



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 01:33 am BST

PDB ID : 2OTJ
Title : 13-deoxytedanolide bound to the large subunit of Haloarcula marismortui
Authors : Blaha, G.; Schroeder, S.J.; Tirado-Rives, J.
Deposited on : 2007-02-08
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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

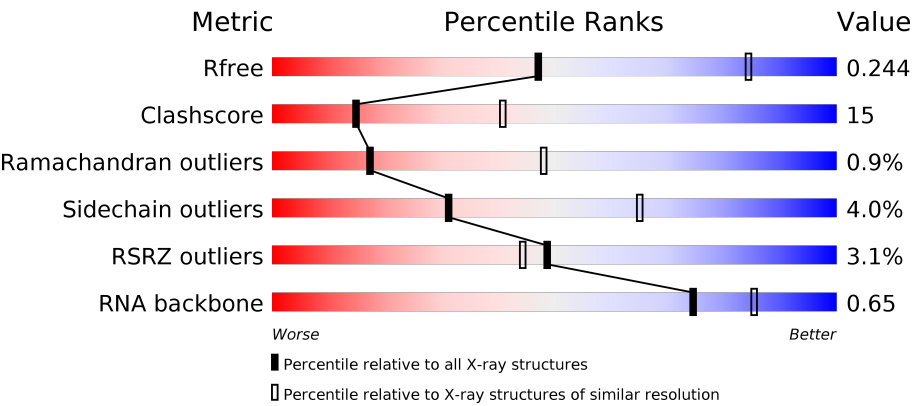
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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.








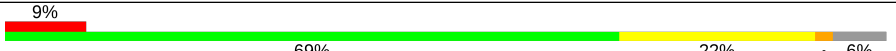
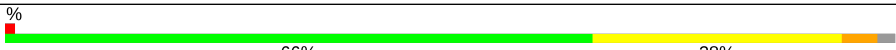

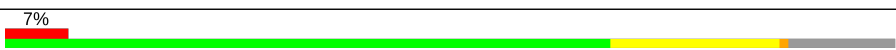

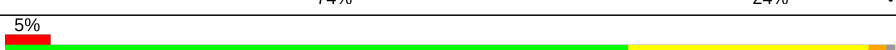
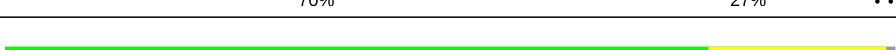

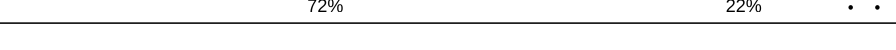
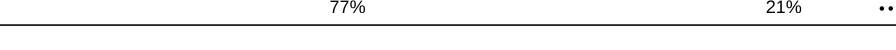

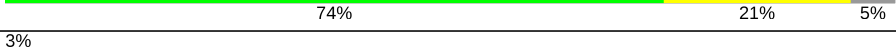
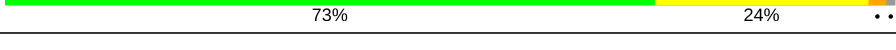




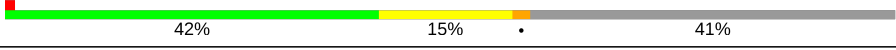


| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R _{free} | 130704 | 1957 (2.90-2.90) |
| Clashscore | 141614 | 2172 (2.90-2.90) |
| Ramachandran outliers | 138981 | 2115 (2.90-2.90) |
| Sidechain outliers | 138945 | 2117 (2.90-2.90) |
| RSRZ outliers | 127900 | 1906 (2.90-2.90) |
| RNA backbone | 3102 | 1007 (3.16-2.64) |

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 respectively. 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 | 0 | 2922 | <div><div></div><div><div>49%</div><div>39%</div><div>6%</div><div>6%</div></div></div> |
| 2 | 9 | 122 | <div><div>2%</div><div><div>38%</div><div>48%</div><div>13%</div></div></div> <div></div> |
| 3 | A | 240 | <div><div>3%</div><div><div>68%</div><div>27%</div></div></div> <div></div> |
| 4 | B | 338 | <div><div><div>62%</div><div>34%</div></div></div> <div></div> |



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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 5 | C | 246 |  |
| 6 | D | 177 |  |
| 7 | E | 178 |  |
| 8 | F | 120 |  |
| 9 | G | 348 |  |
| 10 | H | 171 |  |
| 11 | J | 145 |  |
| 12 | K | 132 |  |
| 13 | L | 165 |  |
| 14 | M | 194 |  |
| 15 | N | 187 |  |
| 16 | O | 116 |  |
| 17 | P | 149 |  |
| 18 | Q | 96 |  |
| 19 | R | 155 |  |
| 20 | S | 85 |  |
| 21 | T | 120 |  |
| 22 | U | 66 |  |
| 23 | V | 71 |  |
| 24 | W | 154 |  |
| 25 | X | 92 |  |
| 26 | Y | 241 |  |
| 27 | Z | 73 |  |
| 28 | 1 | 57 |  |
| 29 | 2 | 50 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 30 | 3 | 92 |  78% 21% |
| 31 | I | 161 |  31% 29% 14% 57% |

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 | 13T | 0 | 9000 | - | - | X | - |
| 35 | NA | 0 | 8506 | - | - | - | X |
| 35 | NA | 0 | 8516 | - | - | - | X |
| 35 | NA | 0 | 8528 | - | - | - | X |
| 35 | NA | 0 | 8542 | - | - | X | - |
| 35 | NA | 0 | 8550 | - | - | - | X |
| 35 | NA | 0 | 8577 | - | - | - | X |
| 35 | NA | 0 | 8584 | - | - | - | X |
| 36 | CL | J | 8801 | - | - | X | - |

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99043 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 1 | 0 | 2754 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 59021 | 26350 | 10878 | 19048 | 2745 | | | |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------------|------------|
| 0 | 560 | C | U | CONFLICT | GB 3377779 |
| 0 | 628 | 1MA | A | MODIFIED RESIDUE | GB 3377779 |
| 0 | 2587 | OMU | U | MODIFIED RESIDUE | GB 3377779 |
| 0 | 2588 | OMG | G | MODIFIED RESIDUE | GB 3377779 |
| 0 | 2619 | UR3 | U | MODIFIED RESIDUE | GB 3377779 |
| 0 | 2621 | PSU | U | MODIFIED RESIDUE | GB 3377779 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 2 | 9 | 122 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2600 | 1160 | 472 | 847 | 121 | | | |

- Molecule 3 is a protein called 50S ribosomal protein L2P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | A | 237 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1753 | 1072 | 352 | 324 | 5 | | | |

- Molecule 4 is a protein called 50S ribosomal protein L3P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4 | B | 337 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2625 | 1616 | 493 | 511 | 5 | | | |

- Molecule 5 is a protein called 50S ribosomal protein L4P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5 | C | 246 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1859 | 1131 | 344 | 383 | 1 | | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| C | 73 | LEU | GLN | CONFLICT | UNP P12735 |

- Molecule 6 is a protein called 50S ribosomal protein L5P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | D | 140 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1094 | 685 | 195 | 210 | 4 | | | |

- Molecule 7 is a protein called 50S ribosomal protein L6P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | E | 172 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1357 | 840 | 224 | 289 | 4 | | | |

- Molecule 8 is a protein called 50S ribosomal protein L7Ae.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | F | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 890 | 551 | 141 | 197 | 1 | | | |

- Molecule 9 is a protein called 50S ribosomal protein L10E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 9 | G | 29 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 240 | 149 | 39 | 51 | 1 | | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| G | 248 | ASP | ALA | CONFLICT | UNP P15825 |

- Molecule 10 is a protein called 50S ribosomal protein L10e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | H | 160 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1266 | 785 | 237 | 238 | 6 | | | |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|------------|
| H | 164 | ASP | - | INSERTION | UNP P60617 |
| H | 165 | SER | - | INSERTION | UNP P60617 |
| H | 166 | SER | - | INSERTION | UNP P60617 |
| H | 167 | PRO | - | INSERTION | UNP P60617 |
| H | 168 | ALA | - | INSERTION | UNP P60617 |
| H | 169 | GLY | - | INSERTION | UNP P60617 |
| H | 170 | ASN | - | INSERTION | UNP P60617 |
| H | 171 | ALA | - | INSERTION | UNP P60617 |

- Molecule 11 is a protein called 50S ribosomal protein L13P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | J | 142 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1120 | 696 | 199 | 222 | 3 | | | |

- Molecule 12 is a protein called 50S ribosomal protein L14P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | K | 132 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 992 | 609 | 187 | 192 | 4 | | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| K | 44 | LEU | HIS | CONFLICT | UNP P22450 |

- Molecule 13 is a protein called 50S ribosomal protein L15P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | L | 145 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1118 | 670 | 222 | 226 | | | | |

- Molecule 14 is a protein called 50S ribosomal protein L15e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14 | M | 194 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1560 | 943 | 332 | 284 | 1 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|------------|
| M | 13 | GLU | LYS | CONFLICT | UNP P60618 |
| M | 194 | ALA | - | INSERTION | UNP P60618 |

- Molecule 15 is a protein called 50S ribosomal protein L18P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15 | N | 186 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1445 | 895 | 262 | 286 | 2 | | | |

- Molecule 16 is a protein called 50S ribosomal protein L18e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 16 | O | 115 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 865 | 529 | 161 | 175 | | | | |

- Molecule 17 is a protein called 50S ribosomal protein L19e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 17 | P | 143 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 1136 | 683 | 229 | 224 | | | | |

- Molecule 18 is a protein called 50S ribosomal protein L21e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 18 | Q | 95 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 735 | 450 | 141 | 144 | | | | |

- Molecule 19 is a protein called 50S ribosomal protein L22P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | R | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1149 | 713 | 209 | 223 | 4 | | | |

- Molecule 20 is a protein called 50S ribosomal protein L23P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | S | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 641 | 389 | 111 | 138 | 3 | | | |

- Molecule 21 is a protein called 50S ribosomal protein L24P.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 21 | T | 119 | Total | C | N | O | | | |
| | | | 950 | 568 | 180 | 202 | 0 | 0 | 0 |

- Molecule 22 is a protein called 50S ribosomal protein L24e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 22 | U | 53 | Total | C | N | O | S | | | |
| | | | 410 | 244 | 75 | 86 | 5 | 0 | 0 | 0 |

- Molecule 23 is a protein called 50S ribosomal protein L29P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|---------|-------|
| 23 | V | 65 | Total | C | N | O | S | | | |
| | | | 499 | 304 | 94 | 100 | 1 | 0 | 0 | 0 |

- Molecule 24 is a protein called 50S ribosomal protein L30P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 24 | W | 154 | Total | C | N | O | S | | | |
| | | | 1196 | 737 | 209 | 244 | 6 | 0 | 0 | 0 |

- Molecule 25 is a protein called 50S ribosomal protein L31e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 25 | X | 82 | Total | C | N | O | S | | | |
| | | | 654 | 402 | 129 | 122 | 1 | 0 | 0 | 0 |

- Molecule 26 is a protein called 50S ribosomal protein L32e.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 26 | Y | 142 | Total | C | N | O | | | |
| | | | 1130 | 686 | 228 | 216 | 0 | 0 | 0 |

- Molecule 27 is a protein called 50S ribosomal protein L37Ae.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 27 | Z | 73 | Total | C | N | O | S | | | |
| | | | 579 | 346 | 116 | 112 | 5 | 0 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|------------|
| Z | 10 | ARG | - | INSERTION | UNP P60619 |

- Molecule 28 is a protein called 50S ribosomal protein L37e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 28 | 1 | 56 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 431 | 258 | 86 | 83 | 4 | | | |

- Molecule 29 is a protein called 50S ribosomal protein L39e.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 29 | 2 | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 396 | 239 | 89 | 67 | 1 | | | |

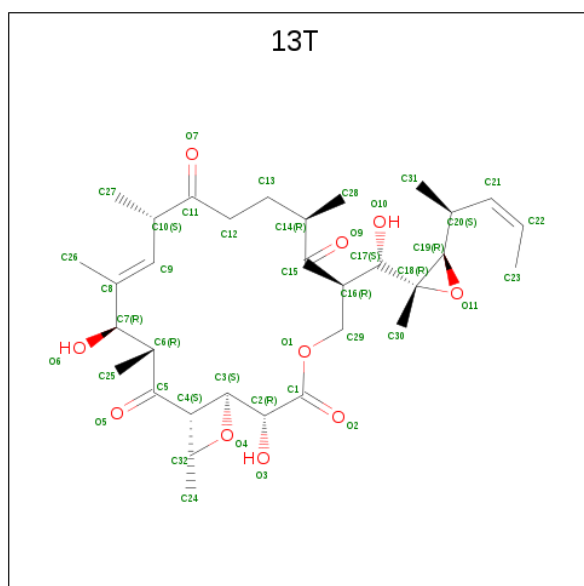
- Molecule 30 is a protein called 50S ribosomal protein L44E.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30 | 3 | 92 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 755 | 458 | 153 | 137 | 7 | | | |

- Molecule 31 is a protein called 50S ribosomal protein L11P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|---------|-------|
| 31 | I | 70 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 519 | 323 | 81 | 114 | 1 | | | |

- Molecule 32 is 13-DEOXYTEDANOLIDE (three-letter code: 13T) (formula: C₃₂H₅₀O₁₀).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 32 | 0 | 1 | Total | C | O | 0 | 0 |
| | | | 42 | 32 | 10 | | |

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 33 | 0 | 108 | Total | Mg | 0 | 0 |
| | | | 108 | 108 | | |
| 33 | Y | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 33 | K | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 33 | B | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 33 | A | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 33 | T | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 33 | 9 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 33 | 3 | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 34 | 0 | 2 | Total | K | 0 | 0 |
| | | | 2 | 2 | | |

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 35 | 0 | 74 | Total | Na | 0 | 0 |
| | | | 74 | 74 | | |
| 35 | J | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 35 | Q | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 35 | H | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 35 | C | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 35 | A | 1 | Total 1 | Na 1 | 0 | 0 |
| 35 | R | 2 | Total 2 | Na 2 | 0 | 0 |
| 35 | 9 | 2 | Total 2 | Na 2 | 0 | 0 |
| 35 | L | 1 | Total 1 | Na 1 | 0 | 0 |
| 35 | S | 1 | Total 1 | Na 1 | 0 | 0 |
| 35 | M | 1 | Total 1 | Na 1 | 0 | 0 |

- Molecule 36 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 36 | 0 | 9 | Total 9 | Cl 9 | 0 | 0 |
| 36 | J | 3 | Total 3 | Cl 3 | 0 | 0 |
| 36 | B | 1 | Total 1 | Cl 1 | 0 | 0 |
| 36 | A | 1 | Total 1 | Cl 1 | 0 | 0 |
| 36 | N | 1 | Total 1 | Cl 1 | 0 | 0 |
| 36 | O | 1 | Total 1 | Cl 1 | 0 | 0 |
| 36 | R | 1 | Total 1 | Cl 1 | 0 | 0 |
| 36 | Y | 2 | Total 2 | Cl 2 | 0 | 0 |
| 36 | L | 1 | Total 1 | Cl 1 | 0 | 0 |
| 36 | 3 | 1 | Total 1 | Cl 1 | 0 | 0 |
| 36 | M | 1 | Total 1 | Cl 1 | 0 | 0 |

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

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

- Molecule 38 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|----------------------|---------|---------|
| 38 | 0 | 5905 | Total O 5905 5905 | 0 | 0 |
| 38 | 9 | 140 | Total O 140 140 | 0 | 0 |
| 38 | A | 112 | Total O 112 112 | 0 | 0 |
| 38 | B | 142 | Total O 142 142 | 0 | 0 |
| 38 | C | 170 | Total O 170 170 | 0 | 0 |
| 38 | D | 45 | Total O 45 45 | 0 | 0 |
| 38 | E | 42 | Total O 42 42 | 0 | 0 |
| 38 | F | 26 | Total O 26 26 | 0 | 0 |
| 38 | G | 19 | Total O 19 19 | 0 | 0 |
| 38 | H | 70 | Total O 70 70 | 0 | 0 |
| 38 | J | 58 | Total O 58 58 | 0 | 0 |
| 38 | K | 59 | Total O 59 59 | 0 | 0 |
| 38 | L | 83 | Total O 83 83 | 0 | 0 |
| 38 | M | 123 | Total O 123 123 | 0 | 0 |
| 38 | N | 63 | Total O 63 63 | 0 | 0 |

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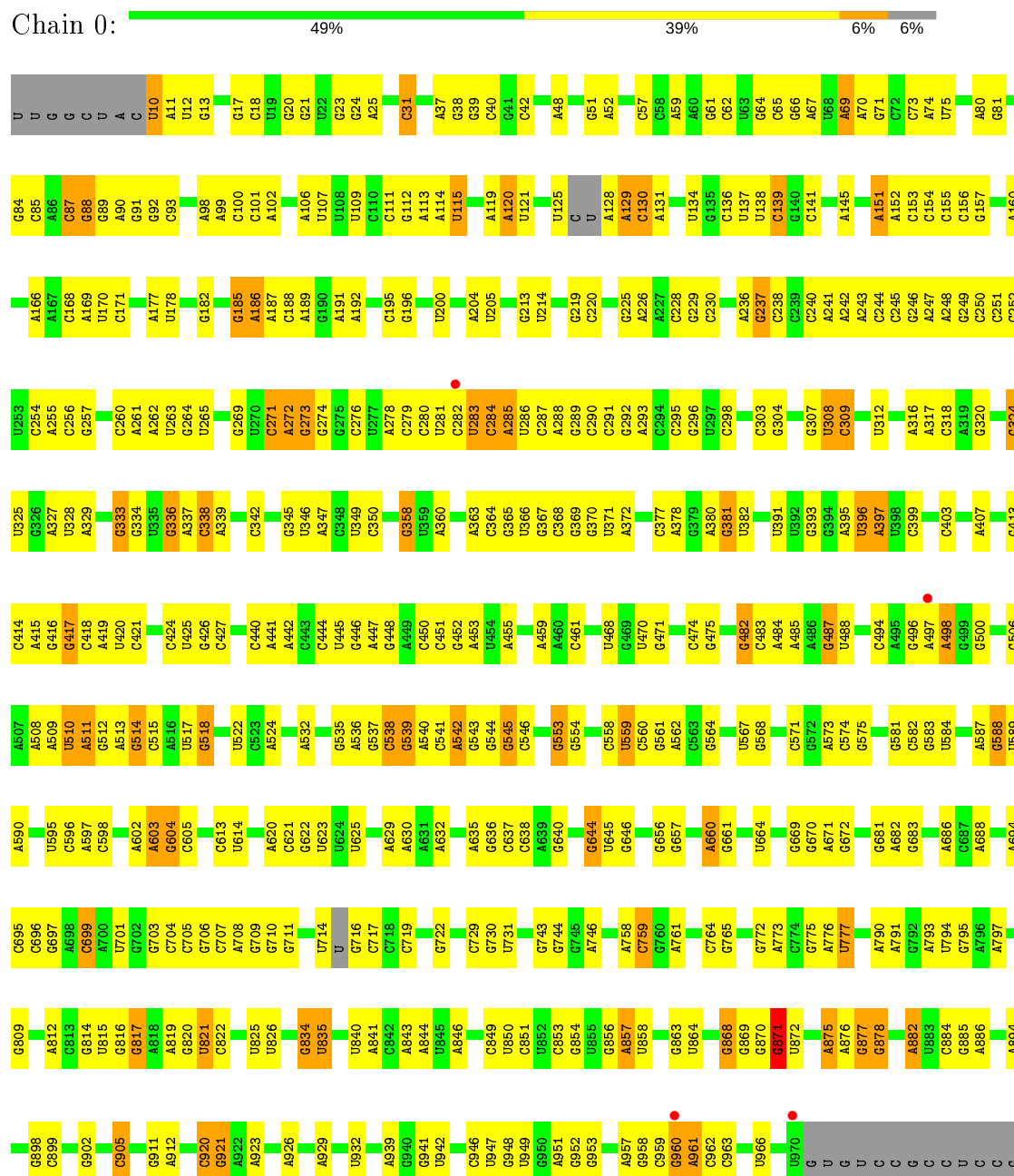
Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 38 | O | 44 | Total 44 | O 44 | 0 | 0 |
| 38 | P | 56 | Total 56 | O 56 | 0 | 0 |
| 38 | Q | 51 | Total 51 | O 51 | 0 | 0 |
| 38 | R | 80 | Total 80 | O 80 | 0 | 0 |
| 38 | S | 36 | Total 36 | O 36 | 0 | 0 |
| 38 | T | 33 | Total 33 | O 33 | 0 | 0 |
| 38 | U | 26 | Total 26 | O 26 | 0 | 0 |
| 38 | V | 11 | Total 11 | O 11 | 0 | 0 |
| 38 | W | 67 | Total 67 | O 67 | 0 | 0 |
| 38 | X | 21 | Total 21 | O 21 | 0 | 0 |
| 38 | Y | 96 | Total 96 | O 96 | 0 | 0 |
| 38 | Z | 31 | Total 31 | O 31 | 0 | 0 |
| 38 | 1 | 56 | Total 56 | O 56 | 0 | 0 |
| 38 | 2 | 45 | Total 45 | O 45 | 0 | 0 |
| 38 | 3 | 66 | Total 66 | O 66 | 0 | 0 |
| 38 | I | 8 | Total 8 | O 8 | 0 | 0 |

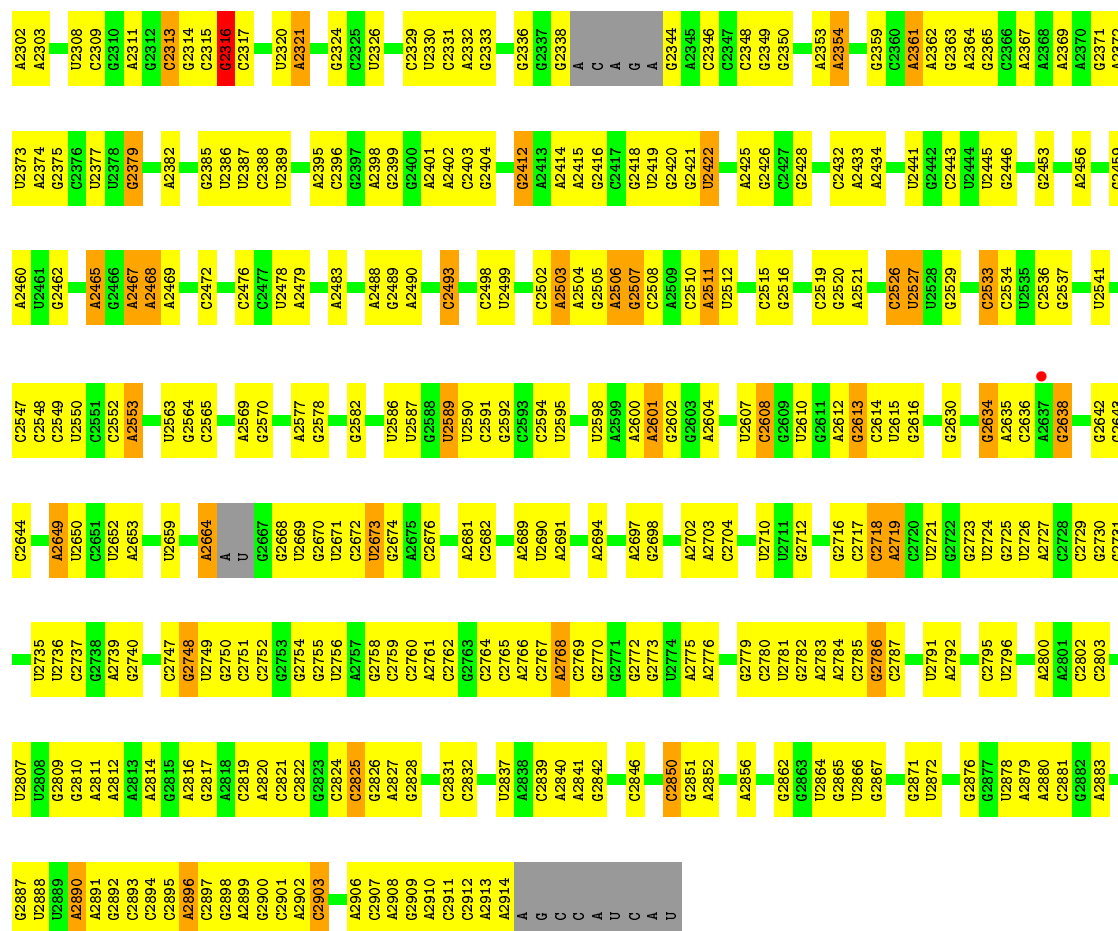
3 Residue-property plots

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

• Molecule 1: 23S ribosomal RNA



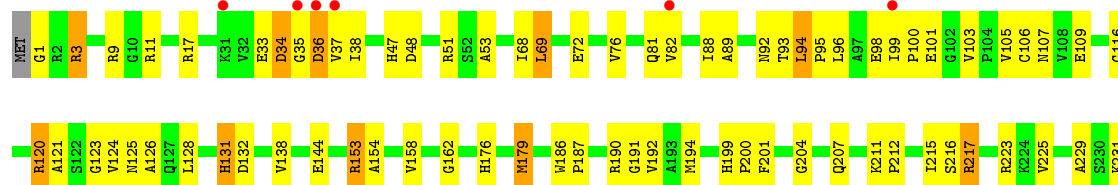




• Molecule 2: 5S ribosomal RNA



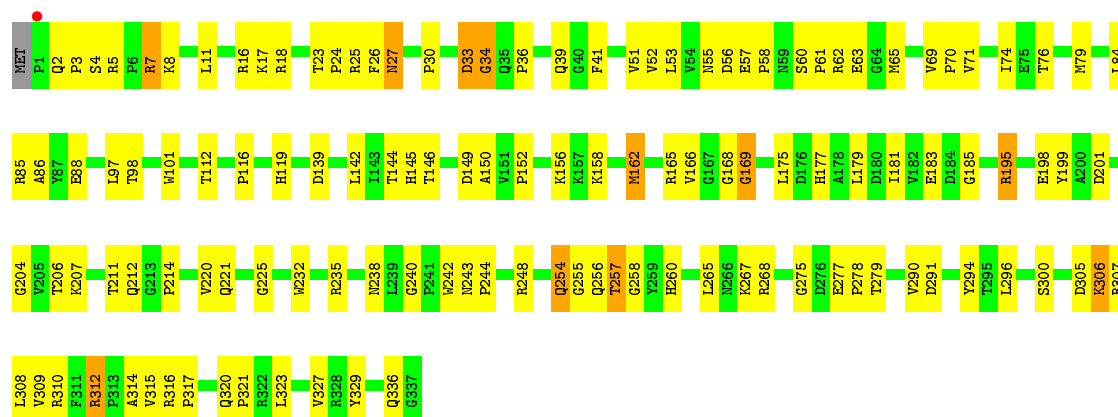
• Molecule 3: 50S ribosomal protein L2P





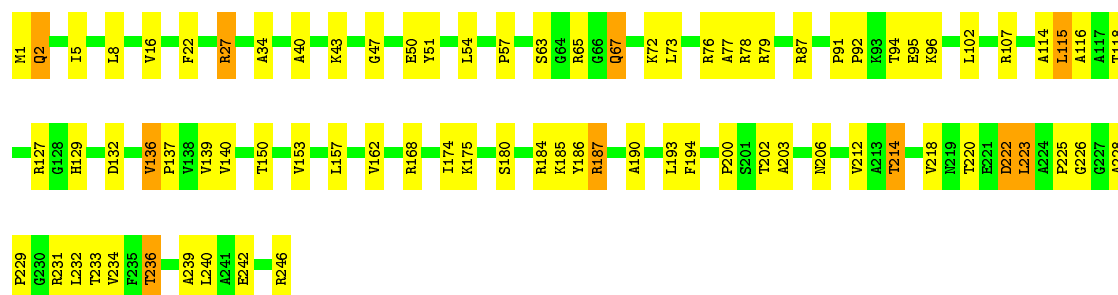
• Molecule 4: 50S ribosomal protein L3P

Chain B: 62% 34%



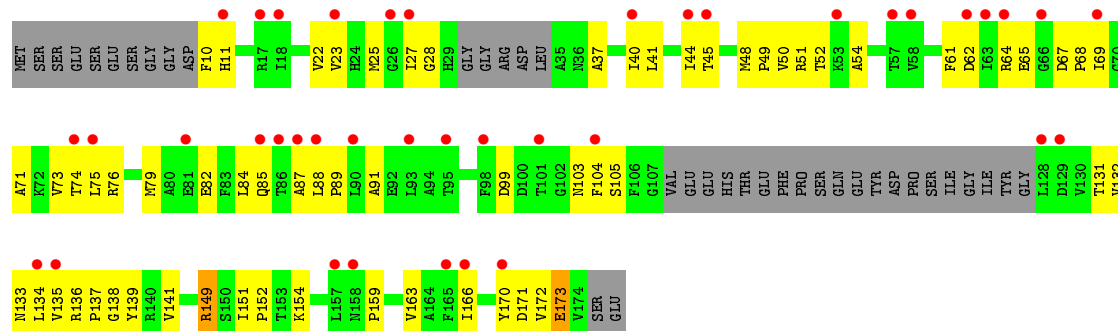
• Molecule 5: 50S ribosomal protein L4P

Chain C: 67% 29%



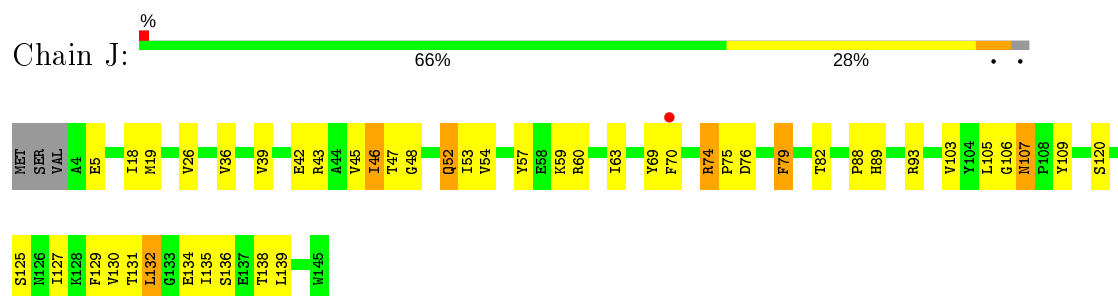
• Molecule 6: 50S ribosomal protein L5P

Chain D: 22% 44% 34% 21%

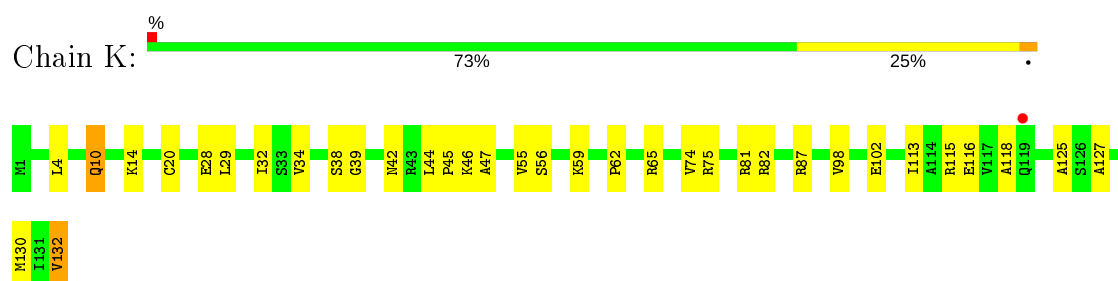


• Molecule 7: 50S ribosomal protein L6P

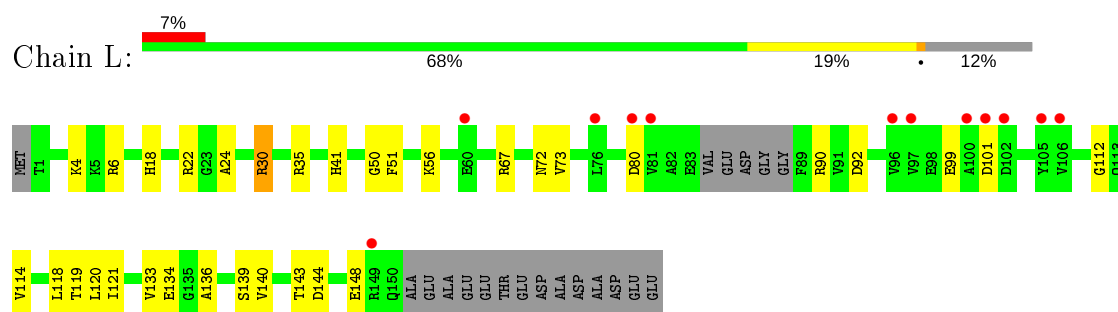
- Molecule 11: 50S ribosomal protein L13P



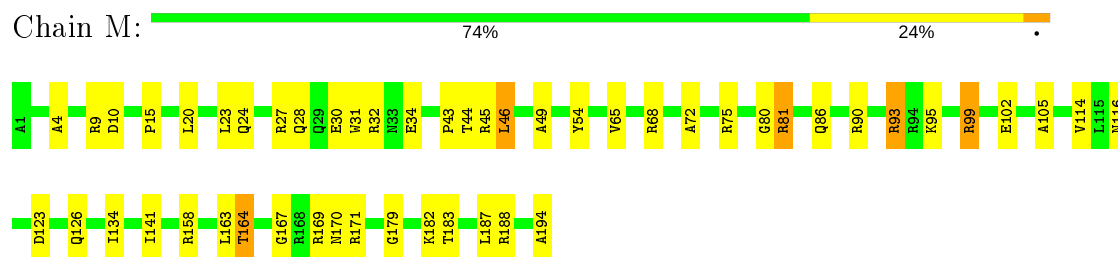
- Molecule 12: 50S ribosomal protein L14P



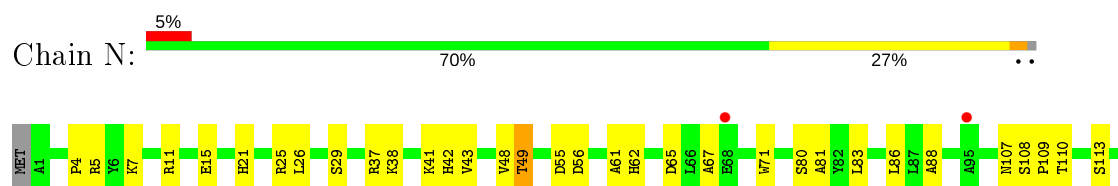
- Molecule 13: 50S ribosomal protein L15P



- Molecule 14: 50S ribosomal protein L15e

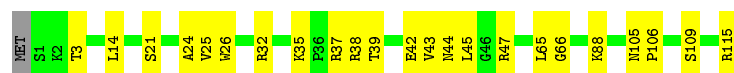
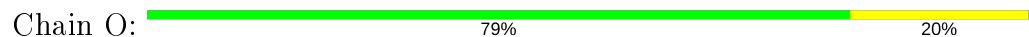


- Molecule 15: 50S ribosomal protein L18P

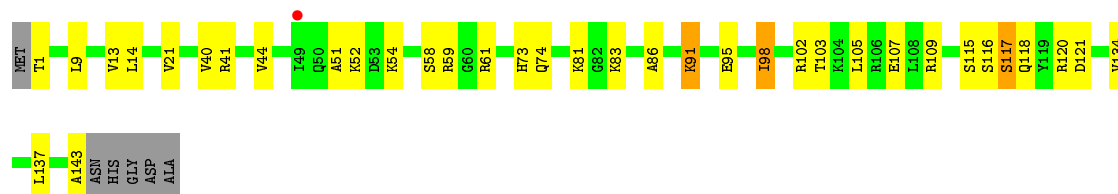




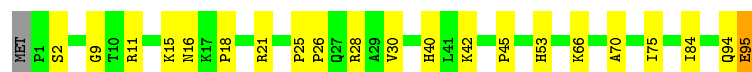
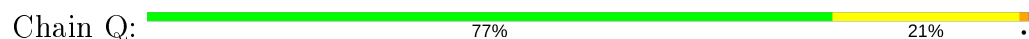
- Molecule 16: 50S ribosomal protein L18e



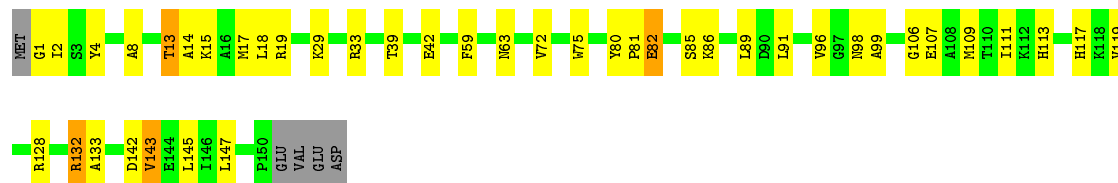
- Molecule 17: 50S ribosomal protein L19e



- Molecule 18: 50S ribosomal protein L21e



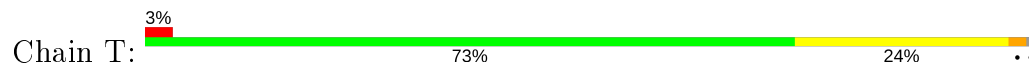
- Molecule 19: 50S ribosomal protein L22P



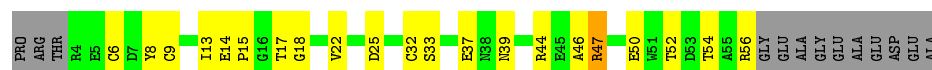
- Molecule 20: 50S ribosomal protein L23P



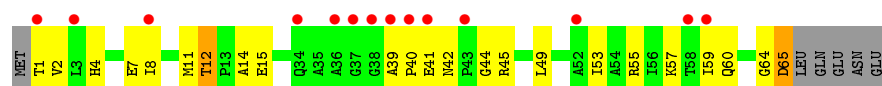
- Molecule 21: 50S ribosomal protein L24P



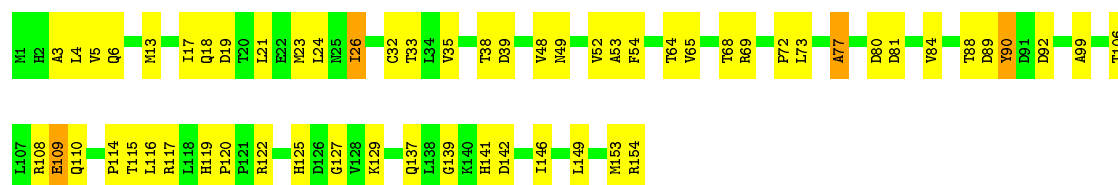
- Molecule 22: 50S ribosomal protein L24e



- Molecule 23: 50S ribosomal protein L29P



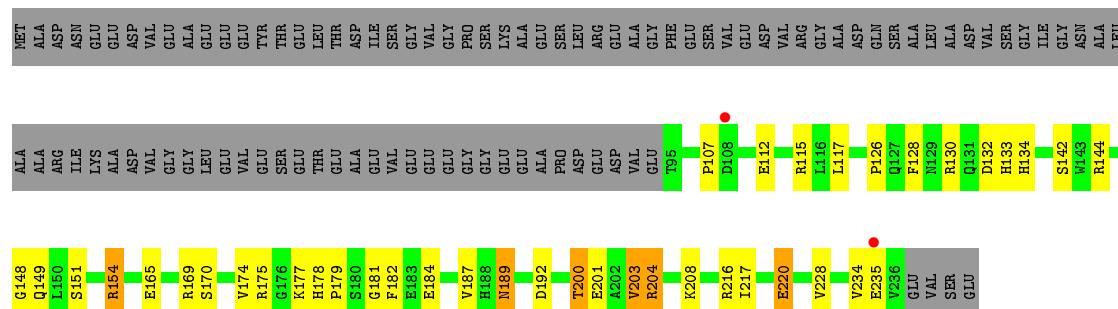
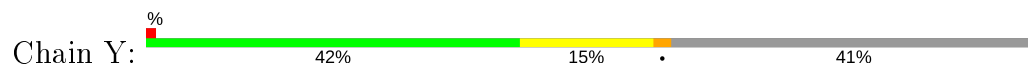
- Molecule 24: 50S ribosomal protein L30P



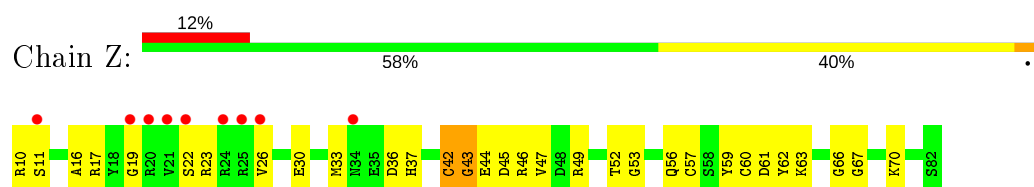
- Molecule 25: 50S ribosomal protein L31e



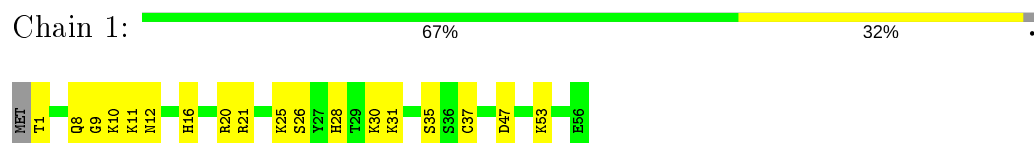
- Molecule 26: 50S ribosomal protein L32e



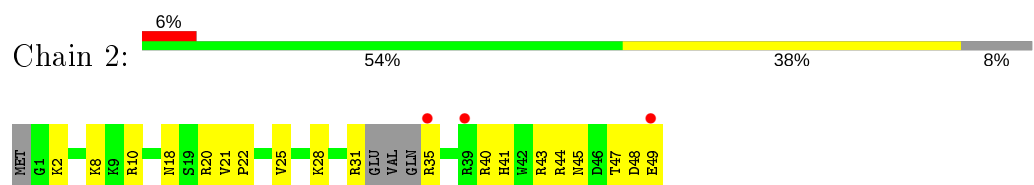
- Molecule 27: 50S ribosomal protein L37Ae



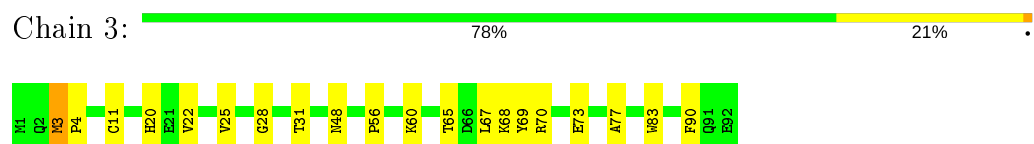
- Molecule 28: 50S ribosomal protein L37e



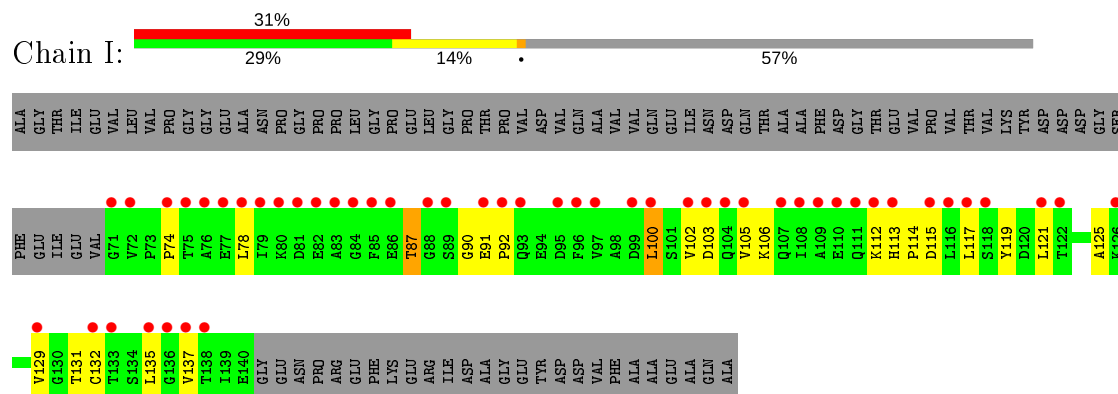
- Molecule 29: 50S ribosomal protein L39e



- Molecule 30: 50S ribosomal protein L44E



- Molecule 31: 50S ribosomal protein L11P



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | C 2 2 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 211.74Å 299.52Å 573.59Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 49.70 – 2.90 85.48 – 2.40 | Depositor EDS |
| % Data completeness (in resolution range) | 99.9 (49.70-2.90) 91.7 (85.48-2.40) | Depositor EDS |
| R_{merge} | 0.16 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 0.00 (at 2.40Å) | Xtriage |
| Refinement program | CNS | Depositor |
| R, R_{free} | 0.193 , 0.238 0.212 , 0.244 | Depositor DCC |
| R_{free} test set | 6547 reflections (0.98%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 50.3 | Xtriage |
| Anisotropy | 0.049 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.32 , 74.2 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.92 | EDS |
| Total number of atoms | 99043 | wwPDB-VP |
| Average B, all atoms (Å ²) | 58.0 | 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, 0.333 respectively for untwinned datasets, and 0.375, 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, NA, K, UR3, CD, OMU, 13T, 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 | 0 | 0.39 | 0/65959 | 0.69 | 14/102870 (0.0%) |
| 2 | 9 | 0.34 | 0/2905 | 0.69 | 1/4528 (0.0%) |
| 3 | A | 0.35 | 0/1786 | 0.66 | 0/2408 |
| 4 | B | 0.34 | 0/2690 | 0.66 | 0/3652 |
| 5 | C | 0.39 | 0/1884 | 0.66 | 0/2551 |
| 6 | D | 0.33 | 0/1111 | 0.58 | 0/1498 |
| 7 | E | 0.34 | 0/1382 | 0.57 | 0/1880 |
| 8 | F | 0.38 | 0/901 | 0.58 | 0/1224 |
| 9 | G | 0.33 | 0/241 | 0.49 | 0/324 |
| 10 | H | 0.38 | 0/1287 | 0.65 | 0/1725 |
| 11 | J | 0.36 | 0/1136 | 0.61 | 0/1530 |
| 12 | K | 0.36 | 0/1001 | 0.68 | 0/1347 |
| 13 | L | 0.35 | 0/1130 | 0.64 | 0/1509 |
| 14 | M | 0.37 | 0/1584 | 0.63 | 0/2119 |
| 15 | N | 0.31 | 0/1474 | 0.65 | 1/1999 (0.1%) |
| 16 | O | 0.36 | 0/874 | 0.61 | 1/1181 (0.1%) |
| 17 | P | 0.35 | 0/1147 | 0.55 | 0/1528 |
| 18 | Q | 0.37 | 0/749 | 0.68 | 0/1005 |
| 19 | R | 0.36 | 0/1172 | 0.64 | 0/1578 |
| 20 | S | 0.35 | 0/648 | 0.59 | 0/875 |
| 21 | T | 0.34 | 0/958 | 0.63 | 0/1289 |
| 22 | U | 0.36 | 0/417 | 0.56 | 0/562 |
| 23 | V | 0.35 | 0/502 | 0.56 | 0/675 |
| 24 | W | 0.34 | 0/1219 | 0.63 | 0/1655 |
| 25 | X | 0.35 | 0/664 | 0.59 | 0/895 |
| 26 | Y | 0.36 | 0/1146 | 0.63 | 0/1536 |
| 27 | Z | 0.39 | 0/590 | 0.64 | 0/787 |
| 28 | 1 | 0.40 | 0/438 | 0.63 | 0/578 |
| 29 | 2 | 0.37 | 0/401 | 0.56 | 0/529 |
| 30 | 3 | 0.37 | 0/771 | 0.57 | 0/1024 |
| 31 | I | 0.35 | 0/526 | 0.57 | 0/716 |
| All | All | 0.38 | 0/98693 | 0.67 | 17/147577 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | 0 | 1 | 42 |
| 2 | 9 | 0 | 2 |
| 24 | W | 0 | 1 |
| All | All | 1 | 45 |

There are no bond length outliers.

