0 | 0 |
| 35 | M | 1 | 0 | 0 | 1 | 0 |
| 35 | N | 1 | 0 | 0 | 1 | 0 |
| 35 | O | 1 | 0 | 0 | 0 | 0 |
| 35 | Q | 1 | 0 | 0 | 0 | 0 |
| 35 | R | 1 | 0 | 0 | 0 | 0 |
| 35 | Y | 1 | 0 | 0 | 0 | 0 |
| 36 | 0 | 93 | 0 | 0 | 0 | 0 |
| 36 | 1 | 2 | 0 | 0 | 0 | 0 |
| 36 | 3 | 2 | 0 | 0 | 0 | 0 |
| 36 | 9 | 3 | 0 | 0 | 0 | 0 |
| 36 | A | 3 | 0 | 0 | 0 | 0 |
| 36 | B | 2 | 0 | 0 | 0 | 0 |
| 36 | F | 1 | 0 | 0 | 0 | 0 |
| 36 | R | 1 | 0 | 0 | 0 | 0 |
| 36 | S | 1 | 0 | 0 | 0 | 0 |
| 37 | 1 | 1 | 0 | 0 | 0 | 0 |
| 37 | 3 | 1 | 0 | 0 | 0 | 0 |
| 37 | O | 1 | 0 | 0 | 0 | 0 |
| 37 | U | 1 | 0 | 0 | 0 | 0 |
| 37 | Z | 1 | 0 | 0 | 0 | 0 |
| 38 | 0 | 5950 | 0 | 0 | 203 | 0 |
| 38 | 1 | 54 | 0 | 0 | 3 | 0 |
| 38 | 2 | 43 | 0 | 0 | 1 | 0 |
| 38 | 3 | 68 | 0 | 0 | 6 | 0 |
| 38 | 9 | 148 | 0 | 0 | 9 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 38 | A | 112 | 0 | 0 | 5 | 0 |
| 38 | B | 142 | 0 | 0 | 14 | 0 |
| 38 | C | 168 | 0 | 0 | 13 | 0 |
| 38 | D | 45 | 0 | 0 | 4 | 0 |
| 38 | E | 42 | 0 | 0 | 4 | 0 |
| 38 | F | 26 | 0 | 0 | 1 | 0 |
| 38 | G | 17 | 0 | 0 | 1 | 0 |
| 38 | H | 65 | 0 | 0 | 5 | 0 |
| 38 | I | 5 | 0 | 0 | 0 | 0 |
| 38 | J | 56 | 0 | 0 | 2 | 0 |
| 38 | K | 60 | 0 | 0 | 5 | 0 |
| 38 | L | 82 | 0 | 0 | 8 | 0 |
| 38 | M | 123 | 0 | 0 | 2 | 0 |
| 38 | N | 59 | 0 | 0 | 3 | 0 |
| 38 | O | 47 | 0 | 0 | 4 | 0 |
| 38 | P | 59 | 0 | 0 | 2 | 0 |
| 38 | Q | 47 | 0 | 0 | 2 | 0 |
| 38 | R | 76 | 0 | 0 | 1 | 0 |
| 38 | S | 33 | 0 | 0 | 0 | 0 |
| 38 | T | 36 | 0 | 0 | 4 | 0 |
| 38 | U | 26 | 0 | 0 | 2 | 0 |
| 38 | V | 12 | 0 | 0 | 1 | 0 |
| 38 | W | 66 | 0 | 0 | 6 | 0 |
| 38 | X | 28 | 0 | 0 | 3 | 0 |
| 38 | Y | 97 | 0 | 0 | 7 | 0 |
| 38 | Z | 31 | 0 | 0 | 4 | 0 |
| All | All | 99120 | 0 | 59910 | 2191 | 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 15.

All (2191) 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) |
|-----------------|-----------------|--------------------------|-------------------|
| 18:R:150:PRO:CG | 18:R:150:PRO:CD | 1.96 | 1.44 |
| 30:0:871:G:C8 | 30:0:871:G:H5' | 1.75 | 1.21 |
| 14:N:37:ARG:NH1 | 31:9:6:C:H5'' | 1.62 | 1.12 |
| 31:9:56:A:H2' | 31:9:57:A:H5'' | 1.21 | 1.11 |
| 30:0:1160:G:C5' | 30:0:1161:A:H5' | 1.79 | 1.11 |
| 30:0:1160:G:H5' | 30:0:1161:A:C5' | 1.83 | 1.09 |
| 30:0:871:G:H8 | 30:0:871:G:H5' | 1.00 | 1.08 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 30:0:545:G:H8 | 30:0:545:G:H5' | 1.12 | 1.08 |
| 18:R:150:PRO:CG | 18:R:150:PRO:C | 2.22 | 1.07 |
| 30:0:1474:C:H6 | 30:0:1474:C:H5' | 1.19 | 1.07 |
| 30:0:1559:A:H1' | 38:0:5888:HOH:O | 1.54 | 1.07 |
| 13:M:171:ARG:HD3 | 30:0:156:C:H5'' | 1.38 | 1.04 |
| 30:0:69:A:H5' | 30:0:69:A:C8 | 1.93 | 1.03 |
| 10:J:82:THR:HG23 | 30:0:1242:A:H5' | 1.38 | 1.02 |
| 30:0:1474:C:C6 | 30:0:1474:C:H5' | 1.96 | 1.01 |
| 4:D:154:LYS:HD2 | 4:D:154:LYS:H | 1.26 | 1.01 |
| 30:0:1666:C:O2' | 30:0:1667:A:H5'' | 1.62 | 0.99 |
| 30:0:2717:C:C2' | 30:0:2718:C:H5'' | 1.93 | 0.99 |
| 31:9:76:G:H3' | 31:9:77:A:H5'' | 1.41 | 0.98 |
| 30:0:69:A:H5' | 30:0:69:A:H8 | 1.28 | 0.97 |
| 30:0:871:G:H8 | 30:0:871:G:C5' | 1.78 | 0.96 |
| 30:0:1205:U:H2' | 30:0:1206:U:C5' | 1.96 | 0.96 |
| 30:0:1116:U:O2' | 30:0:1118:A:H2 | 1.47 | 0.96 |
| 30:0:2717:C:H2' | 30:0:2718:C:H5'' | 1.45 | 0.96 |
| 30:0:2812:A:H2 | 30:0:2814:A:H62 | 1.02 | 0.95 |
| 30:0:1603:A:H5' | 30:0:1605:G:O4' | 1.66 | 0.95 |
| 30:0:545:G:C8 | 30:0:545:G:H5' | 2.00 | 0.95 |
| 30:0:870:G:H2' | 30:0:871:G:H5'' | 1.47 | 0.95 |
| 30:0:1165:G:H21 | 30:0:1173:A:H5'' | 1.30 | 0.95 |
| 15:O:3:THR:HG22 | 30:0:656:G:H5' | 1.45 | 0.95 |
| 30:0:877:G:H5' | 30:0:878:G:OP1 | 1.67 | 0.94 |
| 30:0:2291:A:C8 | 30:0:2309:C:H5' | 2.03 | 0.94 |
| 30:0:2316:G:H5'' | 38:0:6122:HOH:O | 1.66 | 0.94 |
| 30:0:1666:C:C2' | 30:0:1667:A:H5'' | 1.97 | 0.93 |
| 30:0:542:A:H5' | 30:0:542:A:H8 | 1.30 | 0.93 |
| 3:C:236:THR:HG22 | 3:C:239:ALA:H | 1.31 | 0.92 |
| 30:0:1206:U:H5' | 30:0:1206:U:H6 | 1.34 | 0.92 |
| 30:0:2506:A:HO2' | 30:0:2507:G:H8 | 1.10 | 0.92 |
| 30:0:381:G:H5'' | 38:0:4327:HOH:O | 1.68 | 0.92 |
| 30:0:2502:C:C2' | 30:0:2503:A:H5' | 2.00 | 0.92 |
| 11:K:10:GLN:H | 11:K:10:GLN:HE21 | 0.97 | 0.92 |
| 30:0:182:G:H5' | 38:0:5177:HOH:O | 1.68 | 0.92 |
| 16:P:115:SER:H | 16:P:118:GLN:HE21 | 0.99 | 0.92 |
| 30:0:2502:C:H2' | 30:0:2503:A:H5' | 1.50 | 0.91 |
| 31:9:56:A:C2' | 31:9:57:A:H5'' | 2.00 | 0.91 |
| 30:0:1160:G:H5' | 30:0:1161:A:H5' | 0.94 | 0.91 |
| 13:M:99:ARG:HD2 | 13:M:167:GLY:HA2 | 1.51 | 0.91 |
| 30:0:2908:A:H2' | 30:0:2909:G:O4' | 1.69 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 30:0:1187:U:HO2' | 30:0:1189:A:H2 | 1.11 | 0.90 |
| 30:0:2526:C:H5' | 30:0:2526:C:H6 | 1.36 | 0.90 |
| 10:J:52:GLN:NE2 | 30:0:1119:G:H2' | 1.85 | 0.90 |
| 30:0:1835:U:H5 | 30:0:1840:A:N7 | 1.70 | 0.90 |
| 2:B:221:GLN:HE22 | 11:K:42:ASN:HD22 | 1.17 | 0.90 |
| 30:0:2004:U:H4' | 38:0:5326:HOH:O | 1.70 | 0.90 |
| 30:0:1701:A:H4' | 30:0:1702:U:H5'' | 1.51 | 0.89 |
| 30:0:1184:C:H1' | 38:0:7505:HOH:O | 1.70 | 0.89 |
| 6:F:91:VAL:HG12 | 6:F:92:GLY:H | 1.34 | 0.89 |
| 30:0:2526:C:H5' | 30:0:2526:C:C6 | 2.07 | 0.89 |
| 31:9:29:C:H2' | 31:9:30:C:H5' | 1.55 | 0.89 |
| 30:0:506:G:H22 | 30:0:509:A:C5' | 1.86 | 0.89 |
| 30:0:282:C:H1' | 30:0:368:C:N4 | 1.86 | 0.89 |
| 26:Z:70:ARG:HD2 | 26:Z:83:TYR:HB2 | 1.55 | 0.88 |
| 30:0:1189:A:H1' | 30:0:1209:C:O4' | 1.74 | 0.88 |
| 38:B:9099:HOH:O | 30:0:2672:C:H1' | 1.72 | 0.88 |
| 30:0:541:C:H2' | 30:0:542:A:H5'' | 1.56 | 0.88 |
| 30:0:541:C:C2' | 30:0:542:A:H5'' | 2.05 | 0.87 |
| 2:B:238:ASN:HD22 | 2:B:240:GLY:H | 1.20 | 0.87 |
| 30:0:31:C:H2' | 38:0:7724:HOH:O | 1.73 | 0.87 |
| 30:0:1372:A:H3' | 38:0:7228:HOH:O | 1.74 | 0.87 |
| 30:0:2769:C:C2' | 30:0:2770:G:H5' | 2.05 | 0.87 |
| 30:0:2111:G:H1' | 38:0:9054:HOH:O | 1.75 | 0.87 |
| 30:0:214:U:H5' | 38:0:6171:HOH:O | 1.74 | 0.86 |
| 30:0:1205:U:H2' | 30:0:1206:U:H5'' | 1.57 | 0.86 |
| 30:0:1183:C:H2' | 38:0:6275:HOH:O | 1.76 | 0.86 |
| 30:0:1165:G:N2 | 30:0:1173:A:H5'' | 1.89 | 0.86 |
| 31:9:14:G:H5' | 31:9:14:G:H8 | 1.41 | 0.86 |
| 2:B:162:MET:HE3 | 2:B:308:LEU:HD21 | 1.56 | 0.86 |
| 30:0:2586:U:H3 | 30:0:2592:G:H22 | 1.16 | 0.85 |
| 2:B:36:PRO:HA | 2:B:168:GLY:HA3 | 1.59 | 0.85 |
| 24:X:37:LEU:HD13 | 24:X:85:VAL:HG21 | 1.57 | 0.85 |
| 30:0:1165:G:H1' | 30:0:1174:A:H1' | 1.58 | 0.84 |
| 30:0:506:G:H22 | 30:0:509:A:H5' | 1.42 | 0.84 |
| 15:O:3:THR:CG2 | 30:0:656:G:H5' | 2.07 | 0.84 |
| 30:0:2010:A:H2' | 38:0:5984:HOH:O | 1.77 | 0.84 |
| 14:N:83:LEU:HD13 | 14:N:175:LEU:HD23 | 1.58 | 0.83 |
| 13:M:95:LYS:HE2 | 30:0:157:G:H4' | 1.59 | 0.83 |
| 3:C:127:ARG:NH2 | 3:C:225:PRO:HG2 | 1.94 | 0.83 |
| 11:K:39:GLY:HA2 | 38:0:5241:HOH:O | 1.79 | 0.83 |
| 30:0:1667:A:H8 | 30:0:1667:A:H5' | 1.44 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 30:0:1118:A:H3' | 30:0:1118:A:C8 | 2.13 | 0.82 |
| 23:W:137:GLN:HE21 | 23:W:141:HIS:HE1 | 1.24 | 0.82 |
| 30:0:2073:G:H5'' | 38:0:3833:HOH:O | 1.80 | 0.81 |
| 9:I:111:LEU:HD23 | 30:0:1163:G:H4' | 1.60 | 0.81 |
| 30:0:1205:U:H2' | 30:0:1206:U:H5' | 1.62 | 0.81 |
| 8:H:59:GLN:NE2 | 8:H:129:ARG:HE | 1.78 | 0.81 |
| 30:0:1118:A:H3' | 30:0:1118:A:H8 | 1.46 | 0.80 |
| 10:J:52:GLN:HE22 | 30:0:1119:G:H2' | 1.46 | 0.80 |
| 30:0:559:U:H5' | 30:0:559:U:H6 | 1.46 | 0.80 |
| 30:0:1666:C:H2' | 30:0:1667:A:C5' | 2.12 | 0.80 |
| 30:0:871:G:C8 | 30:0:871:G:C5' | 2.57 | 0.79 |
| 30:0:1201:C:H2' | 30:0:1202:A:H5' | 1.65 | 0.79 |
| 30:0:282:C:O2' | 30:0:283:U:H5' | 1.81 | 0.79 |
| 30:0:2769:C:H2' | 30:0:2770:G:H5' | 1.62 | 0.79 |
| 30:0:2766:A:H5' | 38:0:9567:HOH:O | 1.81 | 0.79 |
| 2:B:212:GLN:HB2 | 2:B:257:THR:HG21 | 1.63 | 0.79 |
| 30:0:1377:C:H6 | 30:0:1377:C:H5' | 1.48 | 0.79 |
| 30:0:1300:G:H1' | 38:0:4692:HOH:O | 1.81 | 0.78 |
| 30:0:1119:G:N2 | 30:0:1246:A:C2 | 2.51 | 0.78 |
| 3:C:139:VAL:HG13 | 38:C:8646:HOH:O | 1.83 | 0.78 |
| 2:B:74:ILE:HD13 | 2:B:309:VAL:HG21 | 1.64 | 0.78 |
| 30:0:2748:G:H5' | 38:0:7581:HOH:O | 1.83 | 0.78 |
| 30:0:10:U:H6 | 30:0:10:U:H3' | 1.49 | 0.78 |
| 30:0:1942:A:H5' | 38:0:7387:HOH:O | 1.82 | 0.78 |
| 11:K:10:GLN:H | 11:K:10:GLN:NE2 | 1.79 | 0.78 |
| 23:W:4:LEU:HD23 | 23:W:54:PHE:HB3 | 1.65 | 0.78 |
| 20:T:9:LYS:HE3 | 20:T:13:ARG:NH1 | 1.99 | 0.78 |
| 30:0:308:U:H5' | 30:0:309:C:OP1 | 1.84 | 0.77 |
| 30:0:2103:A:H62 | 30:0:2538:A:H8 | 1.32 | 0.77 |
| 30:0:541:C:H2' | 30:0:542:A:C5' | 2.14 | 0.77 |
| 30:0:396:U:H1' | 38:0:7666:HOH:O | 1.83 | 0.77 |
| 23:W:88:THR:HB | 38:W:6679:HOH:O | 1.84 | 0.77 |
| 16:P:115:SER:H | 16:P:118:GLN:NE2 | 1.81 | 0.77 |
| 30:0:2491:G:H1' | 38:0:6907:HOH:O | 1.86 | 0.76 |
| 26:Z:60:ASP:HB3 | 26:Z:69:ASP:HB3 | 1.68 | 0.76 |
| 30:0:1474:C:C5' | 30:0:1474:C:H6 | 1.98 | 0.76 |
| 30:0:2533:C:H5' | 30:0:2533:C:H6 | 1.50 | 0.76 |
| 30:0:870:G:C2' | 30:0:871:G:H5'' | 2.13 | 0.76 |
| 30:0:2420:G:O2' | 30:0:2421:G:H5' | 1.86 | 0.76 |
| 28:2:43:ARG:HH22 | 30:0:1684:A:H1' | 1.48 | 0.76 |
| 30:0:1205:U:C2' | 30:0:1206:U:H5'' | 2.15 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 31:9:2:U:OP2 | 31:9:3:A:H5' | 1.85 | 0.76 |
| 31:9:92:G:H2' | 31:9:93:A:C8 | 2.21 | 0.76 |
| 30:0:558:C:C2' | 30:0:559:U:H5'' | 2.16 | 0.75 |
| 26:Z:61:HIS:HB2 | 26:Z:71:VAL:HB | 1.66 | 0.75 |
| 22:V:1:THR:HG23 | 22:V:2:VAL:H | 1.51 | 0.75 |
| 30:0:2256:G:O2' | 30:0:2257:G:H5' | 1.85 | 0.75 |
| 30:0:2256:G:C2' | 30:0:2257:G:H5' | 2.16 | 0.75 |
| 30:0:1451:C:H5' | 30:0:1505:U:C5 | 2.21 | 0.75 |
| 30:0:1632:A:H2' | 30:0:1633:C:H5' | 1.69 | 0.75 |
| 30:0:2717:C:O2' | 30:0:2718:C:H5'' | 1.86 | 0.75 |
| 1:A:199:HIS:HD2 | 1:A:201:PHE:H | 1.33 | 0.75 |
| 30:0:558:C:O2' | 30:0:559:U:H5'' | 1.87 | 0.75 |
| 30:0:2787:C:H5 | 38:0:4643:HOH:O | 1.69 | 0.75 |
| 5:E:116:THR:HG22 | 5:E:151:LEU:HD22 | 1.69 | 0.75 |
| 30:0:681:G:N3 | 30:0:681:G:H5' | 2.02 | 0.75 |
| 30:0:1603:A:H5'' | 30:0:1605:G:H5' | 1.68 | 0.74 |
| 5:E:143:GLN:HE21 | 30:0:2780:C:H1' | 1.52 | 0.74 |
| 14:N:113:SER:HB2 | 38:N:8852:HOH:O | 1.87 | 0.74 |
| 30:0:1878:G:H1' | 38:0:6151:HOH:O | 1.87 | 0.74 |
| 14:N:144:GLY:O | 14:N:147:ILE:HG22 | 1.87 | 0.74 |
| 2:B:179:LEU:O | 2:B:183:GLU:HG2 | 1.86 | 0.74 |
| 6:F:58:GLU:HB3 | 13:M:8:ILE:HG23 | 1.69 | 0.74 |
| 30:0:821:U:H3' | 38:0:3779:HOH:O | 1.87 | 0.74 |
| 30:0:2135:A:O2' | 30:0:2136:G:H5' | 1.86 | 0.74 |
| 30:0:1187:U:O2' | 30:0:1189:A:H2 | 1.71 | 0.74 |
| 30:0:1116:U:H3 | 30:0:1246:A:H62 | 1.36 | 0.74 |
| 30:0:2103:A:HO2' | 30:0:2104:C:H6 | 1.36 | 0.74 |
| 5:E:100:ASP:HB2 | 38:E:2789:HOH:O | 1.86 | 0.74 |
| 2:B:98:THR:HG22 | 30:0:2820:A:OP1 | 1.88 | 0.74 |
| 30:0:283:U:H5 | 30:0:284:C:N3 | 1.86 | 0.73 |
| 30:0:107:U:H2' | 30:0:108:U:H5' | 1.70 | 0.73 |
| 19:S:51:GLN:HE21 | 19:S:53:ASN:HD21 | 1.33 | 0.73 |
| 38:C:8660:HOH:O | 30:0:2100:A:H5' | 1.87 | 0.73 |
| 30:0:2426:G:H1' | 38:0:6122:HOH:O | 1.88 | 0.73 |
| 30:0:2768:A:O2' | 30:0:2769:C:H5' | 1.88 | 0.73 |
| 30:0:12:U:H2' | 30:0:13:G:H5' | 1.69 | 0.73 |
| 13:M:171:ARG:CD | 30:0:156:C:H5'' | 2.16 | 0.73 |
| 30:0:1183:C:N4 | 30:0:1184:C:H41 | 1.85 | 0.73 |
| 30:0:1835:U:C5 | 30:0:1840:A:N7 | 2.55 | 0.73 |
| 2:B:336:GLN:O | 30:0:2862:G:H4' | 1.88 | 0.73 |
| 24:X:61:ARG:HH12 | 24:X:67:PRO:HD3 | 1.54 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 30:0:1666:C:C2' | 30:0:1667:A:C5' | 2.67 | 0.72 |
| 30:0:1166:A:H61 | 30:0:1180:U:H3 | 1.37 | 0.72 |
| 30:0:1182:C:H1' | 30:0:1192:A:H8 | 1.54 | 0.72 |
| 30:0:1701:A:H5' | 38:0:6316:HOH:O | 1.89 | 0.72 |
| 30:0:1741:U:H5' | 30:0:1742:A:OP1 | 1.89 | 0.72 |
| 29:3:70:ARG:HG2 | 29:3:77:ALA:HB2 | 1.70 | 0.72 |
| 30:0:2506:A:O2' | 30:0:2507:G:H8 | 1.72 | 0.72 |
| 1:A:35:GLY:O | 1:A:36:ASP:HB3 | 1.87 | 0.72 |
| 30:0:1189:A:H3' | 38:0:7717:HOH:O | 1.89 | 0.72 |
| 22:V:12:THR:HG22 | 22:V:15:GLU:HG3 | 1.72 | 0.72 |
| 30:0:2637:A:H5' | 38:0:9282:HOH:O | 1.88 | 0.72 |
| 22:V:1:THR:HB | 30:0:93:C:H5'' | 1.72 | 0.72 |
| 6:F:63:ILE:HB | 6:F:64:PRO:HD3 | 1.70 | 0.72 |
| 30:0:2896:A:H5'' | 38:0:6129:HOH:O | 1.90 | 0.72 |
| 10:J:70:PHE:CE1 | 30:0:2676:C:H4' | 2.25 | 0.72 |
| 11:K:10:GLN:N | 11:K:10:GLN:HE21 | 1.81 | 0.71 |
| 31:9:14:G:H5' | 31:9:14:G:C8 | 2.24 | 0.71 |
| 11:K:14:LYS:HB2 | 11:K:45:PRO:HG2 | 1.71 | 0.71 |
| 14:N:11:ARG:HD3 | 31:9:114:G:O6 | 1.90 | 0.71 |
| 24:X:71:ARG:HD3 | 38:X:2171:HOH:O | 1.89 | 0.71 |
| 30:0:2102:G:H5' | 30:0:2538:A:C2 | 2.24 | 0.71 |
| 30:0:1973:A:H5' | 30:0:1973:A:H8 | 1.54 | 0.71 |
| 31:9:54:A:O2' | 31:9:55:U:H5' | 1.91 | 0.71 |
| 30:0:542:A:H5' | 30:0:542:A:C8 | 2.20 | 0.71 |
| 4:D:25:MET:HE3 | 4:D:37:ALA:HB1 | 1.72 | 0.71 |
| 30:0:564:G:H1' | 38:0:6343:HOH:O | 1.91 | 0.71 |
| 1:A:211:LYS:HB2 | 38:A:9077:HOH:O | 1.90 | 0.71 |
| 30:0:10:U:C6 | 30:0:10:U:H3' | 2.26 | 0.71 |
| 20:T:61:GLU:HG2 | 38:T:3851:HOH:O | 1.90 | 0.71 |
| 30:0:1187:U:H2' | 38:0:6936:HOH:O | 1.91 | 0.70 |
| 5:E:143:GLN:NE2 | 30:0:2779:G:H21 | 1.89 | 0.70 |
| 4:D:105:SER:OG | 30:0:2338:G:H1' | 1.89 | 0.70 |
| 23:W:88:THR:HG22 | 23:W:89:ASP:H | 1.56 | 0.70 |
| 31:9:23:U:O2' | 31:9:24:U:H4' | 1.91 | 0.70 |
| 30:0:2578:G:H5' | 30:0:2578:G:H8 | 1.57 | 0.70 |
| 38:Y:8860:HOH:O | 35:0:8817:CL:CL | 2.46 | 0.70 |
| 23:W:88:THR:HG23 | 23:W:110:GLN:HB3 | 1.73 | 0.70 |
| 30:0:2256:G:H2' | 30:0:2257:G:H5' | 1.73 | 0.70 |
| 3:C:1:MET:HG2 | 3:C:2:GLN:H | 1.55 | 0.70 |
| 30:0:1205:U:C2' | 30:0:1206:U:C5' | 2.69 | 0.70 |
| 30:0:2781:U:C2' | 30:0:2782:G:H5' | 2.21 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:0:2756:U:H3 | 30:0:2896:A:H2 | 1.37 | 0.70 |
| 31:9:64:C:H2' | 31:9:65:A:H5' | 1.74 | 0.70 |
| 11:K:98:VAL:CG1 | 11:K:102:GLU:HA | 2.21 | 0.70 |
| 6:F:91:VAL:HG12 | 6:F:92:GLY:N | 2.07 | 0.70 |
| 30:0:567:U:H5'' | 38:0:6437:HOH:O | 1.90 | 0.70 |
| 4:D:103:ASN:HD22 | 4:D:134:LEU:H | 1.39 | 0.70 |
| 30:0:545:G:H8 | 30:0:545:G:C5' | 2.00 | 0.69 |
| 3:C:162:VAL:HG22 | 3:C:232:LEU:HD21 | 1.73 | 0.69 |
| 17:Q:11:ARG:HD3 | 38:0:6291:HOH:O | 1.92 | 0.69 |
| 30:0:1058:A:H2' | 30:0:1060:C:H5'' | 1.74 | 0.69 |
| 30:0:1174:A:C5 | 30:0:1201:C:H4' | 2.27 | 0.69 |
| 30:0:794:U:H3 | 30:0:819:A:H61 | 1.40 | 0.69 |
| 30:0:1666:C:H2' | 30:0:1667:A:H5' | 1.75 | 0.69 |
| 30:0:1377:C:H1' | 38:0:9044:HOH:O | 1.91 | 0.69 |
| 30:0:960:G:H3' | 30:0:960:G:N3 | 2.07 | 0.69 |
| 1:A:223:ARG:HH22 | 30:0:2271:G:P | 2.16 | 0.69 |
| 30:0:847:C:H4' | 38:0:3762:HOH:O | 1.92 | 0.69 |
| 30:0:1525:G:H5' | 30:0:1526:A:OP2 | 1.93 | 0.69 |
| 14:N:37:ARG:HH12 | 31:9:6:C:H5'' | 1.51 | 0.69 |
| 11:K:74:VAL:HG12 | 11:K:75:ARG:HG3 | 1.75 | 0.69 |
| 13:M:164:THR:HG22 | 13:M:167:GLY:H | 1.58 | 0.69 |
| 2:B:206:THR:HG21 | 30:0:2716:G:H5'' | 1.74 | 0.69 |
| 30:0:821:U:H5'' | 38:0:3057:HOH:O | 1.93 | 0.68 |
| 30:0:1118:A:H62 | 30:0:1244:U:H3 | 1.39 | 0.68 |
| 30:0:2852:A:H5'' | 38:0:5254:HOH:O | 1.93 | 0.68 |
| 13:M:102:GLU:OE1 | 13:M:164:THR:HG21 | 1.94 | 0.68 |
| 30:0:2769:C:H2' | 30:0:2770:G:C5' | 2.23 | 0.68 |
| 22:V:50:ARG:HH12 | 30:0:56:G:H5'' | 1.59 | 0.68 |
| 30:0:271:C:H41 | 30:0:378:A:H2 | 1.40 | 0.68 |
| 30:0:1701:A:H4' | 30:0:1702:U:C5' | 2.20 | 0.68 |
| 11:K:98:VAL:HG13 | 11:K:102:GLU:HA | 1.74 | 0.68 |
| 30:0:2851:G:O2' | 30:0:2852:A:H5' | 1.92 | 0.68 |
| 23:W:21:LEU:HD21 | 23:W:48:VAL:HG11 | 1.75 | 0.68 |
| 23:W:137:GLN:HE21 | 23:W:141:HIS:CE1 | 2.11 | 0.68 |
| 30:0:1595:G:O2' | 30:0:1596:U:H5' | 1.92 | 0.68 |
| 30:0:2635:A:O2' | 30:0:2636:C:H5' | 1.94 | 0.68 |
| 10:J:19:MET:HE3 | 10:J:132:LEU:HD21 | 1.75 | 0.68 |
| 25:Y:169:ARG:HD2 | 30:0:1328:A:OP1 | 1.93 | 0.68 |
| 18:R:150:PRO:O | 18:R:150:PRO:CG | 2.41 | 0.68 |
| 2:B:97:LEU:HD22 | 2:B:127:GLN:HE21 | 1.57 | 0.68 |
| 35:0:8813:CL:CL | 38:0:4692:HOH:O | 2.48 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:0:1132:A:N6 | 30:0:1229:C:H2' | 2.09 | 0.68 |
| 1:A:135:VAL:HG11 | 1:A:147:ARG:NH2 | 2.09 | 0.68 |
| 18:R:96:VAL:HG13 | 18:R:106:GLY:HA3 | 1.76 | 0.68 |
| 11:K:81:ARG:HB2 | 11:K:87:ARG:HH11 | 1.59 | 0.67 |
| 30:0:559:U:H5' | 30:0:559:U:C6 | 2.29 | 0.67 |
| 30:0:69:A:H8 | 30:0:69:A:C5' | 2.06 | 0.67 |
| 30:0:506:G:H22 | 30:0:509:A:H5'' | 1.58 | 0.67 |
| 23:W:84:VAL:HG12 | 38:W:6679:HOH:O | 1.95 | 0.67 |
| 1:A:153:ARG:HH11 | 1:A:153:ARG:HB2 | 1.58 | 0.67 |
| 25:Y:212:ARG:HD2 | 38:Y:8904:HOH:O | 1.94 | 0.67 |
| 30:0:2812:A:C2 | 30:0:2814:A:N6 | 2.58 | 0.67 |
| 8:H:155:ARG:NH1 | 30:0:2503:A:H5'' | 2.09 | 0.67 |
| 8:H:30:LYS:H | 8:H:62:HIS:HD2 | 1.39 | 0.67 |
| 31:9:22:G:H5' | 31:9:23:U:OP1 | 1.95 | 0.67 |
| 30:0:380:A:H2' | 38:0:7265:HOH:O | 1.93 | 0.67 |
| 30:0:2317:C:C6 | 38:0:6122:HOH:O | 2.46 | 0.67 |
| 14:N:80:SER:HB2 | 38:N:8833:HOH:O | 1.94 | 0.67 |
| 30:0:671:A:O2' | 30:0:672:G:H2' | 1.94 | 0.67 |
| 16:P:117:SER:HB3 | 30:0:1593:C:OP1 | 1.94 | 0.67 |
| 30:0:1279:U:O2 | 30:0:1279:U:H2' | 1.95 | 0.67 |
| 30:0:1183:C:O2 | 30:0:1183:C:H2' | 1.93 | 0.67 |
| 8:H:59:GLN:HE21 | 8:H:129:ARG:HE | 1.41 | 0.67 |
| 5:E:133:VAL:HG12 | 5:E:141:VAL:HG13 | 1.76 | 0.67 |
| 1:A:211:LYS:HB3 | 1:A:212:PRO:HD2 | 1.77 | 0.66 |
| 1:A:199:HIS:CD2 | 1:A:201:PHE:H | 2.12 | 0.66 |
| 3:C:236:THR:HG22 | 3:C:239:ALA:N | 2.08 | 0.66 |
| 23:W:4:LEU:HD22 | 23:W:52:VAL:HG21 | 1.76 | 0.66 |
| 30:0:1159:G:H21 | 30:0:1189:A:H8 | 1.43 | 0.66 |
| 23:W:137:GLN:NE2 | 23:W:141:HIS:HE1 | 1.94 | 0.66 |
| 30:0:2781:U:O2' | 30:0:2782:G:H5' | 1.96 | 0.66 |
| 2:B:5:ARG:HH11 | 2:B:8:LYS:HE2 | 1.61 | 0.66 |
| 12:L:39:GLU:HG2 | 30:0:926:A:H4' | 1.76 | 0.66 |
| 28:2:41:HIS:HD2 | 28:2:44:ARG:H | 1.42 | 0.66 |
| 30:0:2256:G:H2' | 30:0:2257:G:C5' | 2.25 | 0.66 |
| 31:9:64:C:C2' | 31:9:65:A:H5' | 2.26 | 0.66 |
| 10:J:82:THR:CG2 | 30:0:1242:A:H5' | 2.21 | 0.66 |
| 11:K:74:VAL:HG11 | 11:K:113:ILE:HG12 | 1.76 | 0.66 |
| 30:0:2781:U:H2' | 30:0:2782:G:H5' | 1.76 | 0.66 |
| 28:2:18:ASN:HD21 | 28:2:40:ARG:H | 1.41 | 0.66 |
| 31:9:7:G:H5' | 38:9:9100:HOH:O | 1.96 | 0.66 |
| 25:Y:204:ARG:HH22 | 30:0:553:G:P | 2.18 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 21:U:46:ALA:HB1 | 21:U:52:THR:HG21 | 1.78 | 0.66 |
| 30:0:1189:A:H1' | 30:0:1209:C:C1' | 2.25 | 0.66 |
| 30:0:1377:C:H5' | 30:0:1377:C:C6 | 2.31 | 0.66 |
| 4:D:103:ASN:ND2 | 4:D:134:LEU:H | 1.92 | 0.66 |
| 30:0:2001:G:O2' | 30:0:2002:C:H5' | 1.96 | 0.66 |
| 18:R:99:ALA:HB1 | 18:R:109:MET:HE1 | 1.76 | 0.66 |
| 30:0:2251:G:H2' | 30:0:2252:A:C8 | 2.30 | 0.66 |
| 30:0:2769:C:O2' | 30:0:2770:G:H5' | 1.96 | 0.65 |
| 30:0:558:C:H2' | 30:0:559:U:C5' | 2.26 | 0.65 |
| 30:0:1118:A:C8 | 30:0:1118:A:C3' | 2.77 | 0.65 |
| 8:H:72:ALA:HB2 | 8:H:156:ALA:HB2 | 1.78 | 0.65 |
| 30:0:1524:U:OP1 | 30:0:1524:U:H4' | 1.96 | 0.65 |
| 30:0:2768:A:H2' | 30:0:2769:C:O4' | 1.96 | 0.65 |
| 30:0:1634:G:H3' | 38:0:3903:HOH:O | 1.96 | 0.65 |
| 30:0:603:A:H5'' | 30:0:604:G:OP1 | 1.97 | 0.65 |
| 3:C:174:ILE:HD11 | 30:0:338:C:H4' | 1.78 | 0.65 |
| 30:0:2827:A:H2' | 30:0:2828:G:O4' | 1.97 | 0.65 |
| 30:0:1441:G:O2' | 30:0:1442:A:H5' | 1.97 | 0.65 |
| 30:0:2507:G:H2' | 30:0:2510:C:H42 | 1.62 | 0.65 |
| 30:0:1972:U:H2' | 30:0:1973:A:C5' | 2.26 | 0.65 |
| 30:0:2613:G:O2' | 30:0:2614:C:H5' | 1.97 | 0.65 |
| 6:F:21:GLU:O | 6:F:24:ARG:HG2 | 1.97 | 0.65 |
| 15:O:42:GLU:HB2 | 38:O:2176:HOH:O | 1.96 | 0.65 |
| 30:0:635:A:H2' | 30:0:636:G:H5'' | 1.78 | 0.65 |
| 16:P:55:LYS:HG2 | 16:P:56:GLY:N | 2.12 | 0.65 |
| 10:J:88:PRO:HD3 | 30:0:1104:C:H4' | 1.77 | 0.65 |
| 14:N:37:ARG:NH1 | 31:9:6:C:C5' | 2.51 | 0.65 |
| 27:I:20:ARG:HG2 | 30:0:111:C:O2' | 1.97 | 0.65 |
| 30:0:1632:A:C2' | 30:0:1633:C:H5' | 2.27 | 0.64 |
| 30:0:2005:G:OP2 | 30:0:2005:G:H3' | 1.97 | 0.64 |
| 30:0:485:A:N3 | 30:0:487:G:H5'' | 2.12 | 0.64 |
| 30:0:2281:C:H2' | 30:0:2282:U:H5' | 1.80 | 0.64 |
| 30:0:1834:C:H2' | 30:0:1840:A:N6 | 2.11 | 0.64 |
| 30:0:283:U:C5 | 30:0:284:C:N3 | 2.65 | 0.64 |
| 12:L:39:GLU:HG2 | 30:0:926:A:C4' | 2.27 | 0.64 |
| 38:T:2217:HOH:O | 30:0:317:A:H5' | 1.97 | 0.64 |
| 30:0:1667:A:C8 | 30:0:1667:A:H5' | 2.29 | 0.64 |
| 30:0:2717:C:H2' | 30:0:2718:C:C5' | 2.22 | 0.64 |
| 30:0:1185:U:H2' | 30:0:1186:C:C6 | 2.33 | 0.64 |
| 30:0:283:U:H5 | 30:0:284:C:C2 | 2.15 | 0.64 |
| 8:H:30:LYS:H | 8:H:62:HIS:CD2 | 2.14 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 30:0:363:C:O2' | 30:0:364:U:H5' | 1.97 | 0.64 |
| 30:0:613:C:H2' | 30:0:614:U:H6 | 1.62 | 0.64 |
| 14:N:12:ARG:HD3 | 14:N:18:THR:OG1 | 1.97 | 0.64 |
| 21:U:17:THR:HG22 | 21:U:18:GLY:N | 2.13 | 0.64 |
| 30:0:272:A:H5' | 30:0:273:G:OP2 | 1.97 | 0.64 |
| 8:H:168:VAL:HG13 | 38:H:213:HOH:O | 1.98 | 0.64 |
| 30:0:2563:U:H2' | 30:0:2565:C:O5' | 1.98 | 0.64 |
| 30:0:2638:G:H5' | 38:0:4946:HOH:O | 1.98 | 0.64 |
| 30:0:2371:G:H5' | 38:0:5029:HOH:O | 1.98 | 0.64 |
| 21:U:17:THR:HG22 | 21:U:18:GLY:H | 1.62 | 0.64 |
| 3:C:184:ARG:NH2 | 30:0:450:C:OP1 | 2.31 | 0.64 |
| 30:0:644:G:N3 | 30:0:644:G:H5' | 2.13 | 0.64 |
| 30:0:952:G:H4' | 38:0:4042:HOH:O | 1.97 | 0.63 |
| 30:0:333:G:O2' | 30:0:334:G:H5' | 1.97 | 0.63 |
