



Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 07:25 pm BST

PDB ID : 5LMR / pdb_00005lmr
EMDB ID : EMD-4077
Title : Structure of bacterial 30S-IF1-IF3-mRNA-tRNA translation pre-initiation complex(state-2B)
Authors : Hussain, T.; Llacer, J.L.; Wimberly, B.T.; Ramakrishnan, V.
Deposited on : 2016-08-01
Resolution : 4.45 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

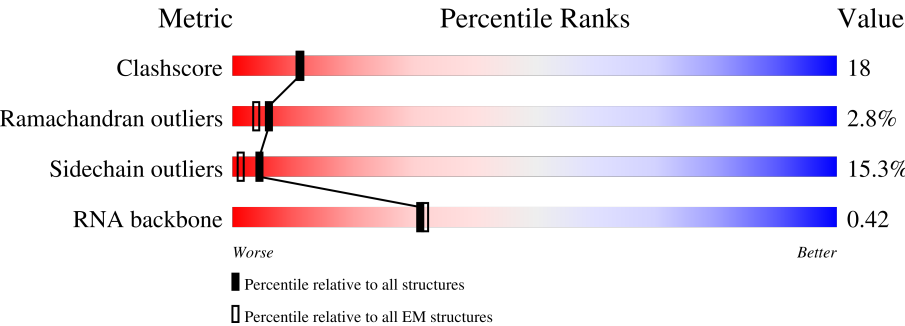
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.45 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.





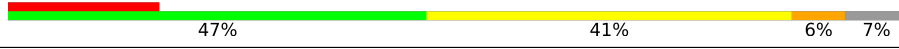




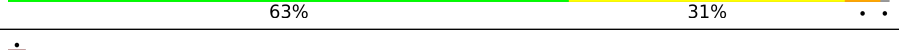
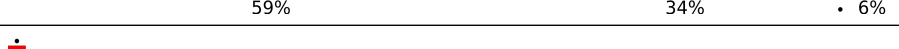
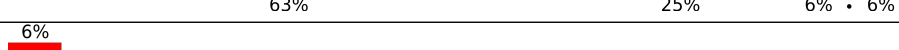

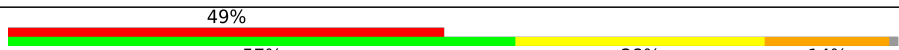

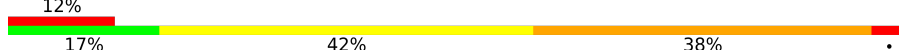

| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 210492 | 15764 |
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |
| RNA backbone | 6643 | 2191 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | A | 1522 | <div> <div>27%</div> <div>55%</div> <div>17%</div> <div>.</div> </div> |
| 2 | B | 256 | <div> <div>62%</div> <div>56%</div> <div>30%</div> <div>5%</div> <div>9%</div> </div> |
| 3 | C | 239 | <div> <div>5%</div> <div>46%</div> <div>33%</div> <div>7%</div> <div>14%</div> </div> |
| 4 | D | 209 | <div> <div>5%</div> <div>57%</div> <div>38%</div> <div>.</div> </div> |
| 5 | E | 162 | <div> <div>59%</div> <div>27%</div> <div>6%</div> <div>7%</div> </div> |
| 6 | F | 101 | <div> <div>66%</div> <div>31%</div> <div>..</div> </div> |
| 7 | G | 156 | <div> <div>8%</div> <div>73%</div> <div>26%</div> <div>.</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 8 | H | 138 |  |
| 9 | I | 128 |  |
| 10 | J | 105 |  |
| 11 | K | 129 |  |
| 12 | L | 132 |  |
| 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 | V | 27 |  |
| 22 | W | 72 |  |
| 23 | X | 171 |  |
| 24 | Y | 42 |  |
| 25 | Z | 77 |  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 26 | ZN | D | 300 | - | - | X | - |

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 55662 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 1 | A | 1515 | Total | C | N | O | P | 0 | 0 |
| | | | 32542 | 14490 | 6022 | 10519 | 1511 | | |

- Molecule 2 is a protein called 30S ribosomal protein S2.

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

- Molecule 3 is a protein called 30S ribosomal protein S3.

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

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

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

- Molecule 6 is a protein called 30S ribosomal protein S6.

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

- Molecule 7 is a protein called 30S ribosomal protein S7.

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

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

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

- Molecule 11 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11 | K | 119 | Total | C | N | O | S | 0 | 0 |
| | | | 885 | 549 | 168 | 165 | 3 | | |

- Molecule 12 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12 | L | 124 | Total | C | N | O | S | 0 | 0 |
| | | | 970 | 611 | 195 | 163 | 1 | | |

- Molecule 13 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13 | M | 121 | Total | C | N | O | S | 0 | 0 |
| | | | 964 | 597 | 199 | 166 | 2 | | |

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15 | O | 88 | Total | C | N | O | S | 0 | 0 |
| | | | 734 | 459 | 147 | 126 | 2 | | |

- Molecule 16 is a protein called 30S ribosomal protein S16.

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

- Molecule 17 is a protein called 30S ribosomal protein S17.

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

- Molecule 18 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|-------|
| 18 | R | 73 | Total | C | N | O | 0 | 0 |
| | | | 598 | 381 | 118 | 99 | | |

- Molecule 19 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19 | S | 82 | Total | C | N | O | S | 0 | 0 |
| | | | 655 | 419 | 120 | 114 | 2 | | |

- Molecule 20 is a protein called 30S ribosomal protein S20.

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

- Molecule 21 is a protein called 30S ribosomal protein Thx.

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

- Molecule 22 is a protein called Translation initiation factor IF-1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22 | W | 71 | Total | C | N | O | S | 0 | 0 |
| | | | 570 | 362 | 103 | 103 | 2 | | |

- Molecule 23 is a protein called Translation initiation factor IF-3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23 | X | 168 | Total | C | N | O | S | 0 | 0 |
| | | | 1356 | 853 | 249 | 245 | 9 | | |

- Molecule 24 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 24 | Y | 17 | Total | C | N | O | P | 0 | 0 |
| | | | 373 | 166 | 74 | 116 | 17 | | |

- Molecule 25 is a RNA chain called tRNAi.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|-------|
| 25 | Z | 77 | Total | C | N | O | P | S | 0 | 0 |
| | | | 1646 | 735 | 297 | 536 | 77 | 1 | | |

- Molecule 26 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 26 | D | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 26 | N | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

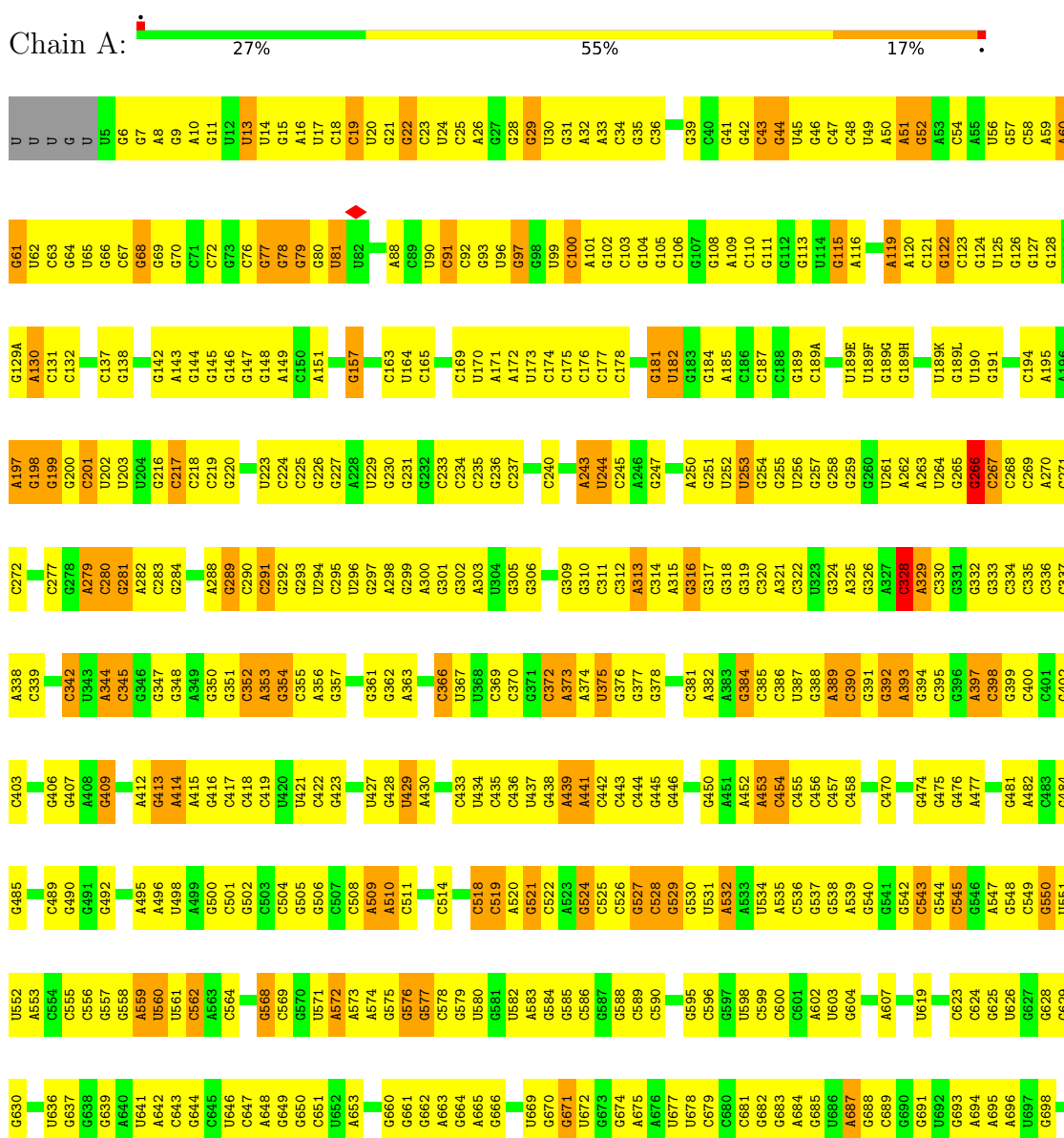
- Molecule 27 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

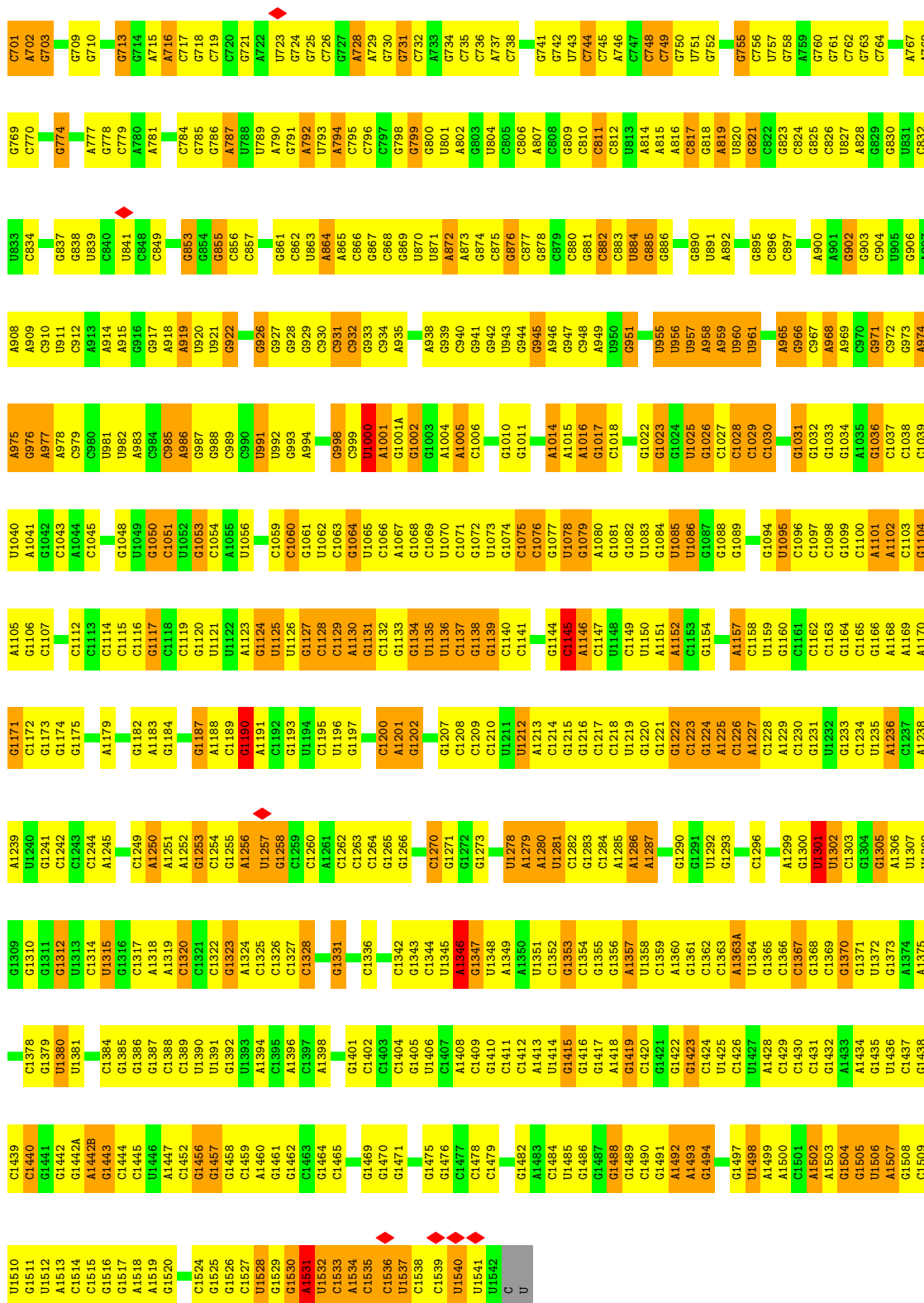
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 27 | W | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 27 | Z | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

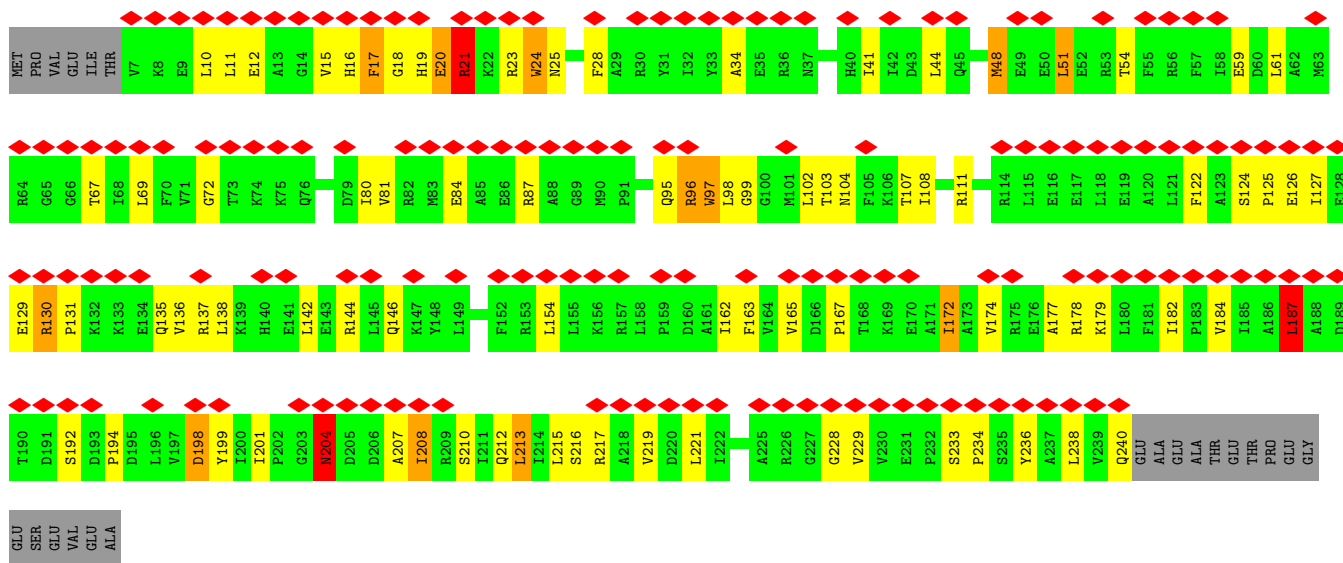
• Molecule 1: 16S rRNA



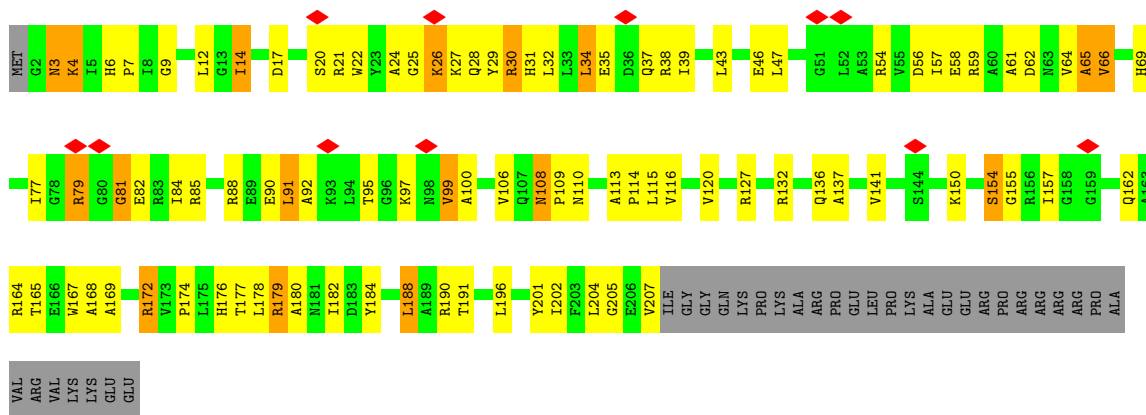


• Molecule 2: 30S ribosomal protein S2

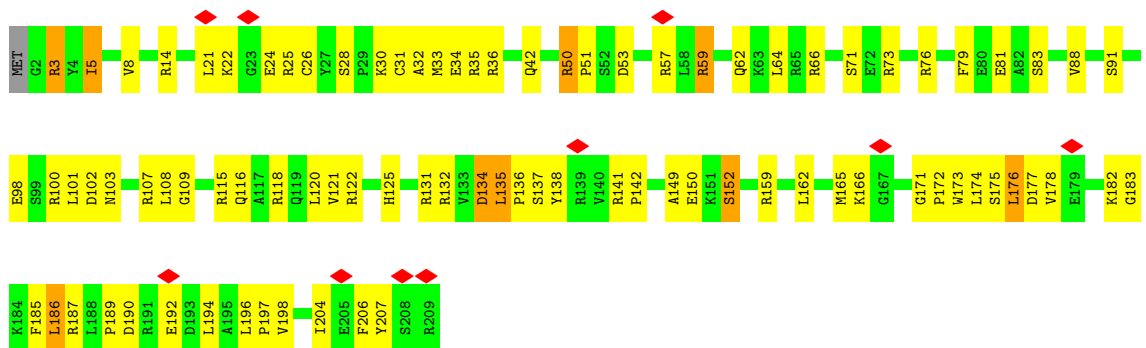




• Molecule 3: 30S ribosomal protein S3

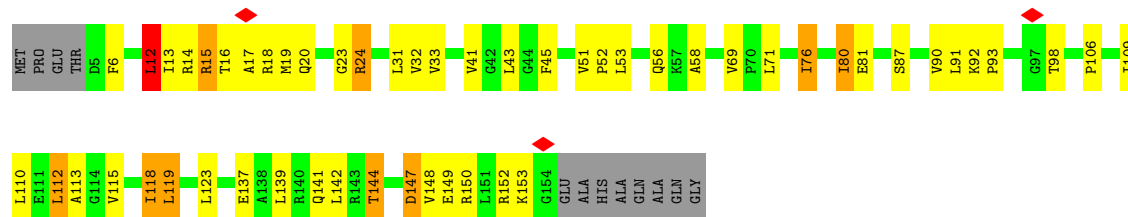


• Molecule 4: 30S ribosomal protein S4



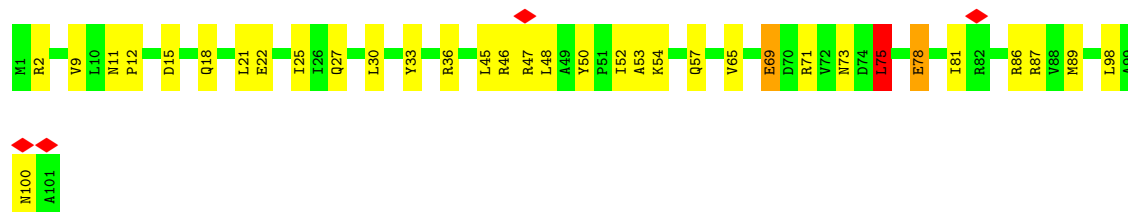
• Molecule 5: 30S ribosomal protein S5

Chain E: 