All (17) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | 0 | 1563 | G | C2'-C3'-O3' | 9.37 | 130.11 | 109.50 |
| 2 | 9 | 3039 | U | N1-C1'-C2' | 6.50 | 122.45 | 114.00 |
| 1 | 0 | 2316 | G | C5'-C4'-C3' | -6.49 | 105.61 | 116.00 |
| 1 | 0 | 1504 | A | C1'-O4'-C4' | -6.21 | 104.93 | 109.90 |
| 1 | 0 | 1942 | A | C5'-C4'-C3' | 6.20 | 125.92 | 116.00 |
| 15 | N | 163 | PHE | N-CA-C | -5.68 | 95.66 | 111.00 |
| 16 | O | 66 | GLY | N-CA-C | 5.59 | 127.06 | 113.10 |
| 1 | 0 | 871 | G | C5'-C4'-O4' | -5.54 | 102.45 | 109.10 |
| 1 | 0 | 1504 | A | N9-C1'-C2' | 5.52 | 121.17 | 114.00 |
| 1 | 0 | 1819 | G | C5'-C4'-C3' | 5.40 | 124.64 | 116.00 |
| 1 | 0 | 1829 | A | N9-C1'-C2' | -5.39 | 106.07 | 112.00 |
| 1 | 0 | 2313 | C | C5'-C4'-O4' | 5.31 | 115.47 | 109.10 |
| 1 | 0 | 2291 | A | N9-C1'-C2' | 5.15 | 120.70 | 114.00 |
| 1 | 0 | 1559 | A | C2'-C3'-O3' | 5.15 | 121.94 | 113.70 |
| 1 | 0 | 2313 | C | O4'-C4'-C3' | -5.07 | 98.93 | 104.00 |
| 1 | 0 | 1878 | G | N9-C1'-C2' | -5.04 | 106.46 | 112.00 |
| 1 | 0 | 777 | U | O4'-C1'-N1 | 5.03 | 112.23 | 108.20 |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 1 | 0 | 1563 | G | C3' |

