



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 05:34 am BST

PDB ID : 4JI7
Title : Crystal Structure of 30S ribosomal subunit from *Thermus thermophilus*
Authors : Demirci, H.; Wang, L.; Murphy IV, F.; Murphy, E.; Carr, J.; Blanchard, S.;
Jogl, G.; Dahlberg, A.E.; Gregory, S.T.
Deposited on : 2013-03-05
Resolution : 3.50 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 |
| 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 |

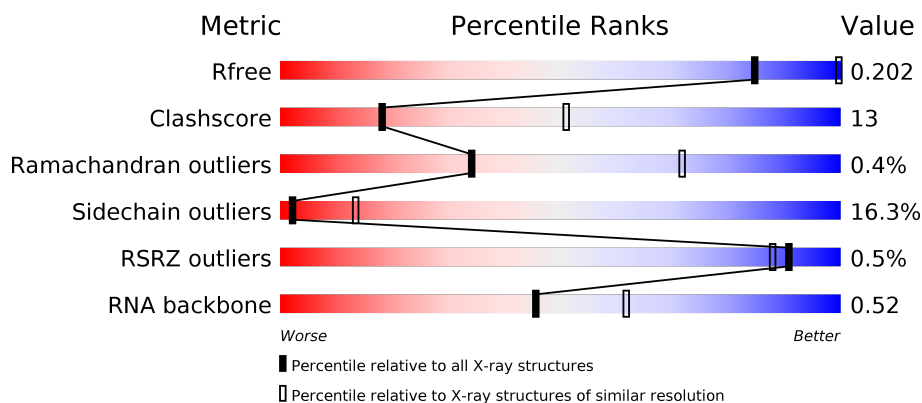
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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 | 1659 (3.60-3.40) |
| Clashscore | 141614 | 1036 (3.58-3.42) |
| Ramachandran outliers | 138981 | 1005 (3.58-3.42) |
| Sidechain outliers | 138945 | 1006 (3.58-3.42) |
| RSRZ outliers | 127900 | 1559 (3.60-3.40) |
| RNA backbone | 3102 | 1002 (4.00-3.00) |

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 | A | 1522 | |
| 2 | B | 256 | |
| 3 | C | 239 | |
| 4 | D | 209 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 5 | E | 162 | |
| 6 | F | 101 | |
| 7 | G | 156 | |
| 8 | H | 138 | |
| 9 | I | 128 | |
| 10 | J | 105 | |
| 11 | K | 129 | |
| 12 | L | 135 | |
| 13 | M | 126 | |
| 14 | N | 61 | |
| 15 | O | 89 | |
| 16 | P | 88 | |
| 17 | Q | 105 | |
| 18 | R | 88 | |
| 19 | S | 93 | |
| 20 | T | 106 | |
| 21 | U | 27 | |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 22 | MG | A | 1601 | - | - | - | X |
| 22 | MG | A | 1647 | - | - | - | X |
| 22 | MG | A | 1658 | - | - | - | X |
| 22 | MG | A | 1666 | - | - | - | X |
| 22 | MG | A | 1681 | - | - | - | X |
| 22 | MG | A | 1686 | - | - | - | X |
| 22 | MG | A | 1695 | - | - | - | X |
| 22 | MG | A | 1702 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 22 | MG | A | 1705 | - | - | - | X |
| 22 | MG | A | 1709 | - | - | - | X |
| 22 | MG | A | 1724 | - | - | - | X |
| 22 | MG | A | 1738 | - | - | - | X |
| 22 | MG | A | 1741 | - | - | - | X |
| 22 | MG | A | 1744 | - | - | - | X |
| 22 | MG | A | 1754 | - | - | - | X |
| 22 | MG | A | 1766 | - | - | - | X |
| 22 | MG | A | 1777 | - | - | - | X |
| 22 | MG | A | 1778 | - | - | - | X |
| 22 | MG | A | 1782 | - | - | - | X |
| 22 | MG | A | 1784 | - | - | - | X |
| 22 | MG | A | 1787 | - | - | - | X |
| 22 | MG | A | 1791 | - | - | - | X |
| 22 | MG | A | 1792 | - | - | - | X |
| 22 | MG | A | 1793 | - | - | - | X |
| 22 | MG | A | 1809 | - | - | - | X |
| 22 | MG | A | 1814 | - | - | - | X |
| 22 | MG | A | 1852 | - | - | - | X |
| 22 | MG | A | 1854 | - | - | - | X |
| 22 | MG | A | 1874 | - | - | - | X |
| 22 | MG | A | 1888 | - | - | - | X |
| 22 | MG | A | 1903 | - | - | - | X |
| 22 | MG | A | 1905 | - | - | - | X |
| 22 | MG | A | 1952 | - | - | - | X |
| 22 | MG | A | 2005 | - | - | - | X |
| 22 | MG | C | 302 | - | - | - | X |
| 22 | MG | E | 202 | - | - | - | X |
| 22 | MG | E | 204 | - | - | - | X |
| 22 | MG | K | 201 | - | - | - | X |
| 22 | MG | N | 102 | - | - | - | X |
| 22 | MG | P | 103 | - | - | - | X |
| 22 | MG | P | 104 | - | - | - | X |
| 22 | MG | Q | 202 | - | - | - | X |

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 53810 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 16S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1 | A | 1514 | Total | C | N | O | P | 0 | 6 | 0 |
| | | | 32687 | 14559 | 6046 | 10562 | 1520 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|-------------|
| A | 1534 | C | A | CONFLICT | GB M26923.1 |
| A | 1535 | A | C | CONFLICT | GB M26923.1 |

- Molecule 2 is a protein called RIBOSOMAL PROTEIN S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2 | B | 234 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1900 | 1213 | 341 | 341 | 5 | | | |

- Molecule 3 is a protein called RIBOSOMAL PROTEIN S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | C | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1612 | 1016 | 314 | 281 | 1 | | | |

- Molecule 4 is a protein called RIBOSOMAL PROTEIN S4.

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

- Molecule 5 is a protein called RIBOSOMAL PROTEIN S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | E | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1146 | 724 | 217 | 201 | 4 | | | |

- Molecule 6 is a protein called RIBOSOMAL PROTEIN S6.

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

- Molecule 7 is a protein called RIBOSOMAL PROTEIN S7.

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

- Molecule 8 is a protein called RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called RIBOSOMAL PROTEIN S9.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 9 | I | 127 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1010 | 639 | 197 | 174 | | | |

- Molecule 10 is a protein called RIBOSOMAL PROTEIN S10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | J | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 792 | 498 | 156 | 137 | 1 | | | |

- Molecule 11 is a protein called RIBOSOMAL PROTEIN S11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | K | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 864 | 537 | 164 | 160 | 3 | | | |

- Molecule 12 is a protein called RIBOSOMAL PROTEIN S12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | L | 124 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 977 | 617 | 196 | 163 | 1 | | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| L | 94 | TRP | PRO | CONFLICT | UNP F6DEQ7 |

- Molecule 13 is a protein called RIBOSOMAL PROTEIN S13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | M | 118 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 937 | 579 | 193 | 163 | 2 | | | |

- Molecule 14 is a protein called RIBOSOMAL PROTEIN S14.

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

- Molecule 15 is a protein called RIBOSOMAL PROTEIN S15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15 | O | 87 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 729 | 457 | 146 | 124 | 2 | | | |

- Molecule 16 is a protein called RIBOSOMAL PROTEIN S16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | P | 83 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 700 | 443 | 139 | 117 | 1 | | | |

- Molecule 17 is a protein called RIBOSOMAL PROTEIN S17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17 | Q | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 823 | 528 | 151 | 142 | 2 | | | |

- Molecule 18 is a protein called RIBOSOMAL PROTEIN S18.

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

- Molecule 19 is a protein called RIBOSOMAL PROTEIN S19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | S | 80 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 647 | 414 | 119 | 112 | 2 | | | |

- Molecule 20 is a protein called RIBOSOMAL PROTEIN S20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | T | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 763 | 470 | 162 | 129 | 2 | | | |

- Molecule 21 is a protein called RIBOSOMAL PROTEIN THX.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 21 | U | 24 | Total | C | N | O | 0 | 0 | 0 |
| | | | 208 | 128 | 50 | 30 | | | |

- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 22 | P | 4 | Total | Mg | 0 | 0 |
| | | | 4 | 4 | | |
| 22 | Q | 3 | Total | Mg | 0 | 0 |
| | | | 3 | 3 | | |
| 22 | D | 6 | Total | Mg | 0 | 0 |
| | | | 6 | 6 | | |
| 22 | K | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 22 | E | 6 | Total | Mg | 0 | 0 |
| | | | 6 | 6 | | |
| 22 | H | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 22 | B | 3 | Total | Mg | 0 | 0 |
| | | | 3 | 3 | | |
| 22 | C | 4 | Total | Mg | 0 | 0 |
| | | | 4 | 4 | | |
| 22 | A | 418 | Total | Mg | 0 | 0 |
| | | | 418 | 418 | | |
| 22 | N | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 22 | O | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 22 | L | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 22 | S | 1 | Total 1 | Mg 1 | 0 | 0 |
| 22 | F | 1 | Total 1 | Mg 1 | 0 | 0 |

- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 23 | D | 1 | Total 1 | Zn 1 | 0 | 0 |
| 23 | N | 1 | Total 1 | Zn 1 | 0 | 0 |

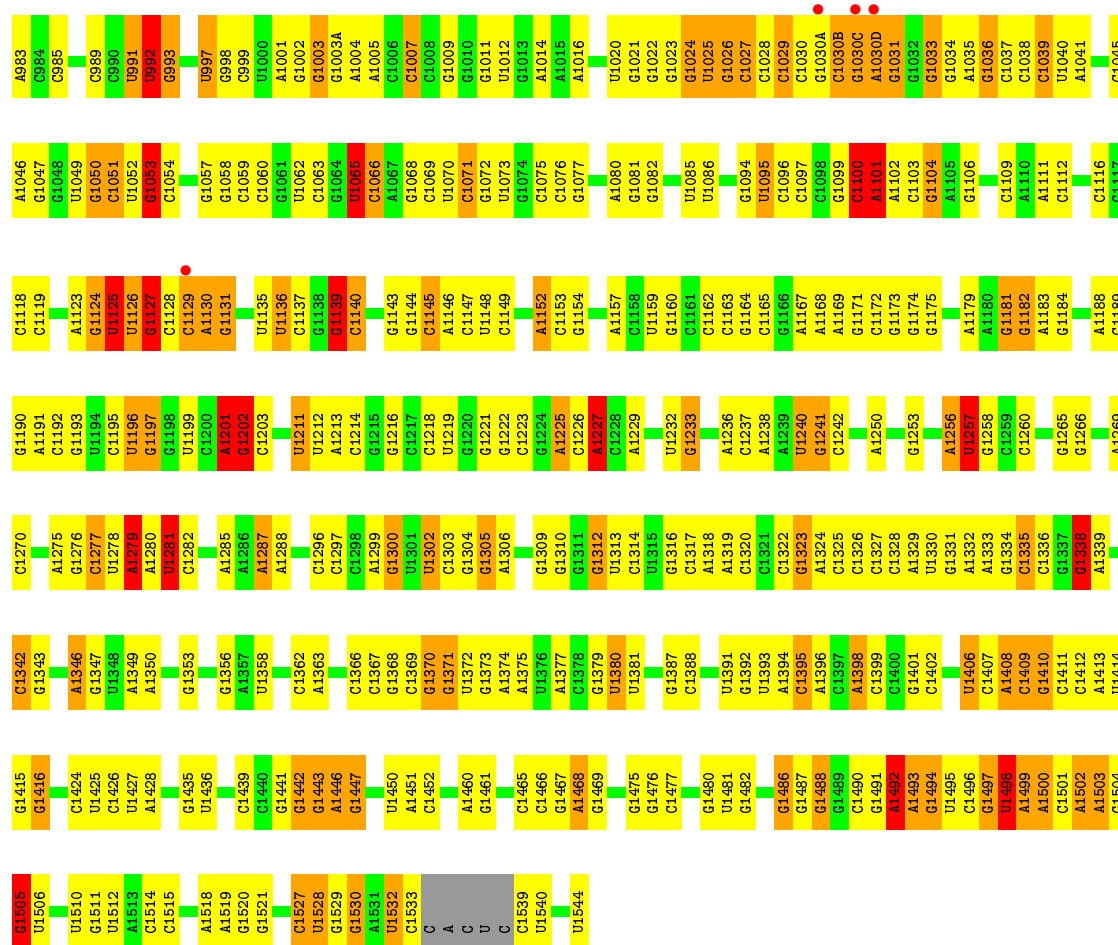
- Molecule 24 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|---------------|-----------|---------|---------|
| 24 | A | 1483 | Total 1483 | O 1483 | 0 | 0 |
| 24 | C | 15 | Total 15 | O 15 | 0 | 0 |
| 24 | D | 26 | Total 26 | O 26 | 0 | 0 |
| 24 | E | 21 | Total 21 | O 21 | 0 | 0 |
| 24 | F | 6 | Total 6 | O 6 | 0 | 0 |
| 24 | H | 3 | Total 3 | O 3 | 0 | 0 |
| 24 | K | 1 | Total 1 | O 1 | 0 | 0 |
| 24 | L | 7 | Total 7 | O 7 | 0 | 0 |
| 24 | M | 2 | Total 2 | O 2 | 0 | 0 |
| 24 | N | 1 | Total 1 | O 1 | 0 | 0 |
| 24 | O | 2 | Total 2 | O 2 | 0 | 0 |
| 24 | P | 2 | Total 2 | O 2 | 0 | 0 |
| 24 | Q | 7 | Total 7 | O 7 | 0 | 0 |

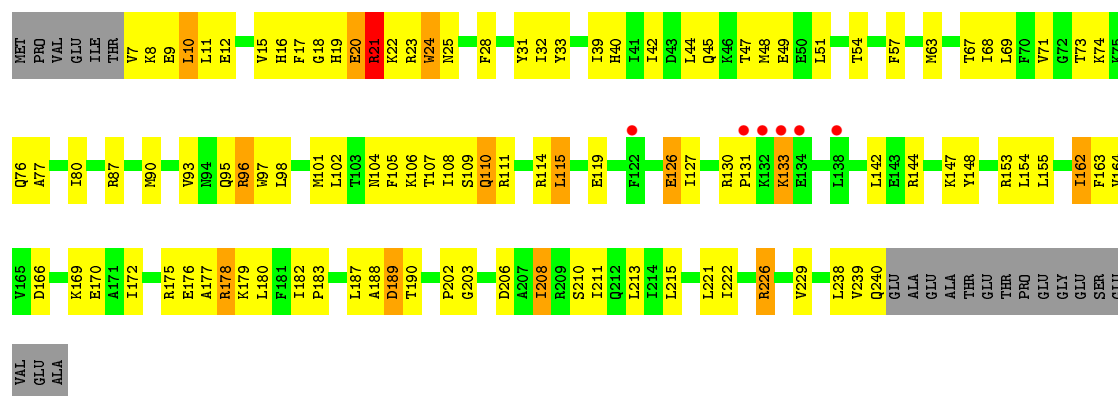
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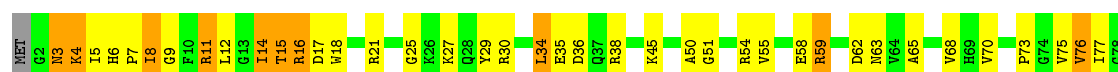
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 24 | T | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |

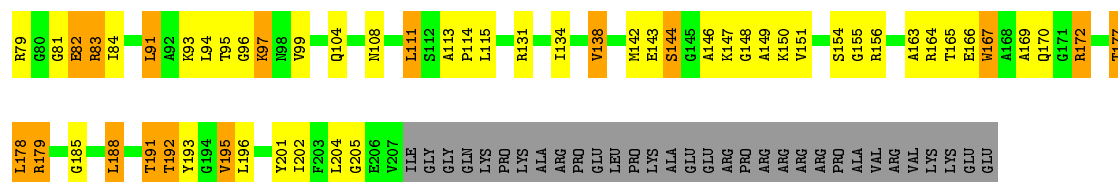


• Molecule 2: RIBOSOMAL PROTEIN S2



• Molecule 3: RIBOSOMAL PROTEIN S3





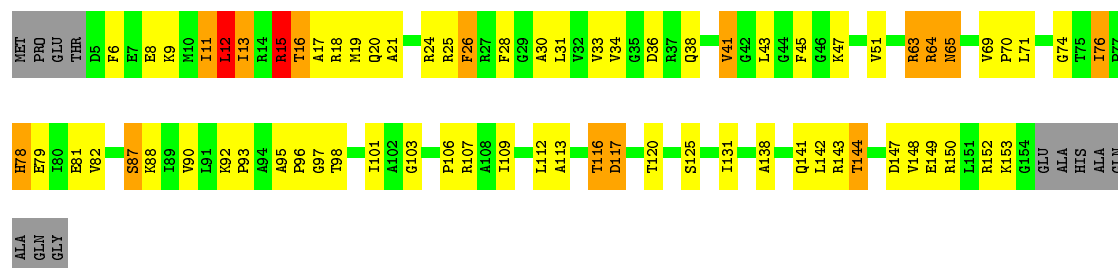
• Molecule 4: RIBOSOMAL PROTEIN S4

Chain D: 56% 34% 8%



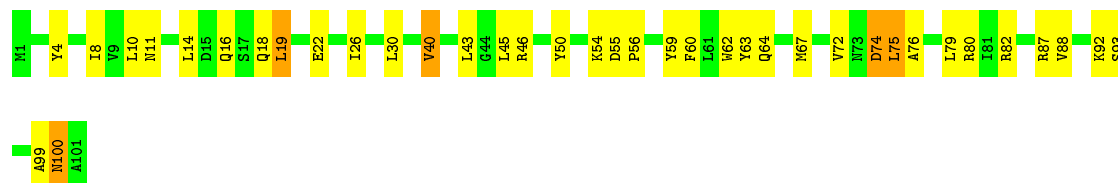
• Molecule 5: RIBOSOMAL PROTEIN S5

Chain E: 48% 35% 9% 7%



• Molecule 6: RIBOSOMAL PROTEIN S6

Chain F: 62% 33% 5%



• Molecule 7: RIBOSOMAL PROTEIN S7

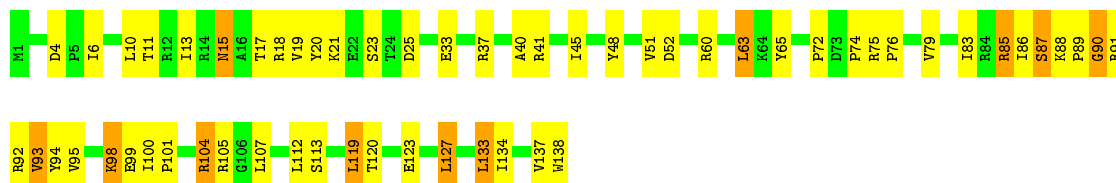
Chain G: 71% 28%





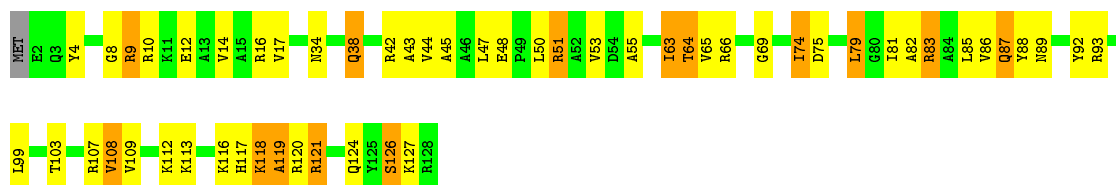
• Molecule 8: RIBOSOMAL PROTEIN S8

Chain H: 58% 34% 8%



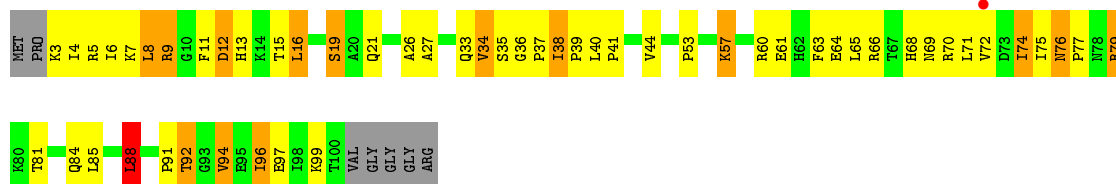
• Molecule 9: RIBOSOMAL PROTEIN S9

Chain I: 57% 31% 11%



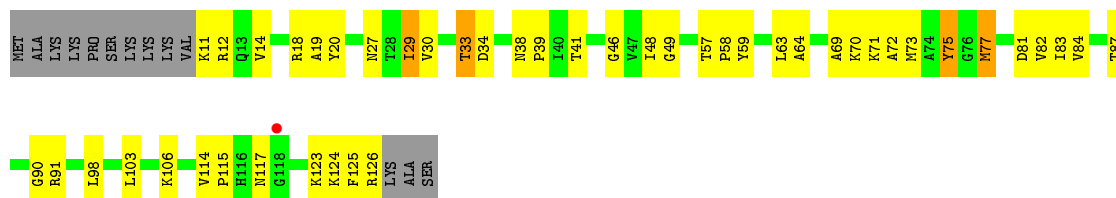
• Molecule 10: RIBOSOMAL PROTEIN S10

Chain J: 42% 37% 13% 7%



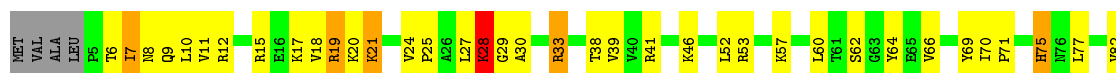
• Molecule 11: RIBOSOMAL PROTEIN S11

Chain K: 54% 33% 10%



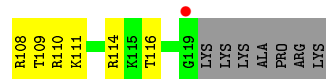
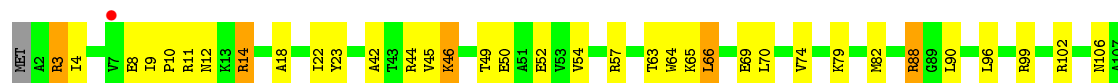
• Molecule 12: RIBOSOMAL PROTEIN S12

Chain L: 49% 36% 6% 8%





• Molecule 13: RIBOSOMAL PROTEIN S13



• Molecule 14: RIBOSOMAL PROTEIN S14



• Molecule 15: RIBOSOMAL PROTEIN S15



• Molecule 16: RIBOSOMAL PROTEIN S16

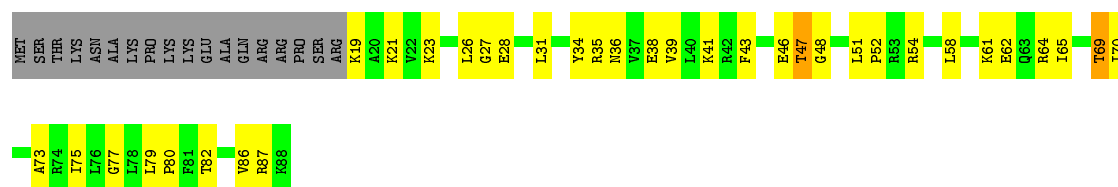


• Molecule 17: RIBOSOMAL PROTEIN S17



• Molecule 18: RIBOSOMAL PROTEIN S18

Chain R: 



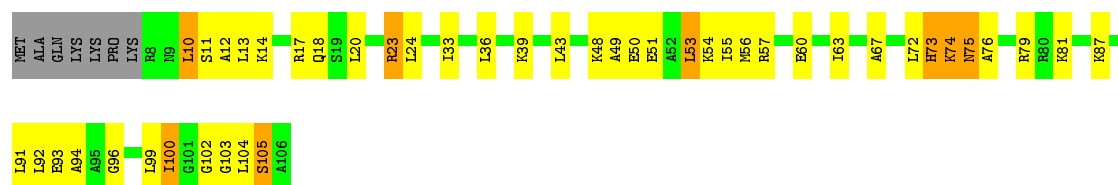
• Molecule 19: RIBOSOMAL PROTEIN S19

Chain S: 



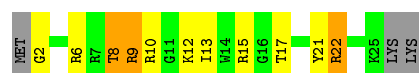
• Molecule 20: RIBOSOMAL PROTEIN S20

Chain T: 



• Molecule 21: RIBOSOMAL PROTEIN THX

Chain U: 



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 41 21 2 | Depositor |
| Cell constants a, b, c, α , β , γ | 397.81Å 397.81Å 214.91Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 49.84 – 3.50 49.84 – 3.50 | Depositor EDS |
| % Data completeness (in resolution range) | 99.6 (49.84-3.50) 99.6 (49.84-3.50) | Depositor EDS |
| R_{merge} | 0.12 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.93 (at 3.48Å) | Xtriage |
| Refinement program | PHENIX dev_1119 | Depositor |
| R, R_{free} | 0.158 , 0.201 0.159 , 0.202 | Depositor DCC |
| R_{free} test set | 10715 reflections (4.99%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 123.2 | Xtriage |
| Anisotropy | 0.088 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.29 , 123.9 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.96 | EDS |
| Total number of atoms | 53810 | wwPDB-VP |
| Average B, all atoms (Å ²) | 116.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% 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: ZN, MA6, MG, 2MG, 5MC, UR3, 4OC, M2G, 7MG, PSU

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|------------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | A | 0.79 | 10/36187 (0.0%) | 1.37 | 377/56471 (0.7%) |
| 2 | B | 0.55 | 0/1935 | 0.77 | 0/2609 |
| 3 | C | 0.56 | 0/1636 | 0.79 | 3/2205 (0.1%) |
| 4 | D | 0.57 | 2/1733 (0.1%) | 0.76 | 1/2318 (0.0%) |
| 5 | E | 0.69 | 0/1162 | 0.94 | 5/1564 (0.3%) |
| 6 | F | 0.57 | 0/856 | 0.78 | 0/1154 |
| 7 | G | 0.47 | 0/1276 | 0.63 | 0/1709 |
| 8 | H | 0.63 | 0/1136 | 0.79 | 0/1527 |
| 9 | I | 0.42 | 0/1029 | 0.69 | 0/1379 |
| 10 | J | 0.52 | 0/805 | 0.81 | 0/1082 |
| 11 | K | 0.49 | 0/879 | 0.75 | 0/1187 |
| 12 | L | 0.67 | 0/994 | 0.93 | 0/1331 |
| 13 | M | 0.45 | 0/947 | 0.68 | 0/1270 |
| 14 | N | 0.59 | 1/501 (0.2%) | 0.74 | 0/664 |
| 15 | O | 0.53 | 0/740 | 0.72 | 1/987 (0.1%) |
| 16 | P | 0.59 | 0/716 | 0.79 | 0/963 |
| 17 | Q | 0.63 | 0/836 | 0.91 | 2/1117 (0.2%) |
| 18 | R | 0.54 | 0/579 | 0.74 | 0/768 |
| 19 | S | 0.47 | 0/661 | 0.82 | 1/890 (0.1%) |
| 20 | T | 0.53 | 0/765 | 0.83 | 1/1007 (0.1%) |
| 21 | U | 0.45 | 0/212 | 0.60 | 0/277 |
| All | All | 0.72 | 13/55585 (0.0%) | 1.22 | 391/82479 (0.5%) |

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 |
|-----|-------|---------------------|---------------------|
| 2 | B | 0 | 3 |
| 3 | C | 0 | 1 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 4 | D | 0 | 2 |
| 8 | H | 0 | 1 |
| 10 | J | 0 | 2 |
| 20 | T | 0 | 2 |
| All | All | 0 | 11 |

All (13) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | A | 279 | A | N9-C4 | -7.59 | 1.33 | 1.37 |
| 1 | A | 1502 | A | C5-C6 | -6.79 | 1.34 | 1.41 |
| 1 | A | 814 | A | N9-C4 | -6.66 | 1.33 | 1.37 |
| 14 | N | 27 | CYS | CB-SG | -6.50 | 1.71 | 1.82 |
| 1 | A | 279 | A | N7-C5 | -5.84 | 1.35 | 1.39 |
| 1 | A | 482 | A | N7-C5 | -5.71 | 1.35 | 1.39 |
| 1 | A | 922 | G | C6-O6 | 5.64 | 1.29 | 1.24 |
| 1 | A | 965 | A | N9-C4 | -5.32 | 1.34 | 1.37 |
| 1 | A | 16 | A | C5-C4 | -5.20 | 1.35 | 1.38 |
| 4 | D | 12 | CYS | CB-SG | 5.19 | 1.91 | 1.82 |
| 4 | D | 9 | CYS | CB-SG | 5.12 | 1.91 | 1.82 |
| 1 | A | 439 | A | N9-C4 | -5.10 | 1.34 | 1.37 |
| 1 | A | 1501 | C | N1-C6 | -5.08 | 1.34 | 1.37 |