| 30:0:1603:A:C5' | 30:0:1605:G:H5' | 2.27 | 0.63 |
| 2:B:162:MET:HG3 | 2:B:310:ARG:HD3 | 1.80 | 0.63 |
| 30:0:2748:G:H2' | 38:0:7581:HOH:O | 1.98 | 0.63 |
| 30:0:1596:U:H2' | 30:0:1598:A:OP2 | 1.99 | 0.63 |
| 30:0:2404:G:H5'' | 38:0:5231:HOH:O | 1.97 | 0.63 |
| 18:R:128:ARG:NH2 | 30:0:2054:A:N3 | 2.46 | 0.63 |
| 23:W:72:PRO:HG2 | 23:W:77:ALA:HB3 | 1.80 | 0.63 |
| 30:0:2718:C:H6 | 30:0:2718:C:H5' | 1.63 | 0.63 |
| 30:0:2610:U:H4' | 38:0:9484:HOH:O | 1.99 | 0.63 |
| 30:0:2344:G:N3 | 30:0:2344:G:H2' | 2.14 | 0.63 |
| 30:0:420:U:H2' | 30:0:421:C:C6 | 2.33 | 0.63 |
| 30:0:544:G:H2' | 30:0:545:G:H5'' | 1.81 | 0.63 |
| 30:0:1166:A:P | 30:0:1174:A:H4' | 2.38 | 0.63 |
| 2:B:238:ASN:HD22 | 2:B:240:GLY:N | 1.93 | 0.63 |
| 16:P:115:SER:N | 16:P:118:GLN:HE21 | 1.84 | 0.63 |
| 30:0:1189:A:O2' | 30:0:1208:C:H2' | 1.98 | 0.63 |
| 5:E:143:GLN:NE2 | 30:0:2780:C:H1' | 2.13 | 0.63 |
| 11:K:81:ARG:HB2 | 11:K:87:ARG:NH1 | 2.14 | 0.63 |
| 14:N:7:LYS:HE3 | 17:Q:21:ARG:O | 1.99 | 0.63 |
| 30:0:1206:U:C5' | 30:0:1206:U:H6 | 2.10 | 0.63 |
| 30:0:1200:A:H3' | 38:0:5774:HOH:O | 1.99 | 0.63 |
| 3:C:140:VAL:HB | 38:C:8649:HOH:O | 1.98 | 0.63 |
| 30:0:10:U:C3' | 30:0:10:U:C6 | 2.82 | 0.63 |
| 22:V:50:ARG:NH1 | 30:0:56:G:H5'' | 2.13 | 0.63 |
| 30:0:2281:C:C2' | 30:0:2282:U:H5' | 2.29 | 0.63 |
| 2:B:307:ARG:HG3 | 2:B:307:ARG:HH11 | 1.64 | 0.63 |
| 12:L:133:VAL:HA | 38:L:8871:HOH:O | 1.99 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:0:1942:A:H3' | 38:0:7387:HOH:O | 1.98 | 0.62 |
| 27:1:16:HIS:HD2 | 30:0:470:U:O2' | 1.81 | 0.62 |
| 30:0:1182:C:H1' | 30:0:1192:A:C8 | 2.34 | 0.62 |
| 30:0:2781:U:H2' | 30:0:2782:G:C5' | 2.29 | 0.62 |
| 1:A:121:ALA:O | 1:A:124:VAL:HG22 | 1.98 | 0.62 |
| 30:0:2502:C:H2' | 30:0:2503:A:C5' | 2.28 | 0.62 |
| 30:0:138:U:OP2 | 30:0:139:C:H5 | 1.82 | 0.62 |
| 10:J:127:ILE:HG22 | 35:J:8801:CL:CL | 2.36 | 0.62 |
| 30:0:2472:C:O2' | 30:0:2634:G:H4' | 1.99 | 0.62 |
| 30:0:420:U:H2' | 30:0:421:C:H6 | 1.64 | 0.62 |
| 3:C:236:THR:HG21 | 38:C:8573:HOH:O | 2.00 | 0.62 |
| 30:0:559:U:C5 | 30:0:560:U:C5 | 2.88 | 0.62 |
| 3:C:27:ARG:NH2 | 30:0:657:G:OP1 | 2.32 | 0.62 |
| 30:0:2241:C:O2' | 30:0:2242:U:H5' | 2.00 | 0.62 |
| 23:W:6:GLN:HB2 | 23:W:26:ILE:HD11 | 1.81 | 0.62 |
| 4:D:22:VAL:HG22 | 4:D:74:THR:HG22 | 1.81 | 0.62 |
| 30:0:1351:G:H1' | 38:0:4064:HOH:O | 1.98 | 0.62 |
| 24:X:43:VAL:HG12 | 24:X:44:ASP:H | 1.63 | 0.62 |
| 28:2:41:HIS:H | 28:2:45:ASN:HD22 | 1.46 | 0.62 |
| 2:B:320:GLN:HE21 | 2:B:321:PRO:HD2 | 1.65 | 0.62 |
| 30:0:1477:C:H5' | 30:0:1868:G:C5' | 2.30 | 0.62 |
| 1:A:191:GLY:HA2 | 1:A:194:MET:CE | 2.30 | 0.62 |
| 20:T:26:THR:HG23 | 20:T:97:ARG:HG3 | 1.82 | 0.62 |
| 28:2:2:LYS:HG3 | 30:0:1486:A:C5 | 2.34 | 0.62 |
| 30:0:107:U:C2' | 30:0:108:U:H5' | 2.29 | 0.62 |
| 30:0:2372:A:H2' | 30:0:2373:U:H6 | 1.65 | 0.62 |
| 29:3:25:VAL:HG22 | 29:3:68:LYS:HG3 | 1.80 | 0.62 |
| 25:Y:189:ASN:HA | 25:Y:217:ILE:HD11 | 1.82 | 0.61 |
| 2:B:18:ARG:HG3 | 2:B:256:GLN:HG3 | 1.82 | 0.61 |
| 30:0:2643:G:H5'' | 38:0:3937:HOH:O | 1.99 | 0.61 |
| 3:C:129:HIS:CE1 | 3:C:231:ARG:HA | 2.35 | 0.61 |
| 21:U:56:ARG:HD2 | 38:0:6278:HOH:O | 1.98 | 0.61 |
| 30:0:958:G:O2' | 30:0:959:C:H5' | 2.01 | 0.61 |
| 30:0:2802:C:H2' | 30:0:2803:C:C6 | 2.35 | 0.61 |
| 30:0:196:G:H2' | 38:0:6690:HOH:O | 2.00 | 0.61 |
| 30:0:2509:A:OP2 | 30:0:2510:C:H5 | 1.82 | 0.61 |
| 30:0:1972:U:H2' | 30:0:1973:A:H5'' | 1.80 | 0.61 |
| 30:0:1015:C:H2' | 30:0:1016:U:H6 | 1.65 | 0.61 |
| 30:0:407:A:H3' | 38:0:4471:HOH:O | 2.00 | 0.61 |
| 31:9:29:C:C2' | 31:9:30:C:H5' | 2.27 | 0.61 |
| 30:0:308:U:C4 | 30:0:342:C:H1' | 2.36 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 23:W:80:ASP:O | 23:W:84:VAL:HG23 | 1.99 | 0.61 |
| 12:L:136:ALA:HB3 | 38:L:8871:HOH:O | 2.00 | 0.61 |
| 11:K:63:GLU:HG2 | 38:K:6344:HOH:O | 2.00 | 0.61 |
| 30:0:705:C:H2' | 30:0:705:C:O2 | 2.01 | 0.61 |
| 30:0:1183:C:H42 | 30:0:1184:C:H41 | 1.47 | 0.61 |
| 18:R:99:ALA:HB1 | 18:R:109:MET:CE | 2.31 | 0.61 |
| 30:0:1174:A:C6 | 30:0:1201:C:H4' | 2.36 | 0.61 |
| 2:B:7:ARG:HG2 | 2:B:7:ARG:HH11 | 1.66 | 0.61 |
| 2:B:201:ASP:HB2 | 2:B:312:ARG:HD2 | 1.82 | 0.61 |
| 27:1:1:THR:HA | 38:1:435:HOH:O | 2.00 | 0.61 |
| 12:L:30:ARG:HD3 | 30:0:164:G:H4' | 1.82 | 0.61 |
| 14:N:11:ARG:HG3 | 14:N:14:ARG:NH1 | 2.15 | 0.61 |
| 31:9:39:U:H3' | 31:9:40:C:H5'' | 1.83 | 0.61 |
| 16:P:91:LYS:O | 16:P:95:GLU:HG3 | 2.00 | 0.61 |
| 30:0:1165:G:N2 | 30:0:1173:A:C5' | 2.63 | 0.61 |
| 30:0:1972:U:C2' | 30:0:1973:A:H5'' | 2.31 | 0.61 |
| 27:1:28:HIS:HE1 | 30:0:776:A:OP1 | 1.84 | 0.61 |
| 30:0:510:U:H6 | 38:0:7477:HOH:O | 1.83 | 0.60 |
| 29:3:15:ASN:O | 30:0:2408:A:H4' | 2.01 | 0.60 |
| 31:9:39:U:H1' | 31:9:44:A:H61 | 1.65 | 0.60 |
| 22:V:39:ALA:N | 22:V:40:PRO:HD2 | 2.14 | 0.60 |
| 30:0:544:G:C2' | 30:0:545:G:H5'' | 2.31 | 0.60 |
| 8:H:6:ALA:HA | 8:H:61:ARG:HH12 | 1.67 | 0.60 |
| 4:D:135:VAL:HG21 | 4:D:139:TYR:CD1 | 2.36 | 0.60 |
| 30:0:2768:A:H5'' | 38:0:4438:HOH:O | 2.00 | 0.60 |
| 30:0:1819:G:H5' | 38:0:5835:HOH:O | 2.01 | 0.60 |
| 30:0:1379:A:H1' | 38:0:9696:HOH:O | 2.01 | 0.60 |
| 30:0:69:A:C8 | 30:0:69:A:C5' | 2.78 | 0.60 |
| 30:0:1116:U:C2' | 30:0:1118:A:H2 | 2.14 | 0.60 |
| 30:0:31:C:H4' | 38:0:7464:HOH:O | 2.00 | 0.60 |
| 30:0:407:A:H5' | 38:0:6054:HOH:O | 2.00 | 0.60 |
| 30:0:2787:C:C5 | 38:0:4643:HOH:O | 2.49 | 0.60 |
| 19:S:55:GLN:NE2 | 30:0:1446:U:H2' | 2.17 | 0.60 |
| 30:0:285:A:H2' | 30:0:286:U:O4' | 2.01 | 0.60 |
| 1:A:47:HIS:HD2 | 30:0:1654:U:H2' | 1.66 | 0.60 |
| 30:0:2581:U:H1' | 38:0:4486:HOH:O | 2.01 | 0.60 |
| 30:0:363:C:H1' | 38:0:5301:HOH:O | 2.01 | 0.60 |
| 18:R:8:ALA:HB1 | 18:R:13:THR:HG21 | 1.82 | 0.60 |
| 25:Y:187:VAL:HG22 | 25:Y:192:ASP:HB3 | 1.84 | 0.60 |
| 2:B:258:GLY:H | 2:B:260:HIS:CE1 | 2.19 | 0.60 |
| 20:T:9:LYS:HE3 | 20:T:13:ARG:CZ | 2.32 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 30:0:960:G:N3 | 30:0:960:G:C2' | 2.65 | 0.60 |
| 11:K:74:VAL:CG1 | 11:K:113:ILE:HG12 | 2.32 | 0.60 |
| 30:0:2893:C:O2' | 30:0:2894:C:H5' | 2.02 | 0.60 |
| 30:0:164:G:H3' | 38:0:3650:HOH:O | 2.02 | 0.60 |
| 30:0:853:C:H3' | 38:0:4563:HOH:O | 2.01 | 0.60 |
| 30:0:2103:A:O2' | 30:0:2104:C:H6 | 1.85 | 0.59 |
| 10:J:75:PRO:HG2 | 10:J:105:LEU:HD21 | 1.83 | 0.59 |
| 30:0:2453:G:H3' | 38:0:5945:HOH:O | 2.01 | 0.59 |
| 25:Y:216:ARG:HD2 | 38:Y:8873:HOH:O | 2.02 | 0.59 |
| 30:0:2637:A:H4' | 38:0:4946:HOH:O | 2.02 | 0.59 |
| 30:0:2134:G:N2 | 30:0:2242:U:C2 | 2.70 | 0.59 |
| 24:X:76:ARG:HH11 | 24:X:76:ARG:HG3 | 1.66 | 0.59 |
| 30:0:941:G:C5 | 30:0:942:U:C4 | 2.91 | 0.59 |
| 19:S:17:ASP:HB3 | 19:S:23:LYS:HB2 | 1.83 | 0.59 |
| 3:C:233:THR:HG22 | 3:C:234:VAL:H | 1.67 | 0.59 |
| 12:L:56:LYS:HE3 | 30:0:2443:C:H1' | 1.84 | 0.59 |
| 13:M:86:GLN:NE2 | 30:0:2274:A:H1' | 2.17 | 0.59 |
| 10:J:18:ILE:HD13 | 30:0:1244:U:OP1 | 2.01 | 0.59 |
| 2:B:162:MET:CE | 2:B:308:LEU:HD21 | 2.32 | 0.59 |
| 17:Q:25:PRO:HB2 | 38:9:9079:HOH:O | 2.01 | 0.59 |
| 30:0:2795:C:O2' | 30:0:2796:U:H5' | 2.02 | 0.59 |
| 30:0:2361:A:H8 | 30:0:2361:A:H5' | 1.68 | 0.59 |
| 6:F:58:GLU:CD | 13:M:27:ARG:HH22 | 2.05 | 0.59 |
| 30:0:821:U:H2' | 30:0:822:C:H6 | 1.67 | 0.59 |
| 30:0:2372:A:H2' | 30:0:2373:U:C6 | 2.37 | 0.59 |
| 30:0:1819:G:H2' | 30:0:1820:G:C5' | 2.32 | 0.59 |
| 5:E:49:ILE:HD11 | 5:E:69:ILE:HD12 | 1.85 | 0.59 |
| 30:0:1527:A:H1' | 30:0:1528:A:C8 | 2.37 | 0.59 |
| 30:0:1249:U:H2' | 30:0:1250:C:C6 | 2.36 | 0.59 |
| 15:O:24:ALA:HB3 | 30:0:710:G:OP1 | 2.02 | 0.59 |
| 13:M:99:ARG:HE | 13:M:170:ASN:HD22 | 1.49 | 0.59 |
| 11:K:45:PRO:HB2 | 38:K:7169:HOH:O | 2.01 | 0.59 |
| 30:0:1625:U:H4' | 38:0:4676:HOH:O | 2.03 | 0.59 |
| 2:B:234:ARG:HG3 | 30:0:1735:C:OP2 | 2.02 | 0.59 |
| 30:0:1202:A:H2' | 30:0:1203:G:O4' | 2.03 | 0.59 |
| 30:0:2073:G:OP2 | 30:0:2490:A:H5' | 2.01 | 0.59 |
| 8:H:174:LEU:HD21 | 30:0:1220:U:H4' | 1.83 | 0.59 |
| 21:U:6:CYS:HB2 | 21:U:32:CYS:HB3 | 1.85 | 0.59 |
| 30:0:1603:A:H5' | 30:0:1605:G:C4' | 2.33 | 0.59 |
| 30:0:2756:U:N3 | 30:0:2896:A:H2 | 2.01 | 0.59 |
| 30:0:905:C:H3' | 38:0:5207:HOH:O | 2.02 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 30:0:2265:U:H2' | 30:0:2266:A:C8 | 2.37 | 0.59 |
| 4:D:54:ALA:HB2 | 4:D:69:ILE:HD12 | 1.84 | 0.59 |
| 30:0:513:A:N3 | 38:0:3665:HOH:O | 2.32 | 0.59 |
| 30:0:2846:C:H4' | 38:0:5100:HOH:O | 2.03 | 0.59 |
| 30:0:1116:U:HO2' | 30:0:1118:A:H2 | 0.68 | 0.59 |
| 30:0:2756:U:N3 | 30:0:2896:A:C2 | 2.67 | 0.59 |
| 11:K:87:ARG:HG3 | 30:0:2721:U:H4' | 1.85 | 0.59 |
| 29:3:60:LYS:HG3 | 29:3:61:PRO:HD2 | 1.83 | 0.59 |
| 30:0:1120:U:H5' | 30:0:1121:G:OP2 | 2.03 | 0.59 |
| 2:B:141:ARG:HD2 | 2:B:163:GLU:OE2 | 2.03 | 0.59 |
| 30:0:137:U:H2' | 30:0:139:C:C5 | 2.38 | 0.58 |
| 1:A:191:GLY:HA2 | 1:A:194:MET:HE3 | 1.84 | 0.58 |
| 30:0:2539:U:H1' | 38:0:7825:HOH:O | 2.02 | 0.58 |
| 30:0:737:A:H2' | 30:0:738:G:O4' | 2.02 | 0.58 |
| 14:N:37:ARG:HH11 | 31:9:6:C:H5'' | 1.61 | 0.58 |
| 30:0:2526:C:C6 | 30:0:2526:C:C5' | 2.85 | 0.58 |
| 2:B:215:VAL:HB | 38:B:9087:HOH:O | 2.02 | 0.58 |
| 30:0:2607:U:H4' | 38:0:9447:HOH:O | 2.03 | 0.58 |
| 29:3:73:GLU:HB3 | 38:3:9052:HOH:O | 2.02 | 0.58 |
| 3:C:236:THR:CG2 | 3:C:239:ALA:H | 2.10 | 0.58 |
| 26:Z:81:CYS:SG | 26:Z:83:TYR:HB3 | 2.43 | 0.58 |
| 5:E:143:GLN:HE22 | 30:0:2779:G:H21 | 1.48 | 0.58 |
| 2:B:145:HIS:HD2 | 2:B:146:THR:O | 1.87 | 0.58 |
| 10:J:76:ASP:HA | 38:J:5907:HOH:O | 2.03 | 0.58 |
| 1:A:23:TYR:HB2 | 30:0:1872:C:C5 | 2.38 | 0.58 |
| 30:0:1641:A:H2' | 30:0:1642:A:H5' | 1.85 | 0.58 |
| 30:0:282:C:O2' | 30:0:283:U:C5' | 2.52 | 0.58 |
| 30:0:368:C:H2' | 30:0:369:G:H5' | 1.85 | 0.58 |
| 29:3:70:ARG:HB3 | 38:3:9064:HOH:O | 2.03 | 0.58 |
| 10:J:107:ASN:HD22 | 10:J:109:TYR:H | 1.50 | 0.58 |
| 30:0:304:G:H1' | 30:0:347:A:N6 | 2.18 | 0.58 |
| 8:H:48:VAL:HA | 8:H:170:ARG:O | 2.02 | 0.58 |
| 2:B:212:GLN:HB2 | 2:B:257:THR:CG2 | 2.32 | 0.58 |
| 30:0:1919:A:H4' | 38:0:4867:HOH:O | 2.03 | 0.58 |
| 30:0:960:G:H4' | 38:0:7470:HOH:O | 2.03 | 0.58 |
| 30:0:1291:A:H2 | 38:0:5311:HOH:O | 1.86 | 0.58 |
| 30:0:899:C:H5' | 38:0:3211:HOH:O | 2.03 | 0.58 |
| 12:L:67:ARG:HB2 | 12:L:112:GLY:HA3 | 1.85 | 0.58 |
| 30:0:638:C:H2' | 30:0:639:A:C8 | 2.39 | 0.58 |
| 30:0:185:G:H4' | 30:0:186:A:OP1 | 2.02 | 0.58 |
| 30:0:1701:A:H5'' | 30:0:1702:U:H3' | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:36:PRO:HG3 | 2:B:169:GLY:H | 1.69 | 0.58 |
| 3:C:2:GLN:HB3 | 38:C:8583:HOH:O | 2.03 | 0.58 |
| 20:T:52:ARG:HD2 | 30:0:317:A:H5' | 1.85 | 0.58 |
| 28:2:2:LYS:HG3 | 30:0:1486:A:C4 | 2.39 | 0.58 |
| 3:C:58:ALA:HA | 3:C:73:GLN:HE21 | 1.69 | 0.58 |
| 3:C:101:ASP:HB2 | 30:0:750:A:O3' | 2.04 | 0.58 |
| 26:Z:40:ALA:HA | 30:0:1773:G:C8 | 2.38 | 0.58 |
| 28:2:11:LEU:HD22 | 30:0:1417:G:O2' | 2.04 | 0.58 |
| 13:M:30:GLU:O | 13:M:34:GLU:HG3 | 2.04 | 0.58 |
| 30:0:1206:U:H5' | 30:0:1206:U:C6 | 2.26 | 0.58 |
| 9:I:107:LYS:HB3 | 9:I:110:ASP:HB2 | 1.85 | 0.58 |
| 14:N:141:ARG:NH2 | 31:9:48:C:H4' | 2.19 | 0.58 |
| 30:0:1507:C:H4' | 38:0:3609:HOH:O | 2.03 | 0.58 |
| 30:0:2670:G:O2' | 30:0:2671:U:H5' | 2.03 | 0.58 |
| 30:0:877:G:C5' | 30:0:878:G:OP1 | 2.48 | 0.58 |
| 30:0:2802:C:H2' | 30:0:2803:C:H6 | 1.66 | 0.58 |
| 9:I:73:LEU:HD12 | 9:I:107:LYS:NZ | 2.19 | 0.58 |
| 1:A:100:PRO:HG2 | 1:A:103:VAL:HG21 | 1.84 | 0.58 |
| 2:B:112:THR:HG23 | 2:B:158:LYS:NZ | 2.18 | 0.58 |
| 30:0:17:G:H2' | 30:0:18:C:H6 | 1.68 | 0.58 |
| 30:0:2842:G:H2' | 30:0:2843:A:H5' | 1.85 | 0.58 |
| 5:E:84:MET:HG2 | 5:E:168:ILE:HA | 1.86 | 0.58 |
| 2:B:207:LYS:HG3 | 30:0:2717:C:OP1 | 2.04 | 0.58 |
| 27:1:25:LYS:HD2 | 28:2:49:GLU:H | 1.68 | 0.58 |
| 17:Q:19:ARG:HH21 | 31:9:11:A:P | 2.27 | 0.58 |
| 30:0:2510:C:H5' | 30:0:2511:A:OP2 | 2.04 | 0.57 |
| 30:0:2445:U:H2' | 30:0:2446:G:C8 | 2.39 | 0.57 |
| 2:B:256:GLN:HG2 | 38:B:9121:HOH:O | 2.04 | 0.57 |
| 7:G:64:ASN:HD22 | 7:G:64:ASN:N | 2.02 | 0.57 |
| 14:N:61:ALA:HB3 | 14:N:88:ALA:HB2 | 1.85 | 0.57 |
| 30:0:2356:A:H5' | 38:0:5655:HOH:O | 2.03 | 0.57 |
| 7:G:16:LYS:O | 7:G:20:VAL:HG23 | 2.03 | 0.57 |
| 12:L:6:ARG:HD3 | 30:0:1299:G:O6 | 2.03 | 0.57 |
| 30:0:2755:G:H1' | 38:0:4691:HOH:O | 2.03 | 0.57 |
| 2:B:5:ARG:NH1 | 2:B:8:LYS:HE2 | 2.19 | 0.57 |
| 31:9:39:U:H1' | 31:9:44:A:N6 | 2.18 | 0.57 |
| 30:0:2238:A:O2' | 30:0:2239:C:H5' | 2.03 | 0.57 |
| 30:0:297:U:H1' | 38:0:3945:HOH:O | 2.04 | 0.57 |
| 30:0:441:A:H1' | 30:0:442:A:N7 | 2.20 | 0.57 |
| 30:0:812:A:H1' | 38:0:3967:HOH:O | 2.03 | 0.57 |
| 30:0:2004:U:H2' | 30:0:2004:U:O2 | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 30:0:1741:U:O2' | 30:0:2723:G:H4' | 2.04 | 0.57 |
| 29:3:48:ASN:HD21 | 30:0:2468:A:H61 | 1.50 | 0.57 |
| 23:W:44:MET:CE | 30:0:944:G:H21 | 2.17 | 0.57 |
| 30:0:1795:G:H2' | 30:0:1796:A:O4' | 2.04 | 0.57 |
| 30:0:2505:G:O2' | 30:0:2506:A:H5' | 2.05 | 0.57 |
| 30:0:1278:A:H4' | 30:0:1279:U:C4 | 2.40 | 0.57 |
| 30:0:232:A:H4' | 38:0:6113:HOH:O | 2.05 | 0.57 |
| 30:0:558:C:H2' | 30:0:559:U:H5'' | 1.84 | 0.57 |
| 19:S:77:VAL:O | 19:S:80:ARG:HG2 | 2.05 | 0.57 |
| 30:0:1167:G:H2' | 30:0:1168:C:O4' | 2.04 | 0.57 |
| 30:0:820:G:O2' | 30:0:856:G:H4' | 2.03 | 0.57 |
| 23:W:52:VAL:HG22 | 23:W:53:ALA:H | 1.68 | 0.57 |
| 31:9:39:U:HO2' | 31:9:42:C:H5 | 1.53 | 0.57 |
| 30:0:558:C:C2' | 30:0:559:U:C5' | 2.83 | 0.57 |
| 12:L:41:HIS:CD2 | 30:0:926:A:O2' | 2.58 | 0.57 |
| 30:0:945:U:H2' | 30:0:946:C:H6 | 1.70 | 0.57 |
| 30:0:2597:U:H2' | 30:0:2598:U:H5' | 1.87 | 0.57 |
| 30:0:1538:C:O2' | 30:0:1539:U:H5' | 2.05 | 0.57 |
| 30:0:2589:U:H2' | 30:0:2590:U:C6 | 2.40 | 0.57 |
| 30:0:168:C:O5' | 30:0:168:C:H6 | 1.88 | 0.57 |
| 10:J:70:PHE:HE1 | 30:0:2676:C:H4' | 1.68 | 0.57 |
| 30:0:2291:A:N9 | 30:0:2309:C:H5' | 2.19 | 0.57 |
| 30:0:483:C:C4 | 30:0:484:A:C6 | 2.93 | 0.57 |
| 14:N:24:LEU:HD13 | 17:Q:26:PRO:HB3 | 1.86 | 0.57 |
| 30:0:292:G:H2' | 30:0:358:G:N2 | 2.20 | 0.57 |
| 1:A:51:ARG:NH1 | 1:A:120:ARG:O | 2.38 | 0.57 |
| 30:0:1205:U:O2' | 30:0:1206:U:H5'' | 2.05 | 0.56 |
| 38:C:8559:HOH:O | 30:0:338:C:H5'' | 2.04 | 0.56 |
| 30:0:287:C:H42 | 30:0:365:G:H1 | 1.53 | 0.56 |
| 23:W:125:HIS:HD2 | 23:W:127:GLY:H | 1.53 | 0.56 |
| 30:0:1214:G:H4' | 38:0:4759:HOH:O | 2.03 | 0.56 |
| 30:0:125:U:H2' | 38:0:3775:HOH:O | 2.04 | 0.56 |
| 31:9:55:U:H4' | 31:9:56:A:C8 | 2.40 | 0.56 |
| 14:N:147:ILE:HD12 | 38:9:9089:HOH:O | 2.04 | 0.56 |
| 30:0:2720:C:H3' | 38:0:6454:HOH:O | 2.05 | 0.56 |
| 30:0:119:A:H2' | 30:0:120:A:H5'' | 1.87 | 0.56 |
| 30:0:334:G:C5 | 30:0:335:U:C5 | 2.94 | 0.56 |
| 30:0:1528:A:H2' | 30:0:1529:G:O4' | 2.05 | 0.56 |
| 30:0:17:G:H2' | 30:0:18:C:C6 | 2.40 | 0.56 |
| 30:0:945:U:H2' | 30:0:946:C:C6 | 2.40 | 0.56 |
| 25:Y:126:PRO:HG2 | 25:Y:128:PHE:CE1 | 2.40 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 16:P:64:GLU:HG2 | 38:P:2495:HOH:O | 2.05 | 0.56 |
| 10:J:69:TYR:CE1 | 30:0:2081:A:H4' | 2.40 | 0.56 |
| 23:W:139:GLY:O | 23:W:141:HIS:HD2 | 1.87 | 0.56 |
| 8:H:15:PRO:HG3 | 30:0:1053:G:OP1 | 2.06 | 0.56 |
| 30:0:1342:C:C2' | 30:0:1343:C:H5' | 2.35 | 0.56 |
| 25:Y:115:ARG:HH21 | 30:0:1266:U:H4' | 1.71 | 0.56 |
| 25:Y:235:GLU:H | 25:Y:235:GLU:CD | 2.08 | 0.56 |
| 30:0:1181:A:C2 | 30:0:1192:A:C8 | 2.94 | 0.56 |
| 2:B:297:VAL:HB | 38:B:9075:HOH:O | 2.05 | 0.56 |
| 30:0:2252:A:C5 | 30:0:2253:G:H1' | 2.40 | 0.56 |
| 30:0:136:C:H2' | 30:0:137:U:O4' | 2.05 | 0.56 |
| 1:A:47:HIS:CD2 | 30:0:1654:U:H2' | 2.41 | 0.56 |
| 18:R:39:THR:HG23 | 18:R:107:GLU:O | 2.04 | 0.56 |
| 8:H:69:ARG:HD3 | 38:H:232:HOH:O | 2.06 | 0.56 |
| 30:0:1679:C:H5' | 38:0:9330:HOH:O | 2.05 | 0.56 |
| 13:M:64:ARG:HD2 | 38:M:8878:HOH:O | 2.04 | 0.56 |
| 12:L:143:THR:HG22 | 12:L:144:ASP:N | 2.21 | 0.56 |
| 11:K:130:MET:SD | 21:U:25:ASP:O | 2.64 | 0.56 |
| 30:0:1903:U:O2' | 30:0:1904:A:N7 | 2.39 | 0.56 |
| 31:9:49:G:H2' | 31:9:50:G:O4' | 2.06 | 0.56 |
| 11:K:118:ALA:HA | 11:K:125:ALA:HB2 | 1.88 | 0.56 |
| 6:F:50:VAL:HG13 | 6:F:60:VAL:HG11 | 1.87 | 0.56 |
| 5:E:149:GLU:HG3 | 5:E:167:TYR:HA | 1.86 | 0.56 |
| 31:9:63:C:O2' | 31:9:64:C:H5' | 2.06 | 0.56 |
| 21:U:9:CYS:HA | 21:U:52:THR:CG2 | 2.36 | 0.56 |
| 2:B:294:TYR:HE2 | 38:B:9114:HOH:O | 1.89 | 0.56 |
| 7:G:20:VAL:O | 7:G:24:VAL:HG23 | 2.06 | 0.56 |
| 31:9:36:C:C5 | 31:9:37:C:C5 | 2.94 | 0.56 |
| 23:W:48:VAL:HG12 | 23:W:52:VAL:HB | 1.87 | 0.55 |
| 30:0:396:U:O2' | 30:0:418:C:H4' | 2.05 | 0.55 |
| 30:0:2253:G:O2' | 30:0:2254:G:H5' | 2.06 | 0.55 |
| 4:D:172:VAL:HG12 | 4:D:173:GLU:H | 1.70 | 0.55 |
| 7:G:12:ILE:HG23 | 38:0:5477:HOH:O | 2.07 | 0.55 |
| 30:0:1198:U:H1' | 30:0:1201:C:H5 | 1.71 | 0.55 |
| 30:0:1183:C:N3 | 30:0:1184:C:C5 | 2.74 | 0.55 |
| 30:0:283:U:C5 | 30:0:284:C:C2 | 2.93 | 0.55 |
| 30:0:960:G:C3' | 30:0:960:G:N3 | 2.70 | 0.55 |
| 30:0:1768:C:H2' | 30:0:1769:C:O4' | 2.06 | 0.55 |
| 30:0:1664:A:H8 | 30:0:1664:A:OP1 | 1.89 | 0.55 |
| 3:C:236:THR:HA | 38:C:8649:HOH:O | 2.05 | 0.55 |
| 30:0:2419:U:H5'' | 30:0:2420:G:H5' | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 10:J:19:MET:HE1 | 10:J:79:PHE:HA | 1.89 | 0.55 |
| 14:N:141:ARG:HH21 | 31:9:48:C:H4' | 1.72 | 0.55 |
| 30:0:2608:C:H2' | 38:0:3579:HOH:O | 2.06 | 0.55 |
| 3:C:47:GLY:HA2 | 3:C:92:PRO:HB2 | 1.87 | 0.55 |
| 9:I:111:LEU:CD2 | 30:0:1163:G:H4' | 2.35 | 0.55 |
| 14:N:11:ARG:HG3 | 14:N:14:ARG:HH12 | 1.71 | 0.55 |
| 30:0:65:C:O2' | 30:0:66:G:H5' | 2.06 | 0.55 |
| 11:K:32:ILE:HD11 | 11:K:56:SER:HB3 | 1.88 | 0.55 |
| 8:H:22:TYR:CZ | 30:0:1007:A:H2' | 2.41 | 0.55 |
| 30:0:628:1MA:H4' | 38:0:3149:HOH:O | 2.06 | 0.55 |
| 6:F:77:VAL:HG21 | 6:F:83:LEU:HD13 | 1.88 | 0.55 |
| 30:0:2509:A:C2 | 30:0:2510:C:H1' | 2.42 | 0.55 |
| 30:0:558:C:H2' | 30:0:559:U:H5' | 1.89 | 0.55 |
| 12:L:22:ARG:HG2 | 38:0:3241:HOH:O | 2.05 | 0.55 |
| 30:0:2478:U:O2' | 30:0:2479:A:H5' | 2.06 | 0.55 |
| 30:0:1666:C:H2' | 30:0:1667:A:H5'' | 1.71 | 0.55 |
| 30:0:2908:A:O5' | 30:0:2908:A:H8 | 1.89 | 0.55 |
| 30:0:2353:A:H4' | 30:0:2354:A:O5' | 2.06 | 0.55 |
| 38:O:1484:HOH:O | 30:0:710:G:H1' | 2.06 | 0.55 |
| 30:0:1787:C:H4' | 30:0:2883:A:O4' | 2.07 | 0.55 |
| 2:B:62:ARG:HA | 2:B:65:MET:CE | 2.36 | 0.55 |
| 30:0:1159:G:H1 | 30:0:1208:C:H42 | 1.54 | 0.55 |
| 30:0:567:U:C5' | 38:0:6437:HOH:O | 2.50 | 0.55 |
| 30:0:960:G:H2' | 30:0:960:G:N3 | 2.22 | 0.55 |
| 30:0:2565:C:H4' | 38:0:4851:HOH:O | 2.06 | 0.55 |
| 8:H:6:ALA:HA | 8:H:61:ARG:NH1 | 2.21 | 0.55 |
| 25:Y:130:ARG:HB2 | 25:Y:142:SER:O | 2.07 | 0.55 |
| 30:0:2320:U:H4' | 30:0:2321:A:O4' | 2.07 | 0.55 |
| 30:0:1127:C:C5 | 30:0:1128:U:C4 | 2.95 | 0.55 |
| 12:L:36:ASP:HB2 | 38:L:8836:HOH:O | 2.07 | 0.55 |
| 23:W:154:ARG:NH1 | 30:0:588:G:O6 | 2.40 | 0.55 |
| 30:0:2896:A:N3 | 30:0:2896:A:H2' | 2.22 | 0.55 |
| 30:0:1120:U:H5'' | 30:0:1120:U:C6 | 2.42 | 0.55 |
| 30:0:89:G:H4' | 38:0:4779:HOH:O | 2.05 | 0.55 |
| 30:0:2249:G:C2 | 30:0:2253:G:C6 | 2.95 | 0.55 |
| 30:0:1819:G:H2' | 30:0:1820:G:H4' | 1.89 | 0.55 |
| 16:P:87:ARG:HG2 | 38:0:5970:HOH:O | 2.07 | 0.55 |
| 30:0:1838:U:H3' | 38:0:5544:HOH:O | 2.07 | 0.55 |
| 30:0:1474:C:C5' | 30:0:1474:C:C6 | 2.79 | 0.54 |
| 31:9:76:G:C3' | 31:9:77:A:H5'' | 2.27 | 0.54 |
| 30:0:1118:A:H8 | 30:0:1119:G:H5'' | 1.73 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 30:0:1066:U:H2' | 30:0:1067:A:C8 | 2.41 | 0.54 |
| 1:A:109:GLU:HG2 | 1:A:116:GLY:H | 1.72 | 0.54 |
| 3:C:174:ILE:CD1 | 30:0:338:C:H4' | 2.36 | 0.54 |
| 24:X:43:VAL:HG11 | 24:X:82:GLU:HA | 1.88 | 0.54 |
| 30:0:1750:C:H5'' | 38:0:3673:HOH:O | 2.07 | 0.54 |
| 9:I:112:LEU:CD1 | 30:0:1162:G:H1' | 2.37 | 0.54 |
| 27:1:9:GLY:HA2 | 30:0:1687:C:O2 | 2.07 | 0.54 |
| 22:V:64:GLY:O | 22:V:65:ASP:HB2 | 2.06 | 0.54 |
| 23:W:142:ASP:HB3 | 23:W:145:GLY:H | 1.71 | 0.54 |
| 2:B:221:GLN:HE22 | 11:K:42:ASN:ND2 | 1.98 | 0.54 |
| 27:1:16:HIS:HE1 | 30:0:775:G:OP1 | 1.91 | 0.54 |
| 16:P:80:ARG:HG2 | 16:P:87:ARG:CZ | 2.37 | 0.54 |
| 38:Z:8707:HOH:O | 30:0:1886:A:H4' | 2.06 | 0.54 |
| 23:W:64:THR:O | 23:W:68:THR:HG22 | 2.06 | 0.54 |
| 30:0:876:A:N3 | 30:0:876:A:H2' | 2.23 | 0.54 |
| 4:D:141:VAL:HG21 | 31:9:57:A:H8 | 1.72 | 0.54 |
| 8:H:59:GLN:HE21 | 8:H:129:ARG:NE | 2.05 | 0.54 |
| 30:0:1016:U:H1' | 38:0:3664:HOH:O | 2.06 | 0.54 |
| 29:3:11:CYS:HB2 | 29:3:20:HIS:CE1 | 2.42 | 0.54 |
| 2:B:305:ASP:O | 2:B:306:LYS:HB2 | 2.08 | 0.54 |
| 30:0:2387:U:H2' | 30:0:2388:C:C6 | 2.42 | 0.54 |
| 2:B:275:GLY:O | 2:B:291:ASP:HA | 2.07 | 0.54 |
| 30:0:138:U:OP1 | 30:0:259:G:H5' | 2.07 | 0.54 |
| 31:9:12:C:H5' | 31:9:70:U:O4' | 2.06 | 0.54 |
| 13:M:66:SER:HB3 | 13:M:128:TRP:CD1 | 2.42 | 0.54 |
| 24:X:23:HIS:HE1 | 30:0:2044:G:OP1 | 1.89 | 0.54 |
| 15:O:105:ASN:HD21 | 15:O:109:SER:N | 2.05 | 0.54 |
| 20:T:68:ASP:HB2 | 38:0:5678:HOH:O | 2.08 | 0.54 |
| 30:0:962:C:H2' | 30:0:963:C:H5' | 1.89 | 0.54 |
| 30:0:711:G:C2 | 30:0:718:C:C2 | 2.96 | 0.54 |
| 23:W:88:THR:HG22 | 23:W:90:TYR:HD1 | 1.72 | 0.54 |
| 31:9:1:U:O3' | 31:9:3:A:H5'' | 2.07 | 0.54 |
| 30:0:2271:G:N3 | 30:0:2271:G:H2' | 2.22 | 0.54 |
| 13:M:159:VAL:HG12 | 35:M:8818:CL:CL | 2.45 | 0.54 |