All (45) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 1 | 0 | 1039 | G | Sidechain |
| 1 | 0 | 1078 | A | Sidechain |
| 1 | 0 | 1131 | G | Sidechain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 1 | 0 | 1309 | U | Sidechain |
| 1 | 0 | 131 | A | Sidechain |
| 1 | 0 | 1376 | G | Sidechain |
| 1 | 0 | 1445 | G | Sidechain |
| 1 | 0 | 1458 | A | Sidechain |
| 1 | 0 | 1635 | U | Sidechain |
| 1 | 0 | 1809 | G | Sidechain |
| 1 | 0 | 1829 | A | Sidechain |
| 1 | 0 | 1863 | G | Sidechain |
| 1 | 0 | 1877 | G | Sidechain |
| 1 | 0 | 1878 | G | Sidechain |
| 1 | 0 | 1970 | G | Sidechain |
| 1 | 0 | 1972 | U | Sidechain |
| 1 | 0 | 1979 | G | Sidechain |
| 1 | 0 | 1993 | C | Sidechain |
| 1 | 0 | 220 | C | Sidechain |
| 1 | 0 | 2308 | U | Sidechain |
| 1 | 0 | 2316 | G | Sidechain |
| 1 | 0 | 2412 | G | Sidechain |
| 1 | 0 | 2465 | A | Sidechain |
| 1 | 0 | 2493 | C | Sidechain |
| 1 | 0 | 2503 | A | Sidechain |
| 1 | 0 | 2506 | A | Sidechain |
| 1 | 0 | 2552 | C | Sidechain |
| 1 | 0 | 2630 | G | Sidechain |
| 1 | 0 | 2673 | U | Sidechain |
| 1 | 0 | 2842 | G | Sidechain |
| 1 | 0 | 324 | G | Sidechain |
| 1 | 0 | 333 | G | Sidechain |
| 1 | 0 | 391 | U | Sidechain |
| 1 | 0 | 396 | U | Sidechain |
| 1 | 0 | 471 | G | Sidechain |
| 1 | 0 | 48 | A | Sidechain |
| 1 | 0 | 482 | G | Sidechain |
| 1 | 0 | 518 | G | Sidechain |
| 1 | 0 | 722 | G | Sidechain |
| 1 | 0 | 795 | G | Sidechain |
| 1 | 0 | 817 | G | Sidechain |
| 1 | 0 | 868 | G | Sidechain |
| 2 | 9 | 3039 | U | Sidechain |
| 2 | 9 | 3090 | G | Sidechain |
| 24 | 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 | 0 | 59021 | 0 | 29812 | 1337 | 0 |
| 2 | 9 | 2600 | 0 | 1326 | 95 | 0 |
| 3 | A | 1753 | 0 | 1766 | 78 | 0 |
| 4 | B | 2625 | 0 | 2533 | 112 | 0 |
| 5 | C | 1859 | 0 | 1816 | 74 | 0 |
| 6 | D | 1094 | 0 | 1085 | 56 | 0 |
| 7 | E | 1357 | 0 | 1266 | 38 | 0 |
| 8 | F | 890 | 0 | 843 | 32 | 0 |
| 9 | G | 240 | 0 | 231 | 9 | 0 |
| 10 | H | 1266 | 0 | 1268 | 39 | 0 |
| 11 | J | 1120 | 0 | 1098 | 49 | 0 |
| 12 | K | 992 | 0 | 1031 | 40 | 0 |
| 13 | L | 1118 | 0 | 1076 | 28 | 0 |
| 14 | M | 1560 | 0 | 1568 | 45 | 0 |
| 15 | N | 1445 | 0 | 1401 | 45 | 0 |
| 16 | O | 865 | 0 | 873 | 21 | 0 |
| 17 | P | 1136 | 0 | 1123 | 33 | 0 |
| 18 | Q | 735 | 0 | 728 | 22 | 0 |
| 19 | R | 1149 | 0 | 1122 | 41 | 0 |
| 20 | S | 641 | 0 | 605 | 14 | 0 |
| 21 | T | 950 | 0 | 923 | 25 | 0 |
| 22 | U | 410 | 0 | 364 | 21 | 0 |
| 23 | V | 499 | 0 | 511 | 19 | 0 |
| 24 | W | 1196 | 0 | 1137 | 57 | 0 |
| 25 | X | 654 | 0 | 653 | 25 | 0 |
| 26 | Y | 1130 | 0 | 1133 | 46 | 0 |
| 27 | Z | 579 | 0 | 539 | 25 | 0 |
| 28 | 1 | 431 | 0 | 426 | 21 | 0 |
| 29 | 2 | 396 | 0 | 413 | 18 | 0 |
| 30 | 3 | 755 | 0 | 728 | 18 | 0 |
| 31 | I | 519 | 0 | 500 | 23 | 0 |
| 32 | 0 | 42 | 0 | 50 | 24 | 0 |
| 33 | 0 | 108 | 0 | 0 | 0 | 0 |
| 33 | 3 | 2 | 0 | 0 | 0 | 0 |
| 33 | 9 | 1 | 0 | 0 | 0 | 0 |
| 33 | A | 2 | 0 | 0 | 0 | 0 |
| 33 | B | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 33 | K | 1 | 0 | 0 | 0 | 0 |
| 33 | T | 1 | 0 | 0 | 0 | 0 |
| 33 | Y | 1 | 0 | 0 | 0 | 0 |
| 34 | 0 | 2 | 0 | 0 | 0 | 0 |
| 35 | 0 | 74 | 0 | 0 | 2 | 0 |
| 35 | 9 | 2 | 0 | 0 | 0 | 0 |
| 35 | A | 1 | 0 | 0 | 0 | 0 |
| 35 | C | 1 | 0 | 0 | 0 | 0 |
| 35 | H | 1 | 0 | 0 | 0 | 0 |
| 35 | J | 1 | 0 | 0 | 0 | 0 |
| 35 | L | 1 | 0 | 0 | 1 | 0 |
| 35 | M | 1 | 0 | 0 | 0 | 0 |
| 35 | Q | 1 | 0 | 0 | 0 | 0 |
| 35 | R | 2 | 0 | 0 | 0 | 0 |
| 35 | S | 1 | 0 | 0 | 0 | 0 |
| 36 | 0 | 9 | 0 | 0 | 2 | 0 |
| 36 | 3 | 1 | 0 | 0 | 0 | 0 |
| 36 | A | 1 | 0 | 0 | 0 | 0 |
| 36 | B | 1 | 0 | 0 | 0 | 0 |
| 36 | J | 3 | 0 | 0 | 2 | 0 |
| 36 | L | 1 | 0 | 0 | 0 | 0 |
| 36 | M | 1 | 0 | 0 | 1 | 0 |
| 36 | N | 1 | 0 | 0 | 0 | 0 |
| 36 | O | 1 | 0 | 0 | 0 | 0 |
| 36 | R | 1 | 0 | 0 | 0 | 0 |
| 36 | Y | 2 | 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 | 5905 | 0 | 0 | 199 | 0 |
| 38 | 1 | 56 | 0 | 0 | 1 | 0 |
| 38 | 2 | 45 | 0 | 0 | 4 | 0 |
| 38 | 3 | 66 | 0 | 0 | 2 | 0 |
| 38 | 9 | 140 | 0 | 0 | 10 | 0 |
| 38 | A | 112 | 0 | 0 | 8 | 0 |
| 38 | B | 142 | 0 | 0 | 21 | 0 |
| 38 | C | 170 | 0 | 0 | 16 | 0 |
| 38 | D | 45 | 0 | 0 | 8 | 0 |
| 38 | E | 42 | 0 | 0 | 5 | 0 |
| 38 | F | 26 | 0 | 0 | 2 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 38 | G | 19 | 0 | 0 | 0 | 0 |
| 38 | H | 70 | 0 | 0 | 6 | 0 |
| 38 | I | 8 | 0 | 0 | 1 | 0 |
| 38 | J | 58 | 0 | 0 | 3 | 0 |
| 38 | K | 59 | 0 | 0 | 1 | 0 |
| 38 | L | 83 | 0 | 0 | 10 | 0 |
| 38 | M | 123 | 0 | 0 | 4 | 0 |
| 38 | N | 63 | 0 | 0 | 6 | 0 |
| 38 | O | 44 | 0 | 0 | 3 | 0 |
| 38 | P | 56 | 0 | 0 | 2 | 0 |
| 38 | Q | 51 | 0 | 0 | 5 | 0 |
| 38 | R | 80 | 0 | 0 | 2 | 0 |
| 38 | S | 36 | 0 | 0 | 2 | 0 |
| 38 | T | 33 | 0 | 0 | 1 | 0 |
| 38 | U | 26 | 0 | 0 | 2 | 0 |
| 38 | V | 11 | 0 | 0 | 1 | 0 |
| 38 | W | 67 | 0 | 0 | 6 | 0 |
| 38 | X | 21 | 0 | 0 | 2 | 0 |
| 38 | Y | 96 | 0 | 0 | 6 | 0 |
| 38 | Z | 31 | 0 | 0 | 2 | 0 |
| All | All | 99043 | 0 | 59948 | 2276 | 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 (2276) 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) |
|-----------------|------------------|--------------------------|-------------------|
| 1:0:871:G:C8 | 1:0:871:G:H5' | 1.77 | 1.19 |
| 1:0:1160:G:C5' | 1:0:1161:A:H5' | 1.73 | 1.18 |
| 1:0:1160:G:H5' | 1:0:1161:A:C5' | 1.79 | 1.12 |
| 1:0:871:G:H8 | 1:0:871:G:H5' | 1.01 | 1.09 |
| 1:0:1002:G:H2' | 1:0:1003:U:H5'' | 1.37 | 1.07 |
| 1:0:1474:C:H6 | 1:0:1474:C:H5' | 1.16 | 1.06 |
| 2:9:3006:C:H5'' | 15:N:37:ARG:NH1 | 1.70 | 1.06 |
| 2:9:3056:A:H2' | 2:9:3057:A:H5'' | 1.34 | 1.05 |
| 1:0:1242:A:H5' | 11:J:82:THR:HG23 | 1.34 | 1.04 |
| 1:0:541:C:H2' | 1:0:542:A:H5'' | 1.41 | 1.03 |
| 10:H:46:GLN:HB3 | 10:H:167:PRO:HD2 | 1.41 | 1.02 |
| 1:0:542:A:H5' | 1:0:542:A:H8 | 1.25 | 1.01 |
| 1:0:1559:A:H1' | 38:0:5876:HOH:O | 1.59 | 1.01 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:0:2717:C:C2' | 1:0:2718:C:H5'' | 1.91 | 1.01 |
| 1:0:381:G:H5'' | 38:0:4329:HOH:O | 1.61 | 1.00 |
| 1:0:1474:C:C6 | 1:0:1474:C:H5' | 1.99 | 0.98 |
| 1:0:1701:A:H4' | 1:0:1702:U:H5'' | 1.44 | 0.98 |
| 1:0:1666:C:O2' | 1:0:1667:A:H5'' | 1.64 | 0.98 |
| 1:0:1162:G:H1' | 31:I:117:LEU:HD11 | 1.45 | 0.98 |
| 1:0:156:C:H5'' | 14:M:171:ARG:HD3 | 1.41 | 0.97 |
| 1:0:1118:A:H62 | 1:0:1244:U:H3 | 1.09 | 0.97 |
| 1:0:2717:C:H2' | 1:0:2718:C:H5'' | 1.46 | 0.96 |
| 1:0:2460:A:H5' | 32:0:9000:13T:C23 | 1.96 | 0.96 |
| 2:9:3092:G:H2' | 2:9:3093:A:C8 | 2.01 | 0.96 |
| 2:9:3076:G:H3' | 2:9:3077:A:H5'' | 1.43 | 0.95 |
| 5:C:236:THR:HG22 | 5:C:239:ALA:H | 1.28 | 0.95 |
| 1:0:871:G:H8 | 1:0:871:G:C5' | 1.80 | 0.95 |
| 10:H:166:SER:HB2 | 10:H:167:PRO:HD3 | 1.49 | 0.94 |
| 1:0:1205:U:H2' | 1:0:1206:U:H5'' | 1.50 | 0.94 |
| 1:0:2460:A:H5' | 32:0:9000:13T:H233 | 1.46 | 0.93 |
| 1:0:1667:A:H8 | 1:0:1667:A:H5' | 1.34 | 0.93 |
| 29:2:41:HIS:H | 29:2:45:ASN:HD22 | 1.16 | 0.93 |
| 26:Y:200:THR:HG22 | 26:Y:201:GLU:HG3 | 1.49 | 0.93 |
| 1:0:289:G:H22 | 1:0:363:A:H2 | 0.97 | 0.93 |
| 1:0:1172:G:H5'' | 38:0:7252:HOH:O | 1.69 | 0.93 |
| 1:0:877:G:H5' | 1:0:878:G:OP1 | 1.69 | 0.93 |
| 1:0:282:C:H1' | 1:0:368:C:N4 | 1.84 | 0.93 |
| 1:0:1372:A:H3' | 38:0:7182:HOH:O | 1.69 | 0.92 |
| 1:0:2710:U:H1' | 38:0:7605:HOH:O | 1.68 | 0.92 |
| 1:0:545:G:H8 | 1:0:545:G:H5' | 1.34 | 0.92 |
| 12:K:10:GLN:H | 12:K:10:GLN:HE21 | 0.93 | 0.92 |
| 1:0:2506:A:HO2' | 1:0:2507:G:H8 | 0.93 | 0.92 |
| 1:0:506:G:H22 | 1:0:509:A:C5' | 1.82 | 0.91 |
| 1:0:1118:A:H3' | 1:0:1118:A:C8 | 2.05 | 0.91 |
| 1:0:1118:A:H3' | 1:0:1118:A:H8 | 1.33 | 0.91 |
| 1:0:2812:A:H2 | 1:0:2814:A:H62 | 1.06 | 0.91 |
| 1:0:541:C:C2' | 1:0:542:A:H5'' | 1.99 | 0.91 |
| 1:0:870:G:H2' | 1:0:871:G:H5'' | 1.50 | 0.90 |
| 1:0:1184:C:H1' | 38:0:7452:HOH:O | 1.70 | 0.90 |
| 1:0:1603:A:H5' | 1:0:1605:G:O4' | 1.72 | 0.90 |
| 1:0:93:C:H5'' | 23:V:1:THR:HB | 1.51 | 0.90 |
| 25:X:37:LEU:HD13 | 25:X:85:VAL:HG21 | 1.54 | 0.89 |
| 24:W:4:LEU:HD22 | 24:W:52:VAL:HG21 | 1.53 | 0.89 |
| 12:K:29:LEU:HB3 | 12:K:55:VAL:HG11 | 1.54 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:0:2529:G:H3' | 38:0:7177:HOH:O | 1.70 | 0.89 |
| 1:0:289:G:N2 | 1:0:363:A:H2 | 1.70 | 0.89 |
| 21:T:71:VAL:HG11 | 21:T:90:PRO:HB3 | 1.55 | 0.88 |
| 1:0:317:A:H4' | 38:0:3775:HOH:O | 1.73 | 0.88 |
| 17:P:115:SER:H | 17:P:118:GLN:HE21 | 1.20 | 0.88 |
| 6:D:134:LEU:HD11 | 6:D:166:ILE:HD11 | 1.56 | 0.88 |
| 1:0:1209:C:H2' | 1:0:1210:G:H8 | 1.39 | 0.87 |
| 1:0:2508:C:H2' | 38:0:6748:HOH:O | 1.72 | 0.87 |
| 1:0:1165:G:H4' | 1:0:1174:A:O2' | 1.74 | 0.87 |
| 1:0:506:G:H22 | 1:0:509:A:H5'' | 1.37 | 0.87 |
| 2:9:3049:G:H5'' | 38:N:8842:HOH:O | 1.73 | 0.87 |
| 1:0:1641:A:H2' | 1:0:1642:A:H5' | 1.55 | 0.86 |
| 1:0:1116:U:H3 | 1:0:1246:A:H62 | 1.21 | 0.86 |
| 1:0:2783:A:H3' | 38:0:5234:HOH:O | 1.75 | 0.84 |
| 1:0:2586:U:H3 | 1:0:2592:G:H22 | 1.25 | 0.84 |
| 1:0:1701:A:H5' | 38:0:6285:HOH:O | 1.77 | 0.84 |
| 12:K:10:GLN:N | 12:K:10:GLN:HE21 | 1.76 | 0.84 |
| 1:0:2769:C:C2' | 1:0:2770:G:H5' | 2.08 | 0.84 |
| 12:K:10:GLN:H | 12:K:10:GLN:NE2 | 1.76 | 0.84 |
| 1:0:182:G:H5' | 38:0:5159:HOH:O | 1.78 | 0.83 |
| 1:0:2291:A:C8 | 1:0:2309:C:H5' | 2.13 | 0.83 |
| 1:0:272:A:H3' | 38:0:7515:HOH:O | 1.79 | 0.83 |
| 1:0:272:A:H5' | 1:0:273:G:OP2 | 1.79 | 0.83 |
| 15:N:113:SER:HB2 | 38:N:8855:HOH:O | 1.78 | 0.83 |
| 1:0:21:G:H5' | 19:R:2:ILE:HA | 1.61 | 0.83 |
| 1:0:1450:C:H4' | 1:0:1451:C:OP2 | 1.76 | 0.83 |
| 10:H:56:GLN:HE21 | 10:H:126:ARG:HE | 1.25 | 0.83 |
| 24:W:21:LEU:HD21 | 24:W:48:VAL:HG11 | 1.61 | 0.83 |
| 1:0:282:C:O2' | 1:0:283:U:H5' | 1.79 | 0.83 |
| 2:9:3056:A:C2' | 2:9:3057:A:H5'' | 2.09 | 0.83 |
| 5:C:5:ILE:HD11 | 5:C:16:VAL:HG23 | 1.59 | 0.82 |
| 4:B:307:ARG:HH11 | 4:B:307:ARG:HG3 | 1.42 | 0.82 |
| 4:B:36:PRO:HA | 4:B:168:GLY:HA3 | 1.61 | 0.82 |
| 1:0:559:U:H5' | 1:0:559:U:H6 | 1.44 | 0.82 |
| 1:0:69:A:H5' | 1:0:69:A:C8 | 2.14 | 0.82 |
| 1:0:797:A:H4' | 27:Z:10:ARG:N | 1.94 | 0.82 |
| 24:W:88:THR:HB | 38:W:6679:HOH:O | 1.79 | 0.82 |
| 1:0:1183:C:H2' | 38:0:6249:HOH:O | 1.79 | 0.81 |
| 6:D:54:ALA:HB2 | 6:D:69:ILE:HD12 | 1.62 | 0.81 |
| 1:0:1187:U:HO2' | 1:0:1189:A:H2 | 1.26 | 0.81 |
| 4:B:221:GLN:HE22 | 12:K:42:ASN:HD22 | 1.23 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 38:0:5223:HOH:O | 12:K:39:GLY:HA2 | 1.81 | 0.81 |
| 1:0:236:A:H4' | 1:0:237:G:H5' | 1.63 | 0.81 |
| 3:A:211:LYS:HB3 | 3:A:212:PRO:HD2 | 1.62 | 0.81 |
| 1:0:2717:C:O2' | 1:0:2718:C:H5'' | 1.80 | 0.81 |
| 15:N:83:LEU:HD13 | 15:N:175:LEU:HD23 | 1.62 | 0.80 |
| 24:W:137:GLN:HE21 | 24:W:141:HIS:HE1 | 1.29 | 0.80 |
| 1:0:515:C:H5'' | 38:0:5657:HOH:O | 1.81 | 0.80 |
| 3:A:199:HIS:HD2 | 3:A:201:PHE:H | 1.27 | 0.80 |
| 1:0:558:C:O2' | 1:0:559:U:H5'' | 1.81 | 0.80 |
| 1:0:1160:G:H5' | 1:0:1161:A:H5' | 0.88 | 0.80 |
| 19:R:8:ALA:HB1 | 19:R:13:THR:HG21 | 1.64 | 0.80 |
| 1:0:541:C:H2' | 1:0:542:A:C5' | 2.12 | 0.80 |
| 1:0:2533:C:H5' | 1:0:2533:C:H6 | 1.46 | 0.79 |
| 1:0:1835:U:H5 | 1:0:1840:A:N7 | 1.79 | 0.79 |
| 1:0:1206:U:H6 | 1:0:1206:U:H5' | 1.47 | 0.79 |
| 4:B:212:GLN:HB2 | 4:B:257:THR:HG21 | 1.63 | 0.79 |
| 1:0:292:G:H2' | 1:0:358:G:N2 | 1.97 | 0.79 |
| 2:9:3029:C:H2' | 2:9:3030:C:H5' | 1.61 | 0.79 |
| 1:0:1116:U:O2' | 1:0:1118:A:H2 | 1.63 | 0.79 |
| 1:0:2716:G:H5'' | 4:B:206:THR:HG21 | 1.63 | 0.79 |
| 12:K:98:VAL:HG13 | 12:K:102:GLU:HA | 1.64 | 0.79 |
| 1:0:1615:A:H5' | 38:0:4195:HOH:O | 1.83 | 0.79 |
| 1:0:2676:C:H4' | 11:J:70:PHE:CE1 | 2.18 | 0.79 |
| 1:0:2054:A:N3 | 19:R:128:ARG:NH2 | 2.30 | 0.79 |
| 1:0:1116:U:HO2' | 1:0:1118:A:H2 | 0.83 | 0.79 |
| 1:0:1119:G:N2 | 1:0:1246:A:C2 | 2.51 | 0.79 |
| 1:0:1667:A:C8 | 1:0:1667:A:H5' | 2.18 | 0.79 |
| 20:S:57:THR:HG22 | 20:S:59:ASP:H | 1.48 | 0.79 |
| 27:Z:46:ARG:HD3 | 27:Z:59:TYR:HB2 | 1.64 | 0.79 |
| 1:0:1002:G:C2' | 1:0:1003:U:H5'' | 2.13 | 0.78 |
| 1:0:1741:U:H5' | 1:0:1742:A:OP1 | 1.83 | 0.78 |
| 1:0:1441:G:H1' | 38:0:7748:HOH:O | 1.82 | 0.78 |
| 32:0:9000:13T:H2 | 32:0:9000:13T:H262 | 1.65 | 0.78 |
| 1:0:1919:A:H4' | 38:0:4858:HOH:O | 1.83 | 0.78 |
| 1:0:514:G:H4' | 38:0:5657:HOH:O | 1.83 | 0.78 |
| 1:0:1878:G:H1' | 38:0:6128:HOH:O | 1.83 | 0.78 |
| 1:0:1666:C:C2' | 1:0:1667:A:H5'' | 2.14 | 0.78 |
| 1:0:2908:A:H2' | 1:0:2909:G:O4' | 1.83 | 0.78 |
| 1:0:681:G:N3 | 1:0:681:G:H5' | 1.99 | 0.77 |
| 1:0:871:G:C8 | 1:0:871:G:C5' | 2.59 | 0.77 |
| 1:0:1474:C:C5' | 1:0:1474:C:H6 | 1.97 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:0:21:G:C5' | 19:R:2:ILE:HA | 2.13 | 0.77 |
| 1:0:130:C:H2' | 38:0:3162:HOH:O | 1.84 | 0.77 |
| 1:0:2426:G:H1' | 38:0:6098:HOH:O | 1.85 | 0.77 |
| 11:J:75:PRO:HG2 | 11:J:105:LEU:HD21 | 1.66 | 0.77 |
| 1:0:1679:C:H5' | 38:0:9320:HOH:O | 1.85 | 0.77 |
| 1:0:542:A:H5' | 1:0:542:A:C8 | 2.15 | 0.77 |
| 5:C:115:LEU:HD13 | 5:C:223:LEU:HD21 | 1.66 | 0.77 |
| 5:C:127:ARG:NH2 | 5:C:225:PRO:HG2 | 2.00 | 0.77 |
| 32:0:9000:13T:H21 | 32:0:9000:13T:C30 | 2.14 | 0.76 |
| 1:0:1205:U:H2' | 1:0:1206:U:C5' | 2.15 | 0.76 |
| 32:0:9000:13T:C2 | 32:0:9000:13T:H262 | 2.14 | 0.76 |
| 1:0:2769:C:H2' | 1:0:2770:G:H5' | 1.68 | 0.76 |
| 6:D:154:LYS:HD2 | 6:D:154:LYS:H | 1.50 | 0.76 |
| 1:0:12:U:H2' | 1:0:13:G:H5' | 1.67 | 0.76 |
| 1:0:1603:A:H5'' | 1:0:1605:G:H5' | 1.67 | 0.75 |
| 1:0:1058:A:H2' | 1:0:1060:C:H5'' | 1.67 | 0.75 |
| 1:0:1701:A:H4' | 1:0:1702:U:C5' | 2.15 | 0.75 |
| 1:0:2851:G:O2' | 1:0:2852:A:H5' | 1.87 | 0.75 |
| 19:R:18:LEU:HB2 | 19:R:143:VAL:HG13 | 1.66 | 0.75 |
| 1:0:2502:C:C2' | 1:0:2503:A:H5' | 2.16 | 0.74 |
| 24:W:4:LEU:HD23 | 24:W:54:PHE:HB3 | 1.68 | 0.74 |
| 1:0:2010:A:H2' | 38:0:5968:HOH:O | 1.86 | 0.74 |
| 1:0:2570:G:H5'' | 38:0:4917:HOH:O | 1.86 | 0.74 |
| 1:0:558:C:C2' | 1:0:559:U:H5'' | 2.17 | 0.74 |
| 1:0:2766:A:H5' | 38:B:8824:HOH:O | 1.87 | 0.74 |
| 1:0:1205:U:C2' | 1:0:1206:U:H5'' | 2.18 | 0.74 |
| 1:0:2756:U:H3 | 1:0:2896:A:H2 | 1.31 | 0.74 |
| 1:0:2005:G:OP2 | 1:0:2005:G:H3' | 1.87 | 0.74 |
| 1:0:2768:A:O2' | 1:0:2769:C:H5' | 1.86 | 0.74 |
| 1:0:396:U:H1' | 38:0:7612:HOH:O | 1.88 | 0.74 |
| 1:0:899:C:H5' | 38:0:3205:HOH:O | 1.86 | 0.74 |
| 24:W:84:VAL:HG12 | 38:W:6679:HOH:O | 1.88 | 0.74 |
| 1:0:949:U:H4' | 18:Q:95:GLU:HA | 1.68 | 0.74 |
| 1:0:69:A:H5' | 1:0:69:A:H8 | 1.52 | 0.74 |
| 7:E:116:THR:HG22 | 7:E:151:LEU:HD22 | 1.70 | 0.74 |
| 1:0:1926:G:H2' | 1:0:1927:A:H8 | 1.53 | 0.73 |
| 1:0:2768:A:H2' | 1:0:2769:C:O4' | 1.87 | 0.73 |
| 1:0:711:G:H1' | 38:0:7092:HOH:O | 1.87 | 0.73 |
| 2:9:3014:G:H8 | 2:9:3014:G:H5' | 1.51 | 0.73 |
| 10:H:56:GLN:NE2 | 10:H:126:ARG:HE | 1.86 | 0.73 |
| 1:0:797:A:C4' | 27:Z:10:ARG:N | 2.51 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:0:2578:G:H5' | 1:0:2578:G:H8 | 1.53 | 0.73 |
| 1:0:2468:A:H61 | 30:3:48:ASN:HD21 | 1.35 | 0.73 |
| 1:0:961:A:H4' | 38:0:6766:HOH:O | 1.89 | 0.73 |
| 3:A:35:GLY:O | 3:A:36:ASP:HB3 | 1.87 | 0.73 |
| 1:0:2748:G:H1' | 38:0:7883:HOH:O | 1.87 | 0.73 |
| 15:N:49:THR:HG22 | 15:N:56:ASP:HB2 | 1.71 | 0.73 |
| 3:A:51:ARG:HB2 | 38:A:8897:HOH:O | 1.89 | 0.73 |
| 11:J:127:ILE:HG22 | 36:J:8801:CL:CL | 2.25 | 0.73 |
| 22:U:14:GLU:O | 22:U:17:THR:HB | 1.88 | 0.73 |
| 1:0:288:A:H61 | 1:0:364:C:H42 | 1.36 | 0.73 |
| 1:0:544:G:H2' | 1:0:545:G:H5'' | 1.70 | 0.72 |
| 5:C:233:THR:HG22 | 5:C:234:VAL:H | 1.54 | 0.72 |
| 1:0:2781:U:C2' | 1:0:2782:G:H5' | 2.19 | 0.72 |
| 1:0:545:G:C8 | 1:0:545:G:H5' | 2.22 | 0.72 |
| 1:0:587:A:H5'' | 38:0:7279:HOH:O | 1.89 | 0.72 |
| 1:0:1926:G:H2' | 1:0:1927:A:C8 | 2.24 | 0.72 |
| 24:W:137:GLN:HE21 | 24:W:141:HIS:CE1 | 2.07 | 0.72 |
| 1:0:2781:U:H2' | 1:0:2782:G:H5' | 1.70 | 0.72 |
| 1:0:1634:G:H3' | 38:0:3901:HOH:O | 1.89 | 0.72 |
| 1:0:1080:C:H4' | 1:0:1081:A:OP1 | 1.89 | 0.72 |
| 1:0:1350:U:H4' | 38:0:5124:HOH:O | 1.88 | 0.72 |
| 1:0:870:G:C2' | 1:0:871:G:H5'' | 2.17 | 0.72 |
| 1:0:2505:G:O2' | 1:0:2506:A:H5' | 1.89 | 0.71 |
| 1:0:2507:G:H2' | 1:0:2510:C:H42 | 1.55 | 0.71 |
| 1:0:1593:C:H5' | 17:P:116:SER:O | 1.89 | 0.71 |
| 1:0:2243:C:H5'' | 38:0:3753:HOH:O | 1.88 | 0.71 |
| 30:3:25:VAL:HG22 | 30:3:68:LYS:HG3 | 1.71 | 0.71 |
| 38:0:3759:HOH:O | 21:T:9:LYS:HD3 | 1.88 | 0.71 |
| 25:X:76:ARG:HH11 | 25:X:76:ARG:HG3 | 1.55 | 0.71 |
| 1:0:1189:A:H1' | 1:0:1209:C:C1' | 2.19 | 0.71 |
| 1:0:1189:A:H1' | 1:0:1209:C:O4' | 1.91 | 0.71 |
| 1:0:2420:G:O2' | 1:0:2421:G:H5' | 1.90 | 0.71 |
| 1:0:2827:A:H2' | 1:0:2828:G:O4' | 1.90 | 0.71 |
| 1:0:2862:G:H4' | 4:B:336:GLN:O | 1.91 | 0.71 |
| 1:0:2878:U:H2' | 1:0:2879:A:O4' | 1.90 | 0.71 |
| 16:O:32:ARG:HE | 16:O:35:LYS:HD2 | 1.56 | 0.71 |
| 19:R:18:LEU:HG | 19:R:91:LEU:HD13 | 1.73 | 0.71 |
| 2:9:3039:U:H3' | 2:9:3040:C:H5'' | 1.73 | 0.71 |
| 1:0:308:U:H5' | 1:0:309:C:OP1 | 1.90 | 0.71 |
| 1:0:156:C:H5'' | 14:M:171:ARG:CD | 2.19 | 0.71 |
| 1:0:271:C:H41 | 1:0:378:A:H2 | 1.36 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:0:2717:C:H2' | 1:0:2718:C:C5' | 2.21 | 0.70 |
| 5:C:236:THR:HG22 | 5:C:239:ALA:N | 2.04 | 0.70 |
| 13:L:133:VAL:HA | 38:L:8872:HOH:O | 1.90 | 0.70 |
| 1:0:1342:C:C2' | 1:0:1343:C:H5' | 2.20 | 0.70 |
| 1:0:2364:A:H5'' | 18:Q:15:LYS:HD3 | 1.73 | 0.70 |
| 19:R:81:PRO:O | 19:R:85:SER:HB2 | 1.91 | 0.70 |
| 6:D:23:VAL:HG22 | 6:D:73:VAL:HB | 1.72 | 0.70 |
| 1:0:214:U:H5' | 38:0:6147:HOH:O | 1.91 | 0.70 |
| 1:0:2526:C:O2' | 1:0:2527:U:H5' | 1.91 | 0.70 |
| 1:0:544:G:C2' | 1:0:545:G:H5'' | 2.22 | 0.70 |
| 8:F:58:GLU:HA | 8:F:61:MET:HE2 | 1.74 | 0.70 |
| 3:A:191:GLY:HA2 | 3:A:194:MET:CE | 2.22 | 0.69 |
| 1:0:962:C:H1' | 15:N:5:ARG:NH1 | 2.07 | 0.69 |
| 17:P:115:SER:H | 17:P:118:GLN:NE2 | 1.90 | 0.69 |
| 1:0:2748:G:H2' | 38:0:7526:HOH:O | 1.91 | 0.69 |
| 17:P:143:ALA:HA | 38:P:5521:HOH:O | 1.93 | 0.69 |
| 24:W:72:PRO:HG2 | 24:W:77:ALA:HB3 | 1.74 | 0.69 |
| 1:0:2748:G:H5' | 38:0:7526:HOH:O | 1.92 | 0.69 |
| 4:B:201:ASP:HB2 | 4:B:312:ARG:HD2 | 1.74 | 0.69 |
| 1:0:338:C:H4' | 5:C:174:ILE:CD1 | 2.21 | 0.69 |
| 1:0:1299:G:O6 | 13:L:6:ARG:HD3 | 1.92 | 0.69 |
| 1:0:960:G:H4' | 38:0:7420:HOH:O | 1.92 | 0.69 |
| 5:C:47:GLY:HA2 | 5:C:92:PRO:HB2 | 1.74 | 0.69 |
| 24:W:80:ASP:O | 24:W:84:VAL:HG23 | 1.92 | 0.69 |
| 4:B:74:ILE:HD13 | 4:B:309:VAL:HG21 | 1.73 | 0.69 |
| 1:0:559:U:H5' | 1:0:559:U:C6 | 2.27 | 0.69 |
| 3:A:191:GLY:HA2 | 3:A:194:MET:HE3 | 1.75 | 0.69 |
| 6:D:103:ASN:ND2 | 6:D:134:LEU:H | 1.90 | 0.69 |
| 1:0:2004:U:H4' | 38:0:5313:HOH:O | 1.93 | 0.69 |
| 24:W:88:THR:HG22 | 24:W:89:ASP:H | 1.58 | 0.69 |
| 1:0:558:C:H2' | 1:0:559:U:C5' | 2.23 | 0.69 |
| 4:B:238:ASN:HD22 | 4:B:240:GLY:H | 1.41 | 0.69 |
| 1:0:1119:G:H2' | 11:J:52:GLN:NE2 | 2.08 | 0.69 |
| 1:0:1189:A:H3' | 38:0:7666:HOH:O | 1.93 | 0.68 |
| 1:0:560:C:H42 | 1:0:597:A:H61 | 1.39 | 0.68 |
| 1:0:1242:A:H5' | 11:J:82:THR:CG2 | 2.18 | 0.68 |
| 32:0:9000:13T:H301 | 32:0:9000:13T:H21 | 1.74 | 0.68 |
| 1:0:657:G:OP1 | 5:C:27:ARG:NH2 | 2.26 | 0.68 |
| 1:0:1641:A:C2' | 1:0:1642:A:H5' | 2.23 | 0.68 |
| 1:0:821:U:H2' | 1:0:822:C:H6 | 1.57 | 0.68 |
| 36:0:8813:CL:CL | 38:0:4691:HOH:O | 2.48 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:9:3054:A:O2' | 2:9:3055:U:H5' | 1.94 | 0.68 |
| 7:E:97:VAL:HG12 | 38:E:4191:HOH:O | 1.94 | 0.68 |
| 10:H:166:SER:HB2 | 10:H:167:PRO:CD | 2.21 | 0.68 |
| 1:0:1183:C:H42 | 1:0:1184:C:H41 | 1.42 | 0.68 |
| 1:0:2635:A:O2' | 1:0:2636:C:H5' | 1.94 | 0.68 |
| 3:A:199:HIS:CD2 | 3:A:201:PHE:H | 2.10 | 0.68 |
| 7:E:81:GLU:HG2 | 7:E:134:SER:HB3 | 1.75 | 0.68 |
| 1:0:2459:G:H2' | 32:0:9000:13T:C23 | 2.24 | 0.68 |
| 3:A:192:VAL:CG1 | 3:A:207:GLN:HB3 | 2.22 | 0.68 |
| 6:D:41:LEU:HA | 6:D:44:ILE:HG22 | 1.76 | 0.68 |
| 1:0:1244:U:OP1 | 11:J:18:ILE:HD13 | 1.93 | 0.68 |
| 1:0:2812:A:C2 | 1:0:2814:A:N6 | 2.55 | 0.68 |
| 1:0:603:A:H5'' | 1:0:604:G:OP1 | 1.93 | 0.68 |
| 24:W:125:HIS:HD2 | 24:W:127:GLY:H | 1.40 | 0.68 |
| 1:0:1183:C:N4 | 1:0:1184:C:H41 | 1.90 | 0.68 |
| 14:M:134:ILE:HG23 | 14:M:141:ILE:HD13 | 1.76 | 0.68 |
| 1:0:138:U:H5'' | 1:0:139:C:OP2 | 1.95 | 0.67 |
| 1:0:500:G:H21 | 19:R:98:ASN:HD21 | 1.41 | 0.67 |
| 1:0:2374:A:H2' | 1:0:2375:G:C8 | 2.29 | 0.67 |
| 1:0:2502:C:H2' | 1:0:2503:A:H5' | 1.76 | 0.67 |
| 29:2:35:ARG:HB2 | 38:2:2691:HOH:O | 1.95 | 0.67 |
| 1:0:1189:A:O2' | 1:0:1208:C:H2' | 1.95 | 0.67 |
| 1:0:1213:C:O2' | 1:0:1214:G:H5' | 1.94 | 0.67 |
| 1:0:1118:A:N6 | 1:0:1244:U:H3 | 1.87 | 0.67 |
| 1:0:506:G:H22 | 1:0:509:A:H5' | 1.57 | 0.67 |
| 5:C:129:HIS:CE1 | 5:C:231:ARG:HA | 2.29 | 0.67 |
| 23:V:57:LYS:HA | 23:V:60:GLN:HE21 | 1.60 | 0.67 |
| 1:0:2533:C:C6 | 1:0:2533:C:H5' | 2.28 | 0.67 |
| 1:0:706:G:HO2' | 1:0:707:C:H6 | 1.43 | 0.67 |
| 11:J:107:ASN:HD22 | 11:J:109:TYR:H | 1.42 | 0.67 |
| 1:0:2717:C:OP1 | 4:B:207:LYS:HG3 | 1.95 | 0.67 |
| 11:J:76:ASP:HA | 38:J:8868:HOH:O | 1.94 | 0.67 |
| 23:V:12:THR:HG22 | 23:V:15:GLU:HG3 | 1.77 | 0.67 |
| 1:0:1973:A:H5' | 1:0:1973:A:H8 | 1.59 | 0.67 |
| 1:0:280:C:H2' | 1:0:281:U:O4' | 1.95 | 0.66 |
| 1:0:2563:U:H2' | 1:0:2565:C:O5' | 1.96 | 0.66 |
| 4:B:267:LYS:HD3 | 38:B:8824:HOH:O | 1.95 | 0.66 |
| 1:0:2100:A:H5' | 38:C:8662:HOH:O | 1.93 | 0.66 |
| 1:0:2256:G:H2' | 1:0:2257:G:C5' | 2.25 | 0.66 |
| 1:0:485:A:N3 | 1:0:487:G:H5'' | 2.10 | 0.66 |
| 11:J:74:ARG:HB3 | 11:J:74:ARG:HH11 | 1.61 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:Z:10:ARG:HA | 38:Z:8715:HOH:O | 1.96 | 0.66 |
| 1:0:2256:G:H2' | 1:0:2257:G:H5' | 1.78 | 0.66 |
| 1:0:2489:G:H1' | 38:0:7268:HOH:O | 1.95 | 0.66 |
| 1:0:284:C:H4' | 1:0:285:A:O5' | 1.96 | 0.66 |
| 5:C:1:MET:HG2 | 5:C:2:GLN:H | 1.61 | 0.66 |
| 30:3:73:GLU:HB3 | 38:3:8854:HOH:O | 1.94 | 0.66 |
| 1:0:1162:G:H1' | 31:I:117:LEU:CD1 | 2.24 | 0.66 |
| 1:0:1209:C:H2' | 1:0:1210:G:C8 | 2.26 | 0.66 |
| 1:0:1328:A:OP1 | 26:Y:169:ARG:HD2 | 1.96 | 0.66 |
| 1:0:1524:U:OP1 | 1:0:1524:U:H4' | 1.94 | 0.66 |
| 1:0:2506:A:O2' | 1:0:2507:G:H8 | 1.72 | 0.66 |
| 1:0:2521:A:OP2 | 10:H:3:ALA:HB3 | 1.96 | 0.66 |
| 1:0:694:A:H2' | 1:0:695:C:H5' | 1.77 | 0.66 |
| 4:B:162:MET:HG3 | 4:B:310:ARG:HD3 | 1.78 | 0.66 |
| 19:R:99:ALA:HB1 | 19:R:109:MET:CE | 2.26 | 0.66 |
| 1:0:21:G:H5'' | 19:R:1:GLY:O | 1.97 | 0.65 |
| 1:0:2638:G:H1' | 38:0:7742:HOH:O | 1.96 | 0.65 |
| 1:0:1684:A:H1' | 29:2:43:ARG:HH22 | 1.61 | 0.65 |
| 15:N:48:VAL:CG1 | 15:N:55:ASP:HB3 | 2.25 | 0.65 |
| 2:9:3029:C:C2' | 2:9:3030:C:H5' | 2.26 | 0.65 |
| 12:K:74:VAL:HG12 | 12:K:75:ARG:HG3 | 1.79 | 0.65 |
| 1:0:2460:A:C5' | 32:0:9000:13T:H233 | 2.23 | 0.65 |
| 26:Y:187:VAL:HG23 | 26:Y:192:ASP:CB | 2.26 | 0.65 |
| 1:0:136:C:H2' | 1:0:137:U:O4' | 1.97 | 0.65 |
| 4:B:179:LEU:O | 4:B:183:GLU:HG2 | 1.95 | 0.65 |
| 5:C:140:VAL:HB | 38:C:8651:HOH:O | 1.94 | 0.65 |
| 1:0:2890:A:H1' | 22:U:56:ARG:NH2 | 2.11 | 0.65 |
| 1:0:1666:C:H2' | 1:0:1667:A:C5' | 2.26 | 0.65 |
| 1:0:2414:A:H2' | 1:0:2415:A:C8 | 2.31 | 0.65 |
| 1:0:447:A:O2' | 1:0:448:G:H5' | 1.97 | 0.65 |
| 1:0:558:C:H2' | 1:0:559:U:H5' | 1.79 | 0.65 |
| 1:0:1187:U:O2' | 1:0:1189:A:H2 | 1.78 | 0.65 |
| 1:0:2795:C:O2' | 1:0:2796:U:H5' | 1.96 | 0.65 |
| 1:0:407:A:H8 | 38:0:4466:HOH:O | 1.79 | 0.65 |
| 1:0:584:U:H3' | 38:0:6101:HOH:O | 1.96 | 0.65 |
| 12:K:14:LYS:HB2 | 12:K:45:PRO:HG2 | 1.79 | 0.65 |
| 2:9:3003:A:N6 | 2:9:3022:G:H1' | 2.12 | 0.65 |
| 1:0:1701:A:H5'' | 1:0:1702:U:H3' | 1.77 | 0.65 |
| 1:0:2320:U:H4' | 1:0:2321:A:O4' | 1.97 | 0.64 |
| 1:0:2780:C:H1' | 7:E:143:GLN:HE21 | 1.62 | 0.64 |
| 10:H:169:GLY:HA3 | 38:H:8591:HOH:O | 1.95 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:0:1342:C:H2' | 1:0:1343:C:H5' | 1.79 | 0.64 |
| 1:0:2241:C:O2' | 1:0:2242:U:H5' | 1.96 | 0.64 |
| 1:0:2787:C:H5 | 38:0:4641:HOH:O | 1.80 | 0.64 |
| 1:0:403:C:H3' | 38:0:6307:HOH:O | 1.97 | 0.64 |
| 12:K:74:VAL:CG1 | 12:K:113:ILE:HG12 | 2.28 | 0.64 |
| 24:W:88:THR:HG23 | 24:W:110:GLN:HE21 | 1.62 | 0.64 |
| 1:0:281:U:O2' | 1:0:282:C:H5' | 1.96 | 0.64 |
| 1:0:2896:A:H5'' | 38:0:6105:HOH:O | 1.97 | 0.64 |
| 1:0:441:A:H1' | 1:0:442:A:N7 | 2.13 | 0.64 |
| 6:D:99:ASP:HB3 | 6:D:103:ASN:H | 1.62 | 0.64 |
| 1:0:958:G:H2' | 1:0:959:C:C6 | 2.32 | 0.64 |
| 38:0:4678:HOH:O | 4:B:300:SER:HB3 | 1.97 | 0.64 |
| 6:D:135:VAL:HG21 | 6:D:139:TYR:CD1 | 2.32 | 0.64 |
| 1:0:2721:U:H4' | 12:K:87:ARG:HG3 | 1.79 | 0.64 |
| 25:X:72:VAL:HG22 | 25:X:85:VAL:HG12 | 1.79 | 0.64 |
| 2:9:3091:C:H2' | 2:9:3092:G:O4' | 1.97 | 0.64 |
| 3:A:121:ALA:O | 3:A:124:VAL:HG22 | 1.97 | 0.64 |
| 12:K:98:VAL:CG1 | 12:K:102:GLU:HA | 2.27 | 0.64 |
| 1:0:1185:U:H2' | 1:0:1186:C:C6 | 2.33 | 0.64 |
| 1:0:2769:C:O2' | 1:0:2770:G:H5' | 1.96 | 0.64 |
| 1:0:2459:G:H2' | 32:0:9000:13T:H233 | 1.80 | 0.64 |
| 1:0:1044:C:H5 | 38:0:6599:HOH:O | 1.81 | 0.64 |
| 2:9:3048:C:H4' | 15:N:141:ARG:HH21 | 1.63 | 0.64 |
| 2:9:3039:U:H1' | 2:9:3044:A:H61 | 1.63 | 0.64 |
| 23:V:42:ASN:HB3 | 38:V:7247:HOH:O | 1.95 | 0.64 |
| 14:M:23:LEU:HD13 | 14:M:27:ARG:NH2 | 2.12 | 0.63 |
| 1:0:1200:A:H3' | 38:0:5765:HOH:O | 1.98 | 0.63 |
| 1:0:1790:C:H2' | 1:0:1791:U:H6 | 1.63 | 0.63 |
| 1:0:2769:C:H2' | 1:0:2770:G:C5' | 2.27 | 0.63 |
| 2:9:3007:G:H5' | 38:9:5071:HOH:O | 1.98 | 0.63 |
| 10:H:46:GLN:HE21 | 10:H:137:TYR:HE2 | 1.45 | 0.63 |
| 5:C:236:THR:HG21 | 38:C:8571:HOH:O | 1.98 | 0.63 |
| 13:L:114:VAL:HG11 | 38:L:8872:HOH:O | 1.99 | 0.63 |
| 1:0:1165:G:H1' | 1:0:1174:A:H1' | 1.79 | 0.63 |
| 1:0:1189:A:H1' | 1:0:1209:C:H1' | 1.79 | 0.63 |
| 1:0:157:G:H4' | 14:M:95:LYS:HE2 | 1.79 | 0.63 |
| 4:B:36:PRO:HG3 | 4:B:169:GLY:H | 1.62 | 0.63 |
| 10:H:166:SER:CB | 10:H:167:PRO:HD3 | 2.27 | 0.63 |
| 16:O:47:ARG:HG3 | 16:O:47:ARG:HH11 | 1.63 | 0.63 |
| 18:Q:26:PRO:O | 18:Q:30:VAL:HG23 | 1.98 | 0.63 |
| 1:0:1185:U:H5' | 38:0:7452:HOH:O | 1.98 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:0:1211:G:H2' | 1:0:1212:C:H6 | 1.63 | 0.63 |
| 1:0:1596:U:H2' | 1:0:1598:A:OP2 | 1.99 | 0.63 |
| 1:0:2443:C:H1' | 13:L:56:LYS:HE3 | 1.81 | 0.63 |
| 13:L:148:GLU:HB2 | 38:L:8889:HOH:O | 1.99 | 0.63 |
| 1:0:447:A:P | 21:T:1:SER:HB2 | 2.39 | 0.63 |
| 27:Z:57:CYS:SG | 27:Z:59:TYR:HB3 | 2.38 | 0.63 |
| 4:B:71:VAL:HG21 | 4:B:296:LEU:HB3 | 1.81 | 0.63 |
| 1:0:20:G:H21 | 19:R:117:HIS:HD2 | 1.47 | 0.63 |
| 1:0:289:G:O2' | 1:0:290:C:H5' | 1.99 | 0.63 |
| 1:0:1164:U:H3 | 1:0:1192:A:H2 | 1.46 | 0.62 |
| 1:0:1666:C:C2' | 1:0:1667:A:C5' | 2.77 | 0.62 |
| 1:0:1878:G:O2' | 1:0:1879:U:C6 | 2.49 | 0.62 |
| 1:0:567:U:H5'' | 38:0:6400:HOH:O | 1.98 | 0.62 |
| 1:0:1313:A:H5' | 26:Y:208:LYS:O | 1.99 | 0.62 |
| 2:9:3092:G:H2' | 2:9:3093:A:H8 | 1.58 | 0.62 |
| 1:0:1307:A:H2' | 1:0:1308:A:C8 | 2.34 | 0.62 |
| 1:0:1666:C:H2' | 1:0:1667:A:H5' | 1.81 | 0.62 |
| 1:0:951:A:C2' | 1:0:952:G:H5' | 2.29 | 0.62 |
| 5:C:67:GLN:HG2 | 38:C:8624:HOH:O | 2.00 | 0.62 |
| 18:Q:25:PRO:HB2 | 38:Q:4350:HOH:O | 1.99 | 0.62 |
| 1:0:1537:C:H1' | 38:0:6583:HOH:O | 1.98 | 0.62 |
| 1:0:396:U:O2' | 1:0:418:C:H4' | 1.99 | 0.62 |
| 2:9:3036:C:C5 | 2:9:3037:C:C5 | 2.88 | 0.62 |
| 1:0:1377:C:H6 | 1:0:1377:C:H5' | 1.64 | 0.62 |
| 1:0:1667:A:H2' | 1:0:1668:U:C6 | 2.34 | 0.62 |
| 1:0:292:G:H2' | 1:0:358:G:H22 | 1.65 | 0.62 |
| 3:A:200:PRO:HG2 | 3:A:225:VAL:HG21 | 1.80 | 0.62 |
| 15:N:80:SER:HB2 | 38:N:8832:HOH:O | 1.99 | 0.62 |
| 1:0:1625:U:H4' | 38:0:4674:HOH:O | 2.00 | 0.62 |
| 1:0:960:G:H2' | 1:0:960:G:N3 | 2.13 | 0.62 |
| 25:X:43:VAL:HG12 | 25:X:44:ASP:N | 2.15 | 0.62 |
| 1:0:1441:G:O2' | 1:0:1442:A:H5' | 2.00 | 0.62 |
| 1:0:1636:G:O2' | 1:0:1637:A:H5' | 1.99 | 0.62 |
| 1:0:2256:G:C2' | 1:0:2257:G:H5' | 2.29 | 0.62 |
| 29:2:22:PRO:HG2 | 29:2:25:VAL:HG23 | 1.82 | 0.62 |
| 14:M:99:ARG:HH21 | 14:M:170:ASN:HD22 | 1.48 | 0.62 |
| 1:0:558:C:C2' | 1:0:559:U:C5' | 2.78 | 0.61 |
| 2:9:3014:G:C8 | 2:9:3014:G:H5' | 2.34 | 0.61 |
| 19:R:96:VAL:HG13 | 19:R:106:GLY:HA3 | 1.82 | 0.61 |
| 23:V:39:ALA:N | 23:V:40:PRO:HD2 | 2.14 | 0.61 |
| 35:L:8580:NA:NA | 38:L:8826:HOH:O | 1.71 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 15:N:67:ALA:HA | 15:N:71:TRP:HB3 | 1.82 | 0.61 |
| 1:0:656:G:H5' | 16:O:3:THR:HB | 1.80 | 0.61 |
| 1:0:597:A:H2' | 1:0:598:C:H6 | 1.65 | 0.61 |
| 35:0:8542:NA:NA | 38:0:5663:HOH:O | 1.71 | 0.61 |
| 15:N:61:ALA:HB3 | 15:N:88:ALA:HB2 | 1.80 | 0.61 |
| 23:V:55:ARG:O | 23:V:59:ILE:HG12 | 1.99 | 0.61 |
| 1:0:1406:A:H4' | 1:0:1407:A:H5'' | 1.81 | 0.61 |
| 1:0:1528:A:H2' | 1:0:1529:G:O4' | 2.00 | 0.61 |
| 1:0:1603:A:C5' | 1:0:1605:G:H5' | 2.30 | 0.61 |
| 1:0:2445:U:H2' | 1:0:2446:G:C8 | 2.36 | 0.61 |
| 1:0:2511:A:H2' | 1:0:2512:U:O4' | 2.00 | 0.61 |
| 1:0:308:U:C4 | 1:0:342:C:H1' | 2.35 | 0.61 |
| 1:0:470:U:O2' | 28:1:16:HIS:HD2 | 1.82 | 0.61 |
| 23:V:1:THR:HG23 | 23:V:2:VAL:H | 1.65 | 0.61 |
| 1:0:1234:U:N3 | 4:B:244:PRO:HB3 | 2.15 | 0.61 |
| 1:0:2338:G:H1' | 6:D:105:SER:OG | 1.99 | 0.61 |
| 1:0:538:C:OP2 | 26:Y:134:HIS:HE1 | 1.84 | 0.61 |
| 38:0:7359:HOH:O | 12:K:45:PRO:HB2 | 2.01 | 0.61 |
| 12:K:81:ARG:HD3 | 12:K:87:ARG:NH2 | 2.15 | 0.61 |
| 18:Q:21:ARG:HA | 38:Q:6597:HOH:O | 2.00 | 0.61 |
| 1:0:128:A:O2' | 1:0:129:A:H5' | 2.01 | 0.61 |
| 2:9:3041:C:O4' | 6:D:50:VAL:HG22 | 2.00 | 0.61 |
| 24:W:13:MET:HE1 | 24:W:18:GLN:HA | 1.82 | 0.61 |
| 1:0:1477:C:H5' | 1:0:1868:G:C5' | 2.30 | 0.61 |
| 2:9:3064:C:H2' | 2:9:3065:A:H5' | 1.83 | 0.61 |
| 6:D:28:GLY:HA2 | 6:D:69:ILE:HG23 | 1.82 | 0.61 |
| 1:0:2507:G:H2' | 1:0:2510:C:N4 | 2.16 | 0.61 |
| 1:0:281:U:H2' | 1:0:282:C:O4' | 2.01 | 0.61 |
| 2:9:3064:C:C2' | 2:9:3065:A:H5' | 2.31 | 0.61 |
| 8:F:50:VAL:HG13 | 8:F:60:VAL:HG11 | 1.82 | 0.61 |
| 24:W:137:GLN:NE2 | 24:W:141:HIS:HE1 | 1.98 | 0.61 |
| 1:0:1762:C:H2' | 1:0:1763:C:H6 | 1.65 | 0.61 |
| 1:0:2433:A:H2' | 1:0:2434:A:C8 | 2.36 | 0.61 |
| 10:H:27:LYS:H | 10:H:59:HIS:CD2 | 2.19 | 0.61 |
| 1:0:2134:G:N2 | 1:0:2242:U:C2 | 2.69 | 0.60 |
| 1:0:656:G:OP2 | 16:O:37:ARG:HD2 | 2.00 | 0.60 |
| 3:A:88:ILE:HD13 | 3:A:100:PRO:HD3 | 1.81 | 0.60 |
| 1:0:1130:U:H2' | 1:0:1131:G:O4' | 2.01 | 0.60 |
| 1:0:517:U:H1' | 38:0:7561:HOH:O | 2.00 | 0.60 |
| 2:9:3006:C:H5'' | 15:N:37:ARG:HH12 | 1.62 | 0.60 |
| 1:0:338:C:H4' | 5:C:174:ILE:HD11 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 20:S:11:THR:H | 20:S:14:ALA:HB3 | 1.65 | 0.60 |
| 1:0:90:A:H2' | 1:0:91:G:O4' | 2.01 | 0.60 |
| 1:0:2659:U:H5'' | 38:0:4135:HOH:O | 2.00 | 0.60 |
| 1:0:669:G:O2' | 1:0:670:G:H5' | 2.01 | 0.60 |
| 32:0:9000:13T:H262 | 32:0:9000:13T:O3 | 2.01 | 0.60 |
| 29:2:20:ARG:HG2 | 29:2:21:VAL:H | 1.66 | 0.60 |
| 30:3:65:THR:HG23 | 30:3:67:LEU:HG | 1.84 | 0.60 |
| 1:0:1118:A:C8 | 1:0:1118:A:C3' | 2.70 | 0.60 |
| 1:0:255:A:H2' | 1:0:256:C:C6 | 2.36 | 0.60 |
| 27:Z:11:SER:HB3 | 27:Z:23:ARG:HB2 | 1.83 | 0.60 |
| 1:0:1819:G:H2' | 1:0:1820:G:H4' | 1.83 | 0.60 |
| 1:0:510:U:H6 | 38:0:7427:HOH:O | 1.85 | 0.60 |
| 1:0:602:A:O2' | 1:0:605:C:H4' | 2.01 | 0.60 |
| 1:0:2359:G:H3' | 38:0:5701:HOH:O | 2.01 | 0.60 |
| 1:0:512:G:O3' | 1:0:513:A:H8 | 1.85 | 0.60 |
| 14:M:187:LEU:CD2 | 14:M:194:ALA:HB3 | 2.32 | 0.60 |
| 3:A:48:ASP:HB3 | 38:A:8897:HOH:O | 2.02 | 0.60 |
| 1:0:2301:A:H5'' | 1:0:2302:A:H5' | 1.84 | 0.59 |
| 1:0:255:A:H2' | 1:0:256:C:H6 | 1.66 | 0.59 |
| 4:B:214:PRO:HD2 | 38:B:8820:HOH:O | 2.02 | 0.59 |
| 6:D:103:ASN:ND2 | 6:D:133:ASN:HA | 2.17 | 0.59 |
| 6:D:65:GLU:HA | 38:D:4069:HOH:O | 2.02 | 0.59 |
| 27:Z:22:SER:O | 27:Z:26:VAL:HG23 | 2.01 | 0.59 |
| 1:0:1202:A:H2' | 1:0:1203:G:H5' | 1.85 | 0.59 |
| 1:0:1525:G:H5' | 1:0:1526:A:OP2 | 2.02 | 0.59 |
| 1:0:450:C:OP1 | 5:C:184:ARG:NH2 | 2.34 | 0.59 |
| 6:D:50:VAL:O | 6:D:71:ALA:HA | 2.02 | 0.59 |
| 1:0:1266:U:H4' | 26:Y:115:ARG:HH21 | 1.66 | 0.59 |
| 1:0:1741:U:O2' | 1:0:2723:G:H4' | 2.02 | 0.59 |
| 32:0:9000:13T:H3 | 30:3:56:PRO:HB2 | 1.83 | 0.59 |
| 2:9:3039:U:H3' | 2:9:3040:C:C5' | 2.32 | 0.59 |
| 4:B:86:ALA:HA | 38:B:8876:HOH:O | 2.01 | 0.59 |
| 7:E:15:GLN:HG3 | 7:E:20:ILE:HG12 | 1.83 | 0.59 |
| 14:M:114:VAL:HG23 | 36:M:8818:CL:CL | 2.39 | 0.59 |
| 19:R:111:ILE:HG23 | 19:R:145:LEU:HD11 | 1.83 | 0.59 |
| 27:Z:42:CYS:SG | 27:Z:43:GLY:N | 2.75 | 0.59 |
| 1:0:1504:A:H5' | 38:0:4423:HOH:O | 2.02 | 0.59 |
| 4:B:212:GLN:HB2 | 4:B:257:THR:CG2 | 2.33 | 0.59 |
| 1:0:1060:C:H6 | 1:0:1060:C:H5' | 1.65 | 0.59 |
| 1:0:2807:U:P | 4:B:27:ASN:HD21 | 2.24 | 0.59 |
| 1:0:966:U:H5' | 38:0:3861:HOH:O | 2.01 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 11:J:45:VAL:HG21 | 11:J:129:PHE:CD1 | 2.38 | 0.59 |
| 1:0:1163:G:H2' | 1:0:1164:U:C5 | 2.37 | 0.59 |
| 1:0:249:G:O2' | 1:0:250:C:H5' | 2.03 | 0.59 |
| 23:V:12:THR:HG23 | 23:V:14:ALA:H | 1.68 | 0.59 |
| 1:0:1167:G:O2' | 1:0:1168:C:H5' | 2.02 | 0.59 |
| 1:0:1183:C:N3 | 1:0:1184:C:C5 | 2.71 | 0.59 |
| 1:0:1736:A:H1' | 38:0:7569:HOH:O | 2.03 | 0.59 |
| 7:E:100:ASP:HB2 | 38:E:2789:HOH:O | 2.02 | 0.59 |
| 8:F:58:GLU:HG3 | 8:F:61:MET:HE1 | 1.85 | 0.59 |
| 23:V:49:LEU:O | 23:V:53:ILE:HG13 | 2.01 | 0.59 |
| 1:0:2781:U:H2' | 1:0:2782:G:C5' | 2.31 | 0.59 |
| 1:0:39:G:N2 | 1:0:444:C:C2 | 2.71 | 0.59 |
| 1:0:84:G:O2' | 1:0:85:C:H5' | 2.02 | 0.59 |
| 38:0:9354:HOH:O | 28:1:1:THR:HA | 2.03 | 0.59 |
| 10:H:3:ALA:HA | 10:H:58:ARG:HH12 | 1.67 | 0.59 |
| 14:M:30:GLU:O | 14:M:34:GLU:HG3 | 2.02 | 0.59 |
| 1:0:121:U:OP2 | 29:2:10:ARG:NH2 | 2.35 | 0.59 |
| 1:0:2851:G:C2' | 1:0:2852:A:H5' | 2.32 | 0.59 |
| 1:0:947:U:H2' | 1:0:948:G:C8 | 2.38 | 0.59 |
| 27:Z:44:GLU:HG2 | 27:Z:46:ARG:HD2 | 1.85 | 0.59 |
| 1:0:316:A:N3 | 1:0:336:G:O2' | 2.34 | 0.59 |
| 35:0:8542:NA:NA | 38:0:3317:HOH:O | 1.75 | 0.59 |
| 1:0:364:C:H2' | 1:0:365:G:O4' | 2.03 | 0.58 |
| 8:F:63:ILE:HB | 8:F:64:PRO:HD3 | 1.84 | 0.58 |
| 15:N:86:LEU:HD12 | 15:N:125:ALA:HB2 | 1.85 | 0.58 |
| 1:0:1014:A:H2' | 1:0:1015:C:H5' | 1.85 | 0.58 |
| 1:0:1015:C:H2' | 1:0:1016:U:H6 | 1.67 | 0.58 |
| 31:I:132:CYS:HB3 | 31:I:137:VAL:HB | 1.83 | 0.58 |
| 11:J:107:ASN:ND2 | 11:J:109:TYR:H | 2.01 | 0.58 |
| 1:0:2676:C:H4' | 11:J:70:PHE:HE1 | 1.66 | 0.58 |
| 12:K:34:VAL:HG22 | 12:K:47:ALA:HB2 | 1.85 | 0.58 |
| 1:0:1202:A:C2' | 1:0:1203:G:H5' | 2.33 | 0.58 |
| 1:0:2252:A:C5 | 1:0:2253:G:H1' | 2.36 | 0.58 |
| 5:C:139:VAL:HG13 | 38:C:8648:HOH:O | 2.02 | 0.58 |
| 25:X:43:VAL:HG12 | 25:X:44:ASP:H | 1.69 | 0.58 |
| 19:R:14:ALA:HB3 | 19:R:147:LEU:HB2 | 1.86 | 0.58 |
| 1:0:1377:C:H5' | 1:0:1377:C:C6 | 2.38 | 0.58 |
| 3:A:94:LEU:HD12 | 3:A:98:GLU:HB2 | 1.84 | 0.58 |
| 5:C:180:SER:HB2 | 38:C:8645:HOH:O | 2.02 | 0.58 |
| 2:9:3035:C:H5'' | 38:9:4078:HOH:O | 2.03 | 0.58 |
| 3:A:100:PRO:HG2 | 3:A:103:VAL:HG21 | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:O:42:GLU:HB2 | 38:O:2176:HOH:O | 2.04 | 0.58 |
| 24:W:21:LEU:HD21 | 24:W:48:VAL:CG1 | 2.32 | 0.58 |
| 1:O:1168:C:H4' | 38:I:5128:HOH:O | 2.04 | 0.58 |
| 1:O:2816:A:H5'' | 1:O:2817:G:H5' | 1.86 | 0.58 |
| 1:O:42:C:H3' | 38:O:4179:HOH:O | 2.03 | 0.58 |
| 1:O:87:C:H2' | 29:2:28:LYS:O | 2.04 | 0.58 |
| 13:L:136:ALA:HB3 | 38:L:8872:HOH:O | 2.03 | 0.58 |
| 4:B:25:ARG:HA | 4:B:310:ARG:HH21 | 1.68 | 0.58 |
| 5:C:5:ILE:HD11 | 5:C:16:VAL:CG2 | 2.31 | 0.58 |
| 13:L:143:THR:HG22 | 13:L:144:ASP:N | 2.18 | 0.58 |
| 1:O:1182:C:H1' | 1:O:1192:A:H8 | 1.69 | 0.58 |
| 1:O:2703:A:H2' | 1:O:2704:C:H6 | 1.67 | 0.58 |
| 1:O:282:C:H1' | 1:O:368:C:H42 | 1.69 | 0.58 |
| 1:O:661:G:C5 | 1:O:686:A:C2 | 2.92 | 0.58 |
| 4:B:195:ARG:HG2 | 4:B:323:LEU:HD22 | 1.86 | 0.58 |
| 6:D:22:VAL:HG22 | 6:D:74:THR:HG22 | 1.84 | 0.58 |
| 11:J:103:VAL:HG12 | 38:J:8868:HOH:O | 2.03 | 0.58 |
| 15:N:144:GLY:O | 15:N:147:ILE:HG22 | 2.02 | 0.58 |
| 1:O:2613:G:O2' | 1:O:2614:C:H5' | 2.04 | 0.57 |
| 28:1:21:ARG:HD2 | 28:1:37:CYS:SG | 2.44 | 0.57 |
| 2:9:3057:A:H8 | 6:D:141:VAL:HG21 | 1.69 | 0.57 |
| 1:O:875:A:C2 | 3:A:194:MET:SD | 2.97 | 0.57 |
| 8:F:53:ASP:OD1 | 8:F:80:GLN:HB2 | 2.05 | 0.57 |
| 1:O:1183:C:O2 | 1:O:1183:C:H2' | 2.03 | 0.57 |
| 7:E:68:HIS:O | 7:E:72:MET:HG3 | 2.04 | 0.57 |
| 10:H:63:GLU:HA | 38:H:8582:HOH:O | 2.03 | 0.57 |
| 1:O:2498:C:O2' | 1:O:2499:U:H5' | 2.04 | 0.57 |
| 4:B:320:GLN:HE21 | 4:B:321:PRO:HD2 | 1.70 | 0.57 |
| 11:J:107:ASN:HD21 | 11:J:109:TYR:HB2 | 1.68 | 0.57 |
| 11:J:131:THR:HB | 11:J:134:GLU:HG3 | 1.85 | 0.57 |
| 38:O:7344:HOH:O | 26:Y:149:GLN:HG3 | 2.02 | 0.57 |
| 1:O:2478:U:O2' | 1:O:2479:A:H5' | 2.04 | 0.57 |
| 1:O:877:G:C5' | 1:O:878:G:OP1 | 2.49 | 0.57 |
| 4:B:258:GLY:H | 4:B:260:HIS:CE1 | 2.21 | 0.57 |
| 1:O:1202:A:H2' | 1:O:1203:G:C5' | 2.34 | 0.57 |
| 1:O:1226:G:H5' | 38:O:4537:HOH:O | 2.05 | 0.57 |
| 1:O:1835:U:C5 | 1:O:1840:A:N7 | 2.67 | 0.57 |
| 1:O:1972:U:H2' | 1:O:1973:A:C5' | 2.35 | 0.57 |
| 1:O:2256:G:O2' | 1:O:2257:G:H5' | 2.04 | 0.57 |
| 2:9:3072:C:O2' | 2:9:3073:G:H5' | 2.05 | 0.57 |
| 14:M:24:GLN:NE2 | 14:M:27:ARG:HH11 | 2.02 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:0:31:C:H2' | 38:0:7673:HOH:O | 2.03 | 0.57 |
| 1:0:92:G:H4' | 23:V:44:GLY:HA3 | 1.87 | 0.57 |
| 30:3:70:ARG:HG2 | 30:3:77:ALA:HB2 | 1.85 | 0.57 |
| 7:E:137:ASP:OD1 | 7:E:139:GLU:HB2 | 2.05 | 0.57 |
| 1:0:671:A:O2' | 1:0:672:G:H2' | 2.05 | 0.57 |
| 23:V:64:GLY:O | 23:V:65:ASP:HB2 | 2.03 | 0.57 |
| 24:W:88:THR:HG23 | 24:W:110:GLN:HB3 | 1.85 | 0.57 |
| 1:0:1028:U:H1' | 38:0:3649:HOH:O | 2.04 | 0.57 |
| 2:9:3095:C:O2' | 2:9:3096:C:H5' | 2.05 | 0.57 |
| 1:0:1654:U:H2' | 3:A:47:HIS:HD2 | 1.70 | 0.57 |
| 4:B:254:GLN:HG2 | 4:B:255:GLY:N | 2.19 | 0.57 |
| 1:0:1015:C:H2' | 1:0:1016:U:C6 | 2.40 | 0.57 |
| 1:0:1118:A:H8 | 1:0:1119:G:H5'' | 1.69 | 0.57 |
| 1:0:1291:A:H2 | 38:0:5297:HOH:O | 1.86 | 0.57 |
| 1:0:1393:A:H2' | 1:0:1394:C:C6 | 2.40 | 0.57 |
| 1:0:88:G:H5' | 1:0:88:G:H8 | 1.70 | 0.57 |
| 30:3:11:CYS:HB2 | 30:3:20:HIS:CE1 | 2.40 | 0.57 |
| 2:9:3091:C:H1' | 38:9:7454:HOH:O | 2.04 | 0.57 |
| 1:0:2676:C:H4' | 11:J:70:PHE:CD1 | 2.39 | 0.57 |
| 16:O:32:ARG:HH21 | 16:O:35:LYS:NZ | 2.03 | 0.57 |
| 1:0:2781:U:O2' | 1:0:2782:G:H5' | 2.05 | 0.57 |
| 4:B:152:PRO:HA | 38:B:8866:HOH:O | 2.04 | 0.57 |
| 10:H:138:CYS:HB2 | 38:H:8544:HOH:O | 2.03 | 0.57 |
| 1:0:1193:A:C2 | 1:0:1194:A:N6 | 2.73 | 0.56 |
| 1:0:2291:A:N9 | 1:0:2309:C:H5' | 2.20 | 0.56 |
| 1:0:820:G:O2' | 1:0:856:G:H4' | 2.05 | 0.56 |
| 2:9:3052:A:H2' | 2:9:3053:G:O4' | 2.05 | 0.56 |
| 1:0:564:G:H1' | 38:0:6311:HOH:O | 2.03 | 0.56 |
| 2:9:3057:A:C8 | 6:D:141:VAL:HG21 | 2.40 | 0.56 |
| 3:A:217:ARG:HG2 | 3:A:229:ALA:HB2 | 1.87 | 0.56 |
| 4:B:225:GLY:HA3 | 38:B:8863:HOH:O | 2.05 | 0.56 |
| 10:H:26:SER:HA | 10:H:59:HIS:HD2 | 1.70 | 0.56 |
| 1:0:1201:C:H2' | 1:0:1202:A:H5' | 1.86 | 0.56 |
| 1:0:2604:A:H5' | 38:0:5801:HOH:O | 2.05 | 0.56 |
| 3:A:99:ILE:O | 3:A:131:HIS:HE1 | 1.87 | 0.56 |
| 21:T:64:ASN:HB3 | 21:T:73:HIS:HB2 | 1.88 | 0.56 |
| 26:Y:187:VAL:HG23 | 26:Y:192:ASP:HB3 | 1.86 | 0.56 |
| 1:0:2385:G:H2' | 1:0:2386:U:C6 | 2.40 | 0.56 |
| 1:0:2445:U:H2' | 1:0:2446:G:H8 | 1.69 | 0.56 |
| 1:0:2756:U:N3 | 1:0:2896:A:H2 | 2.02 | 0.56 |
| 2:9:3044:A:O4' | 6:D:76:ARG:NE | 2.38 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:W:139:GLY:O | 24:W:141:HIS:HD2 | 1.89 | 0.56 |
| 1:0:941:G:O2' | 1:0:942:U:H5' | 2.04 | 0.56 |
| 15:N:147:ILE:HB | 38:N:8842:HOH:O | 2.04 | 0.56 |
| 1:0:1154:A:H2' | 1:0:1155:G:C8 | 2.40 | 0.56 |
| 2:9:3049:G:O2' | 2:9:3050:G:H5' | 2.06 | 0.56 |
| 4:B:254:GLN:HG3 | 38:B:8828:HOH:O | 2.06 | 0.56 |
| 8:F:91:VAL:HG12 | 8:F:92:GLY:N | 2.20 | 0.56 |
| 20:S:43:GLU:HB3 | 38:S:8546:HOH:O | 2.04 | 0.56 |
| 1:0:1717:A:H5'' | 17:P:54:LYS:HB2 | 1.88 | 0.56 |
| 1:0:776:A:OP1 | 28:1:28:HIS:HE1 | 1.87 | 0.56 |
| 1:0:870:G:OP2 | 3:A:3:ARG:HD3 | 2.06 | 0.56 |
| 38:0:5467:HOH:O | 9:G:12:ILE:HA | 2.05 | 0.56 |
| 1:0:1181:A:C2 | 1:0:1192:A:C8 | 2.94 | 0.56 |
| 1:0:1329:A:H2 | 38:0:4691:HOH:O | 1.89 | 0.56 |
| 1:0:2064:U:H5' | 1:0:2652:U:O3' | 2.06 | 0.56 |
| 1:0:380:A:OP2 | 14:M:9:ARG:HD2 | 2.06 | 0.56 |
| 1:0:821:U:H5'' | 38:0:3050:HOH:O | 2.05 | 0.56 |
| 1:0:111:C:O2' | 28:1:20:ARG:HG2 | 2.06 | 0.56 |
| 8:F:36:THR:HG23 | 8:F:97:ALA:HB2 | 1.88 | 0.56 |
| 12:K:29:LEU:HB3 | 12:K:55:VAL:CG1 | 2.31 | 0.56 |
| 16:O:32:ARG:HD3 | 16:O:32:ARG:O | 2.05 | 0.56 |
| 24:W:88:THR:HG23 | 24:W:110:GLN:NE2 | 2.21 | 0.56 |
| 25:X:43:VAL:HG11 | 25:X:82:GLU:HA | 1.86 | 0.56 |
| 1:0:1527:A:H1' | 1:0:1528:A:C8 | 2.41 | 0.56 |
| 1:0:2403:C:H2' | 1:0:2404:G:O5' | 2.06 | 0.56 |
| 1:0:573:A:O2' | 1:0:574:C:H5' | 2.06 | 0.56 |
| 28:1:8:GLN:HE22 | 28:1:11:LYS:HZ2 | 1.54 | 0.56 |
| 1:0:1167:G:H4' | 31:I:135:LEU:HD22 | 1.88 | 0.56 |
| 22:U:47:ARG:HG2 | 38:U:4381:HOH:O | 2.05 | 0.56 |
| 24:W:108:ARG:HH21 | 24:W:114:PRO:HG2 | 1.71 | 0.56 |
| 1:0:1167:G:H2' | 1:0:1168:C:O4' | 2.06 | 0.56 |
| 1:0:2255:A:N1 | 1:0:2256:G:C4 | 2.74 | 0.56 |
| 5:C:114:ALA:HB1 | 5:C:223:LEU:HB3 | 1.88 | 0.56 |
| 21:T:71:VAL:HG11 | 21:T:90:PRO:CB | 2.33 | 0.56 |
| 1:0:1172:G:H1' | 38:0:4978:HOH:O | 2.05 | 0.56 |
| 1:0:21:G:H4' | 19:R:2:ILE:HG22 | 1.88 | 0.56 |
| 10:H:20:ILE:HG23 | 10:H:120:ILE:HD11 | 1.87 | 0.56 |
| 12:K:74:VAL:HG11 | 12:K:113:ILE:HG12 | 1.88 | 0.56 |
| 2:9:3006:C:C5' | 15:N:37:ARG:NH1 | 2.58 | 0.56 |
| 38:0:9539:HOH:O | 17:P:81:LYS:HG2 | 2.05 | 0.56 |
| 1:0:1168:C:H5'' | 31:I:87:THR:HG22 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:0:1377:C:H2' | 1:0:1723:G:O6 | 2.06 | 0.55 |
| 2:9:3106:C:O2' | 2:9:3107:C:H5' | 2.07 | 0.55 |
| 3:A:105:VAL:CG1 | 3:A:154:ALA:HB1 | 2.36 | 0.55 |
| 5:C:65:ARG:HG3 | 5:C:67:GLN:HB2 | 1.88 | 0.55 |
| 1:0:2670:G:O2' | 1:0:2671:U:H5' | 2.05 | 0.55 |
| 1:0:333:G:O2' | 1:0:334:G:H5' | 2.06 | 0.55 |
| 3:A:192:VAL:HG12 | 3:A:207:GLN:HB3 | 1.89 | 0.55 |
| 4:B:62:ARG:HA | 4:B:65:MET:HE3 | 1.87 | 0.55 |
| 6:D:159:PRO:O | 6:D:163:VAL:HG23 | 2.06 | 0.55 |
| 1:0:1309:U:O2' | 1:0:1310:U:H5' | 2.06 | 0.55 |
| 38:0:6860:HOH:O | 3:A:211:LYS:HD3 | 2.07 | 0.55 |
| 4:B:79:MET:HE1 | 38:B:8921:HOH:O | 2.06 | 0.55 |
| 6:D:149:ARG:HH12 | 15:N:15:GLU:HA | 1.72 | 0.55 |
| 20:S:57:THR:HG22 | 20:S:59:ASP:N | 2.18 | 0.55 |
| 22:U:39:ASN:ND2 | 22:U:44:ARG:HH11 | 2.05 | 0.55 |
| 25:X:74:ALA:HB2 | 25:X:85:VAL:HG13 | 1.88 | 0.55 |
| 1:0:2839:C:H2' | 1:0:2840:A:H5'' | 1.88 | 0.55 |
| 2:9:3001:U:H5'' | 2:9:3003:A:OP1 | 2.07 | 0.55 |
| 24:W:6:GLN:HB2 | 24:W:26:ILE:CD1 | 2.36 | 0.55 |
| 1:0:1873:G:H3' | 38:0:5213:HOH:O | 2.06 | 0.55 |
| 24:W:88:THR:HG22 | 24:W:89:ASP:N | 2.20 | 0.55 |
| 26:Y:133:HIS:HD2 | 38:Y:8881:HOH:O | 1.88 | 0.55 |
| 1:0:1169:U:H2' | 1:0:1170:U:O4' | 2.07 | 0.55 |
| 1:0:1180:U:H2' | 1:0:1181:A:O4' | 2.07 | 0.55 |
| 5:C:246:ARG:NE | 38:C:8623:HOH:O | 2.38 | 0.55 |
| 7:E:137:ASP:O | 7:E:141:VAL:HG23 | 2.06 | 0.55 |
| 8:F:27:GLY:HA3 | 8:F:101:ALA:O | 2.07 | 0.55 |
| 1:0:926:A:O2' | 13:L:41:HIS:CD2 | 2.60 | 0.55 |
| 22:U:52:THR:CG2 | 22:U:54:THR:HB | 2.37 | 0.55 |
| 1:0:1687:C:O2 | 28:1:9:GLY:HA2 | 2.06 | 0.55 |
| 1:0:960:G:N3 | 1:0:960:G:C2' | 2.69 | 0.55 |
| 5:C:72:LYS:HG2 | 5:C:77:ALA:HA | 1.88 | 0.55 |
| 1:0:553:G:P | 26:Y:204:ARG:HH22 | 2.30 | 0.55 |
| 1:0:1132:A:N6 | 1:0:1229:C:H2' | 2.22 | 0.55 |
| 1:0:559:U:C5' | 1:0:559:U:H6 | 2.18 | 0.55 |
| 1:0:621:C:H5' | 26:Y:132:ASP:OD2 | 2.07 | 0.55 |
| 1:0:88:G:H2' | 1:0:89:G:C8 | 2.41 | 0.55 |
| 1:0:958:G:H2' | 1:0:959:C:H6 | 1.72 | 0.55 |
| 29:2:20:ARG:HG2 | 29:2:21:VAL:N | 2.22 | 0.55 |
| 4:B:62:ARG:HA | 4:B:65:MET:CE | 2.37 | 0.55 |
| 5:C:77:ALA:O | 5:C:78:ARG:HD2 | 2.06 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:0:1118:A:C8 | 1:0:1119:G:H5'' | 2.41 | 0.55 |
| 1:0:941:G:C5 | 1:0:942:U:C4 | 2.95 | 0.55 |
| 1:0:947:U:H2' | 1:0:948:G:H8 | 1.70 | 0.55 |
| 1:0:856:G:C8 | 38:0:5435:HOH:O | 2.54 | 0.55 |
| 5:C:236:THR:H | 5:C:239:ALA:HB3 | 1.72 | 0.55 |
| 1:0:902:G:N7 | 13:L:18:HIS:HD2 | 2.06 | 0.55 |
| 1:0:1790:C:H2' | 1:0:1791:U:C6 | 2.40 | 0.54 |
| 1:0:2456:A:H5' | 38:0:5705:HOH:O | 2.06 | 0.54 |
| 1:0:65:C:O2' | 1:0:66:G:H5' | 2.07 | 0.54 |
| 5:C:129:HIS:HE1 | 5:C:231:ARG:HA | 1.69 | 0.54 |
| 38:0:4844:HOH:O | 11:J:47:THR:HB | 2.07 | 0.54 |
| 8:F:58:GLU:CD | 14:M:27:ARG:HH22 | 2.10 | 0.54 |
| 1:0:120:A:H2' | 1:0:120:A:N3 | 2.22 | 0.54 |
| 1:0:2090:G:H2' | 1:0:2091:G:C8 | 2.41 | 0.54 |
| 4:B:41:PHE:HA | 4:B:79:MET:HE2 | 1.90 | 0.54 |
| 24:W:125:HIS:HE1 | 38:W:3071:HOH:O | 1.91 | 0.54 |
| 26:Y:187:VAL:HG23 | 26:Y:192:ASP:HB2 | 1.87 | 0.54 |
| 1:0:1137:G:H1' | 38:0:3885:HOH:O | 2.07 | 0.54 |
| 1:0:1588:G:C6 | 1:0:1589:G:N1 | 2.75 | 0.54 |
| 1:0:255:A:C5 | 1:0:256:C:C4 | 2.96 | 0.54 |
| 1:0:468:U:H3' | 38:0:7553:HOH:O | 2.07 | 0.54 |
| 3:A:33:GLU:O | 3:A:34:ASP:HB2 | 2.07 | 0.54 |
| 31:I:113:HIS:N | 31:I:114:PRO:HD2 | 2.22 | 0.54 |
| 14:M:24:GLN:HE22 | 14:M:27:ARG:HH11 | 1.55 | 0.54 |
| 25:X:21:PRO:HG2 | 25:X:24:LYS:HD3 | 1.88 | 0.54 |
| 1:0:2266:A:OP2 | 14:M:90:ARG:NH2 | 2.41 | 0.54 |
| 1:0:2425:A:H2' | 38:0:9228:HOH:O | 2.06 | 0.54 |
| 1:0:2780:C:H1' | 7:E:143:GLN:NE2 | 2.22 | 0.54 |
| 1:0:2826:G:C6 | 1:0:2913:A:N6 | 2.75 | 0.54 |
| 2:9:3076:G:C3' | 2:9:3077:A:H5'' | 2.30 | 0.54 |
| 38:9:3472:HOH:O | 15:N:41:LYS:HD3 | 2.08 | 0.54 |
| 19:R:111:ILE:HG23 | 19:R:145:LEU:CD1 | 2.37 | 0.54 |
| 19:R:39:THR:HB | 19:R:42:GLU:HG3 | 1.90 | 0.54 |
| 1:0:2718:C:H6 | 1:0:2718:C:H5' | 1.73 | 0.54 |
| 1:0:226:A:H1' | 1:0:393:G:C5 | 2.43 | 0.54 |
| 1:0:705:C:H2' | 1:0:705:C:O2 | 2.08 | 0.54 |
| 5:C:22:PHE:HA | 5:C:116:ALA:HA | 1.88 | 0.54 |
| 5:C:233:THR:HG22 | 5:C:234:VAL:N | 2.21 | 0.54 |
| 8:F:29:VAL:HG12 | 8:F:98:VAL:HA | 1.90 | 0.54 |
| 21:T:53:GLY:HA3 | 38:T:6384:HOH:O | 2.08 | 0.54 |
| 1:0:1171:A:H2' | 1:0:1172:G:H5' | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:0:1595:G:O2' | 1:0:1596:U:H5' | 2.08 | 0.54 |
| 1:0:1603:A:H5' | 1:0:1605:G:C4' | 2.38 | 0.54 |
| 1:0:1783:A:O2' | 1:0:1784:U:H5' | 2.08 | 0.54 |
| 1:0:2001:G:O2' | 1:0:2002:C:H5' | 2.07 | 0.54 |
| 1:0:2346:C:O5' | 1:0:2346:C:H6 | 1.90 | 0.54 |
| 1:0:2587:OMU:H2' | 1:0:2589:U:H5'' | 1.88 | 0.54 |
| 1:0:506:G:N2 | 1:0:509:A:H5'' | 2.16 | 0.54 |
| 2:9:3003:A:OP2 | 2:9:3025:G:N2 | 2.40 | 0.54 |
| 5:C:236:THR:CG2 | 5:C:239:ALA:H | 2.11 | 0.54 |
| 8:F:21:GLU:O | 8:F:24:ARG:HG2 | 2.07 | 0.54 |
| 1:0:1667:A:H2' | 1:0:1668:U:H6 | 1.72 | 0.54 |
| 2:9:3076:G:H3' | 2:9:3077:A:C5' | 2.28 | 0.54 |
| 5:C:1:MET:HG2 | 5:C:2:GLN:N | 2.21 | 0.54 |
| 10:H:46:GLN:HG3 | 10:H:137:TYR:CE2 | 2.43 | 0.54 |
| 12:K:118:ALA:HA | 12:K:125:ALA:HB2 | 1.90 | 0.54 |
| 38:0:4623:HOH:O | 16:O:39:THR:HB | 2.07 | 0.54 |
| 1:0:1421:C:H2' | 1:0:1422:U:H6 | 1.73 | 0.54 |
| 1:0:1568:G:O2' | 1:0:1569:U:H5' | 2.07 | 0.54 |
| 2:9:3055:U:H4' | 2:9:3056:A:C8 | 2.43 | 0.54 |
| 38:0:4376:HOH:O | 3:A:212:PRO:HB2 | 2.08 | 0.54 |
| 11:J:75:PRO:HG2 | 11:J:105:LEU:CD2 | 2.38 | 0.54 |
| 1:0:1446:U:H2' | 20:S:55:GLN:NE2 | 2.23 | 0.54 |
| 1:0:1319:G:H1' | 38:0:4701:HOH:O | 2.07 | 0.54 |
| 1:0:1450:C:C4' | 1:0:1451:C:OP2 | 2.53 | 0.54 |
| 1:0:1931:A:H2' | 1:0:1932:G:H5' | 1.90 | 0.54 |
| 8:F:117:GLU:C | 8:F:119:ARG:H | 2.10 | 0.54 |
| 1:0:1173:A:H2 | 38:0:6282:HOH:O | 1.91 | 0.54 |
| 1:0:1762:C:H2' | 1:0:1763:C:C6 | 2.43 | 0.54 |
| 1:0:2064:U:H4' | 1:0:2653:A:OP1 | 2.08 | 0.54 |
| 1:0:328:U:O4' | 5:C:202:THR:HG22 | 2.07 | 0.54 |
| 1:0:794:U:H3 | 1:0:819:A:H61 | 1.54 | 0.54 |
| 3:A:51:ARG:NH1 | 3:A:120:ARG:O | 2.41 | 0.54 |
| 5:C:118:THR:O | 5:C:136:VAL:HG13 | 2.08 | 0.54 |
| 5:C:236:THR:HA | 38:C:8651:HOH:O | 2.08 | 0.54 |
| 1:0:645:U:OP2 | 13:L:4:LYS:HE2 | 2.08 | 0.54 |
| 17:P:91:LYS:O | 17:P:95:GLU:HG3 | 2.08 | 0.54 |
| 1:0:1053:G:OP1 | 10:H:12:PRO:HG3 | 2.08 | 0.53 |
| 1:0:125:U:H2' | 38:0:3769:HOH:O | 2.07 | 0.53 |
| 1:0:1677:U:OP2 | 29:2:8:LYS:NZ | 2.38 | 0.53 |
| 1:0:349:U:O2' | 1:0:350:C:H5' | 2.09 | 0.53 |
| 1:0:424:C:H2' | 1:0:425:U:C6 | 2.43 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:0:820:G:H5' | 1:0:821:U:H5' | 1.90 | 0.53 |
| 1:0:841:A:H5'' | 38:0:6906:HOH:O | 2.08 | 0.53 |
| 4:B:279:THR:OG1 | 4:B:290:VAL:HB | 2.08 | 0.53 |
| 4:B:26:PHE:CE1 | 4:B:310:ARG:HB3 | 2.43 | 0.53 |
| 1:0:1396:C:H1' | 17:P:1:THR:O | 2.08 | 0.53 |
| 1:0:2361:A:H8 | 1:0:2361:A:H5' | 1.73 | 0.53 |
| 1:0:2488:A:H61 | 1:0:2534:C:H42 | 1.54 | 0.53 |
| 4:B:74:ILE:HG22 | 4:B:76:THR:HG23 | 1.91 | 0.53 |
| 1:0:1444:G:O2' | 1:0:1445:G:H5' | 2.08 | 0.53 |
| 19:R:18:LEU:HB2 | 19:R:143:VAL:CG1 | 2.36 | 0.53 |
| 23:V:4:HIS:O | 23:V:8:ILE:HG13 | 2.08 | 0.53 |
| 1:0:2472:C:O2' | 1:0:2634:G:H4' | 2.08 | 0.53 |
| 1:0:2784:A:H1' | 7:E:60:SER:OG | 2.08 | 0.53 |
| 1:0:399:C:H5' | 14:M:179:GLY:O | 2.09 | 0.53 |
| 1:0:40:C:H4' | 38:0:6998:HOH:O | 2.08 | 0.53 |
| 1:0:660:A:H4' | 1:0:661:G:O5' | 2.08 | 0.53 |
| 8:F:56:PRO:HG2 | 14:M:43:PRO:O | 2.08 | 0.53 |
| 20:S:57:THR:HG22 | 20:S:59:ASP:HB2 | 1.90 | 0.53 |
| 22:U:9:CYS:HA | 22:U:52:THR:HG23 | 1.90 | 0.53 |
| 1:0:2064:U:H5' | 1:0:2652:U:H4' | 1.91 | 0.53 |
| 1:0:2526:C:H5' | 1:0:2526:C:C6 | 2.43 | 0.53 |
| 4:B:162:MET:CE | 4:B:308:LEU:HD21 | 2.39 | 0.53 |
| 24:W:64:THR:O | 24:W:68:THR:HG22 | 2.08 | 0.53 |
| 1:0:2382:A:H5' | 38:3:8831:HOH:O | 2.09 | 0.53 |
| 1:0:271:C:H4' | 1:0:272:A:OP1 | 2.08 | 0.53 |
| 1:0:2735:U:H2' | 1:0:2736:U:C6 | 2.44 | 0.53 |
| 1:0:622:G:O2' | 1:0:623:U:H5' | 2.08 | 0.53 |
| 4:B:23:THR:HG23 | 4:B:308:LEU:HD23 | 1.91 | 0.53 |
| 5:C:40:ALA:O | 5:C:43:LYS:HB2 | 2.08 | 0.53 |
| 8:F:96:ALA:HA | 38:F:3111:HOH:O | 2.09 | 0.53 |
| 11:J:46:ILE:HA | 38:J:8828:HOH:O | 2.09 | 0.53 |
| 18:Q:11:ARG:HD3 | 38:Q:5620:HOH:O | 2.08 | 0.53 |
| 24:W:48:VAL:HG12 | 24:W:52:VAL:HB | 1.90 | 0.53 |
| 24:W:68:THR:HG23 | 24:W:69:ARG:HG2 | 1.91 | 0.53 |
| 1:0:1314:U:H2' | 38:0:5885:HOH:O | 2.09 | 0.53 |
| 1:0:2071:C:H5' | 38:0:9529:HOH:O | 2.09 | 0.53 |
| 1:0:420:U:H2' | 1:0:421:C:C6 | 2.44 | 0.53 |
| 1:0:821:U:H2' | 1:0:822:C:C6 | 2.41 | 0.53 |
| 31:I:103:ASP:HA | 31:I:106:LYS:HD2 | 1.91 | 0.53 |
| 17:P:105:LEU:HD21 | 17:P:137:LEU:HD11 | 1.90 | 0.53 |
| 17:P:14:LEU:HD13 | 17:P:51:ALA:HB2 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 20:S:52:VAL:HG22 | 20:S:66:VAL:HG22 | 1.90 | 0.53 |
| 24:W:129:LYS:HG2 | 38:W:1990:HOH:O | 2.07 | 0.53 |
| 1:0:1342:C:O2' | 1:0:1343:C:H5' | 2.09 | 0.53 |
| 1:0:12:U:C2' | 1:0:13:G:H5' | 2.38 | 0.53 |
| 1:0:1456:C:H2' | 1:0:1457:U:C6 | 2.44 | 0.53 |
| 1:0:1855:G:H4' | 1:0:1856:C:O5' | 2.09 | 0.53 |
| 1:0:2781:U:H1' | 7:E:139:GLU:OE2 | 2.09 | 0.53 |
| 1:0:282:C:O2' | 1:0:283:U:C5' | 2.53 | 0.53 |
| 6:D:163:VAL:HA | 38:D:6326:HOH:O | 2.07 | 0.53 |
| 6:D:166:ILE:HB | 38:D:6326:HOH:O | 2.09 | 0.53 |
| 1:0:2081:A:H4' | 11:J:69:TYR:CE1 | 2.44 | 0.53 |
| 1:0:1181:A:N1 | 1:0:1192:A:O2' | 2.38 | 0.53 |
| 1:0:1213:C:C2' | 1:0:1214:G:H5' | 2.39 | 0.53 |
| 1:0:2548:C:OP2 | 4:B:5:ARG:NH2 | 2.42 | 0.53 |
| 1:0:2694:A:H4' | 7:E:91:PHE:CE1 | 2.43 | 0.53 |
| 9:G:64:ASN:N | 9:G:64:ASN:HD22 | 2.06 | 0.53 |
| 21:T:32:ARG:NH1 | 21:T:38:ARG:HH12 | 2.07 | 0.53 |
| 1:0:1104:C:H4' | 11:J:88:PRO:HD3 | 1.89 | 0.53 |
| 1:0:1159:G:H21 | 1:0:1189:A:H8 | 1.55 | 0.53 |
| 1:0:1236:A:H2' | 1:0:1237:U:O4' | 2.09 | 0.53 |
| 1:0:1309:U:C2' | 1:0:1310:U:H5' | 2.40 | 0.53 |
| 1:0:2269:C:C2' | 1:0:2270:G:H5' | 2.39 | 0.53 |
| 28:1:8:GLN:HE22 | 28:1:11:LYS:NZ | 2.06 | 0.53 |
| 6:D:135:VAL:HG22 | 6:D:136:ARG:H | 1.74 | 0.53 |
| 15:N:43:VAL:HG13 | 15:N:118:ILE:HD11 | 1.89 | 0.53 |
| 1:0:625:U:H5'' | 1:0:1044:C:N4 | 2.24 | 0.52 |
| 1:0:1733:A:H4' | 4:B:212:GLN:HA | 1.90 | 0.52 |
| 1:0:204:A:C2' | 1:0:205:U:H5' | 2.38 | 0.52 |
| 1:0:2251:G:H2' | 1:0:2252:A:C8 | 2.43 | 0.52 |
| 1:0:2837:U:H2' | 38:0:6833:HOH:O | 2.08 | 0.52 |
| 2:9:3031:C:H2' | 2:9:3032:G:O4' | 2.10 | 0.52 |
| 5:C:57:PRO:HG2 | 5:C:73:LEU:HD13 | 1.91 | 0.52 |
| 10:H:56:GLN:HE21 | 10:H:126:ARG:NE | 2.00 | 0.52 |
| 12:K:34:VAL:CG2 | 12:K:47:ALA:HB2 | 2.39 | 0.52 |
| 22:U:46:ALA:HB1 | 22:U:52:THR:HG21 | 1.90 | 0.52 |
| 1:0:2737:C:OP2 | 17:P:61:ARG:NH2 | 2.38 | 0.52 |
| 1:0:371:U:H2' | 1:0:372:A:H8 | 1.75 | 0.52 |
| 2:9:3060:C:O2' | 2:9:3061:C:H5' | 2.09 | 0.52 |
| 4:B:16:ARG:NH1 | 38:B:8913:HOH:O | 2.42 | 0.52 |
| 14:M:169:ARG:HD2 | 38:M:8886:HOH:O | 2.09 | 0.52 |
| 1:0:1588:G:C6 | 1:0:1589:G:C6 | 2.98 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:0:603:A:H4' | 1:0:604:G:O5' | 2.09 | 0.52 |
| 10:H:69:ALA:HB2 | 10:H:153:ALA:HB2 | 1.90 | 0.52 |
| 15:N:38:LYS:HE2 | 15:N:107:ASN:ND2 | 2.24 | 0.52 |
| 20:S:76:GLU:HB3 | 38:S:8547:HOH:O | 2.09 | 0.52 |
| 1:0:1010:C:H4' | 15:N:4:PRO:HB2 | 1.91 | 0.52 |
| 1:0:2894:C:O2' | 1:0:2895:C:H5' | 2.09 | 0.52 |
| 1:0:544:G:H2' | 1:0:545:G:C5' | 2.40 | 0.52 |
| 1:0:2601:A:N1 | 12:K:38:SER:HB2 | 2.25 | 0.52 |
| 1:0:1384:C:H5' | 25:X:30:MET:HG2 | 1.92 | 0.52 |
| 1:0:1755:A:H2' | 1:0:1756:G:O4' | 2.09 | 0.52 |
| 1:0:1766:U:O2 | 1:0:1778:A:H5' | 2.09 | 0.52 |
| 1:0:1972:U:C2' | 1:0:1973:A:H5'' | 2.39 | 0.52 |
| 1:0:2237:G:H1' | 38:0:4862:HOH:O | 2.10 | 0.52 |
| 1:0:304:G:H1' | 1:0:347:A:N6 | 2.24 | 0.52 |
| 30:3:3:MET:O | 30:3:90:PHE:HA | 2.10 | 0.52 |
| 19:R:33:ARG:NH1 | 38:R:8838:HOH:O | 2.41 | 0.52 |
| 1:0:1421:C:H2' | 1:0:1422:U:C6 | 2.45 | 0.52 |
| 1:0:2769:C:H2' | 1:0:2770:G:O4' | 2.10 | 0.52 |
| 1:0:289:G:N2 | 1:0:363:A:C2 | 2.57 | 0.52 |
| 2:9:3029:C:H2' | 2:9:3030:C:C5' | 2.36 | 0.52 |
| 6:D:82:GLU:HA | 6:D:85:GLN:HE21 | 1.74 | 0.52 |
| 14:M:24:GLN:NE2 | 14:M:27:ARG:NH1 | 2.57 | 0.52 |
| 21:T:26:THR:HA | 21:T:39:ASN:HB3 | 1.91 | 0.52 |
| 1:0:1169:U:C5 | 1:0:1170:U:C4 | 2.97 | 0.52 |
| 1:0:1641:A:H2' | 1:0:1642:A:C5' | 2.33 | 0.52 |
| 1:0:204:A:H2' | 1:0:205:U:H5' | 1.91 | 0.52 |
| 1:0:346:U:H4' | 38:0:6837:HOH:O | 2.08 | 0.52 |
| 1:0:707:C:C2 | 1:0:708:A:C8 | 2.97 | 0.52 |
| 4:B:312:ARG:HD3 | 4:B:315:VAL:HG13 | 1.90 | 0.52 |
| 7:E:49:ILE:HD11 | 7:E:69:ILE:HD12 | 1.91 | 0.52 |
| 10:H:3:ALA:HA | 10:H:58:ARG:NH1 | 2.25 | 0.52 |
| 13:L:148:GLU:HA | 38:L:8871:HOH:O | 2.10 | 0.52 |
| 22:U:37:GLU:HB3 | 38:U:408:HOH:O | 2.09 | 0.52 |
| 24:W:88:THR:HG22 | 24:W:90:TYR:HD1 | 1.74 | 0.52 |
| 1:0:567:U:C5' | 38:0:6400:HOH:O | 2.57 | 0.52 |
| 1:0:951:A:O2' | 1:0:952:G:H5' | 2.10 | 0.52 |
| 9:G:23:ILE:O | 9:G:27:ILE:HG13 | 2.10 | 0.52 |
| 24:W:21:LEU:HD22 | 24:W:26:ILE:CD1 | 2.40 | 0.52 |
| 1:0:1661:A:C8 | 38:0:5210:HOH:O | 2.55 | 0.52 |
| 1:0:1878:G:O2' | 1:0:1879:U:P | 2.68 | 0.52 |
| 1:0:2460:A:H5' | 32:0:9000:13T:H231 | 1.90 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:0:2766:A:O2' | 1:0:2767:C:H5' | 2.10 | 0.52 |
| 1:0:59:A:H5' | 38:0:4342:HOH:O | 2.09 | 0.52 |
| 4:B:307:ARG:HG3 | 4:B:307:ARG:NH1 | 2.16 | 0.52 |
| 1:0:262:A:OP2 | 8:F:91:VAL:HG11 | 2.10 | 0.52 |
| 1:0:2880:A:H2' | 1:0:2881:C:H5' | 1.92 | 0.52 |
| 4:B:162:MET:HE2 | 4:B:310:ARG:HD3 | 1.92 | 0.52 |
| 5:C:95:GLU:HG3 | 38:C:8673:HOH:O | 2.09 | 0.52 |
| 1:0:1119:G:H22 | 1:0:1246:A:H2 | 1.48 | 0.51 |
| 1:0:475:G:OP1 | 5:C:73:LEU:HD22 | 2.09 | 0.51 |
| 38:0:7541:HOH:O | 30:3:60:LYS:HG3 | 2.10 | 0.51 |
| 2:9:3020:G:O2' | 2:9:3021:G:H5' | 2.10 | 0.51 |
| 14:M:164:THR:HG22 | 14:M:167:GLY:H | 1.74 | 0.51 |
| 24:W:6:GLN:HB2 | 24:W:26:ILE:HD12 | 1.92 | 0.51 |
| 1:0:2010:A:C2' | 38:0:5968:HOH:O | 2.50 | 0.51 |
| 1:0:2361:A:H5'' | 38:0:9001:HOH:O | 2.08 | 0.51 |
| 1:0:2388:C:O2' | 1:0:2389:U:H5' | 2.10 | 0.51 |
| 1:0:2467:A:O2' | 1:0:2468:A:H2' | 2.10 | 0.51 |
| 1:0:291:C:H2' | 1:0:292:G:O4' | 2.10 | 0.51 |
| 5:C:242:GLU:HB2 | 38:C:8579:HOH:O | 2.09 | 0.51 |
| 38:0:4733:HOH:O | 19:R:29:LYS:HD3 | 2.10 | 0.51 |
| 1:0:119:A:H2' | 1:0:120:A:H5'' | 1.93 | 0.51 |
| 1:0:1500:U:P | 17:P:41:ARG:HH22 | 2.33 | 0.51 |
| 1:0:1545:C:H2' | 1:0:1546:G:O4' | 2.10 | 0.51 |
| 1:0:2266:A:H2' | 1:0:2267:G:C8 | 2.45 | 0.51 |
| 1:0:254:C:H2' | 1:0:254:C:O2 | 2.09 | 0.51 |
| 1:0:285:A:H2' | 1:0:286:U:O4' | 2.11 | 0.51 |
| 1:0:64:G:H2' | 1:0:65:C:O4' | 2.10 | 0.51 |
| 1:0:2694:A:H4' | 7:E:91:PHE:HE1 | 1.74 | 0.51 |
| 8:F:91:VAL:HG12 | 8:F:92:GLY:H | 1.76 | 0.51 |
| 1:0:1391:G:H2' | 1:0:1392:A:H5' | 1.93 | 0.51 |
| 1:0:1398:G:O2' | 1:0:1399:A:H5' | 2.11 | 0.51 |
| 2:9:3034:A:H2' | 2:9:3035:C:O4' | 2.11 | 0.51 |
| 2:9:3092:G:C6 | 2:9:3093:A:C6 | 2.98 | 0.51 |
| 1:0:2036:C:O4' | 12:K:44:LEU:HG | 2.10 | 0.51 |
| 14:M:102:GLU:OE1 | 14:M:164:THR:HG21 | 2.09 | 0.51 |
| 1:0:1594:C:OP2 | 17:P:120:ARG:HD2 | 2.11 | 0.51 |
| 18:Q:75:ILE:HD13 | 18:Q:84:ILE:HD11 | 1.93 | 0.51 |
| 26:Y:189:ASN:HD22 | 26:Y:189:ASN:C | 2.14 | 0.51 |
| 27:Z:37:HIS:HB2 | 27:Z:47:VAL:HB | 1.93 | 0.51 |
| 1:0:1249:U:H2' | 1:0:1250:C:C6 | 2.46 | 0.51 |
| 1:0:2887:G:H2' | 1:0:2888:U:C6 | 2.45 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:0:714:U:H3' | 38:0:6939:HOH:O | 2.09 | 0.51 |
| 4:B:85:ARG:NH1 | 38:B:8930:HOH:O | 2.42 | 0.51 |
| 1:0:894:A:C2 | 5:C:87:ARG:NH2 | 2.78 | 0.51 |
| 13:L:72:ASN:HB2 | 38:L:8881:HOH:O | 2.09 | 0.51 |
| 15:N:132:ASN:O | 15:N:135:VAL:HG12 | 2.09 | 0.51 |
| 1:0:2379:G:N3 | 1:0:2418:G:H2' | 2.25 | 0.51 |
| 1:0:2871:G:H2' | 1:0:2872:U:C6 | 2.46 | 0.51 |
| 3:A:101:GLU:OE2 | 3:A:131:HIS:HB2 | 2.10 | 0.51 |
| 11:J:54:VAL:HG11 | 11:J:138:THR:HG21 | 1.93 | 0.51 |
| 17:P:115:SER:N | 17:P:118:GLN:HE21 | 2.00 | 0.51 |
| 17:P:134:VAL:O | 17:P:137:LEU:HB3 | 2.11 | 0.51 |
| 1:0:1314:U:H5'' | 1:0:1316:G:O4' | 2.11 | 0.51 |
| 1:0:1559:A:OP2 | 1:0:1559:A:H8 | 1.92 | 0.51 |
| 1:0:1819:G:H5' | 38:0:4720:HOH:O | 2.09 | 0.51 |
| 1:0:2578:G:C8 | 1:0:2578:G:H5' | 2.41 | 0.51 |
| 1:0:558:C:H2' | 1:0:559:U:H5'' | 1.88 | 0.51 |
| 2:9:3013:A:O2' | 2:9:3014:G:H5'' | 2.11 | 0.51 |
| 2:9:3039:U:H1' | 2:9:3044:A:N6 | 2.26 | 0.51 |
| 6:D:62:ASP:HA | 38:D:4233:HOH:O | 2.11 | 0.51 |
| 7:E:69:ILE:HA | 7:E:72:MET:CE | 2.40 | 0.51 |
| 15:N:169:PRO:O | 15:N:172:PHE:HB3 | 2.11 | 0.51 |
| 1:0:1543:G:N1 | 1:0:1641:A:OP2 | 2.38 | 0.51 |
| 1:0:1856:C:H5' | 1:0:1858:A:O4' | 2.10 | 0.51 |
| 1:0:1787:C:H4' | 1:0:2883:A:O4' | 2.11 | 0.51 |
| 1:0:324:G:C6 | 1:0:325:U:C5 | 2.99 | 0.51 |
| 1:0:482:G:H4' | 1:0:508:A:N1 | 2.26 | 0.51 |
| 1:0:589:U:H2' | 1:0:590:A:H8 | 1.74 | 0.51 |
| 4:B:145:HIS:HD2 | 4:B:146:THR:O | 1.94 | 0.51 |
| 1:0:1163:G:H5' | 31:I:115:ASP:O | 2.10 | 0.51 |
| 20:S:17:ASP:HB3 | 20:S:23:LYS:HB2 | 1.92 | 0.51 |
| 1:0:1116:U:O2' | 1:0:1118:A:C2 | 2.50 | 0.51 |
| 1:0:1878:G:C1' | 38:0:6128:HOH:O | 2.49 | 0.51 |
| 1:0:228:C:H2' | 1:0:229:G:H5' | 1.92 | 0.51 |
| 1:0:2893:C:O2' | 1:0:2894:C:H5' | 2.11 | 0.51 |
| 29:2:40:ARG:HD2 | 29:2:47:THR:HG22 | 1.93 | 0.51 |
| 3:A:105:VAL:HG11 | 3:A:154:ALA:HB1 | 1.93 | 0.51 |
| 7:E:101:GLU:HB3 | 7:E:117:THR:HA | 1.92 | 0.51 |
| 1:0:1600:G:H8 | 1:0:1600:G:OP2 | 1.94 | 0.51 |
| 1:0:168:C:O5' | 1:0:168:C:H6 | 1.93 | 0.51 |
| 1:0:2765:C:H2' | 1:0:2766:A:H8 | 1.76 | 0.51 |
| 1:0:329:A:OP2 | 5:C:206:ASN:HB2 | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:C:132:ASP:HB3 | 38:C:8560:HOH:O | 2.10 | 0.51 |
| 1:0:1119:G:H8 | 11:J:52:GLN:HE22 | 1.59 | 0.51 |
| 26:Y:189:ASN:ND2 | 26:Y:192:ASP:H | 2.08 | 0.51 |
| 1:0:1119:G:H8 | 11:J:52:GLN:NE2 | 2.08 | 0.50 |
| 1:0:1586:G:O2' | 1:0:1587:U:H5' | 2.11 | 0.50 |
| 1:0:2106:C:H5' | 1:0:2284:G:H21 | 1.77 | 0.50 |
| 1:0:2135:A:O2' | 1:0:2136:G:H5' | 2.10 | 0.50 |
| 1:0:2269:C:O2' | 1:0:2270:G:H5' | 2.11 | 0.50 |
| 12:K:20:CYS:HB2 | 12:K:29:LEU:HG | 1.93 | 0.50 |
| 1:0:1556:G:O2' | 1:0:1557:G:H5' | 2.11 | 0.50 |
| 1:0:17:G:H2' | 1:0:18:C:C6 | 2.47 | 0.50 |
| 1:0:1862:C:H1' | 38:0:7211:HOH:O | 2.10 | 0.50 |
| 1:0:2515:C:H2' | 1:0:2516:G:O4' | 2.11 | 0.50 |
| 1:0:588:G:O6 | 24:W:154:ARG:NH1 | 2.43 | 0.50 |
| 1:0:710:G:C2' | 1:0:711:G:H5' | 2.41 | 0.50 |
| 28:1:28:HIS:CE1 | 28:1:31:LYS:HE2 | 2.46 | 0.50 |
| 4:B:314:ALA:HB3 | 4:B:317:PRO:HG3 | 1.93 | 0.50 |
| 6:D:103:ASN:HD22 | 6:D:134:LEU:H | 1.57 | 0.50 |
| 24:W:4:LEU:HB2 | 24:W:33:THR:HG22 | 1.92 | 0.50 |
| 26:Y:117:LEU:HD12 | 26:Y:174:VAL:CG1 | 2.41 | 0.50 |
| 1:0:1287:A:O4' | 24:W:117:ARG:HD3 | 2.12 | 0.50 |
| 1:0:1413:A:H2' | 1:0:1414:A:O4' | 2.11 | 0.50 |
| 1:0:814:G:H4' | 38:0:3133:HOH:O | 2.12 | 0.50 |
| 9:G:12:ILE:HG22 | 9:G:17:GLN:NE2 | 2.27 | 0.50 |
| 19:R:119:VAL:HG21 | 19:R:142:ASP:CG | 2.31 | 0.50 |
| 1:0:1188:A:H5' | 38:0:7415:HOH:O | 2.11 | 0.50 |
| 1:0:1406:A:H4' | 1:0:1407:A:C5' | 2.42 | 0.50 |
| 32:0:9000:13T:C23 | 32:0:9000:13T:C31 | 2.90 | 0.50 |
| 2:9:3023:U:O2' | 2:9:3024:U:H4' | 2.11 | 0.50 |
| 31:I:78:LEU:HD12 | 31:I:112:LYS:NZ | 2.26 | 0.50 |
| 11:J:107:ASN:HD22 | 11:J:107:ASN:C | 2.14 | 0.50 |
| 12:K:82:ARG:NH2 | 12:K:115:ARG:HG2 | 2.26 | 0.50 |
| 1:0:1853:C:O2' | 3:A:217:ARG:NH2 | 2.44 | 0.50 |
| 1:0:1972:U:H2' | 1:0:1973:A:H5' | 1.94 | 0.50 |
| 1:0:1985:U:C2 | 1:0:1996:U:O4' | 2.64 | 0.50 |
| 1:0:2717:C:C2' | 1:0:2718:C:C5' | 2.78 | 0.50 |
| 1:0:2896:A:OP1 | 25:X:15:ARG:NH1 | 2.45 | 0.50 |
| 2:9:3104:A:O2' | 2:9:3105:A:H5' | 2.12 | 0.50 |
| 3:A:191:GLY:HA2 | 3:A:194:MET:HE2 | 1.94 | 0.50 |
| 5:C:102:LEU:HD12 | 38:C:8515:HOH:O | 2.11 | 0.50 |
| 19:R:119:VAL:O | 19:R:119:VAL:HG12 | 2.10 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:0:240:C:O2 | 1:0:240:C:H2' | 2.12 | 0.50 |
| 1:0:2664:A:OP1 | 1:0:2664:A:H8 | 1.95 | 0.50 |
| 1:0:84:G:C2' | 1:0:85:C:H5' | 2.42 | 0.50 |
| 28:1:10:LYS:HG3 | 38:1:8731:HOH:O | 2.11 | 0.50 |
| 3:A:96:LEU:HD22 | 3:A:128:LEU:HD13 | 1.94 | 0.50 |
| 4:B:232:TRP:CD1 | 4:B:235:ARG:HD2 | 2.46 | 0.50 |
| 6:D:172:VAL:HG12 | 6:D:173:GLU:N | 2.27 | 0.50 |
| 12:K:74:VAL:HG13 | 12:K:113:ILE:HG12 | 1.92 | 0.50 |
| 13:L:24:ALA:HB2 | 13:L:30:ARG:HD2 | 1.93 | 0.50 |
| 1:0:793:A:H5'' | 17:P:83:LYS:HG2 | 1.94 | 0.50 |
| 26:Y:189:ASN:HA | 26:Y:217:ILE:HD11 | 1.93 | 0.50 |
| 1:0:370:G:O2' | 1:0:371:U:H5' | 2.12 | 0.50 |
| 3:A:217:ARG:HH11 | 3:A:217:ARG:HG3 | 1.76 | 0.50 |
| 4:B:18:ARG:HG3 | 4:B:256:GLN:HG3 | 1.94 | 0.50 |
| 7:E:23:GLU:HG2 | 7:E:28:SER:HB3 | 1.93 | 0.50 |
| 19:R:59:PHE:O | 19:R:63:ASN:HB3 | 2.12 | 0.50 |
| 21:T:41:ARG:NH1 | 21:T:42:VAL:O | 2.45 | 0.50 |
| 21:T:69:LYS:O | 21:T:71:VAL:HG23 | 2.12 | 0.50 |
| 24:W:125:HIS:CD2 | 24:W:127:GLY:H | 2.25 | 0.50 |
| 26:Y:203:VAL:HG12 | 26:Y:228:VAL:HG22 | 1.94 | 0.50 |
| 1:0:1130:U:H5' | 38:0:7657:HOH:O | 2.11 | 0.50 |
| 1:0:1207:A:C8 | 1:0:1208:C:C5 | 3.00 | 0.50 |
| 1:0:1878:G:O2' | 1:0:1879:U:H6 | 1.93 | 0.50 |
| 1:0:2253:G:C2 | 1:0:2254:G:C8 | 3.00 | 0.50 |
| 1:0:2336:G:H1' | 38:0:6297:HOH:O | 2.12 | 0.50 |
| 1:0:2506:A:N6 | 1:0:2511:A:O2' | 2.44 | 0.50 |
| 1:0:2668:G:H2' | 1:0:2669:U:C6 | 2.46 | 0.50 |
| 1:0:2779:G:H21 | 7:E:143:GLN:NE2 | 2.10 | 0.50 |
| 1:0:363:A:O2' | 1:0:364:C:H5' | 2.12 | 0.50 |
| 3:A:125:ASN:HB3 | 3:A:158:VAL:HG12 | 1.93 | 0.50 |
| 3:A:89:ALA:HB3 | 38:A:8913:HOH:O | 2.11 | 0.50 |
| 5:C:214:THR:HG23 | 38:C:8636:HOH:O | 2.10 | 0.50 |
| 9:G:12:ILE:N | 9:G:13:PRO:HD3 | 2.27 | 0.50 |
| 1:0:1154:A:H2' | 1:0:1155:G:H8 | 1.75 | 0.50 |
| 1:0:1163:G:N2 | 38:0:6056:HOH:O | 2.45 | 0.50 |
| 1:0:424:C:H2' | 1:0:425:U:H6 | 1.77 | 0.50 |
| 10:H:47:ILE:HG12 | 10:H:165:SER:HA | 1.93 | 0.50 |
| 25:X:25:ARG:HD3 | 25:X:64:ALA:O | 2.12 | 0.50 |
| 27:Z:19:GLY:O | 27:Z:23:ARG:HG2 | 2.11 | 0.50 |
| 1:0:2296:C:H2' | 1:0:2297:U:C6 | 2.47 | 0.49 |
| 1:0:2764:C:O2' | 1:0:2765:C:H5' | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:0:2831:C:H2' | 1:0:2832:C:H5' | 1.93 | 0.49 |
| 1:0:635:A:H2' | 1:0:636:G:H5'' | 1.92 | 0.49 |
| 1:0:93:C:H5'' | 23:V:1:THR:CB | 2.33 | 0.49 |
| 8:F:48:VAL:CG2 | 8:F:74:PHE:HB3 | 2.42 | 0.49 |
| 13:L:80:ASP:HB2 | 13:L:90:ARG:O | 2.12 | 0.49 |
| 15:N:43:VAL:HG11 | 15:N:81:ALA:HA | 1.94 | 0.49 |
| 21:T:71:VAL:HG12 | 21:T:72:ILE:N | 2.27 | 0.49 |
| 1:0:1423:C:O2' | 1:0:1424:A:H5' | 2.12 | 0.49 |
| 1:0:2896:A:N3 | 1:0:2896:A:H2' | 2.28 | 0.49 |
| 1:0:710:G:O2' | 1:0:711:G:H5' | 2.12 | 0.49 |
| 2:9:3055:U:H4' | 2:9:3056:A:H8 | 1.77 | 0.49 |
| 4:B:26:PHE:HE1 | 4:B:310:ARG:HB3 | 1.77 | 0.49 |
| 5:C:168:ARG:NH2 | 5:C:190:ALA:O | 2.45 | 0.49 |
| 10:H:162:ARG:HD3 | 38:H:8585:HOH:O | 2.12 | 0.49 |
| 1:0:1497:G:H4' | 1:0:1627:G:O2' | 2.12 | 0.49 |
| 1:0:1909:A:N1 | 1:0:2128:G:H1' | 2.26 | 0.49 |
| 1:0:415:A:O2' | 1:0:416:G:H5' | 2.13 | 0.49 |
| 1:0:775:G:OP1 | 28:1:16:HIS:HE1 | 1.95 | 0.49 |
| 3:A:179:MET:HG2 | 3:A:186:TRP:CG | 2.46 | 0.49 |
| 3:A:190:ARG:NH2 | 3:A:207:GLN:OE1 | 2.45 | 0.49 |
| 9:G:12:ILE:HG22 | 9:G:17:GLN:HE21 | 1.76 | 0.49 |
| 13:L:134:GLU:HG3 | 38:L:8855:HOH:O | 2.12 | 0.49 |
| 1:0:1642:A:C8 | 1:0:1643:C:C5 | 3.00 | 0.49 |
| 1:0:2363:G:O2' | 18:Q:11:ARG:HG3 | 2.13 | 0.49 |