All (391) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 1 | A | 1227 | A | N1-C6-N6 | 14.96 | 127.58 | 118.60 |
| 1 | A | 1502 | A | N1-C6-N6 | 12.28 | 125.97 | 118.60 |
| 1 | A | 117 | G | N1-C6-O6 | 12.17 | 127.20 | 119.90 |
| 1 | A | 814 | A | C2-N3-C4 | -11.85 | 104.67 | 110.60 |
| 1 | A | 1528 | U | O5'-P-OP2 | -10.76 | 96.02 | 105.70 |
| 1 | A | 1227 | A | C6-C5-N7 | -10.33 | 125.07 | 132.30 |
| 1 | A | 1502 | A | C4-C5-N7 | 9.79 | 115.59 | 110.70 |
| 1 | A | 1502 | A | C6-C5-N7 | -9.64 | 125.55 | 132.30 |
| 1 | A | 117 | G | C6-C5-N7 | -9.45 | 124.73 | 130.40 |
| 1 | A | 1502 | A | C5-N7-C8 | -9.42 | 99.19 | 103.90 |
| 1 | A | 279 | A | C5-N7-C8 | -9.40 | 99.20 | 103.90 |
| 1 | A | 144 | G | N1-C6-O6 | 9.38 | 125.53 | 119.90 |
| 1 | A | 1532 | U | C5-C6-N1 | 9.36 | 127.38 | 122.70 |
| 1 | A | 975 | A | C2-N3-C4 | -8.55 | 106.33 | 110.60 |
| 1 | A | 1502 | A | C2-N3-C4 | -8.50 | 106.35 | 110.60 |
| 1 | A | 922 | G | N1-C6-O6 | 8.46 | 124.97 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 1257 | U | C2-N1-C1' | 8.42 | 127.80 | 117.70 |
| 1 | A | 236 | G | N1-C6-O6 | -8.32 | 114.91 | 119.90 |
| 1 | A | 1277 | C | C5-C6-N1 | 8.24 | 125.12 | 121.00 |
| 1 | A | 279 | A | N7-C8-N9 | 8.11 | 117.86 | 113.80 |
| 1 | A | 1530 | G | N3-C4-C5 | 8.11 | 132.66 | 128.60 |
| 1 | A | 526 | C | C6-N1-C2 | 8.09 | 123.53 | 120.30 |
| 3 | C | 179 | ARG | N-CA-C | -8.06 | 89.24 | 111.00 |
| 1 | A | 266 | G | C5-N7-C8 | -8.03 | 100.29 | 104.30 |
| 1 | A | 922 | G | C5-C6-N1 | -8.03 | 107.49 | 111.50 |
| 1 | A | 975 | A | C5-N7-C8 | -8.03 | 99.89 | 103.90 |
| 1 | A | 239 | U | N3-C4-C5 | -8.01 | 109.79 | 114.60 |
| 1 | A | 389 | A | C8-N9-C4 | -8.00 | 102.60 | 105.80 |
| 1 | A | 1416 | G | C4-N9-C1' | 8.00 | 136.90 | 126.50 |
| 1 | A | 862 | C | C6-N1-C2 | 7.98 | 123.49 | 120.30 |
| 1 | A | 144 | G | C5-C6-N1 | -7.97 | 107.51 | 111.50 |
| 1 | A | 108 | G | N1-C6-O6 | 7.94 | 124.66 | 119.90 |
| 1 | A | 1530 | G | C4-N9-C1' | -7.88 | 116.25 | 126.50 |
| 5 | E | 15 | ARG | NE-CZ-NH1 | 7.88 | 124.24 | 120.30 |
| 1 | A | 108 | G | C6-C5-N7 | -7.88 | 125.67 | 130.40 |
| 1 | A | 482 | A | N7-C8-N9 | 7.86 | 117.73 | 113.80 |
| 1 | A | 182 | U | C5-C6-N1 | 7.85 | 126.62 | 122.70 |
| 1 | A | 965 | A | C8-N9-C4 | 7.84 | 108.94 | 105.80 |
| 1 | A | 122 | G | N1-C6-O6 | 7.83 | 124.60 | 119.90 |
| 1 | A | 236 | G | N3-C2-N2 | 7.81 | 125.37 | 119.90 |
| 1 | A | 254 | G | O5'-P-OP1 | -7.79 | 98.69 | 105.70 |
| 1 | A | 328 | C | P-O3'-C3' | 7.75 | 129.00 | 119.70 |
| 1 | A | 583 | A | N1-C6-N6 | 7.73 | 123.24 | 118.60 |
| 1 | A | 518 | C | N1-C2-O2 | 7.72 | 123.53 | 118.90 |
| 1 | A | 333 | G | C5-C6-N1 | -7.68 | 107.66 | 111.50 |
| 1 | A | 1203 | C | C6-N1-C2 | 7.67 | 123.37 | 120.30 |
| 1 | A | 1277 | C | C6-N1-C2 | -7.67 | 117.23 | 120.30 |
| 1 | A | 481 | G | N3-C4-N9 | 7.64 | 130.58 | 126.00 |
| 1 | A | 975 | A | N7-C8-N9 | 7.61 | 117.60 | 113.80 |
| 1 | A | 814 | A | N1-C2-N3 | 7.58 | 133.09 | 129.30 |
| 1 | A | 533 | A | O5'-P-OP2 | -7.56 | 98.89 | 105.70 |
| 1 | A | 484 | G | N3-C4-N9 | 7.54 | 130.53 | 126.00 |
| 1 | A | 922 | G | C4-C5-C6 | 7.54 | 123.33 | 118.80 |
| 1 | A | 1139 | G | C8-N9-C4 | -7.54 | 103.38 | 106.40 |
| 1 | A | 481 | G | N3-C4-C5 | -7.54 | 124.83 | 128.60 |
| 1 | A | 400 | C | C6-N1-C2 | 7.54 | 123.31 | 120.30 |
| 1 | A | 1201 | A | P-O3'-C3' | 7.41 | 128.60 | 119.70 |
| 1 | A | 1227 | A | C4-C5-N7 | 7.41 | 114.40 | 110.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 484 | G | C4-N9-C1' | 7.41 | 136.13 | 126.50 |
| 1 | A | 975 | A | C5-C6-N1 | -7.40 | 114.00 | 117.70 |
| 1 | A | 907 | A | N1-C2-N3 | 7.40 | 133.00 | 129.30 |
| 1 | A | 284 | G | N1-C6-O6 | 7.32 | 124.29 | 119.90 |
| 1 | A | 556 | C | C6-N1-C2 | 7.27 | 123.21 | 120.30 |
| 1 | A | 61 | G | N1-C6-O6 | 7.25 | 124.25 | 119.90 |
| 1 | A | 314 | C | C6-N1-C2 | 7.25 | 123.20 | 120.30 |
| 1 | A | 1505 | G | C8-N9-C4 | -7.22 | 103.51 | 106.40 |
| 1 | A | 1227 | A | C5-N7-C8 | -7.20 | 100.30 | 103.90 |
| 1 | A | 669 | U | O5'-P-OP2 | -7.14 | 99.28 | 105.70 |
| 1 | A | 721 | G | N1-C6-O6 | 7.13 | 124.18 | 119.90 |
| 1 | A | 117 | G | C5-C6-O6 | -7.05 | 124.37 | 128.60 |
| 1 | A | 1227 | A | C4-C5-C6 | 7.05 | 120.53 | 117.00 |
| 1 | A | 1227 | A | N9-C4-C5 | -7.04 | 102.99 | 105.80 |
| 1 | A | 1227 | A | C5-C6-N6 | -7.01 | 118.09 | 123.70 |
| 1 | A | 518 | C | C2-N1-C1' | 7.00 | 126.50 | 118.80 |
| 1 | A | 1502 | A | N9-C4-C5 | -7.00 | 103.00 | 105.80 |
| 1 | A | 1505 | G | N3-C4-C5 | -6.99 | 125.10 | 128.60 |
| 1 | A | 484 | G | N3-C4-C5 | -6.97 | 125.11 | 128.60 |
| 1 | A | 1129 | C | C6-N1-C2 | -6.97 | 117.51 | 120.30 |
| 1 | A | 16 | A | N7-C8-N9 | -6.93 | 110.33 | 113.80 |
| 17 | Q | 98 | LEU | CA-CB-CG | 6.92 | 131.22 | 115.30 |
| 1 | A | 31 | G | O5'-P-OP2 | -6.88 | 99.51 | 105.70 |
| 1 | A | 1442 | G | N3-C4-N9 | 6.87 | 130.12 | 126.00 |
| 1 | A | 722 | A | C2-N3-C4 | -6.86 | 107.17 | 110.60 |
| 1 | A | 1439 | C | C6-N1-C2 | 6.84 | 123.03 | 120.30 |
| 1 | A | 851 | G | N1-C6-O6 | 6.83 | 124.00 | 119.90 |
| 1 | A | 484 | G | C8-N9-C1' | -6.82 | 118.14 | 127.00 |
| 1 | A | 742 | G | C8-N9-C4 | 6.80 | 109.12 | 106.40 |
| 1 | A | 559 | A | C8-N9-C4 | -6.79 | 103.08 | 105.80 |
| 1 | A | 1127 | G | C6-C5-N7 | -6.77 | 126.34 | 130.40 |
| 1 | A | 298 | A | N1-C2-N3 | 6.77 | 132.69 | 129.30 |
| 1 | A | 894 | G | C2-N3-C4 | -6.76 | 108.52 | 111.90 |
| 1 | A | 1139 | G | P-O3'-C3' | 6.76 | 127.81 | 119.70 |
| 1 | A | 509 | A | C8-N9-C4 | -6.74 | 103.10 | 105.80 |
| 5 | E | 41 | VAL | CB-CA-C | -6.74 | 98.59 | 111.40 |
| 1 | A | 1227 | A | C5-C6-N1 | -6.73 | 114.33 | 117.70 |
| 17 | Q | 84 | LEU | CA-CB-CG | -6.73 | 99.83 | 115.30 |
| 1 | A | 557 | G | OP2-P-O3' | 6.72 | 119.99 | 105.20 |
| 1 | A | 144 | G | N3-C2-N2 | -6.71 | 115.20 | 119.90 |
| 1 | A | 362 | G | N1-C6-O6 | 6.70 | 123.92 | 119.90 |
| 1 | A | 116 | A | C2-N3-C4 | -6.68 | 107.26 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 1 | A | 1279 | A | N1-C6-N6 | 6.68 | 122.61 | 118.60 |
| 1 | A | 721 | G | C6-C5-N7 | -6.66 | 126.40 | 130.40 |
| 1 | A | 117 | G | C2-N3-C4 | -6.66 | 108.57 | 111.90 |
| 1 | A | 733 | A | C2-N3-C4 | -6.66 | 107.27 | 110.60 |
| 1 | A | 1442 | G | N3-C4-C5 | -6.64 | 125.28 | 128.60 |
| 1 | A | 830 | G | N3-C4-C5 | 6.62 | 131.91 | 128.60 |
| 1 | A | 1530 | G | N3-C4-N9 | -6.61 | 122.03 | 126.00 |
| 1 | A | 662 | G | N1-C6-O6 | 6.58 | 123.85 | 119.90 |
| 1 | A | 624 | C | C6-N1-C2 | 6.55 | 122.92 | 120.30 |
| 1 | A | 841 | U | C5-C6-N1 | 6.54 | 125.97 | 122.70 |
| 1 | A | 279 | A | C8-N9-C4 | -6.54 | 103.19 | 105.80 |
| 1 | A | 1257 | U | N1-C2-O2 | 6.53 | 127.37 | 122.80 |
| 1 | A | 1416 | G | C8-N9-C1' | -6.53 | 118.51 | 127.00 |
| 4 | D | 12 | CYS | CA-CB-SG | 6.51 | 125.71 | 114.00 |
| 1 | A | 122 | G | N9-C4-C5 | -6.50 | 102.80 | 105.40 |
| 1 | A | 122 | G | C5-C6-O6 | -6.50 | 124.70 | 128.60 |
| 1 | A | 719 | C | N3-C4-C5 | 6.48 | 124.49 | 121.90 |
| 1 | A | 693 | G | N1-C6-O6 | 6.47 | 123.78 | 119.90 |
| 1 | A | 190(D) | U | C5-C6-N1 | -6.46 | 119.47 | 122.70 |
| 1 | A | 1116 | C | C6-N1-C2 | 6.45 | 122.88 | 120.30 |
| 1 | A | 559 | A | N3-C4-C5 | -6.43 | 122.30 | 126.80 |
| 1 | A | 556 | C | N3-C4-C5 | 6.42 | 124.47 | 121.90 |
| 1 | A | 1227 | A | N7-C8-N9 | 6.41 | 117.00 | 113.80 |
| 1 | A | 1065 | U | P-O3'-C3' | 6.40 | 127.38 | 119.70 |
| 1 | A | 812 | C | P-O3'-C3' | 6.39 | 127.37 | 119.70 |
| 1 | A | 284 | G | C5-C6-O6 | -6.36 | 124.79 | 128.60 |
| 1 | A | 313 | A | C8-N9-C4 | 6.35 | 108.34 | 105.80 |
| 1 | A | 310 | G | C8-N9-C4 | 6.33 | 108.93 | 106.40 |
| 1 | A | 578 | C | O5'-P-OP1 | -6.33 | 100.00 | 105.70 |
| 1 | A | 530 | G | P-O3'-C3' | 6.33 | 127.29 | 119.70 |
| 1 | A | 693 | G | C6-C5-N7 | -6.33 | 126.60 | 130.40 |
| 1 | A | 518 | C | N3-C2-O2 | -6.33 | 117.47 | 121.90 |
| 1 | A | 1338 | G | N3-C4-C5 | -6.33 | 125.44 | 128.60 |
| 1 | A | 814 | A | N1-C6-N6 | 6.32 | 122.39 | 118.60 |
| 1 | A | 1145 | C | N1-C2-O2 | 6.31 | 122.69 | 118.90 |
| 1 | A | 333 | G | N1-C6-O6 | 6.29 | 123.68 | 119.90 |
| 1 | A | 1492 | A | O4'-C1'-N9 | 6.26 | 113.21 | 108.20 |
| 1 | A | 484 | G | N1-C2-N2 | -6.26 | 110.57 | 116.20 |
| 1 | A | 662 | G | C2-N3-C4 | -6.25 | 108.77 | 111.90 |
| 1 | A | 1125 | U | C6-N1-C2 | 6.25 | 124.75 | 121.00 |
| 1 | A | 481 | G | C2-N3-C4 | 6.25 | 115.02 | 111.90 |
| 1 | A | 1530 | G | C8-N9-C1' | 6.25 | 135.12 | 127.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 675 | A | C2-N3-C4 | -6.23 | 107.48 | 110.60 |
| 1 | A | 1528 | U | O5'-P-OP1 | 6.23 | 118.18 | 110.70 |
| 1 | A | 1527 | C | C6-N1-C2 | 6.22 | 122.79 | 120.30 |
| 1 | A | 24 | U | C2-N3-C4 | -6.20 | 123.28 | 127.00 |
| 1 | A | 108 | G | C2-N3-C4 | -6.19 | 108.81 | 111.90 |
| 1 | A | 735 | C | C6-N1-C2 | 6.19 | 122.78 | 120.30 |
| 1 | A | 1377 | A | N1-C2-N3 | 6.18 | 132.39 | 129.30 |
| 1 | A | 1371 | G | O5'-P-OP1 | -6.18 | 100.14 | 105.70 |
| 1 | A | 723 | U | N3-C2-O2 | -6.17 | 117.88 | 122.20 |
| 1 | A | 117 | G | C5-C6-N1 | -6.15 | 108.43 | 111.50 |
| 1 | A | 1416 | G | C4-C5-C6 | 6.14 | 122.48 | 118.80 |
| 1 | A | 1395 | C | C6-N1-C2 | 6.14 | 122.75 | 120.30 |
| 1 | A | 898 | G | N1-C6-O6 | 6.13 | 123.58 | 119.90 |
| 1 | A | 1416 | G | N3-C4-C5 | -6.13 | 125.54 | 128.60 |
| 1 | A | 664 | G | N1-C6-O6 | -6.12 | 116.22 | 119.90 |
| 1 | A | 1100 | C | N1-C2-O2 | 6.12 | 122.57 | 118.90 |
| 1 | A | 266 | G | N7-C8-N9 | 6.12 | 116.16 | 113.10 |
| 1 | A | 279 | A | C4-C5-N7 | 6.12 | 113.76 | 110.70 |
| 1 | A | 122 | G | C8-N9-C4 | 6.11 | 108.85 | 106.40 |
| 1 | A | 1069 | C | C6-N1-C2 | 6.11 | 122.75 | 120.30 |
| 1 | A | 1502 | A | N7-C8-N9 | 6.10 | 116.85 | 113.80 |
| 1 | A | 108 | G | C4-C5-N7 | 6.10 | 113.24 | 110.80 |
| 1 | A | 482 | A | N1-C6-N6 | 6.10 | 122.26 | 118.60 |
| 1 | A | 1127 | G | C4-C5-N7 | 6.09 | 113.24 | 110.80 |
| 1 | A | 814 | A | C5-C6-N1 | -6.09 | 114.66 | 117.70 |
| 1 | A | 1139 | G | N3-C4-C5 | -6.07 | 125.56 | 128.60 |
| 1 | A | 536 | C | C6-N1-C2 | -6.07 | 117.87 | 120.30 |
| 1 | A | 975 | A | C6-C5-N7 | -6.06 | 128.06 | 132.30 |
| 1 | A | 279 | A | C2-N3-C4 | -6.05 | 107.58 | 110.60 |
| 1 | A | 1377 | A | C2-N3-C4 | -6.03 | 107.58 | 110.60 |
| 1 | A | 872 | A | N1-C6-N6 | 6.03 | 122.22 | 118.60 |
| 1 | A | 1299 | A | N7-C8-N9 | 6.03 | 116.81 | 113.80 |
| 1 | A | 266 | G | C4-C5-N7 | 6.02 | 113.21 | 110.80 |
| 1 | A | 701 | C | P-O3'-C3' | 6.01 | 126.92 | 119.70 |
| 1 | A | 265 | G | C4-C5-N7 | -6.01 | 108.40 | 110.80 |
| 1 | A | 220 | G | C6-C5-N7 | -6.00 | 126.80 | 130.40 |
| 1 | A | 279 | A | C6-C5-N7 | -6.00 | 128.10 | 132.30 |
| 1 | A | 1460 | A | C8-N9-C4 | 5.99 | 108.20 | 105.80 |
| 1 | A | 1502 | A | C5-C6-N6 | -5.97 | 118.92 | 123.70 |
| 1 | A | 279 | A | N1-C6-N6 | 5.97 | 122.18 | 118.60 |
| 1 | A | 310 | G | N7-C8-N9 | -5.96 | 110.12 | 113.10 |
| 1 | A | 260 | G | C5-C6-N1 | -5.95 | 108.52 | 111.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 781 | A | C8-N9-C4 | 5.95 | 108.18 | 105.80 |
| 3 | C | 4 | LYS | N-CA-C | 5.94 | 127.05 | 111.00 |
| 5 | E | 12 | LEU | CB-CG-CD2 | 5.92 | 121.07 | 111.00 |
| 1 | A | 485 | G | C8-N9-C4 | 5.91 | 108.76 | 106.40 |
| 1 | A | 778 | G | C5-C6-N1 | -5.89 | 108.56 | 111.50 |
| 1 | A | 482 | A | C6-C5-N7 | -5.88 | 128.19 | 132.30 |
| 1 | A | 117 | G | C4-C5-N7 | 5.86 | 113.14 | 110.80 |
| 1 | A | 960 | U | N1-C2-O2 | 5.85 | 126.90 | 122.80 |
| 1 | A | 753 | A | N1-C6-N6 | -5.85 | 115.09 | 118.60 |
| 1 | A | 526 | C | C5-C6-N1 | -5.85 | 118.08 | 121.00 |
| 5 | E | 15 | ARG | NE-CZ-NH2 | -5.85 | 117.38 | 120.30 |
| 1 | A | 1406 | U | N3-C2-O2 | -5.84 | 118.11 | 122.20 |
| 1 | A | 500 | G | C8-N9-C4 | 5.84 | 108.74 | 106.40 |
| 1 | A | 9 | G | C5-C6-O6 | -5.84 | 125.10 | 128.60 |
| 1 | A | 482 | A | C5-N7-C8 | -5.83 | 100.98 | 103.90 |
| 1 | A | 1279 | A | C6-C5-N7 | -5.83 | 128.22 | 132.30 |
| 1 | A | 236 | G | N1-C2-N2 | -5.82 | 110.96 | 116.20 |
| 1 | A | 723 | U | C6-N1-C2 | -5.82 | 117.51 | 121.00 |
| 1 | A | 1528 | U | OP1-P-OP2 | 5.80 | 128.30 | 119.60 |
| 1 | A | 1416 | G | C6-C5-N7 | -5.80 | 126.92 | 130.40 |
| 19 | S | 31 | ILE | N-CA-C | -5.80 | 95.35 | 111.00 |
| 1 | A | 16 | A | C8-N9-C4 | 5.79 | 108.12 | 105.80 |
| 1 | A | 960 | U | P-O3'-C3' | 5.78 | 126.64 | 119.70 |
| 1 | A | 1488 | G | N1-C6-O6 | 5.78 | 123.37 | 119.90 |
| 1 | A | 804 | U | C5-C4-O4 | 5.77 | 129.36 | 125.90 |
| 1 | A | 532 | A | P-O3'-C3' | 5.76 | 126.61 | 119.70 |
| 1 | A | 965 | A | C2-N3-C4 | -5.76 | 107.72 | 110.60 |
| 1 | A | 559 | A | C6-N1-C2 | -5.75 | 115.15 | 118.60 |
| 1 | A | 789 | U | C5-C4-O4 | 5.75 | 129.35 | 125.90 |
| 1 | A | 1335 | C | O4'-C1'-N1 | 5.75 | 112.80 | 108.20 |
| 1 | A | 724 | G | N3-C4-C5 | -5.74 | 125.73 | 128.60 |
| 1 | A | 24 | U | C5-C6-N1 | -5.74 | 119.83 | 122.70 |
| 1 | A | 235 | C | C6-N1-C2 | 5.73 | 122.59 | 120.30 |
| 1 | A | 1053 | G | N3-C4-C5 | 5.73 | 131.46 | 128.60 |
| 1 | A | 350 | G | N7-C8-N9 | 5.71 | 115.96 | 113.10 |
| 1 | A | 869 | G | N1-C6-O6 | -5.71 | 116.47 | 119.90 |
| 1 | A | 1500 | A | O5'-P-OP1 | -5.71 | 100.57 | 105.70 |
| 1 | A | 400 | C | C5-C6-N1 | -5.70 | 118.15 | 121.00 |
| 1 | A | 236 | G | N3-C4-N9 | 5.69 | 129.41 | 126.00 |
| 1 | A | 113 | G | C5-C6-O6 | -5.68 | 125.19 | 128.60 |
| 1 | A | 1442 | G | C4-N9-C1' | 5.67 | 133.88 | 126.50 |
| 1 | A | 350 | G | C8-N9-C4 | -5.67 | 104.13 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 1 | A | 1450 | U | O5'-P-OP2 | -5.66 | 100.61 | 105.70 |
| 1 | A | 1468 | A | C8-N9-C4 | 5.66 | 108.06 | 105.80 |
| 1 | A | 907 | A | C2-N3-C4 | -5.65 | 107.77 | 110.60 |
| 1 | A | 1416 | G | N3-C4-N9 | 5.65 | 129.39 | 126.00 |
| 1 | A | 901 | A | O5'-P-OP1 | -5.64 | 100.63 | 105.70 |
| 1 | A | 1498 | UR3 | P-O3'-C3' | 5.63 | 126.46 | 119.70 |
| 1 | A | 113 | G | N1-C6-O6 | 5.63 | 123.28 | 119.90 |
| 1 | A | 129(A) | G | P-O3'-C3' | 5.63 | 126.45 | 119.70 |
| 20 | T | 94 | ALA | N-CA-C | -5.63 | 95.80 | 111.00 |
| 1 | A | 1227 | A | C2-N3-C4 | -5.63 | 107.79 | 110.60 |
| 1 | A | 662 | G | C6-C5-N7 | -5.62 | 127.03 | 130.40 |
| 1 | A | 250 | A | O5'-P-OP2 | -5.62 | 100.64 | 105.70 |
| 1 | A | 830 | G | N3-C4-N9 | -5.61 | 122.63 | 126.00 |
| 1 | A | 242 | C | C6-N1-C2 | 5.61 | 122.54 | 120.30 |
| 15 | O | 34 | LEU | CA-CB-CG | -5.61 | 102.41 | 115.30 |
| 1 | A | 768 | A | OP2-P-O3' | 5.60 | 117.52 | 105.20 |
| 1 | A | 484 | G | P-O3'-C3' | 5.60 | 126.42 | 119.70 |
| 1 | A | 925 | G | C8-N9-C4 | 5.60 | 108.64 | 106.40 |
| 1 | A | 1145 | C | N3-C2-O2 | -5.59 | 117.99 | 121.90 |
| 3 | C | 25 | GLY | N-CA-C | -5.59 | 99.13 | 113.10 |
| 1 | A | 1227 | A | O4'-C1'-N9 | -5.59 | 103.73 | 108.20 |
| 1 | A | 975 | A | N1-C6-N6 | 5.58 | 121.95 | 118.60 |
| 1 | A | 1257 | U | C5-C6-N1 | 5.56 | 125.48 | 122.70 |
| 1 | A | 122 | G | C6-C5-N7 | -5.56 | 127.07 | 130.40 |
| 1 | A | 576 | G | N3-C4-C5 | -5.55 | 125.83 | 128.60 |
| 1 | A | 922 | G | N1-C2-N3 | 5.55 | 127.23 | 123.90 |
| 1 | A | 1279 | A | N7-C8-N9 | 5.54 | 116.57 | 113.80 |
| 1 | A | 518 | C | C6-N1-C1' | -5.54 | 114.15 | 120.80 |
| 1 | A | 1299 | A | C8-N9-C4 | -5.54 | 103.58 | 105.80 |
| 1 | A | 108 | G | C5-N7-C8 | -5.54 | 101.53 | 104.30 |
| 1 | A | 117 | G | C4-C5-C6 | 5.54 | 122.12 | 118.80 |
| 1 | A | 1127 | G | N1-C6-O6 | 5.53 | 123.22 | 119.90 |
| 1 | A | 115 | G | P-O3'-C3' | 5.53 | 126.33 | 119.70 |
| 1 | A | 1085 | U | N3-C2-O2 | 5.53 | 126.07 | 122.20 |
| 1 | A | 190(E) | U | O5'-P-OP2 | -5.52 | 100.73 | 105.70 |
| 1 | A | 10 | A | N1-C6-N6 | -5.52 | 115.29 | 118.60 |
| 1 | A | 41 | G | C5-C6-O6 | -5.52 | 125.29 | 128.60 |
| 1 | A | 687 | A | P-O3'-C3' | 5.52 | 126.32 | 119.70 |
| 1 | A | 1530 | G | C8-N9-C4 | 5.51 | 108.60 | 106.40 |
| 1 | A | 144 | G | C2-N3-C4 | -5.51 | 109.15 | 111.90 |
| 1 | A | 662 | G | N9-C4-C5 | -5.51 | 103.20 | 105.40 |
| 1 | A | 1163 | C | C6-N1-C2 | -5.50 | 118.10 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-------------|-------|-------------|----------|
| 1 | A | 1257 | U | C6-N1-C1' | -5.49 | 113.51 | 121.20 |
| 1 | A | 855 | G | C5-C6-N1 | -5.49 | 108.76 | 111.50 |
| 1 | A | 365 | U | C2-N1-C1' | 5.47 | 124.27 | 117.70 |
| 1 | A | 128 | G | N1-C6-O6 | 5.46 | 123.18 | 119.90 |
| 1 | A | 922 | G | N3-C2-N2 | -5.46 | 116.08 | 119.90 |
| 5 | E | 78 | HIS | CB-CA-C | -5.46 | 99.48 | 110.40 |
| 1 | A | 314 | C | N3-C4-C5 | 5.45 | 124.08 | 121.90 |
| 1 | A | 482 | A | C8-N9-C4 | -5.45 | 103.62 | 105.80 |
| 1 | A | 881 | G | C8-N9-C4 | 5.45 | 108.58 | 106.40 |
| 1 | A | 1030(B) | C | C6-N1-C2 | -5.44 | 118.12 | 120.30 |
| 1 | A | 484 | G | N3-C2-N2 | 5.44 | 123.71 | 119.90 |
| 1 | A | 839 | U | N1-C2-O2 | 5.43 | 126.60 | 122.80 |
| 1 | A | 1139 | G | C4-C5-N7 | -5.43 | 108.63 | 110.80 |
| 1 | A | 747 | C | C5-C6-N1 | -5.43 | 118.29 | 121.00 |
| 1 | A | 1127 | G | N9-C4-C5 | -5.42 | 103.23 | 105.40 |
| 1 | A | 640 | A | C8-N9-C4 | -5.41 | 103.64 | 105.80 |
| 1 | A | 817 | C | OP1-P-O3' | 5.40 | 117.09 | 105.20 |
| 1 | A | 41 | G | N1-C6-O6 | 5.39 | 123.13 | 119.90 |
| 1 | A | 389 | A | N7-C8-N9 | 5.38 | 116.49 | 113.80 |
| 1 | A | 662 | G | C5-C6-N1 | -5.37 | 108.81 | 111.50 |
| 1 | A | 869 | G | N3-C2-N2 | 5.36 | 123.65 | 119.90 |
| 1 | A | 1127 | G | N3-C4-N9 | 5.36 | 129.22 | 126.00 |
| 1 | A | 35 | G | N1-C6-O6 | 5.34 | 123.11 | 119.90 |
| 1 | A | 1257 | U | N3-C2-O2 | -5.34 | 118.46 | 122.20 |
| 1 | A | 747 | C | C6-N1-C2 | 5.33 | 122.43 | 120.30 |
| 1 | A | 1461 | G | C8-N9-C4 | 5.33 | 108.53 | 106.40 |
| 1 | A | 509 | A | C2'-C3'-O3' | 5.33 | 122.23 | 113.70 |
| 1 | A | 1227 | A | C4-N9-C1' | 5.33 | 135.88 | 126.30 |
| 1 | A | 723 | U | N1-C2-O2 | 5.32 | 126.53 | 122.80 |
| 1 | A | 1505 | G | C4-C5-C6 | 5.32 | 121.99 | 118.80 |
| 1 | A | 1409 | C | C5-C6-N1 | 5.32 | 123.66 | 121.00 |
| 1 | A | 376 | G | N3-C2-N2 | 5.32 | 123.62 | 119.90 |
| 1 | A | 133 | U | N3-C2-O2 | -5.32 | 118.48 | 122.20 |
| 1 | A | 578 | C | N3-C2-O2 | -5.31 | 118.18 | 121.90 |
| 1 | A | 117 | G | N1-C2-N3 | 5.31 | 127.09 | 123.90 |
| 1 | A | 1530 | G | N1-C2-N2 | 5.31 | 120.98 | 116.20 |
| 1 | A | 671 | G | C5-C6-O6 | -5.31 | 125.42 | 128.60 |
| 1 | A | 1030(B) | C | C2-N1-C1' | 5.31 | 124.64 | 118.80 |
| 1 | A | 1101 | A | C5-C6-N1 | -5.30 | 115.05 | 117.70 |
| 1 | A | 1065 | U | OP2-P-O3' | 5.30 | 116.87 | 105.20 |
| 1 | A | 776 | G | OP1-P-O3' | 5.29 | 116.84 | 105.20 |
| 1 | A | 975 | A | C4-C5-N7 | 5.28 | 113.34 | 110.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 329 | A | OP2-P-O3' | 5.28 | 116.81 | 105.20 |
| 1 | A | 242 | C | C5-C6-N1 | -5.28 | 118.36 | 121.00 |
| 1 | A | 248 | C | C6-N1-C2 | 5.28 | 122.41 | 120.30 |
| 1 | A | 276 | G | C8-N9-C4 | 5.28 | 108.51 | 106.40 |
| 1 | A | 897 | C | N3-C4-C5 | 5.28 | 124.01 | 121.90 |
| 1 | A | 736 | C | N3-C2-O2 | -5.27 | 118.21 | 121.90 |
| 1 | A | 1071 | C | C6-N1-C2 | 5.27 | 122.41 | 120.30 |
| 1 | A | 721 | G | N3-C4-N9 | 5.26 | 129.16 | 126.00 |
| 1 | A | 1338 | G | C8-N9-C4 | -5.26 | 104.29 | 106.40 |
| 1 | A | 965 | A | N9-C4-C5 | -5.26 | 103.70 | 105.80 |
| 1 | A | 220 | G | N1-C6-O6 | 5.26 | 123.05 | 119.90 |
| 1 | A | 44 | G | C2-N3-C4 | -5.25 | 109.27 | 111.90 |
| 1 | A | 289 | G | O5'-P-OP2 | -5.25 | 100.98 | 105.70 |
| 1 | A | 653 | A | C8-N9-C4 | -5.25 | 103.70 | 105.80 |
| 1 | A | 408 | A | OP2-P-O3' | 5.25 | 116.74 | 105.20 |
| 1 | A | 25 | C | C6-N1-C2 | 5.24 | 122.40 | 120.30 |
| 1 | A | 814 | A | C5-N7-C8 | -5.23 | 101.28 | 103.90 |
| 1 | A | 248 | C | C5-C6-N1 | -5.23 | 118.39 | 121.00 |
| 1 | A | 653 | A | C2-N3-C4 | 5.23 | 113.21 | 110.60 |
| 1 | A | 310 | G | C5-N7-C8 | 5.22 | 106.91 | 104.30 |
| 1 | A | 1125 | U | N1-C2-N3 | -5.22 | 111.77 | 114.90 |
| 1 | A | 1279 | A | C5-N7-C8 | -5.22 | 101.29 | 103.90 |
| 1 | A | 236 | G | N3-C4-C5 | -5.22 | 125.99 | 128.60 |
| 1 | A | 1530 | G | O5'-P-OP2 | -5.22 | 101.00 | 105.70 |
| 1 | A | 457 | C | C5-C6-N1 | 5.22 | 123.61 | 121.00 |
| 1 | A | 576 | G | N3-C4-N9 | 5.21 | 129.13 | 126.00 |
| 1 | A | 1342 | C | C6-N1-C2 | 5.21 | 122.38 | 120.30 |
| 1 | A | 798 | G | C8-N9-C4 | 5.21 | 108.48 | 106.40 |
| 1 | A | 1139 | G | N9-C4-C5 | 5.21 | 107.48 | 105.40 |
| 1 | A | 855 | G | C2-N3-C4 | -5.20 | 109.30 | 111.90 |
| 1 | A | 374 | A | N1-C2-N3 | 5.20 | 131.90 | 129.30 |
| 1 | A | 556 | C | C5-C6-N1 | -5.19 | 118.40 | 121.00 |
| 1 | A | 720 | C | N3-C2-O2 | -5.19 | 118.27 | 121.90 |
| 1 | A | 921 | U | C5-C6-N1 | -5.19 | 120.10 | 122.70 |
| 1 | A | 1202 | G | N9-C4-C5 | 5.19 | 107.48 | 105.40 |
| 1 | A | 1281 | U | N3-C4-C5 | -5.19 | 111.49 | 114.60 |
| 1 | A | 1502 | A | C5-C6-N1 | -5.19 | 115.11 | 117.70 |
| 1 | A | 277 | C | C5-C6-N1 | -5.18 | 118.41 | 121.00 |
| 1 | A | 814 | A | N3-C4-C5 | 5.18 | 130.42 | 126.80 |
| 1 | A | 117 | G | N9-C4-C5 | -5.16 | 103.33 | 105.40 |
| 1 | A | 122 | G | C4-C5-N7 | 5.16 | 112.86 | 110.80 |
| 1 | A | 236 | G | C5-C6-O6 | 5.16 | 131.69 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | A | 1222 | G | C5-C6-N1 | -5.16 | 108.92 | 111.50 |
| 1 | A | 481 | G | C5-C6-N1 | 5.15 | 114.08 | 111.50 |
| 1 | A | 1468 | A | N9-C4-C5 | -5.15 | 103.74 | 105.80 |
| 1 | A | 578 | C | C5-C6-N1 | -5.15 | 118.42 | 121.00 |
| 1 | A | 721 | G | C4-N9-C1' | 5.15 | 133.20 | 126.50 |
| 1 | A | 144 | G | N3-C4-C5 | 5.15 | 131.17 | 128.60 |
| 1 | A | 566 | G | N3-C4-C5 | 5.14 | 131.17 | 128.60 |
| 1 | A | 781 | A | N9-C4-C5 | -5.13 | 103.75 | 105.80 |
| 1 | A | 530 | G | OP2-P-O3' | 5.13 | 116.48 | 105.20 |
| 1 | A | 965 | A | N3-C4-C5 | 5.13 | 130.39 | 126.80 |
| 1 | A | 1396 | A | OP1-P-OP2 | 5.13 | 127.29 | 119.60 |
| 1 | A | 559 | A | N9-C4-C5 | 5.12 | 107.85 | 105.80 |
| 1 | A | 651 | C | N3-C2-O2 | 5.11 | 125.47 | 121.90 |
| 1 | A | 526 | C | O5'-P-OP1 | 5.11 | 116.83 | 110.70 |
| 1 | A | 748 | C | P-O3'-C3' | 5.11 | 125.83 | 119.70 |
| 1 | A | 1082 | G | C8-N9-C4 | 5.11 | 108.44 | 106.40 |
| 1 | A | 1081 | G | C2-N3-C4 | -5.10 | 109.35 | 111.90 |
| 1 | A | 897 | C | C5-C4-N4 | -5.09 | 116.64 | 120.20 |
| 1 | A | 1131 | G | N1-C6-O6 | 5.08 | 122.95 | 119.90 |
| 1 | A | 482 | A | C2-N3-C4 | -5.08 | 108.06 | 110.60 |
| 1 | A | 1442 | G | C2-N3-C4 | 5.08 | 114.44 | 111.90 |
| 1 | A | 855 | G | C8-N9-C4 | 5.08 | 108.43 | 106.40 |
| 1 | A | 565 | U | N3-C2-O2 | 5.08 | 125.76 | 122.20 |
| 1 | A | 740 | U | C5-C6-N1 | -5.08 | 120.16 | 122.70 |
| 1 | A | 1076 | C | N3-C4-C5 | 5.07 | 123.93 | 121.90 |
| 1 | A | 353 | A | C2-N3-C4 | -5.07 | 108.06 | 110.60 |
| 1 | A | 965 | A | N1-C6-N6 | 5.07 | 121.64 | 118.60 |
| 1 | A | 1530 | G | C4-C5-C6 | -5.04 | 115.78 | 118.80 |
| 1 | A | 735 | C | N3-C4-C5 | 5.03 | 123.91 | 121.90 |
| 1 | A | 1299 | A | C6-C5-N7 | -5.03 | 128.78 | 132.30 |
| 1 | A | 365 | U | N3-C4-O4 | 5.03 | 122.92 | 119.40 |
| 1 | A | 992 | U | P-O3'-C3' | 5.03 | 125.73 | 119.70 |
| 1 | A | 255 | G | C8-N9-C4 | 5.03 | 108.41 | 106.40 |
| 1 | A | 869 | G | N3-C4-N9 | 5.02 | 129.01 | 126.00 |
| 1 | A | 1393 | U | N3-C2-O2 | -5.02 | 118.69 | 122.20 |
| 1 | A | 1380 | U | P-O3'-C3' | 5.02 | 125.72 | 119.70 |
| 1 | A | 1145 | C | C6-N1-C2 | -5.01 | 118.30 | 120.30 |
| 1 | A | 562 | C | OP1-P-O3' | 5.01 | 116.23 | 105.20 |
| 1 | A | 190(D) | U | C2-N1-C1' | -5.01 | 111.69 | 117.70 |

There are no chirality outliers.

All (11) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 2 | B | 11 | LEU | Peptide |
| 2 | B | 8 | LYS | Peptide |
| 2 | B | 9 | GLU | Peptide |
| 3 | C | 166 | GLU | Peptide |
| 4 | D | 3 | ARG | Peptide |
| 4 | D | 35 | ARG | Peptide |
| 8 | H | 90 | GLY | Peptide |
| 10 | J | 12 | ASP | Peptide |
| 10 | J | 88 | LEU | Peptide |
| 20 | T | 12 | ALA | Peptide |
| 20 | T | 93 | GLU | Peptide |

5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 32687 | 0 | 16528 | 553 | 0 |
| 2 | B | 1900 | 0 | 1951 | 69 | 0 |
| 3 | C | 1612 | 0 | 1677 | 65 | 0 |
| 4 | D | 1703 | 0 | 1763 | 66 | 0 |
| 5 | E | 1146 | 0 | 1207 | 52 | 0 |
| 6 | F | 843 | 0 | 857 | 26 | 0 |
| 7 | G | 1257 | 0 | 1296 | 28 | 0 |
| 8 | H | 1116 | 0 | 1177 | 44 | 0 |
| 9 | I | 1010 | 0 | 1037 | 45 | 0 |
| 10 | J | 792 | 0 | 835 | 45 | 0 |
| 11 | K | 864 | 0 | 881 | 33 | 0 |
| 12 | L | 977 | 0 | 1060 | 40 | 0 |
| 13 | M | 937 | 0 | 995 | 25 | 0 |
| 14 | N | 492 | 0 | 529 | 29 | 0 |
| 15 | O | 729 | 0 | 768 | 36 | 0 |
| 16 | P | 700 | 0 | 720 | 15 | 0 |
| 17 | Q | 823 | 0 | 891 | 35 | 0 |
| 18 | R | 574 | 0 | 644 | 28 | 0 |
| 19 | S | 647 | 0 | 673 | 39 | 0 |
| 20 | T | 763 | 0 | 861 | 35 | 0 |
| 21 | U | 208 | 0 | 221 | 11 | 0 |
| 22 | A | 418 | 0 | 0 | 0 | 0 |
| 22 | B | 3 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 22 | C | 4 | 0 | 0 | 0 | 0 |
| 22 | D | 6 | 0 | 0 | 0 | 0 |
| 22 | E | 6 | 0 | 0 | 0 | 0 |
| 22 | F | 1 | 0 | 0 | 0 | 0 |
| 22 | H | 1 | 0 | 0 | 0 | 0 |
| 22 | K | 1 | 0 | 0 | 0 | 0 |
| 22 | L | 1 | 0 | 0 | 0 | 0 |
| 22 | N | 1 | 0 | 0 | 0 | 0 |
| 22 | O | 1 | 0 | 0 | 0 | 0 |
| 22 | P | 4 | 0 | 0 | 0 | 0 |
| 22 | Q | 3 | 0 | 0 | 0 | 0 |
| 22 | S | 1 | 0 | 0 | 0 | 0 |
| 23 | D | 1 | 0 | 0 | 0 | 0 |
| 23 | N | 1 | 0 | 0 | 0 | 0 |
| 24 | A | 1483 | 0 | 0 | 47 | 0 |
| 24 | C | 15 | 0 | 0 | 0 | 0 |
| 24 | D | 26 | 0 | 0 | 0 | 0 |
| 24 | E | 21 | 0 | 0 | 0 | 0 |
| 24 | F | 6 | 0 | 0 | 0 | 0 |
| 24 | H | 3 | 0 | 0 | 1 | 0 |
| 24 | K | 1 | 0 | 0 | 0 | 0 |
| 24 | L | 7 | 0 | 0 | 0 | 0 |
| 24 | M | 2 | 0 | 0 | 1 | 0 |
| 24 | N | 1 | 0 | 0 | 0 | 0 |
| 24 | O | 2 | 0 | 0 | 0 | 0 |
| 24 | P | 2 | 0 | 0 | 0 | 0 |
| 24 | Q | 7 | 0 | 0 | 2 | 0 |
| 24 | T | 1 | 0 | 0 | 0 | 0 |
| All | All | 53810 | 0 | 36571 | 1169 | 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 13.