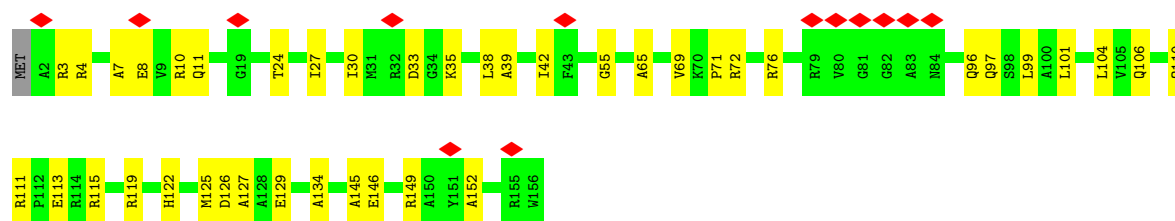
- Molecule 6: 30S ribosomal protein S6

Chain F: 



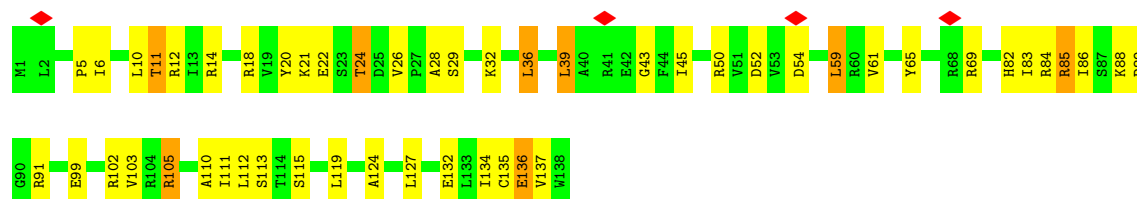
- Molecule 7: 30S ribosomal protein S7

Chain G: 



- Molecule 8: 30S ribosomal protein S8

Chain H: 



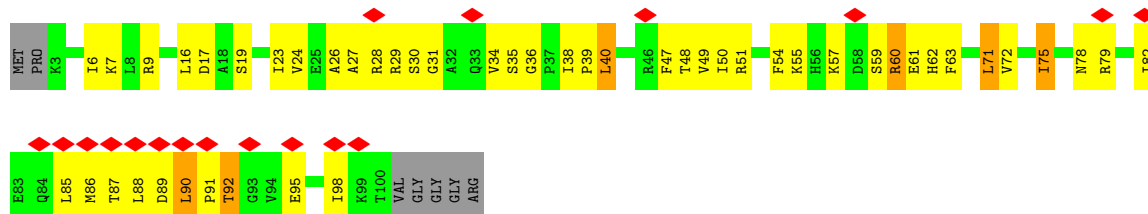
- Molecule 9: 30S ribosomal protein S9

Chain I: 

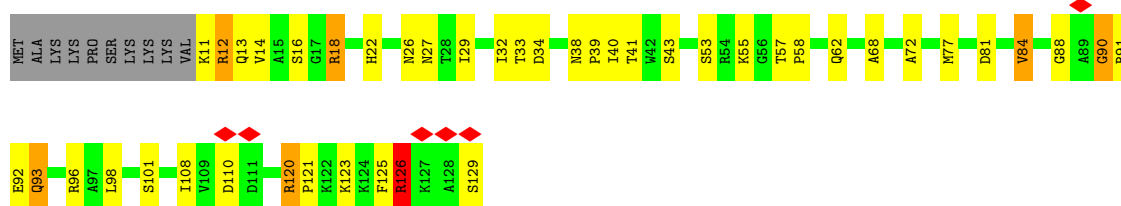




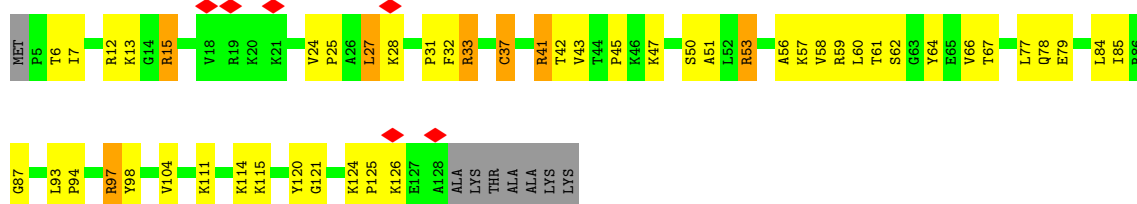
- Molecule 10: 30S ribosomal protein S10



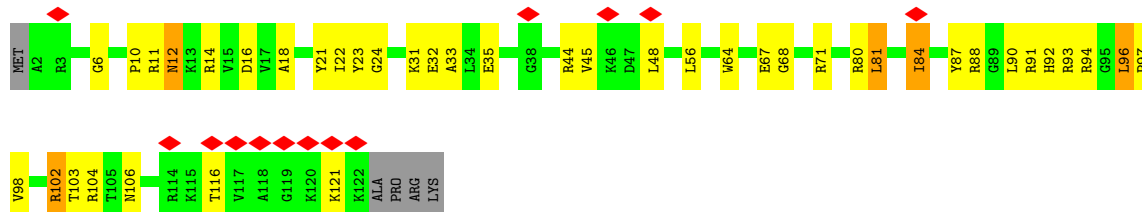
- Molecule 11: 30S ribosomal protein S11



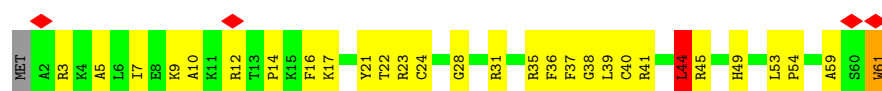
- Molecule 12: 30S ribosomal protein S12



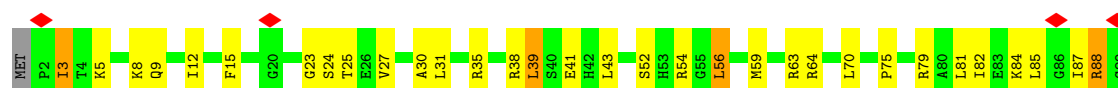
- Molecule 13: 30S ribosomal protein S13



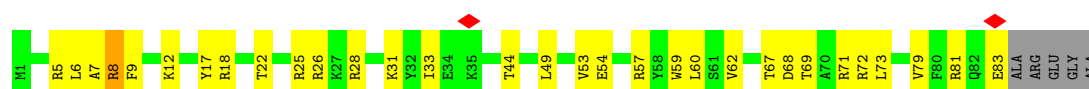
- Molecule 14: 30S ribosomal protein S14 type Z



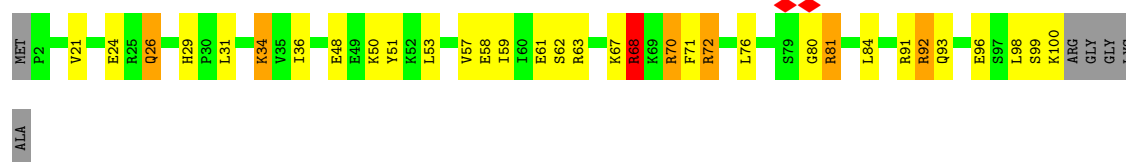
- Molecule 15: 30S ribosomal protein S15



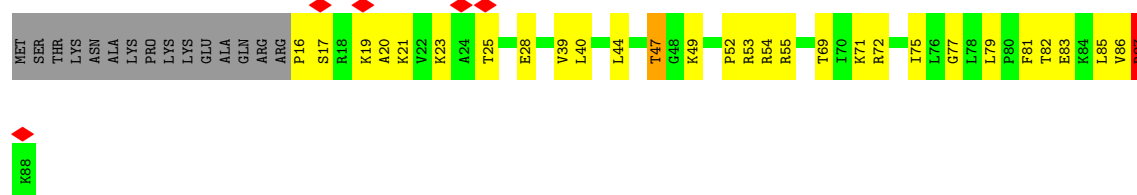
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



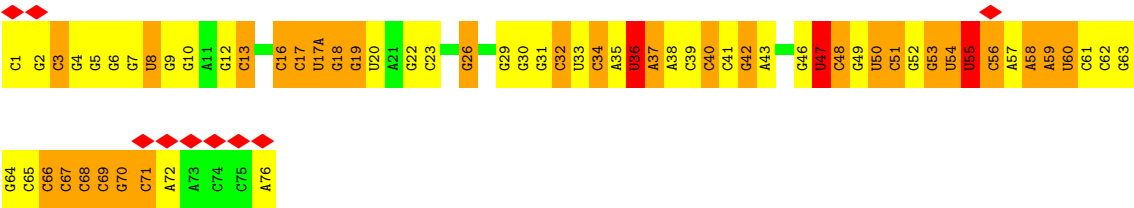
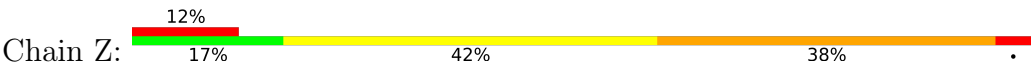
- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19



● Molecule 25: tRNAi



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 17176 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI POLARA 300 | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 30 | Depositor |
| Minimum defocus (nm) | 1500 | Depositor |
| Maximum defocus (nm) | 3500 | Depositor |
| Magnification | 104478 | Depositor |
| Image detector | OTHER | Depositor |
| Maximum map value | 0.438 | Depositor |
| Minimum map value | -0.129 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.022 | Depositor |
| Recommended contour level | 0.075 | Depositor |
| Map size (\AA) | 348.4, 348.4, 348.4 | wwPDB |
| Map dimensions | 260, 260, 260 | wwPDB |
| Map angles ($^\circ$) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (\AA) | 1.34, 1.34, 1.34 | Depositor |

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, ZN, 5MU, G7M, 4SU, MG, PSU

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------|-------------|-----------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | A | 0.33 | 0/36416 | 0.73 | 13/56813 (0.0%) |
| 2 | B | 0.51 | 0/1935 | 0.82 | 2/2609 (0.1%) |
| 3 | C | 0.44 | 0/1636 | 0.88 | 6/2205 (0.3%) |
| 4 | D | 0.42 | 0/1733 | 0.78 | 0/2318 |
| 5 | E | 0.43 | 0/1162 | 0.89 | 3/1564 (0.2%) |
| 6 | F | 0.43 | 0/856 | 0.78 | 1/1154 (0.1%) |
| 7 | G | 0.44 | 0/1276 | 0.77 | 0/1709 |
| 8 | H | 0.40 | 0/1136 | 0.78 | 0/1527 |
| 9 | I | 0.42 | 0/1029 | 0.72 | 0/1379 |
| 10 | J | 0.48 | 0/805 | 0.80 | 2/1082 (0.2%) |
| 11 | K | 0.47 | 0/900 | 0.82 | 0/1213 |
| 12 | L | 0.38 | 0/986 | 0.75 | 0/1320 |
| 13 | M | 0.45 | 0/974 | 0.78 | 1/1303 (0.1%) |
| 14 | N | 0.41 | 0/501 | 0.82 | 1/664 (0.2%) |
| 15 | O | 0.44 | 0/745 | 0.82 | 0/992 |
| 16 | P | 0.42 | 0/716 | 0.77 | 0/963 |
| 17 | Q | 0.40 | 0/836 | 0.75 | 0/1117 |
| 18 | R | 0.45 | 0/604 | 0.81 | 0/801 |
| 19 | S | 0.48 | 0/670 | 0.80 | 1/903 (0.1%) |
| 20 | T | 0.45 | 0/765 | 0.88 | 0/1007 |
| 21 | V | 0.48 | 0/212 | 0.75 | 0/277 |
| 22 | W | 0.53 | 0/580 | 0.90 | 1/782 (0.1%) |
| 23 | X | 0.48 | 0/1375 | 0.78 | 0/1844 |
| 24 | Y | 0.43 | 0/418 | 0.69 | 0/649 |
| 25 | Z | 0.43 | 0/1719 | 0.86 | 2/2674 (0.1%) |
| All | All | 0.38 | 0/59985 | 0.76 | 33/88869 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2 | B | 0 | 1 |
| 23 | X | 0 | 1 |
| All | All | 0 | 2 |

There are no bond length outliers.

All (33) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 3 | C | 65 | ALA | CB-CA-C | -14.85 | 87.83 | 110.10 |
| 5 | E | 15 | ARG | CB-CA-C | -12.38 | 85.65 | 110.40 |
| 22 | W | 23 | ARG | N-CA-C | -11.78 | 79.19 | 111.00 |
| 5 | E | 15 | ARG | N-CA-C | -8.75 | 87.37 | 111.00 |
| 3 | C | 66 | VAL | N-CA-C | -8.72 | 87.46 | 111.00 |
| 10 | J | 61 | GLU | N-CA-CB | -8.33 | 95.61 | 110.60 |
| 13 | M | 81 | LEU | CA-CB-CG | 8.13 | 134.00 | 115.30 |
| 1 | A | 1145 | C | C2'-C3'-O3' | 7.83 | 126.74 | 109.50 |
| 1 | A | 266 | G | C2'-C3'-O3' | 7.73 | 126.51 | 109.50 |
| 3 | C | 65 | ALA | N-CA-C | -7.49 | 90.77 | 111.00 |
| 14 | N | 44 | LEU | CA-CB-CG | 7.28 | 132.05 | 115.30 |
| 1 | A | 1498 | U | C2'-C3'-O3' | 7.08 | 125.08 | 109.50 |
| 1 | A | 1190 | G | C2'-C3'-O3' | 7.04 | 125.00 | 109.50 |
| 3 | C | 34 | LEU | CA-CB-CG | 6.55 | 130.38 | 115.30 |
| 5 | E | 12 | LEU | CA-CB-CG | 6.50 | 130.25 | 115.30 |
| 25 | Z | 47 | U | C2'-C3'-O3' | 6.45 | 124.01 | 113.70 |
| 3 | C | 91 | LEU | CA-CB-CG | 6.43 | 130.10 | 115.30 |
| 1 | A | 1301 | U | C2'-C3'-O3' | 6.43 | 123.99 | 113.70 |
| 2 | B | 221 | LEU | CA-CB-CG | 6.25 | 129.68 | 115.30 |
| 1 | A | 687 | A | C2'-C3'-O3' | 6.17 | 123.57 | 113.70 |
| 6 | F | 75 | LEU | CA-CB-CG | 6.09 | 129.31 | 115.30 |
| 1 | A | 1346 | A | C2'-C3'-O3' | 5.90 | 123.14 | 113.70 |
| 1 | A | 1000 | U | C2'-C3'-O3' | 5.83 | 123.02 | 113.70 |
| 1 | A | 792 | A | C2'-C3'-O3' | 5.82 | 123.01 | 113.70 |
| 25 | Z | 36 | U | C2'-C3'-O3' | 5.69 | 122.80 | 113.70 |
| 1 | A | 328 | C | C2'-C3'-O3' | 5.63 | 122.70 | 113.70 |
| 1 | A | 281 | G | C2'-C3'-O3' | 5.60 | 122.66 | 113.70 |
| 10 | J | 88 | LEU | CA-CB-CG | 5.52 | 127.99 | 115.30 |
| 3 | C | 178 | LEU | CA-CB-CG | 5.45 | 127.84 | 115.30 |
| 1 | A | 965 | A | C2'-C3'-O3' | 5.44 | 122.41 | 113.70 |
| 2 | B | 187 | LEU | CA-CB-CG | 5.34 | 127.58 | 115.30 |
| 19 | S | 20 | LEU | CA-CB-CG | 5.31 | 127.52 | 115.30 |
| 1 | A | 1531 | A | C2'-C3'-O3' | 5.19 | 122.00 | 113.70 |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 2 | B | 16 | HIS | Peptide |
| 23 | X | 53 | ASP | Peptide |

5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 32542 | 0 | 16447 | 1121 | 0 |
| 2 | B | 1900 | 0 | 1951 | 39 | 0 |
| 3 | C | 1612 | 0 | 1674 | 77 | 0 |
| 4 | D | 1703 | 0 | 1766 | 42 | 0 |
| 5 | E | 1146 | 0 | 1207 | 46 | 0 |
| 6 | F | 843 | 0 | 857 | 15 | 0 |
| 7 | G | 1257 | 0 | 1296 | 24 | 0 |
| 8 | H | 1116 | 0 | 1177 | 40 | 0 |
| 9 | I | 1010 | 0 | 1037 | 32 | 0 |
| 10 | J | 792 | 0 | 835 | 48 | 0 |
| 11 | K | 885 | 0 | 904 | 20 | 0 |
| 12 | L | 970 | 0 | 1057 | 32 | 0 |
| 13 | M | 964 | 0 | 1034 | 25 | 0 |
| 14 | N | 492 | 0 | 529 | 28 | 0 |
| 15 | O | 734 | 0 | 771 | 13 | 0 |
| 16 | P | 700 | 0 | 720 | 19 | 0 |
| 17 | Q | 823 | 0 | 891 | 20 | 0 |
| 18 | R | 598 | 0 | 670 | 17 | 0 |
| 19 | S | 655 | 0 | 672 | 35 | 0 |
| 20 | T | 763 | 0 | 861 | 17 | 0 |
| 21 | V | 208 | 0 | 221 | 3 | 0 |
| 22 | W | 570 | 0 | 599 | 25 | 0 |
| 23 | X | 1356 | 0 | 1401 | 15 | 0 |
| 24 | Y | 373 | 0 | 186 | 17 | 0 |
| 25 | Z | 1646 | 0 | 845 | 109 | 0 |
| 26 | D | 1 | 0 | 0 | 4 | 0 |
| 26 | N | 1 | 0 | 0 | 0 | 0 |
| 27 | W | 1 | 0 | 0 | 0 | 0 |
| 27 | Z | 1 | 0 | 0 | 0 | 0 |
| All | All | 55662 | 0 | 39608 | 1690 | 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 18.