| 26:Z:75:GLY:HA3 | 38:Z:8717:HOH:O | 2.06 | 0.54 |
| 31:9:3:A:N6 | 31:9:22:G:H1' | 2.22 | 0.54 |
| 30:0:2414:A:H2' | 30:0:2415:A:C8 | 2.43 | 0.54 |
| 23:W:13:MET:HE1 | 23:W:18:GLN:HA | 1.88 | 0.54 |
| 8:H:87:LYS:NZ | 8:H:87:LYS:HB2 | 2.23 | 0.54 |
| 30:0:1205:U:H5 | 38:0:4451:HOH:O | 1.91 | 0.54 |
| 13:M:24:GLN:NE2 | 13:M:27:ARG:HH11 | 2.06 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 30:0:1342:C:O2' | 30:0:1343:C:H5' | 2.07 | 0.54 |
| 9:I:97:VAL:HG12 | 9:I:101:LYS:HE3 | 1.90 | 0.54 |
| 30:0:2880:A:H2' | 30:0:2881:C:H5' | 1.89 | 0.54 |
| 4:D:18:ILE:HD13 | 4:D:84:LEU:HD12 | 1.89 | 0.54 |
| 30:0:567:U:H5'' | 38:0:5308:HOH:O | 2.08 | 0.54 |
| 30:0:1926:G:H2' | 30:0:1927:A:C8 | 2.42 | 0.54 |
| 19:S:11:THR:H | 19:S:14:ALA:HB3 | 1.73 | 0.54 |
| 30:0:1624:A:H5' | 30:0:1626:A:O4' | 2.07 | 0.54 |
| 30:0:1450:C:H5'' | 38:0:9624:HOH:O | 2.08 | 0.54 |
| 24:X:72:VAL:HG22 | 24:X:85:VAL:HG12 | 1.90 | 0.53 |
| 16:P:7:LYS:HD3 | 16:P:21:VAL:HG22 | 1.90 | 0.53 |
| 30:0:1137:G:H1' | 38:0:3888:HOH:O | 2.07 | 0.53 |
| 24:X:30:MET:HE1 | 24:X:58:ALA:HB3 | 1.90 | 0.53 |
| 2:B:254:GLN:HG2 | 2:B:255:GLY:N | 2.23 | 0.53 |
| 30:0:1201:C:C2' | 30:0:1202:A:H5' | 2.37 | 0.53 |
| 30:0:1973:A:H5' | 30:0:1973:A:C8 | 2.41 | 0.53 |
| 30:0:2697:A:H2' | 30:0:2698:G:O4' | 2.08 | 0.53 |
| 30:0:1766:U:O2 | 30:0:1778:A:H5' | 2.08 | 0.53 |
| 1:A:17:ARG:HD2 | 38:A:9005:HOH:O | 2.07 | 0.53 |
| 17:Q:15:LYS:HD3 | 30:0:2364:A:H5'' | 1.89 | 0.53 |
| 31:9:1:U:O3' | 31:9:3:A:C5' | 2.57 | 0.53 |
| 30:0:644:G:H1' | 38:0:6440:HOH:O | 2.08 | 0.53 |
| 30:0:1304:U:H2' | 30:0:1305:C:C6 | 2.43 | 0.53 |
| 30:0:121:U:H2' | 38:0:9854:HOH:O | 2.08 | 0.53 |
| 30:0:682:A:H2' | 30:0:683:G:O4' | 2.08 | 0.53 |
| 4:D:141:VAL:HG21 | 31:9:57:A:C8 | 2.43 | 0.53 |
| 30:0:280:C:H2' | 30:0:281:U:O4' | 2.07 | 0.53 |
| 30:0:2102:G:C5' | 30:0:2538:A:C2 | 2.91 | 0.53 |
| 30:0:2445:U:H2' | 30:0:2446:G:H8 | 1.72 | 0.53 |
| 30:0:700:A:H5'' | 30:0:701:U:H5' | 1.91 | 0.53 |
| 2:B:154:VAL:HG12 | 2:B:156:LYS:HG2 | 1.89 | 0.53 |
| 19:S:37:VAL:O | 19:S:41:VAL:HG23 | 2.08 | 0.53 |
| 30:0:2311:A:H3' | 38:0:7716:HOH:O | 2.07 | 0.53 |
| 30:0:2354:A:C2 | 30:0:2367:A:C8 | 2.97 | 0.53 |
| 30:0:2002:C:H2' | 30:0:2003:U:H5' | 1.90 | 0.53 |
| 28:2:22:PRO:HG2 | 28:2:25:VAL:HG23 | 1.90 | 0.53 |
| 23:W:5:VAL:HG11 | 23:W:153:MET:CE | 2.39 | 0.53 |
| 30:0:482:G:H4' | 30:0:508:A:N1 | 2.24 | 0.53 |
| 14:N:139:TRP:HA | 14:N:139:TRP:CE3 | 2.44 | 0.53 |
| 30:0:1562:C:N4 | 38:0:5888:HOH:O | 2.41 | 0.53 |
| 30:0:407:A:H2' | 30:0:408:A:C8 | 2.44 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:1:42:SER:HB2 | 38:1:354:HOH:O | 2.08 | 0.53 |
| 30:0:1714:C:O2' | 30:0:1715:C:H5' | 2.09 | 0.53 |
| 3:C:127:ARG:HD3 | 3:C:129:HIS:HE1 | 1.73 | 0.53 |
| 30:0:559:U:C5' | 30:0:559:U:H6 | 2.20 | 0.53 |
| 17:Q:42:LYS:HE2 | 30:0:952:G:OP1 | 2.09 | 0.53 |
| 8:H:6:ALA:HB3 | 30:0:2521:A:OP2 | 2.09 | 0.53 |
| 4:D:23:VAL:HG21 | 4:D:45:THR:HG21 | 1.90 | 0.53 |
| 26:Z:66:CYS:SG | 26:Z:67:GLY:N | 2.82 | 0.53 |
| 30:0:2764:C:O2' | 30:0:2765:C:H5' | 2.08 | 0.53 |
| 30:0:2256:G:C2' | 30:0:2257:G:C5' | 2.86 | 0.53 |
| 30:0:1495:C:H1' | 30:0:1573:A:H1' | 1.91 | 0.53 |
| 25:Y:141:THR:HG23 | 38:Y:8892:HOH:O | 2.08 | 0.53 |
| 14:N:86:LEU:HD12 | 14:N:125:ALA:HB2 | 1.91 | 0.53 |
| 13:M:188:ARG:NH1 | 30:0:154:C:H3' | 2.23 | 0.53 |
| 1:A:190:ARG:NH1 | 30:0:1845:A:OP2 | 2.42 | 0.53 |
| 25:Y:132:ASP:OD2 | 30:0:621:C:H5' | 2.08 | 0.53 |
| 8:H:26:ILE:HA | 8:H:123:ILE:HG21 | 1.91 | 0.53 |
| 1:A:192:VAL:CG1 | 1:A:207:GLN:HB3 | 2.39 | 0.53 |
| 30:0:1060:C:H6 | 30:0:1060:C:H5' | 1.72 | 0.53 |
| 10:J:107:ASN:C | 10:J:107:ASN:HD22 | 2.13 | 0.53 |
| 16:P:115:SER:OG | 16:P:118:GLN:HG3 | 2.09 | 0.52 |
| 30:0:603:A:H1' | 30:0:605:C:C2 | 2.43 | 0.52 |
| 14:N:48:VAL:CG1 | 14:N:55:ASP:HB3 | 2.39 | 0.52 |
| 30:0:1183:C:C2 | 30:0:1184:C:C5 | 2.97 | 0.52 |
| 31:9:13:A:O2' | 31:9:14:G:H5'' | 2.10 | 0.52 |
| 1:A:36:ASP:O | 1:A:38:ILE:N | 2.41 | 0.52 |
| 30:0:138:U:C5 | 30:0:140:G:O6 | 2.62 | 0.52 |
| 30:0:704:C:H2' | 30:0:705:C:H6 | 1.74 | 0.52 |
| 1:A:99:ILE:O | 1:A:131:HIS:HE1 | 1.92 | 0.52 |
| 30:0:2509:A:H2' | 30:0:2510:C:O4' | 2.09 | 0.52 |
| 30:0:282:C:O2' | 30:0:283:U:H4' | 2.09 | 0.52 |
| 4:D:134:LEU:HD11 | 4:D:166:ILE:HD11 | 1.91 | 0.52 |
| 30:0:1014:A:H2' | 30:0:1015:C:H5' | 1.92 | 0.52 |
| 30:0:304:G:H1' | 30:0:347:A:H61 | 1.73 | 0.52 |
| 13:M:134:ILE:HG23 | 13:M:141:ILE:HD13 | 1.92 | 0.52 |
| 18:R:114:VAL:HA | 18:R:144:GLU:O | 2.09 | 0.52 |
| 18:R:18:LEU:HB2 | 18:R:143:VAL:CG1 | 2.40 | 0.52 |
| 30:0:2359:G:H3' | 38:0:5709:HOH:O | 2.09 | 0.52 |
| 20:T:28:SER:O | 20:T:32:ARG:HG3 | 2.08 | 0.52 |
| 23:W:88:THR:HG22 | 23:W:89:ASP:N | 2.23 | 0.52 |
| 17:Q:21:ARG:HH12 | 30:0:2353:A:H1' | 1.74 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:9:42:C:H5' | 31:9:43:G:OP2 | 2.09 | 0.52 |
| 5:E:3:VAL:HG22 | 5:E:49:ILE:HB | 1.91 | 0.52 |
| 30:0:2265:U:H2' | 30:0:2266:A:H8 | 1.75 | 0.52 |
| 7:G:19:GLU:O | 7:G:23:ILE:HG13 | 2.09 | 0.52 |
| 3:C:25:PRO:HG2 | 38:C:8521:HOH:O | 2.08 | 0.52 |
| 18:R:150:PRO:CG | 18:R:150:PRO:CB | 2.87 | 0.52 |
| 14:N:33:ARG:NH2 | 31:9:6:C:O2' | 2.43 | 0.52 |
| 30:0:1180:U:O2' | 30:0:1181:A:H5' | 2.10 | 0.52 |
| 30:0:138:U:OP2 | 30:0:139:C:C5 | 2.62 | 0.52 |
| 30:0:1724:U:H5' | 38:0:3739:HOH:O | 2.09 | 0.52 |
| 6:F:13:GLU:OE2 | 6:F:78:GLU:HG2 | 2.09 | 0.52 |
| 30:0:1289:C:O2' | 30:0:1290:G:H5' | 2.09 | 0.52 |
| 4:D:154:LYS:HD2 | 4:D:154:LYS:N | 2.10 | 0.52 |
| 30:0:1185:U:H5' | 38:0:7505:HOH:O | 2.08 | 0.52 |
| 2:B:267:LYS:HD3 | 38:0:9567:HOH:O | 2.09 | 0.52 |
| 30:0:1249:U:H2' | 30:0:1250:C:H6 | 1.75 | 0.52 |
| 4:D:28:GLY:HA2 | 4:D:69:ILE:HG23 | 1.92 | 0.52 |
| 5:E:5:LEU:HD21 | 5:E:66:GLN:HG3 | 1.91 | 0.52 |
| 30:0:2072:G:C6 | 30:0:2533:C:H1' | 2.45 | 0.52 |
| 4:D:25:MET:CE | 4:D:37:ALA:HB1 | 2.39 | 0.52 |
| 30:0:1477:C:H5' | 30:0:1868:G:H5' | 1.91 | 0.52 |
| 30:0:298:C:H1' | 38:0:3853:HOH:O | 2.09 | 0.52 |
| 30:0:661:G:C5 | 30:0:686:A:C2 | 2.98 | 0.52 |
| 30:0:204:A:H2' | 30:0:205:U:H5' | 1.92 | 0.52 |
| 30:0:2840:A:H3' | 38:0:7686:HOH:O | 2.09 | 0.52 |
| 30:0:1175:G:O2' | 30:0:1193:A:H2' | 2.09 | 0.52 |
| 30:0:1878:G:O2' | 30:0:1879:U:C6 | 2.59 | 0.52 |
| 6:F:2:VAL:HG22 | 6:F:57:GLU:OE1 | 2.09 | 0.52 |
| 30:0:1972:U:H2' | 30:0:1973:A:H5' | 1.91 | 0.52 |
| 13:M:188:ARG:HD3 | 30:0:155:C:OP2 | 2.09 | 0.52 |
| 30:0:2604:A:H4' | 38:0:7644:HOH:O | 2.09 | 0.52 |
| 1:A:217:ARG:HG2 | 1:A:229:ALA:HB2 | 1.91 | 0.52 |
| 12:L:121:ILE:HG12 | 12:L:141:GLU:HB2 | 1.92 | 0.52 |
| 30:0:2498:C:O2' | 30:0:2499:U:H5' | 2.09 | 0.52 |
| 30:0:2526:C:O2' | 30:0:2527:U:H5' | 2.10 | 0.52 |
| 18:R:18:LEU:HB2 | 18:R:143:VAL:HG12 | 1.92 | 0.52 |
| 7:G:23:ILE:O | 7:G:27:ILE:HG13 | 2.09 | 0.52 |
| 3:C:16:VAL:HG12 | 3:C:17:ASP:H | 1.73 | 0.52 |
| 5:E:154:ILE:HD11 | 5:E:157:LYS:HE2 | 1.92 | 0.52 |
| 30:0:545:G:C8 | 30:0:545:G:C5' | 2.83 | 0.52 |
| 30:0:821:U:H2' | 30:0:822:C:C6 | 2.45 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 30:0:734:U:O2' | 30:0:736:A:N7 | 2.37 | 0.52 |
| 17:Q:95:GLU:HA | 30:0:949:U:H4' | 1.92 | 0.52 |
| 4:D:128:LEU:HB2 | 38:D:6007:HOH:O | 2.08 | 0.52 |
| 30:0:999:C:O2' | 30:0:1000:C:H5' | 2.10 | 0.52 |
| 30:0:1419:U:H2' | 30:0:1685:A:C2 | 2.45 | 0.51 |
| 30:0:1675:C:H3' | 38:0:7847:HOH:O | 2.10 | 0.51 |
| 1:A:33:GLU:O | 1:A:34:ASP:HB2 | 2.09 | 0.51 |
| 15:O:37:ARG:HD2 | 30:0:656:G:OP2 | 2.09 | 0.51 |
| 2:B:212:GLN:HA | 30:0:1733:A:H4' | 1.92 | 0.51 |
| 30:0:334:G:C6 | 30:0:335:U:C4 | 2.98 | 0.51 |
| 30:0:137:U:OP1 | 30:0:259:G:O2' | 2.28 | 0.51 |
| 15:O:7:LEU:HD22 | 38:O:5650:HOH:O | 2.10 | 0.51 |
| 30:0:2083:A:H3' | 38:0:7617:HOH:O | 2.10 | 0.51 |
| 30:0:2637:A:OP1 | 30:0:2637:A:H3' | 2.10 | 0.51 |
| 13:M:34:GLU:HB3 | 13:M:38:GLU:HG3 | 1.91 | 0.51 |
| 30:0:1393:A:H2' | 30:0:1394:C:C6 | 2.46 | 0.51 |
| 18:R:14:ALA:HB3 | 18:R:147:LEU:HB2 | 1.93 | 0.51 |
| 30:0:652:G:H8 | 38:0:3020:HOH:O | 1.93 | 0.51 |
| 30:0:432:G:O2' | 30:0:433:C:H5' | 2.10 | 0.51 |
| 27:1:16:HIS:CD2 | 30:0:470:U:O2' | 2.63 | 0.51 |
| 8:H:27:PRO:HD3 | 8:H:123:ILE:HG22 | 1.91 | 0.51 |
| 30:0:2493:C:O2 | 30:0:2493:C:H2' | 2.10 | 0.51 |
| 26:Z:76:THR:HG21 | 30:0:1652:C:H4' | 1.91 | 0.51 |
| 30:0:1307:A:H2' | 30:0:1308:A:C8 | 2.46 | 0.51 |
| 30:0:346:U:H4' | 38:0:6881:HOH:O | 2.10 | 0.51 |
| 26:Z:57:MET:SD | 26:Z:73:ARG:HD2 | 2.51 | 0.51 |
| 30:0:1181:A:H2' | 30:0:1182:C:H5' | 1.93 | 0.51 |
| 2:B:221:GLN:NE2 | 11:K:42:ASN:HD22 | 1.96 | 0.51 |
| 24:X:85:VAL:HG12 | 24:X:86:GLU:N | 2.26 | 0.51 |
| 27:1:8:GLN:HE22 | 27:1:11:LYS:NZ | 2.07 | 0.51 |
| 4:D:62:ASP:HA | 38:D:4233:HOH:O | 2.10 | 0.51 |
| 30:0:1422:U:H2' | 30:0:1423:C:C6 | 2.46 | 0.51 |
| 31:9:95:C:O2' | 31:9:96:C:H5' | 2.11 | 0.51 |
| 30:0:466:A:H2' | 30:0:467:G:O4' | 2.10 | 0.51 |
| 20:T:24:ARG:HH21 | 20:T:39:ASN:HD22 | 1.59 | 0.51 |
| 31:9:3:A:OP2 | 31:9:25:G:N2 | 2.43 | 0.51 |
| 30:0:553:G:H5' | 38:0:3506:HOH:O | 2.11 | 0.51 |
| 30:0:120:A:H2' | 30:0:120:A:N3 | 2.26 | 0.51 |
| 30:0:1477:C:O2' | 30:0:1478:U:H5' | 2.10 | 0.51 |
| 16:P:7:LYS:HG2 | 16:P:23:PHE:CE2 | 2.46 | 0.51 |
| 30:0:2329:C:O2' | 30:0:2330:U:H5' | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:21:THR:HG23 | 5:E:30:THR:OG1 | 2.11 | 0.51 |
| 30:0:2105:C:H2' | 30:0:2106:C:C6 | 2.45 | 0.51 |
| 30:0:281:U:H2' | 30:0:282:C:O4' | 2.10 | 0.51 |
| 30:0:282:C:H2' | 30:0:283:U:O4' | 2.10 | 0.51 |
| 28:2:10:ARG:NH2 | 30:0:121:U:OP2 | 2.42 | 0.51 |
| 28:2:38:LYS:HE3 | 38:0:4239:HOH:O | 2.10 | 0.51 |
| 18:R:40:ALA:O | 18:R:44:VAL:HG23 | 2.11 | 0.51 |
| 30:0:1056:U:H2' | 30:0:1057:A:O4' | 2.11 | 0.51 |
| 10:J:42:GLU:O | 10:J:131:THR:HG23 | 2.11 | 0.51 |
| 30:0:2826:G:C6 | 30:0:2913:A:N6 | 2.78 | 0.51 |
| 23:W:81:ASP:OD1 | 23:W:92:ASP:HB2 | 2.11 | 0.51 |
| 30:0:1166:A:C6 | 30:0:1181:A:C2 | 2.99 | 0.51 |
| 30:0:1181:A:C2' | 30:0:1182:C:H5' | 2.40 | 0.51 |
| 23:W:13:MET:CE | 23:W:17:ILE:HG22 | 2.41 | 0.51 |
| 30:0:764:C:H2' | 30:0:765:G:O4' | 2.11 | 0.51 |
| 2:B:223:ARG:HG3 | 2:B:232:TRP:O | 2.10 | 0.51 |
| 30:0:694:A:H2' | 30:0:695:C:H5' | 1.91 | 0.51 |
| 30:0:1183:C:O2 | 30:0:1183:C:C2' | 2.59 | 0.51 |
| 30:0:1209:C:H2' | 30:0:1210:G:H8 | 1.76 | 0.51 |
| 23:W:80:ASP:HB2 | 38:W:3312:HOH:O | 2.11 | 0.51 |
| 30:0:2786:G:H5'' | 38:0:4643:HOH:O | 2.10 | 0.51 |
| 30:0:951:A:C2' | 30:0:952:G:H5' | 2.40 | 0.51 |
| 30:0:2894:C:O2' | 30:0:2895:C:H5' | 2.11 | 0.51 |
| 18:R:39:THR:HG22 | 18:R:42:GLU:H | 1.75 | 0.51 |
| 31:9:55:U:H4' | 31:9:56:A:H8 | 1.76 | 0.51 |
| 28:2:41:HIS:CD2 | 28:2:44:ARG:H | 2.26 | 0.51 |
| 25:Y:174:VAL:HG23 | 25:Y:177:LYS:HD2 | 1.93 | 0.51 |
| 30:0:90:A:H2' | 30:0:91:G:O4' | 2.11 | 0.51 |
| 30:0:1131:G:C6 | 30:0:1230:A:C4 | 2.99 | 0.51 |
| 30:0:255:A:C5 | 30:0:256:C:C5 | 2.98 | 0.51 |
| 30:0:255:A:H2' | 30:0:256:C:H6 | 1.76 | 0.51 |
| 38:C:8567:HOH:O | 20:T:2:LYS:HE2 | 2.10 | 0.51 |
| 30:0:172:U:H5' | 38:0:4171:HOH:O | 2.11 | 0.51 |
| 3:C:63:SER:OG | 30:0:2101:A:H2' | 2.11 | 0.51 |
| 9:I:114:TYR:CD1 | 9:I:114:TYR:N | 2.80 | 0.50 |
| 23:W:5:VAL:HG11 | 23:W:153:MET:HE1 | 1.92 | 0.50 |
| 30:0:305:A:C5 | 30:0:329:A:C2 | 2.99 | 0.50 |
| 1:A:173:GLY:O | 1:A:176:HIS:HB3 | 2.10 | 0.50 |
| 27:1:10:LYS:HG3 | 38:1:2979:HOH:O | 2.10 | 0.50 |
| 30:0:2553:A:H2' | 30:0:2553:A:N3 | 2.25 | 0.50 |
| 31:9:29:C:H2' | 31:9:30:C:C5' | 2.36 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 30:0:282:C:O2' | 30:0:283:U:C4' | 2.59 | 0.50 |
| 6:F:61:MET:HB3 | 13:M:19:GLN:OE1 | 2.11 | 0.50 |
| 30:0:512:G:O3' | 30:0:513:A:H8 | 1.93 | 0.50 |
| 1:A:192:VAL:HG12 | 1:A:207:GLN:HB3 | 1.93 | 0.50 |
| 30:0:1657:A:H2' | 30:0:1658:A:C8 | 2.46 | 0.50 |
| 30:0:2269:C:C2' | 30:0:2270:G:H5' | 2.40 | 0.50 |
| 1:A:33:GLU:CD | 1:A:33:GLU:H | 2.14 | 0.50 |
| 2:B:41:PHE:CZ | 2:B:79:MET:HG3 | 2.46 | 0.50 |
| 30:0:1594:C:O2' | 30:0:1607:A:H4' | 2.11 | 0.50 |
| 30:0:398:U:H2' | 30:0:399:C:C6 | 2.47 | 0.50 |
| 14:N:37:ARG:NH1 | 31:9:6:C:OP1 | 2.44 | 0.50 |
| 6:F:91:VAL:CG1 | 6:F:92:GLY:H | 2.16 | 0.50 |
| 10:J:19:MET:HE3 | 10:J:132:LEU:HD11 | 1.92 | 0.50 |
| 21:U:6:CYS:HA | 21:U:13:ILE:HD11 | 1.94 | 0.50 |
| 30:0:1515:A:H2' | 30:0:1516:U:C6 | 2.46 | 0.50 |
| 31:9:75:G:H1 | 31:9:106:U:H3 | 1.59 | 0.50 |
| 30:0:23:G:H1' | 30:0:520:A:N6 | 2.26 | 0.50 |
| 31:9:54:A:C2 | 31:9:55:U:N3 | 2.80 | 0.50 |
| 13:M:9:ARG:HD2 | 30:0:380:A:OP2 | 2.11 | 0.50 |
| 30:0:2589:U:H2' | 30:0:2590:U:H6 | 1.76 | 0.50 |
| 30:0:1903:U:O2' | 30:0:1904:A:C8 | 2.63 | 0.50 |
| 5:E:7:ILE:HG22 | 5:E:45:ASP:O | 2.10 | 0.50 |
| 31:9:59:C:H6 | 31:9:59:C:O5' | 1.94 | 0.50 |
| 4:D:159:PRO:O | 4:D:163:VAL:HG23 | 2.12 | 0.50 |
| 30:0:10:U:O4 | 30:0:532:A:OP2 | 2.30 | 0.50 |
| 30:0:602:A:O2' | 30:0:605:C:H4' | 2.11 | 0.50 |
| 30:0:1015:C:H2' | 30:0:1016:U:C6 | 2.47 | 0.50 |
| 8:H:19:ARG:HH12 | 30:0:1008:C:H5'' | 1.76 | 0.50 |
| 26:Z:50:VAL:O | 26:Z:54:GLU:HG3 | 2.11 | 0.50 |
| 30:0:814:G:H4' | 38:0:3140:HOH:O | 2.11 | 0.50 |
| 7:G:63:ARG:NH1 | 30:0:1151:G:OP1 | 2.45 | 0.50 |
| 20:T:38:ARG:NH1 | 38:0:6719:HOH:O | 2.45 | 0.50 |
| 30:0:2878:U:H2' | 30:0:2879:A:O4' | 2.12 | 0.50 |
| 11:K:20:CYS:HB2 | 11:K:29:LEU:HG | 1.94 | 0.50 |
| 16:P:14:LEU:HD13 | 16:P:51:ALA:HB2 | 1.93 | 0.50 |
| 30:0:1883:U:C2' | 30:0:1884:G:H5' | 2.42 | 0.50 |
| 30:0:11:A:N3 | 30:0:11:A:H2' | 2.26 | 0.50 |
| 30:0:1588:G:C6 | 30:0:1589:G:N1 | 2.80 | 0.50 |
| 31:9:1:U:H4' | 31:9:3:A:OP1 | 2.12 | 0.50 |
| 30:0:2842:G:C2' | 30:0:2843:A:H5' | 2.41 | 0.50 |
| 30:0:1186:C:N4 | 30:0:1187:U:C4 | 2.80 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 30:0:1840:A:H4' | 30:0:1841:C:O5' | 2.12 | 0.50 |
| 30:0:319:A:H4' | 30:0:338:C:C4 | 2.47 | 0.50 |
| 14:N:67:ALA:HA | 14:N:71:TRP:HB3 | 1.93 | 0.50 |
| 30:0:2898:G:O2' | 30:0:2899:A:H5' | 2.11 | 0.50 |
| 30:0:1947:G:N2 | 30:0:1966:U:C2 | 2.80 | 0.50 |
| 30:0:1520:G:H2' | 30:0:1521:C:C6 | 2.46 | 0.50 |
| 30:0:1170:U:H2' | 30:0:1172:G:OP2 | 2.12 | 0.50 |
| 30:0:1759:A:N3 | 30:0:1818:C:H2' | 2.27 | 0.50 |
| 23:W:125:HIS:CE1 | 30:0:1097:A:H5'' | 2.47 | 0.49 |
| 30:0:1377:C:H6 | 30:0:1377:C:C5' | 2.19 | 0.49 |
| 2:B:307:ARG:HG3 | 2:B:307:ARG:NH1 | 2.26 | 0.49 |
| 10:J:74:ARG:HH11 | 10:J:74:ARG:HB3 | 1.76 | 0.49 |
| 30:0:1896:G:C6 | 30:0:1897:U:C4 | 3.00 | 0.49 |
| 11:K:4:LEU:HD22 | 11:K:116:GLU:HB3 | 1.93 | 0.49 |
| 24:X:43:VAL:HG12 | 24:X:44:ASP:N | 2.26 | 0.49 |
| 12:L:143:THR:HG22 | 12:L:144:ASP:H | 1.78 | 0.49 |
| 30:0:711:G:O2' | 30:0:712:C:H5' | 2.12 | 0.49 |
| 14:N:5:ARG:HG3 | 14:N:5:ARG:HH11 | 1.77 | 0.49 |
| 30:0:1350:U:H5'' | 38:0:5143:HOH:O | 2.11 | 0.49 |
| 30:0:923:A:H2' | 38:0:5697:HOH:O | 2.12 | 0.49 |
| 23:W:119:HIS:HE1 | 38:0:9559:HOH:O | 1.95 | 0.49 |
| 30:0:2415:A:H2' | 30:0:2416:G:H5' | 1.94 | 0.49 |
| 1:A:217:ARG:NH2 | 30:0:1853:C:O2' | 2.46 | 0.49 |
| 31:9:107:C:O2' | 31:9:108:C:H5' | 2.11 | 0.49 |
| 30:0:1947:G:H2' | 30:0:1948:G:H8 | 1.77 | 0.49 |
| 13:M:75:ARG:HH11 | 30:0:1864:C:H5 | 1.59 | 0.49 |
| 30:0:735:C:C5 | 30:0:736:A:C4 | 2.99 | 0.49 |
| 9:I:73:LEU:HD12 | 9:I:107:LYS:HZ1 | 1.77 | 0.49 |
| 30:0:920:C:H5'' | 30:0:921:G:O5' | 2.13 | 0.49 |
| 30:0:861:A:H4' | 30:0:1697:G:H4' | 1.94 | 0.49 |
| 30:0:2638:G:H1' | 38:0:7796:HOH:O | 2.11 | 0.49 |
| 30:0:2134:G:C6 | 30:0:2258:A:C8 | 3.01 | 0.49 |
| 1:A:51:ARG:HB2 | 38:A:9061:HOH:O | 2.11 | 0.49 |
| 24:X:21:PRO:HG2 | 24:X:24:LYS:HD3 | 1.95 | 0.49 |
| 30:0:1947:G:H2' | 30:0:1948:G:C8 | 2.47 | 0.49 |
| 30:0:939:A:C2 | 30:0:1027:G:N3 | 2.81 | 0.49 |
| 30:0:1221:G:C8 | 38:0:6014:HOH:O | 2.55 | 0.49 |
| 27:1:21:ARG:HD2 | 27:1:37:CYS:SG | 2.53 | 0.49 |
| 30:0:2276:U:H2' | 30:0:2277:U:C6 | 2.47 | 0.49 |
| 16:P:61:ARG:NH2 | 30:0:2737:C:OP2 | 2.37 | 0.49 |
| 30:0:2651:C:H2' | 30:0:2652:U:O4' | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 23:W:125:HIS:CD2 | 23:W:127:GLY:H | 2.31 | 0.49 |
| 31:9:2:U:P | 31:9:3:A:H5' | 2.52 | 0.49 |
| 30:0:1878:G:O2' | 30:0:1879:U:P | 2.71 | 0.49 |
| 10:J:75:PRO:HG2 | 10:J:105:LEU:CD2 | 2.42 | 0.49 |
| 30:0:2345:A:H3' | 30:0:2346:C:C6 | 2.46 | 0.49 |
| 30:0:1119:G:H22 | 30:0:1246:A:H2 | 1.51 | 0.49 |
| 9:I:114:TYR:HD1 | 9:I:114:TYR:N | 2.10 | 0.49 |
| 30:0:370:G:O2' | 30:0:371:U:H5' | 2.12 | 0.49 |
| 27:1:20:ARG:HH21 | 30:0:120:A:H5' | 1.77 | 0.49 |
| 2:B:17:LYS:O | 2:B:260:HIS:HD2 | 1.94 | 0.49 |
| 3:C:233:THR:HG22 | 3:C:234:VAL:N | 2.26 | 0.49 |
| 30:0:291:C:H2' | 30:0:292:G:O4' | 2.12 | 0.49 |
| 14:N:159:TYR:HE1 | 31:9:50:G:H5'' | 1.78 | 0.49 |
| 30:0:711:G:C2' | 30:0:712:C:H5' | 2.42 | 0.49 |
| 16:P:54:LYS:HB2 | 30:0:1717:A:H5'' | 1.94 | 0.49 |
| 30:0:2385:G:H2' | 30:0:2386:U:C6 | 2.47 | 0.49 |
| 15:O:32:ARG:HD3 | 15:O:32:ARG:O | 2.12 | 0.49 |
| 25:Y:186:ARG:HG2 | 25:Y:186:ARG:HH11 | 1.77 | 0.49 |
| 24:X:66:THR:HG23 | 24:X:67:PRO:HD2 | 1.95 | 0.49 |
| 17:Q:18:PRO:O | 17:Q:21:ARG:HB2 | 2.12 | 0.49 |
| 30:0:958:G:H2' | 30:0:959:C:C6 | 2.48 | 0.49 |
| 30:0:941:G:C6 | 30:0:942:U:C4 | 3.01 | 0.49 |
| 30:0:185:G:H4' | 30:0:186:A:H4' | 1.93 | 0.49 |
| 30:0:1298:U:H2' | 30:0:1299:G:C8 | 2.48 | 0.49 |
| 9:I:130:LEU:HD22 | 30:0:1167:G:H4' | 1.95 | 0.49 |
| 8:H:32:ALA:HB3 | 8:H:69:ARG:HH12 | 1.78 | 0.49 |
| 30:0:256:C:H2' | 30:0:257:G:O4' | 2.12 | 0.49 |
| 30:0:699:C:C2 | 30:0:743:G:N2 | 2.81 | 0.49 |
| 17:Q:53:HIS:CD2 | 30:0:2389:U:H4' | 2.47 | 0.49 |
| 30:0:806:A:H2' | 30:0:807:A:O4' | 2.13 | 0.49 |
| 13:M:99:ARG:HD2 | 13:M:167:GLY:CA | 2.35 | 0.49 |
| 30:0:1118:A:C8 | 30:0:1119:G:H5'' | 2.48 | 0.49 |
| 1:A:135:VAL:HG21 | 1:A:147:ARG:HB3 | 1.94 | 0.49 |
| 12:L:41:HIS:HD2 | 30:0:926:A:O2' | 1.95 | 0.49 |
| 31:9:49:G:O2' | 31:9:50:G:H5' | 2.13 | 0.49 |
| 30:0:1849:G:H1' | 30:0:2011:A:N1 | 2.28 | 0.49 |
| 30:0:1755:A:H2' | 30:0:1756:G:O4' | 2.12 | 0.49 |
| 8:H:100:GLU:HB3 | 8:H:124:VAL:HG11 | 1.94 | 0.49 |
| 29:3:3:MET:O | 29:3:90:PHE:HA | 2.12 | 0.49 |
| 30:0:1268:C:H2' | 30:0:1269:G:H8 | 1.77 | 0.49 |
| 30:0:1667:A:H2' | 30:0:1668:U:C6 | 2.48 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 30:0:182:G:H5'' | 38:0:3730:HOH:O | 2.13 | 0.49 |
| 30:0:2103:A:N7 | 30:0:2538:A:N7 | 2.60 | 0.49 |
| 21:U:56:ARG:NH2 | 30:0:2890:A:H1' | 2.28 | 0.49 |
| 30:0:2064:U:H5' | 30:0:2652:U:H4' | 1.95 | 0.49 |
| 30:0:699:C:H6 | 30:0:744:G:O4' | 1.96 | 0.49 |
| 30:0:522:U:O2' | 30:0:1366:C:H5' | 2.13 | 0.49 |
| 30:0:1158:G:O2' | 30:0:1159:G:H5' | 2.13 | 0.48 |
| 24:X:74:ALA:HB2 | 24:X:85:VAL:HG13 | 1.95 | 0.48 |
| 30:0:876:A:N3 | 30:0:876:A:C2' | 2.76 | 0.48 |
| 9:I:101:LYS:O | 9:I:105:GLU:HG3 | 2.12 | 0.48 |
| 2:B:41:PHE:HA | 2:B:79:MET:HE2 | 1.94 | 0.48 |
| 28:2:39:ARG:HG2 | 38:2:3143:HOH:O | 2.13 | 0.48 |
| 14:N:132:ASN:O | 14:N:135:VAL:HG12 | 2.13 | 0.48 |
| 30:0:299:U:H5' | 38:0:7377:HOH:O | 2.12 | 0.48 |
| 30:0:1909:A:N1 | 30:0:2128:G:H1' | 2.27 | 0.48 |
| 31:9:91:C:H2' | 31:9:92:G:O4' | 2.13 | 0.48 |
| 13:M:23:LEU:HD13 | 13:M:27:ARG:NH2 | 2.28 | 0.48 |
| 11:K:34:VAL:HG22 | 11:K:47:ALA:HB2 | 1.94 | 0.48 |
| 1:A:94:LEU:N | 1:A:94:LEU:HD23 | 2.28 | 0.48 |
| 16:P:1:THR:O | 30:0:1396:C:H1' | 2.13 | 0.48 |
| 10:J:5:GLU:HA | 38:J:1652:HOH:O | 2.11 | 0.48 |
| 8:H:64:SER:OG | 30:0:2520:G:H5' | 2.13 | 0.48 |
| 12:L:18:HIS:HD2 | 30:0:902:G:N7 | 2.12 | 0.48 |
| 12:L:138:GLY:HA3 | 38:L:8853:HOH:O | 2.13 | 0.48 |
| 30:0:369:G:O2' | 30:0:370:G:H5' | 2.13 | 0.48 |
| 30:0:2534:C:H1' | 38:0:3502:HOH:O | 2.12 | 0.48 |
| 30:0:2768:A:N3 | 30:0:2768:A:H3' | 2.27 | 0.48 |
| 2:B:262:ARG:HG3 | 30:0:2716:G:H5' | 1.95 | 0.48 |
| 30:0:1634:G:H2' | 30:0:1635:U:C6 | 2.48 | 0.48 |
| 30:0:958:G:H2' | 30:0:959:C:H6 | 1.77 | 0.48 |
| 30:0:1778:A:H2' | 30:0:1779:A:H5' | 1.94 | 0.48 |
| 30:0:652:G:H5'' | 38:0:3020:HOH:O | 2.12 | 0.48 |
| 22:V:56:ILE:O | 22:V:60:GLN:HG3 | 2.14 | 0.48 |
| 13:M:99:ARG:CD | 13:M:167:GLY:HA2 | 2.34 | 0.48 |
| 23:W:125:HIS:HE1 | 38:W:3071:HOH:O | 1.95 | 0.48 |
| 30:0:2032:U:H2' | 30:0:2033:G:C5' | 2.43 | 0.48 |
| 30:0:2851:G:C2' | 30:0:2852:A:H5' | 2.44 | 0.48 |
| 30:0:1592:G:O2' | 30:0:1593:C:O5' | 2.30 | 0.48 |
| 22:V:55:ARG:O | 22:V:59:ILE:HG12 | 2.13 | 0.48 |
| 31:9:54:A:C2' | 31:9:55:U:H5' | 2.43 | 0.48 |
| 30:0:2315:C:O2' | 30:0:2316:G:H5' | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:217:ARG:HG3 | 2:B:257:THR:HG22 | 1.95 | 0.48 |
| 30:0:1972:U:C2' | 30:0:1973:A:C5' | 2.91 | 0.48 |
| 4:D:25:MET:SD | 4:D:40:ILE:HD11 | 2.53 | 0.48 |
| 4:D:99:ASP:HB3 | 4:D:103:ASN:H | 1.79 | 0.48 |
| 30:0:1625:U:H3' | 30:0:1625:U:H6 | 1.79 | 0.48 |
| 9:I:126:THR:O | 9:I:130:LEU:HG | 2.14 | 0.48 |
| 30:0:2899:A:O2' | 30:0:2900:G:H5' | 2.13 | 0.48 |
| 30:0:2900:G:H2' | 30:0:2901:C:O4' | 2.13 | 0.48 |
| 31:9:31:C:H2' | 31:9:32:G:O4' | 2.14 | 0.48 |
| 18:R:47:LEU:HB2 | 18:R:89:LEU:HD21 | 1.95 | 0.48 |
| 30:0:2906:A:H5' | 30:0:2907:C:O4' | 2.14 | 0.48 |
| 30:0:1615:A:H5' | 38:0:4195:HOH:O | 2.13 | 0.48 |
| 30:0:1183:C:H42 | 30:0:1184:C:N4 | 2.11 | 0.48 |