All (1169) 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:A:481:G:HO2' | 1:A:482:A:H8 | 1.13 | 0.90 |
| 14:N:21:TYR:HE2 | 14:N:23:ARG:HE | 1.20 | 0.90 |
| 15:O:64:ARG:HG3 | 15:O:88:ARG:HH22 | 1.36 | 0.89 |
| 1:A:190(L):U:H3 | 20:T:105:SER:HG | 1.21 | 0.88 |
| 1:A:372:C:O2' | 24:A:3555:HOH:O | 1.93 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 13:M:10:PRO:HB2 | 13:M:18:ALA:HB1 | 1.58 | 0.86 |
| 2:B:178:ARG:HH21 | 8:H:74:PRO:HG3 | 1.38 | 0.85 |
| 1:A:745:C:N4 | 24:A:2511:HOH:O | 2.06 | 0.85 |
| 1:A:413:G:H8 | 1:A:428:G:H21 | 1.22 | 0.84 |
| 5:E:12:LEU:HD13 | 5:E:31:LEU:HB2 | 1.59 | 0.84 |
| 1:A:975:A:H5' | 1:A:975:A:H8 | 1.40 | 0.84 |
| 20:T:57:ARG:HH12 | 20:T:100:ILE:HD12 | 1.44 | 0.83 |
| 2:B:16:HIS:HB3 | 2:B:210:SER:HB2 | 1.58 | 0.83 |
| 1:A:1128:C:H5' | 9:I:16:ARG:HH22 | 1.42 | 0.83 |
| 4:D:11:LEU:HD13 | 4:D:66:ARG:HD2 | 1.57 | 0.82 |
| 3:C:35:GLU:HG3 | 3:C:95:THR:HG21 | 1.61 | 0.82 |
| 10:J:57:LYS:HD3 | 10:J:60:ARG:HH12 | 1.43 | 0.82 |
| 1:A:1491:G:H3' | 1:A:1492:A:H5'' | 1.61 | 0.82 |
| 10:J:38:ILE:HG13 | 10:J:71:LEU:HB3 | 1.61 | 0.81 |
| 1:A:677:U:H3 | 1:A:713:G:H22 | 1.27 | 0.80 |
| 8:H:4:ASP:OD2 | 8:H:85:ARG:NH1 | 2.14 | 0.80 |
| 12:L:24:VAL:HG13 | 12:L:98:TYR:HE2 | 1.43 | 0.80 |
| 3:C:91:LEU:HB3 | 3:C:99:VAL:HG11 | 1.62 | 0.80 |
| 1:A:975:A:H4' | 1:A:976:G:H5'' | 1.64 | 0.79 |
| 3:C:14:ILE:HB | 3:C:15:THR:HG23 | 1.65 | 0.79 |
| 1:A:376:G:H5'' | 16:P:5:ARG:HD2 | 1.64 | 0.79 |
| 1:A:1052:U:O2' | 24:A:3216:HOH:O | 2.01 | 0.79 |
| 1:A:337:C:N4 | 24:A:2760:HOH:O | 2.17 | 0.78 |
| 8:H:10:LEU:HD22 | 8:H:83:ILE:HD11 | 1.66 | 0.77 |
| 4:D:25:ARG:HA | 4:D:28:SER:HB3 | 1.67 | 0.77 |
| 11:K:57:THR:HG22 | 11:K:59:TYR:H | 1.49 | 0.77 |
| 12:L:27:LEU:O | 12:L:29:GLY:N | 2.18 | 0.77 |
| 1:A:393:A:N6 | 24:A:2968:HOH:O | 2.18 | 0.77 |
| 18:R:51:LEU:HD23 | 18:R:52:PRO:HD2 | 1.65 | 0.76 |
| 19:S:80:TYR:CE1 | 19:S:81:ARG:HD3 | 2.20 | 0.75 |
| 1:A:1047:G:H5'' | 14:N:4:LYS:HD3 | 1.69 | 0.75 |
| 1:A:279:A:OP2 | 17:Q:95:TYR:OH | 2.00 | 0.75 |
| 20:T:100:ILE:HB | 20:T:102:GLY:H | 1.52 | 0.75 |
| 1:A:1100:C:N4 | 24:A:3186:HOH:O | 2.19 | 0.74 |
| 8:H:17:THR:HG22 | 8:H:63:LEU:HG | 1.70 | 0.74 |
| 1:A:542:G:OP1 | 4:D:10:ARG:NH2 | 2.20 | 0.73 |
| 11:K:18:ARG:HB2 | 11:K:33:THR:HG23 | 1.70 | 0.73 |
| 12:L:33:ARG:HD3 | 12:L:62:SER:HB3 | 1.68 | 0.73 |
| 19:S:50:ALA:HB1 | 19:S:57:HIS:HB3 | 1.69 | 0.73 |
| 9:I:45:ALA:HA | 9:I:48:GLU:HG2 | 1.70 | 0.73 |
| 1:A:481:G:O2' | 1:A:482:A:H8 | 1.71 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1057:G:H5'' | 3:C:154:SER:HB2 | 1.70 | 0.72 |
| 8:H:83:ILE:HG13 | 8:H:137:VAL:HG22 | 1.72 | 0.72 |
| 12:L:28:LYS:HB3 | 12:L:30:ALA:HB2 | 1.71 | 0.72 |
| 18:R:46:GLU:OE2 | 18:R:46:GLU:N | 2.21 | 0.72 |
| 1:A:530:G:N3 | 1:A:530:G:H2' | 2.05 | 0.72 |
| 3:C:147:LYS:HD3 | 3:C:205:GLY:H | 1.55 | 0.72 |
| 1:A:80:G:H2' | 1:A:81:U:H5' | 1.72 | 0.71 |
| 1:A:1427:U:H2' | 1:A:1428:A:C8 | 2.26 | 0.71 |
| 1:A:1499:A:H1' | 1:A:1520[A]:G:H5' | 1.71 | 0.71 |
| 3:C:14:ILE:O | 3:C:16:ARG:N | 2.24 | 0.71 |
| 3:C:77:ILE:HG22 | 3:C:81:GLY:HA2 | 1.73 | 0.71 |
| 5:E:81:GLU:OE1 | 5:E:88:LYS:NZ | 2.20 | 0.71 |
| 14:N:8:GLU:HG2 | 14:N:11:LYS:HE3 | 1.71 | 0.71 |
| 1:A:673:G:H2' | 1:A:674:G:C8 | 2.26 | 0.70 |
| 8:H:41:ARG:NH2 | 8:H:123:GLU:OE2 | 2.24 | 0.70 |
| 21:U:17:THR:O | 21:U:22:ARG:NH1 | 2.24 | 0.70 |
| 1:A:1100:C:OP2 | 2:B:96:ARG:NH1 | 2.25 | 0.70 |
| 3:C:18:TRP:O | 3:C:21:ARG:NH1 | 2.23 | 0.70 |
| 1:A:298:A:N6 | 24:A:2223:HOH:O | 2.23 | 0.70 |
| 15:O:45:VAL:HG23 | 15:O:46:HIS:HD2 | 1.57 | 0.70 |
| 1:A:518:C:H2' | 1:A:530:G:C8 | 2.26 | 0.70 |
| 1:A:1196:U:OP1 | 1:A:1197:G:H5'' | 1.91 | 0.70 |
| 12:L:33:ARG:HB3 | 12:L:60:LEU:HD12 | 1.74 | 0.69 |
| 8:H:19:VAL:HG23 | 8:H:21:LYS:HG3 | 1.75 | 0.69 |
| 13:M:66:LEU:HA | 13:M:70:LEU:HD12 | 1.73 | 0.69 |
| 1:A:1196:U:O2' | 24:A:2229:HOH:O | 2.09 | 0.69 |
| 3:C:58:GLU:H | 3:C:65:ALA:HB3 | 1.56 | 0.69 |
| 1:A:975:A:H5' | 1:A:975:A:C8 | 2.26 | 0.69 |
| 1:A:1124:G:H4' | 10:J:38:ILE:HD13 | 1.74 | 0.68 |
| 10:J:6:ILE:HB | 10:J:72:VAL:HB | 1.74 | 0.68 |
| 15:O:70:LEU:HD21 | 15:O:77:ARG:HB2 | 1.75 | 0.68 |
| 1:A:1195:C:H3' | 1:A:1196:U:H5'' | 1.75 | 0.68 |
| 3:C:95:THR:HB | 3:C:97:LYS:HG2 | 1.75 | 0.68 |
| 12:L:86:ARG:HB3 | 12:L:101:VAL:HG22 | 1.76 | 0.68 |
| 1:A:1443:G:H5'' | 1:A:1446:A:H5' | 1.75 | 0.68 |
| 4:D:175:SER:HB3 | 4:D:186:LEU:HD21 | 1.76 | 0.68 |
| 17:Q:67:LYS:HA | 17:Q:70:ARG:HH12 | 1.59 | 0.68 |
| 2:B:47:THR:HA | 2:B:202:PRO:HG2 | 1.74 | 0.68 |
| 7:G:5:ARG:HG3 | 7:G:7:ALA:H | 1.59 | 0.68 |
| 12:L:38:THR:HG22 | 12:L:39:VAL:HG23 | 1.74 | 0.68 |
| 5:E:116:THR:HG23 | 5:E:117:ASP:OD2 | 1.93 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 16:P:22:THR:HA | 16:P:33:ILE:HG13 | 1.75 | 0.68 |
| 1:A:452:A:HO2' | 1:A:453:A:H8 | 1.41 | 0.67 |
| 1:A:1367:C:H5' | 10:J:60:ARG:HH21 | 1.57 | 0.67 |
| 10:J:53:PRO:HA | 14:N:41:ARG:HH21 | 1.58 | 0.67 |
| 1:A:1502:A:H2 | 1:A:1505:G:H1 | 1.43 | 0.67 |
| 3:C:142:MET:HE1 | 3:C:148:GLY:HA2 | 1.77 | 0.67 |
| 9:I:8:GLY:HA2 | 9:I:79:LEU:HD13 | 1.77 | 0.67 |
| 1:A:983:A:O2' | 1:A:1050:G:OP2 | 2.13 | 0.66 |
| 1:A:1281:U:H5' | 1:A:1282:C:C5 | 2.30 | 0.66 |
| 3:C:6:HIS:CD2 | 14:N:49:HIS:HB3 | 2.30 | 0.66 |
| 2:B:97:TRP:HH2 | 2:B:176:GLU:CD | 1.99 | 0.66 |
| 14:N:5:ALA:O | 14:N:8:GLU:HB3 | 1.95 | 0.66 |
| 2:B:42:ILE:HG13 | 2:B:203:GLY:HA2 | 1.76 | 0.66 |
| 6:F:14:LEU:HD22 | 6:F:18:GLN:HB3 | 1.77 | 0.66 |
| 1:A:972:C:H4' | 10:J:57:LYS:HG2 | 1.76 | 0.66 |
| 15:O:56:LEU:HA | 15:O:59:MET:HE2 | 1.77 | 0.66 |
| 1:A:1059:C:N4 | 24:A:2868:HOH:O | 2.28 | 0.66 |
| 1:A:1391:U:H2' | 1:A:1392:G:C8 | 2.31 | 0.66 |
| 5:E:64:ARG:O | 5:E:65:ASN:ND2 | 2.28 | 0.65 |
| 1:A:1392:G:N2 | 1:A:1502:A:H8 | 1.94 | 0.65 |
| 1:A:250:A:H4' | 1:A:251:G:O5' | 1.96 | 0.65 |
| 19:S:36:ARG:NH2 | 19:S:75:ALA:O | 2.29 | 0.65 |
| 5:E:20:GLN:HG2 | 5:E:25:ARG:HE | 1.62 | 0.65 |
| 20:T:74:LYS:HB2 | 20:T:76:ALA:H | 1.61 | 0.65 |
| 1:A:1128:C:O2' | 1:A:1130:A:OP1 | 2.13 | 0.65 |
| 3:C:36:ASP:OD1 | 3:C:59:ARG:NH2 | 2.30 | 0.65 |
| 4:D:100:ARG:NH2 | 4:D:102:ASP:OD2 | 2.28 | 0.65 |
| 1:A:1001:A:H2' | 1:A:1002:G:H8 | 1.62 | 0.65 |
| 1:A:1104:G:O5' | 2:B:111:ARG:NH1 | 2.29 | 0.65 |
| 4:D:4:TYR:OH | 4:D:7:PRO:O | 2.08 | 0.65 |
| 8:H:86:ILE:HG21 | 8:H:133:LEU:HD13 | 1.78 | 0.65 |
| 1:A:1515[B]:C:N4 | 1:A:1520[B]:G:O6 | 2.29 | 0.64 |
| 10:J:85:LEU:HA | 10:J:88:LEU:HD11 | 1.79 | 0.64 |
| 4:D:111:ALA:HB2 | 4:D:120:LEU:HD12 | 1.79 | 0.64 |
| 8:H:119:LEU:HB3 | 8:H:123:GLU:HB3 | 1.79 | 0.64 |
| 1:A:1103:C:H5'' | 2:B:98:LEU:HD22 | 1.78 | 0.64 |
| 1:A:1241:G:H2' | 1:A:1242:C:C6 | 2.33 | 0.64 |
| 1:A:1392:G:H21 | 1:A:1502:A:H8 | 1.44 | 0.64 |
| 1:A:538:G:H5'' | 12:L:114:LYS:HB2 | 1.80 | 0.64 |
| 1:A:99:C:N4 | 24:A:2677:HOH:O | 2.31 | 0.64 |
| 3:C:73:PRO:O | 3:C:77:ILE:HG12 | 1.98 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1415:G:H2' | 1:A:1416:G:H8 | 1.61 | 0.63 |
| 3:C:50:ALA:HB2 | 3:C:75:VAL:HB | 1.81 | 0.63 |
| 12:L:110:VAL:H | 12:L:122:THR:HG22 | 1.63 | 0.63 |
| 2:B:16:HIS:ND1 | 2:B:17:PHE:O | 2.29 | 0.63 |
| 16:P:74:LEU:HD13 | 16:P:79:VAL:HG21 | 1.80 | 0.63 |
| 19:S:10:PHE:O | 19:S:39:THR:OG1 | 2.15 | 0.63 |
| 2:B:126:GLU:O | 2:B:130:ARG:NH2 | 2.32 | 0.63 |
| 17:Q:40:LYS:HE2 | 17:Q:42:TYR:CZ | 2.33 | 0.63 |
| 1:A:1327:C:OP2 | 21:U:12:LYS:NZ | 2.31 | 0.63 |
| 1:A:1125:U:H3' | 24:A:3301:HOH:O | 1.98 | 0.63 |
| 4:D:150:GLU:H | 4:D:150:GLU:CD | 2.01 | 0.63 |
| 1:A:1226:C:H4' | 1:A:1227:A:OP1 | 1.99 | 0.63 |
| 1:A:1007:C:N4 | 1:A:1023:G:O6 | 2.32 | 0.62 |
| 1:A:1030(C):G:N2 | 1:A:1030(D):A:N1 | 2.45 | 0.62 |
| 11:K:57:THR:HG22 | 11:K:59:TYR:N | 2.13 | 0.62 |
| 21:U:6:ARG:HE | 21:U:15:ARG:CZ | 2.11 | 0.62 |
| 6:F:62:TRP:CH2 | 6:F:64:GLN:HB2 | 2.33 | 0.62 |
| 1:A:951:G:OP2 | 13:M:102:ARG:NH2 | 2.33 | 0.62 |
| 12:L:113:ARG:HH11 | 12:L:116:SER:H | 1.46 | 0.62 |
| 5:E:15:ARG:HG3 | 5:E:15:ARG:HH11 | 1.63 | 0.62 |
| 1:A:1373:G:H5'' | 7:G:36:LYS:HD2 | 1.81 | 0.62 |
| 1:A:598:U:H4' | 8:H:94:TYR:CD1 | 2.35 | 0.62 |
| 1:A:1305:G:OP2 | 21:U:2:GLY:N | 2.33 | 0.62 |
| 2:B:20:GLU:HB3 | 2:B:190:THR:HB | 1.82 | 0.62 |
| 8:H:51:VAL:HG22 | 8:H:52:ASP:H | 1.65 | 0.62 |
| 7:G:70:LYS:HB3 | 7:G:96:GLN:HG2 | 1.82 | 0.61 |
| 4:D:66:ARG:HH11 | 4:D:66:ARG:HG3 | 1.63 | 0.61 |
| 1:A:1281:U:H5' | 1:A:1282:C:H5 | 1.64 | 0.61 |
| 1:A:149:A:H2' | 1:A:150:C:C6 | 2.36 | 0.61 |
| 7:G:85:TYR:HD1 | 7:G:154:TYR:HE1 | 1.49 | 0.61 |
| 8:H:11:THR:HG22 | 8:H:15:ASN:HD21 | 1.65 | 0.61 |
| 4:D:61:LYS:HD2 | 4:D:207:TYR:OH | 2.01 | 0.61 |
| 5:E:11:ILE:HG22 | 5:E:31:LEU:HB3 | 1.82 | 0.61 |
| 10:J:8:LEU:HD22 | 10:J:96:ILE:HG22 | 1.83 | 0.61 |
| 3:C:51:GLY:O | 3:C:115:LEU:HD21 | 2.01 | 0.61 |
| 1:A:1139:G:O2' | 1:A:1140:C:OP2 | 2.16 | 0.61 |
| 5:E:78:HIS:HD2 | 5:E:142:LEU:HA | 1.65 | 0.61 |
| 13:M:49:THR:HB | 13:M:52:GLU:H | 1.66 | 0.61 |
| 3:C:138:VAL:HG23 | 3:C:151:VAL:HG23 | 1.82 | 0.60 |
| 5:E:31:LEU:HD22 | 5:E:43:LEU:HD11 | 1.83 | 0.60 |
| 9:I:16:ARG:HB2 | 9:I:64:THR:HG22 | 1.84 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:172:ILE:H | 2:B:172:ILE:HD12 | 1.65 | 0.60 |
| 5:E:64:ARG:CZ | 5:E:65:ASN:HB3 | 2.31 | 0.60 |
| 4:D:194:LEU:H | 4:D:194:LEU:HD22 | 1.66 | 0.60 |
| 7:G:16:LEU:HD13 | 9:I:44:VAL:HB | 1.82 | 0.60 |
| 11:K:41:THR:HG21 | 11:K:71:LYS:HB3 | 1.84 | 0.60 |
| 19:S:40:ILE:HD13 | 19:S:62:ILE:HD13 | 1.82 | 0.60 |
| 1:A:1435:G:H2' | 1:A:1436:U:C6 | 2.36 | 0.60 |
| 10:J:15:THR:O | 10:J:19:SER:HB2 | 2.02 | 0.60 |
| 13:M:4:ILE:HG23 | 13:M:57:ARG:HA | 1.84 | 0.60 |
| 16:P:34:GLU:OE1 | 16:P:55:ARG:NH1 | 2.30 | 0.60 |
| 3:C:76:VAL:O | 3:C:83:ARG:HG2 | 2.02 | 0.60 |
| 13:M:23:TYR:CD2 | 13:M:70:LEU:HD13 | 2.37 | 0.60 |
| 21:U:6:ARG:HG2 | 21:U:15:ARG:HH11 | 1.66 | 0.60 |
| 1:A:1346:A:N6 | 1:A:1375:A:OP2 | 2.33 | 0.60 |
| 14:N:42:ILE:O | 14:N:46:GLU:HG3 | 2.01 | 0.60 |
| 1:A:1366:C:O3' | 10:J:60:ARG:NH2 | 2.35 | 0.59 |
| 1:A:1054:C:H3' | 24:A:3211:HOH:O | 2.02 | 0.59 |
| 2:B:32:ILE:HD11 | 2:B:190:THR:HG23 | 1.84 | 0.59 |
| 18:R:34:TYR:HB3 | 18:R:69:THR:HG22 | 1.83 | 0.59 |
| 1:A:1174:G:H2' | 1:A:1175:G:H8 | 1.67 | 0.59 |
| 1:A:1241:G:H2' | 1:A:1242:C:H6 | 1.67 | 0.59 |
| 1:A:976:G:H22 | 1:A:1362:C:H5'' | 1.67 | 0.59 |
| 20:T:67:ALA:O | 20:T:73:HIS:ND1 | 2.35 | 0.59 |
| 20:T:33:ILE:HD13 | 20:T:63:ILE:HG12 | 1.84 | 0.59 |
| 1:A:948:C:H42 | 1:A:1233:G:H1 | 1.49 | 0.59 |
| 5:E:78:HIS:CD2 | 5:E:142:LEU:HA | 2.37 | 0.59 |
| 6:F:26:ILE:HG21 | 6:F:63:TYR:HE2 | 1.68 | 0.59 |
| 1:A:3:G:H1 | 4:D:87:GLY:H | 1.50 | 0.59 |
| 2:B:71:VAL:HG13 | 2:B:93:VAL:HB | 1.83 | 0.59 |
| 1:A:1232:U:H5'' | 9:I:124:GLN:O | 2.02 | 0.59 |
| 1:A:1497:G:H2' | 1:A:1498:UR3:H5' | 1.85 | 0.59 |
| 1:A:667:G:H4' | 15:O:51:HIS:ND1 | 2.17 | 0.59 |
| 1:A:371:G:C2' | 1:A:372:C:H5' | 2.32 | 0.59 |
| 1:A:410:G:OP1 | 4:D:30:LYS:NZ | 2.30 | 0.59 |
| 1:A:667:G:H4' | 15:O:51:HIS:CE1 | 2.38 | 0.59 |
| 8:H:21:LYS:O | 8:H:65:TYR:OH | 2.20 | 0.59 |
| 19:S:18:LYS:HD3 | 19:S:31:ILE:HD11 | 1.85 | 0.59 |
| 1:A:1510:U:H2' | 1:A:1511:G:C8 | 2.37 | 0.58 |
| 1:A:547:A:OP2 | 4:D:2:GLY:N | 2.36 | 0.58 |
| 11:K:20:TYR:CZ | 11:K:83:ILE:HD12 | 2.38 | 0.58 |
| 1:A:1277:C:HO2' | 1:A:1279:A:H8 | 1.51 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:682:G:H1 | 1:A:708:C:H42 | 1.50 | 0.58 |
| 2:B:107:THR:O | 2:B:110:GLN:HG3 | 2.03 | 0.58 |
| 7:G:102:ARG:O | 7:G:106:GLN:HG3 | 2.03 | 0.58 |
| 1:A:1126:U:H4' | 24:A:3272:HOH:O | 2.03 | 0.58 |
| 1:A:1126:U:C5 | 1:A:1127:G:N2 | 2.72 | 0.58 |
| 1:A:243:A:C2 | 1:A:246:A:C8 | 2.91 | 0.58 |
| 1:A:1441:G:H4' | 1:A:1442:G:C5 | 2.38 | 0.58 |
| 4:D:70:ILE:HG22 | 4:D:71:SER:O | 2.03 | 0.58 |
| 12:L:84:LEU:HD23 | 12:L:101:VAL:HG21 | 1.84 | 0.58 |
| 1:A:1442:G:N7 | 1:A:1446:A:N6 | 2.52 | 0.58 |
| 1:A:589:C:N4 | 24:A:2443:HOH:O | 2.31 | 0.58 |
| 12:L:24:VAL:HG13 | 12:L:98:TYR:CE2 | 2.32 | 0.58 |
| 2:B:17:PHE:HA | 2:B:44:LEU:HD11 | 1.84 | 0.58 |
| 1:A:1033:G:O6 | 1:A:1034:G:N2 | 2.37 | 0.58 |
| 1:A:827:U:H5'' | 1:A:828:A:OP2 | 2.03 | 0.58 |
| 2:B:21:ARG:HA | 2:B:39:ILE:HA | 1.86 | 0.58 |
| 1:A:524:G:H2' | 1:A:525:C:C6 | 2.39 | 0.58 |
| 1:A:560:U:H4' | 1:A:561:U:H5'' | 1.86 | 0.58 |
| 4:D:8:VAL:O | 4:D:11:LEU:N | 2.33 | 0.58 |
| 1:A:1415:G:H2' | 1:A:1416:G:C8 | 2.38 | 0.58 |
| 1:A:185:A:N6 | 24:A:2739:HOH:O | 2.36 | 0.58 |
| 1:A:371:G:O2' | 1:A:372:C:H5' | 2.03 | 0.58 |
| 4:D:13:ARG:HG2 | 4:D:38:TYR:O | 2.04 | 0.58 |
| 5:E:74:GLY:HA3 | 5:E:116:THR:HG22 | 1.85 | 0.58 |
| 12:L:27:LEU:C | 12:L:29:GLY:H | 2.07 | 0.58 |
| 5:E:17:ALA:HB2 | 5:E:26:PHE:CD2 | 2.38 | 0.57 |
| 13:M:3:ARG:HH12 | 13:M:9:ILE:HD11 | 1.69 | 0.57 |
| 10:J:63:PHE:HE2 | 14:N:58:LYS:HG2 | 1.69 | 0.57 |
| 7:G:26:PHE:HD1 | 7:G:101:LEU:HD22 | 1.68 | 0.57 |
| 15:O:26:GLU:HA | 15:O:81:LEU:HD11 | 1.86 | 0.57 |
| 19:S:39:THR:HG23 | 19:S:70:LYS:HD2 | 1.86 | 0.57 |
| 3:C:6:HIS:ND1 | 3:C:7:PRO:HD2 | 2.18 | 0.57 |
| 4:D:65:ARG:HG3 | 4:D:75:PHE:CG | 2.39 | 0.57 |
| 1:A:530:G:H4' | 1:A:531:U:OP2 | 2.04 | 0.57 |
| 2:B:105:PHE:O | 2:B:109:SER:OG | 2.19 | 0.57 |
| 11:K:123:LYS:HA | 11:K:126:ARG:HG2 | 1.85 | 0.57 |
| 20:T:10:LEU:HD23 | 20:T:13:LEU:H | 1.69 | 0.57 |
| 1:A:869:G:N7 | 24:A:3468:HOH:O | 2.33 | 0.57 |
| 1:A:255:G:N2 | 24:A:3205:HOH:O | 2.14 | 0.57 |
| 1:A:860:A:H2' | 1:A:861:G:O4' | 2.05 | 0.57 |
| 1:A:946:A:H2' | 1:A:947:G:C8 | 2.39 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:141:A:H1' | 1:A:182:U:O2 | 2.05 | 0.57 |
| 9:I:42:ARG:NH2 | 9:I:75:ASP:OD1 | 2.36 | 0.57 |
| 5:E:15:ARG:HH11 | 5:E:15:ARG:CG | 2.18 | 0.57 |
| 1:A:1179:A:OP2 | 9:I:93:ARG:NH2 | 2.38 | 0.56 |
| 3:C:155:GLY:HA3 | 3:C:163:ALA:HB1 | 1.87 | 0.56 |
| 10:J:40:LEU:HB2 | 10:J:69:ASN:HB2 | 1.86 | 0.56 |
| 1:A:235:C:H5' | 17:Q:70:ARG:HG2 | 1.87 | 0.56 |
| 8:H:41:ARG:HB3 | 8:H:41:ARG:NH1 | 2.20 | 0.56 |
| 1:A:1033:G:H2' | 1:A:1034:G:O4' | 2.04 | 0.56 |
| 8:H:113:SER:HB2 | 8:H:134:ILE:HD11 | 1.86 | 0.56 |
| 4:D:187:ARG:CZ | 4:D:188:LEU:H | 2.18 | 0.56 |
| 12:L:46:LYS:HE2 | 12:L:94:TRP:CE3 | 2.40 | 0.56 |
| 1:A:1112:C:N3 | 3:C:178:LEU:HD12 | 2.21 | 0.56 |
| 7:G:37:ASN:O | 7:G:41:ARG:HG2 | 2.06 | 0.56 |
| 18:R:38:GLU:HA | 18:R:41:LYS:HE2 | 1.88 | 0.56 |
| 1:A:1004:A:N6 | 1:A:1037:C:H42 | 2.04 | 0.56 |
| 1:A:296:U:O2' | 1:A:556:C:O2 | 2.18 | 0.56 |
| 2:B:69:LEU:HD21 | 2:B:93:VAL:HG23 | 1.87 | 0.56 |
| 10:J:61:GLU:OE2 | 14:N:45:ARG:NH1 | 2.34 | 0.56 |
| 1:A:1316:G:N1 | 1:A:1319:A:OP2 | 2.38 | 0.56 |
| 1:A:390:C:H2' | 1:A:391:G:C8 | 2.41 | 0.56 |
| 1:A:373:A:H1' | 1:A:481:G:N3 | 2.20 | 0.56 |
| 1:A:975:A:H4' | 1:A:976:G:C5' | 2.35 | 0.56 |
| 2:B:31:TYR:CD2 | 2:B:202:PRO:HG3 | 2.41 | 0.56 |
| 15:O:55:GLY:O | 15:O:59:MET:HG3 | 2.06 | 0.56 |
| 3:C:11:ARG:NH1 | 3:C:177:THR:O | 2.39 | 0.56 |
| 13:M:106:ASN:ND2 | 24:M:202:HOH:O | 2.38 | 0.56 |
| 5:E:97:GLY:N | 5:E:117:ASP:OD1 | 2.39 | 0.56 |
| 20:T:50:GLU:H | 20:T:99:LEU:HD12 | 1.70 | 0.56 |
| 19:S:39:THR:HA | 19:S:70:LYS:HA | 1.87 | 0.55 |
| 1:A:108:G:H5' | 1:A:109:A:H5'' | 1.89 | 0.55 |
| 2:B:101:MET:HA | 2:B:108:ILE:HG13 | 1.87 | 0.55 |
| 10:J:3:LYS:N | 10:J:77:PRO:HG3 | 2.21 | 0.55 |
| 15:O:4:THR:OG1 | 15:O:7:GLU:HG3 | 2.07 | 0.55 |
| 1:A:1040:U:H2' | 1:A:1041:A:C8 | 2.40 | 0.55 |
| 1:A:1149:C:OP1 | 9:I:9:ARG:NH1 | 2.39 | 0.55 |
| 1:A:1490:C:H2' | 1:A:1491:G:H5' | 1.89 | 0.55 |
| 1:A:235:C:N4 | 24:A:2170:HOH:O | 2.38 | 0.55 |
| 1:A:881:G:OP2 | 12:L:12:ARG:NH2 | 2.39 | 0.55 |
| 8:H:13:ILE:O | 8:H:17:THR:HG23 | 2.07 | 0.55 |
| 20:T:39:LYS:HB3 | 20:T:55:ILE:HG21 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 20:T:49:ALA:HB3 | 20:T:99:LEU:HG | 1.89 | 0.55 |
| 1:A:1442:G:N2 | 1:A:1447:G:N7 | 2.44 | 0.55 |
| 9:I:53:VAL:HB | 9:I:92:TYR:CE2 | 2.41 | 0.55 |
| 1:A:130:A:OP2 | 1:A:190(E):U:O2' | 2.19 | 0.55 |
| 1:A:114:U:O2' | 1:A:115:G:H5' | 2.06 | 0.55 |
| 18:R:73:ALA:HB3 | 18:R:79:LEU:HD12 | 1.89 | 0.55 |
| 1:A:1287:A:H2' | 1:A:1288:A:C8 | 2.41 | 0.55 |
| 1:A:537:G:H2' | 1:A:538:G:C8 | 2.41 | 0.55 |
| 1:A:912:C:OP1 | 12:L:46:LYS:NZ | 2.29 | 0.55 |
| 4:D:23:GLY:HA3 | 4:D:112:VAL:HG12 | 1.89 | 0.55 |
| 12:L:25:PRO:C | 12:L:27:LEU:H | 2.07 | 0.55 |
| 13:M:79:LYS:HA | 13:M:82:MET:HE2 | 1.88 | 0.55 |
| 1:A:1127:G:H5'' | 9:I:66:ARG:HH12 | 1.72 | 0.55 |
| 1:A:409:G:N2 | 24:A:3446:HOH:O | 2.39 | 0.55 |
| 20:T:92:LEU:O | 20:T:96:GLY:HA2 | 2.06 | 0.55 |
| 1:A:740:U:O2' | 1:A:741:G:H5' | 2.07 | 0.55 |
| 18:R:38:GLU:OE1 | 18:R:38:GLU:N | 2.39 | 0.55 |
| 1:A:1256:A:H4' | 1:A:1257:U:H5' | 1.89 | 0.55 |
| 1:A:1323:G:H2' | 1:A:1324:A:C8 | 2.42 | 0.55 |
| 3:C:156:ARG:H | 3:C:163:ALA:HA | 1.71 | 0.55 |
| 4:D:25:ARG:O | 4:D:25:ARG:HG2 | 2.07 | 0.55 |
| 9:I:43:ALA:HA | 9:I:74:ILE:HG12 | 1.88 | 0.55 |
| 1:A:974:A:OP1 | 14:N:29:ARG:NH2 | 2.40 | 0.55 |
| 1:A:1086:U:H3 | 1:A:1099:G:H22 | 1.52 | 0.54 |
| 1:A:939:G:H5' | 7:G:102:ARG:HH22 | 1.72 | 0.54 |
| 1:A:1297:C:OP2 | 13:M:44:ARG:NH2 | 2.40 | 0.54 |
| 6:F:100:ASN:H | 18:R:23:LYS:HD2 | 1.72 | 0.54 |
| 1:A:1527:C:H2' | 1:A:1528:U:C6 | 2.42 | 0.54 |
| 1:A:452:A:O2' | 1:A:453:A:H8 | 1.90 | 0.54 |
| 1:A:701:C:H5'' | 1:A:703:G:H5' | 1.89 | 0.54 |
| 1:A:881:G:P | 12:L:12:ARG:HH22 | 2.29 | 0.54 |
| 20:T:67:ALA:HA | 20:T:73:HIS:H | 1.72 | 0.54 |
| 3:C:79:ARG:O | 3:C:82:GLU:HG3 | 2.08 | 0.54 |
| 1:A:412:A:H61 | 4:D:35:ARG:HB3 | 1.73 | 0.54 |
| 13:M:108:ARG:HD3 | 13:M:114:ARG:CZ | 2.37 | 0.54 |
| 14:N:32:SER:O | 14:N:40:CYS:HA | 2.08 | 0.54 |
| 17:Q:86:GLU:O | 17:Q:90:ILE:HG13 | 2.08 | 0.54 |
| 15:O:3:ILE:HA | 15:O:7:GLU:OE1 | 2.08 | 0.54 |
| 18:R:47:THR:OG1 | 18:R:48:GLY:N | 2.39 | 0.54 |
| 3:C:6:HIS:CD2 | 3:C:9:GLY:H | 2.26 | 0.54 |
| 1:A:1126:U:H5' | 24:A:3271:HOH:O | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 8:H:21:LYS:O | 8:H:63:LEU:HD23 | 2.08 | 0.54 |
| 1:A:1406:U:H5' | 1:A:1518[B]:MA6:H1' | 1.90 | 0.53 |
| 10:J:27:ALA:HB1 | 10:J:34:VAL:HG21 | 1.90 | 0.53 |
| 1:A:390:C:O3' | 16:P:28:ARG:NH2 | 2.41 | 0.53 |
| 1:A:551:U:H2' | 1:A:552:U:C6 | 2.43 | 0.53 |
| 1:A:581:G:N7 | 24:A:3575:HOH:O | 2.40 | 0.53 |
| 2:B:18:GLY:HA2 | 2:B:42:ILE:HG12 | 1.90 | 0.53 |
| 1:A:372:C:H4' | 1:A:373:A:O5' | 2.08 | 0.53 |
| 1:A:714:G:H2' | 1:A:715:A:C8 | 2.43 | 0.53 |
| 1:A:957:U:O2 | 1:A:959:A:H8 | 1.90 | 0.53 |
| 1:A:1057:G:H5'' | 3:C:154:SER:CB | 2.39 | 0.53 |
| 1:A:581:G:N2 | 1:A:760:G:N7 | 2.55 | 0.53 |
| 4:D:76:ARG:HD3 | 4:D:207:TYR:CE2 | 2.44 | 0.53 |
| 10:J:4:ILE:HB | 10:J:74:ILE:HG13 | 1.90 | 0.53 |
| 16:P:8:ARG:NH2 | 16:P:15:PRO:HB3 | 2.23 | 0.53 |
| 1:A:1499:A:H1' | 1:A:1520[B]:G:H5' | 1.90 | 0.53 |
| 1:A:350:G:H5'' | 1:A:350:G:H8 | 1.74 | 0.53 |
| 1:A:352:C:H5' | 24:A:3246:HOH:O | 2.08 | 0.53 |
| 1:A:539:A:H2' | 1:A:540:G:C8 | 2.43 | 0.53 |
| 6:F:30:LEU:HD23 | 6:F:75:LEU:HD11 | 1.91 | 0.53 |
| 11:K:126:ARG:HH11 | 11:K:126:ARG:HG3 | 1.73 | 0.53 |
| 1:A:1201:A:H5'' | 24:A:3229:HOH:O | 2.08 | 0.53 |
| 8:H:120:THR:OG1 | 8:H:123:GLU:HB2 | 2.09 | 0.53 |
| 10:J:88:LEU:HD22 | 10:J:88:LEU:N | 2.23 | 0.53 |
| 1:A:1126:U:H2' | 1:A:1127:G:H5' | 1.90 | 0.53 |
| 1:A:748:C:H6 | 1:A:748:C:O5' | 1.92 | 0.53 |
| 4:D:142:PRO:HA | 4:D:185:PHE:HD2 | 1.73 | 0.53 |
| 4:D:64:LEU:HG | 4:D:198:VAL:HG11 | 1.91 | 0.53 |
| 8:H:11:THR:O | 8:H:15:ASN:ND2 | 2.42 | 0.53 |
| 1:A:1147:C:O2' | 9:I:16:ARG:HD3 | 2.09 | 0.53 |
| 1:A:1112:C:O2 | 3:C:179:ARG:HG3 | 2.09 | 0.53 |
| 1:A:1497:G:C2' | 1:A:1498:UR3:H5' | 2.38 | 0.53 |
| 1:A:658:G:H2' | 1:A:659:U:C6 | 2.44 | 0.53 |
| 1:A:836:G:C6 | 1:A:851:G:C6 | 2.97 | 0.53 |
| 1:A:1218:C:H2' | 1:A:1219:U:C6 | 2.44 | 0.52 |
| 1:A:1532:U:H6 | 1:A:1532:U:O5' | 1.92 | 0.52 |
| 1:A:923:A:OP1 | 5:E:21:ALA:HB2 | 2.08 | 0.52 |
| 6:F:45:LEU:HG | 6:F:59:TYR:HD1 | 1.73 | 0.52 |
| 11:K:12:ARG:HB2 | 11:K:75:TYR:HE2 | 1.73 | 0.52 |
| 1:A:748:C:H4' | 1:A:749:C:O5' | 2.08 | 0.52 |
| 1:A:731:G:OP1 | 1:A:766:A:H1' | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 6:F:80:ARG:HD3 | 6:F:88:VAL:HB | 1.92 | 0.52 |
| 16:P:19:ILE:HG22 | 16:P:36:ILE:HG13 | 1.91 | 0.52 |
| 1:A:110:C:H2' | 1:A:111:G:O4' | 2.09 | 0.52 |
| 1:A:658:G:H2' | 1:A:659:U:H6 | 1.72 | 0.52 |
| 1:A:792:A:H4' | 1:A:793:U:H5'' | 1.91 | 0.52 |
| 1:A:1375:A:P | 7:G:28:ASN:HD22 | 2.32 | 0.52 |
| 13:M:11:ARG:HA | 13:M:45:VAL:HG11 | 1.91 | 0.52 |
| 1:A:1196:U:O2' | 1:A:1197:G:OP1 | 2.25 | 0.52 |
| 1:A:1425:U:H2' | 1:A:1426:C:C6 | 2.44 | 0.52 |
| 1:A:1519[B]:MA6:C5 | 1:A:1520[B]:G:H1' | 2.39 | 0.52 |
| 1:A:806:C:H2' | 1:A:807:A:C8 | 2.45 | 0.52 |
| 10:J:16:LEU:HD12 | 10:J:70:ARG:HD2 | 1.90 | 0.52 |
| 10:J:76:ASN:OD1 | 10:J:76:ASN:N | 2.42 | 0.52 |
| 1:A:560:U:H5' | 1:A:566:G:N2 | 2.25 | 0.52 |
| 12:L:25:PRO:HB2 | 12:L:64:TYR:HE2 | 1.73 | 0.52 |
| 13:M:108:ARG:O | 13:M:111:LYS:N | 2.43 | 0.52 |
| 19:S:49:ILE:HD12 | 19:S:71:LEU:HD11 | 1.90 | 0.52 |
| 1:A:1279:A:OP1 | 10:J:99:LYS:NZ | 2.27 | 0.52 |
| 1:A:981:U:H5' | 14:N:21:TYR:CE1 | 2.45 | 0.52 |
| 1:A:1023:G:N2 | 1:A:1024:G:O2' | 2.43 | 0.52 |
| 1:A:1060:C:OP1 | 14:N:45:ARG:NH2 | 2.43 | 0.52 |
| 1:A:551:U:H2' | 1:A:552:U:H6 | 1.75 | 0.52 |
| 1:A:963:G:H5' | 24:A:2803:HOH:O | 2.09 | 0.52 |
| 21:U:6:ARG:HG2 | 21:U:15:ARG:NH1 | 2.25 | 0.52 |
| 1:A:1111:A:N1 | 3:C:177:THR:OG1 | 2.39 | 0.51 |
| 1:A:1191:A:H2' | 1:A:1192:C:C6 | 2.45 | 0.51 |
| 1:A:168:G:N2 | 24:A:3296:HOH:O | 2.26 | 0.51 |
| 2:B:131:PRO:HB2 | 2:B:133:LYS:HD2 | 1.91 | 0.51 |
| 3:C:35:GLU:OE1 | 3:C:59:ARG:NH1 | 2.40 | 0.51 |
| 9:I:4:TYR:CD2 | 9:I:88:TYR:HA | 2.45 | 0.51 |
| 11:K:124:LYS:HD2 | 11:K:125:PHE:CE1 | 2.46 | 0.51 |
| 1:A:1221:G:H4' | 19:S:77:THR:HG21 | 1.92 | 0.51 |
| 20:T:43:LEU:HD22 | 20:T:51:GLU:HB3 | 1.92 | 0.51 |
| 1:A:1511:G:H2' | 1:A:1512:U:O4' | 2.10 | 0.51 |
| 3:C:81:GLY:O | 3:C:84:ILE:HG22 | 2.10 | 0.51 |
| 1:A:434:U:H2' | 1:A:435:C:C6 | 2.45 | 0.51 |
| 3:C:191:THR:HG21 | 3:C:193:TYR:CE2 | 2.45 | 0.51 |
| 1:A:185:A:N3 | 20:T:81:LYS:NZ | 2.56 | 0.51 |
| 1:A:485:G:O2' | 1:A:486:U:P | 2.68 | 0.51 |
| 2:B:74:LYS:HD2 | 2:B:166:ASP:HB2 | 1.93 | 0.51 |
| 16:P:74:LEU:O | 16:P:79:VAL:HG23 | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:187:C:N3 | 20:T:105:SER:HB2 | 2.25 | 0.51 |
| 1:A:45:U:H2' | 1:A:46:G:C8 | 2.45 | 0.51 |
| 1:A:939:G:H5' | 7:G:102:ARG:NH2 | 2.26 | 0.51 |
| 10:J:65:LEU:HD12 | 14:N:56:VAL:HG22 | 1.92 | 0.51 |
| 19:S:38:SER:O | 19:S:71:LEU:N | 2.43 | 0.51 |
| 1:A:1192:C:H2' | 1:A:1193:G:O4' | 2.10 | 0.51 |
| 1:A:485:G:HO2' | 1:A:486:U:P | 2.32 | 0.51 |
| 5:E:78:HIS:O | 5:E:93:PRO:HD3 | 2.11 | 0.51 |
| 10:J:75:ILE:HG22 | 10:J:76:ASN:H | 1.76 | 0.51 |
| 1:A:1029:C:N4 | 1:A:1031:G:N7 | 2.58 | 0.51 |
| 1:A:256:U:H1' | 24:A:3207:HOH:O | 2.10 | 0.51 |
| 1:A:335:C:H2' | 1:A:336:C:C6 | 2.45 | 0.51 |
| 1:A:806:C:H2' | 1:A:807:A:H8 | 1.75 | 0.51 |
| 1:A:811:C:H4' | 1:A:900:A:N6 | 2.26 | 0.51 |
| 2:B:97:TRP:HZ2 | 2:B:102:LEU:HD13 | 1.76 | 0.51 |
| 3:C:17:ASP:O | 3:C:54:ARG:NH2 | 2.43 | 0.51 |
| 5:E:64:ARG:NH2 | 5:E:65:ASN:HB3 | 2.26 | 0.51 |
| 6:F:40:VAL:HB | 6:F:63:TYR:HD1 | 1.76 | 0.51 |
| 1:A:750:G:N3 | 15:O:23:GLY:HA3 | 2.25 | 0.51 |
| 1:A:390:C:H4' | 16:P:28:ARG:HH21 | 1.75 | 0.51 |
| 1:A:222:U:H2' | 1:A:223:U:C6 | 2.45 | 0.51 |
| 1:A:991:U:HO2' | 1:A:992:U:P | 2.33 | 0.51 |
| 2:B:101:MET:HG2 | 2:B:108:ILE:HG21 | 1.92 | 0.51 |
| 3:C:12:LEU:HD11 | 14:N:51:GLY:HA2 | 1.92 | 0.51 |
| 1:A:17:U:H2' | 1:A:18:C:C6 | 2.46 | 0.51 |
| 1:A:4:U:H4' | 1:A:5:U:OP2 | 2.10 | 0.51 |
| 1:A:659:U:OP2 | 15:O:8:LYS:NZ | 2.36 | 0.51 |
| 1:A:949:A:H2' | 1:A:950:U:O4' | 2.11 | 0.51 |
| 3:C:134:ILE:HG23 | 3:C:151:VAL:HB | 1.93 | 0.51 |
| 1:A:1106:G:H5'' | 3:C:172:ARG:HG2 | 1.92 | 0.51 |
| 4:D:35:ARG:O | 4:D:36:ARG:HG2 | 2.10 | 0.51 |
| 17:Q:22:LEU:HD12 | 17:Q:23:VAL:N | 2.26 | 0.51 |
| 19:S:40:ILE:HG23 | 19:S:44:MET:SD | 2.50 | 0.51 |
| 1:A:1269:A:H2 | 1:A:1312:G:N3 | 2.09 | 0.51 |
| 1:A:3:G:O6 | 4:D:86:LYS:HA | 2.11 | 0.51 |
| 3:C:134:ILE:HG21 | 3:C:167:TRP:O | 2.10 | 0.51 |
| 17:Q:27:PHE:CE1 | 17:Q:36:ILE:HD11 | 2.46 | 0.51 |
| 1:A:1277:C:O2' | 1:A:1279:A:H8 | 1.94 | 0.50 |
| 1:A:1350:A:OP1 | 9:I:121:ARG:NH1 | 2.44 | 0.50 |
| 2:B:97:TRP:HH2 | 2:B:176:GLU:OE1 | 1.94 | 0.50 |
| 5:E:98:THR:HB | 5:E:117:ASP:HB3 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:I:17:VAL:HG22 | 9:I:63:ILE:HD13 | 1.93 | 0.50 |
| 13:M:12:ASN:H | 13:M:45:VAL:HB | 1.76 | 0.50 |
| 1:A:1191:A:OP1 | 3:C:4:LYS:NZ | 2.37 | 0.50 |
| 1:A:129:U:O3' | 1:A:129(A):G:H3' | 2.10 | 0.50 |
| 1:A:1305:G:N2 | 1:A:1331:G:H1' | 2.26 | 0.50 |
| 5:E:8:GLU:HG2 | 5:E:34:VAL:HG22 | 1.93 | 0.50 |
| 6:F:16:GLN:HA | 6:F:16:GLN:OE1 | 2.11 | 0.50 |
| 1:A:216:G:H2' | 1:A:217:C:C6 | 2.46 | 0.50 |
| 1:A:436:C:H2' | 1:A:437:U:H6 | 1.76 | 0.50 |
| 1:A:689:C:OP1 | 11:K:27:ASN:ND2 | 2.43 | 0.50 |
| 1:A:1077:G:N2 | 1:A:1080:A:OP2 | 2.40 | 0.50 |
| 1:A:673:G:H5'' | 6:F:87:ARG:NH1 | 2.27 | 0.50 |
| 1:A:665:A:N3 | 1:A:732:C:H2' | 2.26 | 0.50 |
| 1:A:778:G:H8 | 1:A:778:G:O5' | 1.95 | 0.50 |
| 6:F:99:ALA:HB2 | 18:R:31:LEU:HG | 1.93 | 0.50 |
| 1:A:767:A:H2' | 1:A:768:A:O4' | 2.12 | 0.50 |
| 1:A:982:U:OP2 | 14:N:23:ARG:NH2 | 2.44 | 0.50 |
| 5:E:64:ARG:NH1 | 5:E:65:ASN:HB3 | 2.27 | 0.50 |
| 1:A:1174:G:H2' | 1:A:1175:G:C8 | 2.46 | 0.50 |
| 1:A:413:G:H4' | 1:A:413:G:OP1 | 2.12 | 0.50 |
| 1:A:1216:G:H5'' | 14:N:5:ALA:HB2 | 1.93 | 0.50 |
| 1:A:1223:C:OP1 | 19:S:78:ARG:NH2 | 2.41 | 0.50 |
| 1:A:1190:G:OP1 | 3:C:5:ILE:HG22 | 2.12 | 0.50 |
| 1:A:1168:A:H2' | 1:A:1169:A:C8 | 2.47 | 0.50 |
| 1:A:276:G:O2' | 17:Q:68:ARG:NH1 | 2.44 | 0.50 |
| 1:A:579:G:H5' | 1:A:728:A:H1' | 1.94 | 0.50 |
| 1:A:955:U:H2' | 1:A:956:U:H6 | 1.77 | 0.50 |
| 1:A:985:C:N4 | 24:A:2902:HOH:O | 2.45 | 0.50 |
| 17:Q:48:GLU:HB2 | 17:Q:50:LYS:HB3 | 1.94 | 0.50 |
| 17:Q:62:SER:OG | 17:Q:72:ARG:HG2 | 2.11 | 0.50 |
| 18:R:87:ARG:HH11 | 18:R:87:ARG:HA | 1.76 | 0.50 |
| 1:A:1240:U:C2 | 7:G:32:ARG:HD2 | 2.47 | 0.50 |
| 1:A:1328:C:OP1 | 21:U:21:TYR:OH | 2.25 | 0.50 |
| 1:A:1466:C:H2' | 1:A:1467:G:O4' | 2.12 | 0.50 |
| 1:A:520:A:OP1 | 12:L:52:LEU:HD12 | 2.11 | 0.50 |
| 2:B:17:PHE:HD1 | 2:B:18:GLY:H | 1.58 | 0.50 |
| 4:D:201:GLN:O | 4:D:205:GLU:HG3 | 2.11 | 0.50 |
| 10:J:9:ARG:HA | 10:J:68:HIS:O | 2.12 | 0.50 |
| 1:A:1125:U:H5'' | 24:A:3301:HOH:O | 2.12 | 0.49 |
| 1:A:1126:U:C4 | 1:A:1127:G:N3 | 2.79 | 0.49 |
| 1:A:758:G:N7 | 24:A:3576:HOH:O | 2.43 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:H:33:GLU:HG2 | 8:H:48:TYR:OH | 2.12 | 0.49 |
| 9:I:112:LYS:HA | 9:I:119:ALA:HB2 | 1.92 | 0.49 |
| 1:A:1189:C:OP1 | 14:N:58:LYS:NZ | 2.44 | 0.49 |
| 4:D:57:ARG:HB3 | 4:D:206:PHE:HB2 | 1.94 | 0.49 |
| 5:E:16:THR:O | 5:E:16:THR:OG1 | 2.30 | 0.49 |
| 1:A:1314:C:H41 | 19:S:4:SER:HB2 | 1.76 | 0.49 |
| 1:A:1057:G:H2' | 1:A:1058:G:O4' | 2.11 | 0.49 |
| 3:C:6:HIS:NE2 | 3:C:8:ILE:HB | 2.27 | 0.49 |
| 20:T:14:LYS:O | 20:T:17:ARG:HB3 | 2.12 | 0.49 |
| 1:A:1014:A:H4' | 19:S:14:HIS:CD2 | 2.48 | 0.49 |
| 1:A:1148:U:H2' | 1:A:1149:C:O4' | 2.12 | 0.49 |
| 1:A:560:U:H5' | 1:A:566:G:C2 | 2.47 | 0.49 |
| 2:B:240:GLN:OE1 | 2:B:240:GLN:N | 2.46 | 0.49 |
| 2:B:97:TRP:CH2 | 2:B:176:GLU:CD | 2.82 | 0.49 |
| 3:C:111:LEU:HD11 | 3:C:146:ALA:HB2 | 1.94 | 0.49 |
| 5:E:90:VAL:O | 5:E:120:THR:HA | 2.12 | 0.49 |
| 1:A:1118:C:H1' | 1:A:1179:A:C4 | 2.47 | 0.49 |
| 1:A:1502:A:H2 | 1:A:1505:G:N1 | 2.08 | 0.49 |
| 4:D:52:SER:O | 4:D:56:VAL:HG23 | 2.12 | 0.49 |
| 4:D:63:LYS:HD2 | 4:D:197:PRO:O | 2.13 | 0.49 |
| 4:D:3:ARG:HD3 | 4:D:71:SER:HB3 | 1.95 | 0.49 |
| 14:N:14:PRO:HB2 | 14:N:16:PHE:O | 2.12 | 0.49 |
| 1:A:620:C:H2' | 1:A:621:A:O4' | 2.13 | 0.49 |
| 4:D:36:ARG:N | 4:D:37:PRO:HD3 | 2.27 | 0.49 |
| 1:A:1167:A:H2' | 1:A:1168:A:C8 | 2.48 | 0.49 |
| 1:A:1181:G:H1' | 1:A:1182:G:C5 | 2.47 | 0.49 |
| 1:A:1424:C:H42 | 1:A:1476:G:H1 | 1.59 | 0.49 |
| 1:A:298:A:H2' | 1:A:299:G:O4' | 2.13 | 0.49 |
| 1:A:414:A:OP2 | 1:A:428:G:N2 | 2.35 | 0.49 |
| 18:R:58:LEU:HD22 | 18:R:62:GLU:HB3 | 1.95 | 0.49 |
| 1:A:1035:A:H2' | 1:A:1036:G:C8 | 2.48 | 0.49 |
| 1:A:1277:C:C6 | 1:A:1277:C:H3' | 2.48 | 0.49 |
| 14:N:11:LYS:HG3 | 14:N:12:ARG:O | 2.13 | 0.49 |
| 15:O:6:GLU:CD | 15:O:6:GLU:H | 2.16 | 0.49 |
| 17:Q:3:LYS:HD3 | 17:Q:61:GLU:O | 2.13 | 0.49 |
| 1:A:1036:G:N2 | 1:A:1037:C:H1' | 2.28 | 0.49 |
| 1:A:1101:A:H4' | 1:A:1102:A:O5' | 2.13 | 0.49 |
| 1:A:977:A:H2' | 1:A:978:A:H5'' | 1.95 | 0.49 |
| 17:Q:13:ASP:HA | 24:Q:307:HOH:O | 2.12 | 0.49 |
| 4:D:187:ARG:HH22 | 4:D:188:LEU:HD12 | 1.77 | 0.49 |
| 4:D:61:LYS:HD3 | 4:D:206:PHE:CE2 | 2.48 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:G:16:LEU:HD11 | 9:I:45:ALA:HB2 | 1.93 | 0.49 |
| 11:K:69:ALA:O | 11:K:73:MET:HG2 | 2.13 | 0.49 |
| 1:A:956:U:C2 | 1:A:1225:A:C2 | 3.01 | 0.48 |
| 1:A:1330:U:H2' | 1:A:1331:G:H5' | 1.94 | 0.48 |
| 1:A:1399:C:C2 | 1:A:1502:A:N6 | 2.81 | 0.48 |
| 3:C:148:GLY:HA3 | 3:C:172:ARG:O | 2.13 | 0.48 |
| 5:E:76:ILE:O | 5:E:93:PRO:HB3 | 2.12 | 0.48 |
| 1:A:7:G:N7 | 5:E:92:LYS:HD3 | 2.28 | 0.48 |
| 12:L:7:ILE:O | 12:L:11:VAL:HG23 | 2.13 | 0.48 |
| 13:M:22:ILE:HG21 | 13:M:66:LEU:HD13 | 1.94 | 0.48 |
| 17:Q:37:LYS:O | 17:Q:38:ARG:HD3 | 2.13 | 0.48 |
| 1:A:1338:G:H2' | 1:A:1339:A:C8 | 2.49 | 0.48 |
| 1:A:1366:C:H2' | 1:A:1367:C:C6 | 2.49 | 0.48 |
| 1:A:706:A:H1' | 11:K:29:ILE:HD11 | 1.94 | 0.48 |
| 1:A:1237:C:H4' | 1:A:1300:G:H22 | 1.78 | 0.48 |
| 1:A:1401:G:C2 | 1:A:1402:4OC:H1' | 2.48 | 0.48 |
| 1:A:444:C:N4 | 24:A:2334:HOH:O | 2.47 | 0.48 |
| 4:D:100:ARG:HH22 | 4:D:118:ARG:HH22 | 1.60 | 0.48 |
| 6:F:76:ALA:HB1 | 6:F:80:ARG:NH1 | 2.28 | 0.48 |
| 7:G:122:HIS:HA | 7:G:125:MET:HE2 | 1.96 | 0.48 |
| 15:O:3:ILE:HD11 | 15:O:34:LEU:HB3 | 1.95 | 0.48 |
| 1:A:1173:G:H2' | 1:A:1174:G:C8 | 2.48 | 0.48 |
| 1:A:1499:A:C1' | 1:A:1520[A]:G:H5' | 2.41 | 0.48 |
| 1:A:179:A:H2' | 1:A:180:U:C6 | 2.47 | 0.48 |
| 5:E:15:ARG:HG2 | 5:E:16:THR:N | 2.25 | 0.48 |
| 20:T:14:LYS:O | 20:T:18:GLN:HG2 | 2.12 | 0.48 |
| 1:A:1103:C:H2' | 1:A:1104:G:O4' | 2.14 | 0.48 |
| 1:A:1296:C:H4' | 1:A:1302:U:C5 | 2.48 | 0.48 |
| 1:A:182:U:OP2 | 1:A:182:U:H6 | 1.95 | 0.48 |
| 1:A:365:U:H5'' | 1:A:366:C:OP1 | 2.14 | 0.48 |
| 4:D:28:SER:OG | 4:D:30:LYS:N | 2.41 | 0.48 |
| 7:G:12:LEU:H | 7:G:12:LEU:HD12 | 1.77 | 0.48 |
| 9:I:79:LEU:HD22 | 9:I:83:ARG:HG2 | 1.95 | 0.48 |
| 10:J:4:ILE:HD12 | 10:J:74:ILE:HD12 | 1.96 | 0.48 |
| 1:A:739:C:O2' | 15:O:42:HIS:ND1 | 2.40 | 0.48 |
| 15:O:5:LYS:HZ3 | 15:O:5:LYS:H | 1.60 | 0.48 |
| 18:R:43:PHE:C | 18:R:51:LEU:HD12 | 2.34 | 0.48 |
| 4:D:153:ARG:HD3 | 4:D:181:MET:HG3 | 1.96 | 0.48 |
| 11:K:19:ALA:HB3 | 11:K:82:VAL:HG22 | 1.96 | 0.48 |
| 15:O:36:ILE:HG12 | 15:O:59:MET:HE3 | 1.96 | 0.48 |
| 1:A:1265:G:H8 | 1:A:1265:G:O5' | 1.97 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:165:C:H2' | 1:A:166:G:C8 | 2.47 | 0.48 |
| 1:A:403:C:OP1 | 4:D:136:PRO:HD2 | 2.14 | 0.48 |
| 12:L:46:LYS:N | 12:L:92:ASP:O | 2.42 | 0.48 |
| 1:A:1062:U:H2' | 1:A:1063:C:C6 | 2.49 | 0.48 |
| 1:A:1532:U:HO2' | 1:A:1533:C:H5 | 1.62 | 0.48 |
| 1:A:187:C:C2 | 20:T:105:SER:HB2 | 2.49 | 0.48 |
| 16:P:4:ILE:HG23 | 16:P:36:ILE:HD11 | 1.95 | 0.48 |
| 1:A:31:G:N2 | 24:A:3285:HOH:O | 2.46 | 0.48 |
| 2:B:162:ILE:HD13 | 2:B:162:ILE:HA | 1.61 | 0.48 |
| 5:E:63:ARG:HE | 5:E:63:ARG:HB2 | 1.46 | 0.48 |
| 8:H:41:ARG:HH11 | 8:H:41:ARG:HB3 | 1.79 | 0.48 |
| 9:I:89:ASN:HB3 | 9:I:92:TYR:HD1 | 1.78 | 0.48 |
| 1:A:1236:A:H4' | 1:A:1304:G:H4' | 1.96 | 0.48 |
| 1:A:262:A:C6 | 1:A:263:A:C6 | 3.02 | 0.48 |
| 1:A:276:G:O3' | 17:Q:68:ARG:NH1 | 2.43 | 0.48 |
| 1:A:922:G:H1 | 1:A:1395:C:H42 | 1.61 | 0.48 |
| 12:L:70:ILE:HD13 | 12:L:77:LEU:HD12 | 1.96 | 0.48 |
| 15:O:56:LEU:HD22 | 15:O:60:VAL:HG23 | 1.96 | 0.48 |
| 1:A:927:G:O2' | 1:A:1503:A:N7 | 2.46 | 0.47 |
| 1:A:353:A:H5' | 1:A:353:A:C8 | 2.48 | 0.47 |
| 19:S:30:LEU:HD22 | 19:S:50:ALA:HB2 | 1.96 | 0.47 |
| 19:S:64:GLU:O | 19:S:67:VAL:HG23 | 2.14 | 0.47 |
| 20:T:72:LEU:HA | 20:T:72:LEU:HD23 | 1.72 | 0.47 |
| 1:A:295:C:H2' | 1:A:296:U:O4' | 2.14 | 0.47 |
| 13:M:88:ARG:HD3 | 19:S:3:ARG:HH21 | 1.79 | 0.47 |
| 1:A:1317:C:OP2 | 14:N:17:LYS:HE3 | 2.14 | 0.47 |
| 15:O:87:ILE:HG22 | 15:O:88:ARG:N | 2.29 | 0.47 |
| 16:P:28:ARG:HG2 | 16:P:29:ASP:OD2 | 2.15 | 0.47 |
| 1:A:1053:G:H4' | 1:A:1054:C:H5' | 1.96 | 0.47 |
| 1:A:922:G:O2' | 1:A:1398:A:N1 | 2.29 | 0.47 |
| 1:A:750:G:H1' | 15:O:23:GLY:H | 1.79 | 0.47 |
| 11:K:48:ILE:HG22 | 11:K:49:GLY:N | 2.30 | 0.47 |
| 1:A:765:G:H5'' | 1:A:766:A:OP1 | 2.13 | 0.47 |
| 4:D:18:LYS:HD3 | 4:D:20:TYR:HE2 | 1.78 | 0.47 |
| 6:F:74:ASP:OD1 | 6:F:74:ASP:N | 2.47 | 0.47 |
| 9:I:50:LEU:HA | 9:I:53:VAL:HG22 | 1.96 | 0.47 |
| 11:K:29:ILE:HD12 | 11:K:30:VAL:N | 2.30 | 0.47 |
| 3:C:113:ALA:HB2 | 3:C:202:ILE:HG13 | 1.96 | 0.47 |
| 1:A:620:C:N1 | 4:D:135:LEU:HD13 | 2.29 | 0.47 |
| 1:A:878:G:H5' | 8:H:89:PRO:HG2 | 1.96 | 0.47 |
| 15:O:76:GLU:N | 15:O:79:ARG:HH21 | 2.12 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 17:Q:63:ARG:HG2 | 17:Q:64:PRO:HD2 | 1.96 | 0.47 |
| 1:A:1425:U:H3 | 1:A:1475:G:H1 | 1.63 | 0.47 |
| 1:A:165:C:H2' | 1:A:166:G:H8 | 1.79 | 0.47 |
| 7:G:113:GLU:HG2 | 7:G:119:ARG:HG2 | 1.95 | 0.47 |
| 10:J:26:ALA:HB1 | 10:J:84:GLN:HB3 | 1.96 | 0.47 |
| 1:A:1305:G:O2' | 1:A:1331:G:N2 | 2.47 | 0.47 |
| 1:A:499:A:H4' | 1:A:500:G:OP1 | 2.15 | 0.47 |
| 2:B:111:ARG:HH11 | 2:B:111:ARG:HG3 | 1.80 | 0.47 |
| 2:B:69:LEU:HB3 | 2:B:162:ILE:CD1 | 2.45 | 0.47 |
| 2:B:177:ALA:HB1 | 2:B:182:ILE:HB | 1.95 | 0.47 |
| 5:E:82:VAL:HG21 | 5:E:138:ALA:HA | 1.97 | 0.47 |
| 15:O:87:ILE:HG22 | 15:O:88:ARG:HD3 | 1.97 | 0.47 |
| 20:T:54:LYS:HA | 20:T:57:ARG:NH2 | 2.30 | 0.47 |
| 1:A:267:C:H2' | 1:A:268:C:H6 | 1.80 | 0.47 |
| 3:C:114:PRO:HA | 3:C:185:GLY:HA3 | 1.96 | 0.47 |
| 5:E:148:VAL:HG21 | 8:H:107:LEU:HD13 | 1.97 | 0.47 |
| 8:H:85:ARG:NE | 8:H:87:SER:O | 2.48 | 0.47 |
| 9:I:17:VAL:HG11 | 9:I:81:ILE:HA | 1.97 | 0.47 |
| 12:L:60:LEU:HD21 | 12:L:66:VAL:HG22 | 1.97 | 0.47 |
| 15:O:26:GLU:HG3 | 15:O:81:LEU:HG | 1.96 | 0.47 |
| 15:O:87:ILE:HG22 | 15:O:88:ARG:H | 1.80 | 0.47 |
| 17:Q:43:LEU:HD23 | 17:Q:43:LEU:HA | 1.53 | 0.47 |
| 1:A:263:A:OP1 | 20:T:79:ARG:NH1 | 2.48 | 0.47 |
| 1:A:1486:G:H2' | 1:A:1487:G:C8 | 2.50 | 0.47 |
| 1:A:662:G:O2' | 1:A:836:G:OP1 | 2.33 | 0.47 |
| 4:D:66:ARG:NH1 | 4:D:66:ARG:HG3 | 2.29 | 0.47 |
| 17:Q:6:LEU:HD12 | 17:Q:23:VAL:HG21 | 1.97 | 0.47 |
| 4:D:57:ARG:HG3 | 4:D:202:LEU:HD12 | 1.97 | 0.46 |
| 5:E:31:LEU:HA | 5:E:31:LEU:HD23 | 1.68 | 0.46 |
| 8:H:40:ALA:HB2 | 8:H:45:ILE:HD11 | 1.97 | 0.46 |
| 1:A:1277:C:H3' | 1:A:1277:C:H6 | 1.80 | 0.46 |
| 2:B:115:LEU:HD21 | 2:B:153:ARG:CZ | 2.45 | 0.46 |
| 3:C:96:GLY:N | 3:C:97:LYS:HZ2 | 2.13 | 0.46 |
| 8:H:119:LEU:CB | 8:H:123:GLU:HB3 | 2.45 | 0.46 |
| 1:A:1051:C:N4 | 24:A:3238:HOH:O | 2.48 | 0.46 |
| 1:A:1143:G:H2' | 1:A:1144:G:C8 | 2.50 | 0.46 |
| 1:A:976:G:H5' | 1:A:1358:U:O2' | 2.15 | 0.46 |
| 1:A:176:C:H2' | 1:A:177:C:H6 | 1.80 | 0.46 |
| 1:A:616:G:H1' | 1:A:625:G:N2 | 2.30 | 0.46 |
| 1:A:5:U:H4' | 1:A:6:G:O5' | 2.15 | 0.46 |
| 1:A:957:U:O2 | 1:A:959:A:C8 | 2.69 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:21:ARG:H | 2:B:21:ARG:HG2 | 1.42 | 0.46 |
| 3:C:150:LYS:HB3 | 3:C:201:TYR:HB2 | 1.98 | 0.46 |
| 1:A:1313:U:O4 | 19:S:4:SER:OG | 2.24 | 0.46 |
| 1:A:109:A:C6 | 1:A:326:G:C6 | 3.03 | 0.46 |
| 1:A:4:U:H6 | 1:A:4:U:H5'' | 1.81 | 0.46 |
| 18:R:61:LYS:O | 18:R:65:ILE:HG12 | 2.16 | 0.46 |
| 19:S:16:LEU:O | 19:S:20:LEU:HG | 2.15 | 0.46 |
| 20:T:36:LEU:HD23 | 20:T:36:LEU:HA | 1.71 | 0.46 |
| 1:A:1182:G:H4' | 1:A:1183:A:H5'' | 1.97 | 0.46 |
| 2:B:80:ILE:HD11 | 2:B:208:ILE:HG12 | 1.96 | 0.46 |
| 10:J:9:ARG:NH2 | 10:J:97:GLU:OE2 | 2.47 | 0.46 |
| 20:T:50:GLU:O | 20:T:100:ILE:HD11 | 2.16 | 0.46 |
| 1:A:242:C:H2' | 1:A:243:A:H5'' | 1.97 | 0.46 |
| 5:E:9:LYS:HB2 | 5:E:112:LEU:HD11 | 1.98 | 0.46 |
| 8:H:87:SER:HA | 8:H:93:VAL:HG13 | 1.98 | 0.46 |
| 11:K:84:VAL:HG11 | 11:K:91:ARG:HH11 | 1.81 | 0.46 |
| 1:A:1152:A:H2' | 1:A:1153:C:O4' | 2.16 | 0.46 |
| 1:A:299:G:H2' | 1:A:300:A:C8 | 2.50 | 0.46 |
| 1:A:606:G:H1' | 1:A:632:A:N6 | 2.30 | 0.46 |
| 1:A:689:C:H2' | 1:A:690:G:O4' | 2.16 | 0.46 |
| 2:B:23:ARG:HG3 | 2:B:24:TRP:H | 1.79 | 0.46 |
| 20:T:14:LYS:HB2 | 20:T:17:ARG:CZ | 2.45 | 0.46 |
| 1:A:279:A:H8 | 1:A:279:A:H5' | 1.81 | 0.46 |
| 1:A:353:A:H5' | 1:A:353:A:H8 | 1.80 | 0.46 |
| 1:A:448:A:C4 | 1:A:487:A:C2 | 3.04 | 0.46 |
| 1:A:554:C:O2' | 24:A:3278:HOH:O | 2.21 | 0.46 |
| 1:A:833:U:H2' | 1:A:834:C:C6 | 2.51 | 0.46 |
| 1:A:913:A:H4' | 1:A:914:A:H4' | 1.96 | 0.46 |
| 4:D:31:CYS:C | 4:D:33:MET:H | 2.18 | 0.46 |
| 8:H:90:GLY:O | 17:Q:34:LYS:HE2 | 2.15 | 0.46 |
| 1:A:965:A:H3' | 24:A:3435:HOH:O | 2.15 | 0.46 |
| 6:F:14:LEU:HB2 | 6:F:19:LEU:HD12 | 1.97 | 0.46 |
| 6:F:19:LEU:HD21 | 6:F:59:TYR:CZ | 2.51 | 0.46 |
| 7:G:51:GLN:HB2 | 7:G:58:PRO:HG3 | 1.98 | 0.46 |
| 12:L:75:HIS:ND1 | 12:L:75:HIS:C | 2.69 | 0.46 |
| 19:S:19:VAL:HG23 | 19:S:47:HIS:CD2 | 2.50 | 0.46 |
| 1:A:1493:A:H1' | 1:A:1494:G:P | 2.56 | 0.46 |
| 1:A:154:C:H1' | 24:A:3297:HOH:O | 2.16 | 0.46 |
| 1:A:29:G:N2 | 24:A:3277:HOH:O | 2.48 | 0.46 |
| 1:A:439:A:C4 | 1:A:497:A:C2 | 3.04 | 0.46 |
| 1:A:918:A:H2' | 1:A:919:A:C8 | 2.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:F:8:ILE:HD12 | 6:F:26:ILE:HD13 | 1.98 | 0.46 |
| 1:A:136:C:O4' | 16:P:1:MET:HG2 | 2.16 | 0.46 |
| 19:S:53:ASN:O | 19:S:77:THR:HG22 | 2.16 | 0.46 |
| 20:T:53:LEU:HD13 | 20:T:103:GLY:H | 1.81 | 0.46 |
| 1:A:1371:G:OP1 | 9:I:12:GLU:HB2 | 2.16 | 0.45 |
| 5:E:95:ALA:HB1 | 5:E:96:PRO:HD2 | 1.98 | 0.45 |
| 9:I:112:LYS:HG3 | 9:I:118:LYS:HA | 1.98 | 0.45 |
| 21:U:9:ARG:O | 21:U:13:ILE:HG12 | 2.16 | 0.45 |
| 1:A:1004:A:H5'' | 1:A:1025:U:C4 | 2.51 | 0.45 |
| 1:A:489:C:H2' | 1:A:490:G:H8 | 1.81 | 0.45 |
| 4:D:38:TYR:HD2 | 4:D:38:TYR:H | 1.64 | 0.45 |
| 5:E:141:GLN:HA | 5:E:143:ARG:HH12 | 1.79 | 0.45 |
| 8:H:51:VAL:HG21 | 8:H:60:ARG:NH1 | 2.31 | 0.45 |
| 10:J:79:ARG:HA | 10:J:79:ARG:NH1 | 2.31 | 0.45 |
| 1:A:974:A:OP2 | 14:N:41:ARG:NH1 | 2.48 | 0.45 |
| 15:O:5:LYS:CE | 15:O:5:LYS:H | 2.29 | 0.45 |
| 19:S:61:TYR:HD2 | 19:S:62:ILE:N | 2.14 | 0.45 |
| 1:A:691:G:H2' | 1:A:692:U:C6 | 2.50 | 0.45 |
| 18:R:36:ASN:OD1 | 18:R:39:VAL:HG12 | 2.17 | 0.45 |
| 1:A:1096:C:H2' | 1:A:1097:C:H6 | 1.82 | 0.45 |
| 1:A:1392:G:N2 | 1:A:1502:A:C8 | 2.80 | 0.45 |
| 1:A:1486:G:H2' | 1:A:1487:G:H8 | 1.82 | 0.45 |
| 2:B:68:ILE:O | 2:B:90:MET:HB3 | 2.16 | 0.45 |
| 2:B:73:THR:HG23 | 2:B:95:GLN:O | 2.17 | 0.45 |
| 5:E:11:ILE:HD13 | 5:E:11:ILE:HA | 1.51 | 0.45 |
| 11:K:124:LYS:HD2 | 11:K:125:PHE:CZ | 2.51 | 0.45 |
| 19:S:25:LYS:HD3 | 19:S:26:GLY:O | 2.17 | 0.45 |
| 20:T:104:LEU:HD23 | 20:T:104:LEU:HA | 1.66 | 0.45 |
| 1:A:1493:A:O2' | 1:A:1494:G:OP1 | 2.32 | 0.45 |
| 2:B:226:ARG:H | 2:B:226:ARG:HG2 | 1.57 | 0.45 |
| 3:C:191:THR:HG22 | 3:C:192:THR:HG23 | 1.99 | 0.45 |
| 4:D:202:LEU:HD13 | 4:D:202:LEU:HA | 1.70 | 0.45 |
| 8:H:20:TYR:HA | 8:H:65:TYR:CZ | 2.52 | 0.45 |
| 11:K:48:ILE:HD13 | 11:K:63:LEU:HB2 | 1.99 | 0.45 |
| 11:K:70:LYS:HB3 | 11:K:70:LYS:HE2 | 1.80 | 0.45 |
| 1:A:1070:U:H2' | 1:A:1071:C:H6 | 1.81 | 0.45 |
| 1:A:1480:G:C6 | 1:A:1481:U:C4 | 3.05 | 0.45 |
| 1:A:1514:C:H2' | 1:A:1515[A]:C:O4' | 2.17 | 0.45 |
| 1:A:660:G:H1 | 1:A:745:C:H42 | 1.65 | 0.45 |
| 2:B:98:LEU:HB2 | 2:B:101:MET:HG3 | 1.98 | 0.45 |
| 4:D:102:ASP:OD1 | 4:D:103:ASN:N | 2.48 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:28:PHE:CG | 5:E:51:VAL:HG23 | 2.52 | 0.45 |
| 17:Q:45:HIS:HB3 | 17:Q:72:ARG:HB3 | 1.99 | 0.45 |
| 17:Q:81:ARG:HH21 | 17:Q:84:LEU:HD11 | 1.81 | 0.45 |
| 1:A:761:G:H2' | 1:A:762:C:O4' | 2.16 | 0.45 |
| 1:A:828:A:H4' | 1:A:828:A:OP1 | 2.16 | 0.45 |
| 11:K:72:ALA:HB1 | 11:K:77:MET:HE2 | 1.97 | 0.45 |
| 20:T:23:ARG:HH11 | 20:T:23:ARG:HB3 | 1.82 | 0.45 |
| 1:A:1001:A:H2' | 1:A:1002:G:C8 | 2.47 | 0.45 |
| 1:A:1026:G:H3' | 1:A:1027:C:H5'' | 1.99 | 0.45 |
| 1:A:1152:A:O3' | 10:J:13:HIS:NE2 | 2.50 | 0.45 |
| 1:A:872:A:C8 | 1:A:874:G:C8 | 3.04 | 0.45 |
| 1:A:964:A:N6 | 24:A:2817:HOH:O | 2.39 | 0.45 |
| 7:G:91:VAL:HG13 | 7:G:95:ARG:HG2 | 1.99 | 0.45 |
| 14:N:23:ARG:HA | 14:N:29:ARG:O | 2.16 | 0.45 |
| 1:A:1004:A:H5'' | 1:A:1025:U:N3 | 2.31 | 0.45 |
| 1:A:389:A:C6 | 1:A:390:C:H1' | 2.52 | 0.45 |
| 1:A:442:C:H2' | 1:A:443:C:C6 | 2.52 | 0.45 |
| 4:D:65:ARG:HD2 | 4:D:72:GLU:HA | 1.99 | 0.45 |
| 1:A:1075:C:H5'' | 2:B:179:LYS:NZ | 2.31 | 0.45 |
| 1:A:600:C:H2' | 1:A:601:C:C6 | 2.51 | 0.45 |
| 1:A:602:A:H2' | 1:A:603:U:O4' | 2.16 | 0.45 |
| 1:A:614:A:H2' | 1:A:615:C:C6 | 2.52 | 0.45 |
| 1:A:806:C:O2' | 1:A:807:A:H5' | 2.17 | 0.45 |
| 1:A:922:G:H2' | 1:A:923:A:C8 | 2.52 | 0.45 |
| 5:E:30:ALA:O | 5:E:45:PHE:HA | 2.16 | 0.45 |
| 6:F:10:LEU:HD12 | 6:F:59:TYR:HB3 | 1.99 | 0.45 |
| 8:H:127:LEU:HD22 | 8:H:127:LEU:HA | 1.67 | 0.45 |
| 1:A:1233:G:OP2 | 9:I:124:GLN:HB3 | 2.16 | 0.45 |
| 1:A:192:U:O2' | 20:T:57:ARG:HG2 | 2.17 | 0.45 |
| 20:T:87:LYS:O | 20:T:91:LEU:HB2 | 2.17 | 0.45 |
| 1:A:1070:U:H2' | 1:A:1071:C:C6 | 2.53 | 0.44 |
| 1:A:1068:G:N2 | 1:A:1191:A:N3 | 2.53 | 0.44 |
| 1:A:975:A:N6 | 1:A:1366:C:O2' | 2.42 | 0.44 |
| 1:A:176:C:N4 | 24:A:3047:HOH:O | 2.48 | 0.44 |
| 7:G:111:ARG:NH1 | 7:G:113:GLU:OE2 | 2.48 | 0.44 |
| 7:G:26:PHE:CE2 | 7:G:30:ILE:HD11 | 2.52 | 0.44 |
| 1:A:1347:G:C8 | 9:I:107:ARG:HB3 | 2.52 | 0.44 |
| 10:J:39:PRO:HA | 10:J:70:ARG:HG3 | 1.98 | 0.44 |
| 19:S:49:ILE:HG22 | 19:S:51:VAL:HG22 | 2.00 | 0.44 |
| 1:A:1065:U:O2' | 1:A:1066:C:OP2 | 2.26 | 0.44 |
| 1:A:1148:U:O3' | 9:I:14:VAL:HG11 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|---------------------|--------------------------|-------------------|
| 1:A:1413:A:N1 | 1:A:1488:G:C2 | 2.86 | 0.44 |
| 1:A:1442:G:H5'' | 24:A:3034:HOH:O | 2.18 | 0.44 |
| 1:A:1502:A:C2 | 1:A:1504:G:C2 | 3.05 | 0.44 |
| 1:A:1406:U:C5' | 1:A:1518[B]:MA6:H1' | 2.47 | 0.44 |
| 1:A:558:G:C4 | 1:A:559:A:C2 | 3.05 | 0.44 |
| 1:A:663:A:H5'' | 18:R:61:LYS:HE3 | 1.99 | 0.44 |
| 1:A:725:G:O2' | 1:A:726:C:H5' | 2.16 | 0.44 |
| 1:A:973:G:O5' | 1:A:973:G:H8 | 2.00 | 0.44 |
| 14:N:25:VAL:HG12 | 14:N:38:GLY:O | 2.18 | 0.44 |
| 17:Q:57:VAL:HG12 | 17:Q:76:LEU:HA | 2.00 | 0.44 |
| 1:A:1369:C:H2' | 1:A:1370:G:C8 | 2.53 | 0.44 |
| 1:A:273:A:N6 | 1:A:274:A:N6 | 2.65 | 0.44 |
| 4:D:9:CYS:O | 4:D:12:CYS:HB2 | 2.17 | 0.44 |
| 8:H:104:ARG:HG3 | 8:H:138:TRP:CD2 | 2.52 | 0.44 |
| 1:A:103:C:P | 20:T:17:ARG:HH11 | 2.40 | 0.44 |
| 1:A:1332:A:H2' | 1:A:1333:A:C8 | 2.51 | 0.44 |
| 1:A:1465:C:H2' | 1:A:1466:C:O4' | 2.18 | 0.44 |
| 1:A:1491:G:H3' | 1:A:1492:A:C5' | 2.41 | 0.44 |
| 1:A:501:C:H2' | 1:A:502:G:H8 | 1.82 | 0.44 |
| 1:A:959:A:H3' | 1:A:960:U:H5'' | 1.99 | 0.44 |
| 1:A:99:C:H2' | 1:A:101:A:C8 | 2.53 | 0.44 |
| 4:D:127:THR:HG23 | 4:D:147:ALA:HB3 | 1.99 | 0.44 |
| 15:O:21:ASP:OD2 | 15:O:24:SER:HB3 | 2.17 | 0.44 |
| 15:O:8:LYS:O | 15:O:12:ILE:HG13 | 2.18 | 0.44 |
| 24:A:2434:HOH:O | 17:Q:98:LEU:HA | 2.18 | 0.44 |
| 19:S:30:LEU:HB3 | 19:S:31:ILE:H | 1.42 | 0.44 |
| 9:I:113:LYS:HG2 | 9:I:119:ALA:HA | 2.00 | 0.44 |
| 9:I:51:ARG:H | 9:I:51:ARG:HG2 | 1.56 | 0.44 |
| 11:K:58:PRO:HA | 11:K:90:GLY:HA3 | 2.00 | 0.44 |
| 1:A:1029:C:H2' | 1:A:1030:C:C6 | 2.53 | 0.44 |
| 1:A:1410:G:O6 | 1:A:1490:C:N4 | 2.50 | 0.44 |
| 1:A:256:U:OP1 | 17:Q:17:LYS:NZ | 2.33 | 0.44 |
| 7:G:85:TYR:CD1 | 7:G:154:TYR:HE1 | 2.31 | 0.44 |
| 21:U:6:ARG:HE | 21:U:15:ARG:NH1 | 2.15 | 0.44 |
| 1:A:1182:G:H5' | 1:A:1184:G:H5'' | 1.99 | 0.44 |
| 1:A:310:G:C5 | 1:A:311:C:C5 | 3.06 | 0.44 |
| 1:A:489:C:H2' | 1:A:490:G:C8 | 2.53 | 0.44 |
| 1:A:56:U:H2' | 1:A:57:G:C8 | 2.53 | 0.44 |
| 4:D:196:LEU:HA | 4:D:197:PRO:HD3 | 1.83 | 0.44 |
| 4:D:3:ARG:HG2 | 4:D:3:ARG:H | 1.50 | 0.44 |
| 6:F:67:MET:HE3 | 6:F:67:MET:HB2 | 1.87 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:H:104:ARG:HG3 | 8:H:138:TRP:CG | 2.53 | 0.44 |
| 12:L:38:THR:HB | 12:L:57:LYS:HB3 | 2.00 | 0.44 |
| 1:A:1072:G:C5 | 1:A:1073:U:C4 | 3.06 | 0.44 |
| 1:A:289:G:P | 24:A:2104:HOH:O | 2.76 | 0.44 |
| 1:A:325:A:H2' | 1:A:326:G:O4' | 2.17 | 0.44 |
| 2:B:222:ILE:O | 2:B:226:ARG:HG2 | 2.18 | 0.44 |
| 9:I:10:ARG:HG2 | 9:I:75:ASP:HB2 | 2.00 | 0.44 |
| 9:I:4:TYR:HB3 | 9:I:87:GLN:HG2 | 1.99 | 0.44 |
| 1:A:1300:G:C6 | 1:A:1334:G:C5 | 3.06 | 0.44 |
| 1:A:802:A:H2' | 1:A:803:G:O4' | 2.17 | 0.44 |
| 3:C:155:GLY:O | 3:C:196:LEU:HG | 2.18 | 0.44 |
| 10:J:92:THR:C | 10:J:94:VAL:H | 2.20 | 0.44 |
| 13:M:50:GLU:O | 13:M:54:VAL:HG23 | 2.18 | 0.44 |
| 1:A:1338:G:C6 | 1:A:1339:A:C6 | 3.06 | 0.43 |
| 1:A:1505:G:H8 | 1:A:1505:G:H3' | 1.84 | 0.43 |
| 1:A:659:U:H2' | 1:A:660:G:C8 | 2.53 | 0.43 |
| 3:C:108:ASN:HD21 | 3:C:144:SER:CB | 2.31 | 0.43 |
| 3:C:34:LEU:O | 3:C:38:ARG:HG3 | 2.17 | 0.43 |
| 12:L:83:VAL:HG21 | 12:L:100:ILE:HD13 | 1.99 | 0.43 |
| 19:S:30:LEU:HD23 | 19:S:48:THR:HG22 | 1.99 | 0.43 |
| 1:A:1505:G:H3' | 1:A:1505:G:C8 | 2.53 | 0.43 |
| 1:A:503:C:O2' | 1:A:504:C:H5' | 2.18 | 0.43 |
| 2:B:77:ALA:HB2 | 2:B:211:ILE:HD13 | 2.01 | 0.43 |
| 3:C:11:ARG:O | 3:C:14:ILE:O | 2.36 | 0.43 |
| 5:E:15:ARG:HH11 | 5:E:15:ARG:HB2 | 1.83 | 0.43 |
| 6:F:4:TYR:CZ | 6:F:72:VAL:HG21 | 2.53 | 0.43 |
| 1:A:1371:G:O3' | 9:I:69:GLY:HA3 | 2.18 | 0.43 |
| 3:C:58:GLU:HB3 | 10:J:92:THR:HG21 | 2.00 | 0.43 |
| 11:K:98:LEU:HD23 | 11:K:98:LEU:HA | 1.81 | 0.43 |
| 18:R:87:ARG:HA | 18:R:87:ARG:NH1 | 2.33 | 0.43 |
| 1:A:256:U:H2' | 1:A:257:G:C8 | 2.53 | 0.43 |
| 1:A:770:C:N4 | 24:A:2622:HOH:O | 2.34 | 0.43 |
| 1:A:857:C:H5'' | 1:A:857:C:H6 | 1.83 | 0.43 |
| 2:B:119:GLU:OE2 | 2:B:153:ARG:NH2 | 2.50 | 0.43 |
| 1:A:1191:A:H5'' | 3:C:4:LYS:NZ | 2.34 | 0.43 |
| 5:E:103:GLY:O | 5:E:106:PRO:HD2 | 2.18 | 0.43 |
| 6:F:55:ASP:HA | 6:F:56:PRO:HD3 | 1.79 | 0.43 |
| 15:O:33:THR:HG21 | 15:O:85:LEU:HD22 | 2.00 | 0.43 |
| 16:P:51:VAL:O | 16:P:52:ASP:HB3 | 2.18 | 0.43 |
| 1:A:1128:C:H5' | 9:I:16:ARG:NH2 | 2.20 | 0.43 |
| 1:A:1427:U:H2' | 1:A:1428:A:H8 | 1.79 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:216:G:H2' | 1:A:217:C:H6 | 1.83 | 0.43 |
| 1:A:911:U:H2' | 1:A:912:C:C6 | 2.53 | 0.43 |
| 1:A:953:G:H2' | 1:A:954:G:O4' | 2.17 | 0.43 |
| 6:F:46:ARG:HB2 | 6:F:60:PHE:CE1 | 2.53 | 0.43 |
| 19:S:36:ARG:H | 19:S:36:ARG:HG2 | 1.42 | 0.43 |
| 1:A:1356:G:O5' | 1:A:1356:G:H8 | 2.01 | 0.43 |
| 1:A:1411:C:O2' | 1:A:1412:C:H5' | 2.18 | 0.43 |
| 1:A:412:A:N6 | 4:D:35:ARG:HB3 | 2.33 | 0.43 |
| 3:C:111:LEU:HD13 | 3:C:111:LEU:HA | 1.65 | 0.43 |
| 4:D:8:VAL:HG12 | 4:D:21:LEU:HD13 | 1.99 | 0.43 |
| 5:E:13:ILE:HD13 | 5:E:13:ILE:HG21 | 1.76 | 0.43 |
| 7:G:26:PHE:CD1 | 7:G:101:LEU:HD22 | 2.50 | 0.43 |
| 9:I:82:ALA:O | 9:I:86:VAL:HG23 | 2.19 | 0.43 |
| 14:N:27:CYS:SG | 14:N:29:ARG:HB2 | 2.59 | 0.43 |
| 20:T:20:LEU:HD23 | 20:T:20:LEU:HA | 1.86 | 0.43 |
| 1:A:1310:G:N2 | 1:A:1327:C:O2 | 2.48 | 0.43 |
| 1:A:144:G:H1 | 1:A:178:C:H42 | 1.66 | 0.43 |
| 1:A:254:G:OP1 | 17:Q:67:LYS:O | 2.35 | 0.43 |
| 1:A:309:G:H1' | 1:A:608:A:C2 | 2.54 | 0.43 |
| 2:B:15:VAL:HG21 | 2:B:213:LEU:HD12 | 2.00 | 0.43 |
| 8:H:98:LYS:HG2 | 8:H:98:LYS:H | 1.57 | 0.43 |
| 1:A:734:G:H21 | 18:R:75:ILE:HD11 | 1.83 | 0.43 |
| 19:S:44:MET:O | 19:S:47:HIS:HB2 | 2.18 | 0.43 |
| 1:A:1342:C:H2' | 1:A:1343:G:C8 | 2.54 | 0.43 |
| 1:A:1426:C:H2' | 1:A:1427:U:C6 | 2.53 | 0.43 |
| 2:B:45:GLN:O | 2:B:49:GLU:HG3 | 2.19 | 0.43 |
| 3:C:178:LEU:H | 3:C:178:LEU:HD12 | 1.83 | 0.43 |
| 1:A:1232:U:OP1 | 9:I:126:SER:HB2 | 2.18 | 0.43 |
| 17:Q:31:LEU:HA | 17:Q:31:LEU:HD12 | 1.79 | 0.43 |
| 1:A:1073:U:O2 | 2:B:104:ASN:ND2 | 2.51 | 0.43 |
| 1:A:1309:G:N7 | 13:M:99:ARG:NH2 | 2.67 | 0.43 |
| 1:A:1495:U:H2' | 1:A:1496:C:C6 | 2.54 | 0.43 |
| 1:A:501:C:H2' | 1:A:502:G:C8 | 2.53 | 0.43 |
| 4:D:76:ARG:HD2 | 4:D:76:ARG:HA | 1.79 | 0.43 |
| 10:J:36:GLY:HA2 | 10:J:37:PRO:HD3 | 1.81 | 0.43 |
| 13:M:99:ARG:HH12 | 19:S:2:PRO:HG2 | 1.83 | 0.43 |
| 15:O:50:HIS:O | 15:O:53:HIS:HB3 | 2.19 | 0.43 |
| 1:A:1053:G:O2' | 1:A:1199:U:H5 | 2.01 | 0.43 |
| 1:A:115:G:H1' | 1:A:116:A:N7 | 2.34 | 0.43 |
| 1:A:1387:G:C6 | 1:A:1388:C:C4 | 3.07 | 0.43 |
| 1:A:924:C:O2' | 1:A:1502:A:N6 | 2.49 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:166:ASP:HB3 | 2:B:169:LYS:HB3 | 2.01 | 0.43 |
| 3:C:29:TYR:HE1 | 10:J:11:PHE:CE1 | 2.37 | 0.43 |
| 3:C:45:LYS:HB2 | 3:C:45:LYS:HE3 | 1.82 | 0.43 |
| 8:H:100:ILE:HA | 8:H:101:PRO:HD2 | 1.78 | 0.43 |
| 13:M:3:ARG:HB2 | 13:M:3:ARG:HH11 | 1.84 | 0.43 |
| 17:Q:3:LYS:HB3 | 17:Q:61:GLU:HB3 | 2.01 | 0.43 |
| 1:A:1095:U:H5'' | 1:A:1109:C:O2 | 2.19 | 0.43 |
| 1:A:130:A:H1' | 1:A:263:A:O2' | 2.19 | 0.43 |
| 1:A:1367:C:H5' | 10:J:60:ARG:NH2 | 2.28 | 0.43 |
| 1:A:591:U:H2' | 1:A:592:G:C8 | 2.53 | 0.43 |
| 1:A:958:A:C6 | 1:A:959:A:N1 | 2.87 | 0.43 |
| 5:E:131:ILE:HD13 | 5:E:131:ILE:HA | 1.82 | 0.43 |
| 5:E:69:VAL:HA | 5:E:70:PRO:HD3 | 1.78 | 0.43 |
| 7:G:79:ARG:NH2 | 7:G:82:GLY:HA2 | 2.33 | 0.43 |
| 18:R:26:LEU:HD12 | 18:R:27:GLY:H | 1.84 | 0.43 |
| 19:S:40:ILE:HG21 | 19:S:62:ILE:HD11 | 2.01 | 0.43 |
| 1:A:1314:C:C5 | 19:S:6:LYS:HE2 | 2.54 | 0.43 |
| 1:A:1196:U:HO2' | 1:A:1197:G:P | 2.39 | 0.42 |
| 1:A:235:C:N4 | 24:A:2169:HOH:O | 2.52 | 0.42 |
| 1:A:795:C:H5'' | 1:A:796:C:OP2 | 2.19 | 0.42 |
| 11:K:81:ASP:OD2 | 11:K:106:LYS:HE3 | 2.19 | 0.42 |
| 12:L:102:ARG:HE | 12:L:102:ARG:HB3 | 1.67 | 0.42 |
| 1:A:974:A:P | 14:N:41:ARG:HH12 | 2.42 | 0.42 |
| 19:S:31:ILE:HG22 | 19:S:49:ILE:HA | 2.01 | 0.42 |
| 1:A:1468:A:H2' | 1:A:1469:G:O4' | 2.19 | 0.42 |
| 1:A:406:G:N2 | 1:A:437:U:C2 | 2.87 | 0.42 |
| 1:A:485:G:O2' | 1:A:486:U:O5' | 2.36 | 0.42 |
| 1:A:689:C:P | 11:K:46:GLY:HA3 | 2.59 | 0.42 |
| 7:G:111:ARG:HB3 | 7:G:113:GLU:OE2 | 2.19 | 0.42 |
| 17:Q:53:LEU:HD23 | 17:Q:82:MET:SD | 2.59 | 0.42 |
| 1:A:1011:G:H2' | 1:A:1012:U:O4' | 2.19 | 0.42 |
| 1:A:1143:G:H2' | 1:A:1144:G:H8 | 1.83 | 0.42 |
| 1:A:1229:A:OP1 | 13:M:116:THR:OG1 | 2.32 | 0.42 |
| 1:A:1103:C:C5' | 2:B:98:LEU:HD22 | 2.46 | 0.42 |
| 3:C:195:VAL:C | 3:C:196:LEU:HD12 | 2.40 | 0.42 |
| 5:E:36:ASP:O | 5:E:38:GLN:HG2 | 2.18 | 0.42 |
| 8:H:83:ILE:HG23 | 8:H:83:ILE:O | 2.20 | 0.42 |
| 1:A:1171:G:O2' | 1:A:1172:C:H5' | 2.20 | 0.42 |
| 1:A:665:A:H1' | 1:A:733:A:O4' | 2.20 | 0.42 |
| 1:A:765:G:N2 | 1:A:813:U:OP2 | 2.48 | 0.42 |
| 3:C:188:LEU:HD11 | 3:C:195:VAL:HG22 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 4:D:24:GLU:O | 4:D:25:ARG:HB3 | 2.20 | 0.42 |
| 4:D:31:CYS:SG | 4:D:31:CYS:O | 2.77 | 0.42 |
| 9:I:118:LYS:O | 9:I:120:ARG:N | 2.48 | 0.42 |
| 9:I:8:GLY:N | 9:I:83:ARG:HD2 | 2.34 | 0.42 |
| 10:J:57:LYS:O | 10:J:60:ARG:NH1 | 2.53 | 0.42 |
| 1:A:880:C:OP1 | 12:L:8:ASN:ND2 | 2.52 | 0.42 |
| 14:N:22:THR:HB | 14:N:33:VAL:HG21 | 2.02 | 0.42 |
| 18:R:51:LEU:CD2 | 18:R:52:PRO:HD2 | 2.42 | 0.42 |
| 19:S:19:VAL:HG21 | 19:S:44:MET:HA | 2.01 | 0.42 |
| 1:A:1481:U:H2' | 1:A:1482:G:O4' | 2.20 | 0.42 |
| 1:A:149:A:H2' | 1:A:150:C:H6 | 1.83 | 0.42 |
| 1:A:1518[A]:MA6:H93 | 1:A:1519[A]:MA6:H92 | 2.01 | 0.42 |
| 1:A:436:C:H2' | 1:A:437:U:C6 | 2.53 | 0.42 |
| 1:A:875:C:H1' | 8:H:15:ASN:OD1 | 2.19 | 0.42 |
| 4:D:103:ASN:O | 4:D:107:ARG:HB2 | 2.19 | 0.42 |
| 4:D:57:ARG:CG | 4:D:202:LEU:HD12 | 2.49 | 0.42 |
| 5:E:148:VAL:O | 5:E:152:ARG:HG2 | 2.20 | 0.42 |
| 5:E:71:LEU:HD11 | 5:E:113:ALA:O | 2.20 | 0.42 |
| 8:H:51:VAL:HG21 | 8:H:60:ARG:HH12 | 1.85 | 0.42 |
| 10:J:41:PRO:O | 10:J:69:ASN:ND2 | 2.53 | 0.42 |
| 13:M:14:ARG:CZ | 13:M:42:ALA:HA | 2.49 | 0.42 |
| 14:N:14:PRO:O | 14:N:15:LYS:HB3 | 2.19 | 0.42 |
| 17:Q:45:HIS:H | 17:Q:72:ARG:HA | 1.84 | 0.42 |
| 1:A:1325:C:H2' | 1:A:1326:C:H6 | 1.85 | 0.42 |
| 1:A:1325:C:H2' | 1:A:1326:C:C6 | 2.54 | 0.42 |
| 1:A:257:G:H2' | 1:A:258:G:O4' | 2.20 | 0.42 |
| 1:A:517:G:N1 | 1:A:533:A:OP2 | 2.50 | 0.42 |
| 1:A:619:U:N3 | 4:D:134:ASP:OD2 | 2.44 | 0.42 |
| 1:A:737:A:OP1 | 6:F:92:LYS:HG2 | 2.19 | 0.42 |
| 24:A:3306:HOH:O | 10:J:38:ILE:HB | 2.19 | 0.42 |
| 12:L:117:ARG:NH2 | 12:L:124:LYS:HB2 | 2.35 | 0.42 |
| 1:A:1038:C:O2' | 1:A:1039:C:H5' | 2.19 | 0.42 |
| 1:A:1123:A:C2' | 1:A:1124:G:H5' | 2.50 | 0.42 |
| 1:A:997:U:H5' | 1:A:998:G:OP2 | 2.19 | 0.42 |
| 2:B:154:LEU:HA | 2:B:154:LEU:HD23 | 1.91 | 0.42 |
| 8:H:95:VAL:HB | 8:H:99:GLU:HB2 | 2.00 | 0.42 |
| 11:K:38:ASN:HA | 11:K:39:PRO:HD3 | 1.81 | 0.42 |
| 12:L:7:ILE:O | 12:L:10:LEU:N | 2.48 | 0.42 |
| 19:S:80:TYR:HE1 | 19:S:81:ARG:HH11 | 1.68 | 0.42 |
| 1:A:1127:G:H4' | 1:A:1148:U:O2 | 2.19 | 0.42 |
| 1:A:1191:A:OP2 | 3:C:3:ASN:ND2 | 2.53 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1211:U:H2' | 24:A:2779:HOH:O | 2.20 | 0.42 |
| 1:A:1329:A:H2' | 1:A:1330:U:O4' | 2.20 | 0.42 |
| 1:A:1476:G:H2' | 1:A:1477:C:C6 | 2.54 | 0.42 |
| 1:A:229:U:H2' | 1:A:230:G:C8 | 2.55 | 0.42 |
| 1:A:236:G:H2' | 1:A:237:C:O4' | 2.20 | 0.42 |
| 1:A:632:A:H2' | 1:A:633:G:O4' | 2.20 | 0.42 |
| 1:A:659:U:C2 | 1:A:660:G:C8 | 3.08 | 0.42 |
| 1:A:835:U:OP1 | 18:R:64:ARG:NH2 | 2.41 | 0.42 |
| 1:A:977:A:O2' | 1:A:979:C:OP2 | 2.36 | 0.42 |
| 5:E:101:ILE:O | 5:E:120:THR:HB | 2.19 | 0.42 |
| 6:F:19:LEU:HD21 | 6:F:59:TYR:CE2 | 2.55 | 0.42 |
| 10:J:36:GLY:O | 10:J:38:ILE:HG12 | 2.20 | 0.42 |
| 1:A:247:G:OP2 | 17:Q:100:LYS:HB3 | 2.19 | 0.42 |
| 6:F:50:TYR:CE1 | 18:R:77:GLY:HA2 | 2.55 | 0.42 |
| 20:T:92:LEU:HD23 | 20:T:92:LEU:HA | 1.83 | 0.42 |
| 1:A:1004:A:H3' | 1:A:1025:U:H3 | 1.85 | 0.42 |
| 1:A:153:C:O5' | 1:A:153:C:H6 | 2.03 | 0.42 |
| 1:A:187:C:O2 | 20:T:105:SER:HB2 | 2.20 | 0.42 |
| 1:A:262:A:H4' | 20:T:75:ASN:OD1 | 2.20 | 0.42 |
| 3:C:11:ARG:HG3 | 3:C:178:LEU:HB3 | 2.00 | 0.42 |
| 5:E:6:PHE:CE2 | 5:E:36:ASP:HB3 | 2.55 | 0.42 |
| 5:E:87:SER:HB3 | 5:E:131:ILE:HD13 | 2.02 | 0.42 |
| 13:M:96:LEU:HD23 | 13:M:96:LEU:HA | 1.85 | 0.42 |
| 18:R:79:LEU:HA | 18:R:80:PRO:HD3 | 1.88 | 0.42 |
| 1:A:1349:A:H1' | 1:A:1374:A:N6 | 2.34 | 0.42 |
| 1:A:517:G:N2 | 1:A:533:A:OP2 | 2.46 | 0.42 |
| 2:B:10:LEU:O | 2:B:12:GLU:HG2 | 2.20 | 0.42 |
| 3:C:142:MET:HE1 | 3:C:170:GLN:O | 2.20 | 0.42 |
| 8:H:105:ARG:NH2 | 24:H:302:HOH:O | 2.17 | 0.42 |
| 15:O:85:LEU:HD23 | 15:O:85:LEU:HA | 1.73 | 0.42 |
| 1:A:1054:C:H6 | 1:A:1054:C:H2' | 1.69 | 0.41 |
| 1:A:1275:A:H2' | 1:A:1276:G:O4' | 2.20 | 0.41 |
| 1:A:1539:C:H2' | 1:A:1540:PSU:H5'' | 2.01 | 0.41 |
| 1:A:459:G:C6 | 1:A:461:C:H5' | 2.55 | 0.41 |
| 1:A:606:G:H1' | 1:A:632:A:H61 | 1.86 | 0.41 |
| 1:A:7:G:H5' | 1:A:298:A:H5' | 2.02 | 0.41 |
| 2:B:215:LEU:HD23 | 2:B:215:LEU:HA | 1.85 | 0.41 |
| 10:J:91:PRO:HB2 | 10:J:94:VAL:HG11 | 2.02 | 0.41 |
| 11:K:73:MET:HE1 | 11:K:103:LEU:N | 2.35 | 0.41 |
| 17:Q:74:LEU:HD12 | 17:Q:74:LEU:HA | 1.66 | 0.41 |
| 18:R:26:LEU:HA | 18:R:26:LEU:HD12 | 1.82 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 19:S:33:THR:HG22 | 19:S:50:ALA:O | 2.20 | 0.41 |
| 1:A:229:U:O2' | 1:A:230:G:H5' | 2.20 | 0.41 |
| 1:A:688:G:H5' | 11:K:46:GLY:C | 2.40 | 0.41 |
| 1:A:782:A:OP1 | 1:A:1521:G:N2 | 2.51 | 0.41 |
| 2:B:24:TRP:CG | 2:B:25:ASN:N | 2.88 | 0.41 |
| 3:C:59:ARG:HG3 | 3:C:63:ASN:O | 2.21 | 0.41 |
| 4:D:12:CYS:HA | 4:D:19:LEU:HD12 | 2.01 | 0.41 |
| 9:I:34:ASN:O | 9:I:38:GLN:HB2 | 2.20 | 0.41 |
| 9:I:38:GLN:HB3 | 9:I:38:GLN:HE21 | 1.69 | 0.41 |
| 12:L:19:ARG:H | 12:L:19:ARG:HD2 | 1.84 | 0.41 |
| 13:M:46:LYS:H | 13:M:46:LYS:HG3 | 1.62 | 0.41 |
| 15:O:5:LYS:NZ | 15:O:5:LYS:H | 2.18 | 0.41 |
| 1:A:1136:U:H6 | 1:A:1136:U:H2' | 1.64 | 0.41 |
| 1:A:1372:U:H2' | 1:A:1373:G:O4' | 2.20 | 0.41 |
| 3:C:111:LEU:O | 3:C:202:ILE:HD12 | 2.20 | 0.41 |
| 7:G:101:LEU:HA | 7:G:101:LEU:HD23 | 1.77 | 0.41 |
| 8:H:25:ASP:OD1 | 8:H:25:ASP:N | 2.51 | 0.41 |
| 11:K:126:ARG:NH1 | 11:K:126:ARG:HG3 | 2.36 | 0.41 |
| 15:O:16:ALA:HB1 | 15:O:21:ASP:HB3 | 2.03 | 0.41 |
| 1:A:639:G:O2' | 1:A:640:A:H5' | 2.20 | 0.41 |
| 2:B:182:ILE:HA | 2:B:183:PRO:HD3 | 1.95 | 0.41 |
| 4:D:78:LEU:HA | 4:D:78:LEU:HD23 | 1.49 | 0.41 |
| 5:E:144:THR:HB | 5:E:147:ASP:H | 1.85 | 0.41 |
| 9:I:50:LEU:HB3 | 9:I:55:ALA:HB3 | 2.03 | 0.41 |
| 18:R:70:ILE:HG23 | 18:R:79:LEU:HD13 | 2.02 | 0.41 |
| 1:A:106:C:O2 | 1:A:379:C:H4' | 2.21 | 0.41 |
| 1:A:1201:A:H4' | 1:A:1202:G:O5' | 2.21 | 0.41 |
| 2:B:102:LEU:HB3 | 2:B:180:LEU:CD1 | 2.50 | 0.41 |
| 1:A:427:U:OP1 | 4:D:13:ARG:NH2 | 2.52 | 0.41 |
| 5:E:76:ILE:HG22 | 5:E:78:HIS:O | 2.21 | 0.41 |
| 7:G:104:LEU:HA | 7:G:104:LEU:HD23 | 1.88 | 0.41 |
| 1:A:1023:G:N3 | 1:A:1023:G:H2' | 2.35 | 0.41 |
| 1:A:118:U:H3' | 1:A:288:A:H61 | 1.84 | 0.41 |
| 1:A:950:U:H2' | 1:A:951:G:C8 | 2.55 | 0.41 |
| 2:B:19:HIS:HB3 | 2:B:189:ASP:OD2 | 2.21 | 0.41 |
| 2:B:28:PHE:CD2 | 2:B:190:THR:HA | 2.55 | 0.41 |
| 3:C:149:ALA:O | 3:C:169:ALA:HB1 | 2.21 | 0.41 |
| 12:L:21:LYS:H | 12:L:21:LYS:HG2 | 1.62 | 0.41 |
| 12:L:53:ARG:NH1 | 12:L:92:ASP:OD1 | 2.53 | 0.41 |
| 18:R:26:LEU:HD21 | 18:R:39:VAL:HG23 | 2.01 | 0.41 |
| 19:S:49:ILE:HG21 | 19:S:71:LEU:HD11 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1306:A:P | 21:U:6:ARG:HH12 | 2.43 | 0.41 |
| 1:A:1152:A:H4' | 10:J:13:HIS:NE2 | 2.35 | 0.41 |
| 1:A:264:U:H2' | 1:A:265:G:O4' | 2.21 | 0.41 |
| 2:B:19:HIS:CG | 2:B:20:GLU:H | 2.38 | 0.41 |
| 7:G:152:ALA:O | 7:G:155:ARG:HG3 | 2.21 | 0.41 |
| 15:O:33:THR:OG1 | 15:O:63:ARG:NH1 | 2.48 | 0.41 |
| 15:O:67:LEU:HA | 15:O:67:LEU:HD23 | 1.77 | 0.41 |
| 16:P:52:ASP:OD2 | 16:P:55:ARG:HB2 | 2.20 | 0.41 |
| 17:Q:52:LYS:HD3 | 24:Q:305:HOH:O | 2.20 | 0.41 |
| 18:R:34:TYR:CE1 | 18:R:35:ARG:HG3 | 2.55 | 0.41 |
| 1:A:1451:A:H5'' | 1:A:1452:C:H5 | 1.85 | 0.41 |
| 1:A:518:C:H2' | 1:A:530:G:N7 | 2.36 | 0.41 |
| 1:A:562:C:H1' | 12:L:15:ARG:HB3 | 2.02 | 0.41 |
| 1:A:695:A:H2' | 1:A:696:A:C8 | 2.55 | 0.41 |
| 2:B:179:LYS:HA | 8:H:72:PRO:HD3 | 2.02 | 0.41 |
| 5:E:33:VAL:HG11 | 5:E:109:ILE:HA | 2.01 | 0.41 |
| 6:F:11:ASN:HB3 | 6:F:14:LEU:HG | 2.02 | 0.41 |
| 8:H:75:ARG:HA | 8:H:76:PRO:HD3 | 1.70 | 0.41 |
| 9:I:8:GLY:CA | 9:I:79:LEU:HB3 | 2.50 | 0.41 |
| 1:A:538:G:P | 12:L:115:LYS:HB2 | 2.61 | 0.41 |
| 12:L:24:VAL:HG12 | 12:L:24:VAL:O | 2.20 | 0.41 |
| 1:A:1164:G:C6 | 1:A:1165:C:C4 | 3.09 | 0.41 |
| 1:A:1296:C:H4' | 1:A:1302:U:H5 | 1.86 | 0.41 |
| 1:A:563:A:H2' | 1:A:567:G:C8 | 2.56 | 0.41 |
| 2:B:17:PHE:CD1 | 2:B:18:GLY:N | 2.88 | 0.41 |
| 2:B:48:MET:HA | 2:B:51:LEU:HB2 | 2.03 | 0.41 |
| 1:A:1179:A:O3' | 9:I:103:THR:HG23 | 2.21 | 0.41 |
| 9:I:117:HIS:HB2 | 9:I:121:ARG:HG3 | 2.01 | 0.41 |
| 1:A:1402:4OC:O2 | 1:A:1500:A:N1 | 2.53 | 0.41 |
| 1:A:484:G:H5' | 1:A:486:U:O4' | 2.21 | 0.41 |
| 1:A:554:C:H2' | 1:A:555:C:C6 | 2.56 | 0.41 |
| 1:A:659:U:H2' | 1:A:660:G:H8 | 1.85 | 0.41 |
| 1:A:991:U:O2' | 1:A:992:U:O5' | 2.37 | 0.41 |
| 2:B:22:LYS:HG3 | 2:B:40:HIS:NE2 | 2.35 | 0.41 |
| 3:C:59:ARG:HE | 3:C:59:ARG:HB2 | 1.20 | 0.41 |
| 9:I:108:VAL:HG12 | 9:I:109:VAL:H | 1.86 | 0.41 |
| 9:I:127:LYS:HA | 9:I:127:LYS:HD3 | 1.72 | 0.41 |
| 10:J:88:LEU:HD22 | 10:J:88:LEU:H | 1.86 | 0.41 |
| 16:P:40:ASP:HA | 16:P:41:PRO:HD3 | 1.91 | 0.41 |
| 17:Q:84:LEU:HD23 | 17:Q:84:LEU:HA | 1.67 | 0.41 |
| 1:A:1002:G:H2' | 1:A:1003:G:O4' | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:106:C:C2' | 1:A:107:G:H5' | 2.51 | 0.41 |
| 1:A:428:G:H4' | 1:A:429:U:O5' | 2.20 | 0.41 |
| 1:A:566:G:N2 | 24:A:3565:HOH:O | 2.36 | 0.41 |
| 1:A:580:U:H2' | 1:A:581:G:O4' | 2.20 | 0.41 |
| 1:A:631:G:OP2 | 1:A:631:G:H8 | 2.03 | 0.41 |
| 11:K:84:VAL:HG11 | 11:K:91:ARG:HD2 | 2.03 | 0.41 |
| 14:N:31:ARG:O | 14:N:33:VAL:HG22 | 2.21 | 0.41 |
| 20:T:60:GLU:HG3 | 20:T:81:LYS:HD2 | 2.02 | 0.41 |
| 21:U:8:THR:OG1 | 21:U:10:ARG:N | 2.54 | 0.41 |
| 1:A:1196:U:H3' | 1:A:1197:G:H5'' | 2.03 | 0.40 |
| 1:A:838:G:H1 | 1:A:848:C:H42 | 1.69 | 0.40 |
| 1:A:869:G:C8 | 24:A:3466:HOH:O | 2.71 | 0.40 |
| 1:A:961:U:OP1 | 1:A:1223:C:O2' | 2.22 | 0.40 |
| 2:B:188:ALA:O | 2:B:202:PRO:HA | 2.21 | 0.40 |
| 2:B:24:TRP:HB2 | 2:B:190:THR:HG22 | 2.03 | 0.40 |
| 5:E:81:GLU:HB3 | 5:E:88:LYS:HZ2 | 1.86 | 0.40 |
| 6:F:75:LEU:O | 6:F:79:LEU:HG | 2.20 | 0.40 |
| 10:J:79:ARG:HH11 | 10:J:79:ARG:HA | 1.87 | 0.40 |
| 11:K:48:ILE:HD11 | 11:K:64:ALA:HA | 2.02 | 0.40 |
| 15:O:21:ASP:OD1 | 15:O:24:SER:HB3 | 2.21 | 0.40 |
| 18:R:19:LYS:HE2 | 18:R:19:LYS:HB2 | 1.87 | 0.40 |
| 18:R:21:LYS:HD2 | 18:R:54:ARG:O | 2.21 | 0.40 |
| 1:A:1265:G:H2' | 1:A:1266:G:O4' | 2.21 | 0.40 |
| 1:A:1408:A:H2' | 1:A:1409:C:C6 | 2.57 | 0.40 |
| 2:B:147:LYS:HE2 | 2:B:148:TYR:CE1 | 2.56 | 0.40 |
| 4:D:10:ARG:HG2 | 4:D:11:LEU:N | 2.33 | 0.40 |
| 4:D:15:GLU:OE2 | 4:D:15:GLU:HA | 2.21 | 0.40 |
| 12:L:6:THR:HG23 | 12:L:9:GLN:HG3 | 2.03 | 0.40 |
| 13:M:3:ARG:HA | 13:M:8:GLU:O | 2.21 | 0.40 |
| 17:Q:59:ILE:HG23 | 17:Q:71:PHE:HD1 | 1.87 | 0.40 |
| 17:Q:91:ARG:O | 17:Q:94:ASN:HB2 | 2.20 | 0.40 |
| 1:A:1046:A:H3' | 1:A:1047:G:H8 | 1.86 | 0.40 |
| 1:A:244:U:C6 | 1:A:894:G:N2 | 2.89 | 0.40 |
| 1:A:419:C:C2 | 1:A:425:G:C2 | 3.09 | 0.40 |
| 1:A:738:C:H2' | 1:A:739:C:H6 | 1.86 | 0.40 |
| 1:A:664:G:H22 | 1:A:741:G:H1 | 1.69 | 0.40 |
| 1:A:992:U:H4' | 1:A:993:G:O5' | 2.22 | 0.40 |
| 2:B:54:THR:O | 2:B:57:PHE:HB3 | 2.21 | 0.40 |
| 4:D:128:VAL:HG12 | 4:D:129:ASN:HD22 | 1.86 | 0.40 |
| 1:A:1367:C:H5' | 10:J:60:ARG:HE | 1.86 | 0.40 |
| 11:K:115:PRO:C | 11:K:117:ASN:H | 2.23 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1318:A:O2' | 19:S:37:ARG:HG3 | 2.22 | 0.40 |
| 1:A:358:U:H2' | 1:A:359:U:C6 | 2.55 | 0.40 |
| 2:B:208:ILE:HG21 | 2:B:239:VAL:HA | 2.04 | 0.40 |
| 7:G:149:ARG:HD3 | 11:K:59:TYR:CE1 | 2.57 | 0.40 |
| 10:J:64:GLU:OE2 | 10:J:66:ARG:NE | 2.55 | 0.40 |
| 12:L:69:TYR:HE2 | 12:L:71:PRO:HA | 1.87 | 0.40 |
| 12:L:6:THR:HG23 | 12:L:9:GLN:OE1 | 2.22 | 0.40 |
| 15:O:30:ALA:HB2 | 15:O:85:LEU:HD11 | 2.04 | 0.40 |
| 17:Q:40:LYS:HE2 | 17:Q:42:TYR:OH | 2.21 | 0.40 |
| 19:S:11:VAL:HG22 | 19:S:38:SER:HB3 | 2.03 | 0.40 |
| 1:A:877:C:OP1 | 8:H:88:LYS:NZ | 2.40 | 0.40 |
| 1:A:901:A:C5 | 1:A:902:G:H1' | 2.56 | 0.40 |
| 1:A:889:A:N1 | 1:A:907:A:H5'' | 2.36 | 0.40 |
| 1:A:924:C:H2' | 1:A:925:G:C8 | 2.56 | 0.40 |
| 5:E:15:ARG:HG3 | 5:E:15:ARG:NH1 | 2.33 | 0.40 |
| 11:K:34:ASP:OD1 | 11:K:38:ASN:N | 2.48 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 2 | B | 232/256 (91%) | 209 (90%) | 21 (9%) | 2 (1%) | 17 | 56 |
| 3 | C | 204/239 (85%) | 179 (88%) | 24 (12%) | 1 (0%) | 29 | 68 |
| 4 | D | 206/209 (99%) | 199 (97%) | 7 (3%) | 0 | 100 | 100 |
| 5 | E | 148/162 (91%) | 138 (93%) | 10 (7%) | 0 | 100 | 100 |
| 6 | F | 99/101 (98%) | 97 (98%) | 2 (2%) | 0 | 100 | 100 |
| 7 | G | 153/156 (98%) | 143 (94%) | 10 (6%) | 0 | 100 | 100 |
| 8 | H | 136/138 (99%) | 132 (97%) | 4 (3%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 9 | I | 125/128 (98%) | 113 (90%) | 11 (9%) | 1 (1%) | 19 | 58 |
| 10 | J | 96/105 (91%) | 78 (81%) | 16 (17%) | 2 (2%) | 7 | 38 |
| 11 | K | 114/129 (88%) | 103 (90%) | 11 (10%) | 0 | 100 | 100 |
| 12 | L | 122/135 (90%) | 111 (91%) | 10 (8%) | 1 (1%) | 19 | 58 |
| 13 | M | 116/126 (92%) | 104 (90%) | 12 (10%) | 0 | 100 | 100 |
| 14 | N | 58/61 (95%) | 51 (88%) | 7 (12%) | 0 | 100 | 100 |
| 15 | O | 85/89 (96%) | 82 (96%) | 3 (4%) | 0 | 100 | 100 |
| 16 | P | 81/88 (92%) | 79 (98%) | 2 (2%) | 0 | 100 | 100 |
| 17 | Q | 97/105 (92%) | 90 (93%) | 7 (7%) | 0 | 100 | 100 |
| 18 | R | 68/88 (77%) | 63 (93%) | 4 (6%) | 1 (2%) | 10 | 45 |
| 19 | S | 78/93 (84%) | 73 (94%) | 4 (5%) | 1 (1%) | 12 | 48 |
| 20 | T | 97/106 (92%) | 85 (88%) | 12 (12%) | 0 | 100 | 100 |
| 21 | U | 22/27 (82%) | 21 (96%) | 1 (4%) | 0 | 100 | 100 |
| All | All | 2337/2541 (92%) | 2150 (92%) | 178 (8%) | 9 (0%) | 34 | 72 |