| 1:0:2493:C:H2' | 1:0:2493:C:O2 | 2.11 | 0.49 |
| 1:0:451:C:O2' | 1:0:452:G:H5' | 2.12 | 0.49 |
| 3:A:153:ARG:HH11 | 3:A:153:ARG:HB2 | 1.77 | 0.49 |
| 1:0:1008:C:H5'' | 10:H:16:ARG:HH12 | 1.76 | 0.49 |
| 1:0:2866:U:C5 | 22:U:50:GLU:HB2 | 2.47 | 0.49 |
| 1:0:1972:U:H2' | 1:0:1973:A:H5'' | 1.93 | 0.49 |
| 1:0:2004:U:H2' | 1:0:2004:U:O2 | 2.11 | 0.49 |
| 1:0:2533:C:H6 | 1:0:2533:C:C5' | 2.20 | 0.49 |
| 1:0:494:C:H2' | 1:0:496:G:OP2 | 2.13 | 0.49 |
| 1:0:946:C:H2' | 1:0:947:U:C6 | 2.47 | 0.49 |
| 10:H:27:LYS:H | 10:H:59:HIS:HD2 | 1.59 | 0.49 |
| 11:J:19:MET:HE2 | 11:J:79:PHE:HA | 1.94 | 0.49 |
| 26:Y:107:PRO:HD3 | 26:Y:182:PHE:CE1 | 2.47 | 0.49 |
| 27:Z:53:GLY:HA2 | 27:Z:67:GLY:O | 2.12 | 0.49 |
| 1:0:1119:G:H2' | 11:J:52:GLN:HE22 | 1.78 | 0.49 |
| 1:0:1474:C:C5' | 1:0:1474:C:C6 | 2.81 | 0.49 |
| 1:0:2122:C:H3' | 38:0:5295:HOH:O | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:0:251:C:O2' | 1:0:252:C:H5' | 2.12 | 0.49 |
| 1:0:318:C:H5' | 1:0:339:A:C2 | 2.48 | 0.49 |
| 1:0:920:C:H4' | 1:0:921:G:C2 | 2.47 | 0.49 |
| 4:B:36:PRO:CA | 4:B:168:GLY:HA3 | 2.38 | 0.49 |
| 4:B:267:LYS:HA | 38:B:8824:HOH:O | 2.11 | 0.49 |
| 11:J:75:PRO:HD3 | 11:J:136:SER:OG | 2.13 | 0.49 |
| 1:0:1278:A:H4' | 1:0:1279:U:C4 | 2.48 | 0.49 |
| 1:0:1488:U:H4' | 1:0:1489:G:OP1 | 2.12 | 0.49 |
| 1:0:1681:G:H5'' | 1:0:1682:A:H5' | 1.94 | 0.49 |
| 1:0:2270:G:H4' | 3:A:223:ARG:NH1 | 2.27 | 0.49 |
| 8:F:2:VAL:HG22 | 8:F:57:GLU:OE1 | 2.11 | 0.49 |
| 1:0:710:G:OP1 | 16:O:24:ALA:HB3 | 2.13 | 0.49 |
| 1:0:1331:A:OP2 | 26:Y:142:SER:OG | 2.27 | 0.49 |
| 1:0:2694:A:C6 | 1:0:2702:A:C8 | 3.01 | 0.49 |
| 1:0:645:U:O2 | 1:0:761:A:H2 | 1.96 | 0.49 |
| 10:H:51:VAL:HG13 | 10:H:159:PRO:HG3 | 1.95 | 0.49 |
| 38:0:5640:HOH:O | 17:P:58:SER:HB3 | 2.11 | 0.49 |
| 1:0:1422:U:H2' | 1:0:1423:C:C6 | 2.48 | 0.49 |
| 1:0:1484:G:H2' | 38:0:9098:HOH:O | 2.13 | 0.49 |
| 1:0:152:A:O2' | 1:0:153:C:H5' | 2.13 | 0.49 |
| 1:0:2102:G:C2 | 1:0:2104:C:C4 | 3.01 | 0.49 |
| 1:0:2316:G:H4' | 38:0:6098:HOH:O | 2.12 | 0.49 |
| 1:0:2372:A:H2' | 1:0:2373:U:C6 | 2.48 | 0.49 |
| 1:0:514:G:OP1 | 1:0:514:G:H2' | 2.12 | 0.49 |
| 1:0:558:C:H5' | 38:0:5262:HOH:O | 2.13 | 0.49 |
| 28:1:25:LYS:O | 28:1:25:LYS:HG2 | 2.13 | 0.49 |
| 4:B:294:TYR:HE2 | 38:B:8945:HOH:O | 1.95 | 0.49 |
| 4:B:320:GLN:NE2 | 4:B:321:PRO:HD2 | 2.28 | 0.49 |
| 4:B:36:PRO:HA | 4:B:168:GLY:CA | 2.39 | 0.49 |
| 26:Y:126:PRO:HG2 | 26:Y:128:PHE:CE1 | 2.48 | 0.49 |
| 1:0:1098:A:H2' | 1:0:1099:G:O4' | 2.12 | 0.49 |
| 1:0:1311:G:C2 | 1:0:1312:G:C8 | 3.01 | 0.49 |
| 1:0:1333:U:H2' | 1:0:1334:C:C6 | 2.46 | 0.49 |
| 1:0:1421:C:O2' | 1:0:1422:U:H5' | 2.13 | 0.49 |
| 1:0:1834:C:H2' | 1:0:1840:A:N6 | 2.27 | 0.49 |
| 1:0:2300:A:H4' | 1:0:2301:A:O5' | 2.13 | 0.49 |
| 1:0:2387:U:H2' | 1:0:2388:C:C6 | 2.48 | 0.49 |
| 1:0:23:G:C6 | 1:0:24:G:N1 | 2.81 | 0.49 |
| 1:0:2453:G:H3' | 38:0:5931:HOH:O | 2.13 | 0.49 |
| 1:0:949:U:O2' | 18:Q:40:HIS:HE1 | 1.96 | 0.49 |
| 3:A:94:LEU:HG | 3:A:99:ILE:CD1 | 2.43 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:O:6679:HOH:O | 21:T:38:ARG:NH1 | 2.45 | 0.49 |
| 38:O:6699:HOH:O | 26:Y:165:GLU:HB3 | 2.13 | 0.49 |
| 1:O:1165:G:C4' | 1:O:1174:A:O2' | 2.55 | 0.48 |
| 1:O:447:A:OP2 | 21:T:1:SER:HB2 | 2.12 | 0.48 |
| 1:O:522:U:O2' | 1:O:1366:C:H5' | 2.13 | 0.48 |
| 1:O:559:U:C3' | 1:O:559:U:C6 | 2.96 | 0.48 |
| 3:A:211:LYS:HB3 | 3:A:212:PRO:CD | 2.39 | 0.48 |
| 17:P:115:SER:OG | 17:P:118:GLN:HG3 | 2.12 | 0.48 |
| 24:W:115:THR:HG23 | 38:W:5420:HOH:O | 2.13 | 0.48 |
| 1:O:816:G:C6 | 1:O:817:G:N1 | 2.80 | 0.48 |
| 1:O:999:C:H2' | 1:O:1000:C:O4' | 2.14 | 0.48 |
| 30:3:65:THR:HB | 30:3:83:TRP:H | 1.78 | 0.48 |
| 2:9:3002:U:OP2 | 2:9:3003:A:H5' | 2.12 | 0.48 |
| 5:C:200:PRO:HB3 | 5:C:212:VAL:HG23 | 1.95 | 0.48 |
| 13:L:67:ARG:HB2 | 13:L:112:GLY:HA3 | 1.94 | 0.48 |
| 1:O:1477:C:H5' | 1:O:1868:G:H5' | 1.95 | 0.48 |
| 1:O:1947:G:H2' | 1:O:1948:G:H8 | 1.78 | 0.48 |
| 1:O:2349:G:O2' | 1:O:2350:G:H5' | 2.12 | 0.48 |
| 1:O:2703:A:H2' | 1:O:2704:C:C6 | 2.48 | 0.48 |
| 1:O:292:G:H1' | 1:O:360:A:N6 | 2.28 | 0.48 |
| 4:B:30:PRO:HB2 | 4:B:39:GLN:NE2 | 2.28 | 0.48 |
| 5:C:107:ARG:NE | 38:C:8657:HOH:O | 2.35 | 0.48 |
| 1:O:474:C:O2' | 5:C:73:LEU:HD21 | 2.13 | 0.48 |
| 10:H:170:ASN:N | 10:H:170:ASN:HD22 | 2.10 | 0.48 |
| 12:K:130:MET:SD | 22:U:25:ASP:O | 2.71 | 0.48 |
| 14:M:99:ARG:CD | 14:M:167:GLY:HA2 | 2.42 | 0.48 |
| 24:W:4:LEU:HD22 | 24:W:52:VAL:CG2 | 2.34 | 0.48 |
| 25:X:23:HIS:CD2 | 25:X:24:LYS:HG3 | 2.49 | 0.48 |
| 1:O:1056:U:H2' | 1:O:1057:A:O4' | 2.13 | 0.48 |
| 1:O:10:U:O4 | 1:O:532:A:OP2 | 2.32 | 0.48 |
| 1:O:1211:G:O2' | 1:O:1212:C:H5' | 2.14 | 0.48 |
| 1:O:154:C:H2' | 1:O:155:C:H6 | 1.78 | 0.48 |
| 1:O:1589:G:N2 | 1:O:1605:G:H1' | 2.28 | 0.48 |
| 1:O:2374:A:H2' | 1:O:2375:G:H8 | 1.78 | 0.48 |
| 1:O:441:A:O5' | 1:O:441:A:H8 | 1.96 | 0.48 |
| 3:A:53:ALA:HB3 | 38:A:8897:HOH:O | 2.12 | 0.48 |
| 31:I:113:HIS:CE1 | 31:I:121:LEU:HD22 | 2.48 | 0.48 |
| 38:O:9792:HOH:O | 13:L:30:ARG:NH2 | 2.44 | 0.48 |
| 14:M:164:THR:CG2 | 14:M:167:GLY:H | 2.27 | 0.48 |
| 14:M:49:ALA:C | 14:M:54:TYR:HB3 | 2.34 | 0.48 |
| 1:O:1193:A:H2 | 1:O:1194:A:N6 | 2.12 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:0:188:C:H5' | 14:M:163:LEU:HD21 | 1.95 | 0.48 |
| 1:0:2055:A:H4' | 19:R:132:ARG:NH2 | 2.28 | 0.48 |
| 1:0:597:A:C4 | 1:0:598:C:C5 | 3.01 | 0.48 |
| 2:9:3054:A:C2 | 2:9:3055:U:N3 | 2.81 | 0.48 |
| 4:B:17:LYS:O | 4:B:260:HIS:HD2 | 1.95 | 0.48 |
| 10:H:97:GLU:HB3 | 10:H:121:VAL:HG11 | 1.96 | 0.48 |
| 16:O:47:ARG:HG3 | 16:O:47:ARG:NH1 | 2.29 | 0.48 |
| 19:R:39:THR:HB | 19:R:42:GLU:CG | 2.43 | 0.48 |
| 1:0:1081:A:C6 | 1:0:1082:A:N1 | 2.82 | 0.48 |
| 1:0:1495:C:H1' | 1:0:1573:A:H1' | 1.95 | 0.48 |
| 1:0:1942:A:O2' | 1:0:1943:C:H5' | 2.14 | 0.48 |
| 1:0:2403:C:H3' | 38:0:5214:HOH:O | 2.13 | 0.48 |
| 1:0:2616:G:H1' | 38:0:9423:HOH:O | 2.14 | 0.48 |
| 1:0:366:U:H2' | 1:0:367:G:O4' | 2.12 | 0.48 |
| 1:0:597:A:H2' | 1:0:598:C:C6 | 2.46 | 0.48 |
| 1:0:470:U:O2' | 28:1:16:HIS:CD2 | 2.64 | 0.48 |
| 2:9:3058:G:C8 | 2:9:3059:C:C5 | 3.02 | 0.48 |
| 7:E:11:VAL:HG12 | 7:E:12:ASP:N | 2.29 | 0.48 |
| 10:H:20:ILE:HG23 | 10:H:120:ILE:CD1 | 2.44 | 0.48 |
| 1:0:1118:A:N6 | 1:0:1244:U:N3 | 2.57 | 0.48 |
| 1:0:1351:G:OP1 | 5:C:96:LYS:NZ | 2.32 | 0.48 |
| 1:0:1552:G:C6 | 1:0:1553:C:C4 | 3.01 | 0.48 |
| 1:0:1878:G:O2' | 1:0:1879:U:OP2 | 2.32 | 0.48 |
| 1:0:2324:G:N2 | 1:0:2377:U:H1' | 2.29 | 0.48 |
| 1:0:2553:A:H2' | 1:0:2553:A:N3 | 2.28 | 0.48 |
| 1:0:613:C:H2' | 1:0:614:U:H6 | 1.79 | 0.48 |
| 1:0:790:A:H2' | 1:0:791:A:O4' | 2.14 | 0.48 |
| 1:0:963:C:O2 | 1:0:1005:A:N1 | 2.46 | 0.48 |
| 29:2:41:HIS:HD2 | 29:2:44:ARG:H | 1.62 | 0.48 |
| 4:B:221:GLN:HE22 | 12:K:42:ASN:ND2 | 2.03 | 0.48 |
| 11:J:42:GLU:O | 11:J:131:THR:HG23 | 2.14 | 0.48 |
| 11:J:74:ARG:NH1 | 11:J:76:ASP:HB2 | 2.29 | 0.48 |
| 24:W:3:ALA:O | 24:W:54:PHE:HA | 2.14 | 0.48 |
| 27:Z:33:MET:SD | 27:Z:49:ARG:HD2 | 2.53 | 0.48 |
| 1:0:1217:G:C2 | 1:0:1218:U:C2 | 3.02 | 0.48 |
| 1:0:1921:A:O2' | 1:0:1922:A:H5' | 2.14 | 0.48 |
| 1:0:1942:A:H3' | 38:0:7336:HOH:O | 2.12 | 0.48 |
| 1:0:1842:A:C4 | 1:0:1979:G:C6 | 3.01 | 0.48 |
| 1:0:2032:U:H2' | 1:0:2033:G:C5' | 2.44 | 0.48 |
| 1:0:2269:C:H2' | 1:0:2270:G:H5' | 1.96 | 0.48 |
| 1:0:886:A:OP2 | 1:0:2113:G:H5' | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:A:123:GLY:HA3 | 3:A:162:GLY:HA2 | 1.95 | 0.48 |
| 3:A:200:PRO:HD3 | 38:A:8819:HOH:O | 2.14 | 0.48 |
| 4:B:51:VAL:CG2 | 4:B:327:VAL:HG13 | 2.42 | 0.48 |
| 8:F:13:GLU:OE2 | 8:F:78:GLU:HG2 | 2.14 | 0.48 |
| 11:J:45:VAL:HG23 | 11:J:130:VAL:O | 2.14 | 0.48 |
| 15:N:48:VAL:HG11 | 15:N:55:ASP:HB3 | 1.93 | 0.48 |
| 1:0:1044:C:H5'' | 38:0:9021:HOH:O | 2.12 | 0.48 |
| 1:0:1573:A:N7 | 1:0:1574:C:C2 | 2.82 | 0.48 |
| 1:0:1669:A:H2' | 1:0:1670:G:C8 | 2.49 | 0.48 |
| 1:0:1789:G:O6 | 17:P:73:HIS:HE1 | 1.97 | 0.48 |
| 1:0:2070:G:H5'' | 38:0:3786:HOH:O | 2.14 | 0.48 |
| 1:0:2488:A:H2 | 38:0:7268:HOH:O | 1.96 | 0.48 |
| 3:A:94:LEU:HG | 3:A:99:ILE:HD11 | 1.95 | 0.48 |
| 5:C:127:ARG:CZ | 5:C:225:PRO:HG2 | 2.43 | 0.48 |
| 5:C:51:TYR:HA | 5:C:54:LEU:HD12 | 1.96 | 0.48 |
| 1:0:1747:A:C8 | 12:K:44:LEU:HD13 | 2.49 | 0.48 |
| 23:V:39:ALA:C | 23:V:41:GLU:H | 2.16 | 0.48 |
| 1:0:1587:U:H2' | 1:0:1588:G:O4' | 2.13 | 0.48 |
| 1:0:2353:A:H4' | 1:0:2354:A:O5' | 2.12 | 0.48 |
| 1:0:629:A:H2' | 1:0:630:A:O4' | 2.14 | 0.48 |
| 2:9:3051:A:H5' | 15:N:160:SER:HB3 | 1.96 | 0.48 |
| 6:D:51:ARG:HH11 | 6:D:68:PRO:HB3 | 1.79 | 0.48 |
| 7:E:3:VAL:HG22 | 7:E:49:ILE:HB | 1.96 | 0.48 |
| 15:N:67:ALA:HA | 15:N:71:TRP:CB | 2.42 | 0.48 |
| 16:O:39:THR:O | 16:O:115:ARG:NH2 | 2.47 | 0.48 |
| 1:0:2044:G:OP1 | 25:X:23:HIS:HE1 | 1.97 | 0.47 |
| 1:0:2114:C:OP1 | 3:A:1:GLY:HA2 | 2.13 | 0.47 |
| 1:0:2689:A:H2' | 1:0:2690:U:H5' | 1.96 | 0.47 |
| 1:0:2831:C:C2' | 1:0:2832:C:H5' | 2.44 | 0.47 |
| 1:0:324:G:O2' | 1:0:325:U:H5' | 2.14 | 0.47 |
| 1:0:57:C:H5'' | 38:0:6753:HOH:O | 2.14 | 0.47 |
| 1:0:664:U:O4 | 1:0:681:G:H5'' | 2.14 | 0.47 |
| 4:B:84:LEU:HD23 | 4:B:142:LEU:HD23 | 1.95 | 0.47 |
| 7:E:20:ILE:HD11 | 7:E:40:VAL:CG1 | 2.44 | 0.47 |
| 25:X:66:THR:HG23 | 25:X:67:PRO:HD2 | 1.96 | 0.47 |
| 1:0:1188:A:C6 | 1:0:1189:A:C6 | 3.02 | 0.47 |
| 1:0:1477:C:C5' | 1:0:1868:G:H5'' | 2.43 | 0.47 |
| 1:0:2649:A:H5' | 1:0:2649:A:H8 | 1.78 | 0.47 |
| 1:0:2765:C:H2' | 1:0:2766:A:C8 | 2.49 | 0.47 |
| 1:0:709:G:O2' | 16:O:25:VAL:HG12 | 2.14 | 0.47 |
| 1:0:941:G:C6 | 1:0:942:U:C4 | 3.02 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 28:1:25:LYS:HD2 | 29:2:48:ASP:HA | 1.96 | 0.47 |
| 4:B:139:ASP:HB2 | 4:B:165:ARG:HE | 1.79 | 0.47 |
| 7:E:10:ASP:HA | 38:E:6017:HOH:O | 2.14 | 0.47 |
| 1:0:1339:G:C6 | 1:0:1340:G:N1 | 2.82 | 0.47 |
| 1:0:1398:G:H2' | 1:0:1399:A:C8 | 2.49 | 0.47 |
| 1:0:2112:A:H2' | 1:0:2113:G:C8 | 2.49 | 0.47 |
| 1:0:2297:U:H1' | 38:0:5179:HOH:O | 2.13 | 0.47 |
| 1:0:2330:U:H4' | 1:0:2331:C:OP1 | 2.15 | 0.47 |
| 1:0:2506:A:O2' | 1:0:2507:G:O5' | 2.31 | 0.47 |
| 1:0:255:A:C8 | 1:0:256:C:C5 | 3.02 | 0.47 |
| 1:0:264:G:H1' | 1:0:265:U:H5 | 1.79 | 0.47 |
| 1:0:2802:C:H2' | 1:0:2803:C:C6 | 2.50 | 0.47 |
| 3:A:217:ARG:HH11 | 3:A:217:ARG:CG | 2.27 | 0.47 |
| 4:B:150:ALA:O | 4:B:152:PRO:HD3 | 2.14 | 0.47 |
| 1:0:106:A:O2' | 1:0:107:U:H5' | 2.14 | 0.47 |
| 1:0:271:C:C2 | 1:0:273:G:O4' | 2.67 | 0.47 |
| 1:0:293:A:C4 | 1:0:360:A:C2 | 3.03 | 0.47 |
| 2:9:3002:U:H4' | 2:9:3002:U:OP2 | 2.15 | 0.47 |
| 2:9:3049:G:H2' | 2:9:3050:G:O4' | 2.14 | 0.47 |
| 2:9:3114:G:O6 | 15:N:11:ARG:HD3 | 2.13 | 0.47 |
| 38:0:9215:HOH:O | 3:A:11:ARG:HD3 | 2.15 | 0.47 |
| 4:B:112:THR:OG1 | 4:B:158:LYS:HG3 | 2.14 | 0.47 |
| 11:J:135:ILE:O | 11:J:139:LEU:HG | 2.15 | 0.47 |
| 1:0:155:C:OP2 | 14:M:188:ARG:HD3 | 2.13 | 0.47 |
| 21:T:73:HIS:CD2 | 21:T:88:PRO:HG3 | 2.49 | 0.47 |
| 1:0:1503:U:H2' | 1:0:1504:A:O4' | 2.14 | 0.47 |
| 1:0:1592:G:O2' | 1:0:1593:C:O5' | 2.33 | 0.47 |
| 1:0:80:A:H3' | 21:T:43:ASN:OD1 | 2.15 | 0.47 |
| 30:3:3:MET:HG3 | 30:3:4:PRO:HD2 | 1.96 | 0.47 |
| 13:L:143:THR:HG21 | 38:L:8836:HOH:O | 2.14 | 0.47 |
| 1:0:1562:C:O2 | 1:0:1562:C:H2' | 2.12 | 0.47 |
| 1:0:1574:C:H2' | 1:0:1575:C:C6 | 2.50 | 0.47 |
| 1:0:2026:C:O2' | 1:0:2027:U:H5' | 2.15 | 0.47 |
| 1:0:2115:U:H2' | 1:0:2116:U:C6 | 2.49 | 0.47 |
| 1:0:2403:C:C2' | 1:0:2404:G:O5' | 2.62 | 0.47 |
| 1:0:247:A:H2' | 38:0:3931:HOH:O | 2.13 | 0.47 |
| 1:0:69:A:H8 | 1:0:69:A:C5' | 2.25 | 0.47 |
| 1:0:876:A:N3 | 1:0:876:A:H2' | 2.29 | 0.47 |
| 15:N:108:SER:HA | 15:N:109:PRO:HD3 | 1.74 | 0.47 |
| 24:W:52:VAL:HG22 | 24:W:53:ALA:H | 1.79 | 0.47 |
| 26:Y:189:ASN:HD22 | 26:Y:192:ASP:H | 1.63 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:0:1007:A:H2' | 10:H:19:TYR:CZ | 2.50 | 0.47 |
| 1:0:1069:C:C2' | 1:0:1070:A:H5' | 2.44 | 0.47 |
| 1:0:1079:A:H4' | 1:0:2078:U:H5' | 1.97 | 0.47 |
| 1:0:2274:A:O2' | 1:0:2275:G:H5' | 2.14 | 0.47 |
| 1:0:2371:G:H5' | 38:0:5013:HOH:O | 2.14 | 0.47 |
| 1:0:2419:U:H5'' | 1:0:2420:G:H5' | 1.97 | 0.47 |
| 1:0:524:A:C5' | 19:R:29:LYS:HE2 | 2.45 | 0.47 |
| 1:0:644:G:N3 | 1:0:644:G:H5' | 2.30 | 0.47 |
| 1:0:758:A:H2' | 1:0:759:C:O4' | 2.15 | 0.47 |
| 1:0:475:G:H5' | 5:C:73:LEU:CD2 | 2.44 | 0.47 |
| 24:W:90:TYR:CE2 | 24:W:99:ALA:HB2 | 2.50 | 0.47 |
| 1:0:1202:A:O2' | 1:0:1203:G:H5' | 2.14 | 0.47 |
| 1:0:1333:U:H2' | 1:0:1334:C:H6 | 1.79 | 0.47 |
| 1:0:1845:A:OP2 | 3:A:190:ARG:NH1 | 2.47 | 0.47 |
| 1:0:2421:G:H3' | 1:0:2422:U:C5' | 2.45 | 0.47 |
| 1:0:2421:G:H3' | 1:0:2422:U:H5'' | 1.97 | 0.47 |
| 1:0:2615:U:C5 | 1:0:2616:G:C6 | 3.03 | 0.47 |
| 1:0:2754:G:O2' | 1:0:2755:G:H5' | 2.15 | 0.47 |
| 1:0:729:C:C2 | 1:0:743:G:C2 | 3.03 | 0.47 |
| 2:9:3048:C:H4' | 15:N:141:ARG:NH2 | 2.30 | 0.47 |
| 1:0:1845:A:O3' | 3:A:187:PRO:HB2 | 2.15 | 0.47 |
| 4:B:275:GLY:O | 4:B:291:ASP:HA | 2.15 | 0.47 |
| 10:H:2:PRO:HD2 | 10:H:5:MET:SD | 2.55 | 0.47 |
| 31:I:102:VAL:HG12 | 31:I:106:LYS:HE3 | 1.96 | 0.47 |
| 12:K:4:LEU:HD22 | 12:K:116:GLU:HB3 | 1.97 | 0.47 |
| 14:M:65:VAL:HG21 | 14:M:105:ALA:HB2 | 1.97 | 0.47 |
| 16:O:38:ARG:NH1 | 38:O:7674:HOH:O | 2.47 | 0.47 |
| 19:R:18:LEU:HD12 | 19:R:143:VAL:CG1 | 2.45 | 0.47 |
| 24:W:21:LEU:HD22 | 24:W:26:ILE:HD11 | 1.97 | 0.47 |
| 1:0:1731:C:H1' | 38:0:6446:HOH:O | 2.14 | 0.47 |
| 1:0:1746:A:O4' | 1:0:1747:A:C2 | 2.67 | 0.47 |
| 1:0:1819:G:H2' | 1:0:1820:G:C4' | 2.45 | 0.47 |
| 1:0:2111:G:H1' | 38:0:9044:HOH:O | 2.14 | 0.47 |
| 1:0:920:C:H5' | 1:0:921:G:C4 | 2.50 | 0.47 |
| 1:0:951:A:H2' | 1:0:952:G:H5' | 1.96 | 0.47 |
| 28:1:28:HIS:HD2 | 28:1:30:LYS:H | 1.61 | 0.47 |
| 3:A:17:ARG:HD2 | 38:A:8836:HOH:O | 2.13 | 0.47 |
| 4:B:232:TRP:HD1 | 4:B:235:ARG:HD2 | 1.79 | 0.47 |
| 22:U:33:SER:O | 22:U:37:GLU:HG3 | 2.14 | 0.47 |
| 26:Y:117:LEU:HD12 | 26:Y:174:VAL:HG11 | 1.97 | 0.47 |
| 1:0:1013:A:H1' | 38:0:9156:HOH:O | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:0:1114:A:O2' | 1:0:1115:U:H5' | 2.15 | 0.47 |
| 1:0:1268:C:O2' | 1:0:1269:G:H5' | 2.14 | 0.47 |
| 1:0:1921:A:C6 | 1:0:1922:A:C2 | 3.03 | 0.47 |
| 1:0:2244:A:H1' | 38:M:8866:HOH:O | 2.14 | 0.47 |
| 1:0:2274:A:H1' | 14:M:86:GLN:NE2 | 2.30 | 0.47 |
| 1:0:2468:A:H4' | 38:0:3550:HOH:O | 2.14 | 0.47 |
| 1:0:2502:C:H2' | 1:0:2503:A:C5' | 2.43 | 0.47 |
| 1:0:2768:A:C2' | 1:0:2769:C:O4' | 2.61 | 0.47 |
| 1:0:329:A:C5 | 1:0:347:A:C2 | 3.03 | 0.47 |
| 1:0:905:C:H3' | 38:0:5188:HOH:O | 2.15 | 0.47 |
| 2:9:3047:A:C2 | 2:9:3048:C:C2 | 3.03 | 0.47 |
| 3:A:109:GLU:HG2 | 3:A:116:GLY:H | 1.79 | 0.47 |
| 1:0:1593:C:OP1 | 17:P:117:SER:HB3 | 2.15 | 0.47 |
| 38:0:6273:HOH:O | 17:P:59:ARG:HD3 | 2.15 | 0.47 |
| 38:0:6996:HOH:O | 18:Q:9:GLY:HA2 | 2.15 | 0.47 |
| 1:0:524:A:H5' | 19:R:29:LYS:HE2 | 1.97 | 0.47 |
| 24:W:149:LEU:HG | 24:W:153:MET:CE | 2.45 | 0.47 |
| 1:0:1015:C:O5' | 1:0:1015:C:H6 | 1.98 | 0.47 |
| 1:0:1857:A:N6 | 1:0:2247:C:H1' | 2.30 | 0.47 |
| 1:0:1878:G:H5' | 38:0:4380:HOH:O | 2.15 | 0.47 |
| 1:0:312:U:C2 | 1:0:320:G:N2 | 2.83 | 0.47 |
| 1:0:377:C:H5 | 38:0:3309:HOH:O | 1.98 | 0.47 |
| 3:A:215:ILE:HG13 | 3:A:216:SER:N | 2.30 | 0.47 |
| 6:D:135:VAL:HG22 | 6:D:136:ARG:N | 2.29 | 0.47 |
| 6:D:84:LEU:HA | 6:D:87:ALA:HB3 | 1.97 | 0.47 |
| 7:E:37:ASP:OD1 | 11:J:125:SER:HB3 | 2.15 | 0.47 |
| 8:F:34:ASN:HA | 14:M:4:ALA:HB2 | 1.97 | 0.47 |
| 1:0:1058:A:H2' | 1:0:1060:C:C5' | 2.43 | 0.46 |
| 1:0:1773:G:N2 | 1:0:1774:G:C8 | 2.83 | 0.46 |
| 1:0:2047:C:H2' | 1:0:2048:C:H6 | 1.80 | 0.46 |
| 1:0:2063:U:O4 | 1:0:2083:A:H2 | 1.98 | 0.46 |
| 1:0:2255:A:C6 | 1:0:2256:G:C5 | 3.03 | 0.46 |
| 1:0:2809:G:H2' | 1:0:2810:G:O4' | 2.15 | 0.46 |
| 1:0:513:A:N3 | 38:0:3663:HOH:O | 2.36 | 0.46 |
| 1:0:559:U:H3' | 1:0:559:U:C6 | 2.51 | 0.46 |
| 1:0:812:A:H1' | 38:0:3966:HOH:O | 2.14 | 0.46 |
| 1:0:851:C:H5 | 38:0:6802:HOH:O | 1.96 | 0.46 |
| 2:9:3097:U:H2' | 2:9:3098:C:H6 | 1.79 | 0.46 |
| 4:B:55:ASN:HB3 | 4:B:63:GLU:HA | 1.97 | 0.46 |
| 18:Q:28:ARG:HG2 | 38:Q:4350:HOH:O | 2.15 | 0.46 |
| 21:T:71:VAL:HG13 | 21:T:91:LEU:O | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:W:38:THR:HG22 | 24:W:39:ASP:N | 2.30 | 0.46 |
| 26:Y:144:ARG:NH1 | 38:Y:8875:HOH:O | 2.48 | 0.46 |
| 1:0:111:C:O2' | 1:0:112:G:H5' | 2.16 | 0.46 |
| 1:0:1183:C:C2 | 1:0:1184:C:C5 | 3.03 | 0.46 |
| 1:0:1447:U:H3' | 1:0:1506:U:O2 | 2.15 | 0.46 |
| 1:0:1838:U:O2' | 1:0:2644:C:H5' | 2.15 | 0.46 |
| 1:0:2087:C:O2' | 1:0:2088:C:H5' | 2.16 | 0.46 |
| 1:0:2255:A:C2 | 1:0:2256:G:C4 | 3.03 | 0.46 |
| 1:0:31:C:H4' | 38:0:7414:HOH:O | 2.16 | 0.46 |
| 32:0:9000:13T:C23 | 32:0:9000:13T:H311 | 2.46 | 0.46 |
| 2:9:3028:U:H2' | 2:9:3029:C:C6 | 2.50 | 0.46 |
| 1:0:1198:U:C6 | 1:0:1200:A:OP2 | 2.68 | 0.46 |
| 1:0:1207:A:N6 | 38:0:5644:HOH:O | 2.48 | 0.46 |
| 1:0:1211:G:H2' | 1:0:1212:C:C6 | 2.47 | 0.46 |
| 1:0:1523:G:C6 | 1:0:1524:U:O4 | 2.67 | 0.46 |
| 1:0:1850:U:H2' | 1:0:1851:G:H8 | 1.81 | 0.46 |
| 1:0:1878:G:O2' | 1:0:1879:U:C5 | 2.65 | 0.46 |
| 1:0:1913:C:H2' | 1:0:1914:C:H6 | 1.80 | 0.46 |
| 1:0:2269:C:H2' | 1:0:2270:G:C5' | 2.46 | 0.46 |
| 1:0:2764:C:H1' | 38:0:7458:HOH:O | 2.16 | 0.46 |
| 1:0:694:A:C2' | 1:0:695:C:H5' | 2.43 | 0.46 |
| 3:A:126:ALA:HB1 | 3:A:138:VAL:CG1 | 2.45 | 0.46 |
| 8:F:111:ILE:O | 8:F:115:VAL:HG23 | 2.15 | 0.46 |
| 1:0:1913:C:H2' | 1:0:1914:C:C6 | 2.50 | 0.46 |
| 1:0:1931:A:C2' | 1:0:1932:G:H5' | 2.45 | 0.46 |
| 1:0:559:U:H2' | 1:0:560:C:O4' | 2.14 | 0.46 |
| 1:0:704:C:H2' | 1:0:705:C:H6 | 1.81 | 0.46 |
| 1:0:843:A:C2 | 1:0:846:A:C8 | 3.04 | 0.46 |
| 1:0:2459:G:C2' | 32:0:9000:13T:C23 | 2.94 | 0.46 |
| 2:9:3006:C:OP1 | 15:N:37:ARG:NH1 | 2.48 | 0.46 |
| 4:B:5:ARG:HD2 | 4:B:8:LYS:NZ | 2.31 | 0.46 |
| 31:I:100:LEU:HD22 | 31:I:105:VAL:CG2 | 2.46 | 0.46 |
| 16:O:105:ASN:HD21 | 16:O:109:SER:H | 1.62 | 0.46 |
| 1:0:1131:G:C6 | 1:0:1230:A:C4 | 3.04 | 0.46 |
| 1:0:1204:C:H2' | 1:0:1205:U:O4' | 2.16 | 0.46 |
| 1:0:2821:C:H2' | 1:0:2822:C:H6 | 1.80 | 0.46 |
| 1:0:2459:G:H2' | 32:0:9000:13T:H232 | 1.98 | 0.46 |
| 15:N:65:ASP:HB3 | 38:N:8821:HOH:O | 2.14 | 0.46 |
| 1:0:317:A:OP1 | 21:T:52:ARG:O | 2.33 | 0.46 |
| 1:0:1173:A:H3' | 38:0:4360:HOH:O | 2.16 | 0.46 |
| 1:0:1619:G:C5 | 1:0:1620:C:C4 | 3.03 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:0:2114:C:O2' | 1:0:2115:U:H5' | 2.16 | 0.46 |
| 1:0:2332:A:H3' | 1:0:2333:G:H8 | 1.80 | 0.46 |
| 1:0:39:G:C2 | 1:0:444:C:C2 | 3.04 | 0.46 |
| 3:A:179:MET:HG2 | 3:A:186:TRP:CB | 2.45 | 0.46 |
| 3:A:3:ARG:H | 3:A:3:ARG:HG2 | 1.55 | 0.46 |
| 14:M:183:THR:HG22 | 14:M:194:ALA:HB1 | 1.96 | 0.46 |
| 22:U:13:ILE:HG12 | 22:U:32:CYS:HB3 | 1.97 | 0.46 |
| 1:0:1192:A:H3' | 1:0:1193:A:H5' | 1.98 | 0.46 |
| 1:0:1850:U:H2' | 1:0:1851:G:C8 | 2.50 | 0.46 |
| 1:0:281:U:C2' | 1:0:282:C:H5' | 2.46 | 0.46 |
| 1:0:857:A:H4' | 3:A:176:HIS:CD2 | 2.51 | 0.46 |
| 3:A:72:GLU:HG3 | 27:Z:66:GLY:HA2 | 1.98 | 0.46 |
| 6:D:10:PHE:CG | 6:D:11:HIS:N | 2.84 | 0.46 |
| 6:D:88:LEU:HB2 | 6:D:89:PRO:HD3 | 1.96 | 0.46 |
| 19:R:39:THR:HG23 | 19:R:107:GLU:O | 2.16 | 0.46 |
| 1:0:1684:A:O2' | 1:0:1685:A:H5'' | 2.15 | 0.46 |
| 1:0:2121:G:O2' | 1:0:2122:C:H5' | 2.16 | 0.46 |
| 1:0:2729:C:O2' | 1:0:2730:G:H5' | 2.15 | 0.46 |
| 1:0:475:G:H5' | 5:C:73:LEU:HD23 | 1.96 | 0.46 |
| 3:A:36:ASP:O | 3:A:38:ILE:N | 2.49 | 0.46 |
| 31:I:78:LEU:HD12 | 31:I:112:LYS:HZ2 | 1.79 | 0.46 |
| 13:L:56:LYS:NZ | 38:L:8873:HOH:O | 2.49 | 0.46 |
| 22:U:52:THR:HG22 | 22:U:54:THR:N | 2.31 | 0.46 |
| 26:Y:216:ARG:HD2 | 38:Y:8868:HOH:O | 2.14 | 0.46 |
| 1:0:1218:U:H2' | 1:0:1219:U:C6 | 2.51 | 0.46 |
| 1:0:2263:G:H1' | 38:0:6618:HOH:O | 2.16 | 0.46 |
| 1:0:2329:C:O2' | 1:0:2330:U:H5' | 2.16 | 0.46 |
| 26:Y:184:GLU:OE2 | 26:Y:204:ARG:HD2 | 2.15 | 0.46 |
| 1:0:101:C:H2' | 1:0:102:A:C8 | 2.51 | 0.46 |
| 1:0:113:A:H2' | 1:0:115:U:O4 | 2.16 | 0.46 |
| 1:0:1166:A:H1' | 1:0:1192:A:C2 | 2.50 | 0.46 |
| 1:0:1182:C:O2' | 1:0:1183:C:H5 | 1.99 | 0.46 |
| 1:0:17:G:H2' | 1:0:18:C:H6 | 1.81 | 0.46 |
| 1:0:2050:G:H5'' | 19:R:80:TYR:O | 2.16 | 0.46 |
| 1:0:2549:C:H4' | 38:0:7504:HOH:O | 2.16 | 0.46 |
| 1:0:2672:C:H1' | 38:B:8930:HOH:O | 2.15 | 0.46 |
| 1:0:2911:C:H2' | 1:0:2912:C:C6 | 2.51 | 0.46 |
| 29:2:22:PRO:HG2 | 29:2:25:VAL:CG2 | 2.45 | 0.46 |
| 6:D:51:ARG:NH1 | 6:D:68:PRO:HB3 | 2.31 | 0.46 |
| 6:D:75:LEU:HD22 | 6:D:79:MET:HB3 | 1.98 | 0.46 |
| 7:E:69:ILE:HA | 7:E:72:MET:HE3 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:F:107:ASP:O | 8:F:111:ILE:HG13 | 2.15 | 0.46 |
| 10:H:170:ASN:N | 10:H:170:ASN:ND2 | 2.64 | 0.46 |
| 38:O:7403:HOH:O | 31:I:90:GLY:HA2 | 2.16 | 0.46 |
| 11:J:26:VAL:HG13 | 11:J:36:VAL:HG11 | 1.98 | 0.46 |
| 14:M:134:ILE:CG2 | 14:M:141:ILE:HD13 | 2.43 | 0.46 |
| 20:S:57:THR:CG2 | 20:S:59:ASP:HB2 | 2.45 | 0.46 |
| 1:O:1180:U:H4' | 31:I:91:GLU:HG2 | 1.97 | 0.45 |
| 1:O:1583:U:H1' | 38:O:9979:HOH:O | 2.15 | 0.45 |
| 1:O:189:A:OP1 | 14:M:171:ARG:NH2 | 2.49 | 0.45 |
| 1:O:2000:G:O2' | 1:O:2001:G:H5' | 2.16 | 0.45 |
| 1:O:2253:G:O2' | 1:O:2254:G:H5' | 2.16 | 0.45 |
| 1:O:2730:G:O2' | 1:O:2731:G:H5' | 2.15 | 0.45 |
| 1:O:583:G:H2' | 1:O:584:U:C6 | 2.51 | 0.45 |
| 2:9:3107:C:H2' | 2:9:3108:C:C6 | 2.51 | 0.45 |
| 3:A:69:LEU:HD21 | 3:A:120:ARG:HB3 | 1.98 | 0.45 |
| 10:H:1:LYS:HA | 10:H:2:PRO:HD3 | 1.73 | 0.45 |
| 11:J:45:VAL:HG22 | 11:J:46:ILE:N | 2.30 | 0.45 |
| 20:S:77:VAL:O | 20:S:80:ARG:HG2 | 2.17 | 0.45 |
| 1:O:1127:C:C5 | 1:O:1128:U:C4 | 3.04 | 0.45 |
| 1:O:1321:A:H2' | 1:O:1322:G:C8 | 2.51 | 0.45 |
| 1:O:1535:G:H2' | 1:O:1536:C:C6 | 2.51 | 0.45 |
| 1:O:1741:U:C4 | 1:O:2033:G:C8 | 3.04 | 0.45 |
| 1:O:1947:G:N2 | 1:O:1966:U:C2 | 2.84 | 0.45 |
| 1:O:2092:G:H5'' | 1:O:2613:G:OP1 | 2.15 | 0.45 |
| 1:O:2570:G:H8 | 38:O:4917:HOH:O | 2.00 | 0.45 |
| 1:O:2820:A:H2' | 1:O:2821:C:O4' | 2.17 | 0.45 |
| 1:O:939:A:H5' | 38:O:5419:HOH:O | 2.16 | 0.45 |
| 10:H:95:LEU:HD11 | 10:H:124:ALA:HB2 | 1.99 | 0.45 |
| 16:O:32:ARG:HB2 | 38:O:4656:HOH:O | 2.17 | 0.45 |
| 18:Q:66:LYS:HB2 | 18:Q:70:ALA:O | 2.17 | 0.45 |
| 23:V:7:GLU:O | 23:V:11:MET:HG3 | 2.15 | 0.45 |
| 26:Y:220:GLU:HG3 | 38:Y:8849:HOH:O | 2.16 | 0.45 |
| 27:Z:56:GLN:HA | 27:Z:62:TYR:O | 2.16 | 0.45 |
| 1:O:419:A:H1' | 1:O:1921:A:C2 | 2.51 | 0.45 |
| 1:O:2314:G:C2' | 1:O:2315:C:H5' | 2.46 | 0.45 |
| 1:O:2582:G:H5'' | 4:B:3:PRO:HB3 | 1.98 | 0.45 |
| 1:O:2831:C:H2' | 1:O:2832:C:C5' | 2.46 | 0.45 |
| 1:O:365:G:C6 | 1:O:366:U:C4 | 3.04 | 0.45 |
| 1:O:512:G:O3' | 1:O:513:A:C8 | 2.69 | 0.45 |
| 1:O:541:C:C2' | 1:O:542:A:C5' | 2.82 | 0.45 |
| 1:O:706:G:O2' | 1:O:707:C:H6 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:0:814:G:N2 | 1:0:815:U:H1' | 2.31 | 0.45 |
| 1:0:920:C:H5'' | 1:0:921:G:O5' | 2.17 | 0.45 |
| 29:2:20:ARG:HB3 | 38:2:5444:HOH:O | 2.17 | 0.45 |
| 2:9:3107:C:C5 | 38:9:3167:HOH:O | 2.68 | 0.45 |
| 1:0:1855:G:H8 | 3:A:144:GLU:OE2 | 1.99 | 0.45 |
| 15:N:139:TRP:HA | 15:N:139:TRP:CE3 | 2.52 | 0.45 |
| 17:P:83:LYS:O | 17:P:86:ALA:HB3 | 2.16 | 0.45 |
| 23:V:39:ALA:N | 23:V:40:PRO:CD | 2.80 | 0.45 |
| 23:V:45:ARG:HH11 | 23:V:45:ARG:HG3 | 1.82 | 0.45 |
| 25:X:30:MET:HE1 | 25:X:58:ALA:HB3 | 1.98 | 0.45 |
| 27:Z:60:CYS:O | 27:Z:61:ASP:HB2 | 2.16 | 0.45 |
| 1:0:1588:G:C5 | 1:0:1589:G:C6 | 3.05 | 0.45 |
| 1:0:1477:C:H5' | 1:0:1868:G:H5'' | 1.97 | 0.45 |
| 1:0:200:U:H2' | 38:0:3446:HOH:O | 2.15 | 0.45 |
| 1:0:2105:C:H2' | 1:0:2106:C:C6 | 2.52 | 0.45 |
| 1:0:2237:G:O2' | 1:0:2238:A:C8 | 2.69 | 0.45 |
| 1:0:229:G:O2' | 1:0:230:C:H5' | 2.16 | 0.45 |
| 1:0:2428:G:N7 | 30:3:60:LYS:NZ | 2.61 | 0.45 |
| 1:0:2649:A:C8 | 1:0:2649:A:H5' | 2.52 | 0.45 |
| 1:0:51:G:O2' | 1:0:52:A:H5' | 2.16 | 0.45 |
| 3:A:82:VAL:HG13 | 3:A:93:THR:HB | 1.98 | 0.45 |
| 26:Y:130:ARG:HB2 | 26:Y:142:SER:O | 2.16 | 0.45 |
| 1:0:2016:U:H2' | 1:0:2017:U:C6 | 2.51 | 0.45 |
| 1:0:2864:U:C5 | 1:0:2865:G:C6 | 3.04 | 0.45 |
| 1:0:2871:G:H2' | 1:0:2872:U:H6 | 1.81 | 0.45 |
| 1:0:407:A:H5' | 38:0:6034:HOH:O | 2.15 | 0.45 |
| 2:9:3008:G:O6 | 15:N:11:ARG:NH1 | 2.39 | 0.45 |
| 2:9:3026:C:O2' | 2:9:3027:C:H5' | 2.17 | 0.45 |
| 3:A:109:GLU:HG2 | 3:A:116:GLY:N | 2.31 | 0.45 |
| 4:B:162:MET:CE | 4:B:310:ARG:HD3 | 2.47 | 0.45 |
| 5:C:150:THR:HA | 5:C:203:ALA:O | 2.17 | 0.45 |
| 38:0:9988:HOH:O | 13:L:22:ARG:HG2 | 2.15 | 0.45 |
| 1:0:1730:G:H4' | 1:0:1731:C:H6 | 1.82 | 0.45 |
| 1:0:453:A:H4' | 1:0:455:A:N7 | 2.32 | 0.45 |
| 4:B:101:TRP:HB2 | 4:B:119:HIS:CD2 | 2.51 | 0.45 |
| 25:X:76:ARG:NH1 | 25:X:76:ARG:HG3 | 2.28 | 0.45 |
| 25:X:76:ARG:HH11 | 25:X:76:ARG:CG | 2.28 | 0.45 |
| 26:Y:117:LEU:HA | 26:Y:174:VAL:HG11 | 1.98 | 0.45 |
| 1:0:111:C:C2' | 1:0:112:G:H5' | 2.47 | 0.45 |
| 1:0:1544:U:O2' | 1:0:1545:C:H5' | 2.17 | 0.45 |
| 1:0:1771:U:O2' | 1:0:1773:G:N7 | 2.48 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:0:2326:U:H4' | 1:0:2412:G:C4' | 2.46 | 0.45 |
| 1:0:2110:G:C2 | 1:0:2478:U:C2 | 3.04 | 0.45 |
| 1:0:2772:G:O2' | 1:0:2773:G:H5' | 2.16 | 0.45 |
| 1:0:278:A:H2' | 1:0:279:C:O4' | 2.16 | 0.45 |
| 1:0:2891:A:C2 | 1:0:2892:G:C4 | 3.05 | 0.45 |
| 1:0:560:C:H2' | 1:0:561:G:H8 | 1.82 | 0.45 |
| 5:C:153:VAL:O | 5:C:157:LEU:HG | 2.16 | 0.45 |
| 1:0:1164:U:OP1 | 31:I:74:PRO:HA | 2.17 | 0.45 |
| 1:0:1123:A:N1 | 1:0:1238:C:H5' | 2.32 | 0.45 |
| 1:0:1252:A:H2' | 1:0:1253:C:O4' | 2.17 | 0.45 |
| 1:0:1029:U:O2' | 1:0:1273:C:OP1 | 2.32 | 0.45 |
| 1:0:1682:A:O2' | 1:0:1683:G:H5'' | 2.17 | 0.45 |
| 1:0:1819:G:H2' | 1:0:1820:G:C5' | 2.47 | 0.45 |
| 1:0:1940:C:H4' | 38:0:7336:HOH:O | 2.17 | 0.45 |
| 1:0:1973:A:H5' | 1:0:1973:A:C8 | 2.45 | 0.45 |
| 1:0:2073:G:OP2 | 1:0:2490:A:H5' | 2.16 | 0.45 |
| 1:0:289:G:N1 | 1:0:363:A:C2 | 2.81 | 0.45 |
| 1:0:696:C:O2' | 1:0:731:U:OP1 | 2.33 | 0.45 |
| 1:0:834:G:H4' | 1:0:835:U:OP2 | 2.16 | 0.45 |
| 30:3:69:TYR:O | 30:3:77:ALA:HA | 2.16 | 0.45 |
| 7:E:15:GLN:HG2 | 7:E:19:ASP:O | 2.17 | 0.45 |
| 1:0:244:C:OP2 | 8:F:38:LYS:HE3 | 2.17 | 0.45 |
| 1:0:1150:A:C2 | 9:G:20:VAL:HG21 | 2.52 | 0.45 |
| 13:L:143:THR:HG22 | 13:L:144:ASP:H | 1.81 | 0.45 |
| 15:N:110:THR:HB | 15:N:113:SER:OG | 2.17 | 0.45 |
| 24:W:5:VAL:HG11 | 24:W:153:MET:CE | 2.47 | 0.45 |
| 1:0:1076:G:C2 | 1:0:1084:C:C2 | 3.05 | 0.45 |
| 1:0:2075:G:C6 | 1:0:2076:U:C4 | 3.05 | 0.45 |
| 1:0:2505:G:C2' | 1:0:2506:A:H5' | 2.46 | 0.45 |
| 1:0:2614:C:O2' | 1:0:2615:U:H5' | 2.17 | 0.45 |
| 1:0:2906:A:H5' | 1:0:2907:C:O4' | 2.17 | 0.45 |
| 1:0:292:G:H1' | 1:0:360:A:H61 | 1.81 | 0.45 |
| 1:0:542:A:C5' | 1:0:542:A:C8 | 2.95 | 0.45 |
| 4:B:277:GLU:N | 4:B:278:PRO:HD2 | 2.31 | 0.45 |
| 5:C:2:GLN:HB3 | 38:C:8582:HOH:O | 2.15 | 0.45 |
| 1:0:1238:C:H5'' | 1:0:1239:G:OP2 | 2.17 | 0.45 |
| 1:0:2133:U:H4' | 1:0:2134:G:H5' | 1.98 | 0.45 |
| 1:0:488:U:O2' | 21:T:82:THR:HG21 | 2.17 | 0.45 |
| 1:0:670:G:H2' | 1:0:671:A:C8 | 2.52 | 0.45 |
| 1:0:926:A:O2' | 13:L:41:HIS:HD2 | 2.00 | 0.45 |
| 4:B:8:LYS:HG3 | 4:B:220:VAL:HG12 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:C:236:THR:HG22 | 5:C:239:ALA:CB | 2.47 | 0.45 |
| 17:P:9:LEU:O | 17:P:13:VAL:HG23 | 2.17 | 0.45 |
| 24:W:139:GLY:O | 24:W:141:HIS:CD2 | 2.70 | 0.45 |
| 1:0:1188:A:C5 | 1:0:1189:A:C2 | 3.05 | 0.44 |
| 1:0:1279:U:O2 | 1:0:1279:U:H2' | 2.17 | 0.44 |
| 1:0:538:C:N4 | 1:0:2061:C:H1' | 2.32 | 0.44 |
| 1:0:2346:C:O2' | 6:D:52:THR:HG21 | 2.17 | 0.44 |
| 1:0:2354:A:C2 | 1:0:2367:A:C8 | 3.04 | 0.44 |
| 1:0:248:A:H5' | 1:0:249:G:OP2 | 2.18 | 0.44 |
| 1:0:2594:C:O2' | 1:0:2595:U:H5' | 2.17 | 0.44 |
| 1:0:426:G:H2' | 1:0:427:C:O4' | 2.17 | 0.44 |
| 1:0:660:A:N6 | 1:0:746:A:O4' | 2.50 | 0.44 |
| 1:0:703:G:O2' | 1:0:704:C:H5' | 2.18 | 0.44 |
| 6:D:40:ILE:HG23 | 38:D:5583:HOH:O | 2.17 | 0.44 |
| 11:J:53:ILE:O | 11:J:57:TYR:HD1 | 2.00 | 0.44 |
| 15:N:179:LEU:HD23 | 15:N:184:ILE:CD1 | 2.47 | 0.44 |
| 18:Q:75:ILE:CD1 | 18:Q:84:ILE:HD11 | 2.47 | 0.44 |
| 22:U:52:THR:HG22 | 22:U:54:THR:HB | 1.98 | 0.44 |
| 25:X:78:GLU:HG2 | 25:X:79:GLU:H | 1.82 | 0.44 |
| 26:Y:235:GLU:H | 26:Y:235:GLU:CD | 2.21 | 0.44 |
| 1:0:1494:A:O2' | 1:0:1505:U:O2 | 2.34 | 0.44 |
| 1:0:256:C:H2' | 1:0:257:G:O4' | 2.18 | 0.44 |
| 1:0:2719:A:C2 | 4:B:70:PRO:HG3 | 2.52 | 0.44 |
| 1:0:536:A:H3' | 38:0:5051:HOH:O | 2.16 | 0.44 |
| 1:0:957:A:H8 | 1:0:957:A:O5' | 2.00 | 0.44 |
| 2:9:3058:G:H1' | 38:9:3839:HOH:O | 2.16 | 0.44 |
| 2:9:3097:U:H2' | 2:9:3098:C:C6 | 2.51 | 0.44 |
| 3:A:107:ASN:OD1 | 3:A:116:GLY:HA3 | 2.17 | 0.44 |
| 4:B:60:SER:HA | 4:B:61:PRO:HD3 | 1.85 | 0.44 |
| 6:D:104:PHE:CE2 | 6:D:132:VAL:HB | 2.52 | 0.44 |
| 11:J:45:VAL:CG2 | 11:J:129:PHE:HD1 | 2.30 | 0.44 |
| 12:K:32:ILE:HD11 | 12:K:56:SER:HB3 | 1.98 | 0.44 |
| 26:Y:151:SER:HB3 | 26:Y:154:ARG:HB3 | 2.00 | 0.44 |
| 1:0:111:C:H2' | 1:0:112:G:C5' | 2.46 | 0.44 |
| 1:0:1174:A:C5 | 1:0:1201:C:H4' | 2.53 | 0.44 |
| 1:0:1244:U:H4' | 1:0:1246:A:O4' | 2.17 | 0.44 |
| 1:0:1269:G:H2' | 1:0:1270:U:C6 | 2.53 | 0.44 |
| 1:0:1334:C:O2' | 1:0:1335:C:H5' | 2.18 | 0.44 |
| 1:0:1972:U:C2' | 1:0:1973:A:C5' | 2.96 | 0.44 |
| 1:0:2133:U:H4' | 1:0:2134:G:C5' | 2.47 | 0.44 |
| 1:0:263:U:C2 | 8:F:59:ILE:CD1 | 3.01 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:0:2716:G:O2' | 1:0:2717:C:H5' | 2.18 | 0.44 |
| 1:0:2900:G:C2' | 1:0:2901:C:H5' | 2.47 | 0.44 |
| 1:0:697:G:H4' | 1:0:730:G:O3' | 2.17 | 0.44 |
| 1:0:834:G:H3' | 1:0:835:U:H4' | 1.99 | 0.44 |
| 3:A:95:PRO:HA | 3:A:153:ARG:HA | 1.98 | 0.44 |
| 14:M:15:PRO:HA | 14:M:20:LEU:HD23 | 2.00 | 0.44 |
| 15:N:154:LEU:C | 15:N:156:GLU:H | 2.20 | 0.44 |
| 26:Y:126:PRO:HG2 | 26:Y:128:PHE:CZ | 2.52 | 0.44 |
| 1:0:2256:G:H2' | 1:0:2257:G:O5' | 2.17 | 0.44 |
| 1:0:2610:U:H4' | 38:0:9479:HOH:O | 2.18 | 0.44 |
| 4:B:18:ARG:HE | 4:B:256:GLN:NE2 | 2.15 | 0.44 |
| 4:B:307:ARG:HA | 38:B:8850:HOH:O | 2.17 | 0.44 |
| 5:C:34:ALA:HB3 | 5:C:220:THR:HG21 | 2.00 | 0.44 |
| 18:Q:25:PRO:HA | 18:Q:26:PRO:HD3 | 1.85 | 0.44 |
| 1:0:1309:U:C4 | 1:0:1310:U:C5 | 3.06 | 0.44 |
| 1:0:1667:A:H8 | 1:0:1667:A:C5' | 2.18 | 0.44 |
| 1:0:1714:C:O2' | 1:0:1715:C:H5' | 2.18 | 0.44 |
| 1:0:1748:U:C5 | 1:0:1749:U:C4 | 3.06 | 0.44 |
| 1:0:710:G:N2 | 1:0:719:C:C2 | 2.86 | 0.44 |
| 4:B:144:THR:HB | 38:B:8921:HOH:O | 2.18 | 0.44 |
| 1:0:2846:C:H4' | 4:B:156:LYS:HB3 | 1.98 | 0.44 |
| 1:0:1117:A:C2 | 1:0:1244:U:C2 | 3.06 | 0.44 |
| 1:0:1500:U:OP2 | 17:P:41:ARG:NH2 | 2.51 | 0.44 |
| 1:0:1523:G:H2' | 1:0:1524:U:C6 | 2.53 | 0.44 |
| 1:0:1602:C:OP2 | 27:Z:46:ARG:NH2 | 2.51 | 0.44 |
| 1:0:170:U:H2' | 1:0:171:C:H5' | 1.98 | 0.44 |
| 1:0:2819:C:H2' | 1:0:2820:A:C8 | 2.53 | 0.44 |
| 1:0:538:C:H5'' | 1:0:539:G:C8 | 2.53 | 0.44 |
| 1:0:816:G:H5' | 1:0:1598:A:H4' | 2.00 | 0.44 |
| 32:0:9000:13T:O2 | 32:0:9000:13T:H323 | 2.18 | 0.44 |
| 1:0:929:A:O5' | 1:0:929:A:H8 | 2.01 | 0.44 |
| 1:0:1853:C:OP1 | 3:A:231:LYS:HG3 | 2.18 | 0.44 |
| 4:B:199:TYR:CE2 | 4:B:268:ARG:HB2 | 2.53 | 0.44 |
| 7:E:132:THR:HB | 38:E:2227:HOH:O | 2.17 | 0.44 |
| 1:0:2504:A:H4' | 10:H:71:ARG:HH11 | 1.83 | 0.44 |
| 12:K:14:LYS:CB | 12:K:45:PRO:HG2 | 2.46 | 0.44 |
| 19:R:99:ALA:HB1 | 19:R:109:MET:HE1 | 1.97 | 0.44 |
| 23:V:45:ARG:NH1 | 23:V:45:ARG:HG3 | 2.32 | 0.44 |
| 1:0:1419:U:H2' | 1:0:1685:A:C2 | 2.53 | 0.44 |
| 1:0:2416:G:O2' | 15:N:25:ARG:HG2 | 2.17 | 0.44 |
| 1:0:2432:C:H1' | 32:0:9000:13T:O9 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:321:PRO:HA | 38:B:8952:HOH:O | 2.16 | 0.44 |
| 5:C:129:HIS:CE1 | 5:C:232:LEU:H | 2.36 | 0.44 |
| 24:W:13:MET:CE | 24:W:17:ILE:HG22 | 2.48 | 0.44 |
| 24:W:90:TYR:N | 24:W:90:TYR:CD1 | 2.85 | 0.44 |
| 1:0:1069:C:O2' | 1:0:1070:A:H5' | 2.18 | 0.44 |
| 1:0:1280:A:OP1 | 1:0:1280:A:H3' | 2.18 | 0.44 |
| 1:0:1730:G:H4' | 1:0:1731:C:C6 | 2.53 | 0.44 |
| 1:0:2361:A:H2' | 1:0:2362:A:C8 | 2.52 | 0.44 |
| 1:0:2577:A:H5' | 38:0:7734:HOH:O | 2.17 | 0.44 |
| 1:0:2802:C:H2' | 1:0:2803:C:H6 | 1.81 | 0.44 |
| 1:0:2899:A:O2' | 1:0:2900:G:H5' | 2.18 | 0.44 |
| 1:0:413:G:H2' | 1:0:414:C:C6 | 2.52 | 0.44 |
| 1:0:445:U:H2' | 1:0:446:G:H8 | 1.82 | 0.44 |
| 1:0:500:G:H21 | 19:R:98:ASN:ND2 | 2.13 | 0.44 |
| 1:0:622:G:P | 26:Y:148:GLY:HA3 | 2.58 | 0.44 |
| 1:0:637:C:H2' | 1:0:638:C:C6 | 2.52 | 0.44 |
| 1:0:920:C:H4' | 1:0:921:G:N2 | 2.32 | 0.44 |
| 7:E:11:VAL:HG13 | 7:E:23:GLU:O | 2.17 | 0.44 |
| 15:N:171:HIS:CE1 | 38:N:8862:HOH:O | 2.71 | 0.44 |
| 38:0:7396:HOH:O | 21:T:2:LYS:HE2 | 2.17 | 0.44 |
| 1:0:1773:G:C8 | 27:Z:16:ALA:HA | 2.53 | 0.44 |
| 1:0:1236:A:C8 | 11:J:63:ILE:HD11 | 2.53 | 0.44 |
| 1:0:2385:G:H2' | 1:0:2386:U:H6 | 1.79 | 0.44 |
| 1:0:238:C:H4' | 1:0:287:C:OP1 | 2.18 | 0.44 |
| 1:0:2691:A:OP1 | 1:0:2691:A:H8 | 2.01 | 0.44 |
| 1:0:276:C:O5' | 1:0:276:C:H6 | 2.01 | 0.44 |
| 1:0:303:C:O2' | 1:0:304:G:H5' | 2.18 | 0.44 |
| 1:0:307:G:C2 | 1:0:309:C:C4 | 3.05 | 0.44 |
| 1:0:821:U:H4' | 27:Z:17:ARG:NH1 | 2.33 | 0.44 |
| 2:9:3039:U:H3 | 2:9:3042:C:H5'' | 1.83 | 0.44 |
| 4:B:162:MET:HE1 | 4:B:308:LEU:HD21 | 1.99 | 0.44 |
| 4:B:185:GLY:HA2 | 38:B:8929:HOH:O | 2.17 | 0.44 |
| 1:0:1191:A:H2' | 1:0:1193:A:H5' | 2.00 | 0.43 |
| 1:0:1205:U:C2' | 1:0:1206:U:C5' | 2.87 | 0.43 |
| 1:0:1159:G:H1 | 1:0:1208:C:H42 | 1.64 | 0.43 |
| 1:0:699:C:C2 | 1:0:743:G:N2 | 2.86 | 0.43 |
| 1:0:1761:U:H5' | 17:P:81:LYS:O | 2.18 | 0.43 |
| 27:Z:36:ASP:HB3 | 27:Z:45:ASP:HB3 | 1.99 | 0.43 |
| 1:0:106:A:H2' | 1:0:107:U:O4' | 2.18 | 0.43 |
| 1:0:1183:C:H42 | 1:0:1184:C:N4 | 2.12 | 0.43 |
| 1:0:1215:A:O3' | 1:0:1216:G:C4' | 2.66 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:0:1829:A:H5'' | 38:0:3081:HOH:O | 2.17 | 0.43 |
| 1:0:1923:G:H4' | 30:3:31:THR:O | 2.18 | 0.43 |
| 1:0:2821:C:H4' | 4:B:116:PRO:HG3 | 2.00 | 0.43 |
| 1:0:2850:C:H6 | 1:0:2850:C:H5' | 1.83 | 0.43 |
| 1:0:303:C:H2' | 1:0:304:G:O4' | 2.18 | 0.43 |
| 1:0:338:C:H4' | 5:C:174:ILE:HD12 | 1.98 | 0.43 |
| 1:0:37:A:H2' | 1:0:38:G:C8 | 2.52 | 0.43 |
| 5:C:51:TYR:CE2 | 28:1:53:LYS:HB3 | 2.53 | 0.43 |
| 1:0:2101:A:H2' | 5:C:63:SER:OG | 2.18 | 0.43 |
| 12:K:87:ARG:NH1 | 38:K:4066:HOH:O | 2.51 | 0.43 |
| 1:0:1377:C:C5' | 1:0:1377:C:H6 | 2.28 | 0.43 |
| 1:0:1624:A:H5' | 1:0:1626:A:O4' | 2.17 | 0.43 |
| 1:0:195:C:H2' | 1:0:196:G:H5' | 2.00 | 0.43 |
| 1:0:2089:A:O2' | 1:0:2090:G:H5' | 2.18 | 0.43 |
| 1:0:2039:A:H4' | 1:0:2760:C:O2' | 2.19 | 0.43 |
| 32:0:9000:13T:H2 | 32:0:9000:13T:C26 | 2.42 | 0.43 |
| 38:0:7442:HOH:O | 4:B:211:THR:HG21 | 2.19 | 0.43 |
| 1:0:99:A:C8 | 1:0:100:C:C5 | 3.06 | 0.43 |
| 1:0:1118:A:N6 | 1:0:1244:U:C2 | 2.86 | 0.43 |
| 1:0:1343:C:H2' | 1:0:1344:G:O5' | 2.19 | 0.43 |
| 1:0:1409:G:C2 | 1:0:1410:G:C8 | 3.06 | 0.43 |
| 1:0:1903:U:O2' | 1:0:1904:A:N7 | 2.49 | 0.43 |
| 1:0:2002:C:H2' | 1:0:2003:U:H5' | 2.00 | 0.43 |
| 1:0:2252:A:C6 | 1:0:2253:G:H1' | 2.54 | 0.43 |
| 1:0:2326:U:H4' | 1:0:2412:G:H4' | 2.01 | 0.43 |
| 1:0:304:G:H1' | 1:0:347:A:H61 | 1.83 | 0.43 |
| 1:0:772:G:H2' | 1:0:773:A:O4' | 2.17 | 0.43 |
| 5:C:115:LEU:HD12 | 5:C:115:LEU:HA | 1.87 | 0.43 |
| 6:D:170:TYR:O | 6:D:171:ASP:HB3 | 2.18 | 0.43 |
| 7:E:22:VAL:O | 7:E:76:VAL:HG11 | 2.18 | 0.43 |
| 8:F:101:ALA:HA | 38:F:5413:HOH:O | 2.18 | 0.43 |
| 12:K:132:VAL:HG21 | 22:U:22:VAL:HG11 | 2.00 | 0.43 |
| 12:K:34:VAL:HG21 | 12:K:46:LYS:O | 2.19 | 0.43 |
| 17:P:98:ILE:HD12 | 17:P:102:ARG:NE | 2.34 | 0.43 |
| 20:S:33:SER:O | 20:S:37:VAL:HG23 | 2.18 | 0.43 |
| 1:0:137:U:H2' | 1:0:139:C:C5 | 2.53 | 0.43 |
| 1:0:1768:C:H2' | 1:0:1769:C:O4' | 2.18 | 0.43 |
| 1:0:187:A:H3' | 1:0:188:C:H6 | 1.83 | 0.43 |
| 1:0:242:A:N6 | 1:0:269:G:H1' | 2.34 | 0.43 |
| 1:0:2786:G:H2' | 38:0:7180:HOH:O | 2.17 | 0.43 |
| 2:9:3012:C:H5' | 2:9:3070:U:O4' | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:C:185:LYS:HD3 | 5:C:186:TYR:CE1 | 2.53 | 0.43 |
| 5:C:193:LEU:HD13 | 5:C:222:ASP:HB2 | 2.00 | 0.43 |
| 6:D:49:PRO:HA | 6:D:73:VAL:HG22 | 2.01 | 0.43 |
| 7:E:80:TRP:O | 7:E:134:SER:HA | 2.17 | 0.43 |
| 15:N:7:LYS:HE3 | 18:Q:21:ARG:O | 2.19 | 0.43 |
| 19:R:132:ARG:HG2 | 19:R:133:ALA:N | 2.32 | 0.43 |
| 27:Z:30:GLU:HG2 | 27:Z:33:MET:HE2 | 1.99 | 0.43 |
| 1:0:1130:U:H4' | 38:0:6133:HOH:O | 2.18 | 0.43 |
| 1:0:1183:C:O2 | 1:0:1183:C:C2' | 2.67 | 0.43 |
| 1:0:1439:C:H6 | 1:0:1439:C:O5' | 2.01 | 0.43 |
| 1:0:1811:A:C2 | 1:0:2752:C:H1' | 2.52 | 0.43 |
| 1:0:2779:G:N2 | 1:0:2796:U:C2 | 2.87 | 0.43 |
| 1:0:2812:A:H2 | 1:0:2814:A:N6 | 1.91 | 0.43 |
| 1:0:2840:A:OP1 | 4:B:211:THR:HG23 | 2.19 | 0.43 |
| 1:0:645:U:H2' | 1:0:646:G:C8 | 2.54 | 0.43 |
| 1:0:69:A:C8 | 1:0:69:A:C5' | 2.95 | 0.43 |
| 4:B:4:SER:O | 4:B:5:ARG:HB2 | 2.19 | 0.43 |
| 4:B:88:GLU:HG3 | 4:B:88:GLU:O | 2.18 | 0.43 |
| 9:G:20:VAL:O | 9:G:24:VAL:HG23 | 2.19 | 0.43 |
| 1:0:1186:C:H5'' | 31:I:119:TYR:CE1 | 2.53 | 0.43 |
| 8:F:56:PRO:CG | 14:M:44:THR:HA | 2.48 | 0.43 |
| 24:W:26:ILE:HB | 38:W:5420:HOH:O | 2.18 | 0.43 |
| 1:0:1119:G:N2 | 1:0:1246:A:H2 | 2.09 | 0.43 |
| 1:0:1215:A:O3' | 1:0:1216:G:H4' | 2.19 | 0.43 |
| 1:0:1257:C:O2' | 1:0:1258:G:H5' | 2.18 | 0.43 |
| 1:0:1386:G:O2' | 1:0:1387:G:H5' | 2.19 | 0.43 |
| 1:0:1772:C:H5' | 1:0:1773:G:C5 | 2.53 | 0.43 |
| 1:0:1778:A:H2' | 1:0:1779:A:H5' | 2.00 | 0.43 |
| 1:0:1904:A:H2' | 1:0:1905:U:O4' | 2.19 | 0.43 |
| 1:0:1883:U:H5' | 1:0:2012:U:OP2 | 2.19 | 0.43 |
| 1:0:365:G:C5 | 1:0:366:U:C5 | 3.07 | 0.43 |
| 1:0:2460:A:C4 | 32:0:9000:13T:H20 | 2.53 | 0.43 |
| 1:0:947:U:O2' | 1:0:948:G:H5' | 2.18 | 0.43 |
| 3:A:81:GLN:HB2 | 3:A:92:ASN:ND2 | 2.34 | 0.43 |
| 4:B:24:PRO:CG | 4:B:204:GLY:HA2 | 2.49 | 0.43 |
| 11:J:47:THR:HG22 | 11:J:48:GLY:N | 2.34 | 0.43 |
| 14:M:46:LEU:HG | 38:M:8913:HOH:O | 2.18 | 0.43 |
| 24:W:106:THR:OG1 | 24:W:109:GLU:HB2 | 2.19 | 0.43 |
| 1:0:1434:A:H2' | 1:0:1436:C:C5 | 2.53 | 0.43 |
| 1:0:1565:C:O2' | 1:0:1566:C:H5' | 2.19 | 0.43 |
| 1:0:1850:U:O4' | 1:0:1941:A:C2 | 2.71 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:0:2036:C:C4' | 12:K:44:LEU:HG | 2.48 | 0.43 |
| 1:0:2591:C:H2' | 1:0:2592:G:O4' | 2.19 | 0.43 |
| 1:0:2697:A:H2' | 1:0:2698:G:O4' | 2.19 | 0.43 |
| 1:0:2856:A:OP1 | 25:X:15:ARG:NH2 | 2.51 | 0.43 |
| 1:0:241:A:C2 | 1:0:378:A:H4' | 2.53 | 0.43 |
| 1:0:445:U:O2' | 1:0:446:G:H5' | 2.18 | 0.43 |
| 1:0:1415:G:H5' | 28:1:12:ASN:O | 2.18 | 0.43 |
| 2:9:3069:U:OP1 | 15:N:4:PRO:HG3 | 2.18 | 0.43 |
| 38:0:9208:HOH:O | 4:B:248:ARG:NH2 | 2.51 | 0.43 |
| 4:B:33:ASP:HB3 | 4:B:34:GLY:H | 1.60 | 0.43 |
| 31:I:125:ALA:O | 31:I:129:VAL:HG23 | 2.19 | 0.43 |
| 11:J:127:ILE:CG2 | 36:J:8801:CL:CL | 3.00 | 0.43 |
| 38:0:6721:HOH:O | 18:Q:2:SER:HA | 2.19 | 0.43 |
| 26:Y:107:PRO:HB3 | 26:Y:182:PHE:CD2 | 2.54 | 0.43 |
| 1:0:1191:A:H2 | 1:0:1206:U:H3 | 1.67 | 0.43 |
| 1:0:134:U:C2 | 1:0:145:A:C2 | 3.07 | 0.43 |
| 1:0:1825:U:O2' | 1:0:1826:C:H5' | 2.19 | 0.43 |
| 1:0:1943:C:O4' | 3:A:212:PRO:HA | 2.18 | 0.43 |
| 1:0:2088:C:H1' | 1:0:2841:A:N1 | 2.34 | 0.43 |
| 1:0:2254:G:C2 | 1:0:2255:A:C8 | 3.06 | 0.43 |
| 1:0:228:C:C2' | 1:0:229:G:H5' | 2.49 | 0.43 |
| 1:0:2372:A:H2' | 1:0:2373:U:H6 | 1.82 | 0.43 |
| 32:0:9000:13T:H3 | 30:3:56:PRO:CB | 2.48 | 0.43 |
| 6:D:138:GLY:N | 38:D:7597:HOH:O | 2.51 | 0.43 |
| 7:E:20:ILE:HD11 | 7:E:40:VAL:HG11 | 2.01 | 0.43 |
| 8:F:48:VAL:HG12 | 8:F:97:ALA:CB | 2.49 | 0.43 |
| 12:K:125:ALA:C | 12:K:127:ALA:H | 2.22 | 0.43 |
| 24:W:5:VAL:HG11 | 24:W:153:MET:HE3 | 1.99 | 0.43 |
| 1:0:1080:C:O5' | 1:0:1080:C:H6 | 2.02 | 0.43 |
| 1:0:1114:A:H2' | 1:0:1115:U:C6 | 2.54 | 0.43 |
| 1:0:1163:G:H1 | 1:0:1184:C:N4 | 2.17 | 0.43 |
| 1:0:1654:U:H2' | 3:A:47:HIS:CD2 | 2.52 | 0.43 |
| 1:0:1667:A:C2 | 1:0:1668:U:C2 | 3.07 | 0.43 |
| 1:0:1805:G:H2' | 1:0:1806:G:H8 | 1.83 | 0.43 |
| 1:0:213:G:N2 | 1:0:225:G:H2' | 2.34 | 0.43 |
| 1:0:2255:A:H2' | 1:0:2256:G:O4' | 2.18 | 0.43 |
| 1:0:2255:A:O2' | 1:0:2256:G:H5' | 2.18 | 0.43 |
| 1:0:2598:U:O2 | 1:0:2600:A:H8 | 2.00 | 0.43 |
| 1:0:73:C:O2' | 1:0:74:A:H5' | 2.18 | 0.43 |
| 1:0:815:U:O2' | 1:0:1598:A:H4' | 2.18 | 0.43 |
| 29:2:40:ARG:HG3 | 29:2:45:ASN:CB | 2.48 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:B:177:HIS:O | 4:B:181:ILE:HG13 | 2.19 | 0.43 |
| 1:0:2348:C:H1' | 6:D:131:THR:HG21 | 2.01 | 0.43 |
| 11:J:45:VAL:HG21 | 11:J:129:PHE:HD1 | 1.82 | 0.43 |
| 14:M:80:GLY:O | 14:M:81:ARG:HD3 | 2.18 | 0.43 |
| 22:U:17:THR:HG22 | 22:U:18:GLY:N | 2.34 | 0.43 |
| 24:W:4:LEU:O | 24:W:32:CYS:HA | 2.18 | 0.43 |
| 26:Y:107:PRO:HD3 | 26:Y:182:PHE:CD1 | 2.54 | 0.43 |
| 1:0:1181:A:H2' | 1:0:1182:C:H5' | 2.00 | 0.42 |
| 1:0:1242:A:OP2 | 11:J:60:ARG:NH2 | 2.47 | 0.42 |
| 1:0:1930:A:H2' | 1:0:1931:A:C8 | 2.54 | 0.42 |
| 1:0:2291:A:H8 | 38:0:6467:HOH:O | 2.01 | 0.42 |
| 1:0:2504:A:H4' | 10:H:71:ARG:NH1 | 2.34 | 0.42 |
| 1:0:2519:C:O2' | 1:0:2520:G:H5' | 2.19 | 0.42 |
| 1:0:2712:G:H5' | 38:0:5223:HOH:O | 2.18 | 0.42 |
| 1:0:559:U:C5 | 1:0:560:C:C5 | 3.07 | 0.42 |
| 1:0:571:C:O5' | 1:0:571:C:H6 | 2.01 | 0.42 |
| 32:0:9000:13T:H233 | 32:0:9000:13T:H311 | 2.01 | 0.42 |
| 1:0:952:G:N3 | 1:0:2302:A:H2' | 2.34 | 0.42 |
| 28:1:53:LYS:HD3 | 28:1:53:LYS:HA | 1.85 | 0.42 |
| 5:C:194:PHE:HA | 5:C:234:VAL:HG13 | 2.01 | 0.42 |
| 6:D:103:ASN:HD22 | 6:D:133:ASN:HA | 1.84 | 0.42 |
| 38:0:6400:HOH:O | 24:W:122:ARG:NH2 | 2.45 | 0.42 |
| 26:Y:234:VAL:HG12 | 26:Y:235:GLU:N | 2.34 | 0.42 |
| 1:0:1138:G:H4' | 38:0:5719:HOH:O | 2.19 | 0.42 |
| 1:0:1552:G:H2' | 1:0:1553:C:C6 | 2.54 | 0.42 |
| 1:0:169:A:H1' | 30:3:48:ASN:ND2 | 2.34 | 0.42 |
| 1:0:177:A:H2' | 1:0:178:U:O4' | 2.19 | 0.42 |
| 1:0:2072:G:C6 | 1:0:2533:C:H1' | 2.54 | 0.42 |
| 1:0:682:A:H2' | 1:0:683:G:O4' | 2.19 | 0.42 |
| 6:D:44:ILE:HG23 | 6:D:45:THR:HG23 | 2.00 | 0.42 |
| 2:9:3041:C:C2 | 6:D:50:VAL:HG21 | 2.54 | 0.42 |
| 10:H:47:ILE:HG21 | 38:H:8579:HOH:O | 2.20 | 0.42 |
| 16:O:105:ASN:HD21 | 16:O:109:SER:N | 2.18 | 0.42 |
| 16:O:21:SER:OG | 16:O:106:PRO:HB2 | 2.18 | 0.42 |
| 1:0:952:G:OP1 | 18:Q:42:LYS:HE2 | 2.20 | 0.42 |
| 19:R:4:TYR:CE1 | 19:R:15:LYS:HD3 | 2.53 | 0.42 |
| 21:T:28:SER:O | 21:T:32:ARG:HG3 | 2.18 | 0.42 |
| 26:Y:178:HIS:CG | 26:Y:179:PRO:HD2 | 2.54 | 0.42 |
| 1:0:151:A:H2' | 1:0:152:A:O4' | 2.18 | 0.42 |
| 1:0:1544:U:H2' | 1:0:1545:C:C6 | 2.54 | 0.42 |
| 1:0:1970:G:H2' | 1:0:1970:G:N3 | 2.35 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:0:2015:A:H2' | 1:0:2016:U:O4' | 2.19 | 0.42 |
| 1:0:2608:C:H3' | 38:0:7790:HOH:O | 2.18 | 0.42 |
| 1:0:2785:C:H4' | 1:0:2786:G:OP2 | 2.19 | 0.42 |
| 1:0:284:C:C4' | 1:0:285:A:O5' | 2.64 | 0.42 |
| 1:0:644:G:O2' | 36:0:8814:CL:CL | 2.67 | 0.42 |
| 4:B:165:ARG:HG2 | 4:B:166:VAL:N | 2.35 | 0.42 |
| 4:B:204:GLY:HA3 | 38:B:8948:HOH:O | 2.18 | 0.42 |
| 6:D:91:ALA:HB1 | 38:D:5198:HOH:O | 2.19 | 0.42 |
| 38:0:4740:HOH:O | 15:N:21:HIS:HD2 | 2.01 | 0.42 |
| 20:S:37:VAL:O | 20:S:41:VAL:HG23 | 2.19 | 0.42 |
| 25:X:30:MET:HE1 | 25:X:55:ASN:HA | 2.00 | 0.42 |
| 1:0:2296:C:H2' | 1:0:2297:U:H6 | 1.82 | 0.42 |
| 1:0:2415:A:H2' | 1:0:2416:G:H5' | 2.00 | 0.42 |
| 1:0:1486:A:C5 | 29:2:2:LYS:HG3 | 2.55 | 0.42 |
| 2:9:3001:U:H4' | 2:9:3003:A:OP1 | 2.19 | 0.42 |
| 14:M:167:GLY:O | 14:M:171:ARG:HG3 | 2.19 | 0.42 |
| 16:O:44:ASN:HA | 16:O:65:LEU:O | 2.19 | 0.42 |
| 22:U:6:CYS:HB2 | 22:U:32:CYS:HB3 | 2.00 | 0.42 |
| 1:0:2035:C:O5' | 1:0:2035:C:H6 | 2.02 | 0.42 |
| 1:0:2395:A:C6 | 1:0:2396:C:C4 | 3.07 | 0.42 |
| 1:0:2502:C:O2' | 1:0:2503:A:H5' | 2.18 | 0.42 |
| 1:0:263:U:C4 | 8:F:54:VAL:HG13 | 2.54 | 0.42 |
| 1:0:2909:G:O2' | 1:0:2910:A:H5' | 2.20 | 0.42 |
| 1:0:395:A:H4' | 38:0:9964:HOH:O | 2.20 | 0.42 |
| 1:0:853:C:H2' | 1:0:854:G:O4' | 2.19 | 0.42 |
| 1:0:958:G:O2' | 1:0:959:C:H5' | 2.19 | 0.42 |
| 28:1:26:SER:HB3 | 28:1:35:SER:OG | 2.20 | 0.42 |
| 2:9:3031:C:H1' | 38:9:1137:HOH:O | 2.18 | 0.42 |
| 12:K:28:GLU:HB3 | 12:K:59:LYS:HB2 | 2.01 | 0.42 |
| 13:L:73:VAL:HG11 | 13:L:118:LEU:HD21 | 2.01 | 0.42 |
| 15:N:71:TRP:CE3 | 15:N:175:LEU:HD22 | 2.55 | 0.42 |
| 17:P:103:THR:O | 17:P:107:GLU:HG3 | 2.20 | 0.42 |
| 1:0:1046:G:N3 | 1:0:1082:A:H2 | 2.17 | 0.42 |
| 1:0:1175:G:H1' | 1:0:1193:A:H2' | 2.01 | 0.42 |
| 1:0:2105:C:O2' | 1:0:2284:G:N2 | 2.52 | 0.42 |
| 1:0:2265:U:H2' | 1:0:2266:A:C8 | 2.55 | 0.42 |
| 1:0:2607:U:H4' | 38:0:9438:HOH:O | 2.18 | 0.42 |
| 1:0:482:G:O4' | 1:0:511:A:C2 | 2.72 | 0.42 |
| 1:0:764:C:H2' | 1:0:765:G:O4' | 2.19 | 0.42 |
| 2:9:3034:A:O5' | 2:9:3034:A:H8 | 2.02 | 0.42 |
| 3:A:9:ARG:NH1 | 38:A:8822:HOH:O | 2.53 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:0:475:G:C5' | 5:C:73:LEU:HD23 | 2.50 | 0.42 |
| 11:J:39:VAL:HG13 | 11:J:106:GLY:O | 2.20 | 0.42 |
| 14:M:28:GLN:O | 14:M:32:ARG:HG3 | 2.18 | 0.42 |
| 15:N:170:GLU:O | 15:N:174:GLU:HG3 | 2.20 | 0.42 |
| 19:R:82:GLU:O | 19:R:86:LYS:HG3 | 2.20 | 0.42 |
| 25:X:80:GLU:HB3 | 38:X:5564:HOH:O | 2.17 | 0.42 |
| 26:Y:151:SER:HB3 | 26:Y:154:ARG:CB | 2.49 | 0.42 |
| 1:0:1323:G:N2 | 1:0:1335:C:C2 | 2.88 | 0.42 |
| 1:0:316:A:H5' | 21:T:54:ASP:OD2 | 2.20 | 0.42 |
| 1:0:440:C:H2' | 1:0:441:A:C8 | 2.54 | 0.42 |
| 1:0:535:G:C6 | 1:0:2064:U:C5 | 3.08 | 0.42 |
| 1:0:876:A:N3 | 1:0:876:A:C2' | 2.83 | 0.42 |
| 32:0:9000:13T:H323 | 32:0:9000:13T:C1 | 2.49 | 0.42 |
| 30:3:22:VAL:HG11 | 30:3:67:LEU:HD13 | 2.01 | 0.42 |
| 2:9:3059:C:H5' | 38:9:5233:HOH:O | 2.18 | 0.42 |
| 2:9:3110:G:C5 | 2:9:3111:U:C5 | 3.07 | 0.42 |
| 4:B:57:GLU:HA | 4:B:58:PRO:HD2 | 1.96 | 0.42 |
| 11:J:59:LYS:O | 11:J:63:ILE:HG13 | 2.19 | 0.42 |
| 38:0:3186:HOH:O | 14:M:9:ARG:HG3 | 2.19 | 0.42 |
| 1:0:1161:A:H8 | 1:0:1161:A:O5' | 2.02 | 0.42 |
| 1:0:1579:C:H4' | 1:0:1580:A:OP1 | 2.19 | 0.42 |
| 1:0:2078:U:O2' | 1:0:2079:G:H5' | 2.20 | 0.42 |
| 1:0:2256:G:C2' | 1:0:2257:G:C5' | 2.93 | 0.42 |
| 1:0:2900:G:H2' | 1:0:2901:C:O4' | 2.20 | 0.42 |
| 1:0:447:A:OP1 | 21:T:2:LYS:HG2 | 2.20 | 0.42 |
| 1:0:595:U:H2' | 1:0:596:C:H6 | 1.85 | 0.42 |
| 2:9:3013:A:H3' | 2:9:3014:G:H5' | 2.02 | 0.42 |
| 4:B:243:ASN:HA | 4:B:244:PRO:C | 2.40 | 0.42 |
| 5:C:118:THR:HG22 | 5:C:137:PRO:HB3 | 2.02 | 0.42 |
| 5:C:218:VAL:HG12 | 38:C:8623:HOH:O | 2.19 | 0.42 |
| 38:0:4574:HOH:O | 5:C:50:GLU:HG2 | 2.20 | 0.42 |
| 12:K:4:LEU:HD23 | 12:K:4:LEU:HA | 1.83 | 0.42 |
| 13:L:120:LEU:HD12 | 13:L:133:VAL:HG21 | 2.02 | 0.42 |
| 38:0:3652:HOH:O | 16:O:3:THR:HG21 | 2.19 | 0.42 |
| 1:0:1069:C:H2' | 1:0:1070:A:O4' | 2.20 | 0.42 |
| 1:0:1923:G:H2' | 1:0:1924:A:H8 | 1.84 | 0.42 |
| 1:0:2758:G:H2' | 1:0:2759:C:C6 | 2.55 | 0.42 |
| 1:0:282:C:O2' | 1:0:283:U:C4' | 2.68 | 0.42 |
| 1:0:318:C:H5' | 1:0:339:A:N3 | 2.35 | 0.42 |
| 1:0:589:U:H2' | 1:0:590:A:C8 | 2.54 | 0.42 |
| 1:0:825:U:H5'' | 1:0:826:U:OP1 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:0:856:G:H2' | 38:0:5435:HOH:O | 2.18 | 0.42 |
| 2:9:3059:C:H2' | 2:9:3060:C:C6 | 2.55 | 0.42 |
| 6:D:25:MET:HE1 | 6:D:37:ALA:O | 2.20 | 0.42 |
| 6:D:64:ARG:HD3 | 6:D:67:ASP:HB3 | 2.02 | 0.42 |
| 22:U:6:CYS:C | 22:U:8:TYR:H | 2.21 | 0.42 |
| 26:Y:170:SER:OG | 26:Y:175:ARG:HG3 | 2.19 | 0.42 |
| 1:0:1482:A:O2' | 1:0:1483:C:H5' | 2.20 | 0.42 |
| 1:0:1789:G:H2' | 1:0:1790:C:O5' | 2.20 | 0.42 |
| 1:0:2240:U:O2' | 1:0:2241:C:H5' | 2.19 | 0.42 |
| 1:0:2521:A:P | 10:H:3:ALA:HB3 | 2.60 | 0.42 |
| 1:0:2612:A:H4' | 38:0:3685:HOH:O | 2.19 | 0.42 |
| 1:0:2824:C:O3' | 1:0:2825:C:H6 | 2.01 | 0.42 |
| 1:0:561:G:C2 | 1:0:562:A:C5 | 3.08 | 0.42 |
| 2:9:3114:G:H2' | 2:9:3115:C:C6 | 2.55 | 0.42 |
| 4:B:24:PRO:HG3 | 4:B:204:GLY:HA2 | 2.01 | 0.42 |
| 4:B:305:ASP:O | 4:B:306:LYS:CB | 2.68 | 0.42 |
| 4:B:79:MET:HE3 | 4:B:79:MET:HB2 | 1.99 | 0.42 |
| 6:D:23:VAL:HG21 | 6:D:45:THR:HG21 | 2.02 | 0.42 |
| 1:0:1055:G:OP2 | 10:H:96:ARG:NH1 | 2.53 | 0.42 |
| 19:R:132:ARG:NH2 | 38:R:8879:HOH:O | 2.52 | 0.42 |
| 1:0:1762:C:H4' | 38:0:4662:HOH:O | 2.19 | 0.41 |
| 1:0:2032:U:O2' | 1:0:2033:G:H5'' | 2.20 | 0.41 |
| 1:0:2389:U:H4' | 18:Q:53:HIS:CD2 | 2.55 | 0.41 |
| 1:0:2401:A:H2' | 1:0:2402:A:C8 | 2.55 | 0.41 |
| 1:0:2589:U:H2' | 1:0:2590:U:C6 | 2.55 | 0.41 |
| 1:0:2724:U:H2' | 1:0:2725:G:O4' | 2.20 | 0.41 |
| 1:0:517:U:C2' | 1:0:518:G:H5' | 2.50 | 0.41 |
| 1:0:941:G:C2' | 1:0:942:U:H5' | 2.50 | 0.41 |
| 1:0:946:C:H2' | 1:0:947:U:H6 | 1.84 | 0.41 |
| 2:9:3059:C:H6 | 2:9:3059:C:O5' | 2.03 | 0.41 |
| 2:9:3105:A:C2' | 2:9:3106:C:H5' | 2.49 | 0.41 |
| 3:A:131:HIS:O | 3:A:132:ASP:HB2 | 2.20 | 0.41 |
| 4:B:260:HIS:HE1 | 38:B:8883:HOH:O | 2.03 | 0.41 |
| 6:D:25:MET:SD | 6:D:40:ILE:HD11 | 2.60 | 0.41 |
| 6:D:48:MET:HA | 6:D:49:PRO:HD3 | 1.87 | 0.41 |
| 1:0:1019:C:O2 | 18:Q:94:GLN:NE2 | 2.53 | 0.41 |
| 19:R:18:LEU:HD12 | 19:R:143:VAL:HG11 | 2.02 | 0.41 |
| 3:A:76:VAL:HG23 | 27:Z:63:LYS:HB3 | 2.00 | 0.41 |
| 1:0:1904:A:C8 | 1:0:1905:U:C5 | 3.08 | 0.41 |
| 1:0:2112:A:H2' | 1:0:2113:G:H8 | 1.85 | 0.41 |
| 1:0:2254:G:O2' | 1:0:2255:A:H5' | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:0:2402:A:H1' | 38:0:3163:HOH:O | 2.20 | 0.41 |
| 1:0:2689:A:C2' | 1:0:2690:U:H5' | 2.50 | 0.41 |
| 1:0:2754:G:C2' | 1:0:2755:G:H5' | 2.50 | 0.41 |
| 1:0:381:G:OP2 | 14:M:45:ARG:NH2 | 2.50 | 0.41 |
| 1:0:497:A:H2' | 1:0:498:A:C5' | 2.50 | 0.41 |
| 1:0:553:G:H2' | 1:0:554:G:H5' | 2.02 | 0.41 |
| 1:0:699:C:C6 | 1:0:744:G:C4 | 3.08 | 0.41 |
| 28:1:25:LYS:HD2 | 29:2:49:GLU:H | 1.84 | 0.41 |
| 6:D:49:PRO:HG3 | 38:D:5828:HOH:O | 2.21 | 0.41 |
| 8:F:14:ASP:O | 8:F:18:GLU:HG3 | 2.20 | 0.41 |
| 8:F:48:VAL:HG23 | 8:F:74:PHE:HB3 | 2.01 | 0.41 |
| 31:I:100:LEU:HD22 | 31:I:105:VAL:HG23 | 2.02 | 0.41 |
| 14:M:164:THR:HG22 | 14:M:167:GLY:N | 2.35 | 0.41 |
| 22:U:17:THR:CG2 | 22:U:18:GLY:N | 2.83 | 0.41 |
| 1:0:1158:G:O2' | 1:0:1159:G:H5' | 2.20 | 0.41 |
| 1:0:1225:C:H2' | 1:0:1226:G:O4' | 2.21 | 0.41 |
| 1:0:1289:C:O2' | 1:0:1290:G:H5' | 2.19 | 0.41 |
| 1:0:1576:G:H2' | 1:0:1577:U:H6 | 1.85 | 0.41 |
| 1:0:185:G:O3' | 1:0:186:A:H4' | 2.21 | 0.41 |
| 1:0:694:A:H4' | 1:0:2441:U:OP1 | 2.21 | 0.41 |
| 1:0:371:U:H2' | 1:0:372:A:C8 | 2.55 | 0.41 |
| 1:0:459:A:H5'' | 38:0:9047:HOH:O | 2.20 | 0.41 |
| 28:1:25:LYS:HE2 | 38:2:7213:HOH:O | 2.20 | 0.41 |
| 1:0:2434:A:O3' | 30:3:28:GLY:HA3 | 2.20 | 0.41 |
| 2:9:3033:U:H2' | 38:9:3797:HOH:O | 2.19 | 0.41 |
| 2:9:3042:C:O2 | 6:D:76:ARG:NH1 | 2.52 | 0.41 |
| 2:9:3105:A:H2' | 2:9:3106:C:H5' | 2.03 | 0.41 |
| 7:E:84:MET:HG2 | 7:E:168:ILE:HA | 2.02 | 0.41 |
| 10:H:171:ALA:HA | 38:H:8570:HOH:O | 2.20 | 0.41 |
| 31:I:91:GLU:HA | 31:I:92:PRO:HD2 | 1.84 | 0.41 |
| 11:J:19:MET:CE | 11:J:132:LEU:HD11 | 2.51 | 0.41 |
| 1:0:902:G:N7 | 13:L:18:HIS:CD2 | 2.85 | 0.41 |
| 21:T:9:LYS:HE3 | 21:T:13:ARG:NH1 | 2.35 | 0.41 |
| 24:W:4:LEU:CD1 | 24:W:24:LEU:HD13 | 2.50 | 0.41 |
| 26:Y:112:GLU:CD | 26:Y:115:ARG:NH1 | 2.74 | 0.41 |
| 27:Z:30:GLU:HB2 | 38:Z:8715:HOH:O | 2.20 | 0.41 |
| 1:0:1422:U:H4' | 38:0:7732:HOH:O | 2.19 | 0.41 |
| 1:0:1815:A:H4' | 1:0:2751:C:O4' | 2.21 | 0.41 |
| 1:0:2634:G:OP2 | 3:A:204:GLY:N | 2.53 | 0.41 |
| 1:0:2825:C:H4' | 1:0:2826:G:O5' | 2.20 | 0.41 |
| 1:0:695:C:H2' | 1:0:696:C:C6 | 2.54 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:0:81:G:N3 | 1:0:98:A:C2 | 2.89 | 0.41 |
| 1:0:1943:C:C4' | 3:A:212:PRO:HA | 2.50 | 0.41 |
| 1:0:2270:G:H4' | 3:A:223:ARG:HH12 | 1.86 | 0.41 |
| 11:J:19:MET:HE1 | 11:J:132:LEU:HD11 | 2.02 | 0.41 |
| 11:J:74:ARG:HH11 | 11:J:74:ARG:CB | 2.30 | 0.41 |
| 15:N:42:HIS:CG | 15:N:62:HIS:HE1 | 2.38 | 0.41 |
| 25:X:7:GLU:HA | 25:X:74:ALA:O | 2.20 | 0.41 |
| 1:0:1020:A:H2' | 1:0:1021:G:C8 | 2.56 | 0.41 |
| 1:0:1024:G:C6 | 1:0:1025:C:C4 | 3.08 | 0.41 |
| 1:0:1052:G:N3 | 1:0:1052:G:H2' | 2.35 | 0.41 |
| 1:0:1400:C:O2' | 1:0:1401:G:H5' | 2.21 | 0.41 |
| 1:0:1923:G:H2' | 1:0:1924:A:C8 | 2.56 | 0.41 |
| 1:0:308:U:C4 | 1:0:342:C:C1' | 3.03 | 0.41 |
| 1:0:61:G:C6 | 1:0:62:C:C4 | 3.09 | 0.41 |
| 1:0:849:C:O2' | 1:0:850:U:H5' | 2.21 | 0.41 |
| 2:9:3001:U:H5' | 2:9:3121:C:O2 | 2.20 | 0.41 |
| 2:9:3001:U:O3' | 2:9:3003:A:C5' | 2.69 | 0.41 |
| 2:9:3092:G:C6 | 2:9:3093:A:N6 | 2.88 | 0.41 |
| 4:B:69:VAL:HA | 4:B:70:PRO:HD3 | 1.86 | 0.41 |
| 8:F:50:VAL:CG1 | 8:F:60:VAL:HG11 | 2.48 | 0.41 |
| 14:M:182:LYS:HB2 | 14:M:194:ALA:HB2 | 2.01 | 0.41 |
| 24:W:149:LEU:HG | 24:W:153:MET:HE2 | 2.03 | 0.41 |
| 25:X:74:ALA:CB | 25:X:85:VAL:HG22 | 2.51 | 0.41 |
| 27:Z:67:GLY:N | 27:Z:70:LYS:O | 2.54 | 0.41 |
| 1:0:1206:U:C5' | 1:0:1206:U:H6 | 2.23 | 0.41 |
| 1:0:255:A:C5 | 1:0:256:C:C5 | 3.09 | 0.41 |
| 1:0:2775:A:C6 | 1:0:2776:A:C6 | 3.08 | 0.41 |
| 1:0:863:G:C6 | 1:0:864:U:C4 | 3.08 | 0.41 |
| 7:E:145:ALA:HB1 | 7:E:168:ILE:CD1 | 2.51 | 0.41 |
| 31:I:129:VAL:O | 31:I:129:VAL:HG12 | 2.21 | 0.41 |
| 18:Q:16:ASN:OD1 | 18:Q:45:PRO:HB2 | 2.20 | 0.41 |
| 24:W:19:ASP:O | 24:W:23:MET:HG3 | 2.20 | 0.41 |
| 1:0:1181:A:C2' | 1:0:1182:C:H5' | 2.51 | 0.41 |
| 1:0:1224:G:H2' | 1:0:1225:C:C6 | 2.55 | 0.41 |
| 1:0:2549:C:O2' | 1:0:2550:U:H5' | 2.20 | 0.41 |
| 1:0:298:C:H6 | 1:0:298:C:O5' | 2.04 | 0.41 |
| 1:0:25:A:O2' | 1:0:640:G:H5' | 2.21 | 0.41 |
| 4:B:7:ARG:HG2 | 4:B:7:ARG:HH11 | 1.85 | 0.41 |
| 7:E:5:LEU:HD21 | 7:E:66:GLN:HG3 | 2.01 | 0.41 |
| 14:M:123:ASP:OD1 | 14:M:126:GLN:HG2 | 2.19 | 0.41 |
| 24:W:119:HIS:HD2 | 24:W:120:PRO:O | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:0:1021:G:O2' | 1:0:1022:A:H5' | 2.19 | 0.41 |
| 1:0:912:A:C4 | 1:0:1294:A:C2 | 3.09 | 0.41 |
| 1:0:1609:C:H2' | 1:0:1610:G:H8 | 1.84 | 0.41 |
| 1:0:1622:G:H2' | 1:0:1623:C:H5' | 2.02 | 0.41 |
| 1:0:2303:A:H2 | 38:Q:5641:HOH:O | 2.03 | 0.41 |
| 1:0:247:A:H1' | 38:0:3892:HOH:O | 2.21 | 0.41 |
| 1:0:2716:G:H5'' | 4:B:206:THR:CG2 | 2.44 | 0.41 |
| 1:0:295:C:H2' | 1:0:296:G:O4' | 2.20 | 0.41 |
| 1:0:539:G:H2' | 1:0:540:A:C8 | 2.56 | 0.41 |
| 2:9:3003:A:H61 | 2:9:3022:G:H1' | 1.83 | 0.41 |
| 1:0:2036:C:C1' | 12:K:44:LEU:HG | 2.51 | 0.41 |
| 13:L:92:ASP:HA | 13:L:121:ILE:HB | 2.02 | 0.41 |
| 14:M:158:ARG:HB2 | 14:M:163:LEU:HB2 | 2.03 | 0.41 |
| 1:0:2365:G:H4' | 18:Q:45:PRO:O | 2.20 | 0.41 |
| 19:R:72:VAL:CG1 | 19:R:75:TRP:HB3 | 2.50 | 0.41 |
| 20:S:45:TYR:O | 20:S:80:ARG:NH2 | 2.53 | 0.41 |
| 12:K:132:VAL:HG21 | 22:U:22:VAL:CG1 | 2.50 | 0.41 |
| 26:Y:144:ARG:NH2 | 38:Y:8912:HOH:O | 2.54 | 0.41 |
| 1:0:1157:C:O2' | 1:0:1158:G:H5' | 2.20 | 0.41 |
| 1:0:1786:C:OP1 | 17:P:74:GLN:HG2 | 2.21 | 0.41 |
| 1:0:1805:G:O2' | 1:0:1806:G:H5' | 2.21 | 0.41 |
| 1:0:2569:A:H2' | 1:0:2570:G:O5' | 2.20 | 0.41 |
| 1:0:2768:A:H5'' | 38:0:4432:HOH:O | 2.21 | 0.41 |
| 1:0:567:U:O2' | 1:0:568:G:H5' | 2.20 | 0.41 |
| 1:0:66:G:C2 | 1:0:109:U:C4 | 3.08 | 0.41 |
| 2:9:3001:U:C4' | 2:9:3003:A:OP1 | 2.69 | 0.41 |
| 2:9:3040:C:OP1 | 2:9:3041:C:H5 | 2.04 | 0.41 |
| 3:A:105:VAL:HG11 | 3:A:154:ALA:CB | 2.51 | 0.41 |
| 1:0:2607:U:C4 | 4:B:242:TRP:CZ2 | 3.08 | 0.41 |
| 4:B:265:LEU:HD21 | 4:B:316:ARG:HD3 | 2.01 | 0.41 |
| 4:B:52:VAL:O | 4:B:53:LEU:HD12 | 2.21 | 0.41 |
| 5:C:228:ALA:HA | 5:C:229:PRO:HD3 | 1.90 | 0.41 |
| 6:D:151:ILE:HA | 6:D:152:PRO:HD3 | 1.92 | 0.41 |
| 11:J:42:GLU:HG2 | 11:J:43:ARG:HG3 | 2.03 | 0.41 |
| 1:0:2415:A:O2' | 15:N:29:SER:HB3 | 2.21 | 0.41 |
| 21:T:32:ARG:NH1 | 21:T:38:ARG:NH1 | 2.69 | 0.41 |
| 21:T:3:GLN:HA | 21:T:4:PRO:HD3 | 1.76 | 0.41 |
| 4:B:329:TYR:CE2 | 22:U:15:PRO:HG2 | 2.56 | 0.41 |
| 1:0:1115:U:O2' | 1:0:1116:U:H5' | 2.20 | 0.41 |
| 1:0:1116:U:C2 | 1:0:1246:A:N6 | 2.89 | 0.41 |
| 1:0:1166:A:P | 1:0:1174:A:H4' | 2.61 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:0:1619:G:C6 | 1:0:1620:C:N3 | 2.89 | 0.41 |
| 1:0:1630:A:O2' | 1:0:1631:A:H5' | 2.21 | 0.41 |
| 1:0:1666:C:H2' | 1:0:1667:A:H8 | 1.86 | 0.41 |
| 1:0:169:A:H4' | 38:M:8837:HOH:O | 2.20 | 0.41 |
| 1:0:2398:A:H2' | 1:0:2399:G:O4' | 2.21 | 0.41 |
| 1:0:2727:A:N1 | 1:0:2756:U:C2 | 2.89 | 0.41 |
| 1:0:287:C:H6 | 1:0:287:C:O5' | 2.04 | 0.41 |
| 1:0:327:A:H4' | 1:0:329:A:C8 | 2.55 | 0.41 |
| 1:0:368:C:H2' | 1:0:369:G:H5' | 2.02 | 0.41 |
| 1:0:483:C:C4 | 1:0:484:A:C6 | 3.09 | 0.41 |
| 1:0:581:G:O2' | 1:0:582:C:H5' | 2.21 | 0.41 |
| 1:0:911:G:H5' | 1:0:932:U:OP1 | 2.21 | 0.41 |
| 2:9:3065:A:O2' | 2:9:3066:G:P | 2.79 | 0.41 |
| 2:9:3104:A:C2' | 2:9:3105:A:H5' | 2.50 | 0.41 |
| 3:A:186:TRP:CG | 3:A:187:PRO:HA | 2.56 | 0.41 |
| 4:B:23:THR:HG23 | 4:B:308:LEU:CD2 | 2.51 | 0.41 |
| 4:B:41:PHE:CZ | 4:B:79:MET:HG3 | 2.56 | 0.41 |
| 31:I:131:THR:O | 31:I:135:LEU:HG | 2.21 | 0.41 |
| 19:R:113:HIS:O | 19:R:145:LEU:HD12 | 2.20 | 0.41 |
| 24:W:81:ASP:OD1 | 24:W:92:ASP:HB2 | 2.20 | 0.41 |
| 1:0:1182:C:H6 | 1:0:1182:C:O5' | 2.02 | 0.41 |
| 1:0:1299:G:N2 | 38:0:4691:HOH:O | 2.53 | 0.41 |
| 1:0:1594:C:OP1 | 17:P:109:ARG:NH1 | 2.54 | 0.41 |
| 1:0:1662:C:H2' | 1:0:1663:G:O4' | 2.21 | 0.41 |
| 1:0:2004:U:H5'' | 1:0:2005:G:C8 | 2.56 | 0.41 |
| 1:0:2363:G:H2' | 1:0:2364:A:O4' | 2.21 | 0.41 |
| 1:0:2791:U:H1' | 1:0:2792:A:H5'' | 2.03 | 0.41 |
| 1:0:2791:U:H4' | 1:0:2792:A:OP1 | 2.21 | 0.41 |
| 1:0:2897:C:O2' | 1:0:2898:G:H5' | 2.21 | 0.41 |
| 1:0:380:A:O4' | 1:0:382:U:H1' | 2.21 | 0.41 |
| 1:0:397:A:H1' | 1:0:417:G:H1' | 2.02 | 0.41 |
| 1:0:716:G:C6 | 1:0:717:C:N4 | 2.89 | 0.41 |
| 32:0:9000:13T:H261 | 32:0:9000:13T:H10 | 1.80 | 0.41 |
| 3:A:68:ILE:HD11 | 38:A:8863:HOH:O | 2.20 | 0.41 |
| 13:L:119:THR:HA | 13:L:139:SER:O | 2.21 | 0.41 |
| 17:P:115:SER:O | 17:P:117:SER:N | 2.46 | 0.41 |
| 26:Y:144:ARG:NE | 38:Y:8912:HOH:O | 2.54 | 0.41 |
| 1:0:1449:G:N3 | 1:0:1449:G:H2' | 2.36 | 0.40 |
| 1:0:1745:G:H5' | 38:0:4341:HOH:O | 2.20 | 0.40 |
| 1:0:1925:G:O2' | 1:0:1926:G:H5' | 2.21 | 0.40 |
| 1:0:2072:G:H3' | 1:0:2073:G:C5' | 2.52 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:0:228:C:H2' | 1:0:229:G:C5' | 2.51 | 0.40 |
| 1:0:2549:C:H2' | 1:0:2550:U:O4' | 2.22 | 0.40 |
| 1:0:2598:U:O2 | 1:0:2600:A:C8 | 2.74 | 0.40 |
| 1:0:2887:G:H2' | 1:0:2888:U:O4' | 2.21 | 0.40 |
| 1:0:445:U:C1' | 38:0:7326:HOH:O | 2.68 | 0.40 |
| 1:0:545:G:H2' | 1:0:546:C:O4' | 2.21 | 0.40 |
| 3:A:33:GLU:CD | 3:A:33:GLU:H | 2.24 | 0.40 |
| 4:B:198:GLU:HA | 38:B:8952:HOH:O | 2.20 | 0.40 |
| 4:B:305:ASP:O | 4:B:306:LYS:HB2 | 2.21 | 0.40 |
| 4:B:336:GLN:NE2 | 38:B:8822:HOH:O | 2.53 | 0.40 |
| 7:E:172:PRO:HB3 | 38:E:6931:HOH:O | 2.21 | 0.40 |
| 7:E:22:VAL:O | 7:E:28:SER:HA | 2.22 | 0.40 |
| 7:E:69:ILE:HA | 7:E:72:MET:HE2 | 2.03 | 0.40 |
| 9:G:67:LEU:O | 9:G:71:LEU:HG | 2.21 | 0.40 |
| 19:R:89:LEU:HA | 19:R:89:LEU:HD23 | 1.84 | 0.40 |
| 26:Y:189:ASN:ND2 | 26:Y:192:ASP:N | 2.69 | 0.40 |
| 1:0:1310:U:P | 5:C:168:ARG:HH11 | 2.44 | 0.40 |
| 1:0:1457:U:H5 | 38:0:7859:HOH:O | 2.04 | 0.40 |
| 1:0:1494:A:H1' | 1:0:1495:C:C6 | 2.56 | 0.40 |
| 1:0:1574:C:H6 | 1:0:1574:C:O5' | 2.04 | 0.40 |
| 1:0:1642:A:N7 | 1:0:1643:C:C4 | 2.89 | 0.40 |
| 1:0:1657:A:H2' | 1:0:1658:A:C8 | 2.56 | 0.40 |
| 1:0:2064:U:H2' | 1:0:2065:C:H6 | 1.86 | 0.40 |
| 1:0:2344:G:H2' | 1:0:2344:G:N3 | 2.36 | 0.40 |
| 1:0:2361:A:H2' | 1:0:2362:A:O4' | 2.21 | 0.40 |
| 1:0:2547:C:OP2 | 4:B:5:ARG:NH1 | 2.54 | 0.40 |
| 1:0:535:G:O6 | 1:0:2064:U:C6 | 2.75 | 0.40 |
| 1:0:542:A:H2' | 1:0:543:G:O4' | 2.21 | 0.40 |
| 1:0:567:U:O5' | 1:0:567:U:H6 | 2.04 | 0.40 |
| 1:0:699:C:H6 | 1:0:744:G:O4' | 2.03 | 0.40 |
| 1:0:2453:G:O3' | 13:L:50:GLY:HA2 | 2.21 | 0.40 |
| 26:Y:134:HIS:H | 26:Y:134:HIS:CD2 | 2.38 | 0.40 |
| 1:0:1902:G:H2' | 1:0:1903:U:O4' | 2.21 | 0.40 |
| 1:0:2642:G:H2' | 1:0:2643:G:O4' | 2.22 | 0.40 |
| 1:0:2902:A:H4' | 1:0:2903:C:OP1 | 2.21 | 0.40 |
| 1:0:574:C:H2' | 1:0:575:G:O4' | 2.21 | 0.40 |
| 1:0:74:A:H2' | 1:0:75:U:C6 | 2.55 | 0.40 |
| 1:0:844:A:C6 | 1:0:882:A:C6 | 3.09 | 0.40 |
| 3:A:105:VAL:HG12 | 3:A:106:CYS:N | 2.36 | 0.40 |
| 6:D:25:MET:HE3 | 6:D:37:ALA:HB1 | 2.04 | 0.40 |
| 14:M:72:ALA:HB2 | 14:M:93:ARG:HG2 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 17:P:121:ASP:HB2 | 38:P:5891:HOH:O | 2.21 | 0.40 |
| 24:W:13:MET:CE | 24:W:18:GLN:HA | 2.49 | 0.40 |
| 24:W:65:VAL:HG12 | 24:W:116:LEU:HD13 | 2.04 | 0.40 |
| 1:0:1268:C:O2' | 26:Y:169:ARG:HB2 | 2.21 | 0.40 |
| 26:Y:177:LYS:HD3 | 26:Y:181:GLY:O | 2.22 | 0.40 |
| 1:0:1006:A:N1 | 1:0:2311:A:H1' | 2.37 | 0.40 |
| 1:0:1087:G:H4' | 1:0:1088:A:OP1 | 2.22 | 0.40 |
| 1:0:1180:U:O2' | 31:I:92:PRO:HD2 | 2.21 | 0.40 |
| 1:0:1189:A:C3' | 38:0:7666:HOH:O | 2.62 | 0.40 |
| 1:0:1309:U:H2' | 1:0:1310:U:O4' | 2.21 | 0.40 |
| 1:0:1741:U:H3' | 38:0:9763:HOH:O | 2.20 | 0.40 |
| 1:0:243:A:H2 | 1:0:274:G:N3 | 2.19 | 0.40 |
| 1:0:260:C:C4 | 1:0:261:A:C5 | 3.10 | 0.40 |
| 1:0:2673:U:C4 | 1:0:2674:G:C6 | 3.10 | 0.40 |
| 1:0:2754:G:HO2' | 1:0:2755:G:H5' | 1.85 | 0.40 |
| 1:0:485:A:HO2' | 1:0:487:G:H8 | 1.68 | 0.40 |
| 1:0:517:U:H2' | 1:0:518:G:H5' | 2.03 | 0.40 |
| 1:0:559:U:C6 | 1:0:559:U:C4' | 3.04 | 0.40 |
| 1:0:705:C:C2' | 1:0:705:C:O2 | 2.70 | 0.40 |
| 2:9:3110:G:C2' | 2:9:3111:U:H5' | 2.51 | 0.40 |
| 5:C:175:LYS:HD2 | 5:C:187:ARG:HB3 | 2.04 | 0.40 |
| 1:0:1308:A:O4' | 5:C:226:GLY:HA3 | 2.21 | 0.40 |
| 1:0:474:C:O3' | 5:C:73:LEU:HD21 | 2.22 | 0.40 |
| 6:D:25:MET:CE | 6:D:37:ALA:HB1 | 2.51 | 0.40 |
| 6:D:64:ARG:HB3 | 6:D:67:ASP:OD2 | 2.22 | 0.40 |
| 12:K:62:PRO:HG3 | 12:K:65:ARG:NH2 | 2.37 | 0.40 |
| 16:O:14:LEU:HB3 | 16:O:26:TRP:O | 2.21 | 0.40 |
| 16:O:45:LEU:CD1 | 16:O:88:LYS:HD2 | 2.51 | 0.40 |
| 1:0:1705:C:P | 17:P:59:ARG:HH12 | 2.45 | 0.40 |
| 38:9:466:HOH:O | 18:Q:25:PRO:HB3 | 2.21 | 0.40 |
| 25:X:30:MET:CE | 25:X:58:ALA:HB3 | 2.52 | 0.40 |
| 1:0:1329:A:H5'' | 38:0:3790:HOH:O | 2.20 | 0.40 |
| 1:0:1334:C:H2' | 1:0:1335:C:H6 | 1.86 | 0.40 |
| 1:0:1453:G:H2' | 1:0:1454:U:O4' | 2.22 | 0.40 |
| 1:0:1544:U:H2' | 1:0:1545:C:H6 | 1.87 | 0.40 |
| 1:0:1617:C:C4 | 1:0:1643:C:H4' | 2.57 | 0.40 |
| 1:0:160:A:C4 | 1:0:177:A:C2 | 3.09 | 0.40 |
| 1:0:245:C:H2' | 1:0:246:G:H5' | 2.04 | 0.40 |
| 1:0:2739:A:C6 | 1:0:2740:G:C5 | 3.09 | 0.40 |
| 1:0:820:G:H5' | 1:0:821:U:C5' | 2.51 | 0.40 |
| 29:2:49:GLU:HB2 | 38:2:131:HOH:O | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 7:E:6:GLU:HA | 7:E:46:THR:HG22 | 2.03 | 0.40 |
| 8:F:58:GLU:HA | 8:F:61:MET:CE | 2.47 | 0.40 |
| 14:M:28:GLN:HA | 14:M:31:TRP:HB2 | 2.03 | 0.40 |
| 17:P:40:VAL:O | 17:P:44:VAL:HG23 | 2.22 | 0.40 |
| 19:R:17:MET:HE3 | 19:R:19:ARG:HH21 | 1.86 | 0.40 |
| 23:V:39:ALA:O | 23:V:41:GLU:N | 2.51 | 0.40 |
| 25:X:8:ARG:NH1 | 38:X:2479:HOH:O | 2.49 | 0.40 |
| 27:Z:49:ARG:NH2 | 27:Z:52:THR:HA | 2.37 | 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 | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 3 | A | 235/240 (98%) | 212 (90%) | 21 (9%) | 2 (1%) | 17 | 48 |
| 4 | B | 335/338 (99%) | 310 (92%) | 21 (6%) | 4 (1%) | 13 | 40 |
| 5 | C | 244/246 (99%) | 224 (92%) | 18 (7%) | 2 (1%) | 19 | 51 |
| 6 | D | 134/177 (76%) | 113 (84%) | 18 (13%) | 3 (2%) | 6 | 24 |
| 7 | E | 170/178 (96%) | 163 (96%) | 6 (4%) | 1 (1%) | 25 | 58 |
| 8 | F | 117/120 (98%) | 103 (88%) | 11 (9%) | 3 (3%) | 5 | 20 |
| 9 | G | 25/348 (7%) | 25 (100%) | 0 | 0 | 100 | 100 |
| 10 | H | 156/171 (91%) | 142 (91%) | 11 (7%) | 3 (2%) | 8 | 28 |
| 11 | J | 140/145 (97%) | 129 (92%) | 9 (6%) | 2 (1%) | 11 | 36 |
| 12 | K | 130/132 (98%) | 122 (94%) | 8 (6%) | 0 | 100 | 100 |
| 13 | L | 141/165 (86%) | 121 (86%) | 20 (14%) | 0 | 100 | 100 |
| 14 | M | 192/194 (99%) | 183 (95%) | 9 (5%) | 0 | 100 | 100 |
| 15 | N | 184/187 (98%) | 167 (91%) | 13 (7%) | 4 (2%) | 6 | 24 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 16 | O | 113/116 (97%) | 110 (97%) | 3 (3%) | 0 | 100 | 100 |
| 17 | P | 141/149 (95%) | 136 (96%) | 4 (3%) | 1 (1%) | 22 | 54 |
| 18 | Q | 93/96 (97%) | 86 (92%) | 6 (6%) | 1 (1%) | 14 | 42 |
| 19 | R | 148/155 (96%) | 137 (93%) | 11 (7%) | 0 | 100 | 100 |
| 20 | S | 79/85 (93%) | 76 (96%) | 3 (4%) | 0 | 100 | 100 |
| 21 | T | 117/120 (98%) | 109 (93%) | 7 (6%) | 1 (1%) | 17 | 48 |
| 22 | U | 51/66 (77%) | 48 (94%) | 3 (6%) | 0 | 100 | 100 |
| 23 | V | 63/71 (89%) | 58 (92%) | 5 (8%) | 0 | 100 | 100 |
| 24 | W | 152/154 (99%) | 150 (99%) | 0 | 2 (1%) | 12 | 37 |
| 25 | X | 80/92 (87%) | 72 (90%) | 7 (9%) | 1 (1%) | 12 | 37 |
| 26 | Y | 140/241 (58%) | 140 (100%) | 0 | 0 | 100 | 100 |
| 27 | Z | 71/73 (97%) | 60 (84%) | 9 (13%) | 2 (3%) | 5 | 19 |
| 28 | 1 | 54/57 (95%) | 52 (96%) | 2 (4%) | 0 | 100 | 100 |
| 29 | 2 | 42/50 (84%) | 41 (98%) | 1 (2%) | 0 | 100 | 100 |
| 30 | 3 | 90/92 (98%) | 85 (94%) | 5 (6%) | 0 | 100 | 100 |
| 31 | I | 68/161 (42%) | 62 (91%) | 6 (9%) | 0 | 100 | 100 |
| All | All | 3705/4419 (84%) | 3436 (93%) | 237 (6%) | 32 (1%) | 17 | 48 |