All (1690) 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) |
|------------------|------------------|--------------------------|-------------------|
| 22:W:21:THR:CG2 | 22:W:33:LEU:HD11 | 1.53 | 1.36 |
| 10:J:7:LYS:HG3 | 10:J:71:LEU:CD2 | 1.55 | 1.33 |
| 1:A:1358:U:H3 | 1:A:1363(A):A:N6 | 1.36 | 1.24 |
| 1:A:1345:U:N3 | 1:A:1375:A:N6 | 1.87 | 1.21 |
| 5:E:93:PRO:HG3 | 8:H:105:ARG:NH2 | 1.53 | 1.20 |
| 9:I:5:TYR:CE2 | 9:I:7:THR:OG1 | 1.95 | 1.19 |
| 1:A:1358:U:O4 | 1:A:1363(A):A:N1 | 1.75 | 1.19 |
| 5:E:93:PRO:CG | 8:H:105:ARG:NH2 | 2.05 | 1.18 |
| 22:W:21:THR:HG22 | 22:W:33:LEU:CD1 | 1.79 | 1.12 |
| 22:W:21:THR:HG21 | 22:W:33:LEU:HD11 | 1.24 | 1.11 |
| 1:A:92:C:H2' | 1:A:93:G:C8 | 1.85 | 1.11 |
| 10:J:7:LYS:HG3 | 10:J:71:LEU:HD21 | 1.18 | 1.11 |
| 1:A:918:A:H2 | 1:A:1079:G:N2 | 1.46 | 1.11 |
| 1:A:1256:A:H3' | 3:C:27:LYS:NZ | 1.66 | 1.11 |
| 3:C:29:TYR:OH | 14:N:54:PRO:HG2 | 1.50 | 1.09 |
| 1:A:92:C:H2' | 1:A:93:G:H8 | 0.99 | 1.09 |
| 10:J:7:LYS:CG | 10:J:71:LEU:HD21 | 1.84 | 1.07 |
| 22:W:21:THR:CG2 | 22:W:33:LEU:CD1 | 2.31 | 1.07 |
| 25:Z:1:C:H2' | 25:Z:2:G:H8 | 1.14 | 1.06 |
| 5:E:93:PRO:CG | 8:H:105:ARG:HH22 | 1.63 | 1.04 |
| 1:A:827:U:O4 | 1:A:872:A:N1 | 1.91 | 1.04 |
| 1:A:1532:U:H5'' | 1:A:1533:C:OP2 | 1.58 | 1.04 |
| 10:J:7:LYS:HG3 | 10:J:71:LEU:HD23 | 1.37 | 1.02 |
| 1:A:1256:A:H5'' | 3:C:27:LYS:CE | 1.90 | 1.01 |
| 1:A:80:G:H3' | 1:A:81:U:H5'' | 1.39 | 1.01 |
| 1:A:827:U:H3 | 1:A:872:A:N6 | 1.57 | 1.01 |
| 10:J:7:LYS:CG | 10:J:71:LEU:CD2 | 2.39 | 1.00 |
| 1:A:1219:U:H2' | 1:A:1220:G:C8 | 1.97 | 0.97 |
| 4:D:31:CYS:SG | 26:D:300:ZN:ZN | 1.54 | 0.97 |
| 10:J:40:LEU:HD11 | 10:J:71:LEU:HG | 1.44 | 0.97 |
| 1:A:1074:G:H1' | 2:B:104:ASN:HD21 | 1.27 | 0.95 |
| 16:P:59:TRP:O | 16:P:62:VAL:CG2 | 2.14 | 0.94 |
| 1:A:864:A:H2' | 1:A:865:A:C8 | 2.03 | 0.93 |
| 1:A:918:A:C2 | 1:A:1079:G:N2 | 2.33 | 0.93 |
| 1:A:827:U:N3 | 1:A:872:A:N6 | 2.13 | 0.93 |
| 3:C:28:GLN:HA | 3:C:31:HIS:CD2 | 2.04 | 0.93 |
| 9:I:5:TYR:HE2 | 9:I:7:THR:OG1 | 1.40 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:918:A:H2 | 1:A:1079:G:H22 | 1.05 | 0.92 |
| 10:J:50:ILE:HG13 | 10:J:60:ARG:HD2 | 1.51 | 0.92 |
| 1:A:1492:A:H8 | 22:W:19:ASN:HB3 | 1.34 | 0.92 |
| 1:A:1227:A:C2 | 19:S:83:HIS:HB3 | 2.04 | 0.92 |
| 1:A:958:A:N1 | 19:S:55:LYS:HB2 | 1.85 | 0.92 |
| 3:C:92:ALA:O | 3:C:95:THR:O | 1.87 | 0.91 |
| 16:P:59:TRP:O | 16:P:62:VAL:HG22 | 1.71 | 0.90 |
| 5:E:93:PRO:HG2 | 8:H:105:ARG:CZ | 2.01 | 0.90 |
| 1:A:1358:U:N3 | 1:A:1363(A):A:N6 | 2.05 | 0.90 |
| 1:A:13:U:H5' | 1:A:14:U:H5 | 1.38 | 0.89 |
| 1:A:1061:G:H5' | 10:J:59:SER:OG | 1.71 | 0.89 |
| 1:A:664:G:H22 | 1:A:741:G:H1 | 1.19 | 0.88 |
| 1:A:745:C:H2' | 1:A:746:A:C8 | 2.08 | 0.88 |
| 1:A:1256:A:H5'' | 3:C:27:LYS:HE2 | 1.54 | 0.88 |
| 1:A:1071:C:H2' | 1:A:1072:G:H8 | 1.38 | 0.88 |
| 1:A:1345:U:C2 | 1:A:1375:A:N6 | 2.41 | 0.88 |
| 1:A:1535:C:N3 | 1:A:1536:C:C5 | 2.42 | 0.88 |
| 25:Z:50:U:H2' | 25:Z:51:C:C6 | 2.09 | 0.88 |
| 1:A:67:C:H2' | 1:A:68:G:C8 | 2.09 | 0.87 |
| 1:A:1000:U:H2' | 1:A:1001:A:H1' | 1.56 | 0.87 |
| 10:J:62:HIS:HB3 | 14:N:59:ALA:HB3 | 1.56 | 0.87 |
| 3:C:30:ARG:NH1 | 14:N:35:ARG:O | 2.06 | 0.87 |
| 9:I:82:ALA:HB1 | 9:I:96:LEU:HD21 | 1.57 | 0.87 |
| 1:A:966:G:C2 | 25:Z:34:C:H5' | 2.10 | 0.86 |
| 1:A:1073:U:H3 | 1:A:1102:A:H61 | 1.24 | 0.86 |
| 1:A:1227:A:N1 | 19:S:83:HIS:HB3 | 1.89 | 0.86 |
| 25:Z:1:C:H2' | 25:Z:2:G:C8 | 2.06 | 0.86 |
| 1:A:1530:G:H2' | 1:A:1531:A:O4' | 1.76 | 0.86 |
| 5:E:93:PRO:CB | 8:H:105:ARG:HH22 | 1.89 | 0.85 |
| 1:A:1256:A:C3' | 3:C:27:LYS:NZ | 2.38 | 0.85 |
| 1:A:1227:A:C2 | 19:S:83:HIS:CB | 2.59 | 0.85 |
| 1:A:1061:G:C5' | 10:J:59:SER:OG | 2.25 | 0.85 |
| 1:A:1345:U:H3 | 1:A:1375:A:N6 | 1.72 | 0.85 |
| 1:A:1077:G:N2 | 1:A:1079:G:H3' | 1.92 | 0.85 |
| 5:E:93:PRO:CG | 8:H:105:ARG:CZ | 2.56 | 0.84 |
| 1:A:1101:A:H4' | 1:A:1102:A:O5' | 1.76 | 0.84 |
| 10:J:7:LYS:HA | 10:J:71:LEU:HD22 | 1.60 | 0.84 |
| 9:I:5:TYR:CZ | 9:I:7:THR:OG1 | 2.26 | 0.83 |
| 1:A:501:C:H2' | 1:A:502:G:C8 | 2.14 | 0.83 |
| 1:A:920:U:H2' | 1:A:921:U:C6 | 2.13 | 0.83 |
| 9:I:112:LYS:HG2 | 9:I:119:ALA:H | 1.41 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 12:L:33:ARG:HD3 | 12:L:62:SER:HB3 | 1.59 | 0.83 |
| 1:A:1070:U:H2' | 1:A:1071:C:C6 | 2.14 | 0.83 |
| 1:A:67:C:H2' | 1:A:68:G:H8 | 1.43 | 0.82 |
| 1:A:1535:C:C4 | 1:A:1536:C:C5 | 2.68 | 0.82 |
| 1:A:1531:A:H2' | 1:A:1532:U:O4' | 1.79 | 0.82 |
| 1:A:1000:U:H2' | 1:A:1001:A:C1' | 2.09 | 0.82 |
| 1:A:17:U:H2' | 1:A:18:C:C6 | 2.15 | 0.81 |
| 1:A:19:C:H2' | 1:A:20:U:C6 | 2.15 | 0.81 |
| 1:A:1071:C:H2' | 1:A:1072:G:C8 | 2.14 | 0.81 |
| 22:W:32:ILE:HB | 22:W:63:THR:C | 2.01 | 0.81 |
| 1:A:501:C:H2' | 1:A:502:G:H8 | 1.43 | 0.80 |
| 1:A:674:G:H2' | 1:A:675:A:H8 | 1.44 | 0.80 |
| 5:E:93:PRO:HG3 | 8:H:105:ARG:HH22 | 1.23 | 0.80 |
| 1:A:123:C:H2' | 1:A:124:G:H8 | 1.46 | 0.80 |
| 1:A:958:A:C2 | 19:S:55:LYS:HB2 | 2.17 | 0.80 |
| 1:A:13:U:H5' | 1:A:14:U:C5 | 2.16 | 0.80 |
| 25:Z:55:PSU:H3' | 25:Z:56:C:H5'' | 1.63 | 0.80 |
| 1:A:1014:A:H4' | 19:S:14:HIS:HB3 | 1.62 | 0.79 |
| 5:E:93:PRO:HB2 | 8:H:105:ARG:HH12 | 1.47 | 0.79 |
| 1:A:78:G:H2' | 1:A:79:G:O4' | 1.82 | 0.79 |
| 4:D:26:CYS:HG | 26:D:300:ZN:ZN | 0.94 | 0.79 |
| 25:Z:34:C:H2' | 25:Z:35:A:C8 | 2.18 | 0.79 |
| 3:C:29:TYR:HD1 | 14:N:36:PHE:CE2 | 2.02 | 0.78 |
| 1:A:1492:A:C8 | 22:W:19:ASN:HB3 | 2.19 | 0.78 |
| 25:Z:3:C:H2' | 25:Z:4:G:C8 | 2.18 | 0.78 |
| 2:B:72:GLY:HA3 | 2:B:81:VAL:HG21 | 1.66 | 0.78 |
| 25:Z:66:C:H2' | 25:Z:67:C:O4' | 1.82 | 0.78 |
| 1:A:24:U:H2' | 1:A:25:C:C6 | 2.18 | 0.77 |
| 1:A:917:G:H2' | 1:A:918:A:C8 | 2.18 | 0.77 |
| 3:C:9:GLY:HA2 | 3:C:12:LEU:HG | 1.66 | 0.77 |
| 1:A:662:G:H2' | 1:A:663:A:C8 | 2.19 | 0.77 |
| 25:Z:56:C:H2' | 25:Z:57:A:C8 | 2.20 | 0.77 |
| 3:C:29:TYR:OH | 14:N:54:PRO:CG | 2.33 | 0.77 |
| 25:Z:39:C:H2' | 25:Z:40:C:C6 | 2.20 | 0.77 |
| 1:A:745:C:H2' | 1:A:746:A:H8 | 1.49 | 0.76 |
| 1:A:1535:C:C2 | 1:A:1536:C:C6 | 2.73 | 0.76 |
| 1:A:299:G:H2' | 1:A:300:A:C8 | 2.21 | 0.76 |
| 4:D:26:CYS:SG | 26:D:300:ZN:ZN | 1.75 | 0.76 |
| 19:S:34:TRP:HA | 19:S:52:TYR:HB2 | 1.68 | 0.76 |
| 5:E:93:PRO:HG2 | 8:H:105:ARG:NH1 | 2.01 | 0.76 |
| 10:J:40:LEU:HD11 | 10:J:71:LEU:CG | 2.16 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:80:G:H3' | 1:A:81:U:C5' | 2.16 | 0.76 |
| 1:A:21:G:H2' | 1:A:22:G:C8 | 2.21 | 0.75 |
| 1:A:1123:A:H4' | 10:J:36:GLY:HA3 | 1.67 | 0.75 |
| 19:S:11:VAL:HA | 19:S:38:SER:HB2 | 1.68 | 0.75 |
| 1:A:1296:C:H5' | 13:M:14:ARG:HD2 | 1.69 | 0.75 |
| 1:A:316:G:H1 | 1:A:337:C:H42 | 1.33 | 0.74 |
| 1:A:1536:C:H1' | 24:Y:30:G:H22 | 1.50 | 0.74 |
| 3:C:30:ARG:HH21 | 3:C:30:ARG:HB2 | 1.51 | 0.74 |
| 9:I:44:VAL:HG12 | 9:I:51:ARG:HH12 | 1.52 | 0.74 |
| 16:P:59:TRP:O | 16:P:62:VAL:HG23 | 1.85 | 0.74 |
| 1:A:170:U:H2' | 1:A:171:A:H8 | 1.52 | 0.74 |
| 1:A:543:C:H2' | 1:A:544:G:H8 | 1.52 | 0.74 |
| 10:J:16:LEU:HA | 10:J:19:SER:HB3 | 1.69 | 0.74 |
| 1:A:90:U:H2' | 1:A:91:C:C6 | 2.23 | 0.73 |
| 1:A:977:A:N7 | 1:A:1223:C:H2' | 2.03 | 0.73 |
| 1:A:966:G:N3 | 25:Z:34:C:H5' | 2.03 | 0.73 |
| 1:A:1080:A:H5'' | 5:E:16:THR:HB | 1.70 | 0.73 |
| 1:A:524:G:C6 | 1:A:525:C:N4 | 2.57 | 0.73 |
| 1:A:1218:C:H2' | 1:A:1219:U:C6 | 2.22 | 0.73 |
| 1:A:1386:G:H2' | 1:A:1387:G:H8 | 1.54 | 0.72 |
| 1:A:45:U:H2' | 1:A:46:G:H8 | 1.53 | 0.72 |
| 1:A:1219:U:H2' | 1:A:1220:G:H8 | 1.54 | 0.72 |
| 3:C:28:GLN:HA | 3:C:31:HIS:NE2 | 2.04 | 0.72 |
| 11:K:58:PRO:HB2 | 11:K:93:GLN:HG3 | 1.71 | 0.72 |
| 1:A:1270:C:H2' | 1:A:1271:G:H8 | 1.53 | 0.72 |
| 1:A:729:A:H2' | 1:A:730:G:H8 | 1.55 | 0.72 |
| 10:J:6:ILE:HG22 | 10:J:98:ILE:HG12 | 1.71 | 0.72 |
| 4:D:25:ARG:HA | 4:D:28:SER:HB3 | 1.70 | 0.72 |
| 18:R:86:VAL:O | 18:R:87:ARG:HB2 | 1.88 | 0.72 |
| 1:A:69:G:H1 | 1:A:100:C:H42 | 1.38 | 0.71 |
| 1:A:1103:C:H2' | 1:A:1104:G:O4' | 1.89 | 0.71 |
| 3:C:174:PRO:HB2 | 3:C:177:THR:HG22 | 1.72 | 0.71 |
| 22:W:21:THR:HG22 | 22:W:33:LEU:HD12 | 1.71 | 0.71 |
| 1:A:584:G:H2' | 1:A:585:G:H8 | 1.56 | 0.71 |
| 3:C:29:TYR:CZ | 14:N:54:PRO:HG2 | 2.24 | 0.71 |
| 1:A:45:U:H2' | 1:A:46:G:C8 | 2.25 | 0.71 |
| 1:A:19:C:H2' | 1:A:20:U:H6 | 1.53 | 0.71 |
| 1:A:78:G:O2' | 1:A:79:G:O4' | 2.07 | 0.71 |
| 3:C:77:ILE:HA | 3:C:84:ILE:HB | 1.73 | 0.71 |
| 23:X:90:PHE:HB2 | 23:X:120:ILE:HG12 | 1.72 | 0.71 |
| 1:A:584:G:H2' | 1:A:585:G:C8 | 2.24 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 18:R:40:LEU:HB3 | 18:R:79:LEU:HD11 | 1.73 | 0.71 |
| 1:A:1000:U:H3' | 1:A:1000:U:H6 | 1.55 | 0.71 |
| 1:A:1098:C:H1' | 1:A:1168:A:H2 | 1.55 | 0.71 |
| 1:A:1359:C:H3' | 14:N:35:ARG:NH2 | 2.05 | 0.70 |
| 1:A:1475:G:H2' | 1:A:1476:G:H8 | 1.55 | 0.70 |
| 1:A:123:C:H2' | 1:A:124:G:C8 | 2.26 | 0.70 |
| 1:A:743:U:H2' | 1:A:744:C:C6 | 2.26 | 0.70 |
| 1:A:1360:A:H8 | 1:A:1360:A:OP1 | 1.74 | 0.70 |
| 2:B:130:ARG:HB3 | 2:B:131:PRO:HD2 | 1.73 | 0.70 |
| 1:A:1036:G:H2' | 1:A:1037:C:O4' | 1.92 | 0.70 |
| 1:A:1342:C:H2' | 1:A:1343:G:C8 | 2.26 | 0.70 |
| 17:Q:81:ARG:HE | 17:Q:84:LEU:HD12 | 1.55 | 0.70 |
| 24:Y:24:A:H2' | 24:Y:25:A:H8 | 1.57 | 0.69 |
| 25:Z:48:C:H2' | 25:Z:59:A:H4' | 1.74 | 0.69 |
| 1:A:78:G:C2' | 1:A:79:G:O4' | 2.40 | 0.69 |
| 1:A:398:C:H2' | 1:A:399:G:H8 | 1.56 | 0.69 |
| 1:A:1099:G:H5'' | 2:B:96:ARG:HE | 1.58 | 0.69 |
| 4:D:101:LEU:HB2 | 4:D:138:TYR:HB3 | 1.74 | 0.69 |
| 1:A:1064:G:N2 | 1:A:1190:G:H2' | 2.08 | 0.69 |
| 1:A:181:G:H4' | 1:A:182:U:H5' | 1.74 | 0.69 |
| 1:A:1081:G:C8 | 1:A:1081:G:H5'' | 2.27 | 0.69 |
| 1:A:1280:A:H3' | 1:A:1281:U:H5'' | 1.74 | 0.69 |
| 12:L:87:GLY:HA2 | 12:L:98:TYR:HA | 1.75 | 0.69 |
| 10:J:7:LYS:HA | 10:J:71:LEU:CD2 | 2.23 | 0.69 |
| 1:A:536:C:H2' | 1:A:537:G:C8 | 2.28 | 0.69 |
| 1:A:1264:C:H2' | 1:A:1265:G:H8 | 1.58 | 0.68 |
| 25:Z:36:U:H2' | 25:Z:37:A:H8 | 1.58 | 0.68 |
| 1:A:671:G:C2 | 1:A:736:C:N3 | 2.62 | 0.68 |
| 10:J:7:LYS:CB | 10:J:71:LEU:HD21 | 2.22 | 0.68 |