All (9) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 21 | ARG |
| 12 | L | 28 | LYS |
| 19 | S | 31 | ILE |
| 3 | C | 15 | THR |
| 10 | J | 35 | SER |
| 9 | I | 119 | ALA |
| 10 | J | 34 | VAL |
| 18 | R | 86 | VAL |
| 2 | B | 229 | VAL |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 2 | B | 202/220 (92%) | 168 (83%) | 34 (17%) | 2 | 12 |
| 3 | C | 160/188 (85%) | 123 (77%) | 37 (23%) | 1 | 4 |
| 4 | D | 180/181 (99%) | 149 (83%) | 31 (17%) | 2 | 11 |
| 5 | E | 115/123 (94%) | 90 (78%) | 25 (22%) | 1 | 5 |
| 6 | F | 90/90 (100%) | 80 (89%) | 10 (11%) | 6 | 28 |
| 7 | G | 126/127 (99%) | 112 (89%) | 14 (11%) | 6 | 28 |
| 8 | H | 119/119 (100%) | 101 (85%) | 18 (15%) | 3 | 17 |
| 9 | I | 98/99 (99%) | 80 (82%) | 18 (18%) | 1 | 8 |
| 10 | J | 87/92 (95%) | 67 (77%) | 20 (23%) | 1 | 4 |
| 11 | K | 88/99 (89%) | 80 (91%) | 8 (9%) | 9 | 36 |
| 12 | L | 104/111 (94%) | 86 (83%) | 18 (17%) | 2 | 11 |
| 13 | M | 94/101 (93%) | 81 (86%) | 13 (14%) | 3 | 20 |
| 14 | N | 49/50 (98%) | 40 (82%) | 9 (18%) | 1 | 8 |
| 15 | O | 79/80 (99%) | 67 (85%) | 12 (15%) | 3 | 17 |
| 16 | P | 72/74 (97%) | 64 (89%) | 8 (11%) | 6 | 28 |
| 17 | Q | 94/97 (97%) | 80 (85%) | 14 (15%) | 3 | 17 |
| 18 | R | 61/77 (79%) | 57 (93%) | 4 (7%) | 16 | 49 |
| 19 | S | 71/80 (89%) | 56 (79%) | 15 (21%) | 1 | 5 |
| 20 | T | 76/82 (93%) | 64 (84%) | 12 (16%) | 2 | 15 |
| 21 | U | 19/22 (86%) | 16 (84%) | 3 (16%) | 2 | 15 |
| All | All | 1984/2112 (94%) | 1661 (84%) | 323 (16%) | 2 | 13 |