All (32) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | F | 101 | ALA |
| 10 | H | 166 | SER |
| 11 | J | 5 | GLU |
| 15 | N | 154 | LEU |
| 15 | N | 183 | ASP |
| 15 | N | 184 | ILE |
| 3 | A | 34 | ASP |
| 4 | B | 34 | GLY |
| 4 | B | 169 | GLY |
| 6 | D | 27 | ILE |
| 6 | D | 137 | PRO |
| 6 | D | 173 | GLU |
| 8 | F | 44 | SER |
| 24 | W | 49 | ASN |
| 3 | A | 37 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15 | N | 139 | TRP |
| 27 | Z | 42 | CYS |
| 5 | C | 79 | ARG |
| 10 | H | 16 | ARG |
| 10 | H | 168 | ALA |
| 17 | P | 117 | SER |
| 25 | X | 70 | ILE |
| 4 | B | 2 | GLN |
| 5 | C | 8 | LEU |
| 8 | F | 64 | PRO |
| 21 | T | 44 | ALA |
| 24 | W | 77 | ALA |
| 4 | B | 306 | LYS |
| 7 | E | 44 | GLY |
| 11 | J | 89 | HIS |
| 18 | Q | 18 | PRO |
| 27 | Z | 43 | GLY |

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 | |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 3 | A | 179/182 (98%) | 170 (95%) | 9 (5%) | 24 | 57 |
| 4 | B | 282/283 (100%) | 268 (95%) | 14 (5%) | 24 | 57 |
| 5 | C | 193/193 (100%) | 178 (92%) | 15 (8%) | 12 | 34 |
| 6 | D | 117/148 (79%) | 115 (98%) | 2 (2%) | 60 | 86 |
| 7 | E | 152/156 (97%) | 149 (98%) | 3 (2%) | 55 | 82 |
| 8 | F | 93/94 (99%) | 89 (96%) | 4 (4%) | 29 | 62 |
| 9 | G | 27/283 (10%) | 27 (100%) | 0 | 100 | 100 |
| 10 | H | 132/138 (96%) | 126 (96%) | 6 (4%) | 27 | 61 |
| 11 | J | 118/121 (98%) | 110 (93%) | 8 (7%) | 16 | 42 |
| 12 | K | 106/106 (100%) | 104 (98%) | 2 (2%) | 57 | 84 |
| 13 | L | 113/127 (89%) | 107 (95%) | 6 (5%) | 22 | 54 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 14 | M | 158/158 (100%) | 149 (94%) | 9 (6%) | 20 | 51 |
| 15 | N | 149/150 (99%) | 146 (98%) | 3 (2%) | 55 | 82 |
| 16 | O | 93/94 (99%) | 92 (99%) | 1 (1%) | 73 | 92 |
| 17 | P | 113/117 (97%) | 109 (96%) | 4 (4%) | 36 | 70 |
| 18 | Q | 79/80 (99%) | 78 (99%) | 1 (1%) | 69 | 90 |
| 19 | R | 117/122 (96%) | 113 (97%) | 4 (3%) | 37 | 71 |
| 20 | S | 71/74 (96%) | 70 (99%) | 1 (1%) | 67 | 89 |
| 21 | T | 105/106 (99%) | 99 (94%) | 6 (6%) | 20 | 51 |
| 22 | U | 44/52 (85%) | 43 (98%) | 1 (2%) | 50 | 80 |
| 23 | V | 51/57 (90%) | 49 (96%) | 2 (4%) | 32 | 66 |
| 24 | W | 130/130 (100%) | 124 (95%) | 6 (5%) | 27 | 60 |
| 25 | X | 66/74 (89%) | 61 (92%) | 5 (8%) | 13 | 36 |
| 26 | Y | 120/196 (61%) | 114 (95%) | 6 (5%) | 24 | 57 |
| 27 | Z | 60/60 (100%) | 60 (100%) | 0 | 100 | 100 |
| 28 | 1 | 46/47 (98%) | 45 (98%) | 1 (2%) | 52 | 81 |
| 29 | 2 | 42/46 (91%) | 40 (95%) | 2 (5%) | 25 | 58 |
| 30 | 3 | 79/79 (100%) | 78 (99%) | 1 (1%) | 69 | 90 |
| 31 | I | 58/129 (45%) | 56 (97%) | 2 (3%) | 37 | 71 |
| All | All | 3093/3602 (86%) | 2969 (96%) | 124 (4%) | 31 | 65 |