| 1:A:10:A:H2' | 1:A:11:G:C8 | 2.29 | 0.68 |
| 1:A:718:G:H21 | 18:R:49:LYS:HE3 | 1.59 | 0.68 |
| 1:A:1234:C:H2' | 1:A:1235:U:C6 | 2.28 | 0.68 |
| 25:Z:50:U:N3 | 25:Z:51:C:N4 | 2.42 | 0.68 |
| 1:A:736:C:H2' | 1:A:737:A:C8 | 2.27 | 0.68 |
| 1:A:1346:A:H2' | 7:G:10:ARG:HH22 | 1.59 | 0.68 |
| 3:C:62:ASP:HA | 3:C:97:LYS:HD3 | 1.76 | 0.68 |
| 1:A:662:G:H2' | 1:A:663:A:H8 | 1.56 | 0.68 |
| 3:C:28:GLN:O | 3:C:32:LEU:HG | 1.94 | 0.68 |
| 3:C:29:TYR:CD1 | 14:N:36:PHE:CE2 | 2.82 | 0.68 |
| 1:A:398:C:H2' | 1:A:399:G:C8 | 2.29 | 0.68 |
| 2:B:69:LEU:HB3 | 2:B:162:ILE:HG12 | 1.76 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 25:Z:35:A:H2' | 25:Z:36:U:C6 | 2.28 | 0.68 |
| 1:A:16:A:C2 | 1:A:1080:A:H1' | 2.29 | 0.67 |
| 1:A:1073:U:H3 | 1:A:1102:A:N6 | 1.91 | 0.67 |
| 1:A:579:G:H5' | 1:A:728:A:H1' | 1.76 | 0.67 |
| 1:A:1103:C:H5'' | 2:B:98:LEU:HD23 | 1.76 | 0.67 |
| 1:A:1218:C:H2' | 1:A:1219:U:H6 | 1.59 | 0.67 |
| 1:A:701:C:H1' | 1:A:703:G:C5 | 2.30 | 0.67 |
| 5:E:12:LEU:HG | 5:E:31:LEU:HD12 | 1.77 | 0.67 |
| 1:A:1342:C:H2' | 1:A:1343:G:H8 | 1.59 | 0.67 |
| 1:A:1264:C:H2' | 1:A:1265:G:C8 | 2.30 | 0.67 |
| 3:C:30:ARG:NH2 | 14:N:35:ARG:O | 2.26 | 0.67 |
| 1:A:302:G:H2' | 1:A:303:A:C8 | 2.30 | 0.67 |
| 1:A:524:G:C2 | 1:A:525:C:N3 | 2.62 | 0.67 |
| 1:A:1356:G:H2' | 1:A:1357:A:C8 | 2.30 | 0.67 |
| 1:A:1536:C:H1' | 24:Y:30:G:N2 | 2.10 | 0.67 |
| 1:A:1384:C:H2' | 1:A:1385:G:C8 | 2.29 | 0.67 |
| 15:O:75:PRO:O | 15:O:79:ARG:HG3 | 1.95 | 0.67 |
| 1:A:457:C:H2' | 1:A:458:C:C6 | 2.29 | 0.67 |
| 10:J:47:PHE:HB2 | 10:J:63:PHE:HB2 | 1.76 | 0.67 |
| 1:A:674:G:H2' | 1:A:675:A:C8 | 2.30 | 0.66 |
| 1:A:1227:A:C2 | 19:S:83:HIS:HB2 | 2.30 | 0.66 |
| 22:W:15:GLU:HB3 | 22:W:23:ARG:HB2 | 1.76 | 0.66 |
| 1:A:956:U:O2' | 19:S:80:TYR:HB3 | 1.95 | 0.66 |
| 1:A:1280:A:OP1 | 1:A:1281:U:H5 | 1.78 | 0.66 |
| 1:A:6:G:H2' | 5:E:119:LEU:HD21 | 1.76 | 0.66 |
| 7:G:39:ALA:HA | 7:G:42:ILE:HD12 | 1.78 | 0.66 |
| 1:A:562:C:H41 | 1:A:884:U:H2' | 1.61 | 0.66 |
| 1:A:1016:A:H2' | 1:A:1017:G:O4' | 1.95 | 0.65 |
| 3:C:20:SER:HB3 | 3:C:22:TRP:HE1 | 1.61 | 0.65 |
| 24:Y:28:A:H3' | 24:Y:29:G:C8 | 2.32 | 0.65 |
| 1:A:101:A:H2' | 1:A:102:G:H8 | 1.61 | 0.65 |
| 3:C:21:ARG:HG3 | 3:C:58:GLU:HG2 | 1.78 | 0.65 |
| 1:A:1438:G:N2 | 1:A:1439:C:C2 | 2.64 | 0.65 |
| 5:E:149:GLU:O | 5:E:153:LYS:HB2 | 1.97 | 0.65 |
| 6:F:9:VAL:HB | 6:F:87:ARG:HB2 | 1.78 | 0.65 |
| 1:A:1345:U:N3 | 1:A:1375:A:C6 | 2.63 | 0.65 |
| 8:H:105:ARG:NH2 | 8:H:105:ARG:HG2 | 2.10 | 0.65 |
| 12:L:27:LEU:HG | 12:L:28:LYS:HG3 | 1.79 | 0.65 |
| 1:A:543:C:H2' | 1:A:544:G:C8 | 2.31 | 0.65 |
| 1:A:671:G:N2 | 1:A:736:C:C2 | 2.64 | 0.65 |
| 1:A:279:A:H5'' | 1:A:280:C:H3' | 1.77 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:A:1442(A):G:H5'' | 1:A:1442(B):A:H5' | 1.79 | 0.65 |
| 1:A:701:C:H4' | 1:A:702:A:O5' | 1.97 | 0.65 |
| 17:Q:67:LYS:O | 17:Q:68:ARG:HB3 | 1.97 | 0.65 |
| 1:A:189(K):U:H2' | 1:A:189(L):G:C8 | 2.32 | 0.65 |
| 1:A:814:A:H2' | 1:A:816:A:H5'' | 1.78 | 0.65 |
| 1:A:943:U:H2' | 1:A:944:G:H8 | 1.62 | 0.65 |
| 1:A:998:G:N2 | 1:A:999:C:C2 | 2.65 | 0.65 |
| 1:A:1354:C:H2' | 1:A:1355:G:H8 | 1.62 | 0.65 |
| 22:W:32:ILE:HD11 | 22:W:55:VAL:HG11 | 1.79 | 0.65 |
| 1:A:1004:A:H5'' | 1:A:1025:U:C5 | 2.32 | 0.64 |
| 2:B:34:ALA:HB3 | 2:B:41:ILE:HD12 | 1.79 | 0.64 |
| 5:E:93:PRO:CB | 8:H:105:ARG:HH12 | 2.09 | 0.64 |
| 6:F:52:ILE:HD11 | 18:R:77:GLY:HA3 | 1.78 | 0.64 |
| 1:A:1125:U:H5' | 1:A:1126:U:H5 | 1.62 | 0.64 |
| 3:C:58:GLU:HB3 | 10:J:92:THR:HG21 | 1.78 | 0.64 |
| 10:J:50:ILE:CG1 | 10:J:60:ARG:HD2 | 2.26 | 0.64 |
| 1:A:1099:G:C6 | 1:A:1100:C:N3 | 2.65 | 0.64 |
| 1:A:79:G:H2' | 1:A:80:G:H8 | 1.62 | 0.64 |
| 1:A:1443:G:C6 | 1:A:1444:C:N4 | 2.66 | 0.64 |
| 10:J:7:LYS:CB | 10:J:71:LEU:CD2 | 2.76 | 0.64 |
| 25:Z:36:U:H2' | 25:Z:37:A:C8 | 2.32 | 0.64 |
| 1:A:266:G:C8 | 1:A:266:G:H5'' | 2.33 | 0.64 |
| 1:A:1105:A:H2' | 1:A:1106:G:H8 | 1.62 | 0.64 |
| 1:A:61:G:H2' | 1:A:62:U:O4' | 1.98 | 0.64 |
| 1:A:525:C:H2' | 1:A:526:C:C6 | 2.33 | 0.64 |
| 1:A:518:C:O2' | 12:L:50:SER:HB3 | 1.97 | 0.64 |
| 1:A:1081:G:H2' | 1:A:1082:G:C8 | 2.33 | 0.64 |
| 1:A:1392:G:N2 | 1:A:1502:A:H8 | 1.95 | 0.64 |
| 4:D:176:LEU:HA | 4:D:183:GLY:HA2 | 1.79 | 0.64 |
| 1:A:1074:G:C1' | 2:B:104:ASN:HD21 | 2.06 | 0.64 |
| 19:S:6:LYS:HB2 | 19:S:7:LYS:HE3 | 1.80 | 0.64 |
| 1:A:988:G:N1 | 1:A:989:C:C2 | 2.67 | 0.63 |
| 1:A:1070:U:H2' | 1:A:1071:C:H6 | 1.64 | 0.63 |
| 24:Y:28:A:H3' | 24:Y:29:G:H8 | 1.62 | 0.63 |
| 1:A:880:C:H2' | 1:A:881:G:H8 | 1.63 | 0.63 |
| 1:A:1358:U:C4 | 1:A:1363(A):A:N1 | 2.62 | 0.63 |
| 2:B:184:VAL:H | 2:B:198:ASP:HB2 | 1.63 | 0.63 |
| 1:A:335:C:H2' | 1:A:336:C:C6 | 2.33 | 0.63 |
| 1:A:1081:G:H2' | 1:A:1082:G:H8 | 1.64 | 0.63 |
| 1:A:1475:G:H2' | 1:A:1476:G:C8 | 2.33 | 0.63 |
| 1:A:926:G:H3' | 1:A:1505:G:H21 | 1.63 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1128:C:H2' | 1:A:1139:G:N7 | 2.13 | 0.63 |
| 13:M:10:PRO:HB2 | 13:M:18:ALA:HB1 | 1.80 | 0.63 |
| 1:A:919:A:C2 | 1:A:1080:A:H2 | 2.16 | 0.63 |
| 25:Z:51:C:H2' | 25:Z:52:G:O4' | 1.99 | 0.63 |
| 1:A:1391:U:H2' | 1:A:1392:G:C8 | 2.33 | 0.63 |
| 1:A:1445:C:C2 | 1:A:1458:G:C2 | 2.87 | 0.63 |
| 1:A:1048:G:H5'' | 14:N:3:ARG:HG2 | 1.79 | 0.63 |
| 25:Z:52:G:C2 | 25:Z:63:G:C2 | 2.86 | 0.63 |
| 1:A:316:G:H1 | 1:A:337:C:N4 | 1.97 | 0.62 |
| 3:C:154:SER:HA | 3:C:165:THR:HG23 | 1.79 | 0.62 |
| 1:A:920:U:H2' | 1:A:921:U:H6 | 1.63 | 0.62 |
| 1:A:1061:G:H5'' | 10:J:59:SER:OG | 1.99 | 0.62 |
| 1:A:1125:U:H5' | 1:A:1126:U:C5 | 2.34 | 0.62 |
| 25:Z:49:G:C6 | 25:Z:50:U:C2 | 2.87 | 0.62 |
| 1:A:1535:C:N3 | 1:A:1536:C:C6 | 2.67 | 0.62 |
| 2:B:204:ASN:HB3 | 2:B:210:SER:OG | 2.00 | 0.62 |
| 1:A:1354:C:H2' | 1:A:1355:G:C8 | 2.34 | 0.62 |
| 12:L:25:PRO:C | 12:L:27:LEU:H | 2.01 | 0.62 |
| 1:A:877:C:H2' | 1:A:878:G:H8 | 1.64 | 0.62 |
| 1:A:973:G:H3' | 1:A:974:A:H5'' | 1.80 | 0.62 |
| 23:X:4:GLU:HA | 23:X:66:ARG:HH12 | 1.64 | 0.62 |
| 1:A:69:G:H1 | 1:A:100:C:N4 | 1.97 | 0.62 |
| 1:A:1014:A:C2 | 19:S:34:TRP:CG | 2.88 | 0.62 |
| 25:Z:33:U:O2 | 25:Z:36:U:H5 | 1.82 | 0.62 |
| 1:A:234:C:H2' | 1:A:235:C:C6 | 2.34 | 0.62 |
| 1:A:1256:A:N6 | 1:A:1278:U:C2 | 2.68 | 0.62 |
| 10:J:7:LYS:CA | 10:J:71:LEU:HD22 | 2.30 | 0.62 |
| 23:X:64:LYS:O | 23:X:68:GLU:HG2 | 2.00 | 0.62 |
| 1:A:17:U:O2 | 1:A:1079:G:N3 | 2.32 | 0.62 |
| 1:A:313:A:H2' | 1:A:314:C:C6 | 2.34 | 0.62 |
| 1:A:1014:A:C2 | 19:S:34:TRP:CD2 | 2.87 | 0.62 |
| 1:A:1102:A:H2' | 1:A:1103:C:C6 | 2.35 | 0.62 |
| 3:C:108:ASN:HD21 | 3:C:110:ASN:HB2 | 1.65 | 0.62 |
| 23:X:157:LEU:HB2 | 23:X:160:ASP:HB2 | 1.82 | 0.62 |
| 25:Z:55:PSU:H6 | 25:Z:55:PSU:H5' | 1.65 | 0.62 |
| 1:A:868:C:H2' | 1:A:869:G:O4' | 2.00 | 0.62 |
| 1:A:1127:G:H21 | 1:A:1147:C:H41 | 1.47 | 0.62 |
| 8:H:105:ARG:HG2 | 8:H:105:ARG:HH21 | 1.65 | 0.62 |
| 1:A:24:U:H2' | 1:A:25:C:H6 | 1.64 | 0.61 |
| 1:A:694:A:H5' | 11:K:53:SER:HB2 | 1.81 | 0.61 |
| 1:A:695:A:H2' | 1:A:696:A:C8 | 2.35 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 10:J:57:LYS:O | 10:J:60:ARG:HD3 | 2.00 | 0.61 |
| 1:A:939:G:H1' | 1:A:1375:A:C2 | 2.35 | 0.61 |
| 8:H:11:THR:HA | 8:H:14:ARG:NH1 | 2.15 | 0.61 |
| 1:A:582:U:H2' | 1:A:583:A:C8 | 2.35 | 0.61 |
| 1:A:1164:G:N2 | 1:A:1165:C:C2 | 2.69 | 0.61 |
| 10:J:27:ALA:HB2 | 10:J:85:LEU:HD21 | 1.81 | 0.61 |
| 1:A:1386:G:H2' | 1:A:1387:G:C8 | 2.35 | 0.61 |
| 10:J:38:ILE:HD12 | 10:J:71:LEU:O | 1.99 | 0.61 |
| 1:A:588:G:N2 | 1:A:589:C:C2 | 2.68 | 0.61 |
| 1:A:302:G:H2' | 1:A:303:A:H8 | 1.64 | 0.61 |
| 23:X:90:PHE:HE2 | 23:X:118:VAL:HG12 | 1.66 | 0.61 |
| 24:Y:24:A:H2' | 24:Y:25:A:C8 | 2.35 | 0.61 |
| 1:A:509:A:H4' | 1:A:510:A:OP1 | 2.00 | 0.61 |
| 1:A:960:U:H4' | 1:A:961:U:H5'' | 1.82 | 0.61 |
| 1:A:1256:A:H5'' | 3:C:27:LYS:NZ | 2.14 | 0.61 |
| 1:A:1366:C:O2' | 10:J:60:ARG:NH2 | 2.33 | 0.61 |
| 1:A:312:C:H2' | 1:A:313:A:C8 | 2.36 | 0.61 |
| 1:A:1349:A:H5'' | 9:I:121:ARG:HB2 | 1.83 | 0.61 |
| 9:I:17:VAL:HG22 | 9:I:63:ILE:HG12 | 1.82 | 0.61 |
| 9:I:118:LYS:O | 9:I:120:ARG:N | 2.33 | 0.61 |
| 13:M:87:TYR:HA | 13:M:90:LEU:HD12 | 1.83 | 0.61 |
| 1:A:376:G:H2' | 1:A:377:G:H8 | 1.65 | 0.60 |
| 1:A:568:G:N2 | 1:A:883:C:C2 | 2.69 | 0.60 |
| 25:Z:47:U:H4' | 25:Z:48:C:H5' | 1.83 | 0.60 |
| 3:C:28:GLN:CA | 3:C:31:HIS:CD2 | 2.82 | 0.60 |
| 16:P:59:TRP:C | 16:P:62:VAL:HG22 | 2.21 | 0.60 |
| 1:A:623:C:H2' | 1:A:624:C:O4' | 2.01 | 0.60 |
| 14:N:24:CYS:HB3 | 14:N:28:GLY:H | 1.67 | 0.60 |
| 1:A:1132:C:H2' | 1:A:1133:G:C8 | 2.35 | 0.60 |
| 1:A:1384:C:H2' | 1:A:1385:G:H8 | 1.65 | 0.60 |
| 1:A:370:C:C2 | 1:A:392:G:N2 | 2.69 | 0.60 |
| 1:A:1000:U:H3' | 1:A:1000:U:C6 | 2.35 | 0.60 |
| 1:A:96:U:H2' | 1:A:97:G:H8 | 1.66 | 0.60 |
| 1:A:677:U:H2' | 1:A:678:U:C6 | 2.37 | 0.60 |
| 1:A:960:U:H4' | 1:A:961:U:C5' | 2.31 | 0.60 |
| 1:A:1464:G:N2 | 1:A:1465:C:C2 | 2.70 | 0.60 |
| 18:R:52:PRO:HG2 | 18:R:54:ARG:CZ | 2.31 | 0.60 |
| 1:A:399:G:H2' | 1:A:400:C:C6 | 2.37 | 0.60 |
| 1:A:932:C:H5' | 7:G:3:ARG:HB3 | 1.84 | 0.60 |
| 1:A:999:C:O2 | 1:A:1043:C:O2 | 2.18 | 0.60 |
| 3:C:7:PRO:HG2 | 3:C:184:TYR:HB2 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:C:30:ARG:CZ | 14:N:35:ARG:O | 2.49 | 0.60 |
| 4:D:5:ILE:H | 4:D:115:ARG:HH22 | 1.48 | 0.60 |
| 20:T:44:ALA:HB1 | 20:T:91:LEU:HB2 | 1.84 | 0.60 |
| 1:A:884:U:H4' | 1:A:885:G:H5'' | 1.84 | 0.60 |
| 1:A:1532:U:H2' | 1:A:1533:C:H1' | 1.83 | 0.60 |
| 23:X:157:LEU:HD11 | 23:X:162:ASN:HB3 | 1.84 | 0.60 |
| 1:A:390:C:H2' | 1:A:391:G:H8 | 1.67 | 0.59 |
| 1:A:1411:C:H5' | 22:W:64:ARG:HH22 | 1.66 | 0.59 |
| 1:A:1513:A:H2' | 1:A:1514:C:C6 | 2.37 | 0.59 |
| 10:J:9:ARG:HG3 | 10:J:95:GLU:HB3 | 1.82 | 0.59 |
| 14:N:12:ARG:O | 14:N:14:PRO:HD3 | 2.02 | 0.59 |
| 19:S:40:ILE:HG21 | 19:S:62:ILE:HD11 | 1.84 | 0.59 |
| 1:A:170:U:H2' | 1:A:171:A:C8 | 2.35 | 0.59 |
| 1:A:921:U:H5' | 1:A:1081:G:O2' | 2.02 | 0.59 |
| 25:Z:37:A:H2' | 25:Z:38:A:C8 | 2.37 | 0.59 |