All (323) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 7 | VAL |
| 2 | B | 10 | LEU |
| 2 | B | 20 | GLU |
| 2 | B | 21 | ARG |
| 2 | B | 24 | TRP |
| 2 | B | 33 | TYR |
| 2 | B | 63 | MET |
| 2 | B | 67 | THR |
| 2 | B | 76 | GLN |
| 2 | B | 87 | ARG |
| 2 | B | 96 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 106 | LYS |
| 2 | B | 110 | GLN |
| 2 | B | 114 | ARG |
| 2 | B | 115 | LEU |
| 2 | B | 126 | GLU |
| 2 | B | 127 | ILE |
| 2 | B | 133 | LYS |
| 2 | B | 142 | LEU |
| 2 | B | 144 | ARG |
| 2 | B | 155 | LEU |
| 2 | B | 162 | ILE |
| 2 | B | 163 | PHE |
| 2 | B | 164 | VAL |
| 2 | B | 170 | GLU |
| 2 | B | 175 | ARG |
| 2 | B | 178 | ARG |
| 2 | B | 187 | LEU |
| 2 | B | 189 | ASP |
| 2 | B | 206 | ASP |
| 2 | B | 208 | ILE |
| 2 | B | 221 | LEU |
| 2 | B | 226 | ARG |
| 2 | B | 238 | LEU |
| 3 | C | 3 | ASN |
| 3 | C | 8 | ILE |
| 3 | C | 11 | ARG |
| 3 | C | 14 | ILE |
| 3 | C | 16 | ARG |
| 3 | C | 27 | LYS |
| 3 | C | 30 | ARG |
| 3 | C | 34 | LEU |
| 3 | C | 55 | VAL |
| 3 | C | 59 | ARG |
| 3 | C | 62 | ASP |
| 3 | C | 68 | VAL |
| 3 | C | 70 | VAL |
| 3 | C | 76 | VAL |
| 3 | C | 82 | GLU |
| 3 | C | 83 | ARG |
| 3 | C | 91 | LEU |
| 3 | C | 93 | LYS |
| 3 | C | 94 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 97 | LYS |
| 3 | C | 104 | GLN |
| 3 | C | 111 | LEU |
| 3 | C | 131 | ARG |
| 3 | C | 138 | VAL |
| 3 | C | 143 | GLU |
| 3 | C | 144 | SER |
| 3 | C | 164 | ARG |
| 3 | C | 165 | THR |
| 3 | C | 167 | TRP |
| 3 | C | 172 | ARG |
| 3 | C | 177 | THR |
| 3 | C | 178 | LEU |
| 3 | C | 188 | LEU |
| 3 | C | 191 | THR |
| 3 | C | 192 | THR |
| 3 | C | 195 | VAL |
| 3 | C | 204 | LEU |
| 4 | D | 3 | ARG |
| 4 | D | 8 | VAL |
| 4 | D | 10 | ARG |
| 4 | D | 13 | ARG |
| 4 | D | 19 | LEU |
| 4 | D | 26 | CYS |
| 4 | D | 28 | SER |
| 4 | D | 35 | ARG |
| 4 | D | 36 | ARG |
| 4 | D | 38 | TYR |
| 4 | D | 47 | ARG |
| 4 | D | 50 | ARG |
| 4 | D | 64 | LEU |
| 4 | D | 78 | LEU |
| 4 | D | 81 | GLU |
| 4 | D | 96 | LEU |
| 4 | D | 99 | SER |
| 4 | D | 107 | ARG |
| 4 | D | 115 | ARG |
| 4 | D | 122 | ARG |
| 4 | D | 127 | THR |
| 4 | D | 135 | LEU |
| 4 | D | 154 | ASN |
| 4 | D | 159 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | D | 160 | GLN |
| 4 | D | 162 | LEU |
| 4 | D | 169 | LYS |
| 4 | D | 170 | VAL |
| 4 | D | 191 | ARG |
| 4 | D | 194 | LEU |
| 4 | D | 202 | LEU |
| 5 | E | 11 | ILE |
| 5 | E | 12 | LEU |
| 5 | E | 13 | ILE |
| 5 | E | 15 | ARG |
| 5 | E | 16 | THR |
| 5 | E | 18 | ARG |
| 5 | E | 19 | MET |
| 5 | E | 24 | ARG |
| 5 | E | 26 | PHE |
| 5 | E | 41 | VAL |
| 5 | E | 47 | LYS |
| 5 | E | 63 | ARG |
| 5 | E | 64 | ARG |
| 5 | E | 65 | ASN |
| 5 | E | 76 | ILE |
| 5 | E | 79 | GLU |
| 5 | E | 87 | SER |
| 5 | E | 107 | ARG |
| 5 | E | 116 | THR |
| 5 | E | 117 | ASP |
| 5 | E | 125 | SER |
| 5 | E | 144 | THR |
| 5 | E | 149 | GLU |
| 5 | E | 150 | ARG |
| 5 | E | 153 | LYS |
| 6 | F | 19 | LEU |
| 6 | F | 22 | GLU |
| 6 | F | 40 | VAL |
| 6 | F | 43 | LEU |
| 6 | F | 54 | LYS |
| 6 | F | 74 | ASP |
| 6 | F | 75 | LEU |
| 6 | F | 82 | ARG |
| 6 | F | 93 | SER |
| 6 | F | 100 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | G | 12 | LEU |
| 7 | G | 21 | VAL |
| 7 | G | 24 | THR |
| 7 | G | 27 | ILE |
| 7 | G | 38 | LEU |
| 7 | G | 54 | THR |
| 7 | G | 57 | GLU |
| 7 | G | 59 | LEU |
| 7 | G | 73 | MET |
| 7 | G | 75 | VAL |
| 7 | G | 113 | GLU |
| 7 | G | 115 | ARG |
| 7 | G | 146 | GLU |
| 7 | G | 153 | HIS |
| 8 | H | 6 | ILE |
| 8 | H | 15 | ASN |
| 8 | H | 18 | ARG |
| 8 | H | 23 | SER |
| 8 | H | 37 | ARG |
| 8 | H | 63 | LEU |
| 8 | H | 79 | VAL |
| 8 | H | 85 | ARG |
| 8 | H | 87 | SER |
| 8 | H | 91 | ARG |
| 8 | H | 92 | ARG |
| 8 | H | 93 | VAL |
| 8 | H | 98 | LYS |
| 8 | H | 104 | ARG |
| 8 | H | 112 | LEU |
| 8 | H | 119 | LEU |
| 8 | H | 127 | LEU |
| 8 | H | 133 | LEU |
| 9 | I | 9 | ARG |
| 9 | I | 38 | GLN |
| 9 | I | 47 | LEU |
| 9 | I | 51 | ARG |
| 9 | I | 63 | ILE |
| 9 | I | 64 | THR |
| 9 | I | 65 | VAL |
| 9 | I | 74 | ILE |
| 9 | I | 79 | LEU |
| 9 | I | 83 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | I | 85 | LEU |
| 9 | I | 87 | GLN |
| 9 | I | 99 | LEU |
| 9 | I | 108 | VAL |
| 9 | I | 116 | LYS |
| 9 | I | 118 | LYS |
| 9 | I | 121 | ARG |
| 9 | I | 126 | SER |
| 10 | J | 5 | ARG |
| 10 | J | 7 | LYS |
| 10 | J | 8 | LEU |
| 10 | J | 9 | ARG |
| 10 | J | 12 | ASP |
| 10 | J | 16 | LEU |
| 10 | J | 19 | SER |
| 10 | J | 21 | GLN |
| 10 | J | 33 | GLN |
| 10 | J | 38 | ILE |
| 10 | J | 44 | VAL |
| 10 | J | 57 | LYS |
| 10 | J | 74 | ILE |
| 10 | J | 76 | ASN |
| 10 | J | 79 | ARG |
| 10 | J | 81 | THR |
| 10 | J | 88 | LEU |
| 10 | J | 92 | THR |
| 10 | J | 94 | VAL |
| 10 | J | 96 | ILE |
| 11 | K | 11 | LYS |
| 11 | K | 14 | VAL |
| 11 | K | 29 | ILE |
| 11 | K | 33 | THR |
| 11 | K | 75 | TYR |
| 11 | K | 77 | MET |
| 11 | K | 87 | THR |
| 11 | K | 114 | VAL |
| 12 | L | 7 | ILE |
| 12 | L | 17 | LYS |
| 12 | L | 18 | VAL |
| 12 | L | 19 | ARG |
| 12 | L | 20 | LYS |
| 12 | L | 21 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | L | 28 | LYS |
| 12 | L | 33 | ARG |
| 12 | L | 41 | ARG |
| 12 | L | 75 | HIS |
| 12 | L | 82 | VAL |
| 12 | L | 85 | ILE |
| 12 | L | 89 | ARG |
| 12 | L | 97 | ARG |
| 12 | L | 101 | VAL |
| 12 | L | 113 | ARG |
| 12 | L | 122 | THR |
| 12 | L | 126 | LYS |
| 13 | M | 3 | ARG |
| 13 | M | 14 | ARG |
| 13 | M | 46 | LYS |
| 13 | M | 63 | THR |
| 13 | M | 64 | TRP |
| 13 | M | 65 | LYS |
| 13 | M | 66 | LEU |
| 13 | M | 69 | GLU |
| 13 | M | 74 | VAL |
| 13 | M | 88 | ARG |
| 13 | M | 90 | LEU |
| 13 | M | 109 | THR |
| 13 | M | 110 | ARG |
| 14 | N | 6 | LEU |
| 14 | N | 8 | GLU |
| 14 | N | 12 | ARG |
| 14 | N | 18 | VAL |
| 14 | N | 22 | THR |
| 14 | N | 24 | CYS |
| 14 | N | 33 | VAL |
| 14 | N | 45 | ARG |
| 14 | N | 47 | LEU |
| 15 | O | 6 | GLU |
| 15 | O | 8 | LYS |
| 15 | O | 22 | THR |
| 15 | O | 31 | LEU |
| 15 | O | 34 | LEU |
| 15 | O | 39 | LEU |
| 15 | O | 56 | LEU |
| 15 | O | 70 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15 | O | 71 | GLN |
| 15 | O | 77 | ARG |
| 15 | O | 81 | LEU |
| 15 | O | 82 | ILE |
| 16 | P | 1 | MET |
| 16 | P | 2 | VAL |
| 16 | P | 43 | LYS |
| 16 | P | 53 | VAL |
| 16 | P | 55 | ARG |
| 16 | P | 65 | GLN |
| 16 | P | 69 | THR |
| 16 | P | 74 | LEU |
| 17 | Q | 5 | VAL |
| 17 | Q | 6 | LEU |
| 17 | Q | 9 | VAL |
| 17 | Q | 14 | LYS |
| 17 | Q | 15 | MET |
| 17 | Q | 24 | GLU |
| 17 | Q | 35 | VAL |
| 17 | Q | 36 | ILE |
| 17 | Q | 50 | LYS |
| 17 | Q | 58 | GLU |
| 17 | Q | 77 | VAL |
| 17 | Q | 92 | ARG |
| 17 | Q | 98 | LEU |
| 17 | Q | 100 | LYS |
| 18 | R | 28 | GLU |
| 18 | R | 47 | THR |
| 18 | R | 69 | THR |
| 18 | R | 82 | THR |
| 19 | S | 4 | SER |
| 19 | S | 6 | LYS |
| 19 | S | 7 | LYS |
| 19 | S | 15 | LEU |
| 19 | S | 22 | LEU |
| 19 | S | 29 | ARG |
| 19 | S | 32 | LYS |
| 19 | S | 36 | ARG |
| 19 | S | 37 | ARG |
| 19 | S | 39 | THR |
| 19 | S | 41 | VAL |
| 19 | S | 49 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19 | S | 61 | TYR |
| 19 | S | 63 | THR |
| 19 | S | 78 | ARG |
| 20 | T | 10 | LEU |
| 20 | T | 11 | SER |
| 20 | T | 23 | ARG |
| 20 | T | 24 | LEU |
| 20 | T | 48 | LYS |
| 20 | T | 53 | LEU |
| 20 | T | 56 | MET |
| 20 | T | 73 | HIS |
| 20 | T | 74 | LYS |
| 20 | T | 75 | ASN |
| 20 | T | 100 | ILE |
| 20 | T | 105 | SER |
| 21 | U | 8 | THR |
| 21 | U | 9 | ARG |
| 21 | U | 22 | ARG |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 6 | HIS |
| 8 | H | 15 | ASN |
| 12 | L | 8 | ASN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | A | 1505/1522 (98%) | 287 (19%) | 34 (2%) |