| 30:0:368:C:C2' | 30:0:369:G:H5' | 2.43 | 0.48 |
| 30:0:736:A:H2' | 30:0:737:A:O4' | 2.14 | 0.48 |
| 25:Y:142:SER:OG | 30:0:1331:G:OP2 | 2.31 | 0.48 |
| 4:D:10:PHE:CG | 4:D:11:HIS:N | 2.81 | 0.48 |
| 13:M:99:ARG:HE | 13:M:170:ASN:ND2 | 2.10 | 0.48 |
| 23:W:125:HIS:HB2 | 23:W:137:GLN:HG2 | 1.94 | 0.48 |
| 30:0:241:A:C2 | 30:0:378:A:H4' | 2.49 | 0.48 |
| 11:K:87:ARG:NH1 | 38:K:4066:HOH:O | 2.46 | 0.48 |
| 8:H:30:LYS:N | 8:H:62:HIS:HD2 | 2.10 | 0.48 |
| 19:S:33:SER:O | 19:S:37:VAL:HG23 | 2.12 | 0.48 |
| 30:0:318:U:H5' | 30:0:339:A:C2 | 2.49 | 0.48 |
| 25:Y:170:SER:OG | 25:Y:175:ARG:HG3 | 2.13 | 0.48 |
| 14:N:154:LEU:C | 14:N:156:GLU:H | 2.16 | 0.48 |
| 3:C:132:ASP:HB2 | 3:C:161:ASP:HB3 | 1.95 | 0.48 |
| 23:W:130:HIS:O | 23:W:136:GLY:HA3 | 2.13 | 0.48 |
| 30:0:2488:U:O2' | 30:0:2489:G:H5' | 2.14 | 0.48 |
| 30:0:1173:A:C2 | 30:0:1177:A:C8 | 3.02 | 0.48 |
| 30:0:2505:G:C2' | 30:0:2506:A:H5' | 2.44 | 0.48 |
| 30:0:2672:C:O2' | 30:0:2673:U:H5' | 2.14 | 0.48 |
| 2:B:310:ARG:HD2 | 38:B:9112:HOH:O | 2.14 | 0.48 |
| 30:0:559:U:C3' | 30:0:559:U:C6 | 2.97 | 0.48 |
| 30:0:1592:G:H2' | 30:0:1593:C:H6 | 1.78 | 0.48 |
| 30:0:2133:U:H4' | 30:0:2134:G:C5' | 2.44 | 0.48 |
| 30:0:1221:G:H8 | 38:0:6014:HOH:O | 1.94 | 0.48 |
| 30:0:843:A:C2 | 30:0:846:A:C8 | 3.02 | 0.48 |
| 30:0:1692:C:H2' | 38:0:9867:HOH:O | 2.12 | 0.48 |
| 2:B:44:TYR:OH | 2:B:148:PRO:HG3 | 2.13 | 0.48 |
| 30:0:633:C:O2' | 30:0:634:G:H5' | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 30:0:2718:C:H5' | 30:0:2718:C:C6 | 2.46 | 0.48 |
| 30:0:1198:U:C6 | 30:0:1200:A:OP2 | 2.67 | 0.48 |
| 30:0:484:A:N1 | 30:0:506:G:H4' | 2.29 | 0.48 |
| 30:0:281:U:O2' | 30:0:282:C:H5' | 2.14 | 0.48 |
| 30:0:2781:U:C2' | 30:0:2782:G:C5' | 2.91 | 0.48 |
| 23:W:122:ARG:NH2 | 38:0:6437:HOH:O | 2.46 | 0.48 |
| 30:0:334:G:C4 | 30:0:335:U:C6 | 3.02 | 0.48 |
| 30:0:660:A:H4' | 30:0:661:G:O5' | 2.14 | 0.48 |
| 2:B:79:MET:HE1 | 38:B:9092:HOH:O | 2.12 | 0.48 |
| 22:V:4:HIS:HB3 | 38:V:6622:HOH:O | 2.13 | 0.48 |
| 30:0:128:A:O2' | 30:0:129:A:H5' | 2.14 | 0.48 |
| 30:0:1790:C:H2' | 30:0:1791:U:H6 | 1.78 | 0.48 |
| 38:K:992:HOH:O | 30:0:2583:A:H5' | 2.13 | 0.48 |
| 3:C:188:ARG:HD3 | 38:C:8563:HOH:O | 2.13 | 0.48 |
| 30:0:2649:A:H5' | 30:0:2649:A:H8 | 1.79 | 0.48 |
| 30:0:1206:U:H2' | 30:0:1207:A:O4' | 2.14 | 0.47 |
| 30:0:2526:C:H6 | 30:0:2526:C:C5' | 2.18 | 0.47 |
| 4:D:173:GLU:HG3 | 4:D:174:VAL:HG23 | 1.96 | 0.47 |
| 30:0:861:A:C4' | 30:0:1697:G:H4' | 2.44 | 0.47 |
| 15:O:25:VAL:HG12 | 30:0:709:G:O2' | 2.14 | 0.47 |
| 30:0:727:G:H3' | 30:0:728:C:H6 | 1.79 | 0.47 |
| 30:0:559:U:H2' | 30:0:560:U:O4' | 2.15 | 0.47 |
| 1:A:36:ASP:HB2 | 1:A:85:SER:H | 1.79 | 0.47 |
| 31:9:7:G:C5' | 38:9:9100:HOH:O | 2.58 | 0.47 |
| 30:0:1634:G:H2' | 30:0:1635:U:H6 | 1.79 | 0.47 |
| 10:J:107:ASN:ND2 | 10:J:109:TYR:H | 2.11 | 0.47 |
| 4:D:23:VAL:HG21 | 4:D:45:THR:CG2 | 2.44 | 0.47 |
| 2:B:41:PHE:HB3 | 2:B:190:MET:HE3 | 1.95 | 0.47 |
| 30:0:699:C:C2 | 30:0:744:G:C2 | 3.02 | 0.47 |
| 20:T:82:THR:HA | 38:0:3998:HOH:O | 2.12 | 0.47 |
| 30:0:1855:G:H4' | 30:0:1856:C:O5' | 2.13 | 0.47 |
| 2:B:280:VAL:HG13 | 2:B:333:GLU:O | 2.13 | 0.47 |
| 30:0:571:C:H6 | 30:0:571:C:O5' | 1.97 | 0.47 |
| 2:B:85:ARG:NH1 | 38:B:9099:HOH:O | 2.47 | 0.47 |
| 10:J:70:PHE:CD1 | 30:0:2676:C:H4' | 2.49 | 0.47 |
| 30:0:1497:G:H4' | 30:0:1627:G:O2' | 2.14 | 0.47 |
| 15:O:39:THR:HB | 38:0:4627:HOH:O | 2.14 | 0.47 |
| 25:Y:107:PRO:HB3 | 25:Y:182:PHE:CD2 | 2.50 | 0.47 |
| 30:0:619:U:H3' | 38:0:3287:HOH:O | 2.13 | 0.47 |
| 30:0:816:G:C6 | 30:0:817:G:N1 | 2.83 | 0.47 |
| 31:9:76:G:H3' | 31:9:77:A:C5' | 2.30 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 23:W:21:LEU:HD21 | 23:W:48:VAL:CG1 | 2.43 | 0.47 |
| 30:0:12:U:C2' | 30:0:13:G:H5' | 2.40 | 0.47 |
| 2:B:312:ARG:HD3 | 2:B:315:VAL:HG13 | 1.95 | 0.47 |
| 30:0:638:C:H2' | 30:0:639:A:H8 | 1.78 | 0.47 |
| 30:0:963:C:O2 | 30:0:1005:A:N1 | 2.47 | 0.47 |
| 30:0:1172:G:H1' | 38:0:4992:HOH:O | 2.14 | 0.47 |
| 27:1:22:CYS:HB3 | 27:1:37:CYS:SG | 2.55 | 0.47 |
| 30:0:1217:G:C2 | 30:0:1218:U:C2 | 3.03 | 0.47 |
| 16:P:103:THR:HA | 16:P:106:ARG:NH2 | 2.29 | 0.47 |
| 2:B:27:ASN:H | 2:B:27:ASN:HD22 | 1.63 | 0.47 |
| 30:0:1154:A:H2' | 30:0:1155:G:C8 | 2.49 | 0.47 |
| 30:0:2467:A:H8 | 38:0:7512:HOH:O | 1.97 | 0.47 |
| 30:0:350:G:O2' | 30:0:351:A:H5' | 2.13 | 0.47 |
| 30:0:724:G:O2' | 30:0:725:C:H5' | 2.14 | 0.47 |
| 30:0:541:C:C2' | 30:0:542:A:C5' | 2.81 | 0.47 |
| 31:9:1:U:H5'' | 31:9:3:A:OP1 | 2.15 | 0.47 |
| 30:0:1878:G:C1' | 38:0:6151:HOH:O | 2.51 | 0.47 |
| 30:0:1636:G:O2' | 30:0:1637:A:H5' | 2.13 | 0.47 |
| 30:0:2614:C:O2' | 30:0:2615:U:H5' | 2.14 | 0.47 |
| 2:B:307:ARG:HB3 | 38:B:9117:HOH:O | 2.15 | 0.47 |
| 30:0:297:U:H2' | 30:0:298:C:C6 | 2.49 | 0.47 |
| 30:0:255:A:H2' | 30:0:256:C:O4' | 2.14 | 0.47 |
| 30:0:1856:C:H5' | 30:0:1858:A:O4' | 2.15 | 0.47 |
| 30:0:74:G:H2' | 30:0:75:U:C6 | 2.49 | 0.47 |
| 6:F:34:ASN:HA | 13:M:4:ALA:HB2 | 1.95 | 0.47 |
| 30:0:2577:A:H5' | 38:0:7788:HOH:O | 2.14 | 0.47 |
| 1:A:64:ASP:OD2 | 1:A:66:ARG:HD2 | 2.15 | 0.47 |
| 30:0:968:G:C2 | 30:0:1001:U:O2 | 2.67 | 0.47 |
| 30:0:2121:G:O2' | 30:0:2122:C:H5' | 2.14 | 0.47 |
| 30:0:1587:U:H2' | 30:0:1588:G:O4' | 2.14 | 0.47 |
| 30:0:2524:G:H21 | 30:0:2526:C:N4 | 2.12 | 0.47 |
| 30:0:2769:C:H2' | 30:0:2770:G:O4' | 2.15 | 0.47 |
| 30:0:2842:G:H2' | 30:0:2843:A:C5' | 2.44 | 0.47 |
| 16:P:59:ARG:O | 16:P:63:ARG:HG3 | 2.15 | 0.47 |
| 13:M:28:GLN:O | 13:M:32:ARG:HG3 | 2.15 | 0.47 |
| 16:P:16:VAL:CG1 | 16:P:20:ARG:HB2 | 2.45 | 0.47 |
| 20:T:62:VAL:N | 38:T:3851:HOH:O | 2.47 | 0.47 |
| 23:W:122:ARG:NH2 | 38:0:5308:HOH:O | 2.48 | 0.47 |
| 1:A:223:ARG:NH2 | 30:0:2271:G:OP1 | 2.45 | 0.47 |
| 30:0:736:A:H5'' | 38:0:4282:HOH:O | 2.14 | 0.47 |
| 2:B:242:TRP:CZ2 | 30:0:2607:U:C4 | 3.02 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:E:145:ALA:HB1 | 5:E:168:ILE:CD1 | 2.45 | 0.47 |
| 30:0:2587:OMU:O3' | 30:0:2587:OMU:HM22 | 2.15 | 0.47 |
| 30:0:1925:G:O2' | 30:0:1926:G:H5' | 2.15 | 0.47 |
| 2:B:41:PHE:HB3 | 2:B:190:MET:CE | 2.44 | 0.47 |
| 30:0:1268:C:O2' | 30:0:1269:G:H5' | 2.15 | 0.47 |
| 30:0:2649:A:H5' | 30:0:2649:A:C8 | 2.50 | 0.47 |
| 6:F:36:THR:HG23 | 6:F:97:ALA:HB2 | 1.97 | 0.47 |
| 30:0:1339:G:C6 | 30:0:1340:G:N1 | 2.83 | 0.47 |
| 10:J:90:LYS:HB2 | 35:J:8802:CL:CL | 2.51 | 0.47 |
| 3:C:153:VAL:O | 3:C:157:LEU:HG | 2.15 | 0.47 |
| 11:K:66:ARG:HH22 | 30:0:1994:A:P | 2.37 | 0.47 |
| 30:0:27:U:H5 | 38:0:5910:HOH:O | 1.96 | 0.47 |
| 30:0:758:A:H2' | 30:0:759:C:O4' | 2.15 | 0.47 |
| 30:0:772:G:H2' | 30:0:773:A:O4' | 2.15 | 0.47 |
| 2:B:244:PRO:HB3 | 30:0:1234:U:N3 | 2.29 | 0.47 |
| 30:0:1803:C:H2' | 30:0:1804:A:C8 | 2.50 | 0.47 |
| 24:X:78:GLU:HB3 | 38:X:5564:HOH:O | 2.15 | 0.47 |
| 31:9:5:G:O2' | 31:9:6:C:H5' | 2.15 | 0.47 |
| 30:0:1183:C:N3 | 30:0:1184:C:N4 | 2.62 | 0.47 |
| 27:1:28:HIS:O | 27:1:32:LYS:N | 2.47 | 0.47 |
| 30:0:2326:C:H4' | 30:0:2412:G:C4' | 2.45 | 0.47 |
| 30:0:70:A:H4' | 30:0:71:G:O5' | 2.15 | 0.47 |
| 31:9:52:A:O2' | 31:9:53:G:H5' | 2.15 | 0.47 |
| 30:0:24:G:N2 | 30:0:518:G:H1' | 2.30 | 0.47 |
| 3:C:87:ARG:NH2 | 30:0:894:A:C2 | 2.83 | 0.47 |
| 5:E:11:VAL:HG12 | 5:E:12:ASP:N | 2.30 | 0.47 |
| 30:0:1204:C:H2' | 30:0:1205:U:O4' | 2.15 | 0.47 |
| 30:0:2133:U:H4' | 30:0:2134:G:H5' | 1.96 | 0.47 |
| 18:R:18:LEU:HG | 18:R:91:LEU:HD13 | 1.97 | 0.47 |
| 22:V:44:GLY:O | 22:V:48:GLU:HG2 | 2.15 | 0.47 |
| 30:0:834:G:H3' | 30:0:835:U:H4' | 1.97 | 0.47 |
| 30:0:862:U:H2' | 30:0:863:G:H8 | 1.80 | 0.47 |
| 18:R:29:LYS:HE2 | 30:0:524:A:C5' | 2.45 | 0.47 |
| 2:B:139:ASP:HB2 | 38:B:8997:HOH:O | 2.14 | 0.47 |
| 31:9:33:U:H2' | 38:9:9066:HOH:O | 2.15 | 0.47 |
| 1:A:112:PRO:HD3 | 1:A:152:CYS:SG | 2.55 | 0.47 |
| 6:F:46:GLU:OE1 | 6:F:100:ASP:HA | 2.15 | 0.47 |
| 30:0:625:U:H5'' | 30:0:1044:C:N4 | 2.30 | 0.47 |
| 30:0:1181:A:N1 | 30:0:1192:A:O2' | 2.42 | 0.47 |
| 23:W:4:LEU:O | 23:W:32:CYS:HA | 2.15 | 0.47 |
| 30:0:1641:A:C2' | 30:0:1642:A:H5' | 2.45 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:62:ARG:HA | 2:B:65:MET:HE2 | 1.97 | 0.47 |
| 30:0:790:A:H1' | 30:0:1710:A:H2' | 1.97 | 0.47 |
| 30:0:595:U:H2' | 30:0:596:C:H6 | 1.80 | 0.47 |
| 30:0:383:A:H2' | 30:0:384:G:O4' | 2.15 | 0.47 |
| 13:M:184:ARG:HG3 | 13:M:185:PRO:HA | 1.97 | 0.47 |
| 13:M:123:ASP:OD1 | 13:M:126:GLN:HG2 | 2.15 | 0.47 |
| 30:0:1622:G:H2' | 30:0:1623:C:H5' | 1.97 | 0.47 |
| 14:N:4:PRO:HG3 | 31:9:69:U:OP1 | 2.15 | 0.47 |
| 30:0:1116:U:C2' | 30:0:1118:A:C2 | 2.92 | 0.46 |
| 30:0:1589:G:N2 | 30:0:1605:G:H1' | 2.29 | 0.46 |
| 3:C:236:THR:HG22 | 3:C:239:ALA:CB | 2.45 | 0.46 |
| 30:0:2533:C:C6 | 30:0:2533:C:H5' | 2.39 | 0.46 |
| 30:0:737:A:H8 | 30:0:737:A:O5' | 1.98 | 0.46 |
| 1:A:186:TRP:CG | 1:A:187:PRO:HA | 2.50 | 0.46 |
| 30:0:153:C:O2 | 30:0:439:A:H2 | 1.98 | 0.46 |
| 15:O:29:VAL:HG11 | 15:O:98:LEU:HD21 | 1.96 | 0.46 |
| 30:0:1196:C:C2 | 30:0:1197:G:C8 | 3.03 | 0.46 |
| 30:0:541:C:O2' | 30:0:542:A:H5'' | 2.15 | 0.46 |
| 30:0:2511:A:H2' | 30:0:2512:U:O4' | 2.15 | 0.46 |
| 30:0:284:C:H6 | 30:0:284:C:OP2 | 1.98 | 0.46 |
| 30:0:1819:G:H2' | 30:0:1820:G:C4' | 2.45 | 0.46 |
| 30:0:2587:OMU:H2' | 30:0:2589:U:H5'' | 1.96 | 0.46 |
| 23:W:13:MET:HE3 | 23:W:17:ILE:HG22 | 1.95 | 0.46 |
| 10:J:130:VAL:HG12 | 10:J:131:THR:N | 2.30 | 0.46 |
| 16:P:120:ARG:HD2 | 30:0:1594:C:OP2 | 2.16 | 0.46 |
| 30:0:920:C:H4' | 30:0:921:G:C2 | 2.49 | 0.46 |
| 30:0:2791:U:H1' | 30:0:2792:A:H5'' | 1.96 | 0.46 |
| 4:D:77:ASP:HB3 | 4:D:78:GLU:H | 1.55 | 0.46 |
| 31:9:110:G:C6 | 31:9:111:U:C5 | 3.03 | 0.46 |
| 30:0:1666:C:HO2' | 30:0:1667:A:H5'' | 1.72 | 0.46 |
| 30:0:2361:A:H2' | 30:0:2362:A:O4' | 2.15 | 0.46 |
| 2:B:62:ARG:HA | 2:B:65:MET:HE3 | 1.97 | 0.46 |
| 1:A:101:GLU:OE2 | 1:A:131:HIS:HB2 | 2.15 | 0.46 |
| 30:0:2269:C:H2' | 30:0:2270:G:H5' | 1.96 | 0.46 |
| 25:Y:99:ALA:HB2 | 25:Y:233:TYR:CZ | 2.50 | 0.46 |
| 23:W:35:VAL:HA | 23:W:36:PRO:HD3 | 1.80 | 0.46 |
| 30:0:515:C:H5'' | 38:0:5665:HOH:O | 2.13 | 0.46 |
| 30:0:2089:A:O2' | 30:0:2090:G:H5' | 2.15 | 0.46 |
| 30:0:1706:G:C6 | 30:0:1707:G:C6 | 3.04 | 0.46 |
| 30:0:264:G:H1' | 30:0:265:U:H5 | 1.80 | 0.46 |
| 30:0:506:G:N2 | 30:0:509:A:H5' | 2.21 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:D:129:ASP:OD1 | 30:0:2338:G:H2' | 2.16 | 0.46 |
| 10:J:19:MET:CE | 10:J:132:LEU:HD11 | 2.45 | 0.46 |
| 11:K:87:ARG:NH2 | 30:0:2720:C:O2 | 2.49 | 0.46 |
| 30:0:2000:G:O2' | 30:0:2001:G:H5' | 2.15 | 0.46 |
| 2:B:112:THR:HG23 | 2:B:158:LYS:HZ2 | 1.80 | 0.46 |
| 30:0:204:A:C2' | 30:0:205:U:H5' | 2.45 | 0.46 |
| 30:0:1948:G:H1 | 30:0:1964:U:H3 | 1.63 | 0.46 |
| 30:0:1966:U:H6 | 30:0:1966:U:O5' | 1.99 | 0.46 |
| 30:0:128:A:H3' | 30:0:128:A:C8 | 2.50 | 0.46 |
| 30:0:105:G:O2' | 30:0:106:A:H5' | 2.15 | 0.46 |
| 2:B:125:GLU:O | 2:B:129:ARG:HG3 | 2.15 | 0.46 |
| 30:0:890:C:O2' | 30:0:891:G:H5' | 2.16 | 0.46 |
| 30:0:254:C:O2 | 30:0:254:C:H2' | 2.14 | 0.46 |
| 30:0:2506:A:N6 | 30:0:2511:A:O2' | 2.49 | 0.46 |
| 23:W:43:GLY:HA3 | 30:0:945:U:O2' | 2.15 | 0.46 |
| 30:0:2326:C:H4' | 30:0:2412:G:H4' | 1.97 | 0.46 |
| 30:0:1581:A:C5 | 30:0:1582:C:C5 | 3.03 | 0.46 |
| 1:A:71:PRO:HD2 | 1:A:74:VAL:HG21 | 1.98 | 0.46 |
| 30:0:300:U:C4 | 30:0:301:C:C5 | 3.03 | 0.46 |
| 30:0:419:A:H1' | 30:0:1921:A:C2 | 2.51 | 0.46 |
| 16:P:88:GLN:HE22 | 30:0:1799:G:H21 | 1.63 | 0.46 |
| 12:L:148:GLU:HA | 38:L:8870:HOH:O | 2.14 | 0.46 |
| 6:F:101:ALA:HA | 38:F:5413:HOH:O | 2.15 | 0.46 |
| 2:B:177:HIS:O | 2:B:181:ILE:HG13 | 2.15 | 0.46 |
| 13:M:72:ALA:HB2 | 13:M:93:ARG:HG2 | 1.97 | 0.46 |
| 23:W:139:GLY:O | 23:W:141:HIS:CD2 | 2.66 | 0.46 |
| 30:0:1543:G:N1 | 30:0:1641:A:OP2 | 2.35 | 0.46 |
| 30:0:441:A:H8 | 30:0:441:A:O5' | 1.97 | 0.46 |
| 11:K:118:ALA:CA | 11:K:125:ALA:HB2 | 2.45 | 0.46 |
| 30:0:129:A:O2' | 30:0:131:A:OP1 | 2.33 | 0.46 |
| 30:0:2775:A:C6 | 30:0:2799:A:C8 | 3.04 | 0.46 |
| 23:W:73:LEU:HA | 23:W:73:LEU:HD12 | 1.85 | 0.46 |
| 30:0:1588:G:C6 | 30:0:1589:G:C6 | 3.04 | 0.46 |
| 13:M:86:GLN:HE22 | 30:0:2274:A:H1' | 1.79 | 0.46 |
| 30:0:2658:G:H4' | 30:0:2842:G:C8 | 2.51 | 0.46 |
| 30:0:1393:A:N1 | 30:0:1725:C:O2' | 2.39 | 0.46 |
| 15:O:35:LYS:HD3 | 38:O:4627:HOH:O | 2.15 | 0.46 |
| 2:B:214:PRO:HD2 | 38:O:9083:HOH:O | 2.14 | 0.46 |
| 3:C:214:THR:HG23 | 38:C:8635:HOH:O | 2.16 | 0.46 |
| 30:0:1321:A:H2' | 30:0:1322:G:C8 | 2.51 | 0.46 |
| 30:0:2115:U:H2' | 30:0:2116:U:C6 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 15:O:38:ARG:NH1 | 38:O:7674:HOH:O | 2.49 | 0.46 |
| 30:0:1156:C:O5' | 30:0:1156:C:H6 | 1.99 | 0.46 |
| 30:0:1115:U:O2' | 30:0:1116:U:H5' | 2.15 | 0.46 |
| 30:0:1586:G:O2' | 30:0:1587:U:H5' | 2.16 | 0.46 |
| 30:0:1973:A:H2' | 30:0:1974:G:O4' | 2.15 | 0.46 |
| 30:0:2252:A:C6 | 30:0:2253:G:H1' | 2.51 | 0.46 |
| 30:0:1130:U:H2' | 30:0:1131:G:O4' | 2.16 | 0.46 |
| 1:A:6:GLY:O | 30:0:1861:C:H4' | 2.15 | 0.46 |
| 9:I:78:ALA:HB1 | 9:I:93:ALA:HB1 | 1.96 | 0.46 |
| 30:0:2366:C:O5' | 30:0:2366:C:H6 | 1.99 | 0.46 |
| 31:9:20:G:O2' | 31:9:21:G:H5' | 2.16 | 0.46 |
| 23:W:119:HIS:CD2 | 23:W:120:PRO:HD2 | 2.50 | 0.46 |
| 30:0:2385:G:H2' | 30:0:2386:U:H6 | 1.81 | 0.46 |
| 30:0:2710:U:H2' | 30:0:2711:U:C6 | 2.50 | 0.46 |
| 25:Y:133:HIS:HD2 | 38:Y:8884:HOH:O | 1.98 | 0.46 |
| 30:0:2112:A:H2' | 30:0:2113:G:C8 | 2.50 | 0.46 |
| 30:0:2301:A:H5' | 30:0:2302:A:H5' | 1.97 | 0.46 |
| 14:N:110:THR:HB | 14:N:113:SER:OG | 2.16 | 0.46 |
| 30:0:567:U:O2' | 30:0:568:G:H5' | 2.15 | 0.46 |
| 30:0:1598:A:N6 | 35:0:8815:CL:CL | 2.86 | 0.46 |
| 23:W:26:ILE:HB | 38:W:5420:HOH:O | 2.15 | 0.46 |
| 22:V:39:ALA:C | 22:V:41:GLU:H | 2.20 | 0.46 |
| 30:0:440:C:H2' | 30:0:441:A:C8 | 2.51 | 0.46 |
| 30:0:999:C:H2' | 30:0:1000:C:O4' | 2.16 | 0.46 |
| 30:0:1930:A:H2' | 30:0:1931:A:C8 | 2.51 | 0.46 |
| 30:0:1445:G:N2 | 30:0:1678:A:H1' | 2.31 | 0.46 |
| 4:D:131:THR:HG21 | 30:0:2348:C:H1' | 1.96 | 0.46 |
| 16:P:73:HIS:HE1 | 30:0:1789:G:O6 | 1.98 | 0.46 |
| 30:0:417:G:P | 38:0:7458:HOH:O | 2.73 | 0.46 |
| 4:D:75:LEU:HD22 | 4:D:79:MET:HB3 | 1.98 | 0.46 |
| 10:J:54:VAL:HG11 | 10:J:138:THR:HG21 | 1.98 | 0.46 |
| 2:B:140:LEU:HD12 | 2:B:174:ARG:HG3 | 1.97 | 0.46 |
| 30:0:2831:C:C2' | 30:0:2832:C:H5' | 2.46 | 0.46 |
| 18:R:82:GLU:HG3 | 18:R:83:LYS:N | 2.30 | 0.46 |
| 1:A:95:PRO:HA | 1:A:153:ARG:HA | 1.97 | 0.45 |
| 9:I:112:LEU:HG | 30:0:1162:G:O2' | 2.15 | 0.45 |
| 30:0:253:U:H1' | 30:0:256:C:H41 | 1.80 | 0.45 |
| 26:Z:46:SER:O | 26:Z:50:VAL:HG23 | 2.16 | 0.45 |
| 30:0:1169:U:C5 | 30:0:1170:U:C4 | 3.03 | 0.45 |
| 28:2:28:LYS:O | 30:0:87:C:H2' | 2.16 | 0.45 |
| 6:F:53:ASP:OD1 | 6:F:80:GLN:HB2 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 30:0:1456:C:H2' | 30:0:1457:U:C6 | 2.50 | 0.45 |
| 30:0:2299:G:C6 | 30:0:2300:A:C6 | 3.05 | 0.45 |
| 30:0:282:C:H1' | 30:0:368:C:H41 | 1.74 | 0.45 |
| 23:W:88:THR:HG21 | 23:W:96:LEU:HD13 | 1.98 | 0.45 |
| 13:M:90:ARG:NH2 | 30:0:2266:A:OP2 | 2.49 | 0.45 |
| 30:0:2604:A:H5' | 38:0:5810:HOH:O | 2.16 | 0.45 |
| 25:Y:177:LYS:HD3 | 25:Y:181:GLY:O | 2.17 | 0.45 |
| 30:0:1896:G:C5 | 30:0:1897:U:C5 | 3.04 | 0.45 |
| 30:0:861:A:H4' | 30:0:1697:G:C4' | 2.47 | 0.45 |
| 30:0:1669:G:O2' | 30:0:1670:A:H5' | 2.16 | 0.45 |
| 30:0:123:U:O2' | 30:0:124:C:H5' | 2.16 | 0.45 |
| 23:W:56:GLU:O | 23:W:143:THR:HG23 | 2.16 | 0.45 |
| 16:P:36:THR:O | 16:P:39:ASP:HB2 | 2.16 | 0.45 |
| 30:0:851:C:O2 | 30:0:2022:A:H2 | 1.99 | 0.45 |
| 30:0:2869:G:H2' | 30:0:2870:C:C6 | 2.51 | 0.45 |
| 14:N:37:ARG:HD3 | 35:N:8807:CL:CL | 2.54 | 0.45 |
| 30:0:1188:A:C5 | 30:0:1189:A:C2 | 3.03 | 0.45 |
| 30:0:2712:G:O2' | 30:0:2713:G:H5' | 2.16 | 0.45 |
| 20:T:26:THR:HA | 20:T:39:ASN:HB3 | 1.98 | 0.45 |
| 30:0:2421:G:H4' | 38:0:4797:HOH:O | 2.16 | 0.45 |
| 30:0:1314:U:H5'' | 30:0:1316:G:O4' | 2.16 | 0.45 |
| 31:9:39:U:C2' | 31:9:40:C:OP1 | 2.65 | 0.45 |
| 4:D:76:ARG:NE | 31:9:44:A:O4' | 2.49 | 0.45 |
| 22:V:39:ALA:N | 22:V:40:PRO:CD | 2.80 | 0.45 |
| 30:0:1788:U:C2 | 30:0:1805:G:N2 | 2.84 | 0.45 |
| 1:A:109:GLU:HG2 | 1:A:116:GLY:N | 2.30 | 0.45 |
| 1:A:217:ARG:HH11 | 1:A:217:ARG:HG3 | 1.79 | 0.45 |
| 3:C:206:ASN:HB2 | 30:0:329:A:OP2 | 2.16 | 0.45 |
| 15:O:32:ARG:HE | 15:O:35:LYS:HD2 | 1.81 | 0.45 |
| 30:0:2664:A:H8 | 30:0:2664:A:OP1 | 1.99 | 0.45 |
| 30:0:1309:U:O2' | 30:0:1310:U:H5' | 2.16 | 0.45 |
| 30:0:1506:U:H5' | 30:0:1506:U:H6 | 1.82 | 0.45 |
| 14:N:44:ARG:HG3 | 14:N:45:ALA:N | 2.32 | 0.45 |
| 3:C:93:LYS:O | 3:C:98:ARG:NH2 | 2.49 | 0.45 |
| 8:H:52:LEU:HB3 | 8:H:137:PHE:HB2 | 1.99 | 0.45 |
| 30:0:1189:A:C3' | 38:0:7717:HOH:O | 2.59 | 0.45 |
| 17:Q:40:HIS:HE1 | 30:0:949:U:O2' | 1.99 | 0.45 |
| 30:0:1790:C:H2' | 30:0:1791:U:C6 | 2.51 | 0.45 |
| 31:9:110:G:C5 | 31:9:111:U:C5 | 3.04 | 0.45 |
| 30:0:397:A:O2' | 30:0:417:G:N3 | 2.39 | 0.45 |
| 30:0:2594:C:O2' | 30:0:2595:U:H5' | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 30:0:228:C:H2' | 30:0:229:G:H5' | 1.98 | 0.45 |
| 30:0:1116:U:H2' | 30:0:1118:A:C2 | 2.52 | 0.45 |
| 9:I:121:LYS:HB3 | 30:0:1184:C:H4' | 1.97 | 0.45 |
| 3:C:129:HIS:HE1 | 3:C:231:ARG:HA | 1.78 | 0.45 |
| 11:K:81:ARG:HD3 | 11:K:87:ARG:NH1 | 2.31 | 0.45 |
| 16:P:55:LYS:HD3 | 30:0:1716:A:H4' | 1.97 | 0.45 |
| 18:R:128:ARG:HH12 | 30:0:840:U:H2' | 1.80 | 0.45 |
| 23:W:6:GLN:CB | 23:W:26:ILE:HD11 | 2.45 | 0.45 |
| 30:0:482:G:O4' | 30:0:511:A:C2 | 2.70 | 0.45 |
| 4:D:23:VAL:HG12 | 4:D:130:VAL:HG22 | 1.98 | 0.45 |
| 30:0:1002:G:H2' | 30:0:1003:U:O5' | 2.17 | 0.45 |
| 30:0:1398:G:O2' | 30:0:1399:A:H5' | 2.16 | 0.45 |
| 28:2:8:LYS:NZ | 30:0:1677:U:OP2 | 2.43 | 0.45 |
| 30:0:2332:A:H5' | 30:0:2333:G:OP2 | 2.17 | 0.45 |
| 30:0:955:A:C2 | 30:0:1013:A:C4 | 3.05 | 0.45 |
| 30:0:1563:G:H4' | 38:0:4241:HOH:O | 2.16 | 0.45 |
| 30:0:158:A:C2' | 30:0:159:G:H5' | 2.47 | 0.45 |
| 3:C:236:THR:H | 3:C:239:ALA:HB3 | 1.80 | 0.45 |
| 17:Q:11:ARG:HG3 | 30:0:2363:G:O2' | 2.16 | 0.45 |
| 13:M:179:GLY:O | 30:0:399:C:H5' | 2.17 | 0.45 |
| 30:0:1964:U:C2 | 30:0:1965:C:C5 | 3.05 | 0.45 |
| 30:0:228:C:C2' | 30:0:229:G:H5' | 2.46 | 0.45 |
| 30:0:1023:C:H2' | 30:0:1024:G:O4' | 2.16 | 0.45 |
| 9:I:87:PRO:HG3 | 38:0:7157:HOH:O | 2.17 | 0.45 |
| 30:0:1503:U:H2' | 30:0:1504:A:O4' | 2.16 | 0.45 |
| 3:C:35:VAL:HG21 | 3:C:227:GLY:HA2 | 1.98 | 0.45 |
| 6:F:72:VAL:HA | 6:F:73:PRO:HD3 | 1.87 | 0.45 |
| 2:B:162:MET:HE2 | 2:B:310:ARG:HD3 | 1.99 | 0.45 |
| 12:L:30:ARG:HD2 | 30:0:164:G:H5'' | 1.99 | 0.45 |
| 24:X:30:MET:HG2 | 30:0:1384:C:H5' | 1.98 | 0.45 |
| 31:9:60:C:H2' | 31:9:61:C:H6 | 1.81 | 0.45 |
| 25:Y:99:ALA:HB2 | 25:Y:233:TYR:CE2 | 2.51 | 0.45 |
| 30:0:1921:A:O2' | 30:0:1922:A:H5' | 2.17 | 0.45 |
| 23:W:29:VAL:O | 23:W:30:ASN:HB2 | 2.16 | 0.45 |
| 30:0:685:C:O2 | 30:0:748:C:H4' | 2.17 | 0.45 |
| 30:0:559:U:H3' | 30:0:559:U:C6 | 2.52 | 0.45 |
| 30:0:2251:G:H2' | 30:0:2252:A:H8 | 1.79 | 0.45 |
| 30:0:1573:A:N7 | 30:0:1574:C:C2 | 2.85 | 0.45 |
| 30:0:2793:A:H2' | 30:0:2794:G:H5' | 1.98 | 0.45 |
| 19:S:6:LYS:HB2 | 19:S:27:ALA:O | 2.17 | 0.45 |
| 38:3:9030:HOH:O | 30:0:2382:A:H5' | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 14:N:41:LYS:HD3 | 38:9:9060:HOH:O | 2.17 | 0.45 |
| 4:D:15:GLU:HA | 4:D:16:PRO:HD3 | 1.78 | 0.45 |
| 30:0:2316:G:OP1 | 30:0:2317:C:H1' | 2.16 | 0.45 |
| 3:C:127:ARG:HD3 | 3:C:129:HIS:CE1 | 2.52 | 0.45 |
| 30:0:2419:U:H5'' | 30:0:2420:G:C5' | 2.46 | 0.45 |
| 23:W:69:ARG:HD2 | 23:W:117:ARG:O | 2.16 | 0.45 |
| 30:0:962:C:C2' | 30:0:963:C:H5' | 2.47 | 0.45 |
| 28:2:22:PRO:HG2 | 28:2:25:VAL:CG2 | 2.47 | 0.45 |
| 30:0:2897:C:O2' | 30:0:2898:G:H5' | 2.17 | 0.45 |
| 17:Q:3:SER:HB3 | 38:Q:5998:HOH:O | 2.16 | 0.45 |
| 14:N:169:PRO:O | 14:N:172:PHE:HB3 | 2.17 | 0.45 |
| 2:B:199:TYR:HE2 | 2:B:268:ARG:HB2 | 1.82 | 0.45 |
| 26:Z:45:VAL:HG12 | 38:Z:8714:HOH:O | 2.17 | 0.45 |
| 5:E:10:ASP:HA | 38:E:6017:HOH:O | 2.17 | 0.45 |
| 10:J:52:GLN:HE22 | 30:0:1119:G:H8 | 1.65 | 0.45 |
| 30:0:1700:C:H5'' | 30:0:1701:A:OP2 | 2.16 | 0.45 |
| 23:W:119:HIS:CG | 38:0:5308:HOH:O | 2.69 | 0.45 |
| 30:0:2002:C:C2' | 30:0:2003:U:H5' | 2.46 | 0.45 |
| 30:0:1120:U:H6 | 30:0:1120:U:H5'' | 1.81 | 0.45 |
| 29:3:11:CYS:HB2 | 29:3:20:HIS:HE1 | 1.81 | 0.45 |
| 30:0:1268:C:H2' | 30:0:1269:G:C8 | 2.51 | 0.45 |
| 9:I:108:HIS:H | 9:I:109:PRO:HD2 | 1.82 | 0.45 |
| 5:E:23:GLU:HG2 | 5:E:28:SER:HB3 | 1.98 | 0.45 |
| 30:0:249:G:O2' | 30:0:250:C:H5' | 2.17 | 0.45 |
| 30:0:1209:C:O2' | 30:0:1210:G:H5' | 2.16 | 0.44 |
| 23:W:88:THR:HG22 | 23:W:90:TYR:CD1 | 2.50 | 0.44 |
| 8:H:61:ARG:HG3 | 8:H:61:ARG:HH11 | 1.83 | 0.44 |
| 12:L:53:ARG:NH2 | 12:L:57:VAL:HG12 | 2.31 | 0.44 |
| 30:0:1904:A:H2' | 30:0:1905:U:O4' | 2.17 | 0.44 |
| 23:W:68:THR:HG23 | 23:W:69:ARG:HG2 | 1.99 | 0.44 |
| 30:0:2831:C:H2' | 30:0:2832:C:H5' | 1.98 | 0.44 |
| 4:D:140:ARG:HH11 | 4:D:140:ARG:HG3 | 1.82 | 0.44 |
| 30:0:62:C:C4 | 30:0:63:U:C4 | 3.05 | 0.44 |
| 30:0:81:G:N3 | 30:0:98:A:C2 | 2.85 | 0.44 |
| 13:M:6:SER:O | 13:M:10:ASP:HB2 | 2.17 | 0.44 |