All (124) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | A | 3 | ARG |
| 3 | A | 36 | ASP |
| 3 | A | 69 | LEU |
| 3 | A | 94 | LEU |
| 3 | A | 120 | ARG |
| 3 | A | 131 | HIS |
| 3 | A | 153 | ARG |
| 3 | A | 179 | MET |
| 3 | A | 217 | ARG |
| 4 | B | 7 | ARG |
| 4 | B | 11 | LEU |
| 4 | B | 27 | ASN |
| 4 | B | 33 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | B | 56 | ASP |
| 4 | B | 97 | LEU |
| 4 | B | 98 | THR |
| 4 | B | 149 | ASP |
| 4 | B | 162 | MET |
| 4 | B | 175 | LEU |
| 4 | B | 195 | ARG |
| 4 | B | 254 | GLN |
| 4 | B | 257 | THR |
| 4 | B | 312 | ARG |
| 5 | C | 2 | GLN |
| 5 | C | 27 | ARG |
| 5 | C | 67 | GLN |
| 5 | C | 76 | ARG |
| 5 | C | 91 | PRO |
| 5 | C | 94 | THR |
| 5 | C | 115 | LEU |
| 5 | C | 136 | VAL |
| 5 | C | 162 | VAL |
| 5 | C | 187 | ARG |
| 5 | C | 214 | THR |
| 5 | C | 222 | ASP |
| 5 | C | 223 | LEU |
| 5 | C | 236 | THR |
| 5 | C | 240 | LEU |
| 6 | D | 61 | PHE |
| 6 | D | 149 | ARG |
| 7 | E | 16 | ASP |
| 7 | E | 86 | VAL |
| 7 | E | 102 | VAL |
| 8 | F | 12 | LEU |
| 8 | F | 24 | ARG |
| 8 | F | 46 | GLU |
| 8 | F | 103 | GLU |
| 10 | H | 59 | HIS |
| 10 | H | 62 | LEU |
| 10 | H | 84 | LYS |
| 10 | H | 96 | ARG |
| 10 | H | 119 | LYS |
| 10 | H | 154 | TYR |
| 11 | J | 46 | ILE |
| 11 | J | 52 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | J | 74 | ARG |
| 11 | J | 79 | PHE |
| 11 | J | 93 | ARG |
| 11 | J | 107 | ASN |
| 11 | J | 120 | SER |
| 11 | J | 132 | LEU |
| 12 | K | 10 | GLN |
| 12 | K | 132 | VAL |
| 13 | L | 30 | ARG |
| 13 | L | 35 | ARG |
| 13 | L | 51 | PHE |
| 13 | L | 99 | GLU |
| 13 | L | 101 | ASP |
| 13 | L | 140 | VAL |
| 14 | M | 10 | ASP |
| 14 | M | 46 | LEU |
| 14 | M | 68 | ARG |
| 14 | M | 75 | ARG |
| 14 | M | 81 | ARG |
| 14 | M | 93 | ARG |
| 14 | M | 99 | ARG |
| 14 | M | 116 | ASN |
| 14 | M | 164 | THR |
| 15 | N | 26 | LEU |
| 15 | N | 49 | THR |
| 15 | N | 138 | ASP |
| 16 | O | 43 | VAL |
| 17 | P | 21 | VAL |
| 17 | P | 52 | LYS |
| 17 | P | 91 | LYS |
| 17 | P | 98 | ILE |
| 18 | Q | 95 | GLU |
| 19 | R | 13 | THR |
| 19 | R | 82 | GLU |
| 19 | R | 132 | ARG |
| 19 | R | 143 | VAL |
| 20 | S | 72 | ASP |
| 21 | T | 39 | ASN |
| 21 | T | 48 | VAL |
| 21 | T | 73 | HIS |
| 21 | T | 89 | ARG |
| 21 | T | 96 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21 | T | 117 | ASP |
| 22 | U | 47 | ARG |
| 23 | V | 12 | THR |
| 23 | V | 65 | ASP |
| 24 | W | 26 | ILE |
| 24 | W | 35 | VAL |
| 24 | W | 73 | LEU |
| 24 | W | 109 | GLU |
| 24 | W | 142 | ASP |
| 24 | W | 146 | ILE |
| 25 | X | 15 | ARG |
| 25 | X | 27 | ASP |
| 25 | X | 52 | PRO |
| 25 | X | 72 | VAL |
| 25 | X | 82 | GLU |
| 26 | Y | 154 | ARG |
| 26 | Y | 189 | ASN |
| 26 | Y | 200 | THR |
| 26 | Y | 203 | VAL |
| 26 | Y | 204 | ARG |
| 26 | Y | 220 | GLU |
| 28 | 1 | 47 | ASP |
| 29 | 2 | 18 | ASN |
| 29 | 2 | 31 | ARG |
| 30 | 3 | 3 | MET |
| 31 | I | 87 | THR |
| 31 | I | 100 | LEU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | A | 47 | HIS |
| 3 | A | 176 | HIS |
| 3 | A | 199 | HIS |
| 4 | B | 27 | ASN |
| 4 | B | 145 | HIS |
| 4 | B | 238 | ASN |
| 4 | B | 256 | GLN |
| 4 | B | 260 | HIS |
| 4 | B | 320 | GLN |
| 4 | B | 332 | ASN |
| 5 | C | 129 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | D | 85 | GLN |
| 6 | D | 103 | ASN |
| 6 | D | 133 | ASN |
| 7 | E | 119 | HIS |
| 7 | E | 143 | GLN |
| 9 | G | 17 | GLN |
| 9 | G | 64 | ASN |
| 10 | H | 46 | GLN |
| 10 | H | 56 | GLN |
| 10 | H | 59 | HIS |
| 10 | H | 170 | ASN |
| 11 | J | 52 | GLN |
| 11 | J | 107 | ASN |
| 12 | K | 10 | GLN |
| 12 | K | 42 | ASN |
| 13 | L | 18 | HIS |
| 13 | L | 41 | HIS |
| 13 | L | 42 | ASN |
| 13 | L | 116 | HIS |
| 14 | M | 24 | GLN |
| 14 | M | 58 | GLN |
| 14 | M | 137 | ASN |
| 14 | M | 170 | ASN |
| 15 | N | 21 | HIS |
| 15 | N | 107 | ASN |
| 17 | P | 50 | GLN |
| 17 | P | 73 | HIS |
| 17 | P | 118 | GLN |
| 18 | Q | 40 | HIS |
| 19 | R | 94 | ASN |
| 19 | R | 98 | ASN |
| 19 | R | 117 | HIS |
| 19 | R | 123 | GLN |
| 20 | S | 9 | HIS |
| 20 | S | 53 | ASN |
| 21 | T | 39 | ASN |
| 22 | U | 39 | ASN |
| 22 | U | 48 | ASN |
| 23 | V | 60 | GLN |
| 24 | W | 28 | HIS |
| 24 | W | 110 | GLN |
| 24 | W | 119 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24 | W | 125 | HIS |
| 24 | W | 141 | HIS |
| 25 | X | 23 | HIS |
| 26 | Y | 134 | HIS |
| 26 | Y | 149 | GLN |
| 26 | Y | 188 | HIS |
| 26 | Y | 189 | ASN |
| 28 | 1 | 8 | GLN |
| 28 | 1 | 16 | HIS |
| 28 | 1 | 28 | HIS |
| 29 | 2 | 18 | ASN |
| 29 | 2 | 41 | HIS |
| 29 | 2 | 45 | ASN |
| 30 | 3 | 2 | GLN |
| 30 | 3 | 30 | GLN |
| 30 | 3 | 48 | ASN |
| 31 | I | 93 | GLN |
| 31 | I | 107 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | 0 | 2746/2922 (93%) | 241 (8%) | 33 (1%) |
| 2 | 9 | 121/122 (99%) | 18 (14%) | 1 (0%) |
| All | All | 2867/3044 (94%) | 259 (9%) | 34 (1%) |