All (287) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 4 | U |
| 1 | A | 9 | G |
| 1 | A | 32 | A |
| 1 | A | 39 | G |
| 1 | A | 47 | C |
| 1 | A | 48 | C |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | A | 51 | A |
| 1 | A | 80 | G |
| 1 | A | 81 | U |
| 1 | A | 101 | A |
| 1 | A | 115 | G |
| 1 | A | 116 | A |
| 1 | A | 117 | G |
| 1 | A | 121 | C |
| 1 | A | 129(A) | G |
| 1 | A | 130 | A |
| 1 | A | 131 | C |
| 1 | A | 144 | G |
| 1 | A | 163 | C |
| 1 | A | 182 | U |
| 1 | A | 190(E) | U |
| 1 | A | 195 | A |
| 1 | A | 197 | A |
| 1 | A | 201 | C |
| 1 | A | 202 | U |
| 1 | A | 203 | U |
| 1 | A | 216 | G |
| 1 | A | 220 | G |
| 1 | A | 226 | G |
| 1 | A | 247 | G |
| 1 | A | 251 | G |
| 1 | A | 252 | U |
| 1 | A | 254 | G |
| 1 | A | 266 | G |
| 1 | A | 267 | C |
| 1 | A | 289 | G |
| 1 | A | 301 | G |
| 1 | A | 319 | G |
| 1 | A | 321 | A |
| 1 | A | 328 | C |
| 1 | A | 329 | A |
| 1 | A | 345 | C |
| 1 | A | 347 | G |
| 1 | A | 350 | G |
| 1 | A | 352 | C |
| 1 | A | 353 | A |
| 1 | A | 354 | G |
| 1 | A | 356 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 367 | U |
| 1 | A | 371 | G |
| 1 | A | 372 | C |
| 1 | A | 373 | A |
| 1 | A | 374 | A |
| 1 | A | 384 | G |
| 1 | A | 390 | C |
| 1 | A | 398 | C |
| 1 | A | 406 | G |
| 1 | A | 409 | G |
| 1 | A | 412 | A |
| 1 | A | 413 | G |
| 1 | A | 424 | G |
| 1 | A | 429 | U |
| 1 | A | 439 | A |
| 1 | A | 452 | A |
| 1 | A | 461 | C |
| 1 | A | 481 | G |
| 1 | A | 482 | A |
| 1 | A | 483 | C |
| 1 | A | 484 | G |
| 1 | A | 485 | G |
| 1 | A | 486 | U |
| 1 | A | 497 | A |
| 1 | A | 498 | U |
| 1 | A | 505 | G |
| 1 | A | 509 | A |
| 1 | A | 510 | A |
| 1 | A | 511 | C |
| 1 | A | 518 | C |
| 1 | A | 519 | C |
| 1 | A | 527 | 7MG |
| 1 | A | 531 | U |
| 1 | A | 532 | A |
| 1 | A | 533 | A |
| 1 | A | 536 | C |
| 1 | A | 545 | C |
| 1 | A | 547 | A |
| 1 | A | 559 | A |
| 1 | A | 560 | U |
| 1 | A | 562 | C |
| 1 | A | 563 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 564 | C |
| 1 | A | 569 | C |
| 1 | A | 572 | A |
| 1 | A | 573 | A |
| 1 | A | 576 | G |
| 1 | A | 577 | G |
| 1 | A | 579 | G |
| 1 | A | 588 | G |
| 1 | A | 631 | G |
| 1 | A | 651 | C |
| 1 | A | 653 | A |
| 1 | A | 665 | A |
| 1 | A | 666 | G |
| 1 | A | 670 | G |
| 1 | A | 671 | G |
| 1 | A | 687 | A |
| 1 | A | 688 | G |
| 1 | A | 695 | A |
| 1 | A | 701 | C |
| 1 | A | 702 | A |
| 1 | A | 715 | A |
| 1 | A | 721 | G |
| 1 | A | 722 | A |
| 1 | A | 723 | U |
| 1 | A | 731 | G |
| 1 | A | 741 | G |
| 1 | A | 746 | A |
| 1 | A | 749 | C |
| 1 | A | 753 | A |
| 1 | A | 755 | G |
| 1 | A | 759 | A |
| 1 | A | 777 | A |
| 1 | A | 781 | A |
| 1 | A | 782 | A |
| 1 | A | 785 | G |
| 1 | A | 793 | U |
| 1 | A | 794 | A |
| 1 | A | 813 | U |
| 1 | A | 817 | C |
| 1 | A | 818 | G |
| 1 | A | 819 | A |
| 1 | A | 827 | U |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | A | 828 | A |
| 1 | A | 839 | U |
| 1 | A | 840 | C |
| 1 | A | 841 | U |
| 1 | A | 848 | C |
| 1 | A | 857 | C |
| 1 | A | 858 | G |
| 1 | A | 872 | A |
| 1 | A | 873 | A |
| 1 | A | 876 | G |
| 1 | A | 877 | C |
| 1 | A | 889 | A |
| 1 | A | 902 | G |
| 1 | A | 926 | G |
| 1 | A | 927 | G |
| 1 | A | 934 | C |
| 1 | A | 935 | A |
| 1 | A | 939 | G |
| 1 | A | 961 | U |
| 1 | A | 966 | M2G |
| 1 | A | 969 | A |
| 1 | A | 971 | G |
| 1 | A | 975 | A |
| 1 | A | 976 | G |
| 1 | A | 977 | A |
| 1 | A | 982 | U |
| 1 | A | 989 | C |
| 1 | A | 991 | U |
| 1 | A | 992 | U |
| 1 | A | 993 | G |
| 1 | A | 997 | U |
| 1 | A | 999 | C |
| 1 | A | 1003 | G |
| 1 | A | 1003(A) | G |
| 1 | A | 1005 | A |
| 1 | A | 1007 | C |
| 1 | A | 1009 | G |
| 1 | A | 1016 | A |
| 1 | A | 1020 | U |
| 1 | A | 1021 | G |
| 1 | A | 1022 | G |
| 1 | A | 1024 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | A | 1025 | U |
| 1 | A | 1026 | G |
| 1 | A | 1027 | C |
| 1 | A | 1028 | C |
| 1 | A | 1029 | C |
| 1 | A | 1030(A) | G |
| 1 | A | 1030(B) | C |
| 1 | A | 1030(C) | G |
| 1 | A | 1030(D) | A |
| 1 | A | 1031 | G |
| 1 | A | 1033 | G |
| 1 | A | 1036 | G |
| 1 | A | 1039 | C |
| 1 | A | 1045 | C |
| 1 | A | 1049 | U |
| 1 | A | 1050 | G |
| 1 | A | 1051 | C |
| 1 | A | 1053 | G |
| 1 | A | 1065 | U |
| 1 | A | 1066 | C |
| 1 | A | 1094 | G |
| 1 | A | 1095 | U |
| 1 | A | 1100 | C |
| 1 | A | 1101 | A |
| 1 | A | 1104 | G |
| 1 | A | 1119 | C |
| 1 | A | 1124 | G |
| 1 | A | 1125 | U |
| 1 | A | 1126 | U |
| 1 | A | 1127 | G |
| 1 | A | 1129 | C |
| 1 | A | 1130 | A |
| 1 | A | 1131 | G |
| 1 | A | 1135 | U |
| 1 | A | 1136 | U |
| 1 | A | 1137 | C |
| 1 | A | 1139 | G |
| 1 | A | 1140 | C |
| 1 | A | 1146 | A |
| 1 | A | 1152 | A |
| 1 | A | 1154 | G |
| 1 | A | 1157 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1159 | U |
| 1 | A | 1160 | G |
| 1 | A | 1162 | C |
| 1 | A | 1182 | G |
| 1 | A | 1188 | A |
| 1 | A | 1196 | U |
| 1 | A | 1197 | G |
| 1 | A | 1201 | A |
| 1 | A | 1202 | G |
| 1 | A | 1211 | U |
| 1 | A | 1212 | U |
| 1 | A | 1213 | A |
| 1 | A | 1214 | C |
| 1 | A | 1225 | A |
| 1 | A | 1227 | A |
| 1 | A | 1233 | G |
| 1 | A | 1238 | A |
| 1 | A | 1240 | U |
| 1 | A | 1241 | G |
| 1 | A | 1250 | A |
| 1 | A | 1253 | G |
| 1 | A | 1256 | A |
| 1 | A | 1257 | U |
| 1 | A | 1258 | G |
| 1 | A | 1260 | C |
| 1 | A | 1270 | C |
| 1 | A | 1278 | U |
| 1 | A | 1279 | A |
| 1 | A | 1280 | A |
| 1 | A | 1281 | U |
| 1 | A | 1285 | A |
| 1 | A | 1287 | A |
| 1 | A | 1300 | G |
| 1 | A | 1302 | U |
| 1 | A | 1303 | C |
| 1 | A | 1305 | G |
| 1 | A | 1312 | G |
| 1 | A | 1320 | C |
| 1 | A | 1322 | C |
| 1 | A | 1323 | G |
| 1 | A | 1335 | C |
| 1 | A | 1336 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1338 | G |
| 1 | A | 1346 | A |
| 1 | A | 1353 | G |
| 1 | A | 1363 | A |
| 1 | A | 1368 | G |
| 1 | A | 1370 | G |
| 1 | A | 1379 | G |
| 1 | A | 1381 | U |
| 1 | A | 1394 | A |
| 1 | A | 1398 | A |
| 1 | A | 1407 | 5MC |
| 1 | A | 1408 | A |
| 1 | A | 1410 | G |
| 1 | A | 1414 | U |
| 1 | A | 1443 | G |
| 1 | A | 1446 | A |
| 1 | A | 1447 | G |
| 1 | A | 1486 | G |
| 1 | A | 1492 | A |
| 1 | A | 1493 | A |
| 1 | A | 1494 | G |
| 1 | A | 1497 | G |
| 1 | A | 1498 | UR3 |
| 1 | A | 1499 | A |
| 1 | A | 1503 | A |
| 1 | A | 1506 | U |
| 1 | A | 1529 | G |
| 1 | A | 1530 | G |
| 1 | A | 1544 | U |