| 14:N:43:VAL:HG13 | 14:N:118:ILE:HD11 | 1.98 | 0.44 |
| 30:0:2070:G:H2' | 30:0:2072:G:OP1 | 2.17 | 0.44 |
| 30:0:2103:A:N6 | 30:0:2538:A:H8 | 2.09 | 0.44 |
| 30:0:1524:U:H5'' | 30:0:1524:U:C6 | 2.52 | 0.44 |
| 27:1:28:HIS:CD2 | 27:1:31:LYS:HG3 | 2.52 | 0.44 |
| 30:0:812:A:H2' | 30:0:813:C:C6 | 2.52 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 30:0:920:C:H4' | 30:0:921:G:N2 | 2.32 | 0.44 |
| 3:C:54:LEU:HD23 | 3:C:79:ARG:HG3 | 1.99 | 0.44 |
| 30:0:177:A:H2' | 30:0:178:U:O4' | 2.16 | 0.44 |
| 30:0:2072:G:H3' | 30:0:2073:G:C5' | 2.47 | 0.44 |
| 26:Z:61:HIS:O | 26:Z:69:ASP:HA | 2.18 | 0.44 |
| 28:2:43:ARG:NH2 | 30:0:1684:A:H1' | 2.25 | 0.44 |
| 14:N:25:ARG:HG2 | 30:0:2416:G:O2' | 2.17 | 0.44 |
| 30:0:1626:A:H2' | 30:0:1627:G:C5' | 2.48 | 0.44 |
| 30:0:2329:C:H2' | 30:0:2330:U:C6 | 2.52 | 0.44 |
| 31:9:59:C:C4 | 31:9:60:C:N4 | 2.86 | 0.44 |
| 5:E:72:MET:O | 5:E:76:VAL:HG22 | 2.18 | 0.44 |
| 11:K:89:LYS:HE2 | 21:U:19:THR:HG21 | 2.00 | 0.44 |
| 31:9:97:U:O2' | 31:9:98:C:H5' | 2.18 | 0.44 |
| 30:0:2297:U:H1' | 38:0:5197:HOH:O | 2.17 | 0.44 |
| 21:U:37:GLU:HB3 | 38:U:408:HOH:O | 2.18 | 0.44 |
| 1:A:212:PRO:HA | 30:0:1943:C:O4' | 2.18 | 0.44 |
| 1:A:204:GLY:N | 30:0:2634:G:OP2 | 2.51 | 0.44 |
| 24:X:47:ALA:HB1 | 24:X:82:GLU:HB3 | 2.00 | 0.44 |
| 1:A:88:ILE:HD13 | 1:A:100:PRO:HD3 | 1.99 | 0.44 |
| 5:E:19:ASP:HA | 5:E:31:ARG:O | 2.17 | 0.44 |
| 30:0:130:C:H2' | 38:0:3168:HOH:O | 2.17 | 0.44 |
| 30:0:1712:A:H2' | 30:0:1713:G:O4' | 2.18 | 0.44 |
| 3:C:168:ARG:NH2 | 3:C:190:ALA:O | 2.51 | 0.44 |
| 30:0:1190:G:H2' | 38:0:4068:HOH:O | 2.15 | 0.44 |
| 7:G:67:LEU:O | 7:G:71:LEU:HG | 2.18 | 0.44 |
| 13:M:167:GLY:O | 13:M:171:ARG:HG3 | 2.17 | 0.44 |
| 30:0:506:G:N2 | 30:0:509:A:H5'' | 2.30 | 0.44 |
| 30:0:559:U:C4 | 30:0:560:U:C4 | 3.06 | 0.44 |
| 30:0:2104:C:O2 | 30:0:2485:A:N1 | 2.50 | 0.44 |
| 23:W:90:TYR:N | 23:W:90:TYR:CD1 | 2.85 | 0.44 |
| 30:0:2135:A:C2' | 30:0:2136:G:H5' | 2.47 | 0.44 |
| 30:0:1592:G:H2' | 30:0:1593:C:C6 | 2.52 | 0.44 |
| 30:0:1523:G:H2' | 30:0:1524:U:O4' | 2.17 | 0.44 |
| 7:G:64:ASN:N | 7:G:64:ASN:ND2 | 2.66 | 0.44 |
| 1:A:171:LYS:HB2 | 30:0:820:G:C5 | 2.53 | 0.44 |
| 30:0:1902:G:O2' | 30:0:1903:U:H5' | 2.17 | 0.44 |
| 26:Z:78:ILE:HD12 | 38:Z:8717:HOH:O | 2.18 | 0.44 |
| 30:0:1947:G:N2 | 30:0:1965:C:O2 | 2.50 | 0.44 |
| 30:0:1447:U:H3' | 30:0:1506:U:O2 | 2.18 | 0.44 |
| 10:J:39:VAL:HG13 | 10:J:106:GLY:O | 2.17 | 0.44 |
| 30:0:858:U:H2' | 30:0:859:C:C6 | 2.52 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 30:0:677:C:O2' | 30:0:678:G:H5' | 2.17 | 0.44 |
| 5:E:20:ILE:HD11 | 5:E:40:VAL:HG11 | 1.99 | 0.44 |
| 12:L:43:HIS:HD2 | 38:L:8827:HOH:O | 2.00 | 0.44 |
| 30:0:1173:A:H3' | 38:0:4358:HOH:O | 2.16 | 0.44 |
| 30:0:1166:A:OP1 | 30:0:1174:A:H4' | 2.17 | 0.44 |
| 30:0:1182:C:C1' | 30:0:1192:A:C8 | 3.01 | 0.44 |
| 30:0:735:C:H5 | 30:0:736:A:C4 | 2.36 | 0.44 |
| 29:3:48:ASN:ND2 | 30:0:169:A:H1' | 2.33 | 0.44 |
| 11:K:125:ALA:C | 11:K:127:ALA:H | 2.21 | 0.44 |
| 14:N:139:TRP:HA | 14:N:139:TRP:HE3 | 1.81 | 0.44 |
| 30:0:255:A:C4 | 30:0:256:C:C6 | 3.06 | 0.44 |
| 30:0:128:A:C8 | 30:0:128:A:C3' | 3.01 | 0.44 |
| 30:0:594:C:C4 | 30:0:595:U:C4 | 3.06 | 0.44 |
| 5:E:170:ARG:NH2 | 38:E:4761:HOH:O | 2.50 | 0.44 |
| 30:0:113:A:OP2 | 30:0:114:A:H2' | 2.17 | 0.44 |
| 4:D:41:LEU:HA | 4:D:44:ILE:HG22 | 1.99 | 0.44 |
| 30:0:295:C:H2' | 30:0:296:G:O4' | 2.18 | 0.44 |
| 30:0:39:G:N2 | 30:0:444:C:C2 | 2.86 | 0.44 |
| 30:0:1825:U:O2' | 30:0:1826:C:H5' | 2.18 | 0.44 |
| 30:0:645:U:O2 | 30:0:761:A:H2 | 2.00 | 0.44 |
| 30:0:1052:G:H2' | 30:0:1052:G:N3 | 2.31 | 0.44 |
| 20:T:28:SER:HA | 20:T:97:ARG:HD3 | 2.00 | 0.44 |
| 1:A:199:HIS:HE1 | 30:0:1881:A:OP1 | 2.01 | 0.44 |
| 30:0:1318:A:H4' | 30:0:1343:C:H4' | 2.00 | 0.44 |
| 1:A:179:MET:HG2 | 1:A:186:TRP:CB | 2.48 | 0.44 |
| 1:A:94:LEU:HD12 | 1:A:98:GLU:HB2 | 2.00 | 0.44 |
| 30:0:1503:U:C2' | 30:0:1504:A:H5' | 2.48 | 0.44 |
| 24:X:25:ARG:HD2 | 38:X:5356:HOH:O | 2.16 | 0.44 |
| 30:0:1226:G:H5' | 38:0:4543:HOH:O | 2.18 | 0.44 |
| 30:0:2087:C:O2' | 30:0:2088:C:H5' | 2.18 | 0.44 |
| 13:M:80:GLY:O | 13:M:81:ARG:HD2 | 2.17 | 0.44 |
| 30:0:1180:U:H2' | 30:0:1181:A:O4' | 2.18 | 0.44 |
| 30:0:307:G:H3' | 38:0:6719:HOH:O | 2.18 | 0.44 |
| 31:9:2:U:H4' | 38:9:9103:HOH:O | 2.18 | 0.44 |
| 11:K:98:VAL:HG11 | 11:K:102:GLU:HA | 1.98 | 0.44 |
| 18:R:104:PHE:HB3 | 18:R:109:MET:HE1 | 2.00 | 0.44 |
| 2:B:304:PRO:HD2 | 2:B:307:ARG:NE | 2.33 | 0.44 |
| 30:0:734:U:H2' | 30:0:736:A:OP2 | 2.18 | 0.44 |
| 12:L:113:GLN:O | 30:0:700:A:N6 | 2.47 | 0.44 |
| 15:O:105:ASN:HD21 | 15:O:109:SER:H | 1.65 | 0.44 |
| 8:H:39:LYS:HD2 | 30:0:969:G:H5' | 1.98 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 30:0:1882:C:H2' | 30:0:1883:U:H6 | 1.83 | 0.44 |
| 30:0:729:C:C2 | 30:0:743:G:C2 | 3.06 | 0.44 |
| 30:0:1553:C:O5' | 30:0:1553:C:H6 | 2.00 | 0.44 |
| 30:0:1135:G:H5' | 38:0:5953:HOH:O | 2.17 | 0.44 |
| 30:0:696:C:O2' | 30:0:697:G:H5' | 2.17 | 0.44 |
| 5:E:112:ALA:HA | 5:E:113:PRO:HD3 | 1.85 | 0.44 |
| 6:F:1:PRO:H3 | 6:F:4:VAL:HG23 | 1.83 | 0.44 |
| 30:0:2533:C:O2' | 30:0:2534:C:H5' | 2.18 | 0.44 |
| 30:0:2256:G:C6 | 30:0:2257:G:C4 | 3.05 | 0.44 |
| 8:H:29:SER:HA | 8:H:62:HIS:HD2 | 1.82 | 0.44 |
| 30:0:1279:U:O2 | 30:0:1279:U:C2' | 2.64 | 0.44 |
| 30:0:812:A:H2' | 30:0:813:C:O4' | 2.17 | 0.44 |
| 26:Z:66:CYS:SG | 26:Z:68:GLU:HB2 | 2.58 | 0.44 |
| 4:D:52:THR:HG21 | 30:0:2346:C:O2' | 2.17 | 0.44 |
| 30:0:935:G:O2' | 30:0:936:C:H5' | 2.18 | 0.44 |
| 6:F:59:ILE:HD13 | 30:0:263:U:O4' | 2.17 | 0.44 |
| 4:D:167:GLU:C | 4:D:169:THR:H | 2.21 | 0.44 |
| 30:0:2914:A:H5'' | 30:0:2914:A:H8 | 1.83 | 0.44 |
| 30:0:553:G:O4' | 30:0:1325:G:H5' | 2.18 | 0.43 |
| 1:A:191:GLY:HA2 | 1:A:194:MET:HE2 | 1.99 | 0.43 |
| 30:0:2796:U:H2' | 30:0:2797:C:O5' | 2.18 | 0.43 |
| 30:0:1342:C:H2' | 30:0:1343:C:H5' | 2.00 | 0.43 |
| 24:X:23:HIS:CD2 | 24:X:24:LYS:HG3 | 2.53 | 0.43 |
| 30:0:1444:G:O2' | 30:0:1445:G:H5' | 2.18 | 0.43 |
| 14:N:143:ARG:HG2 | 14:N:172:PHE:CD2 | 2.52 | 0.43 |
| 8:H:139:ALA:HB3 | 8:H:149:VAL:HG21 | 2.00 | 0.43 |
| 30:0:1386:G:O2' | 30:0:1387:G:H5' | 2.18 | 0.43 |
| 13:M:47:ASP:CG | 13:M:48:LYS:N | 2.71 | 0.43 |
| 30:0:629:A:H2' | 30:0:630:A:O4' | 2.18 | 0.43 |
| 15:O:47:ARG:HG3 | 15:O:47:ARG:HH11 | 1.82 | 0.43 |
| 30:0:544:G:C3' | 30:0:545:G:H5'' | 2.46 | 0.43 |
| 30:0:2717:C:C2' | 30:0:2718:C:C5' | 2.81 | 0.43 |
| 30:0:282:C:C2' | 30:0:283:U:H5' | 2.47 | 0.43 |
| 17:Q:26:PRO:O | 17:Q:30:VAL:HG23 | 2.17 | 0.43 |
| 17:Q:28:ARG:HG2 | 38:9:9079:HOH:O | 2.17 | 0.43 |
| 12:L:71:GLU:HG2 | 30:0:700:A:C2 | 2.54 | 0.43 |
| 1:A:48:ASP:HB3 | 38:A:9061:HOH:O | 2.18 | 0.43 |
| 30:0:238:C:H4' | 30:0:287:C:OP1 | 2.18 | 0.43 |
| 5:E:8:PRO:HB2 | 5:E:11:VAL:HG23 | 1.99 | 0.43 |
| 30:0:2332:A:H3' | 30:0:2333:G:H8 | 1.83 | 0.43 |
| 30:0:696:C:O2' | 30:0:731:U:OP1 | 2.35 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:O:44:ASN:OD1 | 15:O:65:LEU:HB2 | 2.18 | 0.43 |
| 16:P:100:ALA:HA | 38:O:5526:HOH:O | 2.17 | 0.43 |
| 30:O:1705:C:O2 | 30:O:2735:U:H5'' | 2.18 | 0.43 |
| 30:O:2761:A:C4 | 30:O:2763:G:C8 | 3.06 | 0.43 |
| 30:O:1181:A:H2' | 30:O:1182:C:C5' | 2.49 | 0.43 |
| 20:T:52:ARG:O | 30:O:317:A:OP1 | 2.36 | 0.43 |
| 25:Y:126:PRO:HG2 | 25:Y:128:PHE:CZ | 2.53 | 0.43 |
| 16:P:7:LYS:HD3 | 16:P:21:VAL:CG2 | 2.47 | 0.43 |
| 2:B:232:TRP:CD1 | 2:B:235:ARG:HD2 | 2.52 | 0.43 |
| 9:I:120:ALA:O | 9:I:124:VAL:HG23 | 2.18 | 0.43 |
| 30:O:312:U:C2 | 30:O:320:G:N2 | 2.87 | 0.43 |
| 24:X:34:ARG:NH1 | 24:X:48:VAL:O | 2.51 | 0.43 |
| 30:O:1098:A:H2' | 30:O:1099:G:O4' | 2.18 | 0.43 |
| 20:T:53:GLY:HA3 | 38:T:6384:HOH:O | 2.19 | 0.43 |
| 30:O:483:C:N4 | 30:O:484:A:C6 | 2.87 | 0.43 |
| 30:O:1889:C:O2' | 30:O:1890:U:H5' | 2.18 | 0.43 |
| 30:O:2491:G:H5' | 38:O:9387:HOH:O | 2.19 | 0.43 |
| 6:F:57:GLU:O | 6:F:61:MET:HG3 | 2.18 | 0.43 |
| 1:A:36:ASP:CB | 1:A:85:SER:H | 2.31 | 0.43 |
| 30:O:815:U:O2' | 30:O:1598:A:H4' | 2.19 | 0.43 |
| 23:W:44:MET:HE2 | 30:O:944:G:H21 | 1.83 | 0.43 |
| 13:M:188:ARG:HH11 | 30:O:154:C:H3' | 1.82 | 0.43 |
| 1:A:187:PRO:HB2 | 30:O:1845:A:O3' | 2.19 | 0.43 |
| 30:O:1622:G:C2' | 30:O:1623:C:H5' | 2.48 | 0.43 |
| 30:O:300:U:C2 | 30:O:301:C:C6 | 3.06 | 0.43 |
| 24:X:15:ARG:HH22 | 30:O:2856:A:P | 2.41 | 0.43 |
| 2:B:329:TYR:CE2 | 21:U:15:PRO:HG2 | 2.53 | 0.43 |
| 17:Q:45:PRO:O | 30:O:2365:G:H4' | 2.18 | 0.43 |
| 30:O:912:A:C4 | 30:O:1294:A:C2 | 3.05 | 0.43 |
| 10:J:60:ARG:NH2 | 30:O:1242:A:OP2 | 2.45 | 0.43 |
| 2:B:162:MET:CE | 2:B:310:ARG:HD3 | 2.48 | 0.43 |
| 30:O:2421:G:H3' | 30:O:2422:U:C5' | 2.48 | 0.43 |
| 30:O:2819:C:H2' | 30:O:2820:A:C8 | 2.53 | 0.43 |
| 29:3:70:ARG:HD3 | 38:3:9064:HOH:O | 2.18 | 0.43 |
| 4:D:103:ASN:ND2 | 4:D:133:ASN:HA | 2.33 | 0.43 |
| 18:R:104:PHE:CB | 18:R:109:MET:HE1 | 2.48 | 0.43 |
| 14:N:7:LYS:HB3 | 17:Q:21:ARG:NH2 | 2.33 | 0.43 |
| 25:Y:144:ARG:NE | 38:Y:8914:HOH:O | 2.52 | 0.43 |
| 30:O:962:C:H5'' | 38:O:4933:HOH:O | 2.19 | 0.43 |
| 13:M:147:LEU:O | 13:M:150:ILE:HG22 | 2.18 | 0.43 |
| 30:O:2247:C:O2' | 30:O:2248:C:H5' | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:M:158:ARG:HB2 | 13:M:163:LEU:HB2 | 2.01 | 0.43 |
| 30:0:844:A:C6 | 30:0:882:A:C5 | 3.06 | 0.43 |
| 30:0:213:G:N2 | 30:0:225:G:H2' | 2.34 | 0.43 |
| 23:W:88:THR:CG2 | 23:W:90:TYR:HD1 | 2.32 | 0.43 |
| 30:0:2727:A:N1 | 30:0:2756:U:C2 | 2.87 | 0.43 |
| 17:Q:25:PRO:HA | 17:Q:26:PRO:HD3 | 1.79 | 0.43 |
| 30:0:1735:C:O2' | 30:0:1736:A:H5' | 2.18 | 0.43 |
| 27:1:25:LYS:O | 27:1:25:LYS:HG2 | 2.19 | 0.43 |
| 12:L:6:ARG:NH1 | 30:0:1299:G:N7 | 2.67 | 0.43 |
| 30:0:2869:G:H5' | 38:0:5515:HOH:O | 2.18 | 0.43 |
| 23:W:134:GLU:OE2 | 31:9:97:U:H1' | 2.19 | 0.43 |
| 30:0:1482:A:H1' | 38:0:9428:HOH:O | 2.18 | 0.43 |
| 30:0:653:U:H2' | 30:0:654:A:C8 | 2.53 | 0.43 |
| 30:0:1842:A:C4 | 30:0:1979:G:C6 | 3.06 | 0.43 |
| 30:0:2566:A:C2 | 30:0:2696:G:O4' | 2.71 | 0.43 |
| 1:A:9:ARG:HG2 | 1:A:16:PHE:CD2 | 2.54 | 0.43 |
| 30:0:451:C:O2' | 30:0:452:G:H5' | 2.18 | 0.43 |
| 30:0:2812:A:H2 | 30:0:2814:A:N6 | 1.86 | 0.43 |
| 30:0:1165:G:H1' | 30:0:1174:A:O2' | 2.19 | 0.43 |
| 30:0:1184:C:O2' | 30:0:1185:U:OP2 | 2.33 | 0.43 |
| 30:0:1684:A:O2' | 30:0:1685:A:H5'' | 2.18 | 0.43 |
| 31:9:1:U:C4' | 31:9:3:A:OP1 | 2.67 | 0.43 |
| 5:E:101:GLU:HB2 | 5:E:116:THR:O | 2.18 | 0.43 |
| 11:K:74:VAL:HG13 | 11:K:113:ILE:HG23 | 2.01 | 0.43 |
| 28:2:40:ARG:HD2 | 28:2:47:THR:HG22 | 1.99 | 0.43 |
| 30:0:1524:U:H5'' | 30:0:1524:U:H6 | 1.84 | 0.43 |
| 30:0:1477:C:C5' | 30:0:1868:G:H5'' | 2.48 | 0.43 |
| 30:0:2664:A:C8 | 30:0:2664:A:OP1 | 2.72 | 0.43 |
| 30:0:629:A:C2 | 30:0:2074:A:C2 | 3.07 | 0.43 |
| 13:M:193:LYS:HB3 | 30:0:392:U:H4' | 2.00 | 0.43 |
| 29:3:28:GLY:HA3 | 30:0:2435:U:OP1 | 2.18 | 0.43 |
| 30:0:2075:G:C6 | 30:0:2076:U:C4 | 3.07 | 0.43 |
| 30:0:1248:A:H3' | 38:0:7547:HOH:O | 2.17 | 0.43 |
| 31:9:88:G:N2 | 31:9:89:C:C2 | 2.87 | 0.43 |
| 18:R:124:GLY:HA3 | 18:R:136:TRP:O | 2.18 | 0.43 |
| 30:0:191:A:C4 | 30:0:237:G:N7 | 2.87 | 0.43 |
| 10:J:75:PRO:HD3 | 10:J:136:SER:OG | 2.19 | 0.43 |
| 30:0:111:C:H2' | 30:0:112:G:O4' | 2.18 | 0.43 |
| 12:L:143:THR:HG21 | 38:L:8839:HOH:O | 2.17 | 0.43 |
| 30:0:1882:C:H2' | 30:0:1883:U:C6 | 2.53 | 0.43 |
| 30:0:1482:A:O2' | 30:0:1483:C:H5' | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 30:0:1545:C:H2' | 30:0:1546:G:O4' | 2.18 | 0.43 |
| 8:H:46:TYR:HA | 8:H:47:PRO:HD3 | 1.82 | 0.43 |
| 30:0:1157:C:O2' | 30:0:1158:G:H5' | 2.18 | 0.43 |
| 11:K:41:LYS:HA | 30:0:2582:G:O3' | 2.19 | 0.43 |
| 30:0:212:A:O3' | 30:0:213:G:H4' | 2.19 | 0.43 |
| 30:0:2255:A:O2' | 30:0:2256:G:H5' | 2.18 | 0.43 |
| 13:M:24:GLN:NE2 | 13:M:27:ARG:NH1 | 2.67 | 0.43 |
| 30:0:1132:A:H61 | 30:0:1229:C:H2' | 1.83 | 0.43 |
| 30:0:1819:G:H2' | 30:0:1820:G:H5' | 2.01 | 0.43 |
| 30:0:2096:A:H2' | 30:0:2539:U:O4' | 2.19 | 0.43 |
| 25:Y:125:LYS:HB2 | 25:Y:126:PRO:HD2 | 2.00 | 0.43 |
| 30:0:1883:U:H5' | 30:0:2012:U:OP2 | 2.18 | 0.43 |
| 5:E:40:VAL:HA | 5:E:48:VAL:O | 2.19 | 0.43 |
| 30:0:47:G:N3 | 30:0:114:A:C2 | 2.87 | 0.43 |
| 30:0:2456:A:H2' | 30:0:2457:U:C6 | 2.54 | 0.43 |
| 30:0:1176:C:N4 | 38:0:9957:HOH:O | 2.52 | 0.43 |
| 26:Z:43:GLY:O | 26:Z:47:ARG:HG2 | 2.19 | 0.43 |
| 30:0:1815:A:H4' | 30:0:2751:C:O4' | 2.19 | 0.43 |
| 30:0:722:G:H22 | 30:0:938:G:P | 2.42 | 0.43 |
| 6:F:48:VAL:CG2 | 6:F:74:PHE:HB3 | 2.48 | 0.43 |
| 30:0:2482:G:H4' | 30:0:2483:A:C5' | 2.48 | 0.43 |
| 30:0:1029:U:O2' | 30:0:1273:C:OP1 | 2.33 | 0.43 |
| 31:9:2:U:OP2 | 31:9:2:U:H4' | 2.19 | 0.43 |
| 6:F:57:GLU:HB2 | 13:M:23:LEU:HD11 | 1.99 | 0.43 |
| 14:N:11:ARG:NH1 | 31:9:8:G:O6 | 2.52 | 0.43 |
| 21:U:17:THR:CG2 | 21:U:18:GLY:N | 2.82 | 0.43 |
| 30:0:169:A:H5'' | 38:0:9693:HOH:O | 2.18 | 0.43 |
| 30:0:1787:C:O2' | 30:0:1788:U:H5' | 2.19 | 0.43 |
| 30:0:1520:G:C6 | 30:0:1521:C:N4 | 2.87 | 0.43 |
| 30:0:790:A:H2' | 30:0:791:A:O4' | 2.19 | 0.43 |
| 2:B:148:PRO:HD2 | 38:B:9048:HOH:O | 2.19 | 0.43 |
| 6:F:27:GLY:HA3 | 6:F:101:ALA:O | 2.18 | 0.43 |
| 14:N:164:ASP:OD2 | 14:N:168:LEU:HG | 2.19 | 0.43 |
| 30:0:2729:C:O2' | 30:0:2730:G:H5' | 2.19 | 0.43 |
| 14:N:116:PHE:HB3 | 14:N:136:LEU:HD23 | 2.00 | 0.43 |
| 8:H:65:LEU:HD12 | 8:H:65:LEU:HA | 1.84 | 0.43 |
| 31:9:14:G:O2' | 31:9:15:C:H5' | 2.19 | 0.42 |
| 30:0:2756:U:H1' | 38:0:5024:HOH:O | 2.19 | 0.42 |
| 30:0:1315:G:H4' | 30:0:1316:G:OP2 | 2.19 | 0.42 |
| 30:0:365:G:C6 | 30:0:366:U:C4 | 3.07 | 0.42 |
| 30:0:1787:C:C4' | 30:0:2883:A:O4' | 2.67 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 30:0:1521:C:H2' | 30:0:1522:A:H8 | 1.84 | 0.42 |
| 30:0:1044:C:H5'' | 38:0:9030:HOH:O | 2.18 | 0.42 |
| 30:0:1706:G:C5 | 30:0:1707:G:C6 | 3.06 | 0.42 |
| 1:A:6:GLY:HA3 | 38:0:4633:HOH:O | 2.19 | 0.42 |
| 18:R:82:GLU:O | 18:R:86:LYS:HG3 | 2.19 | 0.42 |
| 30:0:1894:C:N4 | 30:0:1939:U:H2' | 2.33 | 0.42 |
| 30:0:2866:U:H4' | 30:0:2867:G:H5' | 2.01 | 0.42 |
| 30:0:85:C:H3' | 30:0:86:A:H2' | 2.01 | 0.42 |
| 30:0:162:C:H2' | 30:0:163:U:H5' | 2.01 | 0.42 |
| 30:0:2026:C:O2' | 30:0:2027:U:H5' | 2.19 | 0.42 |
| 30:0:1189:A:H1' | 30:0:1209:C:H1' | 2.01 | 0.42 |
| 30:0:1741:U:C4 | 30:0:2033:G:C8 | 3.06 | 0.42 |
| 30:0:907:A:H2' | 30:0:908:A:C8 | 2.53 | 0.42 |
| 30:0:1976:G:O2' | 30:0:1977:U:H5' | 2.19 | 0.42 |
| 2:B:112:THR:HG23 | 2:B:158:LYS:HZ1 | 1.84 | 0.42 |
| 30:0:366:U:H2' | 30:0:367:G:O4' | 2.19 | 0.42 |
| 7:G:12:ILE:N | 7:G:13:PRO:HD3 | 2.35 | 0.42 |
| 2:B:232:TRP:HD1 | 2:B:235:ARG:HD2 | 1.83 | 0.42 |
| 30:0:2783:A:H5'' | 38:0:5252:HOH:O | 2.19 | 0.42 |
| 3:C:107:ARG:O | 3:C:111:VAL:HG23 | 2.19 | 0.42 |
| 19:S:10:VAL:HG11 | 22:V:36:ALA:HA | 2.00 | 0.42 |
| 30:0:1603:A:C8 | 30:0:1605:G:C2 | 3.07 | 0.42 |
| 4:D:76:ARG:NH1 | 31:9:42:C:O2 | 2.49 | 0.42 |
| 29:3:71:CYS:SG | 38:3:9052:HOH:O | 2.61 | 0.42 |
| 30:0:255:A:H2' | 30:0:256:C:C6 | 2.54 | 0.42 |
| 10:J:74:ARG:O | 10:J:78:ILE:HG13 | 2.19 | 0.42 |
| 15:O:65:LEU:HD13 | 30:0:746:A:C6 | 2.54 | 0.42 |
| 30:0:844:A:C6 | 30:0:882:A:C6 | 3.07 | 0.42 |
| 26:Z:84:CYS:O | 26:Z:85:ASP:HB2 | 2.19 | 0.42 |
| 30:0:1381:A:N3 | 30:0:1382:G:H1' | 2.34 | 0.42 |
| 5:E:68:HIS:CE1 | 38:0:6506:HOH:O | 2.72 | 0.42 |
| 4:D:104:PHE:CE2 | 4:D:132:VAL:HB | 2.54 | 0.42 |
| 3:C:22:PHE:HA | 3:C:116:ALA:HA | 2.00 | 0.42 |
| 14:N:108:SER:HA | 14:N:109:PRO:HD3 | 1.82 | 0.42 |
| 30:0:2506:A:O2' | 30:0:2507:G:P | 2.78 | 0.42 |
| 8:H:158:ASN:ND2 | 30:0:2502:C:H4' | 2.35 | 0.42 |
| 30:0:2780:C:C4 | 30:0:2781:U:C4 | 3.08 | 0.42 |
| 30:0:590:A:H2' | 30:0:591:A:H5' | 2.01 | 0.42 |
| 30:0:2244:A:C4 | 30:0:2258:A:C2 | 3.08 | 0.42 |
| 30:0:2414:A:N1 | 30:0:2415:A:C6 | 2.87 | 0.42 |
| 1:A:97:ALA:HA | 1:A:131:HIS:NE2 | 2.33 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 17:Q:94:GLN:O | 17:Q:95:GLU:HB2 | 2.19 | 0.42 |
| 30:0:26:U:H3' | 38:0:5910:HOH:O | 2.18 | 0.42 |
| 18:R:29:LYS:HE2 | 30:0:524:A:H5' | 2.01 | 0.42 |
| 2:B:51:VAL:HG23 | 2:B:329:TYR:O | 2.20 | 0.42 |
| 20:T:64:ASN:HB3 | 20:T:73:HIS:HB2 | 2.01 | 0.42 |
| 14:N:73:ALA:HB1 | 14:N:74:PRO:CD | 2.49 | 0.42 |
| 30:0:1681:G:H4' | 30:0:1682:A:N3 | 2.34 | 0.42 |
| 16:P:143:ALA:HA | 38:P:5521:HOH:O | 2.18 | 0.42 |
| 4:D:156:ARG:NH1 | 38:D:5234:HOH:O | 2.51 | 0.42 |
| 18:R:98:ASN:HD21 | 30:0:500:G:H21 | 1.66 | 0.42 |
| 4:D:146:LYS:NZ | 14:N:107:ASN:ND2 | 2.67 | 0.42 |
| 8:H:157:TYR:C | 8:H:157:TYR:CD1 | 2.93 | 0.42 |
| 14:N:37:ARG:HH11 | 31:9:6:C:C5' | 2.28 | 0.42 |
| 13:M:164:THR:CG2 | 13:M:165:GLY:N | 2.82 | 0.42 |
| 31:9:1:U:O3' | 31:9:3:A:OP1 | 2.37 | 0.42 |
| 30:0:2727:A:C5 | 30:0:2756:U:C4 | 3.07 | 0.42 |
| 11:K:14:LYS:CB | 11:K:45:PRO:HG2 | 2.43 | 0.42 |
| 23:W:115:THR:HG23 | 38:W:5420:HOH:O | 2.18 | 0.42 |
| 1:A:53:ALA:HB3 | 38:A:9061:HOH:O | 2.18 | 0.42 |
| 30:0:255:A:C5 | 30:0:256:C:C4 | 3.08 | 0.42 |
| 31:9:74:G:C6 | 31:9:75:G:N7 | 2.87 | 0.42 |
| 30:0:1964:U:O2 | 30:0:1964:U:H2' | 2.18 | 0.42 |
| 30:0:858:U:H2' | 30:0:859:C:H6 | 1.84 | 0.42 |
| 30:0:583:C:H2' | 30:0:584:U:H6 | 1.85 | 0.42 |
| 30:0:2708:G:H2' | 30:0:2709:G:O4' | 2.19 | 0.42 |
| 3:C:193:LEU:HA | 3:C:211:ASP:O | 2.20 | 0.42 |
| 5:E:162:PHE:CD1 | 5:E:162:PHE:N | 2.88 | 0.42 |
| 4:D:137:PRO:O | 31:9:30:C:OP1 | 2.37 | 0.42 |
| 22:V:12:THR:HG23 | 22:V:14:ALA:H | 1.85 | 0.42 |
| 30:0:960:G:C8 | 38:0:5997:HOH:O | 2.57 | 0.42 |
| 17:Q:19:ARG:HH22 | 31:9:11:A:H3' | 1.84 | 0.42 |
| 31:9:106:U:O2' | 31:9:107:C:H5' | 2.20 | 0.42 |
| 30:0:1791:U:O2' | 30:0:1792:C:H5' | 2.20 | 0.42 |
| 30:0:595:U:O2' | 30:0:596:C:H5' | 2.20 | 0.42 |
| 21:U:50:GLU:HB2 | 30:0:2866:U:C5 | 2.55 | 0.42 |
| 30:0:1748:U:C5 | 30:0:1749:U:C5 | 3.08 | 0.42 |
| 13:M:187:LEU:CD2 | 13:M:194:GLY:HA3 | 2.49 | 0.42 |
| 30:0:445:U:O2' | 30:0:446:G:H5' | 2.19 | 0.42 |
| 29:3:91:GLN:O | 29:3:92:GLU:HB2 | 2.19 | 0.42 |
| 30:0:1185:U:C5' | 38:0:7505:HOH:O | 2.66 | 0.42 |
| 2:B:217:ARG:CD | 2:B:257:THR:HG22 | 2.50 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 20:T:32:ARG:NH1 | 20:T:38:ARG:HH12 | 2.18 | 0.42 |
| 30:0:1878:G:H5' | 38:0:4379:HOH:O | 2.19 | 0.42 |
| 30:0:2637:A:C5' | 38:0:9282:HOH:O | 2.57 | 0.42 |
| 4:D:40:ILE:HG23 | 38:D:5583:HOH:O | 2.20 | 0.42 |
| 4:D:27:ILE:HB | 4:D:69:ILE:O | 2.20 | 0.42 |
| 4:D:23:VAL:CG2 | 4:D:73:VAL:HB | 2.50 | 0.42 |
| 30:0:699:C:H2' | 30:0:744:G:N3 | 2.34 | 0.42 |
| 4:D:151:ILE:HB | 4:D:156:ARG:HE | 1.85 | 0.42 |
| 30:0:2450:C:C2' | 30:0:2451:G:O5' | 2.67 | 0.42 |
| 30:0:1063:G:H8 | 38:0:9865:HOH:O | 2.02 | 0.42 |
| 30:0:800:G:H2' | 30:0:801:U:C6 | 2.55 | 0.42 |
| 30:0:1555:G:H4' | 30:0:1630:A:H2 | 1.85 | 0.42 |
| 2:B:55:ASN:HB3 | 2:B:63:GLU:HA | 2.00 | 0.42 |
| 14:N:33:ARG:NH1 | 14:N:103:ASP:OD2 | 2.51 | 0.42 |
| 13:M:171:ARG:NH2 | 30:0:189:A:OP1 | 2.52 | 0.42 |
| 30:0:1119:G:N2 | 30:0:1246:A:H2 | 2.10 | 0.42 |
| 31:9:3:A:H2 | 31:9:21:G:N3 | 2.18 | 0.42 |
| 30:0:1878:G:O2' | 30:0:1879:U:OP2 | 2.37 | 0.42 |
| 30:0:2135:A:O4' | 30:0:2243:C:N4 | 2.53 | 0.42 |
| 30:0:907:A:H2' | 30:0:908:A:H8 | 1.85 | 0.42 |
| 1:A:153:ARG:CB | 1:A:153:ARG:HH11 | 2.28 | 0.42 |
| 8:H:31:ILE:HG23 | 38:H:232:HOH:O | 2.19 | 0.42 |
| 1:A:217:ARG:CG | 1:A:217:ARG:HH11 | 2.32 | 0.42 |
| 7:G:63:ARG:N | 38:G:2569:HOH:O | 2.53 | 0.42 |
| 17:Q:55:ARG:HD2 | 38:Q:2875:HOH:O | 2.19 | 0.42 |
| 16:P:41:ARG:NH2 | 30:0:1500:U:OP2 | 2.51 | 0.42 |
| 30:0:336:G:H5' | 38:0:7404:HOH:O | 2.20 | 0.42 |
| 25:Y:134:HIS:HE1 | 30:0:538:C:OP2 | 2.02 | 0.42 |
| 6:F:107:ASP:O | 6:F:111:ILE:HG13 | 2.19 | 0.42 |
| 30:0:907:A:H4' | 30:0:1328:A:C2 | 2.54 | 0.42 |
| 30:0:1477:C:H5' | 30:0:1868:G:H5'' | 1.99 | 0.42 |
| 30:0:1167:G:O2' | 30:0:1168:C:H5' | 2.20 | 0.42 |
| 30:0:1178:G:C6 | 30:0:1179:C:N4 | 2.87 | 0.42 |
| 30:0:1343:C:H2' | 30:0:1344:G:O5' | 2.20 | 0.42 |
| 27:1:8:GLN:HE22 | 27:1:11:LYS:HZ2 | 1.68 | 0.42 |
| 30:0:1515:A:H2' | 30:0:1516:U:H6 | 1.83 | 0.42 |
| 30:0:939:A:H2 | 30:0:1027:G:N3 | 2.16 | 0.42 |
| 30:0:807:A:C6 | 30:0:808:A:C6 | 3.07 | 0.42 |
| 30:0:2113:G:C6 | 30:0:2114:C:C4 | 3.08 | 0.42 |
| 21:U:33:SER:O | 21:U:37:GLU:HG3 | 2.18 | 0.42 |
| 30:0:1762:C:H2' | 30:0:1763:C:H6 | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 30:0:947:U:O2' | 30:0:948:G:H5' | 2.20 | 0.42 |
| 14:N:171:HIS:CE1 | 38:N:8858:HOH:O | 2.71 | 0.42 |
| 30:0:2007:A:N3 | 30:0:2627:G:O2' | 2.48 | 0.42 |
| 13:M:61:ILE:HG22 | 13:M:62:VAL:N | 2.35 | 0.42 |
| 3:C:129:HIS:HD2 | 3:C:165:ASP:OD2 | 2.03 | 0.42 |
| 30:0:2765:C:H2' | 30:0:2766:A:C8 | 2.54 | 0.42 |
| 30:0:470:U:H2' | 30:0:471:G:O4' | 2.20 | 0.42 |
| 8:H:123:ILE:HD12 | 8:H:123:ILE:N | 2.35 | 0.42 |
| 30:0:920:C:H5' | 30:0:921:G:C4 | 2.55 | 0.42 |
| 30:0:1992:U:H2' | 30:0:1994:A:OP2 | 2.19 | 0.42 |
| 18:R:17:MET:HE3 | 18:R:19:ARG:NH2 | 2.35 | 0.42 |
| 31:9:26:C:H2' | 31:9:27:C:C6 | 2.55 | 0.42 |
| 30:0:382:U:O2' | 30:0:430:A:H1' | 2.19 | 0.42 |
| 4:D:88:LEU:N | 4:D:89:PRO:CD | 2.83 | 0.42 |
| 30:0:1433:G:O2' | 30:0:1434:A:H5' | 2.20 | 0.42 |