| 25:Z:40:C:H2' | 25:Z:41:C:C6 | 2.37 | 0.59 |
| 1:A:189(L):G:H2' | 1:A:190:U:C6 | 2.38 | 0.59 |
| 1:A:735:C:H5' | 18:R:71:LYS:HD3 | 1.84 | 0.59 |
| 1:A:1005:A:O4' | 1:A:1036:G:N2 | 2.35 | 0.59 |
| 1:A:1430:C:C2 | 1:A:1471:G:N2 | 2.71 | 0.59 |
| 1:A:556:C:H2' | 1:A:557:G:O4' | 2.02 | 0.59 |
| 25:Z:64:G:H2' | 25:Z:65:C:O4' | 2.03 | 0.59 |
| 1:A:59:A:H5'' | 1:A:387:U:H5'' | 1.83 | 0.59 |
| 1:A:521:G:N2 | 1:A:522:C:C2 | 2.71 | 0.59 |
| 5:E:33:VAL:HG21 | 5:E:109:ILE:HG12 | 1.84 | 0.59 |
| 1:A:691:G:H3' | 11:K:26:ASN:HD21 | 1.66 | 0.59 |
| 1:A:1074:G:O2' | 1:A:1101:A:N1 | 2.35 | 0.59 |
| 1:A:1081:G:H5'' | 1:A:1081:G:H8 | 1.66 | 0.59 |
| 25:Z:53:G:C2 | 25:Z:62:C:C2 | 2.90 | 0.59 |
| 1:A:1435:G:H2' | 1:A:1436:U:C6 | 2.38 | 0.59 |
| 5:E:18:ARG:HD3 | 5:E:20:GLN:HE21 | 1.67 | 0.59 |
| 1:A:17:U:H2' | 1:A:18:C:C5 | 2.38 | 0.58 |
| 1:A:1310:G:N2 | 1:A:1328:C:C2 | 2.71 | 0.58 |
| 1:A:1493:A:C2 | 22:W:46:ARG:HA | 2.38 | 0.58 |
| 2:B:17:PHE:HD1 | 2:B:18:GLY:H | 1.51 | 0.58 |
| 8:H:105:ARG:HH21 | 8:H:105:ARG:CG | 2.14 | 0.58 |
| 1:A:258:G:N2 | 1:A:269:C:C2 | 2.71 | 0.58 |
| 3:C:26:LYS:HE3 | 3:C:26:LYS:H | 1.68 | 0.58 |
| 1:A:216:G:C6 | 1:A:217:C:N4 | 2.71 | 0.58 |
| 1:A:757:U:H2' | 1:A:758:G:O4' | 2.03 | 0.58 |
| 1:A:1022:G:H2' | 1:A:1023:G:C8 | 2.39 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:1025:U:H2' | 1:A:1026:G:C8 | 2.39 | 0.58 |
| 3:C:20:SER:HB3 | 3:C:22:TRP:NE1 | 2.18 | 0.58 |
| 13:M:87:TYR:O | 13:M:91:ARG:HG2 | 2.03 | 0.58 |
| 1:A:820:U:H3' | 1:A:821:G:C5' | 2.34 | 0.58 |
| 1:A:1162:C:C2 | 1:A:1175:G:C2 | 2.92 | 0.58 |
| 2:B:135:GLN:HA | 2:B:138:LEU:HD12 | 1.84 | 0.58 |
| 4:D:196:LEU:HB3 | 4:D:198:VAL:HG12 | 1.84 | 0.58 |
| 25:Z:50:U:H3 | 25:Z:51:C:N4 | 2.01 | 0.58 |
| 10:J:57:LYS:HB2 | 10:J:60:ARG:NH1 | 2.19 | 0.58 |
| 1:A:576:G:H3' | 1:A:577:G:H5'' | 1.85 | 0.58 |
| 1:A:824:C:H2' | 1:A:825:G:C8 | 2.39 | 0.58 |
| 1:A:1216:G:H5'' | 14:N:5:ALA:HB2 | 1.86 | 0.58 |
| 1:A:109:A:H2' | 1:A:326:G:N2 | 2.18 | 0.58 |
| 25:Z:3:C:H2' | 25:Z:4:G:H8 | 1.69 | 0.58 |
| 1:A:1456:G:C2 | 1:A:1457:G:C8 | 2.92 | 0.58 |
| 2:B:122:PHE:HA | 2:B:127:ILE:HG12 | 1.85 | 0.58 |
| 1:A:725:G:N2 | 1:A:726:C:C2 | 2.72 | 0.58 |
| 1:A:1241:G:N2 | 1:A:1242:C:C2 | 2.71 | 0.58 |
| 25:Z:17:C:OP1 | 25:Z:18:G:H5' | 2.04 | 0.58 |
| 1:A:243:A:H4' | 1:A:244:U:O5' | 2.04 | 0.57 |
| 1:A:928:G:H1 | 1:A:1389:C:H42 | 1.51 | 0.57 |
| 5:E:93:PRO:CG | 8:H:105:ARG:NH1 | 2.66 | 0.57 |
| 1:A:911:U:H2' | 1:A:912:C:C6 | 2.40 | 0.57 |
| 1:A:1515:C:H2' | 1:A:1516:G:C8 | 2.39 | 0.57 |
| 9:I:10:ARG:HE | 9:I:11:LYS:HB2 | 1.69 | 0.57 |
| 10:J:50:ILE:HA | 10:J:59:SER:O | 2.04 | 0.57 |
| 1:A:1106:G:N2 | 1:A:1107:C:C2 | 2.73 | 0.57 |
| 25:Z:64:G:C5 | 25:Z:65:C:C4 | 2.92 | 0.57 |
| 1:A:354:G:N2 | 1:A:355:C:C2 | 2.72 | 0.57 |
| 4:D:166:LYS:HG3 | 4:D:178:VAL:HG11 | 1.87 | 0.57 |
| 9:I:26:VAL:HB | 9:I:33:PHE:HB2 | 1.86 | 0.57 |
| 9:I:96:LEU:HG | 9:I:101:PHE:HB2 | 1.86 | 0.57 |
| 15:O:24:SER:HB3 | 15:O:27:VAL:HG23 | 1.87 | 0.57 |
| 1:A:769:G:N2 | 1:A:770:C:C2 | 2.73 | 0.57 |
| 1:A:1347:G:N2 | 1:A:1373:G:H2' | 2.20 | 0.57 |
| 8:H:12:ARG:HB3 | 8:H:24:THR:HG21 | 1.87 | 0.57 |
| 10:J:6:ILE:HG13 | 10:J:72:VAL:O | 2.05 | 0.57 |
| 1:A:524:G:C2 | 1:A:525:C:C4 | 2.93 | 0.57 |
| 1:A:551:U:H2' | 1:A:552:U:C6 | 2.39 | 0.57 |
| 1:A:1391:U:H2' | 1:A:1392:G:H8 | 1.68 | 0.57 |
| 1:A:558:G:H3' | 1:A:559:A:H5'' | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:958:A:H8 | 1:A:958:A:O5' | 1.88 | 0.57 |
| 4:D:26:CYS:HA | 4:D:31:CYS:HB2 | 1.87 | 0.57 |
| 1:A:18:C:H4' | 1:A:1078:U:H1' | 1.87 | 0.57 |
| 1:A:384:G:H2' | 1:A:385:C:C6 | 2.40 | 0.57 |
| 1:A:1095:U:H2' | 1:A:1096:C:C6 | 2.40 | 0.57 |
| 1:A:1530:G:C2' | 1:A:1531:A:O4' | 2.50 | 0.57 |
| 5:E:14:ARG:HE | 5:E:45:PHE:HZ | 1.53 | 0.57 |
| 25:Z:50:U:C2 | 25:Z:51:C:C5 | 2.93 | 0.57 |
| 1:A:1106:G:C6 | 1:A:1107:C:N4 | 2.73 | 0.57 |
| 3:C:106:VAL:HG21 | 3:C:115:LEU:HD11 | 1.86 | 0.57 |
| 25:Z:1:C:H42 | 25:Z:72:A:H61 | 1.50 | 0.57 |
| 25:Z:39:C:H2' | 25:Z:40:C:H6 | 1.66 | 0.57 |
| 1:A:874:G:N2 | 1:A:875:C:C2 | 2.73 | 0.57 |
| 1:A:943:U:H2' | 1:A:944:G:C8 | 2.40 | 0.57 |
| 1:A:1464:G:N1 | 1:A:1465:C:C4 | 2.73 | 0.57 |
| 2:B:130:ARG:HH22 | 3:C:207:VAL:HG22 | 1.70 | 0.57 |
| 1:A:128:G:N2 | 1:A:234:C:C2 | 2.73 | 0.56 |
| 1:A:590:C:C2 | 1:A:650:G:C2 | 2.93 | 0.56 |
| 1:A:1076:C:H2' | 1:A:1077:G:C8 | 2.40 | 0.56 |
| 1:A:1270:C:H2' | 1:A:1271:G:C8 | 2.37 | 0.56 |
| 5:E:33:VAL:HG12 | 5:E:112:LEU:HD12 | 1.86 | 0.56 |
| 10:J:23:ILE:HG23 | 10:J:85:LEU:HD22 | 1.87 | 0.56 |
| 23:X:122:PHE:HE2 | 23:X:161:MET:HB2 | 1.69 | 0.56 |
| 25:Z:37:A:H3' | 25:Z:38:A:H8 | 1.70 | 0.56 |
| 25:Z:55:PSU:C3' | 25:Z:56:C:H5'' | 2.34 | 0.56 |
| 1:A:763:G:H2' | 1:A:764:C:C6 | 2.40 | 0.56 |
| 1:A:90:U:O2' | 1:A:91:C:H5' | 2.05 | 0.56 |
| 1:A:253:U:H2' | 1:A:254:G:H8 | 1.70 | 0.56 |
| 1:A:589:C:O2 | 1:A:651:C:O2 | 2.24 | 0.56 |
| 1:A:598:U:H2' | 1:A:599:C:C6 | 2.40 | 0.56 |
| 1:A:810:C:H2' | 1:A:811:C:O4' | 2.05 | 0.56 |
| 1:A:974:A:H8 | 1:A:974:A:OP1 | 1.88 | 0.56 |
| 1:A:975:A:H4' | 1:A:976:G:O5' | 2.05 | 0.56 |
| 1:A:1222:G:C6 | 1:A:1223:C:N4 | 2.73 | 0.56 |
| 1:A:1314:C:H2' | 1:A:1315:U:C6 | 2.40 | 0.56 |
| 1:A:1404:C:H42 | 1:A:1497:G:H1 | 1.51 | 0.56 |
| 1:A:1438:G:N1 | 1:A:1439:C:C4 | 2.73 | 0.56 |
| 5:E:106:PRO:HA | 5:E:109:ILE:HD12 | 1.87 | 0.56 |
| 16:P:54:GLU:HA | 16:P:57:ARG:HD2 | 1.87 | 0.56 |
| 17:Q:51:TYR:HE1 | 17:Q:76:LEU:HB2 | 1.70 | 0.56 |
| 1:A:755:G:N2 | 1:A:756:C:C2 | 2.73 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1164:G:N1 | 1:A:1165:C:C4 | 2.74 | 0.56 |
| 1:A:1323:G:H2' | 1:A:1324:A:C8 | 2.41 | 0.56 |
| 1:A:1500:A:H5'' | 1:A:1508:G:H5'' | 1.88 | 0.56 |
| 20:T:43:LEU:HD22 | 20:T:51:GLU:HG3 | 1.88 | 0.56 |
| 22:W:32:ILE:HB | 22:W:63:THR:O | 2.05 | 0.56 |
| 25:Z:41:C:H2' | 25:Z:42:G:C8 | 2.40 | 0.56 |
| 1:A:417:C:N4 | 1:A:418:C:N4 | 2.54 | 0.56 |
| 6:F:22:GLU:HA | 6:F:25:ILE:HD12 | 1.88 | 0.56 |
| 1:A:96:U:H2' | 1:A:97:G:C8 | 2.39 | 0.56 |
| 1:A:930:C:H2' | 1:A:931:C:O4' | 2.05 | 0.56 |
| 7:G:115:ARG:O | 7:G:119:ARG:HG3 | 2.05 | 0.56 |
| 1:A:255:G:H2' | 1:A:256:U:C6 | 2.41 | 0.56 |
| 1:A:678:U:H2' | 1:A:679:C:C6 | 2.41 | 0.56 |
| 1:A:914:A:H2' | 1:A:915:A:H8 | 1.69 | 0.56 |
| 1:A:998:G:N1 | 1:A:999:C:C4 | 2.74 | 0.56 |
| 1:A:1537:U:H3 | 24:Y:28:A:H61 | 1.52 | 0.56 |
| 2:B:84:GLU:HB3 | 2:B:219:VAL:HG21 | 1.87 | 0.56 |
| 1:A:78:G:HO2' | 1:A:79:G:C4' | 2.19 | 0.56 |
| 1:A:538:G:H2' | 1:A:539:A:H8 | 1.71 | 0.56 |
| 1:A:790:A:H2' | 1:A:791:G:C8 | 2.40 | 0.56 |
| 1:A:939:G:H1' | 1:A:1375:A:H2 | 1.71 | 0.56 |
| 1:A:999:C:C2' | 1:A:1000:U:H5' | 2.36 | 0.56 |
| 1:A:1233:G:C6 | 1:A:1234:C:N4 | 2.73 | 0.56 |
| 1:A:377:G:H1 | 1:A:386:C:H42 | 1.53 | 0.56 |
| 1:A:891:U:H2' | 1:A:892:A:H8 | 1.71 | 0.56 |
| 25:Z:4:G:H2' | 25:Z:5:G:C8 | 2.41 | 0.56 |
| 1:A:1005:A:OP1 | 1:A:1006:C:C5 | 2.58 | 0.55 |
| 1:A:1353:G:N2 | 1:A:1354:C:C2 | 2.74 | 0.55 |
| 13:M:10:PRO:CB | 13:M:18:ALA:HB1 | 2.35 | 0.55 |
| 25:Z:54:5MU:H73 | 25:Z:55:PSU:C2 | 2.42 | 0.55 |
| 1:A:60:A:H4' | 1:A:61:G:O5' | 2.06 | 0.55 |
| 1:A:1098:C:H1' | 1:A:1168:A:C2 | 2.39 | 0.55 |
| 1:A:1515:C:H2' | 1:A:1516:G:H8 | 1.70 | 0.55 |
| 8:H:113:SER:HB3 | 8:H:132:GLU:HB3 | 1.87 | 0.55 |
| 18:R:47:THR:HA | 18:R:83:GLU:HB2 | 1.87 | 0.55 |
| 25:Z:63:G:N1 | 25:Z:64:G:C5 | 2.75 | 0.55 |
| 2:B:97:TRP:HZ2 | 2:B:102:LEU:HD13 | 1.70 | 0.55 |
| 1:A:128:G:C2 | 1:A:234:C:C2 | 2.95 | 0.55 |
| 1:A:910:C:H4' | 1:A:1413:A:H4' | 1.88 | 0.55 |
| 1:A:1227:A:N1 | 19:S:83:HIS:CB | 2.67 | 0.55 |
| 1:A:189(K):U:H2' | 1:A:189(L):G:H8 | 1.72 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:279:A:H4' | 1:A:280:C:OP2 | 2.06 | 0.55 |
| 1:A:1540:U:H3 | 24:Y:25:A:H61 | 1.53 | 0.55 |
| 19:S:50:ALA:HB1 | 19:S:57:HIS:HB3 | 1.87 | 0.55 |
| 1:A:233:C:H2' | 1:A:234:C:H6 | 1.72 | 0.55 |
| 1:A:390:C:H2' | 1:A:391:G:C8 | 2.42 | 0.55 |
| 1:A:457:C:H2' | 1:A:458:C:H6 | 1.71 | 0.55 |
| 1:A:1127:G:H21 | 1:A:1147:C:N4 | 2.05 | 0.55 |
| 1:A:1485:U:H2' | 1:A:1486:G:H8 | 1.72 | 0.55 |
| 2:B:54:THR:HG21 | 2:B:201:ILE:HD11 | 1.89 | 0.55 |
| 5:E:93:PRO:HB2 | 8:H:105:ARG:NH1 | 2.21 | 0.55 |
| 8:H:85:ARG:HH21 | 8:H:134:ILE:HG23 | 1.72 | 0.55 |
| 1:A:530:G:O2' | 22:W:39:LYS:HG2 | 2.07 | 0.55 |
| 1:A:774:G:N2 | 1:A:806:C:C2 | 2.74 | 0.55 |
| 1:A:1223:C:H5'' | 1:A:1224:G:H5'' | 1.89 | 0.55 |
| 1:A:939:G:C6 | 1:A:940:C:N4 | 2.74 | 0.55 |
| 1:A:1166:G:N2 | 1:A:1170:A:OP2 | 2.30 | 0.55 |
| 7:G:24:THR:HA | 7:G:27:ILE:HD12 | 1.89 | 0.55 |
| 13:M:88:ARG:HG3 | 13:M:98:VAL:CG1 | 2.37 | 0.55 |
| 1:A:397:A:H3' | 1:A:397:A:N3 | 2.21 | 0.54 |
| 1:A:695:A:H2' | 1:A:696:A:H8 | 1.71 | 0.54 |
| 1:A:1000:U:H2' | 1:A:1001:A:O4' | 2.06 | 0.54 |
| 3:C:30:ARG:HH21 | 3:C:30:ARG:CB | 2.20 | 0.54 |
| 10:J:7:LYS:CA | 10:J:71:LEU:CD2 | 2.86 | 0.54 |
| 25:Z:56:C:H2' | 25:Z:57:A:H8 | 1.66 | 0.54 |
| 1:A:683:G:H2' | 1:A:684:A:C8 | 2.42 | 0.54 |
| 1:A:1005:A:OP1 | 1:A:1006:C:H5 | 1.91 | 0.54 |
| 1:A:1010:G:H2' | 1:A:1011:G:C8 | 2.42 | 0.54 |
| 1:A:1134:G:N2 | 1:A:1141:C:C2 | 2.75 | 0.54 |
| 1:A:1491:G:H5'' | 12:L:47:LYS:HE2 | 1.89 | 0.54 |
| 8:H:88:LYS:HB2 | 8:H:91:ARG:HB3 | 1.89 | 0.54 |
| 22:W:10:GLU:HG2 | 22:W:54:VAL:HG22 | 1.88 | 0.54 |
| 24:Y:36:A:C2 | 24:Y:37:U:C2 | 2.95 | 0.54 |
| 1:A:691:G:H8 | 11:K:26:ASN:HD22 | 1.53 | 0.54 |
| 1:A:1368:G:N2 | 1:A:1369:C:C2 | 2.76 | 0.54 |
| 25:Z:48:C:H2' | 25:Z:59:A:C4' | 2.38 | 0.54 |
| 1:A:729:A:H2' | 1:A:730:G:C8 | 2.38 | 0.54 |
| 1:A:878:G:H5' | 8:H:89:PRO:HG2 | 1.89 | 0.54 |
| 1:A:946:A:H2' | 1:A:947:G:C8 | 2.42 | 0.54 |
| 1:A:1079:G:H5'' | 5:E:14:ARG:NH2 | 2.22 | 0.54 |
| 1:A:1359:C:H3' | 14:N:35:ARG:HH22 | 1.71 | 0.54 |
| 5:E:81:GLU:HG2 | 5:E:90:VAL:HG22 | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 25:Z:17:C:O2 | 25:Z:17:C:C2' | 2.55 | 0.54 |
| 1:A:33:A:H2' | 1:A:34:C:C6 | 2.43 | 0.54 |