All (259) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 0 | 11 | A |
| 1 | 0 | 31 | C |
| 1 | 0 | 67 | A |
| 1 | 0 | 69 | A |
| 1 | 0 | 70 | A |
| 1 | 0 | 71 | G |
| 1 | 0 | 87 | C |
| 1 | 0 | 88 | G |
| 1 | 0 | 114 | A |
| 1 | 0 | 115 | U |
| 1 | 0 | 120 | A |
| 1 | 0 | 130 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 0 | 139 | C |
| 1 | 0 | 141 | C |
| 1 | 0 | 151 | A |
| 1 | 0 | 166 | A |
| 1 | 0 | 185 | G |
| 1 | 0 | 186 | A |
| 1 | 0 | 191 | A |
| 1 | 0 | 192 | A |
| 1 | 0 | 219 | G |
| 1 | 0 | 237 | G |
| 1 | 0 | 271 | C |
| 1 | 0 | 272 | A |
| 1 | 0 | 273 | G |
| 1 | 0 | 283 | U |
| 1 | 0 | 284 | C |
| 1 | 0 | 285 | A |
| 1 | 0 | 308 | U |
| 1 | 0 | 309 | C |
| 1 | 0 | 336 | G |
| 1 | 0 | 337 | A |
| 1 | 0 | 345 | G |
| 1 | 0 | 358 | G |
| 1 | 0 | 381 | G |
| 1 | 0 | 397 | A |
| 1 | 0 | 417 | G |
| 1 | 0 | 461 | C |
| 1 | 0 | 487 | G |
| 1 | 0 | 498 | A |
| 1 | 0 | 510 | U |
| 1 | 0 | 511 | A |
| 1 | 0 | 514 | G |
| 1 | 0 | 537 | G |
| 1 | 0 | 538 | C |
| 1 | 0 | 539 | G |
| 1 | 0 | 542 | A |
| 1 | 0 | 545 | G |
| 1 | 0 | 553 | G |
| 1 | 0 | 559 | U |
| 1 | 0 | 588 | G |
| 1 | 0 | 604 | G |
| 1 | 0 | 620 | A |
| 1 | 0 | 632 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 0 | 644 | G |
| 1 | 0 | 660 | A |
| 1 | 0 | 688 | A |
| 1 | 0 | 701 | U |
| 1 | 0 | 759 | C |
| 1 | 0 | 777 | U |
| 1 | 0 | 809 | G |
| 1 | 0 | 821 | U |
| 1 | 0 | 835 | U |
| 1 | 0 | 840 | U |
| 1 | 0 | 857 | A |
| 1 | 0 | 858 | U |
| 1 | 0 | 868 | G |
| 1 | 0 | 869 | G |
| 1 | 0 | 872 | U |
| 1 | 0 | 875 | A |
| 1 | 0 | 877 | G |
| 1 | 0 | 878 | G |
| 1 | 0 | 882 | A |
| 1 | 0 | 884 | C |
| 1 | 0 | 885 | G |
| 1 | 0 | 898 | G |
| 1 | 0 | 905 | C |
| 1 | 0 | 920 | C |
| 1 | 0 | 921 | G |
| 1 | 0 | 923 | A |
| 1 | 0 | 953 | G |
| 1 | 0 | 960 | G |
| 1 | 0 | 961 | A |
| 1 | 0 | 1003 | U |
| 1 | 0 | 1006 | A |
| 1 | 0 | 1008 | C |
| 1 | 0 | 1029 | U |
| 1 | 0 | 1045 | G |
| 1 | 0 | 1059 | G |
| 1 | 0 | 1060 | C |
| 1 | 0 | 1072 | G |
| 1 | 0 | 1081 | A |
| 1 | 0 | 1087 | G |
| 1 | 0 | 1088 | A |
| 1 | 0 | 1109 | U |
| 1 | 0 | 1110 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 0 | 1119 | G |
| 1 | 0 | 1130 | U |
| 1 | 0 | 1137 | G |
| 1 | 0 | 1151 | G |
| 1 | 0 | 1164 | U |
| 1 | 0 | 1165 | G |
| 1 | 0 | 1166 | A |
| 1 | 0 | 1174 | A |
| 1 | 0 | 1175 | G |
| 1 | 0 | 1185 | U |
| 1 | 0 | 1192 | A |
| 1 | 0 | 1193 | A |
| 1 | 0 | 1205 | U |
| 1 | 0 | 1206 | U |
| 1 | 0 | 1216 | G |
| 1 | 0 | 1237 | U |
| 1 | 0 | 1238 | C |
| 1 | 0 | 1239 | G |
| 1 | 0 | 1279 | U |
| 1 | 0 | 1289 | C |
| 1 | 0 | 1331 | A |
| 1 | 0 | 1342 | C |
| 1 | 0 | 1353 | C |
| 1 | 0 | 1360 | C |
| 1 | 0 | 1377 | C |
| 1 | 0 | 1407 | A |
| 1 | 0 | 1451 | C |
| 1 | 0 | 1474 | C |
| 1 | 0 | 1492 | A |
| 1 | 0 | 1505 | U |
| 1 | 0 | 1506 | U |
| 1 | 0 | 1524 | U |
| 1 | 0 | 1525 | G |
| 1 | 0 | 1526 | A |
| 1 | 0 | 1559 | A |
| 1 | 0 | 1564 | C |
| 1 | 0 | 1580 | A |
| 1 | 0 | 1592 | G |
| 1 | 0 | 1625 | U |
| 1 | 0 | 1626 | A |
| 1 | 0 | 1633 | C |
| 1 | 0 | 1634 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 0 | 1656 | A |
| 1 | 0 | 1667 | A |
| 1 | 0 | 1682 | A |
| 1 | 0 | 1684 | A |
| 1 | 0 | 1685 | A |
| 1 | 0 | 1692 | C |
| 1 | 0 | 1701 | A |
| 1 | 0 | 1722 | U |
| 1 | 0 | 1723 | G |
| 1 | 0 | 1725 | C |
| 1 | 0 | 1730 | G |
| 1 | 0 | 1731 | C |
| 1 | 0 | 1732 | A |
| 1 | 0 | 1742 | A |
| 1 | 0 | 1752 | G |
| 1 | 0 | 1778 | A |
| 1 | 0 | 1798 | C |
| 1 | 0 | 1819 | G |
| 1 | 0 | 1820 | G |
| 1 | 0 | 1829 | A |
| 1 | 0 | 1856 | C |
| 1 | 0 | 1879 | U |
| 1 | 0 | 1919 | A |
| 1 | 0 | 1942 | A |
| 1 | 0 | 1971 | G |
| 1 | 0 | 1973 | A |
| 1 | 0 | 1979 | G |
| 1 | 0 | 1996 | U |
| 1 | 0 | 2006 | C |
| 1 | 0 | 2008 | U |
| 1 | 0 | 2011 | A |
| 1 | 0 | 2012 | U |
| 1 | 0 | 2013 | G |
| 1 | 0 | 2033 | G |
| 1 | 0 | 2034 | U |
| 1 | 0 | 2064 | U |
| 1 | 0 | 2072 | G |
| 1 | 0 | 2073 | G |
| 1 | 0 | 2074 | A |
| 1 | 0 | 2096 | A |
| 1 | 0 | 2101 | A |
| 1 | 0 | 2102 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 0 | 2110 | G |
| 1 | 0 | 2238 | A |
| 1 | 0 | 2243 | C |
| 1 | 0 | 2258 | A |
| 1 | 0 | 2271 | G |
| 1 | 0 | 2272 | G |
| 1 | 0 | 2291 | A |
| 1 | 0 | 2317 | C |
| 1 | 0 | 2321 | A |
| 1 | 0 | 2354 | A |
| 1 | 0 | 2361 | A |
| 1 | 0 | 2369 | A |
| 1 | 0 | 2379 | G |
| 1 | 0 | 2422 | U |
| 1 | 0 | 2462 | G |
| 1 | 0 | 2465 | A |
| 1 | 0 | 2467 | A |
| 1 | 0 | 2468 | A |
| 1 | 0 | 2469 | A |
| 1 | 0 | 2476 | C |
| 1 | 0 | 2483 | A |
| 1 | 0 | 2507 | G |
| 1 | 0 | 2511 | A |
| 1 | 0 | 2526 | C |
| 1 | 0 | 2527 | U |
| 1 | 0 | 2533 | C |
| 1 | 0 | 2537 | G |
| 1 | 0 | 2541 | U |
| 1 | 0 | 2553 | A |
| 1 | 0 | 2564 | G |
| 1 | 0 | 2589 | U |
| 1 | 0 | 2601 | A |
| 1 | 0 | 2602 | G |
| 1 | 0 | 2608 | C |
| 1 | 0 | 2613 | G |
| 1 | 0 | 2634 | G |
| 1 | 0 | 2638 | G |
| 1 | 0 | 2649 | A |
| 1 | 0 | 2650 | U |
| 1 | 0 | 2664 | A |
| 1 | 0 | 2681 | A |
| 1 | 0 | 2682 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 0 | 2719 | A |
| 1 | 0 | 2726 | U |
| 1 | 0 | 2747 | C |
| 1 | 0 | 2748 | G |
| 1 | 0 | 2749 | U |
| 1 | 0 | 2750 | G |
| 1 | 0 | 2762 | C |
| 1 | 0 | 2768 | A |
| 1 | 0 | 2786 | G |
| 1 | 0 | 2800 | A |
| 1 | 0 | 2811 | A |
| 1 | 0 | 2825 | C |
| 1 | 0 | 2850 | C |
| 1 | 0 | 2867 | G |
| 1 | 0 | 2876 | G |
| 1 | 0 | 2890 | A |
| 1 | 0 | 2896 | A |
| 1 | 0 | 2903 | C |
| 1 | 0 | 2914 | A |
| 2 | 9 | 3002 | U |
| 2 | 9 | 3007 | G |
| 2 | 9 | 3014 | G |
| 2 | 9 | 3022 | G |
| 2 | 9 | 3023 | U |
| 2 | 9 | 3024 | U |
| 2 | 9 | 3025 | G |
| 2 | 9 | 3039 | U |
| 2 | 9 | 3040 | C |
| 2 | 9 | 3041 | C |
| 2 | 9 | 3043 | G |
| 2 | 9 | 3044 | A |
| 2 | 9 | 3052 | A |
| 2 | 9 | 3057 | A |
| 2 | 9 | 3066 | G |
| 2 | 9 | 3077 | A |
| 2 | 9 | 3114 | G |
| 2 | 9 | 3122 | C |

All (34) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 0 | 10 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 0 | 69 | A |
| 1 | 0 | 129 | A |
| 1 | 0 | 338 | C |
| 1 | 0 | 603 | A |
| 1 | 0 | 644 | G |
| 1 | 0 | 699 | C |
| 1 | 0 | 834 | G |
| 1 | 0 | 857 | A |
| 1 | 0 | 871 | G |
| 1 | 0 | 877 | G |
| 1 | 0 | 1080 | C |
| 1 | 0 | 1165 | G |
| 1 | 0 | 1232 | A |
| 1 | 0 | 1237 | U |
| 1 | 0 | 1246 | A |
| 1 | 0 | 1352 | A |
| 1 | 0 | 1377 | C |
| 1 | 0 | 1450 | C |
| 1 | 0 | 1474 | C |
| 1 | 0 | 1506 | U |
| 1 | 0 | 1563 | G |
| 1 | 0 | 1667 | A |
| 1 | 0 | 1685 | A |
| 1 | 0 | 1942 | A |
| 1 | 0 | 2313 | C |
| 1 | 0 | 2361 | A |
| 1 | 0 | 2467 | A |
| 1 | 0 | 2526 | C |
| 1 | 0 | 2536 | C |
| 1 | 0 | 2649 | A |
| 1 | 0 | 2718 | C |
| 1 | 0 | 2761 | A |
| 2 | 9 | 3065 | 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 | $\# Z > 2$ |
| 1 | PSU | 0 | 2621 | 1 | 17,21,22 | 1.64 | 3 (17%) | 20,30,33 | 5.46 | 4 (20%) |
| 1 | OMG | 0 | 2588 | 1 | 18,26,27 | 1.04 | 2 (11%) | 20,38,41 | 2.60 | 4 (20%) |
| 1 | UR3 | 0 | 2619 | 1 | 14,22,23 | 0.75 | 0 | 15,32,35 | 0.65 | 0 |
| 1 | OMU | 0 | 2587 | 1 | 14,22,23 | 0.95 | 1 (7%) | 14,31,34 | 1.19 | 1 (7%) |
| 1 | 1MA | 0 | 628 | 1 | 15,25,26 | 0.74 | 0 | 15,37,40 | 1.45 | 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 |
|-----|------|-------|------|------|---------|-----------|---------|
| 1 | PSU | 0 | 2621 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMG | 0 | 2588 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | UR3 | 0 | 2619 | 1 | - | 0/5/25/26 | 0/2/2/2 |
| 1 | OMU | 0 | 2587 | 1 | - | 0/7/27/28 | 0/2/2/2 |
| 1 | 1MA | 0 | 628 | 1 | - | 0/3/25/26 | 0/3/3/3 |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1 | 0 | 2621 | PSU | C5-C1' | -5.16 | 1.47 | 1.52 |
| 1 | 0 | 2588 | OMG | C6-N1 | 3.32 | 1.38 | 1.33 |
| 1 | 0 | 2621 | PSU | C2-N1 | 2.67 | 1.43 | 1.38 |
| 1 | 0 | 2621 | PSU | C4-N3 | 2.57 | 1.37 | 1.33 |
| 1 | 0 | 2587 | OMU | C4-N3 | 2.50 | 1.37 | 1.33 |
| 1 | 0 | 2588 | OMG | C8-N7 | -2.08 | 1.31 | 1.34 |

All (10) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 0 | 2621 | PSU | N1-C2-N3 | -17.33 | 114.65 | 128.43 |
| 1 | 0 | 2621 | PSU | C4-N3-C2 | 14.37 | 127.28 | 115.14 |
| 1 | 0 | 2588 | OMG | C5-C6-N1 | -8.62 | 111.64 | 123.43 |
| 1 | 0 | 2621 | PSU | C5-C4-N3 | -8.18 | 114.81 | 125.36 |
| 1 | 0 | 2588 | OMG | C6-N1-C2 | 5.86 | 125.24 | 115.93 |
| 1 | 0 | 628 | 1MA | C2-N3-C4 | -4.79 | 110.59 | 116.58 |
| 1 | 0 | 2587 | OMU | C5-C4-N3 | -3.95 | 114.61 | 123.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | 0 | 2588 | OMG | C2-N3-C4 | -3.16 | 111.75 | 115.36 |
| 1 | 0 | 2621 | PSU | C6-N1-C2 | 2.66 | 119.75 | 115.36 |
| 1 | 0 | 2588 | OMG | N3-C2-N1 | -2.50 | 123.89 | 127.22 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1 | 0 | 2587 | OMU | 1 | 0 |

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 233 ligands modelled in this entry, 232 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 32 | 13T | 0 | 9000 | - | 41,43,43 | 2.02 | 10 (24%) | 51,63,63 | 1.75 | 9 (17%) |

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 |
|-----|------|-------|------|------|---------|-------------|---------|
| 32 | 13T | 0 | 9000 | - | - | 15/73/81/81 | 0/1/2/2 |

All (10) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 32 | 0 | 9000 | 13T | C18-C19 | 7.20 | 1.56 | 1.47 |
| 32 | 0 | 9000 | 13T | C10-C9 | 3.89 | 1.57 | 1.51 |
| 32 | 0 | 9000 | 13T | O2-C1 | 3.33 | 1.29 | 1.21 |
| 32 | 0 | 9000 | 13T | O5-C5 | 3.27 | 1.26 | 1.21 |
| 32 | 0 | 9000 | 13T | C9-C8 | 3.21 | 1.40 | 1.33 |
| 32 | 0 | 9000 | 13T | O7-C11 | 2.98 | 1.26 | 1.21 |
| 32 | 0 | 9000 | 13T | C29-C16 | 2.69 | 1.55 | 1.52 |
| 32 | 0 | 9000 | 13T | C27-C10 | 2.37 | 1.57 | 1.54 |
| 32 | 0 | 9000 | 13T | C26-C8 | 2.25 | 1.54 | 1.50 |
| 32 | 0 | 9000 | 13T | O1-C1 | 2.11 | 1.37 | 1.33 |

All (9) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 32 | 0 | 9000 | 13T | C18-O11-C19 | 7.60 | 65.36 | 60.79 |
| 32 | 0 | 9000 | 13T | O4-C3-C4 | 4.13 | 115.61 | 105.83 |
| 32 | 0 | 9000 | 13T | O11-C18-C19 | -4.10 | 56.62 | 59.38 |
| 32 | 0 | 9000 | 13T | C27-C10-C9 | 2.56 | 113.14 | 110.75 |
| 32 | 0 | 9000 | 13T | O11-C19-C18 | -2.55 | 58.01 | 59.83 |
| 32 | 0 | 9000 | 13T | C7-C6-C5 | -2.21 | 106.74 | 109.48 |
| 32 | 0 | 9000 | 13T | C19-C20-C21 | -2.21 | 108.45 | 113.94 |
| 32 | 0 | 9000 | 13T | C29-O1-C1 | 2.15 | 121.09 | 116.84 |
| 32 | 0 | 9000 | 13T | O1-C1-O2 | 2.11 | 128.12 | 124.13 |

There are no chirality outliers.

All (15) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 32 | 0 | 9000 | 13T | C2-C3-O4-C32 |
| 32 | 0 | 9000 | 13T | C1-C2-C3-O4 |
| 32 | 0 | 9000 | 13T | O6-C7-C8-C9 |
| 32 | 0 | 9000 | 13T | O6-C7-C8-C26 |
| 32 | 0 | 9000 | 13T | C6-C7-C8-C9 |
| 32 | 0 | 9000 | 13T | C6-C7-C8-C26 |
| 32 | 0 | 9000 | 13T | C18-C19-C20-C21 |
| 32 | 0 | 9000 | 13T | O11-C19-C20-C21 |
| 32 | 0 | 9000 | 13T | O11-C19-C20-C31 |
| 32 | 0 | 9000 | 13T | C14-C15-C16-C29 |
| 32 | 0 | 9000 | 13T | O9-C15-C16-C17 |
| 32 | 0 | 9000 | 13T | C14-C15-C16-C17 |
| 32 | 0 | 9000 | 13T | O9-C15-C16-C29 |

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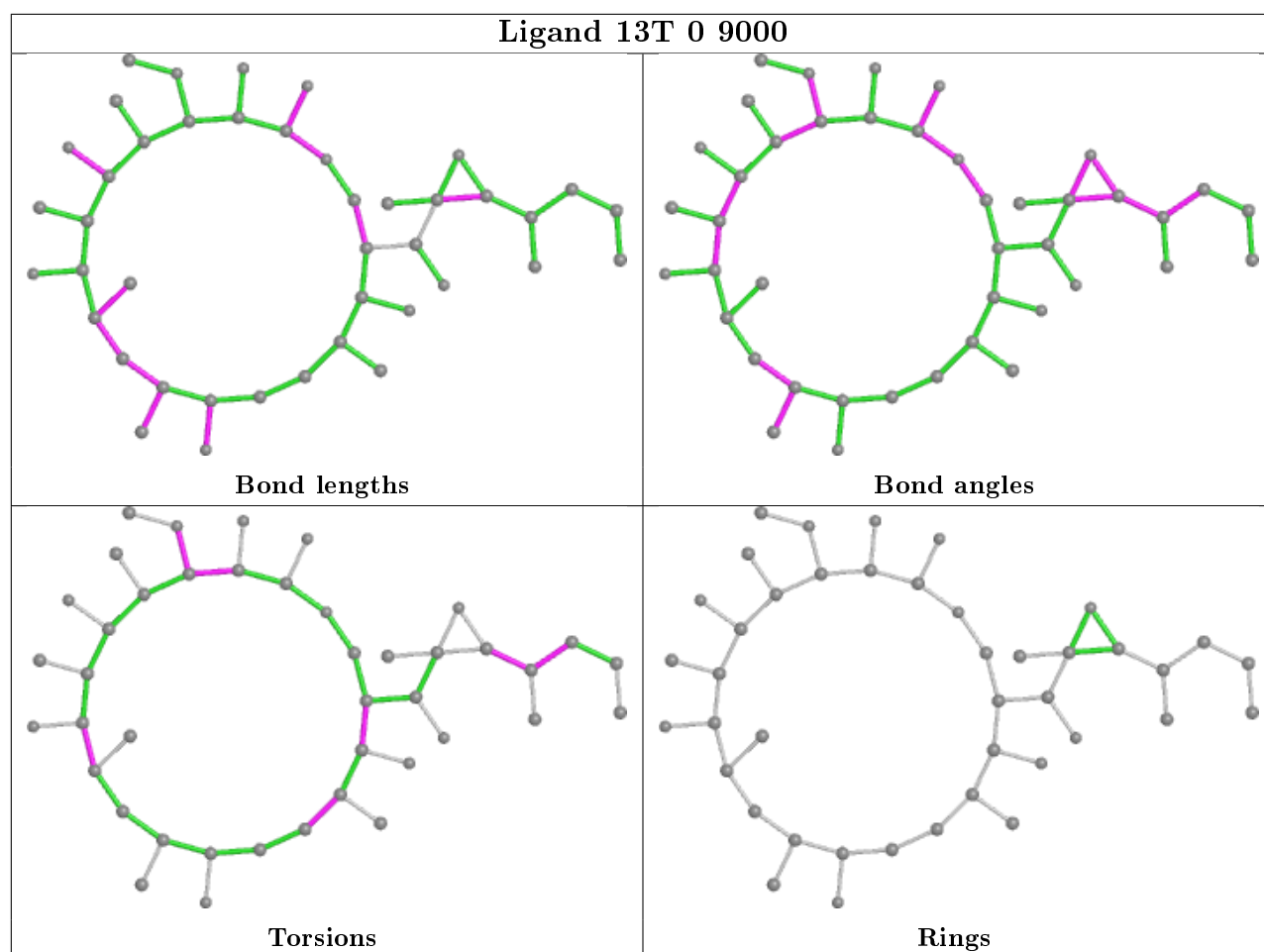
| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 32 | 0 | 9000 | 13T | C12-C13-C14-C15 |
| 32 | 0 | 9000 | 13T | C31-C20-C21-C22 |

There are no ring outliers.