| 5:E:95:VAL:HG11 | 5:E:131:LEU:HD11 | 2.02 | 0.42 |
| 30:0:536:A:H4' | 38:0:5552:HOH:O | 2.18 | 0.42 |
| 27:1:12:ASN:O | 30:0:1415:G:H5' | 2.19 | 0.42 |
| 30:0:2502:C:O2' | 30:0:2503:A:H5' | 2.17 | 0.41 |
| 30:0:213:G:O2' | 30:0:214:U:OP2 | 2.38 | 0.41 |
| 2:B:162:MET:HG3 | 2:B:310:ARG:NH1 | 2.35 | 0.41 |
| 13:M:58:GLN:NE2 | 30:0:259:G:H21 | 2.17 | 0.41 |
| 12:L:57:VAL:HG21 | 30:0:2443:C:H5' | 2.02 | 0.41 |
| 30:0:152:A:H1' | 30:0:440:C:O2' | 2.21 | 0.41 |
| 1:A:94:LEU:HG | 1:A:99:ILE:CD1 | 2.50 | 0.41 |
| 2:B:27:ASN:HD21 | 30:0:2807:U:P | 2.43 | 0.41 |
| 30:0:2112:A:H2' | 30:0:2113:G:H8 | 1.85 | 0.41 |
| 4:D:146:LYS:NZ | 14:N:107:ASN:HD21 | 2.18 | 0.41 |
| 3:C:8:LEU:HD13 | 3:C:147:LEU:HD21 | 2.01 | 0.41 |
| 1:A:72:GLU:HG3 | 26:Z:90:GLY:HA2 | 2.01 | 0.41 |
| 6:F:14:ASP:O | 6:F:18:GLU:HG3 | 2.20 | 0.41 |
| 30:0:1950:G:H2' | 30:0:1951:G:C8 | 2.55 | 0.41 |
| 4:D:51:ARG:HH11 | 4:D:68:PRO:HB3 | 1.84 | 0.41 |
| 8:H:99:ARG:NH1 | 30:0:1055:G:OP2 | 2.53 | 0.41 |
| 11:K:78:LYS:HA | 11:K:79:PRO:HD3 | 1.94 | 0.41 |
| 6:F:118:LEU:O | 6:F:119:ARG:HB3 | 2.20 | 0.41 |
| 14:N:26:LEU:HA | 14:N:26:LEU:HD12 | 1.93 | 0.41 |
| 30:0:1667:A:C2 | 30:0:1668:U:C2 | 3.07 | 0.41 |
| 30:0:1890:U:H4' | 30:0:2010:A:C6 | 2.55 | 0.41 |
| 31:9:24:U:H3' | 31:9:25:G:C5' | 2.51 | 0.41 |
| 6:F:58:GLU:HA | 6:F:61:MET:HG3 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:88:GLU:HB3 | 2:B:97:LEU:HG | 2.01 | 0.41 |
| 30:0:1524:U:C5' | 30:0:1524:U:H6 | 2.33 | 0.41 |
| 12:L:57:VAL:HG12 | 12:L:57:VAL:O | 2.20 | 0.41 |
| 25:Y:144:ARG:NH1 | 30:0:905:C:OP1 | 2.54 | 0.41 |
| 12:L:67:ARG:O | 12:L:71:GLU:HG3 | 2.20 | 0.41 |
| 30:0:969:G:H1 | 30:0:999:C:N4 | 2.18 | 0.41 |
| 30:0:1883:U:H2' | 30:0:1884:G:H5' | 2.02 | 0.41 |
| 30:0:158:A:H2' | 30:0:159:G:H5' | 2.02 | 0.41 |
| 10:J:39:VAL:HG12 | 10:J:40:ASN:ND2 | 2.35 | 0.41 |
| 18:R:9:ASP:HA | 18:R:10:PRO:HD2 | 1.91 | 0.41 |
| 3:C:61:PHE:HB3 | 38:C:8643:HOH:O | 2.20 | 0.41 |
| 30:0:1409:G:H5' | 38:0:3732:HOH:O | 2.20 | 0.41 |
| 30:0:1871:U:O4' | 30:0:1873:G:C8 | 2.73 | 0.41 |
| 30:0:1414:A:H2 | 38:0:4921:HOH:O | 2.03 | 0.41 |
| 3:C:118:THR:HG22 | 3:C:137:PRO:HB3 | 2.00 | 0.41 |
| 10:J:45:VAL:HG11 | 10:J:121:LEU:HD22 | 2.02 | 0.41 |
| 30:0:526:U:H2' | 30:0:527:U:C6 | 2.55 | 0.41 |
| 13:M:46:LEU:HG | 38:M:8913:HOH:O | 2.20 | 0.41 |
| 13:M:49:ALA:C | 13:M:54:TYR:HB3 | 2.40 | 0.41 |
| 23:W:11:VAL:O | 23:W:12:ASN:HB2 | 2.19 | 0.41 |
| 30:0:51:G:O2' | 30:0:52:A:H5' | 2.20 | 0.41 |
| 30:0:539:G:H2' | 30:0:540:A:C8 | 2.55 | 0.41 |
| 30:0:2245:C:H6 | 30:0:2245:C:O5' | 2.02 | 0.41 |
| 30:0:1119:G:C5 | 30:0:1243:C:C4 | 3.08 | 0.41 |
| 30:0:2506:A:O2' | 30:0:2507:G:O5' | 2.38 | 0.41 |
| 30:0:372:A:H2' | 30:0:373:G:C8 | 2.55 | 0.41 |
| 20:T:21:LYS:HA | 20:T:24:ARG:HG3 | 2.03 | 0.41 |
| 13:M:24:GLN:HE22 | 13:M:27:ARG:HH11 | 1.67 | 0.41 |
| 25:Y:212:ARG:HB2 | 30:0:1315:G:C4 | 2.55 | 0.41 |
| 30:0:2344:G:N7 | 38:0:4937:HOH:O | 2.49 | 0.41 |
| 25:Y:189:ASN:HD22 | 25:Y:189:ASN:C | 2.23 | 0.41 |
| 30:0:1015:C:O5' | 30:0:1015:C:H6 | 2.02 | 0.41 |
| 30:0:2379:G:N7 | 30:0:2408:A:N1 | 2.67 | 0.41 |
| 30:0:2598:U:O2 | 30:0:2600:A:H8 | 2.03 | 0.41 |
| 8:H:66:GLU:HA | 38:H:232:HOH:O | 2.19 | 0.41 |
| 30:0:2330:U:H4' | 30:0:2331:C:OP1 | 2.20 | 0.41 |
| 30:0:708:A:H2' | 30:0:709:G:O4' | 2.20 | 0.41 |
| 5:E:95:VAL:O | 5:E:126:ILE:HD12 | 2.20 | 0.41 |
| 30:0:2500:C:H1' | 38:0:4674:HOH:O | 2.20 | 0.41 |
| 30:0:2508:C:H2' | 38:0:6793:HOH:O | 2.19 | 0.41 |
| 25:Y:151:SER:HB3 | 25:Y:154:ARG:CB | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 12:L:125:PHE:CE1 | 12:L:140:VAL:HG13 | 2.55 | 0.41 |
| 18:R:59:PHE:O | 18:R:63:ASN:HB3 | 2.20 | 0.41 |
| 30:0:2512:U:H4' | 30:0:2514:U:O4 | 2.20 | 0.41 |
| 11:K:41:LYS:O | 11:K:42:ASN:HB2 | 2.20 | 0.41 |
| 11:K:34:VAL:HB | 38:K:7169:HOH:O | 2.20 | 0.41 |
| 30:0:1058:A:H2' | 30:0:1060:C:C5' | 2.48 | 0.41 |
| 30:0:485:A:O2' | 30:0:487:G:H5' | 2.19 | 0.41 |
| 30:0:735:C:C5 | 30:0:736:A:N3 | 2.89 | 0.41 |
| 30:0:1213:C:O2' | 30:0:1214:G:H5' | 2.21 | 0.41 |
| 30:0:2269:C:H2' | 30:0:2270:G:C5' | 2.50 | 0.41 |
| 30:0:2011:A:H4' | 30:0:2012:U:O5' | 2.20 | 0.41 |
| 30:0:2791:U:H4' | 30:0:2792:A:OP1 | 2.20 | 0.41 |
| 2:B:24:PRO:CG | 2:B:204:GLY:HA2 | 2.50 | 0.41 |
| 30:0:393:G:C6 | 30:0:394:G:C6 | 3.08 | 0.41 |
| 30:0:2237:G:H1' | 38:0:4871:HOH:O | 2.20 | 0.41 |
| 30:0:1427:A:O2' | 30:0:1428:C:H5' | 2.20 | 0.41 |
| 30:0:2375:A:H2' | 30:0:2376:C:C6 | 2.56 | 0.41 |
| 30:0:1603:A:C5' | 30:0:1605:G:O4' | 2.53 | 0.41 |
| 30:0:284:C:C6 | 30:0:284:C:OP2 | 2.73 | 0.41 |
| 2:B:74:ILE:HG13 | 38:B:9075:HOH:O | 2.20 | 0.41 |
| 30:0:1132:A:H2' | 30:0:1133:A:C8 | 2.56 | 0.41 |
| 30:0:1976:G:H1' | 30:0:2005:G:N2 | 2.36 | 0.41 |
| 13:M:133:LEU:O | 13:M:134:ILE:HD13 | 2.21 | 0.41 |
| 31:9:73:A:N1 | 31:9:108:C:O2 | 2.54 | 0.41 |
| 30:0:1883:U:O2' | 30:0:1884:G:H5' | 2.20 | 0.41 |
| 30:0:1522:A:C2 | 30:0:1665:G:C6 | 3.09 | 0.41 |
| 30:0:699:C:C6 | 30:0:744:G:O4' | 2.73 | 0.41 |
| 25:Y:182:PHE:HD2 | 25:Y:200:THR:O | 2.03 | 0.41 |
| 2:B:51:VAL:CG2 | 2:B:327:VAL:HG13 | 2.50 | 0.41 |
| 30:0:1748:U:C4 | 30:0:1749:U:C4 | 3.09 | 0.41 |
| 30:0:1488:U:H4' | 30:0:1489:G:OP1 | 2.21 | 0.41 |
| 30:0:491:C:O2' | 30:0:492:C:H5' | 2.21 | 0.41 |
| 30:0:2067:A:H2' | 30:0:2068:G:O4' | 2.20 | 0.41 |
| 1:A:125:ASN:HB3 | 1:A:158:VAL:HG12 | 2.02 | 0.41 |
| 23:W:108:ARG:HE | 23:W:114:PRO:HG3 | 1.85 | 0.41 |
| 30:0:1388:U:H2' | 30:0:1389:G:O4' | 2.20 | 0.41 |
| 4:D:96:SER:C | 4:D:98:PHE:H | 2.24 | 0.41 |
| 3:C:140:VAL:HG12 | 3:C:141:SER:N | 2.35 | 0.41 |
| 30:0:284:C:H4' | 30:0:285:A:H8 | 1.85 | 0.41 |
| 31:9:2:U:C4' | 38:9:9103:HOH:O | 2.67 | 0.41 |
| 3:C:184:ARG:HD2 | 30:0:1306:U:H5'' | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 30:0:259:G:O2' | 30:0:260:C:H5' | 2.20 | 0.41 |
| 2:B:7:ARG:CG | 2:B:7:ARG:HH11 | 2.31 | 0.41 |
| 25:Y:216:ARG:NH1 | 38:Y:8834:HOH:O | 2.53 | 0.41 |
| 30:0:2478:U:H2' | 30:0:2479:A:C8 | 2.55 | 0.41 |
| 30:0:1926:G:H2' | 30:0:1927:A:H8 | 1.84 | 0.41 |
| 30:0:523:C:H2' | 30:0:524:A:C8 | 2.56 | 0.41 |
| 30:0:300:U:N3 | 30:0:301:C:C5 | 2.88 | 0.41 |
| 30:0:1761:U:H2' | 30:0:1762:C:C6 | 2.55 | 0.41 |
| 13:M:139:PRO:HA | 13:M:142:GLN:HB2 | 2.03 | 0.41 |
| 29:3:30:GLN:NE2 | 38:3:9046:HOH:O | 2.51 | 0.41 |
| 30:0:1319:G:H1' | 38:0:4701:HOH:O | 2.19 | 0.41 |
| 9:I:91:PHE:HD2 | 9:I:131:GLY:HA2 | 1.85 | 0.41 |
| 12:L:117:GLU:HG2 | 38:L:8860:HOH:O | 2.20 | 0.41 |
| 30:0:240:C:O2 | 30:0:240:C:H2' | 2.21 | 0.41 |
| 31:9:5:G:C2' | 31:9:6:C:H5' | 2.50 | 0.41 |
| 4:D:154:LYS:H | 4:D:154:LYS:CD | 2.09 | 0.41 |
| 30:0:1206:U:C3' | 30:0:1206:U:C6 | 3.04 | 0.41 |
| 30:0:2421:G:H3' | 30:0:2422:U:H5'' | 2.02 | 0.41 |
| 30:0:1523:G:C6 | 30:0:1524:U:C4 | 3.09 | 0.41 |
| 10:J:127:ILE:O | 10:J:127:ILE:HG12 | 2.21 | 0.41 |
| 30:0:853:C:H2' | 30:0:854:G:O4' | 2.21 | 0.41 |
| 30:0:1662:C:H2' | 30:0:1663:G:O4' | 2.21 | 0.41 |
| 30:0:1417:G:N3 | 30:0:1417:G:H2' | 2.35 | 0.41 |
| 30:0:2597:U:C2' | 30:0:2598:U:H5' | 2.50 | 0.41 |
| 30:0:64:G:H2' | 30:0:65:C:O4' | 2.21 | 0.41 |
| 30:0:2878:U:OP1 | 30:0:2878:U:H6 | 2.03 | 0.41 |
| 24:X:78:GLU:HG2 | 24:X:79:GLU:H | 1.86 | 0.41 |
| 2:B:137:LEU:HD21 | 2:B:140:LEU:HD21 | 2.03 | 0.41 |
| 5:E:111:LYS:HE3 | 30:0:2690:U:H4' | 2.02 | 0.41 |
| 10:J:47:THR:O | 10:J:53:ILE:HD11 | 2.21 | 0.41 |
| 30:0:541:C:H2' | 30:0:542:A:H5' | 1.95 | 0.41 |
| 9:I:114:TYR:HE1 | 30:0:1186:C:H4' | 1.85 | 0.41 |
| 6:F:91:VAL:CG1 | 6:F:92:GLY:N | 2.78 | 0.41 |
| 26:Z:70:ARG:CD | 26:Z:83:TYR:HB2 | 2.36 | 0.41 |
| 1:A:212:PRO:HB2 | 38:0:4373:HOH:O | 2.20 | 0.41 |
| 30:0:1265:G:H1' | 38:0:5020:HOH:O | 2.21 | 0.41 |
| 30:0:466:A:C2 | 30:0:476:A:C4 | 3.09 | 0.41 |
| 30:0:862:U:H2' | 30:0:863:G:C8 | 2.56 | 0.41 |
| 30:0:2090:G:H2' | 30:0:2091:G:C8 | 2.55 | 0.41 |
| 30:0:123:U:H5' | 38:0:6689:HOH:O | 2.20 | 0.41 |
| 9:I:108:HIS:N | 9:I:109:PRO:HD2 | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:Z:35:SER:HB3 | 26:Z:47:ARG:HB2 | 2.03 | 0.41 |
| 30:0:1762:C:H2' | 30:0:1763:C:C6 | 2.56 | 0.41 |
| 30:0:1576:G:H2' | 30:0:1577:U:O4' | 2.21 | 0.41 |
| 30:0:60:A:C2 | 30:0:61:G:C8 | 3.09 | 0.41 |
| 23:W:59:GLN:NE2 | 23:W:97:ALA:HB3 | 2.36 | 0.41 |
| 3:C:84:VAL:HG12 | 3:C:85:LYS:HG2 | 2.02 | 0.41 |
| 17:Q:66:LYS:HB2 | 17:Q:70:ALA:O | 2.21 | 0.41 |
| 5:E:91:PHE:HA | 5:E:92:PRO:HD3 | 1.87 | 0.41 |
| 30:0:1589:G:H22 | 30:0:1605:G:H1' | 1.85 | 0.41 |
| 30:0:2511:A:H4' | 38:0:5487:HOH:O | 2.21 | 0.41 |
| 30:0:1632:A:C3' | 30:0:1633:C:H5' | 2.51 | 0.41 |
| 30:0:1878:G:C4' | 38:0:6151:HOH:O | 2.69 | 0.41 |
| 22:V:12:THR:HB | 22:V:15:GLU:OE2 | 2.20 | 0.41 |
| 1:A:211:LYS:HB3 | 1:A:212:PRO:CD | 2.49 | 0.41 |
| 23:W:122:ARG:HH11 | 23:W:122:ARG:HG3 | 1.85 | 0.41 |
| 10:J:75:PRO:HB3 | 10:J:132:LEU:HB3 | 2.02 | 0.41 |
| 10:J:132:LEU:HA | 10:J:132:LEU:HD23 | 1.92 | 0.41 |
| 30:0:1592:G:O2' | 30:0:1593:C:O4' | 2.32 | 0.41 |
| 2:B:307:ARG:HG3 | 30:0:2837:U:O2 | 2.21 | 0.41 |
| 30:0:1486:A:H4' | 30:0:1487:A:OP2 | 2.20 | 0.41 |
| 30:0:1250:C:O2' | 30:0:1251:C:H5' | 2.20 | 0.41 |
| 30:0:711:G:N2 | 30:0:718:C:C2 | 2.89 | 0.41 |
| 30:0:2063:U:O4 | 30:0:2083:A:H2 | 2.03 | 0.41 |
| 20:T:2:LYS:HG2 | 30:0:447:A:OP1 | 2.21 | 0.41 |
| 29:3:3:MET:HG3 | 29:3:4:PRO:HD2 | 2.03 | 0.41 |
| 13:M:61:ILE:N | 13:M:61:ILE:HD12 | 2.36 | 0.41 |
| 23:W:11:VAL:HG11 | 30:0:1086:A:C6 | 2.56 | 0.41 |
| 12:L:11:ARG:O | 30:0:903:U:C2 | 2.73 | 0.41 |
| 28:2:5:LYS:O | 28:2:9:LYS:HG3 | 2.21 | 0.41 |
| 5:E:132:THR:HB | 38:E:2227:HOH:O | 2.21 | 0.41 |
| 13:M:65:VAL:HG21 | 13:M:105:ALA:HB2 | 2.03 | 0.41 |
| 2:B:195:ARG:HG2 | 2:B:323:LEU:HD22 | 2.03 | 0.41 |
| 2:B:150:ALA:O | 2:B:152:PRO:HD3 | 2.21 | 0.41 |
| 30:0:2543:G:H2' | 30:0:2544:G:O4' | 2.21 | 0.41 |
| 19:S:57:THR:HG22 | 19:S:58:MET:N | 2.35 | 0.41 |
| 23:W:61:THR:HG23 | 23:W:151:GLU:HG3 | 2.03 | 0.41 |
| 21:U:44:ARG:HB3 | 38:U:3805:HOH:O | 2.21 | 0.41 |
| 31:9:76:G:O5' | 31:9:76:G:H8 | 2.04 | 0.41 |
| 30:0:1119:G:N2 | 30:0:1246:A:N1 | 2.68 | 0.41 |
| 30:0:2712:G:H5' | 38:0:5241:HOH:O | 2.19 | 0.41 |
| 1:A:233:THR:HB | 30:0:1942:A:H5'' | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:9:93:A:H8 | 31:9:93:A:O5' | 2.04 | 0.41 |
| 30:0:1525:G:OP1 | 30:0:1525:G:H4' | 2.21 | 0.41 |
| 30:0:2361:A:H2' | 30:0:2362:A:C8 | 2.55 | 0.41 |
| 30:0:1771:U:O2' | 30:0:1773:G:N7 | 2.53 | 0.41 |
| 30:0:1167:G:H1 | 30:0:1179:C:H42 | 1.69 | 0.41 |
| 1:A:48:ASP:HA | 1:A:49:PRO:HD3 | 1.89 | 0.41 |
| 14:N:154:LEU:O | 14:N:155:GLU:HB3 | 2.21 | 0.41 |
| 12:L:145:LEU:O | 12:L:148:GLU:HG3 | 2.21 | 0.41 |
| 30:0:2088:C:H1' | 30:0:2841:A:C2 | 2.56 | 0.41 |
| 30:0:2680:A:O2' | 30:0:2681:A:C4 | 2.72 | 0.41 |
| 30:0:2887:G:H2' | 30:0:2888:U:O4' | 2.20 | 0.41 |
| 17:Q:34:ASP:O | 17:Q:37:GLU:HB2 | 2.21 | 0.41 |
| 12:L:32:ASP:HB3 | 30:0:222:A:H5'' | 2.03 | 0.41 |
| 18:R:33:ARG:NH2 | 38:R:8935:HOH:O | 2.54 | 0.41 |
| 30:0:2824:C:H5'' | 30:0:2825:C:H5' | 2.02 | 0.41 |
| 30:0:2318:C:H2' | 30:0:2319:C:H6 | 1.86 | 0.41 |
| 30:0:613:C:C2 | 30:0:614:U:C5 | 3.09 | 0.40 |
| 30:0:371:U:H2' | 30:0:372:A:H8 | 1.85 | 0.40 |
| 30:0:1635:U:O2' | 30:0:1636:G:H5' | 2.19 | 0.40 |
| 28:2:11:LEU:HA | 28:2:11:LEU:HD23 | 1.91 | 0.40 |
| 30:0:1265:G:C5 | 30:0:1266:U:C5 | 3.09 | 0.40 |
| 27:1:21:ARG:HD2 | 27:1:39:PHE:HB2 | 2.03 | 0.40 |
| 22:V:42:ASN:O | 22:V:44:GLY:N | 2.55 | 0.40 |
| 13:M:138:HIS:O | 13:M:142:GLN:HG3 | 2.21 | 0.40 |
| 30:0:932:U:O2' | 30:0:1296:A:H1' | 2.21 | 0.40 |
| 30:0:488:U:H2' | 38:0:4016:HOH:O | 2.21 | 0.40 |
| 14:N:34:LEU:HD22 | 14:N:129:ILE:HD13 | 2.02 | 0.40 |
| 3:C:80:VAL:HA | 3:C:81:PRO:HD3 | 1.88 | 0.40 |
| 30:0:2531:U:O2' | 30:0:2532:A:H5' | 2.21 | 0.40 |
| 17:Q:64:GLU:HG3 | 17:Q:74:ASP:OD2 | 2.21 | 0.40 |
| 13:M:164:THR:HG22 | 13:M:166:ALA:N | 2.36 | 0.40 |
| 14:N:1:ALA:HB2 | 31:9:14:G:O2' | 2.21 | 0.40 |
| 30:0:2010:A:C2' | 38:0:5984:HOH:O | 2.51 | 0.40 |
| 30:0:1505:U:H4' | 38:0:5200:HOH:O | 2.22 | 0.40 |
| 30:0:1632:A:H2' | 30:0:1633:C:C5' | 2.46 | 0.40 |
| 30:0:2716:G:H1' | 38:0:3037:HOH:O | 2.21 | 0.40 |
| 30:0:1838:U:O2' | 30:0:2644:C:H5' | 2.21 | 0.40 |
| 30:0:1573:A:H2' | 30:0:1574:C:O4' | 2.21 | 0.40 |
| 30:0:154:C:H2' | 30:0:155:C:H6 | 1.86 | 0.40 |
| 8:H:100:GLU:HG2 | 8:H:102:LYS:HB3 | 2.03 | 0.40 |
| 30:0:634:G:O2' | 30:0:1358:A:OP1 | 2.36 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 30:0:625:U:H5' | 38:0:3194:HOH:O | 2.20 | 0.40 |
| 30:0:2348:C:O2' | 30:0:2349:G:H5' | 2.21 | 0.40 |
| 30:0:1413:A:H2' | 30:0:1414:A:O4' | 2.20 | 0.40 |
| 3:C:124:VAL:HA | 3:C:230:GLY:O | 2.21 | 0.40 |
| 30:0:1252:A:H2' | 30:0:1253:C:O4' | 2.21 | 0.40 |
| 30:0:2119:C:O2' | 30:0:2120:U:H5' | 2.22 | 0.40 |
| 25:Y:219:GLU:HG3 | 25:Y:220:GLU:N | 2.36 | 0.40 |
| 30:0:1202:A:C2' | 30:0:1203:G:H5' | 2.52 | 0.40 |
| 30:0:613:C:H2' | 30:0:614:U:C6 | 2.49 | 0.40 |
| 30:0:2765:C:H2' | 30:0:2766:A:H8 | 1.86 | 0.40 |
| 31:9:47:A:C2 | 31:9:48:C:C2 | 3.09 | 0.40 |
| 27:1:25:LYS:HD2 | 28:2:48:ASP:HA | 2.03 | 0.40 |
| 25:Y:182:PHE:CG | 25:Y:202:ALA:HB2 | 2.57 | 0.40 |
| 30:0:2467:A:H3' | 38:0:5475:HOH:O | 2.22 | 0.40 |
| 23:W:22:GLU:HG2 | 23:W:27:HIS:CD2 | 2.56 | 0.40 |
| 5:E:1:PRO:HG2 | 5:E:59:MET:SD | 2.61 | 0.40 |
| 30:0:1511:U:O2' | 30:0:1512:G:H5' | 2.22 | 0.40 |
| 2:B:16:ARG:NH2 | 38:B:9021:HOH:O | 2.49 | 0.40 |
| 30:0:622:G:O2' | 30:0:623:U:H5' | 2.21 | 0.40 |
| 3:C:43:LYS:HG2 | 30:0:449:A:N7 | 2.36 | 0.40 |
| 21:U:20:MET:CG | 21:U:28:THR:HG23 | 2.51 | 0.40 |
| 18:R:132:ARG:HG2 | 18:R:133:ALA:N | 2.36 | 0.40 |
| 13:M:176:LYS:HB3 | 13:M:176:LYS:HE2 | 1.95 | 0.40 |
| 30:0:1588:G:C5 | 30:0:1589:G:C6 | 3.09 | 0.40 |
| 30:0:1603:A:C5' | 30:0:1605:G:C5' | 2.98 | 0.40 |
| 20:T:97:ARG:NH2 | 30:0:309:C:OP1 | 2.54 | 0.40 |
| 5:E:116:THR:CG2 | 5:E:151:LEU:HD22 | 2.43 | 0.40 |
| 8:H:6:ALA:HB3 | 30:0:2521:A:P | 2.61 | 0.40 |
| 2:B:141:ARG:N | 38:B:9047:HOH:O | 2.54 | 0.40 |
| 30:0:2598:U:O2 | 30:0:2600:A:C8 | 2.74 | 0.40 |
| 16:P:2:ASP:OD1 | 30:0:1396:C:H4' | 2.21 | 0.40 |
| 30:0:596:C:H2' | 30:0:597:A:C8 | 2.56 | 0.40 |
| 16:P:81:LYS:HB3 | 30:0:1707:G:O3' | 2.21 | 0.40 |
| 30:0:645:U:H2' | 30:0:646:G:C8 | 2.56 | 0.40 |
| 4:D:151:ILE:HA | 4:D:152:PRO:HD3 | 1.95 | 0.40 |
| 30:0:1576:G:H2' | 30:0:1577:U:C6 | 2.56 | 0.40 |
| 30:0:222:A:H2' | 30:0:223:G:O4' | 2.21 | 0.40 |
| 30:0:1565:C:H2' | 30:0:1566:C:H6 | 1.86 | 0.40 |
| 30:0:1996:U:O2' | 30:0:1997:A:H5' | 2.21 | 0.40 |
| 30:0:37:A:H2' | 30:0:38:G:C8 | 2.57 | 0.40 |
| 30:0:1915:U:O2' | 30:0:1916:C:H5' | 2.22 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 17:Q:16:ASN:HD22 | 17:Q:16:ASN:HA | 1.71 | 0.40 |
| 8:H:155:ARG:NE | 38:H:198:HOH:O | 2.54 | 0.40 |
| 30:0:1188:A:C6 | 30:0:1189:A:C6 | 3.09 | 0.40 |
| 26:Z:70:ARG:NH2 | 30:0:1602:C:OP2 | 2.53 | 0.40 |
| 30:0:535:G:C5 | 30:0:2063:U:C4 | 3.09 | 0.40 |
| 14:N:44:ARG:NH1 | 31:9:4:G:H21 | 2.20 | 0.40 |
| 6:F:59:ILE:CD1 | 30:0:263:U:C2 | 3.04 | 0.40 |
| 8:H:74:ARG:NH1 | 30:0:2504:A:H4' | 2.36 | 0.40 |
| 3:C:135:GLU:HB3 | 38:C:8576:HOH:O | 2.22 | 0.40 |
| 20:T:16:LEU:HB2 | 30:0:100:C:H4' | 2.03 | 0.40 |
| 11:K:64:MET:HA | 11:K:67:GLN:HE21 | 1.87 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1 | A | 235/240 (98%) | 213 (91%) | 18 (8%) | 4 (2%) | 11 | 38 |
| 2 | B | 335/338 (99%) | 309 (92%) | 22 (7%) | 4 (1%) | 16 | 48 |
| 3 | C | 244/246 (99%) | 222 (91%) | 22 (9%) | 0 | 100 | 100 |
| 4 | D | 134/177 (76%) | 107 (80%) | 22 (16%) | 5 (4%) | 4 | 17 |
| 5 | E | 170/178 (96%) | 156 (92%) | 14 (8%) | 0 | 100 | 100 |
| 6 | F | 117/120 (98%) | 104 (89%) | 9 (8%) | 4 (3%) | 5 | 19 |
| 7 | G | 25/348 (7%) | 23 (92%) | 2 (8%) | 0 | 100 | 100 |
| 8 | H | 156/177 (88%) | 145 (93%) | 11 (7%) | 0 | 100 | 100 |
| 9 | I | 68/162 (42%) | 54 (79%) | 13 (19%) | 1 (2%) | 13 | 42 |
| 10 | J | 140/145 (97%) | 132 (94%) | 8 (6%) | 0 | 100 | 100 |
| 11 | K | 130/132 (98%) | 124 (95%) | 6 (5%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 12 | L | 141/165 (86%) | 124 (88%) | 14 (10%) | 3 (2%) | 9 | 32 |
| 13 | M | 192/196 (98%) | 182 (95%) | 10 (5%) | 0 | 100 | 100 |
| 14 | N | 184/187 (98%) | 169 (92%) | 11 (6%) | 4 (2%) | 8 | 31 |
| 15 | O | 113/116 (97%) | 108 (96%) | 5 (4%) | 0 | 100 | 100 |
| 16 | P | 141/149 (95%) | 138 (98%) | 3 (2%) | 0 | 100 | 100 |
| 17 | Q | 93/96 (97%) | 89 (96%) | 4 (4%) | 0 | 100 | 100 |
| 18 | R | 148/155 (96%) | 137 (93%) | 11 (7%) | 0 | 100 | 100 |
| 19 | S | 79/85 (93%) | 72 (91%) | 7 (9%) | 0 | 100 | 100 |
| 20 | T | 117/120 (98%) | 107 (92%) | 9 (8%) | 1 (1%) | 21 | 57 |
| 21 | U | 51/67 (76%) | 48 (94%) | 3 (6%) | 0 | 100 | 100 |
| 22 | V | 63/71 (89%) | 58 (92%) | 3 (5%) | 2 (3%) | 5 | 20 |
| 23 | W | 152/154 (99%) | 145 (95%) | 6 (4%) | 1 (1%) | 26 | 63 |
| 24 | X | 80/92 (87%) | 71 (89%) | 8 (10%) | 1 (1%) | 15 | 46 |
| 25 | Y | 140/241 (58%) | 140 (100%) | 0 | 0 | 100 | 100 |
| 26 | Z | 71/116 (61%) | 62 (87%) | 8 (11%) | 1 (1%) | 14 | 44 |
| 27 | 1 | 54/57 (95%) | 51 (94%) | 3 (6%) | 0 | 100 | 100 |
| 28 | 2 | 42/50 (84%) | 37 (88%) | 5 (12%) | 0 | 100 | 100 |
| 29 | 3 | 90/92 (98%) | 89 (99%) | 1 (1%) | 0 | 100 | 100 |
| All | All | 3705/4472 (83%) | 3416 (92%) | 258 (7%) | 31 (1%) | 24 | 60 |

All (31) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 27 | LEU |
| 1 | A | 36 | ASP |
| 1 | A | 37 | VAL |
| 6 | F | 101 | ALA |
| 14 | N | 154 | LEU |
| 14 | N | 183 | ASP |
| 14 | N | 184 | ILE |
| 1 | A | 34 | ASP |
| 4 | D | 27 | ILE |
| 6 | F | 44 | SER |
| 24 | X | 70 | ILE |
| 4 | D | 97 | GLN |
| 12 | L | 149 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14 | N | 139 | TRP |
| 26 | Z | 44 | ARG |
| 2 | B | 2 | GLN |
| 2 | B | 184 | ASP |
| 4 | D | 56 | ARG |
| 6 | F | 100 | ASP |
| 12 | L | 80 | ASP |
| 22 | V | 43 | PRO |
| 6 | F | 61 | MET |
| 9 | I | 83 | GLY |
| 20 | T | 53 | GLY |
| 23 | W | 49 | ASN |
| 12 | L | 82 | ALA |
| 2 | B | 34 | GLY |
| 2 | B | 169 | GLY |
| 4 | D | 28 | GLY |
| 4 | D | 137 | PRO |
| 22 | V | 40 | 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.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1 | A | 179/182 (98%) | 171 (96%) | 8 (4%) | 34 | 70 |
| 2 | B | 282/283 (100%) | 268 (95%) | 14 (5%) | 30 | 65 |
| 3 | C | 193/193 (100%) | 180 (93%) | 13 (7%) | 20 | 50 |
| 4 | D | 117/148 (79%) | 113 (97%) | 4 (3%) | 44 | 79 |
| 5 | E | 152/156 (97%) | 148 (97%) | 4 (3%) | 54 | 85 |
| 6 | F | 93/94 (99%) | 91 (98%) | 2 (2%) | 60 | 88 |
| 7 | G | 27/282 (10%) | 26 (96%) | 1 (4%) | 41 | 77 |
| 8 | H | 134/145 (92%) | 128 (96%) | 6 (4%) | 34 | 70 |
| 9 | I | 58/130 (45%) | 56 (97%) | 2 (3%) | 44 | 79 |
| 10 | J | 118/121 (98%) | 110 (93%) | 8 (7%) | 20 | 49 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 11 | K | 106/106 (100%) | 103 (97%) | 3 (3%) | 51 | 84 |
| 12 | L | 113/127 (89%) | 108 (96%) | 5 (4%) | 35 | 70 |
| 13 | M | 158/160 (99%) | 151 (96%) | 7 (4%) | 35 | 70 |
| 14 | N | 149/150 (99%) | 147 (99%) | 2 (1%) | 76 | 94 |
| 15 | O | 93/94 (99%) | 92 (99%) | 1 (1%) | 80 | 95 |
| 16 | P | 113/117 (97%) | 111 (98%) | 2 (2%) | 66 | 90 |
| 17 | Q | 79/80 (99%) | 75 (95%) | 4 (5%) | 29 | 65 |
| 18 | R | 117/122 (96%) | 112 (96%) | 5 (4%) | 35 | 71 |
| 19 | S | 71/74 (96%) | 71 (100%) | 0 | 100 | 100 |
| 20 | T | 105/106 (99%) | 101 (96%) | 4 (4%) | 40 | 76 |
| 21 | U | 44/53 (83%) | 42 (96%) | 2 (4%) | 34 | 70 |
| 22 | V | 51/57 (90%) | 48 (94%) | 3 (6%) | 24 | 58 |
| 23 | W | 130/130 (100%) | 127 (98%) | 3 (2%) | 58 | 87 |
| 24 | X | 66/74 (89%) | 63 (96%) | 3 (4%) | 34 | 70 |
| 25 | Y | 120/196 (61%) | 116 (97%) | 4 (3%) | 45 | 80 |
| 26 | Z | 60/94 (64%) | 59 (98%) | 1 (2%) | 68 | 91 |
| 27 | 1 | 46/47 (98%) | 46 (100%) | 0 | 100 | 100 |
| 28 | 2 | 42/46 (91%) | 41 (98%) | 1 (2%) | 57 | 86 |
| 29 | 3 | 79/79 (100%) | 78 (99%) | 1 (1%) | 76 | 94 |
| All | All | 3095/3646 (85%) | 2982 (96%) | 113 (4%) | 41 | 77 |

All (113) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 3 | ARG |
| 1 | A | 36 | ASP |
| 1 | A | 69 | LEU |
| 1 | A | 94 | LEU |
| 1 | A | 131 | HIS |
| 1 | A | 153 | ARG |
| 1 | A | 179 | MET |
| 1 | A | 217 | ARG |
| 2 | B | 7 | ARG |
| 2 | B | 11 | LEU |
| 2 | B | 27 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 49 | THR |
| 2 | B | 56 | ASP |
| 2 | B | 71 | VAL |
| 2 | B | 132 | HIS |
| 2 | B | 162 | MET |
| 2 | B | 175 | LEU |
| 2 | B | 190 | MET |
| 2 | B | 195 | ARG |
| 2 | B | 254 | GLN |
| 2 | B | 256 | GLN |
| 2 | B | 277 | GLU |
| 3 | C | 2 | GLN |
| 3 | C | 27 | ARG |
| 3 | C | 78 | ARG |
| 3 | C | 94 | THR |
| 3 | C | 136 | VAL |
| 3 | C | 162 | VAL |
| 3 | C | 187 | ARG |
| 3 | C | 214 | THR |
| 3 | C | 234 | VAL |
| 3 | C | 236 | THR |
| 3 | C | 237 | GLU |
| 3 | C | 240 | LEU |
| 3 | C | 243 | VAL |
| 4 | D | 24 | HIS |
| 4 | D | 50 | VAL |
| 4 | D | 100 | ASP |
| 4 | D | 153 | THR |