All (34) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | A | 115 | G |
| 1 | A | 129(A) | G |
| 1 | A | 181 | G |
| 1 | A | 250 | A |
| 1 | A | 251 | G |
| 1 | A | 328 | C |
| 1 | A | 353 | A |
| 1 | A | 372 | C |
| 1 | A | 428 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 484 | G |
| 1 | A | 485 | G |
| 1 | A | 509 | A |
| 1 | A | 518 | C |
| 1 | A | 530 | G |
| 1 | A | 532 | A |
| 1 | A | 559 | A |
| 1 | A | 687 | A |
| 1 | A | 701 | C |
| 1 | A | 748 | C |
| 1 | A | 793 | U |
| 1 | A | 812 | C |
| 1 | A | 960 | U |
| 1 | A | 991 | U |
| 1 | A | 992 | U |
| 1 | A | 1049 | U |
| 1 | A | 1065 | U |
| 1 | A | 1129 | C |
| 1 | A | 1139 | G |
| 1 | A | 1145 | C |
| 1 | A | 1181 | G |
| 1 | A | 1201 | A |
| 1 | A | 1380 | U |
| 1 | A | 1493 | A |
| 1 | A | 1505 | G |

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

16 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 | 5MC | A | 1404 | 1 | 15,22,23 | 0.96 | 0 | 19,32,35 | 0.99 | 1 (5%) |
| 1 | 7MG | A | 527 | 1 | 22,26,27 | 2.21 | 8 (36%) | 28,39,42 | 1.42 | 7 (25%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|---------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | MA6 | A | 1519[A] | 1 | 19,26,27 | 0.81 | 0 | 18,38,41 | 0.92 | 1 (5%) |
| 1 | 5MC | A | 1400 | 1 | 15,22,23 | 0.90 | 0 | 19,32,35 | 1.24 | 3 (15%) |
| 1 | MA6 | A | 1519[B] | 1 | 19,26,27 | 1.33 | 3 (15%) | 18,38,41 | 0.57 | 0 |
| 1 | PSU | A | 1541 | 1 | 17,21,22 | 1.09 | 3 (17%) | 20,30,33 | 3.07 | 6 (30%) |
| 1 | 5MC | A | 967 | 1 | 15,22,23 | 1.00 | 0 | 19,32,35 | 1.06 | 0 |
| 1 | M2G | A | 966 | 1 | 20,27,28 | 1.57 | 2 (10%) | 22,40,43 | 2.33 | 3 (13%) |
| 1 | PSU | A | 516 | 1,22 | 17,21,22 | 1.42 | 3 (17%) | 20,30,33 | 2.74 | 8 (40%) |
| 1 | UR3 | A | 1498 | 1 | 14,22,23 | 0.91 | 0 | 15,32,35 | 1.15 | 1 (6%) |
| 1 | MA6 | A | 1518[B] | 1 | 19,26,27 | 1.14 | 1 (5%) | 18,38,41 | 0.62 | 0 |
| 1 | 4OC | A | 1402 | 1 | 16,23,24 | 0.75 | 0 | 17,32,35 | 0.92 | 1 (5%) |
| 1 | 5MC | A | 1407 | 1 | 15,22,23 | 1.01 | 1 (6%) | 19,32,35 | 1.07 | 1 (5%) |
| 1 | MA6 | A | 1518[A] | 1 | 19,26,27 | 0.67 | 0 | 18,38,41 | 0.86 | 1 (5%) |
| 1 | PSU | A | 1540 | 1 | 17,21,22 | 0.99 | 1 (5%) | 20,30,33 | 3.28 | 7 (35%) |
| 1 | 2MG | A | 1207 | 1 | 19,26,27 | 2.34 | 3 (15%) | 21,38,41 | 2.29 | 6 (28%) |

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 | 5MC | A | 1404 | 1 | - | 0/5/25/26 | 0/2/2/2 |
| 1 | 7MG | A | 527 | 1 | - | 2/7/37/38 | 0/3/3/3 |
| 1 | MA6 | A | 1519[A] | 1 | - | 3/7/29/30 | 0/3/3/3 |
| 1 | 5MC | A | 1400 | 1 | - | 1/5/25/26 | 0/2/2/2 |
| 1 | MA6 | A | 1519[B] | 1 | - | 5/7/29/30 | 0/3/3/3 |
| 1 | PSU | A | 1541 | 1 | - | 1/7/25/26 | 0/2/2/2 |
| 1 | 5MC | A | 967 | 1 | - | 0/5/25/26 | 0/2/2/2 |
| 1 | M2G | A | 966 | 1 | - | 2/7/29/30 | 0/3/3/3 |
| 1 | PSU | A | 516 | 1,22 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | UR3 | A | 1498 | 1 | - | 0/5/25/26 | 0/2/2/2 |
| 1 | MA6 | A | 1518[B] | 1 | - | 5/7/29/30 | 0/3/3/3 |
| 1 | 4OC | A | 1402 | 1 | - | 2/9/29/30 | 0/2/2/2 |
| 1 | 5MC | A | 1407 | 1 | - | 2/5/25/26 | 0/2/2/2 |
| 1 | MA6 | A | 1518[A] | 1 | - | 2/7/29/30 | 0/3/3/3 |
| 1 | PSU | A | 1540 | 1 | - | 1/7/25/26 | 0/2/2/2 |
| 1 | 2MG | A | 1207 | 1 | - | 2/5/27/28 | 0/3/3/3 |

All (25) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|---------|-------|-------------|----------|
| 1 | A | 1207 | 2MG | C2-N2 | 8.10 | 1.41 | 1.34 |
| 1 | A | 966 | M2G | C6-N1 | 5.12 | 1.42 | 1.33 |
| 1 | A | 527 | 7MG | C8-N9 | -5.05 | 1.33 | 1.45 |
| 1 | A | 1207 | 2MG | C6-N1 | 4.36 | 1.40 | 1.33 |
| 1 | A | 527 | 7MG | C2-N2 | 3.95 | 1.41 | 1.33 |
| 1 | A | 516 | PSU | C5-C1' | -3.94 | 1.48 | 1.52 |
| 1 | A | 527 | 7MG | C4-N3 | 3.90 | 1.39 | 1.34 |
| 1 | A | 1519[B] | MA6 | C6-N1 | 3.65 | 1.38 | 1.33 |
| 1 | A | 527 | 7MG | CM7-N7 | -3.53 | 1.40 | 1.46 |
| 1 | A | 1540 | PSU | C4-N3 | 3.27 | 1.38 | 1.33 |
| 1 | A | 966 | M2G | C2-N1 | 3.24 | 1.40 | 1.34 |
| 1 | A | 516 | PSU | C4-N3 | 3.09 | 1.38 | 1.33 |
| 1 | A | 527 | 7MG | C2-N3 | -3.07 | 1.29 | 1.35 |
| 1 | A | 1518[B] | MA6 | C6-N1 | 2.91 | 1.37 | 1.33 |
| 1 | A | 527 | 7MG | C6-N1 | 2.85 | 1.38 | 1.33 |
| 1 | A | 1541 | PSU | C4-N3 | 2.78 | 1.37 | 1.33 |
| 1 | A | 527 | 7MG | C4-N9 | -2.60 | 1.33 | 1.38 |
| 1 | A | 1207 | 2MG | C6-C5 | -2.57 | 1.36 | 1.41 |
| 1 | A | 1519[B] | MA6 | C2-N1 | 2.51 | 1.38 | 1.33 |
| 1 | A | 516 | PSU | O4'-C1' | -2.39 | 1.41 | 1.44 |
| 1 | A | 1407 | 5MC | C5-C4 | 2.34 | 1.45 | 1.41 |
| 1 | A | 1541 | PSU | O4'-C1' | -2.30 | 1.41 | 1.44 |
| 1 | A | 1519[B] | MA6 | C2-N3 | 2.07 | 1.35 | 1.32 |
| 1 | A | 1541 | PSU | C5-C1' | -2.04 | 1.50 | 1.52 |
| 1 | A | 527 | 7MG | C5-C4 | -2.01 | 1.34 | 1.39 |

All (46) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | A | 1540 | PSU | N1-C2-N3 | -10.97 | 119.71 | 128.43 |
| 1 | A | 1541 | PSU | N1-C2-N3 | -10.63 | 119.98 | 128.43 |
| 1 | A | 966 | M2G | C5-C6-N1 | -8.69 | 111.54 | 123.43 |
| 1 | A | 516 | PSU | N1-C2-N3 | -7.85 | 122.19 | 128.43 |
| 1 | A | 1207 | 2MG | C5-C6-N1 | -7.27 | 113.49 | 123.43 |
| 1 | A | 1540 | PSU | C4-N3-C2 | 6.33 | 120.49 | 115.14 |
| 1 | A | 516 | PSU | C5-C4-N3 | -5.50 | 118.28 | 125.36 |
| 1 | A | 966 | M2G | C6-N1-C2 | 5.26 | 122.45 | 116.18 |
| 1 | A | 1541 | PSU | C4-N3-C2 | 4.90 | 119.28 | 115.14 |
| 1 | A | 1540 | PSU | C5-C4-N3 | -4.64 | 119.38 | 125.36 |
| 1 | A | 516 | PSU | C4-N3-C2 | 4.33 | 118.80 | 115.14 |
| 1 | A | 1541 | PSU | C5-C4-N3 | -3.82 | 120.44 | 125.36 |
| 1 | A | 1207 | 2MG | C6-N1-C2 | 3.82 | 122.01 | 115.18 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-------------|-------|-------------|----------|
| 1 | A | 1541 | PSU | C5-C6-N1 | -3.67 | 119.93 | 124.44 |
| 1 | A | 1541 | PSU | C6-N1-C2 | 3.41 | 120.98 | 115.36 |
| 1 | A | 1207 | 2MG | C4-C5-N7 | 3.32 | 112.86 | 109.40 |
| 1 | A | 1207 | 2MG | N2-C2-N3 | 3.27 | 120.10 | 116.96 |
| 1 | A | 516 | PSU | C5-C6-N1 | -3.24 | 120.45 | 124.44 |
| 1 | A | 1540 | PSU | C6-N1-C2 | 3.14 | 120.53 | 115.36 |
| 1 | A | 516 | PSU | O4'-C1'-C5 | -3.03 | 105.24 | 109.93 |
| 1 | A | 527 | 7MG | C4-N9-C1' | -2.96 | 119.58 | 126.60 |
| 1 | A | 1407 | 5MC | N4-C4-N3 | -2.86 | 113.00 | 117.03 |
| 1 | A | 527 | 7MG | C6-N1-C2 | 2.72 | 120.25 | 115.93 |
| 1 | A | 1402 | 4OC | CM4-N4-C4 | -2.70 | 120.65 | 122.97 |
| 1 | A | 1540 | PSU | C5-C6-N1 | -2.66 | 121.17 | 124.44 |
| 1 | A | 1400 | 5MC | CM5-C5-C4 | -2.55 | 119.14 | 121.72 |
| 1 | A | 966 | M2G | C2-N3-C4 | -2.50 | 112.44 | 115.28 |
| 1 | A | 527 | 7MG | N3-C4-N9 | 2.45 | 130.06 | 126.91 |
| 1 | A | 1498 | UR3 | O3'-C3'-C2' | 2.43 | 119.68 | 111.82 |
| 1 | A | 1400 | 5MC | CM5-C5-C6 | 2.40 | 123.73 | 118.68 |
| 1 | A | 1540 | PSU | C5-C1'-C2' | -2.39 | 111.06 | 115.32 |
| 1 | A | 1519[A] | MA6 | N1-C6-N6 | -2.38 | 114.55 | 117.06 |
| 1 | A | 527 | 7MG | N7-C8-N9 | 2.35 | 106.74 | 103.38 |
| 1 | A | 516 | PSU | O4'-C1'-C2' | 2.34 | 108.45 | 104.66 |
| 1 | A | 516 | PSU | C6-N1-C2 | 2.31 | 119.17 | 115.36 |
| 1 | A | 527 | 7MG | C5-C4-N3 | -2.27 | 122.79 | 126.49 |
| 1 | A | 1518[A] | MA6 | N1-C6-N6 | -2.25 | 114.69 | 117.06 |
| 1 | A | 527 | 7MG | N2-C2-N1 | 2.20 | 120.68 | 117.25 |
| 1 | A | 1207 | 2MG | C6-C5-C4 | 2.16 | 122.86 | 120.80 |
| 1 | A | 1541 | PSU | O4'-C1'-C2' | 2.12 | 108.10 | 104.66 |
| 1 | A | 1207 | 2MG | C2-N3-C4 | -2.12 | 112.87 | 115.28 |
| 1 | A | 1540 | PSU | O4'-C1'-C2' | 2.07 | 108.01 | 104.66 |
| 1 | A | 516 | PSU | C5-C1'-C2' | -2.06 | 111.64 | 115.32 |
| 1 | A | 527 | 7MG | C2-N3-C4 | 2.06 | 119.58 | 113.89 |
| 1 | A | 1400 | 5MC | N4-C4-N3 | -2.06 | 114.13 | 117.03 |
| 1 | A | 1404 | 5MC | N4-C4-N3 | -2.01 | 114.19 | 117.03 |

There are no chirality outliers.

All (28) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|---------|------|-----------------|
| 1 | A | 1519[A] | MA6 | O4'-C4'-C5'-O5' |
| 1 | A | 1519[A] | MA6 | C3'-C4'-C5'-O5' |
| 1 | A | 1519[B] | MA6 | C3'-C4'-C5'-O5' |
| 1 | A | 1519[B] | MA6 | C5-C6-N6-C9 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|---------|------|-----------------|
| 1 | A | 966 | M2G | O4'-C4'-C5'-O5' |
| 1 | A | 1402 | 4OC | O4'-C4'-C5'-O5' |
| 1 | A | 1518[B] | MA6 | O4'-C4'-C5'-O5' |
| 1 | A | 1518[B] | MA6 | C3'-C4'-C5'-O5' |
| 1 | A | 1518[B] | MA6 | C5-C6-N6-C9 |
| 1 | A | 1518[B] | MA6 | C5-C6-N6-C10 |
| 1 | A | 527 | 7MG | O4'-C4'-C5'-O5' |
| 1 | A | 527 | 7MG | C3'-C4'-C5'-O5' |
| 1 | A | 1407 | 5MC | O4'-C4'-C5'-O5' |
| 1 | A | 1407 | 5MC | C3'-C4'-C5'-O5' |
| 1 | A | 1207 | 2MG | N1-C2-N2-CM2 |
| 1 | A | 1207 | 2MG | N3-C2-N2-CM2 |
| 1 | A | 1518[A] | MA6 | O4'-C4'-C5'-O5' |
| 1 | A | 966 | M2G | C3'-C4'-C5'-O5' |
| 1 | A | 1402 | 4OC | C3'-C4'-C5'-O5' |
| 1 | A | 1519[B] | MA6 | O4'-C4'-C5'-O5' |
| 1 | A | 1519[B] | MA6 | N1-C6-N6-C9 |
| 1 | A | 1518[B] | MA6 | N1-C6-N6-C9 |
| 1 | A | 1518[A] | MA6 | C3'-C4'-C5'-O5' |
| 1 | A | 1519[B] | MA6 | C5-C6-N6-C10 |
| 1 | A | 1519[A] | MA6 | C4'-C5'-O5'-P |
| 1 | A | 1541 | PSU | O4'-C1'-C5-C4 |
| 1 | A | 1540 | PSU | C2'-C1'-C5-C6 |
| 1 | A | 1400 | 5MC | O4'-C4'-C5'-O5' |

There are no ring outliers.

7 monomers are involved in 9 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|---------|------|---------|--------------|
| 1 | A | 1519[A] | MA6 | 1 | 0 |
| 1 | A | 1519[B] | MA6 | 1 | 0 |
| 1 | A | 1498 | UR3 | 2 | 0 |
| 1 | A | 1518[B] | MA6 | 2 | 0 |
| 1 | A | 1402 | 4OC | 2 | 0 |
| 1 | A | 1518[A] | MA6 | 1 | 0 |
| 1 | A | 1540 | PSU | 1 | 0 |

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 453 ligands modelled in this entry, 453 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

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

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1 | A | 1500/1522 (98%) | -0.28 | 6 (0%) 92 90 | 66, 103, 182, 297 | 0 |
| 2 | B | 234/256 (91%) | -0.25 | 6 (2%) 56 49 | 83, 115, 192, 217 | 0 |
| 3 | C | 206/239 (86%) | -0.50 | 0 100 100 | 87, 114, 150, 183 | 0 |
| 4 | D | 208/209 (99%) | -0.35 | 1 (0%) 91 88 | 71, 103, 143, 192 | 0 |
| 5 | E | 150/162 (92%) | -0.36 | 0 100 100 | 64, 90, 123, 150 | 0 |
| 6 | F | 101/101 (100%) | -0.25 | 0 100 100 | 92, 120, 150, 213 | 0 |
| 7 | G | 155/156 (99%) | -0.29 | 0 100 100 | 109, 133, 184, 220 | 0 |
| 8 | H | 138/138 (100%) | -0.42 | 0 100 100 | 66, 92, 122, 155 | 0 |
| 9 | I | 127/128 (99%) | -0.18 | 0 100 100 | 100, 139, 175, 200 | 0 |
| 10 | J | 98/105 (93%) | -0.07 | 1 (1%) 82 77 | 91, 140, 161, 196 | 0 |
| 11 | K | 116/129 (89%) | -0.22 | 1 (0%) 84 79 | 92, 119, 157, 183 | 0 |
| 12 | L | 124/135 (91%) | -0.05 | 1 (0%) 86 81 | 70, 89, 121, 192 | 0 |
| 13 | M | 118/126 (93%) | -0.05 | 2 (1%) 70 64 | 110, 144, 180, 242 | 0 |
| 14 | N | 60/61 (98%) | -0.24 | 0 100 100 | 98, 119, 153, 198 | 0 |
| 15 | O | 87/89 (97%) | -0.32 | 0 100 100 | 92, 115, 137, 157 | 0 |
| 16 | P | 83/88 (94%) | 0.02 | 0 100 100 | 79, 97, 125, 165 | 0 |
| 17 | Q | 99/105 (94%) | -0.21 | 0 100 100 | 75, 97, 125, 145 | 0 |
| 18 | R | 70/88 (79%) | -0.25 | 0 100 100 | 81, 114, 195, 226 | 0 |
| 19 | S | 80/93 (86%) | 0.26 | 2 (2%) 57 51 | 117, 155, 191, 207 | 0 |
| 20 | T | 99/106 (93%) | -0.20 | 0 100 100 | 79, 105, 146, 169 | 0 |
| 21 | U | 24/27 (88%) | -0.02 | 0 100 100 | 129, 142, 156, 169 | 0 |
| All | All | 3877/4063 (95%) | -0.25 | 20 (0%) 91 88 | 64, 111, 173, 297 | 0 |

All (20) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 12 | L | 128 | ALA | 5.6 |
| 1 | A | 1129 | C | 4.9 |
| 4 | D | 35 | ARG | 4.3 |
| 1 | A | 1030(D) | A | 3.6 |
| 2 | B | 134 | GLU | 3.0 |
| 19 | S | 32 | LYS | 2.8 |
| 2 | B | 122 | PHE | 2.8 |
| 1 | A | 1030(C) | G | 2.7 |
| 19 | S | 33 | THR | 2.6 |
| 2 | B | 132 | LYS | 2.5 |
| 13 | M | 7 | VAL | 2.5 |
| 1 | A | 723 | U | 2.4 |
| 2 | B | 133 | LYS | 2.4 |
| 1 | A | 81 | U | 2.2 |
| 2 | B | 131 | PRO | 2.2 |
| 10 | J | 72 | VAL | 2.2 |
| 13 | M | 119 | GLY | 2.1 |
| 1 | A | 1030(A) | G | 2.0 |
| 2 | B | 138 | LEU | 2.0 |
| 11 | K | 118 | GLY | 2.0 |