| 1:A:35:G:H2' | 1:A:36:C:C6 | 2.42 | 0.54 |
| 1:A:999:C:N3 | 1:A:1043:C:N3 | 2.55 | 0.54 |
| 1:A:1169:A:H2' | 1:A:1170:A:O4' | 2.07 | 0.54 |
| 1:A:1370:G:H4' | 9:I:12:GLU:OE2 | 2.07 | 0.54 |
| 8:H:28:ALA:HA | 8:H:59:LEU:HD12 | 1.90 | 0.54 |
| 8:H:111:ILE:HG22 | 8:H:134:ILE:HD12 | 1.89 | 0.54 |
| 1:A:34:C:H2' | 1:A:35:G:C8 | 2.43 | 0.54 |
| 1:A:235:C:H5' | 17:Q:70:ARG:HG2 | 1.90 | 0.54 |
| 1:A:761:G:C2 | 1:A:762:C:C2 | 2.96 | 0.54 |
| 1:A:1098:C:C1' | 1:A:1168:A:H2 | 2.20 | 0.54 |
| 1:A:1112:C:H1' | 3:C:179:ARG:HH21 | 1.72 | 0.54 |
| 1:A:1244:C:H2' | 1:A:1245:A:C8 | 2.43 | 0.54 |
| 1:A:1378:C:N3 | 7:G:76:ARG:NH2 | 2.56 | 0.54 |
| 3:C:113:ALA:HA | 3:C:202:ILE:HD12 | 1.89 | 0.54 |
| 4:D:102:ASP:HB3 | 4:D:136:PRO:HB3 | 1.88 | 0.54 |
| 17:Q:68:ARG:HG3 | 17:Q:68:ARG:O | 2.08 | 0.54 |
| 1:A:1230:C:C5' | 25:Z:30:G:H5'' | 2.38 | 0.54 |
| 9:I:46:ALA:HB2 | 9:I:74:ILE:HG23 | 1.89 | 0.54 |
| 1:A:530:G:H8 | 22:W:38:GLY:HA3 | 1.73 | 0.54 |
| 1:A:434:U:H2' | 1:A:435:C:C6 | 2.43 | 0.54 |
| 1:A:582:U:H2' | 1:A:583:A:H8 | 1.72 | 0.54 |
| 1:A:1262:C:H2' | 1:A:1263:C:C6 | 2.43 | 0.54 |
| 1:A:1325:C:H2' | 1:A:1326:C:C6 | 2.43 | 0.54 |
| 3:C:113:ALA:N | 3:C:114:PRO:CD | 2.71 | 0.54 |
| 8:H:91:ARG:HD3 | 12:L:7:ILE:HG21 | 1.90 | 0.54 |
| 12:L:37:CYS:SG | 12:L:58:VAL:HG22 | 2.48 | 0.54 |
| 1:A:504:C:N3 | 1:A:542:G:C2 | 2.76 | 0.53 |
| 1:A:555:C:H2' | 1:A:556:C:C6 | 2.43 | 0.53 |
| 1:A:827:U:C4 | 1:A:872:A:N1 | 2.72 | 0.53 |
| 1:A:1312:G:C2 | 1:A:1326:C:C2 | 2.95 | 0.53 |
| 1:A:500:G:C6 | 1:A:501:C:N4 | 2.76 | 0.53 |
| 1:A:522:C:H5'' | 12:L:120:TYR:OH | 2.08 | 0.53 |
| 9:I:104:ARG:HH11 | 9:I:106:ALA:HA | 1.73 | 0.53 |
| 23:X:110:LEU:HD13 | 23:X:148:ALA:HB2 | 1.89 | 0.53 |
| 25:Z:70:G:H2' | 25:Z:71:C:O4' | 2.08 | 0.53 |
| 1:A:948:C:H2' | 1:A:949:A:H8 | 1.74 | 0.53 |
| 1:A:1133:G:H1 | 1:A:1141:C:H42 | 1.55 | 0.53 |
| 1:A:79:G:H2' | 1:A:80:G:C8 | 2.42 | 0.53 |
| 1:A:532:A:N6 | 3:C:127:ARG:HB3 | 2.23 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 12:L:58:VAL:HG21 | 12:L:85:ILE:HD11 | 1.91 | 0.53 |
| 25:Z:37:A:H2' | 25:Z:38:A:O4' | 2.09 | 0.53 |
| 1:A:521:G:N1 | 1:A:522:C:C4 | 2.77 | 0.53 |
| 1:A:910:C:H5'' | 12:L:97:ARG:NH2 | 2.24 | 0.53 |
| 1:A:975:A:H5'' | 1:A:975:A:C8 | 2.44 | 0.53 |
| 1:A:1027:C:H2' | 1:A:1028:C:H5' | 1.89 | 0.53 |
| 1:A:1314:C:H42 | 19:S:4:SER:HB2 | 1.74 | 0.53 |
| 8:H:36:LEU:HD21 | 8:H:61:VAL:HG22 | 1.91 | 0.53 |
| 1:A:975:A:H4' | 1:A:976:G:C5' | 2.39 | 0.53 |
| 4:D:109:GLY:HA3 | 4:D:165:MET:HG3 | 1.91 | 0.53 |
| 7:G:33:ASP:HB2 | 7:G:35:LYS:HG3 | 1.90 | 0.53 |
| 1:A:138:G:H1 | 1:A:225:C:H42 | 1.57 | 0.53 |
| 1:A:216:G:C2 | 1:A:217:C:N3 | 2.77 | 0.53 |
| 1:A:1414:U:H2' | 1:A:1415:G:C8 | 2.43 | 0.53 |
| 1:A:1418:A:N6 | 1:A:1482:G:O2' | 2.40 | 0.53 |
| 1:A:1437:C:H2' | 1:A:1438:G:H8 | 1.74 | 0.53 |
| 25:Z:48:C:H5'' | 25:Z:50:U:OP2 | 2.09 | 0.53 |
| 1:A:974:A:H4' | 1:A:975:A:H3' | 1.90 | 0.53 |
| 1:A:1510:U:H2' | 1:A:1511:G:C8 | 2.44 | 0.53 |
| 2:B:10:LEU:HG | 2:B:48:MET:HG3 | 1.89 | 0.53 |
| 1:A:376:G:H5'' | 16:P:5:ARG:HD2 | 1.90 | 0.53 |
| 1:A:598:U:H2' | 1:A:599:C:H6 | 1.74 | 0.53 |
| 1:A:662:G:C2 | 1:A:744:C:O2 | 2.62 | 0.53 |
| 1:A:928:G:H1 | 1:A:1389:C:N4 | 2.07 | 0.53 |
| 5:E:20:GLN:HB2 | 5:E:23:GLY:O | 2.09 | 0.53 |
| 23:X:112:GLU:HB3 | 23:X:114:HIS:CD2 | 2.43 | 0.53 |
| 1:A:46:G:H2' | 1:A:366:C:C5 | 2.43 | 0.52 |
| 1:A:1105:A:H2' | 1:A:1106:G:C8 | 2.44 | 0.52 |
| 10:J:90:LEU:H | 10:J:91:PRO:HD2 | 1.74 | 0.52 |
| 1:A:266:G:O2' | 1:A:267:C:OP2 | 2.22 | 0.52 |
| 1:A:317:G:P | 1:A:353:A:H61 | 2.33 | 0.52 |
| 1:A:369:C:H2' | 1:A:370:C:C6 | 2.44 | 0.52 |
| 1:A:529:G:H5' | 1:A:530:G:OP2 | 2.09 | 0.52 |
| 1:A:1050:G:C6 | 1:A:1051:C:N4 | 2.77 | 0.52 |
| 1:A:1106:G:C2 | 1:A:1107:C:C4 | 2.98 | 0.52 |
| 1:A:1456:G:N2 | 1:A:1457:G:N7 | 2.57 | 0.52 |
| 2:B:80:ILE:O | 2:B:84:GLU:HG2 | 2.09 | 0.52 |
| 1:A:122:G:C2 | 1:A:123:C:C2 | 2.96 | 0.52 |
| 1:A:148:G:C2 | 1:A:175:C:C2 | 2.98 | 0.52 |
| 1:A:312:C:H2' | 1:A:313:A:H8 | 1.75 | 0.52 |
| 1:A:392:G:H2' | 1:A:393:A:C8 | 2.44 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1114:C:H2' | 1:A:1115:C:C6 | 2.45 | 0.52 |
| 1:A:1125:U:C5' | 1:A:1126:U:H5 | 2.20 | 0.52 |
| 1:A:1525:G:H2' | 1:A:1526:G:H8 | 1.75 | 0.52 |
| 1:A:568:G:C2 | 1:A:883:C:C2 | 2.98 | 0.52 |
| 1:A:890:G:O2' | 1:A:906:G:O6 | 2.24 | 0.52 |
| 1:A:1251:A:H2' | 1:A:1252:A:O4' | 2.09 | 0.52 |
| 1:A:1534:A:C4 | 1:A:1535:C:C5 | 2.98 | 0.52 |
| 13:M:94:ARG:HB3 | 13:M:96:LEU:HD12 | 1.92 | 0.52 |
| 15:O:82:ILE:HA | 15:O:87:ILE:HD12 | 1.90 | 0.52 |
| 1:A:437:U:H2' | 1:A:438:G:O4' | 2.09 | 0.52 |
| 1:A:1124:G:H1 | 1:A:1149:C:H42 | 1.57 | 0.52 |
| 1:A:1162:C:C2 | 1:A:1175:G:N2 | 2.77 | 0.52 |
| 4:D:108:LEU:HD21 | 4:D:174:LEU:HD22 | 1.91 | 0.52 |
| 25:Z:52:G:C4 | 25:Z:53:G:C8 | 2.97 | 0.52 |
| 25:Z:64:G:C2 | 25:Z:65:C:C2 | 2.98 | 0.52 |
| 1:A:145:G:N2 | 1:A:178:C:C2 | 2.78 | 0.52 |
| 1:A:876:G:C6 | 1:A:877:C:N4 | 2.77 | 0.52 |
| 1:A:1096:C:H2' | 1:A:1097:C:C6 | 2.44 | 0.52 |
| 8:H:6:ILE:O | 8:H:10:LEU:HG | 2.09 | 0.52 |
| 1:A:333:G:N2 | 1:A:334:C:C2 | 2.77 | 0.52 |
| 1:A:505:G:H2' | 1:A:506:G:H8 | 1.74 | 0.52 |
| 1:A:674:G:O5' | 1:A:674:G:H8 | 1.93 | 0.52 |
| 1:A:1229:A:H2' | 1:A:1230:C:H6 | 1.75 | 0.52 |
| 3:C:26:LYS:N | 3:C:26:LYS:CE | 2.73 | 0.52 |
| 1:A:99:U:H2' | 1:A:100:C:C6 | 2.45 | 0.52 |
| 1:A:1001(A):G:N1 | 1:A:1002:G:C6 | 2.78 | 0.52 |
| 1:A:1365:G:C2 | 1:A:1366:C:C2 | 2.98 | 0.52 |
| 1:A:1365:G:C6 | 1:A:1366:C:C4 | 2.98 | 0.52 |
| 1:A:1424:C:H42 | 1:A:1476:G:H1 | 1.56 | 0.52 |
| 25:Z:17(A):U:C3' | 25:Z:18:G:H5'' | 2.40 | 0.52 |
| 1:A:130:A:H8 | 1:A:130:A:OP1 | 1.93 | 0.52 |
| 1:A:200:G:C2 | 1:A:218:C:C2 | 2.98 | 0.52 |
| 1:A:269:C:H2' | 1:A:270:A:C8 | 2.44 | 0.52 |
| 1:A:413:G:N2 | 1:A:429:U:OP2 | 2.38 | 0.52 |
| 1:A:1129:C:O5' | 1:A:1130:A:H5' | 2.10 | 0.52 |
| 5:E:139:LEU:HA | 5:E:142:LEU:HD12 | 1.91 | 0.52 |
| 9:I:10:ARG:CD | 9:I:105:ASP:HB3 | 2.40 | 0.52 |
| 1:A:100:C:H2' | 1:A:101:A:C8 | 2.45 | 0.52 |
| 1:A:124:G:H2' | 1:A:125:U:O4' | 2.10 | 0.52 |
| 1:A:1010:G:H2' | 1:A:1011:G:H8 | 1.74 | 0.52 |
| 1:A:1434:A:H2' | 1:A:1435:G:O4' | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 8:H:11:THR:HA | 8:H:14:ARG:HH12 | 1.75 | 0.52 |
| 13:M:33:ALA:HB2 | 13:M:64:TRP:HH2 | 1.74 | 0.52 |
| 19:S:6:LYS:HD2 | 19:S:7:LYS:H | 1.75 | 0.52 |
| 1:A:70:G:C2 | 1:A:100:C:C2 | 2.98 | 0.51 |
| 10:J:57:LYS:HB2 | 10:J:60:ARG:HH12 | 1.74 | 0.51 |
| 19:S:17:GLU:HA | 19:S:20:LEU:HG | 1.91 | 0.51 |
| 1:A:560:U:H2' | 5:E:123:LEU:HD22 | 1.91 | 0.51 |
| 1:A:1029:C:H2' | 1:A:1030:C:C6 | 2.45 | 0.51 |
| 1:A:1137:C:H4' | 1:A:1138:G:C2 | 2.45 | 0.51 |
| 1:A:1392:G:H21 | 1:A:1502:A:H8 | 1.59 | 0.51 |
| 5:E:92:LYS:HG2 | 5:E:93:PRO:HD2 | 1.91 | 0.51 |
| 15:O:30:ALA:HA | 15:O:85:LEU:HD11 | 1.92 | 0.51 |
| 17:Q:34:LYS:HG3 | 17:Q:36:ILE:HG23 | 1.91 | 0.51 |
| 25:Z:68:C:H2' | 25:Z:69:C:C6 | 2.45 | 0.51 |
| 1:A:967:C:H2' | 1:A:968:A:C8 | 2.45 | 0.51 |
| 1:A:1280:A:OP1 | 1:A:1281:U:C5 | 2.62 | 0.51 |
| 23:X:67:TYR:O | 23:X:71:MET:HG2 | 2.11 | 0.51 |
| 1:A:223:U:H5' | 20:T:68:LYS:HZ1 | 1.76 | 0.51 |
| 1:A:277:C:H5' | 17:Q:68:ARG:NH1 | 2.25 | 0.51 |
| 1:A:476:G:H2' | 1:A:477:A:C8 | 2.45 | 0.51 |
| 1:A:681:C:H42 | 1:A:709:G:H1 | 1.58 | 0.51 |
| 1:A:1068:G:N2 | 1:A:1069:C:C2 | 2.78 | 0.51 |
| 1:A:1369:C:H2' | 1:A:1370:G:O4' | 2.10 | 0.51 |
| 1:A:1389:C:H2' | 1:A:1390:U:O4' | 2.11 | 0.51 |
| 3:C:30:ARG:NH2 | 3:C:30:ARG:CB | 2.73 | 0.51 |
| 7:G:111:ARG:CZ | 7:G:122:HIS:HB3 | 2.41 | 0.51 |
| 1:A:184:G:H2' | 1:A:185:A:H8 | 1.75 | 0.51 |
| 1:A:522:C:H41 | 12:L:53:ARG:HH21 | 1.59 | 0.51 |
| 1:A:737:A:H2' | 1:A:738:C:C6 | 2.46 | 0.51 |
| 1:A:838:G:C2 | 1:A:849:C:C2 | 2.99 | 0.51 |
| 1:A:1126:U:O2 | 1:A:1126:U:H2' | 2.09 | 0.51 |
| 1:A:1431:C:C2 | 1:A:1470:G:N2 | 2.79 | 0.51 |
| 1:A:1443:G:N2 | 1:A:1444:C:C2 | 2.79 | 0.51 |
| 1:A:1493:A:H2' | 22:W:20:ALA:H | 1.75 | 0.51 |
| 5:E:19:MET:SD | 5:E:24:ARG:HB3 | 2.51 | 0.51 |
| 1:A:1244:C:H2' | 1:A:1245:A:H8 | 1.75 | 0.51 |
| 1:A:1367:C:H4' | 10:J:48:THR:HG21 | 1.91 | 0.51 |
| 1:A:1464:G:C2 | 1:A:1465:C:C4 | 2.98 | 0.51 |
| 3:C:26:LYS:N | 3:C:26:LYS:CD | 2.73 | 0.51 |
| 6:F:78:GLU:HA | 6:F:81:ILE:HD12 | 1.92 | 0.51 |
| 13:M:90:LEU:HA | 13:M:93:ARG:HD2 | 1.91 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 22:W:13:VAL:HB | 22:W:50:GLY:H | 1.75 | 0.51 |
| 1:A:880:C:H2' | 1:A:881:G:C8 | 2.46 | 0.51 |
| 1:A:1405:G:H2' | 1:A:1406:U:H6 | 1.75 | 0.51 |
| 20:T:45:GLN:HG2 | 20:T:91:LEU:HD22 | 1.93 | 0.51 |
| 1:A:70:G:C2 | 1:A:100:C:O2 | 2.64 | 0.51 |
| 1:A:264:U:H2' | 1:A:265:G:O4' | 2.11 | 0.51 |
| 1:A:1048:G:H1 | 1:A:1209:C:H42 | 1.59 | 0.51 |
| 1:A:1230:C:H5'' | 25:Z:30:G:H5'' | 1.92 | 0.51 |
| 1:A:1283:G:N2 | 1:A:1284:C:C2 | 2.79 | 0.51 |
| 4:D:30:LYS:C | 4:D:32:ALA:H | 2.14 | 0.51 |
| 1:A:173:U:H5' | 1:A:197:A:O4' | 2.11 | 0.51 |
| 1:A:824:C:H2' | 1:A:825:G:H8 | 1.74 | 0.51 |
| 1:A:864:A:C2 | 1:A:865:A:C2 | 2.99 | 0.51 |
| 1:A:1027:C:C2' | 1:A:1028:C:H5' | 2.40 | 0.51 |
| 1:A:1064:G:H21 | 1:A:1190:G:H2' | 1.75 | 0.51 |
| 1:A:1079:G:H2' | 1:A:1080:A:C8 | 2.46 | 0.51 |
| 1:A:1325:C:H2' | 1:A:1326:C:H6 | 1.75 | 0.51 |
| 1:A:1363(A):A:H1' | 1:A:1365:G:C5 | 2.45 | 0.51 |
| 25:Z:70:G:C6 | 25:Z:71:C:C4 | 2.99 | 0.51 |
| 1:A:504:C:C2 | 1:A:542:G:N2 | 2.79 | 0.51 |
| 1:A:1201:A:H4' | 1:A:1202:G:O5' | 2.11 | 0.51 |
| 1:A:1534:A:C4 | 1:A:1535:C:C6 | 2.99 | 0.51 |
| 25:Z:31:G:H2' | 25:Z:32:OMC:H6 | 1.76 | 0.51 |
| 1:A:1360:A:OP2 | 14:N:35:ARG:NH2 | 2.44 | 0.50 |
| 17:Q:93:GLN:O | 17:Q:96:GLU:HB2 | 2.12 | 0.50 |
| 25:Z:29:G:H2' | 25:Z:30:G:O4' | 2.11 | 0.50 |
| 1:A:17:U:O2 | 1:A:1079:G:C2 | 2.64 | 0.50 |
| 1:A:876:G:H2' | 1:A:877:C:C6 | 2.45 | 0.50 |
| 1:A:1130:A:H2' | 1:A:1131:G:C8 | 2.46 | 0.50 |
| 1:A:1229:A:H2' | 1:A:1230:C:C6 | 2.46 | 0.50 |
| 1:A:10:A:H2' | 1:A:11:G:H8 | 1.72 | 0.50 |