| 5 | E | 86 | VAL |
| 5 | E | 102 | VAL |
| 5 | E | 126 | ILE |
| 5 | E | 156 | ASP |
| 6 | F | 12 | LEU |
| 6 | F | 119 | ARG |
| 7 | G | 73 | ASP |
| 8 | H | 21 | GLU |
| 8 | H | 65 | LEU |
| 8 | H | 87 | LYS |
| 8 | H | 91 | ARG |
| 8 | H | 157 | TYR |
| 8 | H | 173 | GLU |
| 9 | I | 110 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | I | 114 | TYR |
| 10 | J | 45 | VAL |
| 10 | J | 46 | ILE |
| 10 | J | 52 | GLN |
| 10 | J | 74 | ARG |
| 10 | J | 79 | PHE |
| 10 | J | 107 | ASN |
| 10 | J | 127 | ILE |
| 10 | J | 131 | THR |
| 11 | K | 7 | ASP |
| 11 | K | 10 | GLN |
| 11 | K | 55 | VAL |
| 12 | L | 32 | ASP |
| 12 | L | 35 | ARG |
| 12 | L | 43 | HIS |
| 12 | L | 101 | ASP |
| 12 | L | 104 | ASP |
| 13 | M | 46 | LEU |
| 13 | M | 68 | ARG |
| 13 | M | 93 | ARG |
| 13 | M | 99 | ARG |
| 13 | M | 116 | ASN |
| 13 | M | 130 | GLU |
| 13 | M | 164 | THR |
| 14 | N | 26 | LEU |
| 14 | N | 138 | ASP |
| 15 | O | 67 | SER |
| 16 | P | 91 | LYS |
| 16 | P | 98 | ILE |
| 17 | Q | 16 | ASN |
| 17 | Q | 18 | PRO |
| 17 | Q | 20 | ASP |
| 17 | Q | 57 | ASP |
| 18 | R | 13 | THR |
| 18 | R | 39 | THR |
| 18 | R | 119 | VAL |
| 18 | R | 123 | GLN |
| 18 | R | 132 | ARG |
| 20 | T | 39 | ASN |
| 20 | T | 48 | VAL |
| 20 | T | 89 | ARG |
| 20 | T | 117 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21 | U | 52 | THR |
| 21 | U | 53 | ASP |
| 22 | V | 12 | THR |
| 22 | V | 22 | ASP |
| 22 | V | 65 | ASP |
| 23 | W | 35 | VAL |
| 23 | W | 76 | ASP |
| 23 | W | 146 | ILE |
| 24 | X | 27 | ASP |
| 24 | X | 46 | ASP |
| 24 | X | 88 | GLU |
| 25 | Y | 163 | THR |
| 25 | Y | 186 | ARG |
| 25 | Y | 189 | ASN |
| 25 | Y | 203 | VAL |
| 26 | Z | 106 | SER |
| 28 | 2 | 18 | ASN |
| 29 | 3 | 3 | MET |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 199 | HIS |
| 2 | B | 27 | ASN |
| 2 | B | 127 | GLN |
| 2 | B | 145 | HIS |
| 2 | B | 221 | GLN |
| 2 | B | 238 | ASN |
| 2 | B | 260 | HIS |
| 2 | B | 320 | GLN |
| 3 | C | 2 | GLN |
| 3 | C | 39 | GLN |
| 3 | C | 73 | GLN |
| 3 | C | 129 | HIS |
| 3 | C | 151 | GLN |
| 4 | D | 103 | ASN |
| 5 | E | 74 | HIS |
| 5 | E | 119 | HIS |
| 5 | E | 143 | GLN |
| 7 | G | 17 | GLN |
| 7 | G | 64 | ASN |
| 8 | H | 34 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | H | 59 | GLN |
| 8 | H | 62 | HIS |
| 8 | H | 158 | ASN |
| 9 | I | 106 | GLN |
| 10 | J | 52 | GLN |
| 10 | J | 107 | ASN |
| 10 | J | 126 | ASN |
| 11 | K | 10 | GLN |
| 11 | K | 44 | HIS |
| 11 | K | 67 | GLN |
| 12 | L | 18 | HIS |
| 12 | L | 41 | HIS |
| 12 | L | 116 | HIS |
| 13 | M | 24 | GLN |
| 13 | M | 58 | GLN |
| 13 | M | 137 | ASN |
| 13 | M | 170 | ASN |
| 14 | N | 53 | ASN |
| 14 | N | 93 | GLN |
| 14 | N | 107 | ASN |
| 16 | P | 50 | GLN |
| 16 | P | 66 | GLN |
| 16 | P | 73 | HIS |
| 16 | P | 88 | GLN |
| 16 | P | 118 | GLN |
| 17 | Q | 40 | HIS |
| 18 | R | 94 | ASN |
| 18 | R | 98 | ASN |
| 18 | R | 113 | HIS |
| 18 | R | 117 | HIS |
| 19 | S | 9 | HIS |
| 19 | S | 44 | GLN |
| 19 | S | 53 | ASN |
| 20 | T | 39 | ASN |
| 21 | U | 39 | ASN |
| 21 | U | 48 | ASN |
| 22 | V | 4 | HIS |
| 22 | V | 34 | GLN |
| 22 | V | 60 | GLN |
| 23 | W | 2 | HIS |
| 23 | W | 27 | HIS |
| 23 | W | 110 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23 | W | 119 | HIS |
| 23 | W | 125 | HIS |
| 23 | W | 141 | HIS |
| 24 | X | 23 | HIS |
| 25 | Y | 134 | HIS |
| 25 | Y | 149 | GLN |
| 25 | Y | 189 | ASN |
| 27 | 1 | 8 | GLN |
| 27 | 1 | 16 | HIS |
| 27 | 1 | 28 | HIS |
| 28 | 2 | 18 | ASN |
| 28 | 2 | 37 | HIS |
| 28 | 2 | 41 | HIS |
| 28 | 2 | 45 | ASN |
| 29 | 3 | 48 | ASN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 30 | 0 | 2745/2923 (93%) | 242 (8%) | 22 (0%) |
| 31 | 9 | 121/122 (99%) | 18 (14%) | 1 (0%) |
| All | All | 2866/3045 (94%) | 260 (9%) | 23 (0%) |

All (260) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30 | 0 | 31 | C |
| 30 | 0 | 67 | A |
| 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 | 131 | A |
| 30 | 0 | 138 | U |
| 30 | 0 | 139 | C |
| 30 | 0 | 141 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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 | 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 | 337 | A |
| 30 | 0 | 358 | G |
| 30 | 0 | 368 | C |
| 30 | 0 | 381 | G |
| 30 | 0 | 417 | G |
| 30 | 0 | 461 | C |
| 30 | 0 | 487 | G |
| 30 | 0 | 510 | U |
| 30 | 0 | 511 | A |
| 30 | 0 | 514 | G |
| 30 | 0 | 537 | G |
| 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 | 581 | G |
| 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 |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 30 | 0 | 701 | U |
| 30 | 0 | 702 | G |
| 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 | 885 | G |
| 30 | 0 | 898 | G |
| 30 | 0 | 905 | C |
| 30 | 0 | 920 | C |
| 30 | 0 | 921 | G |
| 30 | 0 | 953 | G |
| 30 | 0 | 960 | G |
| 30 | 0 | 961 | A |
| 30 | 0 | 1006 | A |
| 30 | 0 | 1008 | C |
| 30 | 0 | 1015 | C |
| 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 | 1088 | A |
| 30 | 0 | 1109 | U |
| 30 | 0 | 1110 | G |
| 30 | 0 | 1119 | G |
| 30 | 0 | 1130 | U |
| 30 | 0 | 1137 | G |
| 30 | 0 | 1151 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 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 | 1206 | U |
| 30 | 0 | 1208 | C |
| 30 | 0 | 1216 | G |
| 30 | 0 | 1237 | U |
| 30 | 0 | 1238 | C |
| 30 | 0 | 1239 | G |
| 30 | 0 | 1242 | A |
| 30 | 0 | 1279 | U |
| 30 | 0 | 1289 | C |
| 30 | 0 | 1331 | G |
| 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 | 1409 | G |
| 30 | 0 | 1474 | C |
| 30 | 0 | 1492 | A |
| 30 | 0 | 1505 | U |
| 30 | 0 | 1506 | U |
| 30 | 0 | 1524 | U |
| 30 | 0 | 1525 | G |
| 30 | 0 | 1526 | A |
| 30 | 0 | 1528 | A |
| 30 | 0 | 1535 | G |
| 30 | 0 | 1559 | A |
| 30 | 0 | 1592 | G |
| 30 | 0 | 1625 | U |
| 30 | 0 | 1626 | A |
| 30 | 0 | 1634 | G |
| 30 | 0 | 1656 | A |
| 30 | 0 | 1667 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 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 | 1730 | G |
| 30 | 0 | 1731 | C |
| 30 | 0 | 1752 | G |
| 30 | 0 | 1774 | 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 | 1879 | U |
| 30 | 0 | 1919 | A |
| 30 | 0 | 1942 | A |
| 30 | 0 | 1965 | C |
| 30 | 0 | 1971 | G |
| 30 | 0 | 1973 | A |
| 30 | 0 | 1979 | G |
| 30 | 0 | 1996 | U |
| 30 | 0 | 2004 | U |
| 30 | 0 | 2008 | U |
| 30 | 0 | 2011 | A |
| 30 | 0 | 2012 | U |
| 30 | 0 | 2013 | G |
| 30 | 0 | 2033 | 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 | 2110 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 30 | 0 | 2243 | C |
| 30 | 0 | 2258 | A |
| 30 | 0 | 2271 | G |
| 30 | 0 | 2272 | G |
| 30 | 0 | 2291 | A |
| 30 | 0 | 2317 | C |
| 30 | 0 | 2321 | A |
| 30 | 0 | 2345 | 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 | 2465 | A |
| 30 | 0 | 2467 | A |
| 30 | 0 | 2469 | A |
| 30 | 0 | 2476 | C |
| 30 | 0 | 2483 | A |
| 30 | 0 | 2507 | G |
| 30 | 0 | 2509 | A |
| 30 | 0 | 2511 | A |
| 30 | 0 | 2526 | C |
| 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 | 2570 | G |
| 30 | 0 | 2589 | U |
| 30 | 0 | 2601 | A |
| 30 | 0 | 2602 | G |
| 30 | 0 | 2608 | C |
| 30 | 0 | 2613 | G |
| 30 | 0 | 2638 | G |
| 30 | 0 | 2649 | A |
| 30 | 0 | 2664 | A |
| 30 | 0 | 2676 | C |
| 30 | 0 | 2681 | A |
| 30 | 0 | 2682 | C |
| 30 | 0 | 2718 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 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 | 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 | 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 |
| 31 | 9 | 25 | G |
| 31 | 9 | 39 | U |
| 31 | 9 | 40 | C |
| 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 |

All (23) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30 | 0 | 69 | A |
| 30 | 0 | 129 | A |
| 30 | 0 | 603 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 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 | 1237 | U |
| 30 | 0 | 1246 | A |
| 30 | 0 | 1352 | A |
| 30 | 0 | 1377 | C |
| 30 | 0 | 1474 | C |
| 30 | 0 | 1506 | U |
| 30 | 0 | 1692 | C |
| 30 | 0 | 2467 | A |
| 30 | 0 | 2526 | C |
| 30 | 0 | 2536 | C |
| 30 | 0 | 2649 | A |
| 30 | 0 | 2681 | A |
| 30 | 0 | 2718 | C |
| 31 | 9 | 65 | A |

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

5 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 | 1.03 | 1 (8%) | 19,31,34 | 3.15 | 2 (10%) |
| 30 | OMG | 0 | 2588 | 30 | 17,26,27 | 1.04 | 1 (5%) | 21,38,41 | 2.53 | 3 (14%) |
| 30 | UR3 | 0 | 2619 | 30 | 12,22,23 | 0.76 | 0 | 16,32,35 | 0.77 | 0 |
| 30 | PSU | 0 | 2621 | 30 | 13,21,22 | 1.61 | 2 (15%) | 18,30,33 | 6.13 | 4 (22%) |
| 30 | 1MA | 0 | 628 | 30,34 | 14,25,26 | 0.98 | 1 (7%) | 15,37,40 | 1.14 | 1 (6%) |

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 | 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 | 30,34 | - | 0/3/25/26 | 0/3/3/3 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 30 | 0 | 2621 | PSU | C5-C1' | -4.85 | 1.48 | 1.52 |
| 30 | 0 | 628 | 1MA | C6-N6 | 2.50 | 1.33 | 1.29 |
| 30 | 0 | 2621 | PSU | C4-N3 | 2.52 | 1.37 | 1.33 |
| 30 | 0 | 2587 | OMU | C4-N3 | 2.55 | 1.37 | 1.33 |
| 30 | 0 | 2588 | OMG | C6-N1 | 3.21 | 1.39 | 1.33 |

All (10) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 30 | 0 | 2621 | PSU | N1-C2-N3 | -21.44 | 114.66 | 128.33 |
| 30 | 0 | 2588 | OMG | C5-C6-N1 | -8.73 | 111.66 | 123.59 |
| 30 | 0 | 628 | 1MA | C2-N3-C4 | -3.74 | 110.61 | 116.40 |
| 30 | 0 | 2587 | OMU | C5-C4-N3 | -3.31 | 114.63 | 123.12 |
| 30 | 0 | 2588 | OMG | N3-C2-N1 | -2.38 | 123.81 | 127.44 |
| 30 | 0 | 2621 | PSU | C5-C1'-C2' | -2.04 | 111.90 | 115.52 |
| 30 | 0 | 2621 | PSU | C6-N1-C2 | 2.73 | 119.86 | 115.47 |
| 30 | 0 | 2588 | OMG | C6-N1-C2 | 6.68 | 125.21 | 115.94 |
| 30 | 0 | 2587 | OMU | C4-N3-C2 | 13.10 | 127.12 | 114.14 |
| 30 | 0 | 2621 | PSU | C4-N3-C2 | 13.95 | 127.31 | 115.25 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 30 | 0 | 2587 | OMU | 2 | 0 |
| 30 | 0 | 628 | 1MA | 1 | 0 |

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 305 ligands modelled in this entry, 305 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%) | -0.21 | 7 (2%) 54 47 | 34, 56, 94, 116 | 0 |
| 2 | B | 337/338 (99%) | -0.41 | 2 (0%) 90 89 | 34, 58, 89, 99 | 0 |
| 3 | C | 246/246 (100%) | -0.23 | 4 (1%) 74 72 | 32, 51, 75, 87 | 0 |
| 4 | D | 140/177 (79%) | 1.67 | 51 (36%) 0 0 | 69, 106, 134, 144 | 0 |
| 5 | E | 172/178 (96%) | -0.09 | 9 (5%) 31 24 | 49, 73, 97, 102 | 0 |
| 6 | F | 119/120 (99%) | -0.00 | 6 (5%) 32 26 | 52, 76, 109, 124 | 0 |
| 7 | G | 29/348 (8%) | 0.54 | 2 (6%) 20 14 | 79, 103, 110, 113 | 0 |
| 8 | H | 160/177 (90%) | -0.33 | 2 (1%) 79 78 | 53, 73, 107, 111 | 0 |
| 9 | I | 70/162 (43%) | 3.88 | 49 (70%) 0 0 | 137, 155, 173, 175 | 0 |
| 10 | J | 142/145 (97%) | -0.64 | 0 100 100 | 43, 57, 77, 99 | 0 |
| 11 | K | 132/132 (100%) | -0.61 | 0 100 100 | 39, 54, 79, 83 | 0 |
| 12 | L | 145/165 (87%) | 0.35 | 5 (3%) 49 41 | 32, 71, 123, 134 | 0 |
| 13 | M | 194/196 (98%) | -0.47 | 1 (0%) 91 90 | 35, 49, 64, 71 | 0 |
| 14 | N | 186/187 (99%) | 0.26 | 17 (9%) 11 7 | 51, 74, 121, 131 | 0 |
| 15 | O | 115/116 (99%) | -0.48 | 0 100 100 | 44, 61, 78, 85 | 0 |
| 16 | P | 143/149 (95%) | -0.41 | 1 (0%) 89 88 | 47, 61, 74, 83 | 0 |
| 17 | Q | 95/96 (98%) | -0.48 | 0 100 100 | 44, 55, 72, 85 | 0 |
| 18 | R | 150/155 (96%) | -0.50 | 0 100 100 | 37, 51, 73, 84 | 0 |
| 19 | S | 81/85 (95%) | -0.04 | 2 (2%) 61 55 | 49, 64, 87, 97 | 0 |
| 20 | T | 119/120 (99%) | -0.16 | 3 (2%) 61 55 | 42, 62, 92, 121 | 0 |
| 21 | U | 53/67 (79%) | 0.03 | 1 (1%) 70 66 | 51, 64, 83, 91 | 0 |
| 22 | V | 65/71 (91%) | 1.10 | 14 (21%) 1 0 | 53, 76, 130, 134 | 0 |
| 23 | W | 154/154 (100%) | -0.69 | 0 100 100 | 41, 56, 74, 88 | 0 |
| 24 | X | 82/92 (89%) | -0.31 | 0 100 100 | 49, 66, 91, 108 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 25 | Y | 142/241 (58%) | -0.50 | 1 (0%) 89 88 | 34, 48, 72, 94 | 0 |
| 26 | Z | 73/116 (62%) | 0.20 | 6 (8%) 14 9 | 59, 77, 92, 101 | 0 |
| 27 | 1 | 56/57 (98%) | -0.23 | 0 100 100 | 33, 39, 48, 56 | 0 |
| 28 | 2 | 46/50 (92%) | -0.13 | 1 (2%) 65 60 | 41, 69, 102, 114 | 0 |
| 29 | 3 | 92/92 (100%) | -0.11 | 1 (1%) 82 80 | 43, 65, 78, 91 | 0 |
| 30 | 0 | 2749/2923 (94%) | -0.27 | 46 (1%) 73 70 | 28, 51, 95, 171 | 0 |
| 31 | 9 | 122/122 (100%) | -0.23 | 2 (1%) 74 72 | 45, 72, 95, 154 | 0 |
| All | All | 6646/7517 (88%) | -0.17 | 233 (3%) 48 40 | 28, 57, 106, 175 | 0 |

All (233) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 9 | I | 71 | ALA | 15.2 |
| 9 | I | 74 | ILE | 13.4 |
| 22 | V | 1 | THR | 12.2 |
| 9 | I | 72 | GLU | 11.3 |
| 22 | V | 43 | PRO | 11.0 |
| 9 | I | 70 | THR | 10.1 |
| 9 | I | 80 | PHE | 8.9 |
| 9 | I | 82 | THR | 8.8 |
| 31 | 9 | 1 | U | 8.6 |
| 9 | I | 83 | GLY | 8.4 |
| 9 | I | 88 | GLN | 8.1 |
| 14 | N | 166 | ALA | 7.9 |
| 9 | I | 132 | VAL | 7.1 |
| 9 | I | 81 | GLU | 6.9 |
| 9 | I | 112 | LEU | 6.9 |
| 9 | I | 79 | GLY | 6.9 |
| 9 | I | 128 | THR | 6.5 |
| 9 | I | 69 | PRO | 6.1 |
| 22 | V | 40 | PRO | 5.9 |
| 4 | D | 18 | ILE | 5.7 |
| 9 | I | 84 | SER | 5.7 |
| 9 | I | 92 | VAL | 5.4 |
| 22 | V | 39 | ALA | 5.4 |
| 4 | D | 10 | PHE | 5.4 |
| 4 | D | 63 | ILE | 5.4 |
| 14 | N | 147 | ILE | 5.4 |
| 9 | I | 75 | LYS | 5.3 |
| 9 | I | 111 | LEU | 5.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 30 | 0 | 1172 | G | 5.3 |
| 12 | L | 60 | GLU | 5.3 |
| 4 | D | 69 | ILE | 5.2 |
| 22 | V | 46 | ILE | 5.2 |
| 30 | 0 | 735 | C | 5.2 |
| 9 | I | 86 | GLU | 5.2 |
| 9 | I | 66 | GLY | 5.0 |
| 4 | D | 57 | THR | 5.0 |
| 26 | Z | 35 | SER | 4.9 |
| 20 | T | 119 | ALA | 4.8 |
| 4 | D | 26 | GLY | 4.8 |
| 30 | 0 | 1175 | G | 4.7 |
| 9 | I | 130 | LEU | 4.6 |
| 9 | I | 131 | GLY | 4.6 |
| 4 | D | 134 | LEU | 4.6 |
| 9 | I | 93 | ALA | 4.6 |
| 26 | Z | 46 | SER | 4.5 |
| 14 | N | 138 | ASP | 4.5 |
| 14 | N | 75 | THR | 4.5 |
| 1 | A | 37 | VAL | 4.4 |
| 30 | 0 | 1168 | C | 4.4 |
| 4 | D | 75 | LEU | 4.3 |
| 30 | 0 | 1169 | U | 4.3 |
| 30 | 0 | 1171 | A | 4.2 |
| 1 | A | 237 | GLY | 4.2 |
| 9 | I | 126 | THR | 4.2 |
| 9 | I | 109 | PRO | 4.2 |
| 9 | I | 127 | CYS | 4.2 |
| 9 | I | 91 | PHE | 4.1 |
| 9 | I | 113 | SER | 4.1 |
| 30 | 0 | 1176 | C | 4.0 |
| 4 | D | 101 | THR | 4.0 |
| 30 | 0 | 1195 | G | 4.0 |
| 4 | D | 27 | ILE | 4.0 |
| 9 | I | 129 | SER | 3.9 |
| 4 | D | 104 | PHE | 3.9 |
| 30 | 0 | 1173 | A | 3.9 |
| 4 | D | 85 | GLN | 3.8 |
| 9 | I | 76 | ASP | 3.8 |
| 30 | 0 | 1166 | A | 3.8 |
| 30 | 0 | 1174 | A | 3.8 |
| 26 | Z | 58 | ASN | 3.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 30 | 0 | 1177 | A | 3.8 |
| 4 | D | 44 | ILE | 3.8 |
| 1 | A | 35 | GLY | 3.7 |
| 4 | D | 25 | MET | 3.7 |
| 4 | D | 23 | VAL | 3.7 |
| 4 | D | 90 | LEU | 3.7 |
| 1 | A | 236 | GLY | 3.7 |
| 30 | 0 | 1170 | U | 3.7 |
| 4 | D | 135 | VAL | 3.6 |
| 7 | G | 27 | ILE | 3.6 |
| 4 | D | 128 | LEU | 3.6 |
| 14 | N | 113 | SER | 3.6 |
| 6 | F | 106 | ALA | 3.6 |
| 14 | N | 165 | ALA | 3.6 |
| 4 | D | 102 | GLY | 3.6 |
| 4 | D | 107 | GLY | 3.6 |
| 30 | 0 | 1192 | A | 3.6 |
| 12 | L | 106 | VAL | 3.6 |
| 30 | 0 | 1181 | A | 3.6 |
| 30 | 0 | 1193 | A | 3.5 |
| 4 | D | 154 | LYS | 3.5 |
| 9 | I | 97 | VAL | 3.5 |
| 30 | 0 | 1167 | G | 3.5 |
| 4 | D | 17 | ARG | 3.5 |
| 22 | V | 51 | LYS | 3.5 |
| 30 | 0 | 1190 | G | 3.4 |
| 9 | I | 106 | GLN | 3.4 |
| 30 | 0 | 1165 | G | 3.4 |
| 30 | 0 | 1178 | G | 3.4 |
| 4 | D | 70 | GLY | 3.4 |
| 30 | 0 | 1199 | A | 3.4 |
| 4 | D | 73 | VAL | 3.4 |
| 4 | D | 93 | LEU | 3.4 |
| 22 | V | 44 | GLY | 3.4 |
| 8 | H | 158 | ASN | 3.4 |
| 20 | T | 118 | SER | 3.4 |
| 14 | N | 158 | LEU | 3.4 |
| 9 | I | 73 | LEU | 3.4 |
| 30 | 0 | 1207 | A | 3.3 |
| 30 | 0 | 1947 | G | 3.3 |
| 9 | I | 67 | VAL | 3.3 |
| 30 | 0 | 1202 | A | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 9 | I | 103 | ILE | 3.2 |
| 9 | I | 104 | ALA | 3.2 |
| 5 | E | 157 | LYS | 3.2 |
| 30 | 0 | 1163 | G | 3.2 |
| 30 | 0 | 2237 | G | 3.2 |
| 4 | D | 92 | GLU | 3.2 |
| 9 | I | 85 | GLY | 3.1 |
| 5 | E | 108 | LEU | 3.1 |
| 9 | I | 125 | GLY | 3.1 |
| 22 | V | 52 | ALA | 3.1 |
| 4 | D | 165 | PHE | 3.1 |
| 4 | D | 130 | VAL | 3.1 |
| 4 | D | 106 | PHE | 3.1 |
| 16 | P | 67 | LYS | 3.1 |
| 9 | I | 87 | PRO | 3.1 |
| 9 | I | 100 | VAL | 3.0 |
| 4 | D | 98 | PHE | 3.0 |
| 4 | D | 19 | GLU | 3.0 |
| 4 | D | 89 | PRO | 3.0 |
| 22 | V | 2 | VAL | 3.0 |
| 30 | 0 | 1951 | G | 3.0 |
| 5 | E | 10 | ASP | 3.0 |
| 9 | I | 108 | HIS | 3.0 |
| 4 | D | 40 | ILE | 2.9 |
| 5 | E | 45 | ASP | 2.9 |
| 5 | E | 154 | ILE | 2.9 |
| 14 | N | 80 | SER | 2.8 |
| 19 | S | 81 | ILE | 2.8 |
| 30 | 0 | 1200 | A | 2.8 |
| 12 | L | 99 | GLU | 2.8 |
| 22 | V | 48 | GLU | 2.8 |
| 28 | 2 | 39 | ARG | 2.8 |
| 30 | 0 | 282 | C | 2.8 |
| 9 | I | 110 | ASP | 2.7 |
| 20 | T | 82 | THR | 2.7 |
| 30 | 0 | 1198 | U | 2.7 |
| 9 | I | 133 | THR | 2.7 |
| 19 | S | 76 | GLU | 2.7 |
| 4 | D | 56 | ARG | 2.7 |
| 6 | F | 49 | PHE | 2.7 |
| 2 | B | 337 | GLY | 2.7 |
| 30 | 0 | 1162 | G | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 99 | ILE | 2.6 |
| 4 | D | 24 | HIS | 2.6 |
| 9 | I | 99 | GLN | 2.6 |
| 4 | D | 41 | LEU | 2.6 |
| 12 | L | 105 | TYR | 2.6 |
| 4 | D | 74 | THR | 2.6 |
| 4 | D | 81 | GLU | 2.6 |
| 4 | D | 11 | HIS | 2.6 |
| 7 | G | 26 | MET | 2.6 |
| 30 | 0 | 1164 | U | 2.6 |
| 9 | I | 94 | ASP | 2.6 |
| 14 | N | 134 | ASP | 2.6 |
| 6 | F | 44 | SER | 2.6 |
| 30 | 0 | 1191 | A | 2.6 |
| 13 | M | 194 | GLY | 2.5 |
| 5 | E | 11 | VAL | 2.5 |
| 30 | 0 | 1179 | C | 2.5 |
| 14 | N | 159 | TYR | 2.5 |
| 30 | 0 | 1203 | G | 2.5 |
| 3 | C | 60 | SER | 2.5 |
| 9 | I | 90 | ASP | 2.5 |
| 4 | D | 158 | ASN | 2.5 |
| 30 | 0 | 1208 | C | 2.5 |
| 3 | C | 64 | GLY | 2.5 |
| 1 | A | 31 | LYS | 2.4 |
| 4 | D | 45 | THR | 2.4 |
| 14 | N | 160 | SER | 2.4 |
| 2 | B | 115 | VAL | 2.4 |
| 30 | 0 | 1201 | C | 2.4 |
| 4 | D | 157 | LEU | 2.4 |
| 5 | E | 6 | GLU | 2.4 |
| 14 | N | 41 | LYS | 2.4 |
| 5 | E | 156 | ASP | 2.4 |
| 6 | F | 15 | ASP | 2.4 |
| 30 | 0 | 1204 | C | 2.4 |
| 30 | 0 | 280 | C | 2.3 |
| 9 | I | 68 | PRO | 2.3 |
| 4 | D | 95 | THR | 2.3 |
| 9 | I | 102 | GLN | 2.3 |
| 30 | 0 | 1194 | A | 2.3 |
| 4 | D | 172 | VAL | 2.3 |
| 22 | V | 41 | GLU | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 110 | SER | 2.3 |
| 22 | V | 37 | GLY | 2.3 |
| 30 | 0 | 970 | U | 2.3 |
| 4 | D | 88 | LEU | 2.3 |
| 22 | V | 3 | LEU | 2.3 |
| 9 | I | 78 | ALA | 2.3 |
| 30 | 0 | 1182 | C | 2.3 |
| 29 | 3 | 13 | HIS | 2.2 |
| 4 | D | 84 | LEU | 2.2 |
| 26 | Z | 50 | VAL | 2.2 |
| 8 | H | 40 | GLN | 2.2 |
| 25 | Y | 235 | GLU | 2.2 |
| 6 | F | 16 | ALA | 2.2 |
| 6 | F | 75 | ILE | 2.2 |
| 3 | C | 135 | GLU | 2.2 |
| 4 | D | 138 | GLY | 2.2 |
| 30 | 0 | 1196 | C | 2.2 |
| 21 | U | 51 | TRP | 2.2 |
| 4 | D | 13 | MET | 2.2 |
| 14 | N | 140 | GLN | 2.2 |
| 30 | 0 | 1965 | C | 2.1 |
| 14 | N | 112 | GLY | 2.1 |
| 14 | N | 146 | HIS | 2.1 |
| 14 | N | 145 | ALA | 2.1 |
| 4 | D | 105 | SER | 2.1 |
| 30 | 0 | 1948 | G | 2.1 |
| 31 | 9 | 2 | U | 2.1 |
| 26 | Z | 44 | ARG | 2.1 |
| 30 | 0 | 1161 | A | 2.1 |
| 5 | E | 161 | VAL | 2.1 |
| 12 | L | 149 | ARG | 2.1 |
| 26 | Z | 83 | TYR | 2.1 |
| 14 | N | 137 | ALA | 2.1 |
| 3 | C | 66 | GLY | 2.0 |
| 22 | V | 49 | LEU | 2.0 |
| 4 | D | 141 | VAL | 2.0 |
| 4 | D | 166 | ILE | 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 | 1MA | 0 | 628 | 23/24 | 0.98 | 0.18 | - | 33,37,38,39 | 0 |
| 30 | OMG | 0 | 2588 | 24/25 | 0.99 | 0.14 | - | 36,39,42,43 | 0 |
| 30 | OMU | 0 | 2587 | 21/22 | 0.99 | 0.13 | - | 38,40,44,45 | 0 |
| 30 | PSU | 0 | 2621 | 20/21 | 0.98 | 0.18 | - | 34,35,47,48 | 0 |
| 30 | UR3 | 0 | 2619 | 21/22 | 0.98 | 0.15 | - | 42,44,47,47 | 0 |

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 34 | NA | 0 | 8565 | 1/1 | 0.87 | 1.24 | 97.52 | 79,79,79,79 | 0 |
| 34 | NA | 0 | 8547 | 1/1 | 0.91 | 0.70 | 73.51 | 80,80,80,80 | 0 |
| 34 | NA | 0 | 8562 | 1/1 | 0.69 | 1.31 | 72.93 | 78,78,78,78 | 0 |
| 34 | NA | 0 | 8560 | 1/1 | 0.19 | 0.89 | 36.93 | 101,101,101,101 | 0 |
| 33 | K | 0 | 8401 | 1/1 | 0.41 | 0.78 | 30.06 | 128,128,128,128 | 0 |
| 34 | NA | 0 | 8564 | 1/1 | 0.93 | 0.39 | 27.90 | 68,68,68,68 | 0 |
| 34 | NA | 0 | 8555 | 1/1 | 0.96 | 0.81 | 25.22 | 75,75,75,75 | 0 |
| 34 | NA | 9 | 8572 | 1/1 | 0.96 | 0.89 | 21.13 | 81,81,81,81 | 0 |
| 34 | NA | 0 | 8559 | 1/1 | 0.92 | 0.29 | 16.79 | 91,91,91,91 | 0 |
| 34 | NA | 0 | 8528 | 1/1 | 0.65 | 0.55 | 13.46 | 66,66,66,66 | 0 |
| 34 | NA | 0 | 8553 | 1/1 | 0.98 | 0.46 | 12.64 | 65,65,65,65 | 0 |
| 32 | MG | 0 | 8085 | 1/1 | 0.98 | 0.53 | 12.56 | 97,97,97,97 | 0 |