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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 | PSU | A | 1540 | 20/21 | 0.84 | 0.42 | 210,230,255,256 | 0 |
| 1 | PSU | A | 1541 | 20/21 | 0.89 | 0.21 | 209,230,242,244 | 0 |
| 1 | MA6 | A | 1518[B] | 24/25 | 0.91 | 0.24 | 80,83,91,94 | 24 |
| 1 | MA6 | A | 1518[A] | 24/25 | 0.91 | 0.24 | 73,79,83,87 | 24 |
| 1 | MA6 | A | 1519[B] | 24/25 | 0.92 | 0.28 | 69,74,75,77 | 24 |
| 1 | MA6 | A | 1519[A] | 24/25 | 0.92 | 0.28 | 68,73,77,81 | 24 |
| 1 | 5MC | A | 1404 | 21/22 | 0.94 | 0.26 | 70,87,96,102 | 0 |
| 1 | 7MG | A | 527 | 24/25 | 0.94 | 0.20 | 81,89,105,113 | 0 |
| 1 | 4OC | A | 1402 | 22/23 | 0.94 | 0.26 | 80,92,108,108 | 0 |
| 1 | 5MC | A | 1407 | 21/22 | 0.95 | 0.16 | 93,104,118,120 | 0 |
| 1 | 5MC | A | 1400 | 21/22 | 0.96 | 0.20 | 65,79,104,105 | 0 |
| 1 | UR3 | A | 1498 | 21/22 | 0.96 | 0.24 | 76,85,96,100 | 0 |
| 1 | M2G | A | 966 | 25/26 | 0.96 | 0.17 | 85,98,120,126 | 0 |
| 1 | 2MG | A | 1207 | 24/25 | 0.96 | 0.12 | 111,117,122,131 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 1 | 5MC | A | 967 | 21/22 | 0.97 | 0.22 | 94,105,113,116 | 0 |
| 1 | PSU | A | 516 | 20/21 | 0.97 | 0.12 | 88,102,114,116 | 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(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 22 | MG | A | 1777 | 1/1 | 0.27 | 0.84 | 112,112,112,112 | 0 |
| 22 | MG | A | 1694 | 1/1 | 0.28 | 0.31 | 94,94,94,94 | 0 |
| 22 | MG | A | 1666 | 1/1 | 0.39 | 0.52 | 100,100,100,100 | 0 |
| 22 | MG | A | 1715 | 1/1 | 0.50 | 0.32 | 109,109,109,109 | 0 |
| 22 | MG | E | 204 | 1/1 | 0.53 | 0.55 | 74,74,74,74 | 0 |
| 22 | MG | A | 1669 | 1/1 | 0.54 | 0.23 | 99,99,99,99 | 0 |
| 22 | MG | A | 1764 | 1/1 | 0.54 | 0.21 | 148,148,148,148 | 0 |
| 22 | MG | A | 1784 | 1/1 | 0.55 | 1.04 | 109,109,109,109 | 0 |
| 22 | MG | A | 1790 | 1/1 | 0.57 | 0.31 | 115,115,115,115 | 0 |
| 22 | MG | A | 1786 | 1/1 | 0.57 | 0.18 | 115,115,115,115 | 0 |
| 22 | MG | A | 2005 | 1/1 | 0.60 | 0.45 | 327,327,327,327 | 0 |
| 22 | MG | D | 302 | 1/1 | 0.61 | 0.27 | 87,87,87,87 | 0 |
| 22 | MG | Q | 201 | 1/1 | 0.61 | 0.39 | 64,64,64,64 | 0 |
| 22 | MG | E | 202 | 1/1 | 0.62 | 1.07 | 105,105,105,105 | 0 |
| 22 | MG | A | 1620 | 1/1 | 0.62 | 0.36 | 83,83,83,83 | 0 |
| 22 | MG | A | 1882 | 1/1 | 0.63 | 0.19 | 443,443,443,443 | 0 |
| 22 | MG | P | 104 | 1/1 | 0.63 | 0.45 | 89,89,89,89 | 0 |
| 22 | MG | A | 1806 | 1/1 | 0.63 | 0.21 | 444,444,444,444 | 0 |
| 22 | MG | A | 1905 | 1/1 | 0.64 | 0.78 | 506,506,506,506 | 0 |
| 22 | MG | A | 1724 | 1/1 | 0.65 | 0.53 | 74,74,74,74 | 0 |
| 22 | MG | A | 1681 | 1/1 | 0.65 | 0.44 | 115,115,115,115 | 0 |
| 22 | MG | A | 1803 | 1/1 | 0.65 | 0.17 | 447,447,447,447 | 0 |
| 22 | MG | E | 205 | 1/1 | 0.66 | 0.39 | 550,550,550,550 | 0 |
| 22 | MG | A | 1912 | 1/1 | 0.67 | 0.22 | 429,429,429,429 | 0 |
| 22 | MG | A | 1648 | 1/1 | 0.67 | 0.17 | 109,109,109,109 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 22 | MG | A | 1678 | 1/1 | 0.67 | 0.27 | 105,105,105,105 | 0 |
| 22 | MG | A | 1709 | 1/1 | 0.67 | 0.90 | 105,105,105,105 | 0 |
| 22 | MG | A | 1839 | 1/1 | 0.67 | 0.18 | 533,533,533,533 | 0 |
| 22 | MG | A | 1787 | 1/1 | 0.68 | 0.52 | 98,98,98,98 | 0 |
| 22 | MG | Q | 203 | 1/1 | 0.68 | 0.18 | 406,406,406,406 | 0 |
| 22 | MG | A | 1700 | 1/1 | 0.68 | 0.36 | 97,97,97,97 | 0 |
| 22 | MG | A | 1778 | 1/1 | 0.69 | 0.93 | 111,111,111,111 | 0 |
| 22 | MG | A | 1871 | 1/1 | 0.69 | 0.25 | 417,417,417,417 | 0 |
| 22 | MG | A | 1686 | 1/1 | 0.69 | 0.67 | 99,99,99,99 | 0 |
| 22 | MG | A | 1873 | 1/1 | 0.69 | 0.26 | 473,473,473,473 | 0 |
| 22 | MG | A | 1952 | 1/1 | 0.69 | 0.51 | 397,397,397,397 | 0 |
| 22 | MG | C | 302 | 1/1 | 0.69 | 0.48 | 95,95,95,95 | 0 |
| 22 | MG | A | 1771 | 1/1 | 0.69 | 0.35 | 101,101,101,101 | 0 |
| 22 | MG | A | 1727 | 1/1 | 0.70 | 0.19 | 97,97,97,97 | 0 |
| 22 | MG | A | 1741 | 1/1 | 0.70 | 0.53 | 87,87,87,87 | 0 |
| 22 | MG | A | 1837 | 1/1 | 0.70 | 0.39 | 500,500,500,500 | 0 |
| 22 | MG | A | 1814 | 1/1 | 0.70 | 0.70 | 481,481,481,481 | 0 |
| 22 | MG | A | 1936 | 1/1 | 0.70 | 0.19 | 388,388,388,388 | 0 |
| 22 | MG | K | 201 | 1/1 | 0.70 | 0.46 | 74,74,74,74 | 0 |
| 22 | MG | A | 1782 | 1/1 | 0.71 | 0.40 | 89,89,89,89 | 0 |
| 22 | MG | A | 1918 | 1/1 | 0.72 | 0.22 | 441,441,441,441 | 0 |
| 22 | MG | A | 1695 | 1/1 | 0.72 | 0.99 | 127,127,127,127 | 0 |
| 22 | MG | A | 1601 | 1/1 | 0.72 | 0.45 | 101,101,101,101 | 0 |
| 22 | MG | A | 1702 | 1/1 | 0.73 | 1.14 | 105,105,105,105 | 0 |
| 22 | MG | A | 1852 | 1/1 | 0.73 | 0.45 | 473,473,473,473 | 0 |
| 22 | MG | A | 1793 | 1/1 | 0.74 | 0.62 | 124,124,124,124 | 0 |
| 22 | MG | A | 1862 | 1/1 | 0.75 | 0.18 | 474,474,474,474 | 0 |
| 22 | MG | A | 1888 | 1/1 | 0.75 | 0.51 | 481,481,481,481 | 0 |
| 22 | MG | A | 1779 | 1/1 | 0.75 | 0.29 | 101,101,101,101 | 0 |
| 22 | MG | A | 1738 | 1/1 | 0.75 | 0.72 | 88,88,88,88 | 0 |
| 22 | MG | A | 1792 | 1/1 | 0.75 | 0.50 | 93,93,93,93 | 0 |
| 22 | MG | A | 1815 | 1/1 | 0.75 | 0.32 | 516,516,516,516 | 0 |
| 22 | MG | A | 1945 | 1/1 | 0.75 | 0.20 | 436,436,436,436 | 0 |
| 22 | MG | A | 1705 | 1/1 | 0.76 | 0.53 | 99,99,99,99 | 0 |
| 22 | MG | A | 1760 | 1/1 | 0.76 | 0.15 | 115,115,115,115 | 0 |
| 22 | MG | A | 1805 | 1/1 | 0.76 | 0.18 | 503,503,503,503 | 0 |
| 22 | MG | A | 1844 | 1/1 | 0.77 | 0.22 | 415,415,415,415 | 0 |
| 22 | MG | A | 1878 | 1/1 | 0.77 | 0.29 | 455,455,455,455 | 0 |
| 22 | MG | A | 1809 | 1/1 | 0.77 | 0.69 | 517,517,517,517 | 0 |
| 22 | MG | A | 1706 | 1/1 | 0.77 | 0.31 | 114,114,114,114 | 0 |
| 22 | MG | A | 1874 | 1/1 | 0.77 | 0.45 | 384,384,384,384 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 22 | MG | Q | 202 | 1/1 | 0.77 | 0.57 | 538,538,538,538 | 0 |
| 22 | MG | A | 1667 | 1/1 | 0.78 | 0.12 | 103,103,103,103 | 0 |
| 22 | MG | A | 1903 | 1/1 | 0.78 | 1.06 | 475,475,475,475 | 0 |
| 22 | MG | B | 302 | 1/1 | 0.78 | 0.14 | 88,88,88,88 | 0 |
| 22 | MG | A | 1813 | 1/1 | 0.78 | 0.18 | 438,438,438,438 | 0 |
| 22 | MG | A | 1658 | 1/1 | 0.78 | 0.69 | 99,99,99,99 | 0 |
| 22 | MG | A | 1870 | 1/1 | 0.78 | 0.26 | 449,449,449,449 | 0 |
| 22 | MG | A | 1854 | 1/1 | 0.78 | 0.50 | 364,364,364,364 | 0 |
| 22 | MG | A | 1737 | 1/1 | 0.78 | 0.29 | 68,68,68,68 | 0 |
| 22 | MG | N | 102 | 1/1 | 0.78 | 0.53 | 79,79,79,79 | 0 |
| 22 | MG | A | 1647 | 1/1 | 0.78 | 0.45 | 70,70,70,70 | 0 |
| 22 | MG | P | 103 | 1/1 | 0.79 | 0.49 | 60,60,60,60 | 0 |
| 22 | MG | A | 1926 | 1/1 | 0.79 | 0.19 | 439,439,439,439 | 0 |
| 22 | MG | A | 1817 | 1/1 | 0.79 | 0.16 | 499,499,499,499 | 0 |
| 22 | MG | A | 1766 | 1/1 | 0.79 | 0.53 | 93,93,93,93 | 0 |
| 22 | MG | A | 1634 | 1/1 | 0.79 | 0.28 | 88,88,88,88 | 0 |
| 22 | MG | A | 1746 | 1/1 | 0.79 | 0.36 | 86,86,86,86 | 0 |
| 22 | MG | A | 1791 | 1/1 | 0.79 | 0.44 | 114,114,114,114 | 0 |
| 22 | MG | A | 1802 | 1/1 | 0.79 | 0.08 | 464,464,464,464 | 0 |
| 22 | MG | A | 1744 | 1/1 | 0.79 | 0.61 | 94,94,94,94 | 0 |
| 22 | MG | A | 1887 | 1/1 | 0.80 | 0.10 | 321,321,321,321 | 0 |
| 22 | MG | A | 2006 | 1/1 | 0.80 | 0.08 | 302,302,302,302 | 0 |
| 22 | MG | A | 1616 | 1/1 | 0.80 | 0.18 | 91,91,91,91 | 0 |
| 22 | MG | A | 1661 | 1/1 | 0.80 | 0.57 | 115,115,115,115 | 0 |
| 22 | MG | A | 1754 | 1/1 | 0.80 | 0.40 | 108,108,108,108 | 0 |
| 22 | MG | A | 1740 | 1/1 | 0.80 | 0.71 | 81,81,81,81 | 0 |
| 22 | MG | A | 1742 | 1/1 | 0.80 | 0.76 | 81,81,81,81 | 0 |
| 22 | MG | A | 1984 | 1/1 | 0.80 | 0.55 | 360,360,360,360 | 0 |
| 22 | MG | A | 1902 | 1/1 | 0.80 | 0.28 | 395,395,395,395 | 0 |
| 22 | MG | A | 1904 | 1/1 | 0.81 | 0.47 | 469,469,469,469 | 0 |
| 22 | MG | A | 1751 | 1/1 | 0.81 | 0.55 | 69,69,69,69 | 0 |
| 22 | MG | A | 1622 | 1/1 | 0.81 | 0.92 | 81,81,81,81 | 0 |
| 22 | MG | A | 1626 | 1/1 | 0.81 | 0.42 | 70,70,70,70 | 0 |
| 22 | MG | A | 1795 | 1/1 | 0.81 | 0.55 | 534,534,534,534 | 0 |
| 22 | MG | A | 1833 | 1/1 | 0.81 | 0.30 | 497,497,497,497 | 0 |
| 22 | MG | A | 1769 | 1/1 | 0.81 | 0.31 | 134,134,134,134 | 0 |
| 22 | MG | A | 1714 | 1/1 | 0.81 | 0.74 | 104,104,104,104 | 0 |
| 22 | MG | A | 1807 | 1/1 | 0.81 | 0.31 | 511,511,511,511 | 0 |
| 22 | MG | A | 1763 | 1/1 | 0.81 | 0.96 | 94,94,94,94 | 0 |
| 22 | MG | A | 1842 | 1/1 | 0.81 | 0.38 | 424,424,424,424 | 0 |
| 22 | MG | A | 1968 | 1/1 | 0.82 | 1.52 | 503,503,503,503 | 0 |
| 22 | MG | A | 1845 | 1/1 | 0.82 | 0.08 | 521,521,521,521 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 22 | MG | A | 1893 | 1/1 | 0.82 | 0.20 | 453,453,453,453 | 0 |
| 22 | MG | A | 1923 | 1/1 | 0.82 | 0.12 | 427,427,427,427 | 0 |
| 22 | MG | A | 1753 | 1/1 | 0.82 | 0.40 | 103,103,103,103 | 0 |
| 22 | MG | A | 1914 | 1/1 | 0.82 | 0.30 | 376,376,376,376 | 0 |
| 22 | MG | A | 1911 | 1/1 | 0.82 | 0.15 | 425,425,425,425 | 0 |
| 22 | MG | A | 1890 | 1/1 | 0.82 | 0.27 | 469,469,469,469 | 0 |
| 22 | MG | A | 1750 | 1/1 | 0.82 | 0.46 | 109,109,109,109 | 0 |
| 22 | MG | A | 1980 | 1/1 | 0.82 | 0.57 | 340,340,340,340 | 0 |
| 22 | MG | A | 1652 | 1/1 | 0.82 | 0.56 | 76,76,76,76 | 0 |
| 22 | MG | A | 1684 | 1/1 | 0.82 | 0.25 | 86,86,86,86 | 0 |
| 22 | MG | A | 1720 | 1/1 | 0.83 | 0.36 | 100,100,100,100 | 0 |
| 22 | MG | A | 1785 | 1/1 | 0.83 | 0.58 | 103,103,103,103 | 0 |
| 22 | MG | A | 1959 | 1/1 | 0.83 | 0.18 | 382,382,382,382 | 0 |
| 22 | MG | A | 1627 | 1/1 | 0.83 | 0.24 | 333,333,333,333 | 0 |
| 22 | MG | A | 1708 | 1/1 | 0.83 | 0.34 | 117,117,117,117 | 0 |
| 22 | MG | A | 1752 | 1/1 | 0.83 | 0.38 | 115,115,115,115 | 0 |
| 22 | MG | A | 1947 | 1/1 | 0.84 | 0.36 | 440,440,440,440 | 0 |
| 22 | MG | A | 1880 | 1/1 | 0.84 | 0.29 | 498,498,498,498 | 0 |
| 22 | MG | A | 1981 | 1/1 | 0.84 | 0.35 | 451,451,451,451 | 0 |
| 22 | MG | A | 1969 | 1/1 | 0.84 | 1.20 | 550,550,550,550 | 0 |
| 22 | MG | A | 1610 | 1/1 | 0.84 | 0.12 | 94,94,94,94 | 0 |
| 22 | MG | A | 1922 | 1/1 | 0.84 | 0.60 | 433,433,433,433 | 0 |
| 22 | MG | A | 1773 | 1/1 | 0.84 | 0.30 | 69,69,69,69 | 0 |
| 22 | MG | A | 1665 | 1/1 | 0.85 | 0.61 | 81,81,81,81 | 0 |
| 22 | MG | A | 1884 | 1/1 | 0.85 | 0.78 | 546,546,546,546 | 0 |
| 22 | MG | A | 1726 | 1/1 | 0.85 | 0.33 | 77,77,77,77 | 0 |
| 22 | MG | A | 1810 | 1/1 | 0.85 | 0.42 | 460,460,460,460 | 0 |
| 22 | MG | A | 1606 | 1/1 | 0.85 | 0.30 | 69,69,69,69 | 0 |
| 22 | MG | A | 1707 | 1/1 | 0.85 | 1.06 | 99,99,99,99 | 0 |
| 22 | MG | A | 1827 | 1/1 | 0.85 | 0.25 | 515,515,515,515 | 0 |
| 22 | MG | A | 1829 | 1/1 | 0.85 | 0.29 | 436,436,436,436 | 0 |
| 22 | MG | A | 1743 | 1/1 | 0.85 | 0.45 | 88,88,88,88 | 0 |
| 22 | MG | A | 1965 | 1/1 | 0.85 | 0.22 | 296,296,296,296 | 0 |
| 22 | MG | A | 1774 | 1/1 | 0.85 | 0.10 | 263,263,263,263 | 0 |
| 22 | MG | A | 1858 | 1/1 | 0.85 | 0.46 | 473,473,473,473 | 0 |
| 22 | MG | A | 1711 | 1/1 | 0.85 | 0.09 | 68,68,68,68 | 0 |
| 22 | MG | B | 303 | 1/1 | 0.85 | 0.26 | 88,88,88,88 | 0 |
| 22 | MG | A | 1879 | 1/1 | 0.86 | 0.09 | 396,396,396,396 | 0 |
| 22 | MG | A | 1830 | 1/1 | 0.86 | 0.05 | 331,331,331,331 | 0 |
| 22 | MG | A | 1930 | 1/1 | 0.86 | 0.39 | 510,510,510,510 | 0 |
| 22 | MG | A | 1950 | 1/1 | 0.86 | 0.26 | 424,424,424,424 | 0 |
| 22 | MG | A | 1621 | 1/1 | 0.86 | 0.35 | 130,130,130,130 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 22 | MG | A | 1836 | 1/1 | 0.86 | 0.69 | 424,424,424,424 | 0 |
| 22 | MG | A | 1662 | 1/1 | 0.86 | 0.39 | 111,111,111,111 | 0 |
| 22 | MG | A | 1816 | 1/1 | 0.86 | 0.15 | 458,458,458,458 | 0 |
| 22 | MG | A | 1631 | 1/1 | 0.86 | 0.49 | 173,173,173,173 | 0 |
| 22 | MG | A | 1683 | 1/1 | 0.86 | 0.33 | 110,110,110,110 | 0 |
| 22 | MG | A | 1974 | 1/1 | 0.87 | 0.21 | 503,503,503,503 | 0 |
| 22 | MG | A | 2016 | 1/1 | 0.87 | 0.14 | 104,104,104,104 | 0 |
| 22 | MG | A | 1835 | 1/1 | 0.87 | 0.20 | 516,516,516,516 | 0 |
| 22 | MG | A | 1998 | 1/1 | 0.87 | 0.91 | 464,464,464,464 | 0 |
| 22 | MG | A | 1977 | 1/1 | 0.87 | 0.45 | 419,419,419,419 | 0 |
| 22 | MG | A | 1962 | 1/1 | 0.87 | 0.55 | 273,273,273,273 | 0 |
| 22 | MG | A | 1701 | 1/1 | 0.87 | 0.69 | 106,106,106,106 | 0 |
| 22 | MG | A | 1838 | 1/1 | 0.87 | 0.21 | 350,350,350,350 | 0 |
| 22 | MG | A | 1759 | 1/1 | 0.87 | 0.22 | 111,111,111,111 | 0 |
| 22 | MG | A | 1804 | 1/1 | 0.87 | 0.41 | 506,506,506,506 | 0 |
| 22 | MG | A | 1654 | 1/1 | 0.87 | 0.24 | 127,127,127,127 | 0 |
| 22 | MG | A | 1875 | 1/1 | 0.88 | 0.61 | 451,451,451,451 | 0 |
| 22 | MG | A | 1682 | 1/1 | 0.88 | 0.09 | 187,187,187,187 | 0 |
| 22 | MG | A | 1826 | 1/1 | 0.88 | 0.12 | 441,441,441,441 | 0 |
| 22 | MG | A | 1723 | 1/1 | 0.88 | 0.33 | 81,81,81,81 | 0 |
| 22 | MG | A | 1851 | 1/1 | 0.88 | 0.08 | 365,365,365,365 | 0 |
| 22 | MG | A | 2017 | 1/1 | 0.88 | 0.21 | 80,80,80,80 | 0 |
| 22 | MG | A | 2018 | 1/1 | 0.88 | 0.15 | 82,82,82,82 | 0 |
| 22 | MG | A | 2015 | 1/1 | 0.88 | 0.40 | 414,414,414,414 | 0 |
| 22 | MG | A | 1831 | 1/1 | 0.88 | 0.07 | 233,233,233,233 | 0 |
| 22 | MG | A | 1846 | 1/1 | 0.88 | 0.49 | 490,490,490,490 | 0 |
| 22 | MG | B | 301 | 1/1 | 0.89 | 0.26 | 76,76,76,76 | 0 |
| 22 | MG | A | 1788 | 1/1 | 0.89 | 0.20 | 81,81,81,81 | 0 |
| 22 | MG | P | 101 | 1/1 | 0.89 | 0.25 | 78,78,78,78 | 0 |
| 22 | MG | A | 1992 | 1/1 | 0.89 | 0.51 | 495,495,495,495 | 0 |
| 22 | MG | A | 1691 | 1/1 | 0.89 | 0.22 | 160,160,160,160 | 0 |
| 22 | MG | A | 1901 | 1/1 | 0.89 | 0.23 | 536,536,536,536 | 0 |
| 22 | MG | A | 1958 | 1/1 | 0.89 | 0.10 | 431,431,431,431 | 0 |
| 22 | MG | A | 1927 | 1/1 | 0.89 | 0.25 | 440,440,440,440 | 0 |
| 22 | MG | A | 1820 | 1/1 | 0.89 | 0.17 | 382,382,382,382 | 0 |
| 22 | MG | A | 1919 | 1/1 | 0.89 | 0.32 | 440,440,440,440 | 0 |
| 22 | MG | A | 1964 | 1/1 | 0.89 | 0.13 | 382,382,382,382 | 0 |
| 22 | MG | A | 1864 | 1/1 | 0.89 | 0.40 | 450,450,450,450 | 0 |
| 22 | MG | A | 1798 | 1/1 | 0.89 | 0.06 | 374,374,374,374 | 0 |
| 22 | MG | A | 1840 | 1/1 | 0.90 | 0.17 | 525,525,525,525 | 0 |
| 22 | MG | A | 1999 | 1/1 | 0.90 | 0.26 | 438,438,438,438 | 0 |
| 22 | MG | A | 1676 | 1/1 | 0.90 | 0.26 | 63,63,63,63 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 22 | MG | A | 1770 | 1/1 | 0.90 | 0.51 | 122,122,122,122 | 0 |
| 22 | MG | A | 1731 | 1/1 | 0.90 | 0.19 | 68,68,68,68 | 0 |
| 22 | MG | A | 1866 | 1/1 | 0.90 | 0.08 | 354,354,354,354 | 0 |
| 22 | MG | A | 1756 | 1/1 | 0.90 | 0.46 | 132,132,132,132 | 0 |
| 22 | MG | C | 301 | 1/1 | 0.90 | 0.20 | 77,77,77,77 | 0 |
| 22 | MG | A | 1913 | 1/1 | 0.90 | 0.26 | 432,432,432,432 | 0 |
| 22 | MG | A | 1944 | 1/1 | 0.90 | 0.40 | 461,461,461,461 | 0 |
| 22 | MG | A | 1948 | 1/1 | 0.90 | 0.48 | 503,503,503,503 | 0 |
| 22 | MG | D | 306 | 1/1 | 0.90 | 0.17 | 350,350,350,350 | 0 |
| 22 | MG | A | 1637 | 1/1 | 0.90 | 0.31 | 94,94,94,94 | 0 |
| 22 | MG | A | 1630 | 1/1 | 0.90 | 0.27 | 100,100,100,100 | 0 |
| 22 | MG | A | 1768 | 1/1 | 0.90 | 0.27 | 119,119,119,119 | 0 |
| 22 | MG | A | 1653 | 1/1 | 0.90 | 0.24 | 114,114,114,114 | 0 |
| 22 | MG | A | 1972 | 1/1 | 0.90 | 0.21 | 420,420,420,420 | 0 |
| 22 | MG | A | 1638 | 1/1 | 0.90 | 0.20 | 180,180,180,180 | 0 |
| 22 | MG | A | 1745 | 1/1 | 0.90 | 0.24 | 88,88,88,88 | 0 |
| 22 | MG | A | 1808 | 1/1 | 0.90 | 0.12 | 335,335,335,335 | 0 |
| 22 | MG | A | 1672 | 1/1 | 0.90 | 0.11 | 121,121,121,121 | 0 |
| 22 | MG | A | 1739 | 1/1 | 0.90 | 0.30 | 74,74,74,74 | 0 |
| 22 | MG | A | 1671 | 1/1 | 0.91 | 0.45 | 153,153,153,153 | 0 |
| 22 | MG | A | 1733 | 1/1 | 0.91 | 0.26 | 85,85,85,85 | 0 |
| 22 | MG | A | 1797 | 1/1 | 0.91 | 0.18 | 427,427,427,427 | 0 |
| 22 | MG | A | 1693 | 1/1 | 0.91 | 0.13 | 209,209,209,209 | 0 |
| 22 | MG | A | 1861 | 1/1 | 0.91 | 0.21 | 444,444,444,444 | 0 |
| 22 | MG | A | 1868 | 1/1 | 0.91 | 0.27 | 452,452,452,452 | 0 |
| 22 | MG | A | 1818 | 1/1 | 0.91 | 0.26 | 391,391,391,391 | 0 |
| 22 | MG | A | 1951 | 1/1 | 0.91 | 0.46 | 476,476,476,476 | 0 |
| 22 | MG | A | 1729 | 1/1 | 0.91 | 0.30 | 106,106,106,106 | 0 |
| 22 | MG | A | 1819 | 1/1 | 0.91 | 0.14 | 508,508,508,508 | 0 |
| 22 | MG | A | 1960 | 1/1 | 0.91 | 0.33 | 293,293,293,293 | 0 |
| 22 | MG | A | 1898 | 1/1 | 0.91 | 0.24 | 406,406,406,406 | 0 |
| 22 | MG | A | 1990 | 1/1 | 0.91 | 0.32 | 259,259,259,259 | 0 |
| 22 | MG | A | 1941 | 1/1 | 0.91 | 0.38 | 457,457,457,457 | 0 |
| 22 | MG | L | 201 | 1/1 | 0.91 | 0.27 | 342,342,342,342 | 0 |
| 22 | MG | A | 1748 | 1/1 | 0.91 | 0.65 | 98,98,98,98 | 0 |
| 22 | MG | A | 2010 | 1/1 | 0.92 | 0.42 | 87,87,87,87 | 0 |
| 22 | MG | A | 1651 | 1/1 | 0.92 | 0.30 | 112,112,112,112 | 0 |
| 22 | MG | A | 1971 | 1/1 | 0.92 | 0.49 | 410,410,410,410 | 0 |
| 22 | MG | A | 1687 | 1/1 | 0.92 | 0.33 | 81,81,81,81 | 0 |
| 22 | MG | A | 1853 | 1/1 | 0.92 | 1.01 | 543,543,543,543 | 0 |
| 22 | MG | D | 307 | 1/1 | 0.92 | 0.19 | 376,376,376,376 | 0 |
| 22 | MG | A | 1891 | 1/1 | 0.92 | 0.18 | 308,308,308,308 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 22 | MG | A | 1645 | 1/1 | 0.92 | 0.29 | 137,137,137,137 | 0 |
| 22 | MG | A | 2002 | 1/1 | 0.92 | 0.16 | 176,176,176,176 | 0 |
| 22 | MG | A | 1897 | 1/1 | 0.92 | 0.26 | 424,424,424,424 | 0 |
| 22 | MG | A | 1970 | 1/1 | 0.92 | 0.40 | 394,394,394,394 | 0 |
| 22 | MG | A | 1670 | 1/1 | 0.92 | 0.14 | 92,92,92,92 | 0 |
| 22 | MG | A | 1696 | 1/1 | 0.92 | 0.34 | 94,94,94,94 | 0 |
| 22 | MG | A | 1921 | 1/1 | 0.92 | 0.64 | 412,412,412,412 | 0 |
| 22 | MG | A | 1704 | 1/1 | 0.92 | 0.18 | 66,66,66,66 | 0 |
| 22 | MG | A | 1732 | 1/1 | 0.92 | 0.38 | 98,98,98,98 | 0 |
| 22 | MG | A | 1618 | 1/1 | 0.92 | 0.12 | 71,71,71,71 | 0 |
| 22 | MG | A | 1855 | 1/1 | 0.92 | 0.63 | 525,525,525,525 | 0 |
| 22 | MG | A | 1794 | 1/1 | 0.92 | 0.47 | 103,103,103,103 | 0 |
| 22 | MG | E | 203 | 1/1 | 0.92 | 0.11 | 72,72,72,72 | 0 |
| 22 | MG | A | 1758 | 1/1 | 0.92 | 0.13 | 96,96,96,96 | 0 |
| 22 | MG | A | 1949 | 1/1 | 0.92 | 0.24 | 481,481,481,481 | 0 |
| 22 | MG | A | 1986 | 1/1 | 0.92 | 0.06 | 225,225,225,225 | 0 |
| 22 | MG | A | 1857 | 1/1 | 0.92 | 0.31 | 436,436,436,436 | 0 |
| 22 | MG | A | 1935 | 1/1 | 0.93 | 0.26 | 363,363,363,363 | 0 |
| 22 | MG | A | 1991 | 1/1 | 0.93 | 0.66 | 473,473,473,473 | 0 |
| 22 | MG | A | 1674 | 1/1 | 0.93 | 0.64 | 146,146,146,146 | 0 |
| 22 | MG | A | 1608 | 1/1 | 0.93 | 0.16 | 165,165,165,165 | 0 |
| 22 | MG | A | 1633 | 1/1 | 0.93 | 0.35 | 124,124,124,124 | 0 |
| 22 | MG | A | 1703 | 1/1 | 0.93 | 0.08 | 187,187,187,187 | 0 |
| 22 | MG | D | 305 | 1/1 | 0.93 | 0.10 | 418,418,418,418 | 0 |
| 22 | MG | A | 1943 | 1/1 | 0.93 | 0.12 | 341,341,341,341 | 0 |
| 22 | MG | A | 1996 | 1/1 | 0.93 | 0.79 | 445,445,445,445 | 0 |
| 22 | MG | A | 1825 | 1/1 | 0.93 | 0.14 | 409,409,409,409 | 0 |
| 22 | MG | A | 1856 | 1/1 | 0.93 | 0.13 | 461,461,461,461 | 0 |
| 22 | MG | A | 1677 | 1/1 | 0.93 | 0.22 | 125,125,125,125 | 0 |
| 22 | MG | D | 304 | 1/1 | 0.93 | 0.26 | 526,526,526,526 | 0 |
| 22 | MG | A | 1668 | 1/1 | 0.93 | 0.09 | 165,165,165,165 | 0 |
| 22 | MG | A | 1821 | 1/1 | 0.93 | 0.26 | 377,377,377,377 | 0 |
| 22 | MG | E | 206 | 1/1 | 0.93 | 0.28 | 412,412,412,412 | 0 |
| 22 | MG | O | 1001 | 1/1 | 0.93 | 0.17 | 183,183,183,183 | 0 |
| 22 | MG | A | 1872 | 1/1 | 0.93 | 0.15 | 378,378,378,378 | 0 |
| 22 | MG | A | 1725 | 1/1 | 0.93 | 0.66 | 98,98,98,98 | 0 |
| 22 | MG | A | 2001 | 1/1 | 0.93 | 0.15 | 346,346,346,346 | 0 |
| 22 | MG | A | 1812 | 1/1 | 0.93 | 0.10 | 484,484,484,484 | 0 |
| 22 | MG | A | 1916 | 1/1 | 0.94 | 0.22 | 445,445,445,445 | 0 |
| 22 | MG | A | 1920 | 1/1 | 0.94 | 0.46 | 444,444,444,444 | 0 |
| 22 | MG | A | 1946 | 1/1 | 0.94 | 0.37 | 503,503,503,503 | 0 |
| 22 | MG | A | 1712 | 1/1 | 0.94 | 0.30 | 96,96,96,96 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 22 | MG | A | 1989 | 1/1 | 0.94 | 0.42 | 475,475,475,475 | 0 |
| 22 | MG | A | 1895 | 1/1 | 0.94 | 0.56 | 472,472,472,472 | 0 |
| 22 | MG | A | 1883 | 1/1 | 0.94 | 0.13 | 304,304,304,304 | 0 |
| 22 | MG | D | 303 | 1/1 | 0.94 | 0.15 | 81,81,81,81 | 0 |
| 22 | MG | A | 1799 | 1/1 | 0.94 | 0.22 | 446,446,446,446 | 0 |
| 22 | MG | A | 1604 | 1/1 | 0.94 | 0.19 | 89,89,89,89 | 0 |
| 22 | MG | A | 1865 | 1/1 | 0.94 | 0.14 | 484,484,484,484 | 0 |
| 22 | MG | A | 1937 | 1/1 | 0.94 | 0.17 | 443,443,443,443 | 0 |
| 22 | MG | A | 1843 | 1/1 | 0.94 | 0.16 | 393,393,393,393 | 0 |
| 22 | MG | H | 201 | 1/1 | 0.94 | 0.16 | 281,281,281,281 | 0 |
| 22 | MG | A | 1933 | 1/1 | 0.94 | 0.14 | 374,374,374,374 | 0 |
| 22 | MG | A | 1877 | 1/1 | 0.94 | 0.64 | 407,407,407,407 | 0 |
| 22 | MG | A | 1735 | 1/1 | 0.94 | 0.23 | 73,73,73,73 | 0 |
| 22 | MG | A | 1967 | 1/1 | 0.94 | 0.73 | 459,459,459,459 | 0 |
| 22 | MG | A | 1776 | 1/1 | 0.94 | 0.26 | 460,460,460,460 | 0 |
| 22 | MG | A | 1988 | 1/1 | 0.94 | 0.67 | 402,402,402,402 | 0 |
| 22 | MG | A | 1639 | 1/1 | 0.94 | 0.25 | 92,92,92,92 | 0 |
| 22 | MG | A | 1767 | 1/1 | 0.94 | 0.20 | 61,61,61,61 | 0 |
| 22 | MG | A | 1801 | 1/1 | 0.94 | 0.05 | 392,392,392,392 | 0 |
| 22 | MG | A | 1822 | 1/1 | 0.94 | 0.10 | 229,229,229,229 | 0 |
| 22 | MG | A | 1734 | 1/1 | 0.94 | 0.15 | 84,84,84,84 | 0 |
| 22 | MG | A | 1783 | 1/1 | 0.94 | 0.13 | 69,69,69,69 | 0 |
| 22 | MG | A | 1780 | 1/1 | 0.94 | 0.09 | 119,119,119,119 | 0 |
| 22 | MG | A | 1609 | 1/1 | 0.94 | 0.12 | 125,125,125,125 | 0 |
| 22 | MG | P | 102 | 1/1 | 0.94 | 0.19 | 89,89,89,89 | 0 |
| 22 | MG | A | 1954 | 1/1 | 0.94 | 0.54 | 459,459,459,459 | 0 |
| 22 | MG | A | 1859 | 1/1 | 0.95 | 0.10 | 151,151,151,151 | 0 |
| 22 | MG | A | 1659 | 1/1 | 0.95 | 0.16 | 72,72,72,72 | 0 |
| 22 | MG | A | 1664 | 1/1 | 0.95 | 0.10 | 95,95,95,95 | 0 |
| 22 | MG | A | 1899 | 1/1 | 0.95 | 0.06 | 345,345,345,345 | 0 |
| 22 | MG | S | 101 | 1/1 | 0.95 | 0.07 | 101,101,101,101 | 0 |
| 22 | MG | A | 1624 | 1/1 | 0.95 | 0.18 | 100,100,100,100 | 0 |
| 22 | MG | C | 303 | 1/1 | 0.95 | 0.14 | 429,429,429,429 | 0 |
| 22 | MG | A | 1625 | 1/1 | 0.95 | 0.15 | 96,96,96,96 | 0 |
| 22 | MG | A | 1924 | 1/1 | 0.95 | 0.18 | 336,336,336,336 | 0 |
| 22 | MG | A | 1757 | 1/1 | 0.95 | 0.27 | 163,163,163,163 | 0 |
| 22 | MG | A | 1869 | 1/1 | 0.95 | 0.34 | 339,339,339,339 | 0 |
| 22 | MG | A | 1995 | 1/1 | 0.95 | 0.17 | 355,355,355,355 | 0 |
| 22 | MG | A | 1982 | 1/1 | 0.95 | 0.24 | 340,340,340,340 | 0 |
| 22 | MG | A | 1765 | 1/1 | 0.95 | 0.23 | 84,84,84,84 | 0 |
| 22 | MG | A | 1834 | 1/1 | 0.95 | 0.06 | 265,265,265,265 | 0 |
| 22 | MG | A | 1663 | 1/1 | 0.95 | 0.15 | 125,125,125,125 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 22 | MG | A | 1747 | 1/1 | 0.95 | 0.09 | 70,70,70,70 | 0 |
| 22 | MG | A | 2004 | 1/1 | 0.95 | 0.66 | 402,402,402,402 | 0 |
| 22 | MG | A | 1717 | 1/1 | 0.95 | 0.21 | 87,87,87,87 | 0 |
| 22 | MG | A | 1860 | 1/1 | 0.95 | 0.24 | 411,411,411,411 | 0 |
| 22 | MG | A | 1929 | 1/1 | 0.95 | 0.11 | 346,346,346,346 | 0 |
| 22 | MG | A | 1849 | 1/1 | 0.95 | 0.33 | 412,412,412,412 | 0 |
| 22 | MG | A | 1656 | 1/1 | 0.95 | 0.14 | 100,100,100,100 | 0 |
| 22 | MG | A | 1623 | 1/1 | 0.95 | 0.34 | 112,112,112,112 | 0 |
| 22 | MG | A | 1811 | 1/1 | 0.95 | 0.14 | 181,181,181,181 | 0 |
| 22 | MG | A | 1957 | 1/1 | 0.95 | 0.61 | 482,482,482,482 | 0 |
| 22 | MG | A | 1823 | 1/1 | 0.95 | 0.12 | 337,337,337,337 | 0 |
| 22 | MG | A | 1781 | 1/1 | 0.96 | 0.18 | 95,95,95,95 | 0 |
| 22 | MG | A | 1649 | 1/1 | 0.96 | 0.18 | 79,79,79,79 | 0 |
| 22 | MG | A | 1867 | 1/1 | 0.96 | 0.29 | 364,364,364,364 | 0 |
| 22 | MG | A | 2011 | 1/1 | 0.96 | 1.21 | 96,96,96,96 | 0 |
| 22 | MG | A | 1973 | 1/1 | 0.96 | 0.41 | 446,446,446,446 | 0 |
| 22 | MG | A | 1643 | 1/1 | 0.96 | 0.23 | 132,132,132,132 | 0 |
| 22 | MG | A | 1688 | 1/1 | 0.96 | 0.15 | 178,178,178,178 | 0 |
| 22 | MG | A | 1928 | 1/1 | 0.96 | 1.20 | 490,490,490,490 | 0 |
| 22 | MG | A | 2000 | 1/1 | 0.96 | 0.43 | 441,441,441,441 | 0 |
| 22 | MG | A | 1953 | 1/1 | 0.96 | 0.07 | 295,295,295,295 | 0 |
| 22 | MG | A | 1692 | 1/1 | 0.96 | 0.18 | 231,231,231,231 | 0 |
| 22 | MG | A | 1892 | 1/1 | 0.96 | 0.11 | 329,329,329,329 | 0 |
| 22 | MG | A | 1863 | 1/1 | 0.96 | 0.11 | 413,413,413,413 | 0 |
| 22 | MG | A | 1615 | 1/1 | 0.96 | 0.20 | 93,93,93,93 | 0 |
| 22 | MG | A | 1635 | 1/1 | 0.96 | 0.63 | 66,66,66,66 | 0 |
| 22 | MG | A | 1749 | 1/1 | 0.96 | 0.13 | 123,123,123,123 | 0 |
| 22 | MG | A | 1915 | 1/1 | 0.96 | 0.18 | 185,185,185,185 | 0 |
| 22 | MG | A | 1713 | 1/1 | 0.96 | 0.34 | 85,85,85,85 | 0 |
| 22 | MG | A | 1761 | 1/1 | 0.96 | 0.59 | 57,57,57,57 | 0 |
| 22 | MG | A | 1979 | 1/1 | 0.96 | 0.18 | 113,113,113,113 | 0 |
| 22 | MG | A | 1697 | 1/1 | 0.96 | 0.19 | 106,106,106,106 | 0 |
| 22 | MG | A | 2008 | 1/1 | 0.96 | 0.28 | 373,373,373,373 | 0 |
| 22 | MG | A | 1942 | 1/1 | 0.96 | 0.33 | 487,487,487,487 | 0 |
| 22 | MG | A | 1909 | 1/1 | 0.96 | 0.27 | 312,312,312,312 | 0 |
| 22 | MG | A | 1939 | 1/1 | 0.96 | 0.57 | 392,392,392,392 | 0 |
| 22 | MG | A | 1824 | 1/1 | 0.96 | 0.21 | 354,354,354,354 | 0 |
| 22 | MG | A | 1641 | 1/1 | 0.96 | 0.14 | 122,122,122,122 | 0 |
| 22 | MG | A | 1755 | 1/1 | 0.96 | 0.49 | 83,83,83,83 | 0 |
| 22 | MG | A | 1650 | 1/1 | 0.96 | 0.48 | 112,112,112,112 | 0 |
| 22 | MG | A | 1614 | 1/1 | 0.96 | 0.13 | 100,100,100,100 | 0 |
| 22 | MG | A | 1894 | 1/1 | 0.96 | 0.40 | 227,227,227,227 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 22 | MG | A | 1617 | 1/1 | 0.96 | 0.37 | 85,85,85,85 | 0 |
| 22 | MG | A | 1917 | 1/1 | 0.96 | 0.12 | 430,430,430,430 | 0 |
| 22 | MG | A | 1963 | 1/1 | 0.96 | 0.51 | 335,335,335,335 | 0 |
| 22 | MG | A | 1896 | 1/1 | 0.97 | 0.29 | 172,172,172,172 | 0 |
| 22 | MG | A | 1730 | 1/1 | 0.97 | 0.45 | 85,85,85,85 | 0 |
| 22 | MG | A | 1716 | 1/1 | 0.97 | 0.18 | 53,53,53,53 | 0 |
| 22 | MG | A | 1955 | 1/1 | 0.97 | 0.65 | 374,374,374,374 | 0 |
| 22 | MG | A | 1938 | 1/1 | 0.97 | 0.38 | 496,496,496,496 | 0 |
| 22 | MG | A | 1789 | 1/1 | 0.97 | 0.10 | 118,118,118,118 | 0 |
| 22 | MG | A | 1685 | 1/1 | 0.97 | 0.20 | 87,87,87,87 | 0 |
| 22 | MG | A | 1841 | 1/1 | 0.97 | 0.08 | 315,315,315,315 | 0 |
| 22 | MG | A | 1657 | 1/1 | 0.97 | 0.24 | 110,110,110,110 | 0 |
| 22 | MG | A | 1925 | 1/1 | 0.97 | 0.28 | 447,447,447,447 | 0 |
| 22 | MG | A | 1881 | 1/1 | 0.97 | 0.10 | 357,357,357,357 | 0 |
| 22 | MG | A | 1985 | 1/1 | 0.97 | 0.10 | 278,278,278,278 | 0 |
| 22 | MG | C | 304 | 1/1 | 0.97 | 0.07 | 475,475,475,475 | 0 |
| 22 | MG | A | 1886 | 1/1 | 0.97 | 0.24 | 361,361,361,361 | 0 |
| 22 | MG | A | 1775 | 1/1 | 0.97 | 0.14 | 168,168,168,168 | 0 |
| 22 | MG | A | 1847 | 1/1 | 0.97 | 0.11 | 414,414,414,414 | 0 |
| 22 | MG | A | 1719 | 1/1 | 0.97 | 0.26 | 102,102,102,102 | 0 |
| 22 | MG | E | 201 | 1/1 | 0.97 | 0.37 | 115,115,115,115 | 0 |
| 22 | MG | A | 1690 | 1/1 | 0.97 | 0.26 | 137,137,137,137 | 0 |
| 22 | MG | A | 1828 | 1/1 | 0.97 | 0.36 | 417,417,417,417 | 0 |
| 22 | MG | A | 1931 | 1/1 | 0.97 | 0.14 | 397,397,397,397 | 0 |
| 22 | MG | A | 1640 | 1/1 | 0.97 | 0.22 | 49,49,49,49 | 0 |
| 22 | MG | A | 1612 | 1/1 | 0.97 | 0.32 | 145,145,145,145 | 0 |
| 22 | MG | A | 1772 | 1/1 | 0.97 | 0.08 | 72,72,72,72 | 0 |
| 22 | MG | A | 1997 | 1/1 | 0.97 | 0.77 | 172,172,172,172 | 0 |
| 22 | MG | A | 1848 | 1/1 | 0.97 | 0.21 | 330,330,330,330 | 0 |
| 22 | MG | A | 1718 | 1/1 | 0.97 | 0.14 | 65,65,65,65 | 0 |
| 22 | MG | A | 1956 | 1/1 | 0.97 | 0.43 | 322,322,322,322 | 0 |
| 22 | MG | A | 1632 | 1/1 | 0.97 | 0.16 | 73,73,73,73 | 0 |
| 22 | MG | A | 1994 | 1/1 | 0.97 | 0.13 | 158,158,158,158 | 0 |
| 22 | MG | A | 2012 | 1/1 | 0.97 | 0.14 | 196,196,196,196 | 0 |
| 22 | MG | A | 1889 | 1/1 | 0.97 | 0.10 | 392,392,392,392 | 0 |
| 22 | MG | A | 1655 | 1/1 | 0.98 | 0.14 | 72,72,72,72 | 0 |
| 22 | MG | A | 1978 | 1/1 | 0.98 | 0.19 | 184,184,184,184 | 0 |
| 22 | MG | A | 1646 | 1/1 | 0.98 | 0.21 | 80,80,80,80 | 0 |
| 22 | MG | A | 1636 | 1/1 | 0.98 | 0.17 | 63,63,63,63 | 0 |
| 22 | MG | A | 1605 | 1/1 | 0.98 | 0.08 | 112,112,112,112 | 0 |
| 22 | MG | A | 1800 | 1/1 | 0.98 | 0.09 | 124,124,124,124 | 0 |
| 22 | MG | A | 1736 | 1/1 | 0.98 | 0.20 | 142,142,142,142 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 22 | MG | A | 1908 | 1/1 | 0.98 | 0.17 | 354,354,354,354 | 0 |
| 22 | MG | A | 2003 | 1/1 | 0.98 | 0.45 | 400,400,400,400 | 0 |
| 22 | MG | A | 1796 | 1/1 | 0.98 | 0.19 | 383,383,383,383 | 0 |
| 22 | MG | A | 1721 | 1/1 | 0.98 | 0.17 | 77,77,77,77 | 0 |
| 22 | MG | F | 201 | 1/1 | 0.98 | 0.18 | 351,351,351,351 | 0 |
| 22 | MG | A | 1961 | 1/1 | 0.98 | 0.09 | 379,379,379,379 | 0 |
| 22 | MG | A | 1934 | 1/1 | 0.98 | 0.26 | 349,349,349,349 | 0 |
| 22 | MG | A | 1876 | 1/1 | 0.98 | 0.10 | 460,460,460,460 | 0 |
| 22 | MG | A | 1680 | 1/1 | 0.98 | 0.11 | 81,81,81,81 | 0 |
| 22 | MG | A | 1983 | 1/1 | 0.98 | 0.31 | 393,393,393,393 | 0 |
| 22 | MG | A | 1619 | 1/1 | 0.98 | 0.47 | 95,95,95,95 | 0 |
| 22 | MG | A | 1976 | 1/1 | 0.98 | 0.13 | 127,127,127,127 | 0 |
| 22 | MG | A | 1762 | 1/1 | 0.98 | 0.12 | 69,69,69,69 | 0 |
| 22 | MG | A | 1722 | 1/1 | 0.98 | 0.07 | 89,89,89,89 | 0 |
| 22 | MG | A | 1900 | 1/1 | 0.98 | 0.35 | 410,410,410,410 | 0 |
| 22 | MG | A | 1602 | 1/1 | 0.98 | 0.07 | 155,155,155,155 | 0 |
| 22 | MG | A | 1613 | 1/1 | 0.98 | 0.29 | 58,58,58,58 | 0 |
| 22 | MG | A | 1698 | 1/1 | 0.98 | 0.21 | 138,138,138,138 | 0 |
| 22 | MG | A | 1910 | 1/1 | 0.98 | 0.16 | 222,222,222,222 | 0 |
| 22 | MG | A | 1906 | 1/1 | 0.98 | 0.17 | 180,180,180,180 | 0 |
| 22 | MG | A | 1710 | 1/1 | 0.98 | 0.12 | 124,124,124,124 | 0 |
| 22 | MG | A | 2009 | 1/1 | 0.98 | 0.16 | 79,79,79,79 | 0 |
| 22 | MG | A | 2013 | 1/1 | 0.98 | 0.17 | 227,227,227,227 | 0 |
| 22 | MG | A | 1975 | 1/1 | 0.98 | 0.15 | 459,459,459,459 | 0 |
| 22 | MG | A | 1644 | 1/1 | 0.99 | 0.21 | 96,96,96,96 | 0 |
| 22 | MG | A | 1660 | 1/1 | 0.99 | 0.03 | 160,160,160,160 | 0 |
| 22 | MG | A | 1642 | 1/1 | 0.99 | 0.16 | 81,81,81,81 | 0 |
| 22 | MG | A | 1885 | 1/1 | 0.99 | 0.06 | 132,132,132,132 | 0 |
| 22 | MG | A | 1932 | 1/1 | 0.99 | 0.14 | 402,402,402,402 | 0 |
| 22 | MG | A | 1629 | 1/1 | 0.99 | 0.21 | 71,71,71,71 | 0 |
| 22 | MG | A | 1679 | 1/1 | 0.99 | 0.17 | 102,102,102,102 | 0 |
| 22 | MG | A | 1611 | 1/1 | 0.99 | 0.13 | 104,104,104,104 | 0 |
| 22 | MG | A | 1675 | 1/1 | 0.99 | 0.17 | 150,150,150,150 | 0 |
| 22 | MG | A | 1689 | 1/1 | 0.99 | 0.21 | 138,138,138,138 | 0 |
| 22 | MG | A | 1850 | 1/1 | 0.99 | 0.13 | 96,96,96,96 | 0 |
| 23 | ZN | N | 101 | 1/1 | 0.99 | 0.19 | 100,100,100,100 | 0 |
| 23 | ZN | D | 301 | 1/1 | 0.99 | 0.37 | 97,97,97,97 | 0 |
| 22 | MG | A | 1993 | 1/1 | 0.99 | 0.18 | 36,36,36,36 | 0 |
| 22 | MG | A | 1907 | 1/1 | 0.99 | 0.11 | 310,310,310,310 | 0 |
| 22 | MG | A | 1987 | 1/1 | 0.99 | 0.16 | 238,238,238,238 | 0 |
| 22 | MG | A | 1673 | 1/1 | 0.99 | 0.34 | 121,121,121,121 | 0 |
| 22 | MG | A | 2014 | 1/1 | 0.99 | 0.21 | 75,75,75,75 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 22 | MG | A | 1628 | 1/1 | 0.99 | 0.13 | 130,130,130,130 | 0 |
| 22 | MG | A | 1832 | 1/1 | 0.99 | 0.33 | 453,453,453,453 | 0 |
| 22 | MG | A | 1966 | 1/1 | 0.99 | 0.28 | 349,349,349,349 | 0 |
| 22 | MG | A | 2007 | 1/1 | 0.99 | 0.06 | 159,159,159,159 | 0 |
| 22 | MG | A | 1607 | 1/1 | 0.99 | 0.18 | 65,65,65,65 | 0 |
| 22 | MG | A | 1940 | 1/1 | 0.99 | 0.29 | 425,425,425,425 | 0 |
| 22 | MG | A | 1728 | 1/1 | 0.99 | 0.63 | 91,91,91,91 | 0 |
| 22 | MG | A | 1603 | 1/1 | 1.00 | 0.15 | 90,90,90,90 | 0 |
| 22 | MG | A | 1699 | 1/1 | 1.00 | 0.18 | 89,89,89,89 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.