1 monomer is involved in 24 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 32 | 0 | 9000 | 13T | 24 | 0 |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1 | 0 | 2749/2922 (94%) | -0.50 | 14 (0%) 91 91 | 23, 50, 93, 150 | 0 |
| 2 | 9 | 122/122 (100%) | -0.69 | 3 (2%) 57 55 | 43, 69, 91, 151 | 0 |
| 3 | A | 237/240 (98%) | -0.21 | 7 (2%) 50 45 | 32, 55, 86, 105 | 0 |
| 4 | B | 337/338 (99%) | -0.28 | 1 (0%) 94 94 | 33, 60, 82, 90 | 0 |
| 5 | C | 246/246 (100%) | -0.44 | 0 100 100 | 30, 50, 73, 82 | 0 |
| 6 | D | 140/177 (79%) | 1.26 | 39 (27%) 0 0 | 63, 103, 124, 130 | 0 |
| 7 | E | 172/178 (96%) | -0.13 | 2 (1%) 79 79 | 55, 73, 90, 96 | 0 |
| 8 | F | 119/120 (99%) | 0.38 | 6 (5%) 28 25 | 57, 74, 96, 106 | 0 |
| 9 | G | 29/348 (8%) | 0.78 | 4 (13%) 2 2 | 81, 94, 103, 103 | 0 |
| 10 | H | 160/171 (93%) | 0.44 | 15 (9%) 8 6 | 52, 67, 93, 100 | 0 |
| 11 | J | 142/145 (97%) | -0.36 | 1 (0%) 87 87 | 45, 56, 74, 94 | 0 |
| 12 | K | 132/132 (100%) | -0.44 | 1 (0%) 86 86 | 41, 54, 75, 81 | 0 |
| 13 | L | 145/165 (87%) | 0.27 | 12 (8%) 11 8 | 32, 71, 107, 118 | 0 |
| 14 | M | 194/194 (100%) | -0.52 | 0 100 100 | 36, 47, 60, 64 | 0 |
| 15 | N | 186/187 (99%) | 0.10 | 9 (4%) 30 27 | 50, 67, 110, 119 | 0 |
| 16 | O | 115/116 (99%) | -0.34 | 0 100 100 | 44, 59, 71, 76 | 0 |
| 17 | P | 143/149 (95%) | -0.30 | 1 (0%) 87 87 | 46, 60, 70, 75 | 0 |
| 18 | Q | 95/96 (98%) | -0.44 | 0 100 100 | 43, 52, 64, 72 | 0 |
| 19 | R | 150/155 (96%) | -0.43 | 0 100 100 | 38, 50, 68, 73 | 0 |
| 20 | S | 81/85 (95%) | -0.05 | 1 (1%) 79 79 | 52, 65, 81, 85 | 0 |
| 21 | T | 119/120 (99%) | -0.08 | 3 (2%) 57 55 | 47, 62, 83, 96 | 0 |
| 22 | U | 53/66 (80%) | -0.20 | 0 100 100 | 51, 61, 75, 81 | 0 |
| 23 | V | 65/71 (91%) | 1.28 | 14 (21%) 0 0 | 59, 79, 109, 114 | 0 |
| 24 | W | 154/154 (100%) | -0.39 | 0 100 100 | 42, 56, 70, 77 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 25 | X | 82/92 (89%) | 0.17 | 7 (8%) 10 8 | 52, 64, 87, 97 | 0 |
| 26 | Y | 142/241 (58%) | -0.57 | 2 (1%) 75 75 | 30, 51, 70, 86 | 0 |
| 27 | Z | 73/73 (100%) | 0.30 | 9 (12%) 4 3 | 58, 69, 80, 94 | 0 |
| 28 | 1 | 56/57 (98%) | -0.44 | 0 100 100 | 31, 37, 43, 51 | 0 |
| 29 | 2 | 46/50 (92%) | 0.16 | 3 (6%) 18 14 | 41, 69, 90, 99 | 0 |
| 30 | 3 | 92/92 (100%) | -0.35 | 0 100 100 | 42, 60, 71, 82 | 0 |
| 31 | I | 70/161 (43%) | 3.20 | 50 (71%) 0 0 | 109, 119, 135, 135 | 0 |
| All | All | 6646/7463 (89%) | -0.24 | 204 (3%) 49 44 | 23, 57, 100, 151 | 0 |

All (204) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 31 | I | 75 | THR | 9.2 |
| 31 | I | 79 | ILE | 8.7 |
| 23 | V | 1 | THR | 8.2 |
| 31 | I | 109 | ALA | 8.2 |
| 6 | D | 63 | ILE | 7.9 |
| 31 | I | 113 | HIS | 7.7 |
| 31 | I | 71 | GLY | 7.7 |
| 31 | I | 118 | SER | 7.5 |
| 13 | L | 100 | ALA | 6.7 |
| 23 | V | 40 | PRO | 6.7 |
| 23 | V | 39 | ALA | 6.7 |
| 31 | I | 96 | PHE | 6.7 |
| 15 | N | 166 | ALA | 6.6 |
| 23 | V | 43 | PRO | 6.4 |
| 13 | L | 97 | VAL | 6.4 |
| 31 | I | 93 | GLN | 5.9 |
| 31 | I | 102 | VAL | 5.8 |
| 25 | X | 88 | GLU | 5.8 |
| 31 | I | 137 | VAL | 5.6 |
| 6 | D | 57 | THR | 5.6 |
| 31 | I | 76 | ALA | 5.5 |
| 6 | D | 64 | ARG | 5.3 |
| 31 | I | 105 | VAL | 5.3 |
| 10 | H | 73 | LEU | 5.2 |
| 31 | I | 133 | THR | 5.0 |
| 25 | X | 80 | GLU | 4.8 |
| 23 | V | 38 | GLY | 4.7 |
| 31 | I | 103 | ASP | 4.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 31 | I | 107 | GLN | 4.5 |
| 6 | D | 85 | GLN | 4.5 |
| 31 | I | 77 | GLU | 4.5 |
| 31 | I | 85 | PHE | 4.4 |
| 6 | D | 18 | ILE | 4.4 |
| 27 | Z | 22 | SER | 4.3 |
| 20 | S | 81 | ILE | 4.3 |
| 6 | D | 90 | LEU | 4.3 |
| 4 | B | 1 | PRO | 4.3 |
| 27 | Z | 26 | VAL | 4.2 |
| 27 | Z | 11 | SER | 4.2 |
| 23 | V | 41 | GLU | 4.2 |
| 3 | A | 37 | VAL | 4.0 |
| 31 | I | 111 | GLN | 4.0 |
| 1 | 0 | 1172 | G | 4.0 |
| 31 | I | 83 | ALA | 4.0 |
| 13 | L | 102 | ASP | 3.9 |
| 31 | I | 84 | GLY | 3.8 |
| 29 | 2 | 39 | ARG | 3.8 |
| 8 | F | 17 | LEU | 3.7 |
| 31 | I | 115 | ASP | 3.7 |
| 31 | I | 116 | LEU | 3.7 |
| 27 | Z | 21 | VAL | 3.7 |
| 23 | V | 37 | GLY | 3.7 |
| 6 | D | 69 | ILE | 3.6 |
| 31 | I | 104 | GLN | 3.5 |
| 10 | H | 138 | CYS | 3.5 |
| 6 | D | 88 | LEU | 3.4 |
| 31 | I | 108 | ILE | 3.4 |
| 10 | H | 32 | LYS | 3.4 |
| 6 | D | 87 | ALA | 3.4 |
| 8 | F | 49 | PHE | 3.4 |
| 31 | I | 121 | LEU | 3.3 |
| 31 | I | 74 | PRO | 3.3 |
| 1 | 0 | 1198 | U | 3.3 |
| 9 | G | 27 | ILE | 3.2 |
| 31 | I | 132 | CYS | 3.2 |
| 29 | 2 | 35 | ARG | 3.2 |
| 6 | D | 23 | VAL | 3.2 |
| 27 | Z | 19 | GLY | 3.2 |
| 3 | A | 237 | GLY | 3.2 |
| 2 | 9 | 3001 | U | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 13 | L | 76 | LEU | 3.1 |
| 15 | N | 165 | ALA | 3.1 |
| 23 | V | 52 | ALA | 3.1 |
| 6 | D | 157 | LEU | 3.1 |
| 31 | I | 91 | GLU | 3.1 |
| 10 | H | 65 | SER | 3.1 |
| 25 | X | 71 | ARG | 3.1 |
| 2 | 9 | 3024 | U | 3.1 |
| 31 | I | 117 | LEU | 3.0 |
| 10 | H | 37 | GLN | 3.0 |
| 6 | D | 17 | ARG | 3.0 |
| 15 | N | 183 | ASP | 3.0 |
| 31 | I | 81 | ASP | 3.0 |
| 6 | D | 66 | GLY | 3.0 |
| 3 | A | 31 | LYS | 3.0 |
| 6 | D | 81 | GLU | 3.0 |
| 8 | F | 106 | ALA | 2.9 |
| 1 | 0 | 1199 | A | 2.9 |
| 15 | N | 185 | GLU | 2.9 |
| 29 | 2 | 49 | GLU | 2.9 |
| 31 | I | 126 | LYS | 2.8 |
| 6 | D | 95 | THR | 2.8 |
| 31 | I | 122 | THR | 2.8 |
| 7 | E | 45 | ASP | 2.8 |
| 23 | V | 34 | GLN | 2.8 |
| 1 | 0 | 1177 | A | 2.8 |
| 26 | Y | 108 | ASP | 2.8 |
| 1 | 0 | 960 | G | 2.8 |
| 21 | T | 116 | ASP | 2.8 |
| 31 | I | 97 | VAL | 2.8 |
| 31 | I | 110 | GLU | 2.8 |
| 9 | G | 23 | ILE | 2.7 |
| 10 | H | 79 | GLU | 2.7 |
| 13 | L | 101 | ASP | 2.7 |
| 6 | D | 135 | VAL | 2.7 |
| 6 | D | 53 | LYS | 2.7 |
| 31 | I | 72 | VAL | 2.7 |
| 9 | G | 25 | GLU | 2.7 |
| 6 | D | 45 | THR | 2.7 |
| 25 | X | 65 | ASN | 2.7 |
| 1 | 0 | 1171 | A | 2.7 |
| 6 | D | 134 | LEU | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 31 | I | 99 | ASP | 2.7 |
| 6 | D | 166 | ILE | 2.6 |
| 31 | I | 89 | SER | 2.6 |
| 31 | I | 138 | THR | 2.6 |
| 31 | I | 82 | GLU | 2.6 |
| 23 | V | 59 | ILE | 2.6 |
| 6 | D | 128 | LEU | 2.6 |
| 10 | H | 86 | THR | 2.6 |
| 1 | 0 | 497 | A | 2.6 |
| 10 | H | 171 | ALA | 2.6 |
| 1 | 0 | 970 | U | 2.6 |
| 13 | L | 80 | ASP | 2.6 |
| 10 | H | 146 | VAL | 2.5 |
| 13 | L | 105 | TYR | 2.5 |
| 6 | D | 40 | ILE | 2.5 |
| 6 | D | 101 | THR | 2.5 |
| 6 | D | 62 | ASP | 2.5 |
| 31 | I | 86 | GLU | 2.5 |
| 6 | D | 44 | ILE | 2.5 |
| 6 | D | 11 | HIS | 2.5 |
| 6 | D | 58 | VAL | 2.5 |
| 8 | F | 29 | VAL | 2.5 |
| 6 | D | 75 | LEU | 2.5 |
| 10 | H | 36 | LYS | 2.5 |
| 13 | L | 60 | GLU | 2.5 |
| 8 | F | 16 | ALA | 2.5 |
| 6 | D | 93 | LEU | 2.5 |
| 15 | N | 95 | ALA | 2.4 |
| 21 | T | 119 | ALA | 2.4 |
| 1 | 0 | 1169 | U | 2.4 |
| 31 | I | 78 | LEU | 2.4 |
| 13 | L | 106 | VAL | 2.4 |
| 25 | X | 74 | ALA | 2.4 |
| 25 | X | 10 | VAL | 2.4 |
| 26 | Y | 235 | GLU | 2.3 |
| 6 | D | 26 | GLY | 2.3 |
| 6 | D | 165 | PHE | 2.3 |
| 31 | I | 136 | GLY | 2.3 |
| 7 | E | 100 | ASP | 2.3 |
| 31 | I | 129 | VAL | 2.3 |
| 10 | H | 29 | ALA | 2.3 |
| 6 | D | 74 | THR | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 6 | D | 104 | PHE | 2.3 |
| 6 | D | 129 | ASP | 2.3 |
| 3 | A | 35 | GLY | 2.2 |
| 21 | T | 118 | SER | 2.2 |
| 31 | I | 135 | LEU | 2.2 |
| 23 | V | 8 | ILE | 2.2 |
| 6 | D | 158 | ASN | 2.2 |
| 10 | H | 63 | GLU | 2.2 |
| 6 | D | 170 | TYR | 2.2 |
| 13 | L | 149 | ARG | 2.2 |
| 1 | 0 | 2637 | A | 2.2 |
| 2 | 9 | 3023 | U | 2.2 |
| 17 | P | 49 | ILE | 2.2 |
| 6 | D | 98 | PHE | 2.2 |
| 31 | I | 80 | LYS | 2.2 |
| 15 | N | 68 | GLU | 2.2 |
| 27 | Z | 20 | ARG | 2.2 |
| 6 | D | 86 | THR | 2.2 |
| 15 | N | 178 | THR | 2.2 |
| 10 | H | 81 | GLY | 2.2 |
| 10 | H | 74 | ILE | 2.2 |
| 3 | A | 82 | VAL | 2.2 |
| 23 | V | 3 | LEU | 2.1 |
| 6 | D | 27 | ILE | 2.1 |
| 12 | K | 119 | GLN | 2.1 |
| 27 | Z | 34 | ASN | 2.1 |
| 23 | V | 36 | ALA | 2.1 |
| 31 | I | 92 | PRO | 2.1 |
| 23 | V | 58 | THR | 2.1 |
| 31 | I | 100 | LEU | 2.1 |
| 15 | N | 137 | ALA | 2.1 |
| 1 | 0 | 1202 | A | 2.1 |
| 13 | L | 81 | VAL | 2.1 |
| 13 | L | 96 | VAL | 2.1 |
| 27 | Z | 25 | ARG | 2.0 |
| 11 | J | 70 | PHE | 2.0 |
| 1 | 0 | 282 | C | 2.0 |
| 10 | H | 34 | GLY | 2.0 |
| 31 | I | 88 | GLY | 2.0 |
| 31 | I | 112 | LYS | 2.0 |
| 25 | X | 72 | VAL | 2.0 |
| 27 | Z | 24 | ARG | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 3 | A | 36 | ASP | 2.0 |
| 3 | A | 99 | ILE | 2.0 |
| 8 | F | 75 | ILE | 2.0 |
| 1 | 0 | 1173 | A | 2.0 |
| 15 | N | 138 | ASP | 2.0 |
| 31 | I | 95 | ASP | 2.0 |
| 1 | 0 | 1200 | A | 2.0 |
| 9 | G | 26 | MET | 2.0 |

6.2 Non-standard residues in protein, DNA, RNA chains [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. 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 | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 1 | OMU | 0 | 2587 | 21/22 | 0.95 | 0.12 | 38,39,40,41 | 0 |
| 1 | UR3 | 0 | 2619 | 21/22 | 0.96 | 0.15 | 36,38,39,40 | 0 |
| 1 | 1MA | 0 | 628 | 23/24 | 0.96 | 0.17 | 33,35,36,37 | 0 |
| 1 | OMG | 0 | 2588 | 24/25 | 0.97 | 0.13 | 37,38,39,40 | 0 |
| 1 | PSU | 0 | 2621 | 20/21 | 0.97 | 0.12 | 30,32,39,40 | 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. 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 | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 33 | MG | 0 | 8113 | 1/1 | 0.23 | 0.16 | 44,44,44,44 | 0 |
| 35 | NA | 9 | 8551 | 1/1 | 0.38 | 0.38 | 92,92,92,92 | 0 |
| 35 | NA | 0 | 8538 | 1/1 | 0.47 | 0.09 | 55,55,55,55 | 0 |
| 33 | MG | 0 | 8096 | 1/1 | 0.48 | 0.11 | 48,48,48,48 | 0 |
| 35 | NA | 0 | 8559 | 1/1 | 0.48 | 0.37 | 53,53,53,53 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 35 | NA | 0 | 8507 | 1/1 | 0.53 | 0.24 | 69,69,69,69 | 0 |
| 35 | NA | 0 | 8513 | 1/1 | 0.54 | 0.07 | 72,72,72,72 | 0 |
| 33 | MG | 0 | 8104 | 1/1 | 0.54 | 0.37 | 78,78,78,78 | 0 |
| 35 | NA | 0 | 8531 | 1/1 | 0.55 | 0.39 | 57,57,57,57 | 0 |
| 35 | NA | 0 | 8585 | 1/1 | 0.60 | 0.38 | 65,65,65,65 | 0 |
| 35 | NA | 0 | 8571 | 1/1 | 0.61 | 0.30 | 59,59,59,59 | 0 |
| 35 | NA | 0 | 8577 | 1/1 | 0.63 | 0.75 | 81,81,81,81 | 0 |
| 36 | CL | 0 | 8815 | 1/1 | 0.64 | 0.14 | 89,89,89,89 | 0 |
| 33 | MG | 0 | 8080 | 1/1 | 0.64 | 0.15 | 39,39,39,39 | 0 |
| 35 | NA | 0 | 8502 | 1/1 | 0.66 | 0.20 | 57,57,57,57 | 0 |
| 35 | NA | 0 | 8550 | 1/1 | 0.66 | 0.61 | 65,65,65,65 | 0 |
| 33 | MG | 0 | 8111 | 1/1 | 0.68 | 0.08 | 46,46,46,46 | 0 |
| 35 | NA | 0 | 8528 | 1/1 | 0.68 | 0.50 | 54,54,54,54 | 0 |
| 35 | NA | 0 | 8569 | 1/1 | 0.69 | 0.25 | 64,64,64,64 | 0 |
| 33 | MG | 0 | 8117 | 1/1 | 0.69 | 0.09 | 34,34,34,34 | 0 |
| 33 | MG | 0 | 8102 | 1/1 | 0.71 | 0.29 | 50,50,50,50 | 0 |
| 33 | MG | 0 | 8100 | 1/1 | 0.71 | 0.10 | 42,42,42,42 | 0 |
| 33 | MG | 0 | 8046 | 1/1 | 0.72 | 0.07 | 56,56,56,56 | 0 |
| 35 | NA | 0 | 8509 | 1/1 | 0.72 | 0.11 | 48,48,48,48 | 0 |
| 35 | NA | 0 | 8582 | 1/1 | 0.72 | 0.21 | 85,85,85,85 | 0 |
| 35 | NA | 0 | 8510 | 1/1 | 0.72 | 0.15 | 45,45,45,45 | 0 |
| 35 | NA | 0 | 8560 | 1/1 | 0.74 | 0.24 | 60,60,60,60 | 0 |
| 35 | NA | 9 | 8583 | 1/1 | 0.74 | 0.15 | 73,73,73,73 | 0 |
| 35 | NA | 0 | 8535 | 1/1 | 0.74 | 0.35 | 54,54,54,54 | 0 |
| 35 | NA | 0 | 8575 | 1/1 | 0.75 | 0.32 | 72,72,72,72 | 0 |
| 35 | NA | J | 8546 | 1/1 | 0.76 | 0.25 | 39,39,39,39 | 0 |
| 33 | MG | 0 | 8045 | 1/1 | 0.76 | 0.12 | 67,67,67,67 | 0 |
| 35 | NA | 0 | 8506 | 1/1 | 0.77 | 0.71 | 49,49,49,49 | 0 |
| 33 | MG | 0 | 8075 | 1/1 | 0.77 | 0.05 | 56,56,56,56 | 0 |
| 35 | NA | 0 | 8517 | 1/1 | 0.77 | 0.13 | 37,37,37,37 | 0 |
| 35 | NA | 0 | 8584 | 1/1 | 0.77 | 0.70 | 90,90,90,90 | 0 |
| 33 | MG | 9 | 8095 | 1/1 | 0.77 | 0.15 | 77,77,77,77 | 0 |
| 35 | NA | 0 | 8516 | 1/1 | 0.78 | 0.42 | 49,49,49,49 | 0 |
| 35 | NA | 0 | 8564 | 1/1 | 0.78 | 0.37 | 49,49,49,49 | 0 |
| 35 | NA | 0 | 8527 | 1/1 | 0.78 | 0.24 | 61,61,61,61 | 0 |
| 35 | NA | H | 8522 | 1/1 | 0.79 | 0.35 | 77,77,77,77 | 0 |
| 36 | CL | 0 | 8816 | 1/1 | 0.80 | 0.13 | 69,69,69,69 | 0 |
| 33 | MG | 0 | 8094 | 1/1 | 0.80 | 0.15 | 59,59,59,59 | 0 |
| 35 | NA | 0 | 8581 | 1/1 | 0.81 | 0.08 | 42,42,42,42 | 0 |
| 35 | NA | 0 | 8565 | 1/1 | 0.81 | 0.57 | 47,47,47,47 | 0 |
| 35 | NA | 0 | 8524 | 1/1 | 0.81 | 0.11 | 48,48,48,48 | 0 |
| 35 | NA | 0 | 8562 | 1/1 | 0.81 | 0.49 | 70,70,70,70 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 33 | MG | 0 | 8052 | 1/1 | 0.81 | 0.13 | 68,68,68,68 | 0 |
| 33 | MG | 0 | 8063 | 1/1 | 0.82 | 0.09 | 63,63,63,63 | 0 |
| 33 | MG | 0 | 8071 | 1/1 | 0.82 | 0.07 | 50,50,50,50 | 0 |
| 33 | MG | K | 8069 | 1/1 | 0.82 | 0.06 | 51,51,51,51 | 0 |
| 33 | MG | 0 | 8084 | 1/1 | 0.82 | 0.14 | 58,58,58,58 | 0 |
| 35 | NA | 0 | 8521 | 1/1 | 0.83 | 0.41 | 77,77,77,77 | 0 |
| 33 | MG | 0 | 8047 | 1/1 | 0.83 | 0.12 | 57,57,57,57 | 0 |
| 33 | MG | 0 | 8061 | 1/1 | 0.84 | 0.16 | 44,44,44,44 | 0 |
| 35 | NA | 0 | 8566 | 1/1 | 0.84 | 0.18 | 48,48,48,48 | 0 |
| 36 | CL | L | 8810 | 1/1 | 0.84 | 0.10 | 59,59,59,59 | 0 |
| 35 | NA | 0 | 8568 | 1/1 | 0.84 | 0.20 | 87,87,87,87 | 0 |
| 33 | MG | 0 | 8112 | 1/1 | 0.84 | 0.07 | 39,39,39,39 | 0 |
| 35 | NA | 0 | 8529 | 1/1 | 0.84 | 0.09 | 68,68,68,68 | 0 |
| 33 | MG | 0 | 8035 | 1/1 | 0.84 | 0.11 | 46,46,46,46 | 0 |
| 33 | MG | 0 | 8024 | 1/1 | 0.84 | 1.00 | 65,65,65,65 | 0 |
| 35 | NA | C | 8504 | 1/1 | 0.84 | 0.08 | 35,35,35,35 | 0 |
| 35 | NA | 0 | 8579 | 1/1 | 0.85 | 0.23 | 65,65,65,65 | 0 |
| 33 | MG | 0 | 8057 | 1/1 | 0.85 | 0.05 | 41,41,41,41 | 0 |
| 33 | MG | 0 | 8072 | 1/1 | 0.85 | 0.09 | 57,57,57,57 | 0 |
| 36 | CL | 0 | 8822 | 1/1 | 0.85 | 0.48 | 90,90,90,90 | 0 |
| 33 | MG | 0 | 8015 | 1/1 | 0.85 | 0.17 | 35,35,35,35 | 0 |
| 33 | MG | 0 | 8097 | 1/1 | 0.85 | 0.07 | 45,45,45,45 | 0 |
| 35 | NA | 0 | 8515 | 1/1 | 0.86 | 0.22 | 49,49,49,49 | 0 |
| 33 | MG | 0 | 8116 | 1/1 | 0.86 | 0.10 | 56,56,56,56 | 0 |
| 32 | 13T | 0 | 9000 | 42/42 | 0.86 | 0.25 | 58,67,73,74 | 0 |
| 33 | MG | 0 | 8058 | 1/1 | 0.86 | 0.11 | 42,42,42,42 | 0 |
| 35 | NA | 0 | 8544 | 1/1 | 0.86 | 0.07 | 29,29,29,29 | 0 |
| 34 | K | 0 | 8401 | 1/1 | 0.87 | 0.73 | 84,84,84,84 | 0 |
| 36 | CL | J | 8821 | 1/1 | 0.87 | 0.21 | 77,77,77,77 | 0 |
| 35 | NA | 0 | 8556 | 1/1 | 0.87 | 0.44 | 61,61,61,61 | 0 |
| 35 | NA | 0 | 8561 | 1/1 | 0.87 | 0.32 | 50,50,50,50 | 0 |
| 35 | NA | S | 8512 | 1/1 | 0.87 | 0.42 | 57,57,57,57 | 0 |
| 33 | MG | 0 | 8076 | 1/1 | 0.87 | 0.06 | 49,49,49,49 | 0 |
| 36 | CL | 0 | 8812 | 1/1 | 0.87 | 0.09 | 49,49,49,49 | 0 |
| 35 | NA | 0 | 8555 | 1/1 | 0.88 | 0.99 | 85,85,85,85 | 0 |
| 36 | CL | N | 8807 | 1/1 | 0.88 | 0.14 | 71,71,71,71 | 0 |
| 36 | CL | O | 8808 | 1/1 | 0.88 | 0.09 | 67,67,67,67 | 0 |
| 35 | NA | 0 | 8572 | 1/1 | 0.88 | 0.39 | 73,73,73,73 | 0 |
| 37 | CD | O | 8705 | 1/1 | 0.88 | 0.10 | 186,186,186,186 | 0 |
| 35 | NA | 0 | 8557 | 1/1 | 0.88 | 0.13 | 45,45,45,45 | 0 |
| 33 | MG | 0 | 8013 | 1/1 | 0.88 | 0.19 | 38,38,38,38 | 0 |
| 33 | MG | Y | 8109 | 1/1 | 0.89 | 0.16 | 44,44,44,44 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 35 | NA | 0 | 8518 | 1/1 | 0.89 | 0.34 | 58,58,58,58 | 0 |
| 33 | MG | 0 | 8029 | 1/1 | 0.89 | 0.12 | 42,42,42,42 | 0 |
| 35 | NA | 0 | 8558 | 1/1 | 0.89 | 0.56 | 75,75,75,75 | 0 |
| 33 | MG | 0 | 8011 | 1/1 | 0.89 | 0.18 | 39,39,39,39 | 0 |
| 33 | MG | 0 | 8008 | 1/1 | 0.89 | 0.08 | 29,29,29,29 | 0 |
| 33 | MG | 0 | 8022 | 1/1 | 0.90 | 0.08 | 37,37,37,37 | 0 |
| 33 | MG | 0 | 8081 | 1/1 | 0.90 | 0.13 | 43,43,43,43 | 0 |
| 33 | MG | 0 | 8018 | 1/1 | 0.90 | 0.15 | 39,39,39,39 | 0 |
| 33 | MG | 0 | 8028 | 1/1 | 0.90 | 0.06 | 33,33,33,33 | 0 |
| 33 | MG | 0 | 8062 | 1/1 | 0.90 | 0.22 | 13,13,13,13 | 0 |
| 35 | NA | M | 8547 | 1/1 | 0.90 | 0.07 | 41,41,41,41 | 0 |
| 35 | NA | 0 | 8532 | 1/1 | 0.90 | 0.23 | 44,44,44,44 | 0 |
| 33 | MG | 0 | 8020 | 1/1 | 0.90 | 0.12 | 39,39,39,39 | 0 |
| 35 | NA | 0 | 8563 | 1/1 | 0.90 | 0.42 | 68,68,68,68 | 0 |
| 33 | MG | 0 | 8090 | 1/1 | 0.90 | 0.23 | 73,73,73,73 | 0 |
| 33 | MG | 0 | 8115 | 1/1 | 0.90 | 0.07 | 45,45,45,45 | 0 |
| 35 | NA | 0 | 8554 | 1/1 | 0.90 | 0.15 | 42,42,42,42 | 0 |
| 36 | CL | J | 8802 | 1/1 | 0.91 | 0.15 | 76,76,76,76 | 0 |
| 33 | MG | 0 | 8091 | 1/1 | 0.91 | 0.10 | 65,65,65,65 | 0 |
| 35 | NA | 0 | 8552 | 1/1 | 0.91 | 0.13 | 68,68,68,68 | 0 |
| 35 | NA | 0 | 8542 | 1/1 | 0.91 | 0.29 | 15,15,15,15 | 0 |
| 33 | MG | 0 | 8114 | 1/1 | 0.91 | 0.35 | 54,54,54,54 | 0 |
| 35 | NA | 0 | 8567 | 1/1 | 0.91 | 0.46 | 61,61,61,61 | 0 |
| 33 | MG | 0 | 8040 | 1/1 | 0.91 | 0.34 | 53,53,53,53 | 0 |
| 35 | NA | 0 | 8505 | 1/1 | 0.91 | 0.23 | 37,37,37,37 | 0 |
| 33 | MG | 0 | 8031 | 1/1 | 0.91 | 0.10 | 30,30,30,30 | 0 |
| 36 | CL | B | 8819 | 1/1 | 0.91 | 0.10 | 53,53,53,53 | 0 |
| 33 | MG | 0 | 8088 | 1/1 | 0.92 | 0.10 | 33,33,33,33 | 0 |
| 33 | MG | 0 | 8103 | 1/1 | 0.92 | 0.19 | 78,78,78,78 | 0 |
| 33 | MG | 0 | 8023 | 1/1 | 0.92 | 0.24 | 61,61,61,61 | 0 |
| 33 | MG | 0 | 8070 | 1/1 | 0.92 | 0.15 | 43,43,43,43 | 0 |
| 35 | NA | 0 | 8574 | 1/1 | 0.92 | 0.60 | 67,67,67,67 | 0 |
| 33 | MG | 0 | 8010 | 1/1 | 0.92 | 0.16 | 11,11,11,11 | 0 |
| 33 | MG | 0 | 8050 | 1/1 | 0.92 | 0.19 | 74,74,74,74 | 0 |
| 33 | MG | 0 | 8036 | 1/1 | 0.92 | 0.06 | 41,41,41,41 | 0 |
| 33 | MG | 0 | 8093 | 1/1 | 0.92 | 0.10 | 61,61,61,61 | 0 |
| 35 | NA | 0 | 8533 | 1/1 | 0.92 | 0.12 | 39,39,39,39 | 0 |
| 33 | MG | 0 | 8044 | 1/1 | 0.93 | 0.08 | 55,55,55,55 | 0 |
| 33 | MG | 0 | 8079 | 1/1 | 0.93 | 0.15 | 27,27,27,27 | 0 |
| 33 | MG | 0 | 8049 | 1/1 | 0.93 | 0.17 | 36,36,36,36 | 0 |
| 33 | MG | 0 | 8067 | 1/1 | 0.93 | 0.09 | 37,37,37,37 | 0 |
| 33 | MG | 0 | 8025 | 1/1 | 0.93 | 0.10 | 43,43,43,43 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 33 | MG | 0 | 8001 | 1/1 | 0.93 | 0.12 | 44,44,44,44 | 0 |
| 35 | NA | 0 | 8549 | 1/1 | 0.93 | 0.26 | 53,53,53,53 | 0 |
| 35 | NA | 0 | 8526 | 1/1 | 0.93 | 0.30 | 70,70,70,70 | 0 |
| 33 | MG | 0 | 8083 | 1/1 | 0.93 | 0.07 | 41,41,41,41 | 0 |
| 36 | CL | 0 | 8803 | 1/1 | 0.93 | 0.15 | 56,56,56,56 | 0 |
| 35 | NA | 0 | 8539 | 1/1 | 0.93 | 0.30 | 40,40,40,40 | 0 |
| 35 | NA | 0 | 8540 | 1/1 | 0.93 | 0.26 | 50,50,50,50 | 0 |
| 33 | MG | 0 | 8089 | 1/1 | 0.93 | 0.13 | 62,62,62,62 | 0 |
| 33 | MG | 0 | 8037 | 1/1 | 0.93 | 0.07 | 42,42,42,42 | 0 |
| 33 | MG | 0 | 8019 | 1/1 | 0.94 | 0.04 | 34,34,34,34 | 0 |
| 35 | NA | 0 | 8541 | 1/1 | 0.94 | 0.09 | 46,46,46,46 | 0 |
| 35 | NA | 0 | 8570 | 1/1 | 0.94 | 0.39 | 65,65,65,65 | 0 |
| 35 | NA | R | 8537 | 1/1 | 0.94 | 0.14 | 45,45,45,45 | 0 |
| 35 | NA | A | 8545 | 1/1 | 0.94 | 0.16 | 61,61,61,61 | 0 |
| 33 | MG | 0 | 8006 | 1/1 | 0.94 | 0.09 | 36,36,36,36 | 0 |
| 35 | NA | Q | 8548 | 1/1 | 0.94 | 0.11 | 46,46,46,46 | 0 |
| 35 | NA | 0 | 8534 | 1/1 | 0.94 | 0.07 | 40,40,40,40 | 0 |
| 33 | MG | 0 | 8021 | 1/1 | 0.94 | 0.09 | 37,37,37,37 | 0 |
| 33 | MG | 0 | 8033 | 1/1 | 0.94 | 0.04 | 38,38,38,38 | 0 |
| 33 | MG | 3 | 8078 | 1/1 | 0.94 | 0.10 | 16,16,16,16 | 0 |
| 33 | MG | 0 | 8051 | 1/1 | 0.95 | 0.12 | 56,56,56,56 | 0 |
| 36 | CL | A | 8809 | 1/1 | 0.95 | 0.19 | 82,82,82,82 | 0 |
| 35 | NA | R | 8586 | 1/1 | 0.95 | 0.35 | 23,23,23,23 | 0 |
| 33 | MG | 0 | 8042 | 1/1 | 0.95 | 0.05 | 33,33,33,33 | 0 |
| 33 | MG | B | 8055 | 1/1 | 0.95 | 0.15 | 64,64,64,64 | 0 |
| 36 | CL | 0 | 8813 | 1/1 | 0.95 | 0.06 | 54,54,54,54 | 0 |
| 35 | NA | 0 | 8536 | 1/1 | 0.95 | 0.07 | 54,54,54,54 | 0 |
| 33 | MG | 0 | 8043 | 1/1 | 0.95 | 0.13 | 47,47,47,47 | 0 |
| 33 | MG | 0 | 8092 | 1/1 | 0.95 | 0.12 | 72,72,72,72 | 0 |
| 33 | MG | 0 | 8098 | 1/1 | 0.95 | 0.11 | 42,42,42,42 | 0 |
| 33 | MG | 0 | 8038 | 1/1 | 0.95 | 0.12 | 31,31,31,31 | 0 |
| 36 | CL | Y | 8817 | 1/1 | 0.95 | 0.15 | 70,70,70,70 | 0 |
| 33 | MG | 0 | 8085 | 1/1 | 0.95 | 0.12 | 48,48,48,48 | 0 |
| 34 | K | 0 | 8402 | 1/1 | 0.95 | 0.13 | 61,61,61,61 | 0 |
| 33 | MG | 0 | 8099 | 1/1 | 0.95 | 0.33 | 70,70,70,70 | 0 |
| 35 | NA | 0 | 8530 | 1/1 | 0.95 | 0.09 | 45,45,45,45 | 0 |
| 33 | MG | 0 | 8074 | 1/1 | 0.95 | 0.04 | 30,30,30,30 | 0 |
| 36 | CL | J | 8801 | 1/1 | 0.95 | 0.06 | 58,58,58,58 | 0 |
| 33 | MG | 0 | 8034 | 1/1 | 0.96 | 0.10 | 25,25,25,25 | 0 |
| 33 | MG | 0 | 8004 | 1/1 | 0.96 | 0.18 | 37,37,37,37 | 0 |
| 33 | MG | A | 8065 | 1/1 | 0.96 | 0.14 | 45,45,45,45 | 0 |
| 33 | MG | 0 | 8086 | 1/1 | 0.96 | 0.07 | 42,42,42,42 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 36 | CL | 0 | 8814 | 1/1 | 0.96 | 0.11 | 57,57,57,57 | 0 |
| 37 | CD | Z | 8703 | 1/1 | 0.96 | 0.09 | 71,71,71,71 | 0 |
| 33 | MG | T | 8073 | 1/1 | 0.96 | 0.10 | 57,57,57,57 | 0 |
| 36 | CL | 3 | 8804 | 1/1 | 0.96 | 0.09 | 56,56,56,56 | 0 |
| 33 | MG | 0 | 8041 | 1/1 | 0.96 | 0.23 | 68,68,68,68 | 0 |
| 33 | MG | 0 | 8005 | 1/1 | 0.96 | 0.10 | 32,32,32,32 | 0 |
| 33 | MG | 0 | 8101 | 1/1 | 0.96 | 0.08 | 45,45,45,45 | 0 |
| 33 | MG | 0 | 8048 | 1/1 | 0.96 | 0.09 | 49,49,49,49 | 0 |
| 35 | NA | 0 | 8508 | 1/1 | 0.96 | 0.26 | 58,58,58,58 | 0 |
| 36 | CL | M | 8818 | 1/1 | 0.96 | 0.09 | 44,44,44,44 | 0 |
| 33 | MG | 0 | 8087 | 1/1 | 0.96 | 0.09 | 63,63,63,63 | 0 |
| 33 | MG | 0 | 8077 | 1/1 | 0.96 | 0.16 | 36,36,36,36 | 0 |
| 33 | MG | 0 | 8053 | 1/1 | 0.96 | 0.13 | 43,43,43,43 | 0 |
| 35 | NA | 0 | 8520 | 1/1 | 0.96 | 0.23 | 36,36,36,36 | 0 |
| 35 | NA | 0 | 8514 | 1/1 | 0.96 | 0.10 | 38,38,38,38 | 0 |
| 33 | MG | A | 8066 | 1/1 | 0.96 | 0.05 | 73,73,73,73 | 0 |
| 33 | MG | 0 | 8108 | 1/1 | 0.96 | 0.03 | 77,77,77,77 | 0 |
| 33 | MG | 0 | 8056 | 1/1 | 0.97 | 0.10 | 56,56,56,56 | 0 |
| 33 | MG | 0 | 8017 | 1/1 | 0.97 | 0.16 | 31,31,31,31 | 0 |
| 33 | MG | 0 | 8059 | 1/1 | 0.97 | 0.05 | 39,39,39,39 | 0 |
| 33 | MG | 0 | 8054 | 1/1 | 0.97 | 0.16 | 30,30,30,30 | 0 |
| 33 | MG | 0 | 8016 | 1/1 | 0.97 | 0.07 | 18,18,18,18 | 0 |
| 33 | MG | 0 | 8003 | 1/1 | 0.97 | 0.10 | 36,36,36,36 | 0 |
| 33 | MG | 0 | 8002 | 1/1 | 0.97 | 0.03 | 40,40,40,40 | 0 |
| 35 | NA | 0 | 8578 | 1/1 | 0.97 | 0.10 | 57,57,57,57 | 0 |
| 33 | MG | 0 | 8007 | 1/1 | 0.97 | 0.17 | 26,26,26,26 | 0 |
| 35 | NA | 0 | 8573 | 1/1 | 0.97 | 0.20 | 56,56,56,56 | 0 |
| 33 | MG | 0 | 8032 | 1/1 | 0.97 | 0.07 | 35,35,35,35 | 0 |
| 33 | MG | 0 | 8082 | 1/1 | 0.97 | 0.34 | 84,84,84,84 | 0 |
| 33 | MG | 0 | 8009 | 1/1 | 0.97 | 0.15 | 36,36,36,36 | 0 |
| 35 | NA | 0 | 8553 | 1/1 | 0.98 | 0.11 | 44,44,44,44 | 0 |
| 35 | NA | L | 8580 | 1/1 | 0.98 | 0.24 | 1,1,1,1 | 0 |
| 35 | NA | 0 | 8543 | 1/1 | 0.98 | 0.20 | 35,35,35,35 | 0 |
| 33 | MG | 0 | 8107 | 1/1 | 0.98 | 0.12 | 38,38,38,38 | 0 |
| 33 | MG | 0 | 8068 | 1/1 | 0.98 | 0.09 | 56,56,56,56 | 0 |
| 33 | MG | 3 | 8118 | 1/1 | 0.98 | 0.21 | 50,50,50,50 | 0 |
| 36 | CL | Y | 8820 | 1/1 | 0.98 | 0.05 | 44,44,44,44 | 0 |
| 35 | NA | 0 | 8576 | 1/1 | 0.98 | 0.16 | 33,33,33,33 | 0 |
| 35 | NA | 0 | 8525 | 1/1 | 0.98 | 0.39 | 59,59,59,59 | 0 |
| 37 | CD | 3 | 8704 | 1/1 | 0.98 | 0.08 | 65,65,65,65 | 0 |
| 33 | MG | 0 | 8060 | 1/1 | 0.98 | 0.17 | 45,45,45,45 | 0 |
| 33 | MG | 0 | 8026 | 1/1 | 0.98 | 0.09 | 33,33,33,33 | 0 |

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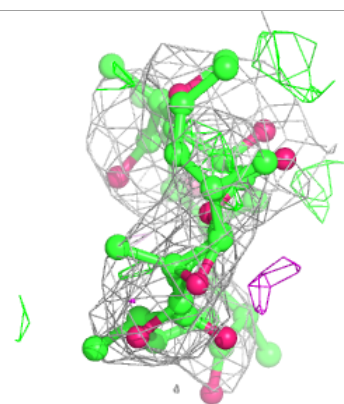
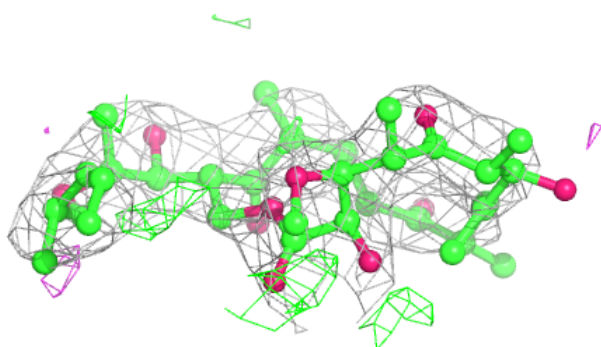
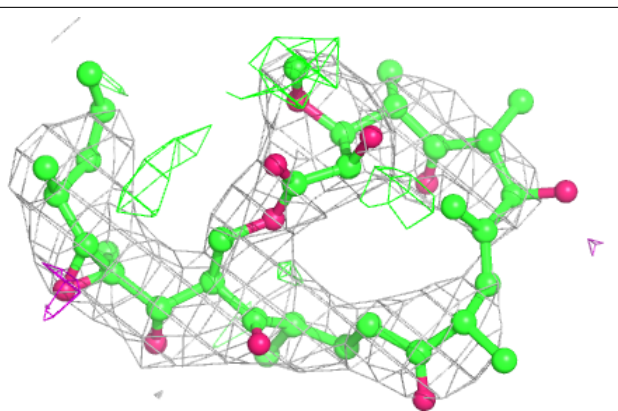
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 35 | NA | 0 | 8511 | 1/1 | 0.98 | 0.12 | 56,56,56,56 | 0 |
| 35 | NA | 0 | 8523 | 1/1 | 0.99 | 0.22 | 38,38,38,38 | 0 |
| 33 | MG | 0 | 8030 | 1/1 | 0.99 | 0.07 | 35,35,35,35 | 0 |
| 37 | CD | 1 | 8702 | 1/1 | 0.99 | 0.08 | 65,65,65,65 | 0 |
| 33 | MG | 0 | 8027 | 1/1 | 0.99 | 0.03 | 40,40,40,40 | 0 |
| 33 | MG | 0 | 8106 | 1/1 | 0.99 | 0.07 | 71,71,71,71 | 0 |
| 36 | CL | 0 | 8805 | 1/1 | 0.99 | 0.13 | 71,71,71,71 | 0 |
| 33 | MG | 0 | 8039 | 1/1 | 0.99 | 0.07 | 64,64,64,64 | 0 |
| 33 | MG | 0 | 8064 | 1/1 | 0.99 | 0.09 | 41,41,41,41 | 0 |
| 35 | NA | 0 | 8503 | 1/1 | 0.99 | 0.30 | 1,1,1,1 | 0 |
| 36 | CL | R | 8806 | 1/1 | 0.99 | 0.03 | 49,49,49,49 | 0 |
| 35 | NA | 0 | 8501 | 1/1 | 0.99 | 0.06 | 50,50,50,50 | 0 |
| 36 | CL | 0 | 8811 | 1/1 | 0.99 | 0.11 | 58,58,58,58 | 0 |
| 33 | MG | 0 | 8110 | 1/1 | 0.99 | 0.10 | 53,53,53,53 | 0 |
| 35 | NA | 0 | 8519 | 1/1 | 0.99 | 0.16 | 17,17,17,17 | 0 |
| 37 | CD | U | 8701 | 1/1 | 0.99 | 0.10 | 67,67,67,67 | 0 |
| 33 | MG | 0 | 8012 | 1/1 | 0.99 | 0.14 | 39,39,39,39 | 0 |
| 33 | MG | 0 | 8014 | 1/1 | 1.00 | 0.10 | 41,41,41,41 | 0 |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 13T 0 9000:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.