| 36 | SR | B | 8987 | 1/1 | 0.80 | 0.56 | 10.79 | 200,200,200,200 | 0 |
| 34 | NA | 0 | 8521 | 1/1 | 0.91 | 0.39 | 9.53 | 61,61,61,61 | 0 |
| 34 | NA | 0 | 8542 | 1/1 | 0.96 | 0.45 | 9.03 | 49,49,49,49 | 0 |
| 34 | NA | 0 | 8567 | 1/1 | 0.88 | 0.36 | 8.01 | 76,76,76,76 | 0 |
| 34 | NA | 0 | 8556 | 1/1 | 0.96 | 0.82 | 7.68 | 64,64,64,64 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 36 | SR | 0 | 8903 | 1/1 | 1.00 | 0.19 | 7.63 | 59,59,59,59 | 0 |
| 32 | MG | A | 8051 | 1/1 | 0.93 | 0.65 | 7.37 | 70,70,70,70 | 0 |
| 34 | NA | 0 | 8546 | 1/1 | 0.84 | 0.40 | 7.31 | 65,65,65,65 | 0 |
| 32 | MG | 0 | 8047 | 1/1 | 0.96 | 0.32 | 6.31 | 51,51,51,51 | 0 |
| 34 | NA | 0 | 8527 | 1/1 | 0.81 | 0.27 | 5.82 | 71,71,71,71 | 0 |
| 34 | NA | 0 | 8563 | 1/1 | 0.69 | 0.28 | 4.99 | 88,88,88,88 | 0 |
| 36 | SR | 0 | 8949 | 1/1 | 0.98 | 0.16 | 4.90 | 122,122,122,122 | 0 |
| 34 | NA | R | 8575 | 1/1 | 0.93 | 0.25 | 4.29 | 99,99,99,99 | 0 |
| 32 | MG | 0 | 8014 | 1/1 | 0.95 | 0.20 | 3.99 | 33,33,33,33 | 0 |
| 32 | MG | 0 | 8009 | 1/1 | 0.98 | 0.25 | 3.75 | 36,36,36,36 | 0 |
| 34 | NA | 0 | 8530 | 1/1 | 0.74 | 0.32 | 3.55 | 59,59,59,59 | 0 |
| 33 | K | 0 | 8402 | 1/1 | 0.98 | 0.25 | 3.53 | 76,76,76,76 | 0 |
| 32 | MG | 0 | 8041 | 1/1 | 0.96 | 0.21 | 3.23 | 29,29,29,29 | 0 |
| 36 | SR | 0 | 8904 | 1/1 | 0.99 | 0.18 | 3.08 | 65,65,65,65 | 0 |
| 32 | MG | 0 | 8028 | 1/1 | 0.98 | 0.16 | 2.27 | 26,26,26,26 | 0 |
| 32 | MG | 0 | 8084 | 1/1 | 0.99 | 0.15 | 2.17 | 33,33,33,33 | 0 |
| 34 | NA | M | 8539 | 1/1 | 0.99 | 0.18 | 1.97 | 34,34,34,34 | 0 |
| 36 | SR | A | 8929 | 1/1 | 0.92 | 0.23 | 1.84 | 144,144,144,144 | 0 |
| 34 | NA | 0 | 8537 | 1/1 | 0.95 | 0.18 | 1.65 | 38,38,38,38 | 0 |
| 36 | SR | 0 | 8918 | 1/1 | 0.99 | 0.15 | 1.59 | 80,80,80,80 | 0 |
| 32 | MG | 0 | 8003 | 1/1 | 0.96 | 0.19 | 1.54 | 45,45,45,45 | 0 |
| 32 | MG | 0 | 8004 | 1/1 | 1.00 | 0.19 | 1.41 | 32,32,32,32 | 0 |
| 36 | SR | 0 | 8944 | 1/1 | 0.79 | 0.14 | 1.21 | 169,169,169,169 | 0 |
| 34 | NA | 0 | 8558 | 1/1 | 0.97 | 0.23 | 1.14 | 49,49,49,49 | 0 |
| 32 | MG | 0 | 8088 | 1/1 | 0.98 | 0.21 | 1.12 | 52,52,52,52 | 0 |
| 36 | SR | R | 8912 | 1/1 | 0.99 | 0.17 | 0.80 | 92,92,92,92 | 0 |
| 36 | SR | 0 | 8985 | 1/1 | 0.90 | 0.13 | 0.72 | 134,134,134,134 | 0 |
| 32 | MG | 0 | 8044 | 1/1 | 0.92 | 0.16 | 0.60 | 50,50,50,50 | 0 |
| 32 | MG | K | 8054 | 1/1 | 0.99 | 0.16 | 0.39 | 46,46,46,46 | 0 |
| 34 | NA | C | 8503 | 1/1 | 0.97 | 0.21 | 0.28 | 36,36,36,36 | 0 |
| 34 | NA | 0 | 8519 | 1/1 | 0.96 | 0.20 | 0.28 | 43,43,43,43 | 0 |
| 34 | NA | 0 | 8515 | 1/1 | 0.94 | 0.20 | 0.26 | 41,41,41,41 | 0 |
| 34 | NA | 0 | 8504 | 1/1 | 0.88 | 0.18 | 0.22 | 44,44,44,44 | 0 |
| 32 | MG | 0 | 8053 | 1/1 | 0.95 | 0.20 | 0.15 | 47,47,47,47 | 0 |
| 32 | MG | 0 | 8011 | 1/1 | 0.92 | 0.23 | 0.08 | 25,25,25,25 | 0 |
| 34 | NA | 0 | 8568 | 1/1 | 0.79 | 0.21 | 0.02 | 52,52,52,52 | 0 |
| 34 | NA | J | 8538 | 1/1 | 0.83 | 0.18 | -0.02 | 56,56,56,56 | 0 |
| 32 | MG | 0 | 8034 | 1/1 | 0.98 | 0.16 | -0.07 | 46,46,46,46 | 0 |
| 32 | MG | 0 | 8010 | 1/1 | 0.99 | 0.22 | -0.15 | 45,45,45,45 | 0 |
| 32 | MG | 0 | 8015 | 1/1 | 0.99 | 0.13 | -0.20 | 30,30,30,30 | 0 |
| 36 | SR | 0 | 8992 | 1/1 | 0.88 | 0.15 | -0.21 | 136,136,136,136 | 0 |
| 37 | CD | Z | 8703 | 1/1 | 0.99 | 0.13 | -0.35 | 75,75,75,75 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 36 | SR | 0 | 8972 | 1/1 | 0.90 | 0.14 | -0.54 | 146,146,146,146 | 0 |
| 35 | CL | J | 8821 | 1/1 | 0.95 | 0.14 | -0.63 | 67,67,67,67 | 0 |
| 37 | CD | 1 | 8702 | 1/1 | 0.99 | 0.13 | -0.66 | 67,67,67,67 | 0 |
| 32 | MG | 0 | 8002 | 1/1 | 0.97 | 0.15 | -0.67 | 36,36,36,36 | 0 |
| 32 | MG | 0 | 8067 | 1/1 | 0.83 | 0.16 | -0.75 | 40,40,40,40 | 0 |
| 36 | SR | 0 | 8975 | 1/1 | 0.91 | 0.14 | -0.77 | 130,130,130,130 | 0 |
| 34 | NA | 0 | 8517 | 1/1 | 0.99 | 0.15 | -0.93 | 31,31,31,31 | 0 |
| 32 | MG | 0 | 8062 | 1/1 | 0.91 | 0.15 | -1.12 | 59,59,59,59 | 0 |
| 34 | NA | Q | 8540 | 1/1 | 0.78 | 0.11 | -1.14 | 64,64,64,64 | 0 |
| 34 | NA | 0 | 8569 | 1/1 | 0.93 | 0.15 | -1.15 | 48,48,48,48 | 0 |
| 37 | CD | 3 | 8704 | 1/1 | 1.00 | 0.10 | -1.17 | 74,74,74,74 | 0 |
| 34 | NA | 0 | 8520 | 1/1 | 0.95 | 0.07 | -1.19 | 49,49,49,49 | 0 |
| 32 | MG | 0 | 8058 | 1/1 | 1.00 | 0.10 | -1.22 | 22,22,22,22 | 0 |
| 32 | MG | T | 8057 | 1/1 | 0.94 | 0.12 | -1.22 | 60,60,60,60 | 0 |
| 32 | MG | 0 | 8043 | 1/1 | 0.99 | 0.06 | -1.23 | 52,52,52,52 | 0 |
| 36 | SR | 1 | 8913 | 1/1 | 0.97 | 0.14 | -1.41 | 95,95,95,95 | 0 |
| 36 | SR | 0 | 8936 | 1/1 | 0.91 | 0.11 | -1.42 | 94,94,94,94 | 0 |
| 32 | MG | 0 | 8025 | 1/1 | 0.98 | 0.12 | -1.42 | 37,37,37,37 | 0 |
| 36 | SR | F | 9005 | 1/1 | 0.99 | 0.08 | -1.45 | 133,133,133,133 | 0 |
| 36 | SR | 0 | 8902 | 1/1 | 0.99 | 0.17 | -1.55 | 66,66,66,66 | 0 |
| 37 | CD | U | 8701 | 1/1 | 0.99 | 0.10 | -1.57 | 63,63,63,63 | 0 |
| 36 | SR | 0 | 8935 | 1/1 | 0.99 | 0.09 | -1.62 | 79,79,79,79 | 0 |
| 34 | NA | 0 | 8534 | 1/1 | 0.97 | 0.14 | -1.65 | 44,44,44,44 | 0 |
| 34 | NA | 0 | 8533 | 1/1 | 0.95 | 0.10 | -1.68 | 55,55,55,55 | 0 |
| 35 | CL | L | 8810 | 1/1 | 0.94 | 0.09 | -1.84 | 68,68,68,68 | 0 |
| 32 | MG | 0 | 8045 | 1/1 | 0.92 | 0.09 | -1.92 | 44,44,44,44 | 0 |
| 35 | CL | O | 8808 | 1/1 | 0.91 | 0.08 | -1.93 | 70,70,70,70 | 0 |
| 36 | SR | 0 | 8969 | 1/1 | 0.94 | 0.12 | -2.02 | 159,159,159,159 | 0 |
| 32 | MG | 0 | 8012 | 1/1 | 0.98 | 0.14 | -2.02 | 18,18,18,18 | 0 |
| 34 | NA | 0 | 8557 | 1/1 | 0.82 | 0.06 | -2.02 | 53,53,53,53 | 0 |
| 35 | CL | M | 8818 | 1/1 | 0.96 | 0.09 | -2.03 | 40,40,40,40 | 0 |
| 32 | MG | 0 | 8008 | 1/1 | 1.00 | 0.09 | -2.10 | 28,28,28,28 | 0 |
| 32 | MG | 0 | 8050 | 1/1 | 0.97 | 0.09 | -2.13 | 32,32,32,32 | 0 |
| 35 | CL | 0 | 8813 | 1/1 | 0.93 | 0.09 | -2.26 | 66,66,66,66 | 0 |
| 32 | MG | 0 | 8016 | 1/1 | 0.96 | 0.14 | -2.26 | 48,48,48,48 | 0 |
| 34 | NA | 0 | 8523 | 1/1 | 0.96 | 0.09 | -2.51 | 50,50,50,50 | 0 |
| 35 | CL | 0 | 8816 | 1/1 | 0.99 | 0.08 | -2.53 | 79,79,79,79 | 0 |
| 35 | CL | 3 | 8804 | 1/1 | 0.98 | 0.06 | -2.60 | 63,63,63,63 | 0 |
| 34 | NA | 0 | 8512 | 1/1 | 0.94 | 0.15 | -2.69 | 52,52,52,52 | 0 |
| 32 | MG | 0 | 8056 | 1/1 | 0.93 | 0.11 | -2.89 | 47,47,47,47 | 0 |
| 32 | MG | 0 | 8079 | 1/1 | 0.97 | 0.11 | -2.98 | 51,51,51,51 | 0 |
| 36 | SR | A | 8930 | 1/1 | 0.99 | 0.06 | -2.98 | 97,97,97,97 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 36 | SR | 0 | 8948 | 1/1 | 0.99 | 0.10 | -3.14 | 92,92,92,92 | 0 |
| 35 | CL | 0 | 8812 | 1/1 | 0.98 | 0.06 | -3.18 | 58,58,58,58 | 0 |
| 34 | NA | 0 | 8507 | 1/1 | 0.98 | 0.11 | -3.20 | 37,37,37,37 | 0 |
| 36 | SR | 0 | 8943 | 1/1 | 0.96 | 0.04 | -3.33 | 124,124,124,124 | 0 |
| 35 | CL | 0 | 8805 | 1/1 | 0.98 | 0.06 | -3.47 | 67,67,67,67 | 0 |
| 32 | MG | 0 | 8021 | 1/1 | 0.97 | 0.05 | -3.62 | 40,40,40,40 | 0 |
| 32 | MG | 0 | 8006 | 1/1 | 0.93 | 0.10 | -3.62 | 32,32,32,32 | 0 |
| 32 | MG | Y | 8086 | 1/1 | 0.99 | 0.08 | -3.72 | 44,44,44,44 | 0 |
| 32 | MG | 0 | 8001 | 1/1 | 0.96 | 0.11 | -3.88 | 33,33,33,33 | 0 |
| 32 | MG | 0 | 8052 | 1/1 | 0.98 | 0.07 | -3.98 | 56,56,56,56 | 0 |
| 32 | MG | 0 | 8013 | 1/1 | 0.97 | 0.06 | -4.46 | 25,25,25,25 | 0 |
| 32 | MG | 0 | 8065 | 1/1 | 0.98 | 0.06 | -4.68 | 57,57,57,57 | 0 |
| 34 | NA | B | 8552 | 1/1 | 0.98 | 0.10 | -5.15 | 83,83,83,83 | 0 |
| 36 | SR | 0 | 8970 | 1/1 | 0.99 | 0.01 | -6.07 | 123,123,123,123 | 0 |
| 32 | MG | 0 | 8075 | 1/1 | 0.93 | 0.03 | -6.54 | 42,42,42,42 | 0 |
| 36 | SR | 0 | 8945 | 1/1 | 0.97 | 0.07 | -6.57 | 106,106,106,106 | 0 |
| 36 | SR | 0 | 8910 | 1/1 | 0.98 | 0.04 | -7.09 | 100,100,100,100 | 0 |
| 36 | SR | 0 | 8984 | 1/1 | 0.98 | 0.03 | -9.15 | 121,121,121,121 | 0 |
| 35 | CL | B | 8819 | 1/1 | 0.98 | 0.09 | -9.73 | 58,58,58,58 | 0 |
| 32 | MG | 0 | 8089 | 1/1 | 0.93 | 0.17 | - | 72,72,72,72 | 0 |
| 36 | SR | 0 | 8955 | 1/1 | 0.68 | 0.21 | - | 199,199,199,199 | 0 |
| 36 | SR | 9 | 8978 | 1/1 | 0.99 | 0.08 | - | 135,135,135,135 | 0 |
| 36 | SR | 0 | 8941 | 1/1 | 0.98 | 0.14 | - | 108,108,108,108 | 0 |
| 35 | CL | 0 | 8822 | 1/1 | 0.97 | 0.45 | - | 81,81,81,81 | 0 |
| 36 | SR | 0 | 8914 | 1/1 | 0.98 | 0.32 | - | 120,120,120,120 | 0 |
| 32 | MG | 0 | 8035 | 1/1 | 0.96 | 0.10 | - | 54,54,54,54 | 0 |
| 36 | SR | 3 | 8999 | 1/1 | 0.98 | 0.10 | - | 110,110,110,110 | 0 |
| 34 | NA | 0 | 8561 | 1/1 | 0.94 | 0.22 | - | 68,68,68,68 | 0 |
| 36 | SR | B | 8950 | 1/1 | 0.98 | 0.14 | - | 116,116,116,116 | 0 |
| 35 | CL | 0 | 8814 | 1/1 | 0.94 | 0.21 | - | 72,72,72,72 | 0 |
| 32 | MG | 0 | 8023 | 1/1 | 0.98 | 0.10 | - | 37,37,37,37 | 0 |
| 32 | MG | 0 | 8072 | 1/1 | 0.81 | 0.18 | - | 63,63,63,63 | 0 |
| 34 | NA | 0 | 8536 | 1/1 | 0.91 | 0.24 | - | 61,61,61,61 | 0 |
| 36 | SR | 0 | 8954 | 1/1 | 0.97 | 0.10 | - | 109,109,109,109 | 0 |
| 36 | SR | 0 | 9002 | 1/1 | 0.92 | 0.29 | - | 177,177,177,177 | 0 |
| 32 | MG | 0 | 8033 | 1/1 | 0.94 | 0.09 | - | 55,55,55,55 | 0 |
| 36 | SR | 0 | 8966 | 1/1 | 0.95 | 0.10 | - | 107,107,107,107 | 0 |
| 32 | MG | 0 | 8063 | 1/1 | 0.98 | 0.14 | - | 80,80,80,80 | 0 |
| 32 | MG | 0 | 8020 | 1/1 | 0.97 | 0.07 | - | 40,40,40,40 | 0 |
| 35 | CL | 0 | 8803 | 1/1 | 0.95 | 0.10 | - | 58,58,58,58 | 0 |
| 32 | MG | 0 | 8078 | 1/1 | 0.98 | 0.27 | - | 69,69,69,69 | 0 |
| 32 | MG | 0 | 8024 | 1/1 | 0.97 | 0.12 | - | 49,49,49,49 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|-------|------|------|-----------------------------|-------|
| 34 | NA | 0 | 8550 | 1/1 | 0.86 | 0.96 | - | 57,57,57,57 | 0 |
| 36 | SR | 0 | 8983 | 1/1 | 0.98 | 0.24 | - | 170,170,170,170 | 0 |
| 32 | MG | 0 | 8080 | 1/1 | 0.99 | 0.12 | - | 75,75,75,75 | 0 |
| 36 | SR | 0 | 8981 | 1/1 | 0.98 | 0.34 | - | 178,178,178,178 | 0 |
| 34 | NA | 0 | 8509 | 1/1 | 0.70 | 0.92 | - | 85,85,85,85 | 0 |
| 32 | MG | 0 | 8073 | 1/1 | 0.99 | 0.34 | - | 73,73,73,73 | 0 |
| 32 | MG | 0 | 8083 | 1/1 | 0.91 | 0.10 | - | 60,60,60,60 | 0 |
| 36 | SR | 0 | 8921 | 1/1 | 0.96 | 0.15 | - | 96,96,96,96 | 0 |
| 32 | MG | 9 | 8074 | 1/1 | 0.84 | 0.09 | - | 86,86,86,86 | 0 |
| 36 | SR | 0 | 8920 | 1/1 | 0.97 | 0.08 | - | 135,135,135,135 | 0 |
| 36 | SR | 0 | 8982 | 1/1 | 0.73 | 2.26 | - | 200,200,200,200 | 0 |
| 36 | SR | 0 | 9000 | 1/1 | 0.94 | 0.07 | - | 176,176,176,176 | 0 |
| 36 | SR | 0 | 8905 | 1/1 | 1.00 | 0.27 | - | 61,61,61,61 | 0 |
| 32 | MG | 0 | 8018 | 1/1 | 1.00 | 0.24 | - | 40,40,40,40 | 0 |
| 32 | MG | 0 | 8059 | 1/1 | 0.99 | 0.07 | - | 57,57,57,57 | 0 |
| 36 | SR | 0 | 8938 | 1/1 | 0.98 | 0.02 | - | 147,147,147,147 | 0 |
| 36 | SR | 0 | 8946 | 1/1 | 0.91 | 0.22 | - | 123,123,123,123 | 0 |
| 32 | MG | 0 | 8060 | 1/1 | 0.94 | 0.08 | - | 53,53,53,53 | 0 |
| 32 | MG | 0 | 8036 | 1/1 | 0.94 | 0.12 | - | 56,56,56,56 | 0 |
| 34 | NA | 0 | 8501 | 1/1 | 0.87 | 0.08 | - | 40,40,40,40 | 0 |
| 36 | SR | 0 | 8906 | 1/1 | 0.99 | 0.23 | - | 64,64,64,64 | 0 |
| 35 | CL | Y | 8820 | 1/1 | 0.97 | 0.04 | - | 48,48,48,48 | 0 |
| 36 | SR | 0 | 8947 | 1/1 | 0.54 | 0.51 | - | 200,200,200,200 | 0 |
| 32 | MG | 0 | 8069 | 1/1 | 0.98 | 0.30 | - | 73,73,73,73 | 0 |
| 34 | NA | 0 | 8524 | 1/1 | 0.97 | 0.25 | - | 58,58,58,58 | 0 |
| 34 | NA | 0 | 8573 | 1/1 | 0.88 | 0.35 | - | 73,73,73,73 | 0 |
| 36 | SR | 0 | 8933 | 1/1 | 0.98 | 0.16 | - | 139,139,139,139 | 0 |
| 32 | MG | 0 | 8070 | 1/1 | 0.95 | 0.12 | - | 46,46,46,46 | 0 |
| 32 | MG | 0 | 8082 | 1/1 | 0.95 | 0.78 | - | 89,89,89,89 | 0 |
| 36 | SR | 0 | 8963 | 1/1 | 0.96 | 0.17 | - | 112,112,112,112 | 0 |
| 35 | CL | A | 8809 | 1/1 | 0.91 | 0.11 | - | 80,80,80,80 | 0 |
| 32 | MG | 0 | 8066 | 1/1 | 0.92 | 0.18 | - | 70,70,70,70 | 0 |
| 34 | NA | 0 | 8514 | 1/1 | 0.98 | 0.50 | - | 56,56,56,56 | 0 |
| 36 | SR | 0 | 9006 | 1/1 | -0.20 | 2.27 | - | 200,200,200,200 | 0 |
| 32 | MG | 0 | 8039 | 1/1 | 0.92 | 0.27 | - | 76,76,76,76 | 0 |
| 36 | SR | 0 | 8931 | 1/1 | 0.99 | 0.07 | - | 113,113,113,113 | 0 |
| 36 | SR | 0 | 8973 | 1/1 | 0.94 | 0.05 | - | 130,130,130,130 | 0 |
| 35 | CL | 0 | 8817 | 1/1 | 0.99 | 0.15 | - | 67,67,67,67 | 0 |
| 34 | NA | 0 | 8531 | 1/1 | 0.97 | 0.06 | - | 40,40,40,40 | 0 |
| 37 | CD | O | 8705 | 1/1 | 0.99 | 0.06 | - | 118,118,118,118 | 0 |
| 35 | CL | N | 8807 | 1/1 | 0.93 | 0.17 | - | 69,69,69,69 | 0 |
| 34 | NA | 0 | 8571 | 1/1 | 0.82 | 0.16 | - | 76,76,76,76 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 36 | SR | 0 | 8997 | 1/1 | 0.84 | 0.84 | - | 200,200,200,200 | 0 |
| 36 | SR | 0 | 8998 | 1/1 | 0.82 | 0.19 | - | 173,173,173,173 | 0 |
| 32 | MG | 0 | 8064 | 1/1 | 0.99 | 0.18 | - | 44,44,44,44 | 0 |
| 32 | MG | 0 | 8040 | 1/1 | 0.96 | 0.21 | - | 96,96,96,96 | 0 |
| 32 | MG | 0 | 8077 | 1/1 | 0.93 | 0.06 | - | 45,45,45,45 | 0 |
| 32 | MG | 0 | 8037 | 1/1 | 0.93 | 0.14 | - | 88,88,88,88 | 0 |
| 36 | SR | 0 | 9008 | 1/1 | 0.95 | 0.17 | - | 95,95,95,95 | 0 |
| 36 | SR | 0 | 8959 | 1/1 | 0.91 | 0.37 | - | 163,163,163,163 | 0 |
| 36 | SR | 0 | 8926 | 1/1 | 0.98 | 0.17 | - | 108,108,108,108 | 0 |
| 34 | NA | 0 | 8549 | 1/1 | 0.91 | 0.51 | - | 52,52,52,52 | 0 |
| 36 | SR | 0 | 8958 | 1/1 | 0.96 | 0.06 | - | 122,122,122,122 | 0 |
| 36 | SR | 0 | 8901 | 1/1 | 0.94 | 0.08 | - | 91,91,91,91 | 0 |
| 36 | SR | 0 | 8951 | 1/1 | 0.90 | 0.04 | - | 148,148,148,148 | 0 |
| 32 | MG | 0 | 8076 | 1/1 | 0.99 | 0.08 | - | 40,40,40,40 | 0 |
| 36 | SR | 0 | 9001 | 1/1 | 0.81 | 0.08 | - | 173,173,173,173 | 0 |
| 36 | SR | S | 8961 | 1/1 | 0.94 | 0.06 | - | 121,121,121,121 | 0 |
| 32 | MG | 0 | 8022 | 1/1 | 0.97 | 0.21 | - | 44,44,44,44 | 0 |
| 32 | MG | 0 | 8049 | 1/1 | 0.88 | 0.30 | - | 69,69,69,69 | 0 |
| 36 | SR | 0 | 8957 | 1/1 | 0.97 | 0.14 | - | 195,195,195,195 | 0 |
| 32 | MG | 0 | 8091 | 1/1 | 0.93 | 0.07 | - | 57,57,57,57 | 0 |
| 32 | MG | 0 | 8019 | 1/1 | 0.99 | 0.20 | - | 28,28,28,28 | 0 |
| 36 | SR | 0 | 8990 | 1/1 | 0.99 | 0.10 | - | 139,139,139,139 | 0 |
| 32 | MG | 0 | 8017 | 1/1 | 0.98 | 0.19 | - | 52,52,52,52 | 0 |
| 32 | MG | 0 | 8055 | 1/1 | 0.94 | 0.16 | - | 53,53,53,53 | 0 |
| 36 | SR | 0 | 8939 | 1/1 | 0.97 | 0.09 | - | 149,149,149,149 | 0 |
| 34 | NA | 0 | 8535 | 1/1 | 0.83 | 0.53 | - | 61,61,61,61 | 0 |
| 36 | SR | 9 | 9003 | 1/1 | 0.94 | 0.09 | - | 171,171,171,171 | 0 |
| 34 | NA | 0 | 8506 | 1/1 | 0.69 | 0.16 | - | 64,64,64,64 | 0 |
| 36 | SR | 0 | 8991 | 1/1 | 0.64 | 0.07 | - | 199,199,199,199 | 0 |
| 36 | SR | 0 | 8956 | 1/1 | 0.99 | 0.06 | - | 155,155,155,155 | 0 |
| 34 | NA | 0 | 8522 | 1/1 | 0.90 | 1.14 | - | 79,79,79,79 | 0 |
| 36 | SR | 0 | 8994 | 1/1 | 0.75 | 0.43 | - | 200,200,200,200 | 0 |
| 36 | SR | 0 | 8907 | 1/1 | 1.00 | 0.15 | - | 56,56,56,56 | 0 |
| 36 | SR | 0 | 8911 | 1/1 | 0.99 | 0.08 | - | 85,85,85,85 | 0 |
| 32 | MG | 0 | 8026 | 1/1 | 0.97 | 0.08 | - | 35,35,35,35 | 0 |
| 35 | CL | J | 8802 | 1/1 | 0.95 | 0.21 | - | 75,75,75,75 | 0 |
| 36 | SR | 0 | 8908 | 1/1 | 0.96 | 0.08 | - | 116,116,116,116 | 0 |
| 34 | NA | 0 | 8574 | 1/1 | 0.89 | 0.26 | - | 59,59,59,59 | 0 |
| 35 | CL | Q | 8811 | 1/1 | 0.93 | 0.15 | - | 82,82,82,82 | 0 |
| 34 | NA | 0 | 8570 | 1/1 | 0.91 | 0.09 | - | 52,52,52,52 | 0 |
| 36 | SR | 0 | 8962 | 1/1 | 0.53 | 0.19 | - | 169,169,169,169 | 0 |
| 36 | SR | 0 | 8916 | 1/1 | 1.00 | 0.03 | - | 120,120,120,120 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 34 | NA | 0 | 8526 | 1/1 | 0.93 | 0.08 | - | 47,47,47,47 | 0 |
| 36 | SR | 0 | 8942 | 1/1 | 0.93 | 0.08 | - | 122,122,122,122 | 0 |
| 32 | MG | 0 | 8068 | 1/1 | 0.98 | 0.08 | - | 51,51,51,51 | 0 |
| 32 | MG | B | 8042 | 1/1 | 0.99 | 0.07 | - | 44,44,44,44 | 0 |
| 32 | MG | 0 | 8081 | 1/1 | 0.90 | 0.23 | - | 73,73,73,73 | 0 |
| 36 | SR | 0 | 8993 | 1/1 | 0.74 | 0.10 | - | 176,176,176,176 | 0 |
| 36 | SR | 3 | 8932 | 1/1 | 0.99 | 0.14 | - | 76,76,76,76 | 0 |
| 36 | SR | 0 | 8928 | 1/1 | 0.93 | 0.06 | - | 135,135,135,135 | 0 |
| 36 | SR | 0 | 8971 | 1/1 | 0.96 | 0.07 | - | 171,171,171,171 | 0 |
| 32 | MG | 0 | 8048 | 1/1 | 0.98 | 0.24 | - | 33,33,33,33 | 0 |
| 36 | SR | 0 | 8934 | 1/1 | 0.98 | 0.25 | - | 134,134,134,134 | 0 |
| 34 | NA | 0 | 8554 | 1/1 | 0.90 | 1.00 | - | 65,65,65,65 | 0 |
| 32 | MG | 0 | 8046 | 1/1 | 0.96 | 0.14 | - | 43,43,43,43 | 0 |
| 36 | SR | 0 | 9004 | 1/1 | 0.96 | 0.30 | - | 200,200,200,200 | 0 |
| 32 | MG | 0 | 8038 | 1/1 | 0.90 | 0.15 | - | 70,70,70,70 | 0 |
| 34 | NA | 0 | 8541 | 1/1 | 0.98 | 0.18 | - | 75,75,75,75 | 0 |
| 34 | NA | 0 | 8518 | 1/1 | 0.85 | 0.59 | - | 88,88,88,88 | 0 |
| 34 | NA | 0 | 8566 | 1/1 | 0.98 | 0.12 | - | 64,64,64,64 | 0 |
| 34 | NA | 0 | 8529 | 1/1 | 0.92 | 0.15 | - | 39,39,39,39 | 0 |
| 36 | SR | 0 | 8967 | 1/1 | 0.99 | 0.06 | - | 133,133,133,133 | 0 |
| 32 | MG | 0 | 8030 | 1/1 | 0.98 | 0.30 | - | 68,68,68,68 | 0 |
| 34 | NA | 0 | 8513 | 1/1 | 0.98 | 0.21 | - | 54,54,54,54 | 0 |
| 32 | MG | 0 | 8005 | 1/1 | 0.99 | 0.23 | - | 35,35,35,35 | 0 |
| 36 | SR | 0 | 8995 | 1/1 | 0.94 | 0.15 | - | 136,136,136,136 | 0 |
| 32 | MG | 0 | 8087 | 1/1 | 0.92 | 0.12 | - | 51,51,51,51 | 0 |
| 36 | SR | 0 | 8960 | 1/1 | 0.83 | 0.10 | - | 141,141,141,141 | 0 |
| 36 | SR | 0 | 8968 | 1/1 | 0.94 | 0.03 | - | 160,160,160,160 | 0 |
| 32 | MG | 0 | 8090 | 1/1 | 0.99 | 0.10 | - | 65,65,65,65 | 0 |
| 36 | SR | 0 | 8986 | 1/1 | 0.78 | 0.42 | - | 200,200,200,200 | 0 |
| 36 | SR | A | 8977 | 1/1 | 0.83 | 0.06 | - | 160,160,160,160 | 0 |
| 36 | SR | 0 | 8917 | 1/1 | 0.96 | 0.10 | - | 107,107,107,107 | 0 |
| 36 | SR | 0 | 9007 | 1/1 | 0.97 | 0.67 | - | 200,200,200,200 | 0 |
| 34 | NA | 0 | 8508 | 1/1 | 0.98 | 0.20 | - | 35,35,35,35 | 0 |
| 36 | SR | 9 | 8980 | 1/1 | 0.93 | 0.15 | - | 175,175,175,175 | 0 |
| 32 | MG | 0 | 8093 | 1/1 | 0.95 | 0.08 | - | 42,42,42,42 | 0 |
| 34 | NA | S | 8510 | 1/1 | 0.81 | 0.48 | - | 64,64,64,64 | 0 |
| 36 | SR | 0 | 8979 | 1/1 | 0.76 | 0.13 | - | 200,200,200,200 | 0 |
| 34 | NA | 0 | 8525 | 1/1 | 0.29 | 0.25 | - | 92,92,92,92 | 0 |
| 36 | SR | 1 | 8952 | 1/1 | 0.98 | 0.15 | - | 89,89,89,89 | 0 |
| 36 | SR | 0 | 8925 | 1/1 | 1.00 | 0.08 | - | 86,86,86,86 | 0 |
| 34 | NA | R | 8532 | 1/1 | 0.96 | 0.11 | - | 58,58,58,58 | 0 |
| 34 | NA | 0 | 8516 | 1/1 | 0.96 | 0.11 | - | 45,45,45,45 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 32 | MG | 0 | 8061 | 1/1 | 0.99 | 0.23 | - | 37,37,37,37 | 0 |
| 32 | MG | 0 | 8031 | 1/1 | 0.91 | 0.11 | - | 62,62,62,62 | 0 |
| 34 | NA | 0 | 8505 | 1/1 | 0.93 | 0.86 | - | 48,48,48,48 | 0 |
| 35 | CL | 0 | 8815 | 1/1 | 0.91 | 0.12 | - | 77,77,77,77 | 0 |
| 32 | MG | 0 | 8027 | 1/1 | 0.99 | 0.11 | - | 51,51,51,51 | 0 |
| 34 | NA | 0 | 8551 | 1/1 | 0.94 | 0.38 | - | 52,52,52,52 | 0 |
| 32 | MG | 0 | 8032 | 1/1 | 0.99 | 0.05 | - | 44,44,44,44 | 0 |
| 36 | SR | 0 | 8996 | 1/1 | 0.78 | 1.20 | - | 200,200,200,200 | 0 |
| 32 | MG | 0 | 8007 | 1/1 | 0.99 | 0.15 | - | 32,32,32,32 | 0 |
| 34 | NA | 0 | 8548 | 1/1 | 0.74 | 0.26 | - | 58,58,58,58 | 0 |
| 35 | CL | R | 8806 | 1/1 | 0.99 | 0.17 | - | 57,57,57,57 | 0 |
| 36 | SR | 0 | 8909 | 1/1 | 0.99 | 0.15 | - | 88,88,88,88 | 0 |
| 36 | SR | 0 | 8988 | 1/1 | 0.93 | 0.05 | - | 158,158,158,158 | 0 |
| 36 | SR | 0 | 8915 | 1/1 | 0.92 | 0.08 | - | 121,121,121,121 | 0 |
| 32 | MG | 0 | 8071 | 1/1 | 0.97 | 0.10 | - | 72,72,72,72 | 0 |
| 34 | NA | 0 | 8545 | 1/1 | 0.88 | 0.26 | - | 47,47,47,47 | 0 |
| 34 | NA | 0 | 8502 | 1/1 | 0.72 | 0.15 | - | 66,66,66,66 | 0 |
| 34 | NA | 0 | 8511 | 1/1 | 0.75 | 0.29 | - | 69,69,69,69 | 0 |
| 36 | SR | 0 | 8940 | 1/1 | 0.98 | 0.07 | - | 97,97,97,97 | 0 |
| 36 | SR | 0 | 8919 | 1/1 | 0.97 | 0.07 | - | 170,170,170,170 | 0 |
| 36 | SR | 0 | 8927 | 1/1 | 0.90 | 0.09 | - | 153,153,153,153 | 0 |
| 34 | NA | 0 | 8544 | 1/1 | 0.86 | 0.17 | - | 67,67,67,67 | 0 |
| 32 | MG | 0 | 8092 | 1/1 | 0.89 | 0.18 | - | 53,53,53,53 | 0 |
| 36 | SR | 0 | 8923 | 1/1 | 0.98 | 0.11 | - | 101,101,101,101 | 0 |
| 36 | SR | 0 | 8964 | 1/1 | 0.99 | 0.09 | - | 131,131,131,131 | 0 |
| 36 | SR | 0 | 8937 | 1/1 | 0.98 | 0.27 | - | 112,112,112,112 | 0 |
| 36 | SR | 0 | 8976 | 1/1 | 0.88 | 0.28 | - | 194,194,194,194 | 0 |
| 36 | SR | 0 | 8922 | 1/1 | 0.88 | 0.47 | - | 161,161,161,161 | 0 |
| 36 | SR | 0 | 8953 | 1/1 | 0.96 | 0.13 | - | 144,144,144,144 | 0 |
| 34 | NA | 9 | 8543 | 1/1 | 0.77 | 0.11 | - | 74,74,74,74 | 0 |
| 36 | SR | 0 | 8989 | 1/1 | 0.92 | 0.16 | - | 168,168,168,168 | 0 |
| 36 | SR | 0 | 8924 | 1/1 | 0.34 | 0.09 | - | 154,154,154,154 | 0 |
| 32 | MG | 0 | 8029 | 1/1 | 0.99 | 0.15 | - | 49,49,49,49 | 0 |
| 36 | SR | 0 | 8974 | 1/1 | 0.87 | 0.24 | - | 165,165,165,165 | 0 |
| 36 | SR | 0 | 8965 | 1/1 | 0.93 | 0.09 | - | 132,132,132,132 | 0 |
| 35 | CL | J | 8801 | 1/1 | 0.99 | 0.07 | - | 79,79,79,79 | 0 |

6.5 Other polymers

There are no such residues in this entry.