| 1:A:967:C:H4' | 9:I:128:ARG:NE | 2.26 | 0.50 |
| 1:A:1507:A:H2' | 1:A:1508:G:C8 | 2.45 | 0.50 |
| 5:E:152:ARG:HB3 | 8:H:43:GLY:HA3 | 1.94 | 0.50 |
| 7:G:65:ALA:O | 7:G:69:VAL:HG23 | 2.12 | 0.50 |
| 25:Z:69:C:H2' | 25:Z:70:G:O4' | 2.11 | 0.50 |
| 1:A:132:C:C2 | 1:A:231:G:N2 | 2.80 | 0.50 |
| 1:A:309:G:H2' | 1:A:310:G:H8 | 1.76 | 0.50 |
| 1:A:558:G:H3' | 1:A:559:A:C5' | 2.42 | 0.50 |
| 1:A:914:A:H2' | 1:A:915:A:C8 | 2.46 | 0.50 |
| 4:D:149:ALA:HB3 | 4:D:152:SER:HB2 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:G:97:GLN:O | 7:G:101:LEU:HG | 2.11 | 0.50 |
| 24:Y:36:A:H2' | 24:Y:37:U:O4' | 2.12 | 0.50 |
| 1:A:56:U:H2' | 1:A:57:G:C8 | 2.45 | 0.50 |
| 1:A:236:G:C2 | 1:A:237:C:C2 | 3.00 | 0.50 |
| 1:A:381:C:H2' | 1:A:382:A:O4' | 2.12 | 0.50 |
| 1:A:1106:G:H5'' | 3:C:172:ARG:HD2 | 1.92 | 0.50 |
| 1:A:1128:C:H1' | 1:A:1146:A:H61 | 1.77 | 0.50 |
| 3:C:188:LEU:HD12 | 3:C:190:ARG:HG3 | 1.92 | 0.50 |
| 4:D:79:PHE:CZ | 4:D:204:ILE:HA | 2.47 | 0.50 |
| 1:A:777:A:H2' | 1:A:778:G:C8 | 2.46 | 0.50 |
| 1:A:966:G:C4 | 25:Z:34:C:H5' | 2.46 | 0.50 |
| 1:A:1255:G:H2' | 1:A:1279:A:N6 | 2.26 | 0.50 |
| 1:A:1361:G:C6 | 1:A:1362:C:N3 | 2.80 | 0.50 |
| 2:B:51:LEU:HG | 2:B:201:ILE:HG23 | 1.93 | 0.50 |
| 4:D:121:VAL:O | 4:D:134:ASP:HA | 2.12 | 0.50 |
| 10:J:51:ARG:N | 10:J:59:SER:O | 2.37 | 0.50 |
| 1:A:16:A:N3 | 1:A:1080:A:H1' | 2.27 | 0.50 |
| 1:A:229:U:H2' | 1:A:230:G:C8 | 2.47 | 0.50 |
| 1:A:648:A:H2' | 1:A:649:G:H8 | 1.77 | 0.50 |
| 1:A:1081:G:O5' | 5:E:18:ARG:HB2 | 2.12 | 0.50 |
| 14:N:24:CYS:HB2 | 14:N:40:CYS:HB3 | 1.93 | 0.50 |
| 25:Z:53:G:N2 | 25:Z:62:C:C2 | 2.80 | 0.50 |
| 1:A:22:G:C6 | 1:A:23:C:C4 | 2.99 | 0.50 |
| 1:A:142:G:H2' | 1:A:143:A:C8 | 2.47 | 0.50 |
| 1:A:474:G:H2' | 1:A:475:G:C8 | 2.47 | 0.50 |
| 1:A:1028:C:H2' | 1:A:1029:C:O4' | 2.12 | 0.50 |
| 1:A:1132:C:H2' | 1:A:1133:G:H8 | 1.76 | 0.50 |
| 1:A:1532:U:H5'' | 1:A:1533:C:P | 2.51 | 0.50 |
| 6:F:27:GLN:HA | 6:F:30:LEU:HD12 | 1.93 | 0.50 |
| 1:A:399:G:C6 | 1:A:400:C:N4 | 2.80 | 0.50 |
| 1:A:784:C:C2 | 1:A:799:G:N2 | 2.80 | 0.50 |
| 1:A:939:G:H2' | 1:A:940:C:C6 | 2.47 | 0.50 |
| 1:A:1000:U:C6 | 1:A:1000:U:C3' | 2.95 | 0.50 |
| 1:A:1017:G:C2 | 1:A:1018:C:C2 | 2.99 | 0.50 |
| 1:A:1280:A:C3' | 1:A:1281:U:H5'' | 2.41 | 0.50 |
| 1:A:1518:A:H2' | 1:A:1519:A:C8 | 2.47 | 0.50 |
| 7:G:145:ALA:O | 7:G:146:GLU:HB2 | 2.11 | 0.50 |
| 1:A:1135:U:H4' | 1:A:1136:U:C5 | 2.47 | 0.49 |
| 10:J:62:HIS:CB | 14:N:59:ALA:HB3 | 2.37 | 0.49 |
| 14:N:7:ILE:HG22 | 14:N:10:ALA:HB2 | 1.93 | 0.49 |
| 16:P:22:THR:HA | 16:P:33:ILE:HD12 | 1.93 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 25:Z:22:G:N2 | 25:Z:23:C:C2 | 2.79 | 0.49 |
| 1:A:416:G:C6 | 1:A:417:C:C4 | 3.00 | 0.49 |
| 1:A:538:G:H2' | 1:A:539:A:C8 | 2.46 | 0.49 |
| 1:A:1059:C:O3' | 14:N:45:ARG:NH2 | 2.45 | 0.49 |
| 1:A:1172:C:H2' | 1:A:1173:G:H8 | 1.77 | 0.49 |
| 1:A:1220:G:H2' | 1:A:1221:G:C8 | 2.47 | 0.49 |
| 1:A:1385:G:H2' | 1:A:1386:G:H8 | 1.77 | 0.49 |
| 1:A:1525:G:H2' | 1:A:1526:G:C8 | 2.47 | 0.49 |
| 2:B:174:VAL:HG13 | 2:B:184:VAL:HG11 | 1.94 | 0.49 |
| 8:H:12:ARG:HD3 | 8:H:26:VAL:HG12 | 1.94 | 0.49 |
| 10:J:57:LYS:HA | 10:J:60:ARG:HH11 | 1.77 | 0.49 |
| 1:A:105:G:H2' | 1:A:106:C:C6 | 2.46 | 0.49 |
| 1:A:115:G:O2' | 1:A:289:G:H5'' | 2.13 | 0.49 |
| 1:A:384:G:C6 | 1:A:385:C:N4 | 2.80 | 0.49 |
| 1:A:1405:G:H2' | 1:A:1406:U:C6 | 2.46 | 0.49 |
| 25:Z:52:G:H2' | 25:Z:53:G:O4' | 2.13 | 0.49 |
| 1:A:41:G:H2' | 1:A:42:G:H8 | 1.78 | 0.49 |
| 1:A:293:G:C6 | 1:A:294:U:C4 | 3.00 | 0.49 |
| 1:A:919:A:C2 | 1:A:1080:A:C2 | 2.99 | 0.49 |
| 1:A:1114:C:C2 | 1:A:1187:G:C2 | 3.00 | 0.49 |
| 1:A:1222:G:OP1 | 19:S:77:THR:HG23 | 2.12 | 0.49 |
| 1:A:1256:A:H1' | 1:A:1258:G:C4 | 2.48 | 0.49 |
| 1:A:1493:A:H4' | 1:A:1494:G:OP1 | 2.13 | 0.49 |
| 3:C:25:GLY:O | 3:C:29:TYR:HB2 | 2.12 | 0.49 |
| 15:O:39:LEU:HD22 | 15:O:56:LEU:HB2 | 1.94 | 0.49 |
| 25:Z:37:A:H3' | 25:Z:38:A:C8 | 2.47 | 0.49 |
| 1:A:270:A:H2' | 1:A:271:C:C6 | 2.47 | 0.49 |
| 1:A:416:G:C2 | 1:A:417:C:C2 | 3.01 | 0.49 |
| 1:A:544:G:OP1 | 4:D:62:GLN:HG3 | 2.12 | 0.49 |
| 1:A:1262:C:H42 | 1:A:1273:G:H1 | 1.60 | 0.49 |
| 1:A:1345:U:H4' | 1:A:1346:A:O5' | 2.12 | 0.49 |
| 1:A:1416:G:H2' | 1:A:1417:G:O4' | 2.12 | 0.49 |
| 1:A:1428:A:H2' | 1:A:1429:C:C6 | 2.48 | 0.49 |
| 5:E:139:LEU:O | 5:E:142:LEU:HB2 | 2.12 | 0.49 |
| 12:L:37:CYS:SG | 12:L:56:ALA:HB1 | 2.52 | 0.49 |
| 20:T:22:ARG:HG2 | 20:T:25:ARG:HH22 | 1.76 | 0.49 |
| 1:A:22:G:C2 | 1:A:23:C:C2 | 3.01 | 0.49 |
| 1:A:122:G:C6 | 1:A:123:C:C4 | 3.00 | 0.49 |
| 1:A:132:C:N3 | 1:A:231:G:C2 | 2.81 | 0.49 |
| 1:A:744:C:H2' | 1:A:745:C:C6 | 2.48 | 0.49 |
| 1:A:1409:C:H2' | 1:A:1410:G:H8 | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1443:G:C2 | 1:A:1444:C:C4 | 3.00 | 0.49 |
| 11:K:33:THR:HA | 11:K:39:PRO:HA | 1.94 | 0.49 |
| 20:T:43:LEU:HB3 | 20:T:52:ALA:HB2 | 1.94 | 0.49 |
| 22:W:56:GLU:HB3 | 22:W:66:ARG:HH11 | 1.76 | 0.49 |
| 23:X:141:THR:HG22 | 23:X:165:LEU:HD11 | 1.93 | 0.49 |
| 1:A:940:C:H2' | 1:A:941:G:C8 | 2.48 | 0.49 |
| 1:A:20:U:H2' | 1:A:21:G:O4' | 2.13 | 0.49 |
| 1:A:125:U:H2' | 1:A:126:G:C8 | 2.47 | 0.49 |
| 1:A:552:U:H2' | 1:A:553:A:C8 | 2.48 | 0.49 |
| 1:A:864:A:O2' | 1:A:865:A:O4' | 2.31 | 0.49 |
| 1:A:1456:G:N2 | 1:A:1457:G:C8 | 2.81 | 0.49 |
| 1:A:15:G:H2' | 1:A:16:A:H8 | 1.78 | 0.49 |
| 1:A:28:G:O2' | 1:A:296:U:OP1 | 2.31 | 0.49 |
| 1:A:148:G:H2' | 1:A:149:A:C8 | 2.47 | 0.49 |
| 1:A:940:C:H2' | 1:A:941:G:H8 | 1.78 | 0.49 |
| 5:E:51:VAL:HG13 | 5:E:52:PRO:HD3 | 1.95 | 0.49 |
| 13:M:94:ARG:HH22 | 19:S:80:TYR:HA | 1.77 | 0.49 |
| 25:Z:64:G:C6 | 25:Z:65:C:C4 | 3.00 | 0.49 |
| 1:A:189:G:C2 | 1:A:189(A):C:C2 | 3.00 | 0.49 |
| 1:A:224:C:H2' | 1:A:225:C:C6 | 2.48 | 0.49 |
| 1:A:1217:C:N4 | 1:A:1218:C:N4 | 2.61 | 0.49 |
| 1:A:1484:C:H2' | 1:A:1485:U:O4' | 2.13 | 0.49 |
| 1:A:977:A:H2' | 1:A:978:A:H5'' | 1.95 | 0.48 |
| 1:A:1030:C:C2 | 1:A:1032:G:N2 | 2.81 | 0.48 |
| 1:A:1357:A:N6 | 1:A:1363(A):A:C2 | 2.80 | 0.48 |
| 18:R:69:THR:HA | 18:R:72:ARG:HD2 | 1.94 | 0.48 |
| 25:Z:36:U:H2' | 25:Z:37:A:O4' | 2.12 | 0.48 |
| 25:Z:64:G:H2' | 25:Z:65:C:C6 | 2.48 | 0.48 |
| 1:A:427:U:OP2 | 4:D:36:ARG:NH2 | 2.46 | 0.48 |
| 1:A:568:G:C6 | 1:A:569:C:N4 | 2.81 | 0.48 |
| 1:A:648:A:H2' | 1:A:649:G:C8 | 2.48 | 0.48 |
| 1:A:1266:G:N2 | 1:A:1270:C:C2 | 2.81 | 0.48 |
| 10:J:7:LYS:CG | 10:J:71:LEU:HD23 | 2.24 | 0.48 |
| 12:L:32:PHE:HB3 | 12:L:84:LEU:HD11 | 1.95 | 0.48 |
| 25:Z:70:G:C2 | 25:Z:71:C:C2 | 3.01 | 0.48 |
| 1:A:130:A:H5' | 17:Q:63:ARG:HE | 1.79 | 0.48 |
| 1:A:198:G:H2' | 1:A:199:G:C8 | 2.48 | 0.48 |
| 1:A:229:U:H2' | 1:A:230:G:H8 | 1.78 | 0.48 |
| 1:A:261:U:N3 | 1:A:264:U:OP2 | 2.39 | 0.48 |
| 1:A:442:C:H2' | 1:A:443:C:C6 | 2.49 | 0.48 |
| 1:A:778:G:C6 | 1:A:779:C:C4 | 3.01 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:778:G:C2 | 1:A:779:C:C2 | 3.02 | 0.48 |
| 1:A:823:G:N2 | 1:A:824:C:C2 | 2.81 | 0.48 |
| 1:A:1147:C:HO2' | 9:I:5:TYR:HH | 1.61 | 0.48 |
| 1:A:1226:C:H2' | 13:M:103:THR:HB | 1.94 | 0.48 |
| 3:C:29:TYR:CE2 | 14:N:54:PRO:HG2 | 2.48 | 0.48 |
| 5:E:71:LEU:HD21 | 5:E:115:VAL:HG22 | 1.96 | 0.48 |
| 12:L:57:LYS:HG2 | 12:L:67:THR:HG22 | 1.96 | 0.48 |
| 1:A:588:G:N1 | 1:A:589:C:C4 | 2.81 | 0.48 |
| 1:A:719:C:H1' | 18:R:49:LYS:HG2 | 1.94 | 0.48 |
| 1:A:877:C:H2' | 1:A:878:G:C8 | 2.46 | 0.48 |
| 1:A:947:G:H2' | 1:A:948:C:O4' | 2.13 | 0.48 |
| 1:A:951:G:C6 | 1:A:1231:G:C6 | 3.02 | 0.48 |
| 2:B:21:ARG:HD3 | 2:B:21:ARG:H | 1.79 | 0.48 |
| 1:A:35:G:O2' | 12:L:121:GLY:HA2 | 2.12 | 0.48 |
| 1:A:253:U:H2' | 1:A:254:G:C8 | 2.48 | 0.48 |
| 1:A:361:G:H2' | 1:A:362:G:O4' | 2.13 | 0.48 |
| 1:A:1345:U:O4 | 1:A:1375:A:N1 | 2.47 | 0.48 |
| 10:J:26:ALA:HA | 10:J:29:ARG:HH21 | 1.78 | 0.48 |
| 19:S:32:LYS:HA | 19:S:50:ALA:HB3 | 1.95 | 0.48 |
| 25:Z:1:C:N4 | 25:Z:72:A:H61 | 2.12 | 0.48 |
| 1:A:1385:G:H2' | 1:A:1386:G:C8 | 2.49 | 0.48 |
| 1:A:1443:G:C2 | 1:A:1444:C:N3 | 2.81 | 0.48 |
| 25:Z:50:U:H2' | 25:Z:51:C:H6 | 1.71 | 0.48 |
| 1:A:434:U:H2' | 1:A:435:C:H6 | 1.79 | 0.48 |
| 1:A:518:C:O2' | 1:A:519:C:OP2 | 2.25 | 0.48 |
| 1:A:600:C:C2 | 1:A:639:G:C2 | 3.01 | 0.48 |
| 1:A:602:A:H2' | 1:A:603:U:O4' | 2.13 | 0.48 |
| 1:A:750:G:N3 | 15:O:23:GLY:HA3 | 2.28 | 0.48 |
| 1:A:988:G:C6 | 1:A:989:C:N3 | 2.82 | 0.48 |
| 1:A:1216:G:N2 | 1:A:1217:C:C2 | 2.81 | 0.48 |
| 3:C:54:ARG:H | 3:C:69:HIS:HB2 | 1.79 | 0.48 |
| 3:C:132:ARG:HG2 | 3:C:136:GLN:HE21 | 1.79 | 0.48 |
| 4:D:57:ARG:HB3 | 4:D:206:PHE:HB2 | 1.94 | 0.48 |
| 5:E:33:VAL:HG11 | 5:E:109:ILE:HA | 1.94 | 0.48 |
| 10:J:24:VAL:HG22 | 10:J:72:VAL:HG21 | 1.95 | 0.48 |
| 15:O:9:GLN:HA | 15:O:12:ILE:HD12 | 1.95 | 0.48 |
| 1:A:169:C:H2' | 1:A:170:U:C6 | 2.49 | 0.48 |
| 1:A:568:G:C2 | 1:A:883:C:N3 | 2.82 | 0.48 |
| 1:A:603:U:H2' | 1:A:604:G:H8 | 1.78 | 0.48 |
| 1:A:1077:G:H22 | 1:A:1079:G:H3' | 1.78 | 0.48 |
| 25:Z:62:C:H2' | 25:Z:63:G:C8 | 2.48 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:110:C:H4' | 16:P:25:ARG:HB3 | 1.96 | 0.48 |
| 1:A:296:U:H2' | 1:A:297:G:C8 | 2.49 | 0.48 |
| 1:A:715:A:H2' | 1:A:716:A:O4' | 2.14 | 0.48 |
| 1:A:1038:C:H2' | 1:A:1039:C:H6 | 1.79 | 0.48 |
| 3:C:57:ILE:HA | 3:C:65:ALA:O | 2.13 | 0.48 |
| 4:D:22:LYS:HB2 | 4:D:26:CYS:SG | 2.54 | 0.48 |
| 21:V:14:TRP:HZ3 | 21:V:15:ARG:HE | 1.62 | 0.48 |
| 25:Z:63:G:C2 | 25:Z:64:G:C5 | 3.01 | 0.48 |
| 1:A:761:G:C6 | 1:A:762:C:C4 | 3.01 | 0.47 |
| 1:A:1508:G:C2 | 1:A:1509:C:C2 | 3.02 | 0.47 |
| 7:G:125:MET:O | 7:G:129:GLU:HG2 | 2.14 | 0.47 |
| 1:A:403:C:H5'' | 4:D:136:PRO:HD2 | 1.96 | 0.47 |
| 1:A:577:G:C2 | 1:A:578:C:C2 | 3.01 | 0.47 |
| 1:A:784:C:H42 | 1:A:798:G:H1 | 1.60 | 0.47 |
| 1:A:1301:U:H1' | 1:A:1302:U:OP1 | 2.13 | 0.47 |
| 12:L:114:LYS:HE2 | 12:L:125:PRO:HB3 | 1.96 | 0.47 |
| 25:Z:16:C:O4' | 25:Z:59:A:C2 | 2.67 | 0.47 |
| 1:A:263:A:OP1 | 20:T:79:ARG:HD3 | 2.14 | 0.47 |
| 1:A:538:G:OP2 | 12:L:115:LYS:HB2 | 2.14 | 0.47 |
| 1:A:636:U:H2' | 1:A:637:G:C8 | 2.49 | 0.47 |
| 1:A:975:A:H4' | 1:A:976:G:H5' | 1.95 | 0.47 |
| 3:C:116:VAL:O | 3:C:120:VAL:HG23 | 2.13 | 0.47 |
| 3:C:155:GLY:O | 3:C:196:LEU:HG | 2.13 | 0.47 |
| 5:E:32:VAL:HB | 5:E:58:ALA:HB1 | 1.95 | 0.47 |
| 1:A:669:U:H2' | 1:A:670:G:H8 | 1.79 | 0.47 |
| 1:A:988:G:H2' | 1:A:989:C:O4' | 2.14 | 0.47 |
| 1:A:1305:G:HO2' | 1:A:1306:A:H8 | 1.62 | 0.47 |
| 3:C:77:ILE:HG22 | 3:C:81:GLY:HA2 | 1.96 | 0.47 |
| 4:D:31:CYS:HG | 26:D:300:ZN:ZN | 1.24 | 0.47 |
| 8:H:86:ILE:HD11 | 8:H:136:GLU:HB3 | 1.96 | 0.47 |
| 1:A:377:G:H1 | 1:A:386:C:N4 | 2.12 | 0.47 |
| 1:A:669:U:H2' | 1:A:670:G:C8 | 2.49 | 0.47 |
| 1:A:681:C:C2 | 1:A:710:G:N2 | 2.82 | 0.47 |
| 1:A:875:C:O2' | 8:H:14:ARG:HD2 | 2.14 | 0.47 |
| 1:A:881:G:C2 | 1:A:882:C:C2 | 3.02 | 0.47 |
| 1:A:1444:C:O5' | 1:A:1444:C:H6 | 1.97 | 0.47 |
| 3:C:64:VAL:O | 3:C:99:VAL:HG23 | 2.14 | 0.47 |
| 8:H:20:TYR:HA | 8:H:65:TYR:CZ | 2.49 | 0.47 |
| 25:Z:12:G:N1 | 25:Z:13:C:C2 | 2.83 | 0.47 |
| 25:Z:53:G:H3' | 25:Z:54:5MU:H71 | 1.97 | 0.47 |
| 1:A:172:A:H2' | 1:A:174:C:H5 | 1.78 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:189:G:C6 | 1:A:189(A):C:C4 | 3.03 | 0.47 |
| 1:A:883:C:H2' | 1:A:884:U:C6 | 2.50 | 0.47 |
| 1:A:945:G:H2' | 1:A:945:G:N3 | 2.30 | 0.47 |
| 1:A:949:A:OP2 | 13:M:106:ASN:HB2 | 2.13 | 0.47 |
| 1:A:1084:G:H1' | 1:A:1103:C:H41 | 1.78 | 0.47 |
| 1:A:1188:A:H2' | 1:A:1189:C:O4' | 2.15 | 0.47 |
| 1:A:1283:G:C6 | 1:A:1284:C:N4 | 2.82 | 0.47 |
| 1:A:1346:A:H2' | 7:G:10:ARG:NH2 | 2.26 | 0.47 |
| 11:K:72:ALA:HB1 | 11:K:77:MET:HG3 | 1.95 | 0.47 |
| 25:Z:31:G:C2 | 25:Z:40:C:C2 | 3.02 | 0.47 |
| 25:Z:52:G:C5 | 25:Z:53:G:N7 | 2.82 | 0.47 |
| 1:A:333:G:C6 | 1:A:334:C:N4 | 2.82 | 0.47 |
| 1:A:590:C:N3 | 1:A:650:G:C2 | 2.83 | 0.47 |
| 1:A:960:U:H4' | 1:A:961:U:O5' | 2.13 | 0.47 |
| 1:A:1119:C:H2' | 1:A:1120:G:H8 | 1.78 | 0.47 |
| 1:A:1228:C:H4' | 13:M:116:THR:HA | 1.96 | 0.47 |
| 2:B:187:LEU:HA | 2:B:201:ILE:HB | 1.97 | 0.47 |
| 3:C:54:ARG:HB3 | 3:C:69:HIS:CD2 | 2.50 | 0.47 |
| 8:H:103:VAL:HG21 | 8:H:110:ALA:HB2 | 1.95 | 0.47 |
| 24:Y:28:A:H5' | 24:Y:29:G:OP2 | 2.15 | 0.47 |
| 25:Z:4:G:H2' | 25:Z:5:G:H8 | 1.80 | 0.47 |
| 1:A:362:G:H5'' | 12:L:61:THR:HB | 1.97 | 0.47 |
| 1:A:1050:G:N2 | 1:A:1051:C:C2 | 2.83 | 0.47 |
| 3:C:99:VAL:CG2 | 3:C:100:ALA:N | 2.78 | 0.47 |
| 4:D:120:LEU:HA | 4:D:125:HIS:HD2 | 1.79 | 0.47 |
| 15:O:15:PHE:HE2 | 15:O:84:LYS:HB3 | 1.79 | 0.47 |
| 16:P:49:LEU:HD13 | 16:P:73:LEU:HD22 | 1.97 | 0.47 |
| 1:A:236:G:C6 | 1:A:237:C:C4 | 3.03 | 0.47 |
| 1:A:628:G:H2' | 1:A:629:G:C8 | 2.50 | 0.47 |
| 1:A:643:C:H2' | 1:A:644:G:H8 | 1.80 | 0.47 |
| 1:A:823:G:H2' | 1:A:824:C:C6 | 2.50 | 0.47 |
| 1:A:928:G:H2' | 1:A:929:G:C8 | 2.49 | 0.47 |
| 1:A:957:U:H4' | 19:S:79:THR:HG23 | 1.96 | 0.47 |
| 1:A:1030:C:H42 | 1:A:1031:G:H1 | 1.62 | 0.47 |
| 1:A:1038:C:H2' | 1:A:1039:C:C6 | 2.49 | 0.47 |
| 2:B:177:ALA:HA | 2:B:182:ILE:HD12 | 1.96 | 0.47 |
| 3:C:34:LEU:O | 3:C:38:ARG:HG2 | 2.15 | 0.47 |
| 1:A:988:G:C6 | 1:A:989:C:C2 | 3.03 | 0.47 |
| 1:A:1533:C:H2' | 1:A:1534:A:N1 | 2.30 | 0.47 |
| 6:F:53:ALA:HB3 | 6:F:86:ARG:HH11 | 1.79 | 0.47 |
| 19:S:36:ARG:HD3 | 19:S:72:GLY:HA3 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 22:W:32:ILE:HG22 | 22:W:63:THR:HA | 1.97 | 0.47 |
| 1:A:14:U:H1' | 1:A:17:U:H5 | 1.80 | 0.46 |
| 1:A:199:G:N2 | 1:A:219:C:C2 | 2.83 | 0.46 |
| 2:B:80:ILE:HG21 | 2:B:212:GLN:HA | 1.96 | 0.46 |
| 13:M:11:ARG:HG3 | 13:M:12:ASN:HB2 | 1.97 | 0.46 |
| 1:A:199:G:C2 | 1:A:219:C:N3 | 2.83 | 0.46 |
| 1:A:201:C:H42 | 1:A:216:G:H1 | 1.63 | 0.46 |
| 1:A:269:C:H2' | 1:A:270:A:H8 | 1.79 | 0.46 |
| 1:A:1119:C:OP2 | 9:I:9:ARG:NH2 | 2.44 | 0.46 |
| 1:A:1171:G:N2 | 1:A:1172:C:C2 | 2.82 | 0.46 |
| 1:A:1320:C:OP1 | 19:S:70:LYS:HE3 | 2.15 | 0.46 |
| 17:Q:61:GLU:HA | 17:Q:71:PHE:CE1 | 2.50 | 0.46 |
| 1:A:290:C:H2' | 1:A:291:C:O4' | 2.16 | 0.46 |
| 1:A:585:G:C2 | 1:A:586:C:C2 | 3.04 | 0.46 |
| 1:A:908:A:H2' | 1:A:909:A:H8 | 1.80 | 0.46 |
| 1:A:1084:G:H2' | 1:A:1085:U:C5 | 2.51 | 0.46 |
| 1:A:1127:G:N2 | 1:A:1145:C:C2 | 2.83 | 0.46 |
| 3:C:137:ALA:O | 3:C:141:VAL:HG23 | 2.15 | 0.46 |
| 5:E:110:LEU:HD13 | 5:E:118:ILE:HD12 | 1.97 | 0.46 |
| 9:I:7:THR:O | 9:I:83:ARG:CD | 2.64 | 0.46 |
| 1:A:23:C:C4 | 1:A:24:U:C4 | 3.03 | 0.46 |
| 1:A:35:G:C6 | 1:A:36:C:N4 | 2.84 | 0.46 |
| 1:A:277:C:H5' | 17:Q:68:ARG:HH12 | 1.79 | 0.46 |
| 1:A:725:G:N1 | 1:A:726:C:C4 | 2.83 | 0.46 |
| 1:A:806:C:H2' | 1:A:807:A:C8 | 2.51 | 0.46 |
| 1:A:834:C:C2 | 1:A:853:G:C2 | 3.02 | 0.46 |
| 1:A:1535:C:C4 | 1:A:1536:C:H5 | 2.29 | 0.46 |
| 6:F:100:ASN:HB3 | 18:R:28:GLU:HA | 1.96 | 0.46 |
| 10:J:31:GLY:HA2 | 10:J:78:ASN:HD22 | 1.81 | 0.46 |
| 13:M:88:ARG:HG3 | 13:M:98:VAL:HG11 | 1.97 | 0.46 |
| 16:P:7:ALA:O | 16:P:17:TYR:HA | 2.15 | 0.46 |
| 25:Z:49:G:C8 | 25:Z:49:G:O5' | 2.68 | 0.46 |
| 1:A:194:C:H4' | 20:T:64:ASP:HB3 | 1.96 | 0.46 |
| 1:A:376:G:H5'' | 16:P:5:ARG:HB2 | 1.96 | 0.46 |
| 1:A:895:G:H1 | 1:A:904:C:H42 | 1.63 | 0.46 |
| 1:A:1431:C:H3' | 1:A:1432:G:H8 | 1.81 | 0.46 |
| 2:B:213:LEU:O | 2:B:217:ARG:HG2 | 2.15 | 0.46 |
| 11:K:22:HIS:HB3 | 11:K:29:ILE:HG23 | 1.98 | 0.46 |
| 1:A:259:G:C2 | 1:A:268:C:C2 | 3.04 | 0.46 |
| 1:A:663:A:H2' | 1:A:664:G:O4' | 2.16 | 0.46 |
| 1:A:838:G:N2 | 1:A:849:C:C2 | 2.83 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:977:A:O2' | 1:A:979:C:OP2 | 2.21 | 0.46 |
| 1:A:1077:G:N2 | 1:A:1080:A:OP2 | 2.41 | 0.46 |
| 14:N:44:LEU:HD22 | 14:N:53:LEU:HD11 | 1.98 | 0.46 |
| 1:A:289:G:N2 | 1:A:290:C:C2 | 2.84 | 0.46 |
| 1:A:931:C:H3' | 1:A:932:C:H5'' | 1.98 | 0.46 |
| 1:A:1050:G:C2 | 1:A:1209:C:C2 | 3.04 | 0.46 |
| 17:Q:92:ARG:HB3 | 17:Q:92:ARG:HH11 | 1.81 | 0.46 |
| 1:A:127:G:N2 | 1:A:235:C:C2 | 2.84 | 0.46 |
| 1:A:389:A:H3' | 1:A:390:C:C6 | 2.51 | 0.46 |
| 1:A:392:G:H5' | 16:P:12:LYS:HG3 | 1.98 | 0.46 |
| 1:A:1078:U:H5 | 1:A:1079:G:N1 | 2.14 | 0.46 |
| 1:A:1419:G:C2 | 1:A:1420:C:C2 | 3.04 | 0.46 |
| 1:A:1533:C:H4' | 24:Y:32:A:H61 | 1.80 | 0.46 |
| 5:E:93:PRO:CB | 8:H:105:ARG:NH1 | 2.78 | 0.46 |
| 22:W:26:LEU:HD12 | 22:W:30:PRO:HD2 | 1.98 | 0.46 |
| 25:Z:58:A:O2' | 25:Z:60:U:OP2 | 2.34 | 0.46 |
| 1:A:919:A:N3 | 1:A:1080:A:H2 | 2.13 | 0.46 |
| 1:A:971:G:OP1 | 1:A:972:C:H5'' | 2.16 | 0.46 |
| 1:A:986:A:H2' | 1:A:987:G:C8 | 2.50 | 0.46 |
| 1:A:1119:C:H42 | 1:A:1154:G:H1 | 1.63 | 0.46 |
| 1:A:1440:C:H42 | 1:A:1461:G:H1 | 1.63 | 0.46 |
| 1:A:1508:G:C6 | 1:A:1509:C:C4 | 3.04 | 0.46 |
| 3:C:26:LYS:H | 3:C:26:LYS:CE | 2.28 | 0.46 |
| 11:K:88:GLY:O | 11:K:90:GLY:N | 2.47 | 0.46 |
| 1:A:200:G:N2 | 1:A:218:C:C2 | 2.84 | 0.46 |
| 1:A:917:G:H2' | 1:A:918:A:H8 | 1.79 | 0.46 |
| 1:A:928:G:H2' | 1:A:929:G:H8 | 1.80 | 0.46 |
| 1:A:1074:G:C6 | 1:A:1075:C:C4 | 3.03 | 0.46 |
| 1:A:1430:C:C2 | 1:A:1471:G:C2 | 3.03 | 0.46 |
| 4:D:59:ARG:HH12 | 4:D:62:GLN:HG3 | 1.81 | 0.46 |
| 12:L:41:ARG:HD2 | 12:L:43:VAL:HG22 | 1.98 | 0.46 |
| 1:A:18:C:H2' | 1:A:19:C:C6 | 2.51 | 0.45 |
| 1:A:21:G:H21 | 1:A:914:A:H62 | 1.62 | 0.45 |
| 1:A:113:G:H1' | 1:A:354:G:H5' | 1.98 | 0.45 |
| 1:A:763:G:C2 | 1:A:764:C:C2 | 3.04 | 0.45 |
| 1:A:908:A:H2' | 1:A:909:A:C8 | 2.50 | 0.45 |
| 1:A:932:C:O5' | 7:G:4:ARG:HG2 | 2.15 | 0.45 |
| 1:A:988:G:C6 | 1:A:989:C:C4 | 3.04 | 0.45 |
| 3:C:157:ILE:HD12 | 3:C:164:ARG:HB2 | 1.97 | 0.45 |
| 4:D:116:GLN:O | 4:D:120:LEU:HG | 2.16 | 0.45 |
| 7:G:101:LEU:HA | 7:G:104:LEU:HD12 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:579:G:H2' | 1:A:580:U:C6 | 2.51 | 0.45 |
| 1:A:781:A:N6 | 1:A:802:A:H1' | 2.31 | 0.45 |
| 1:A:1256:A:C5' | 3:C:27:LYS:CE | 2.81 | 0.45 |
| 5:E:144:THR:HB | 5:E:147:ASP:H | 1.81 | 0.45 |
| 14:N:37:PHE:HB3 | 14:N:39:LEU:HD12 | 1.97 | 0.45 |
| 17:Q:48:GLU:HB2 | 17:Q:50:LYS:HB2 | 1.97 | 0.45 |
| 25:Z:70:G:N1 | 25:Z:71:C:C2 | 2.85 | 0.45 |
| 1:A:291:C:H2' | 1:A:292:G:H8 | 1.81 | 0.45 |
| 1:A:548:G:C2 | 1:A:549:C:C2 | 3.04 | 0.45 |
| 1:A:1033:G:H2' | 1:A:1034:G:C8 | 2.52 | 0.45 |
| 2:B:87:ARG:HE | 2:B:219:VAL:CG1 | 2.29 | 0.45 |
| 11:K:32:ILE:HG22 | 11:K:40:ILE:HD12 | 1.98 | 0.45 |
| 16:P:6:LEU:HD11 | 16:P:73:LEU:HD12 | 1.98 | 0.45 |
| 1:A:184:G:H2' | 1:A:185:A:C8 | 2.51 | 0.45 |
| 1:A:233:C:H2' | 1:A:234:C:C6 | 2.52 | 0.45 |
| 1:A:399:G:C2 | 1:A:400:C:C2 | 3.04 | 0.45 |
| 1:A:662:G:N1 | 1:A:744:C:C2 | 2.84 | 0.45 |
| 1:A:671:G:C2 | 1:A:736:C:C2 | 3.04 | 0.45 |
| 1:A:774:G:C2 | 1:A:806:C:N3 | 2.84 | 0.45 |
| 11:K:84:VAL:HG23 | 11:K:110:ASP:HA | 1.98 | 0.45 |
| 1:A:122:G:N1 | 1:A:123:C:C2 | 2.85 | 0.45 |
| 1:A:439:A:C6 | 1:A:441:A:H1' | 2.51 | 0.45 |
| 1:A:865:A:H2' | 1:A:866:C:C6 | 2.51 | 0.45 |
| 1:A:872:A:C4 | 1:A:874:G:N7 | 2.84 | 0.45 |
| 1:A:1081:G:H8 | 1:A:1081:G:OP2 | 2.00 | 0.45 |
| 1:A:1401:G:H2' | 1:A:1402:C:O4' | 2.16 | 0.45 |
| 1:A:1459:C:H2' | 1:A:1460:A:H8 | 1.82 | 0.45 |
| 1:A:1536:C:C2 | 24:Y:30:G:N1 | 2.85 | 0.45 |
| 13:M:68:GLY:HA2 | 13:M:71:ARG:HD2 | 1.98 | 0.45 |
| 1:A:19:C:O2 | 1:A:917:G:C2 | 2.69 | 0.45 |
| 1:A:226:G:H2' | 1:A:227:G:O4' | 2.17 | 0.45 |
| 1:A:500:G:C2 | 1:A:501:C:N3 | 2.84 | 0.45 |
| 1:A:968:A:H8 | 1:A:968:A:OP1 | 1.99 | 0.45 |
| 1:A:991:U:C4 | 1:A:1212:U:H1' | 2.51 | 0.45 |
| 1:A:1106:G:N1 | 1:A:1107:C:C4 | 2.85 | 0.45 |
| 3:C:30:ARG:NH2 | 14:N:38:GLY:N | 2.65 | 0.45 |
| 11:K:43:SER:HB3 | 11:K:68:ALA:HB2 | 1.98 | 0.45 |
| 12:L:25:PRO:C | 12:L:27:LEU:N | 2.69 | 0.45 |
| 20:T:63:ILE:HG21 | 20:T:81:LYS:HG3 | 1.99 | 0.45 |
| 25:Z:10:G:N2 | 25:Z:26:G:H1' | 2.32 | 0.45 |
| 25:Z:17:C:OP1 | 25:Z:60:U:O2' | 2.26 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:63:C:H42 | 1:A:104:G:H1 | 1.65 | 0.45 |
| 1:A:571:U:H3' | 1:A:572:A:H5'' | 1.98 | 0.45 |
| 1:A:767:A:H2' | 1:A:768:A:O4' | 2.17 | 0.45 |
| 1:A:880:C:H5'' | 12:L:12:ARG:HH21 | 1.81 | 0.45 |
| 1:A:977:A:H3' | 1:A:977:A:N3 | 2.32 | 0.45 |
| 1:A:1017:G:C6 | 1:A:1018:C:C4 | 3.04 | 0.45 |
| 1:A:1305:G:OP2 | 21:V:5:ASP:HB2 | 2.17 | 0.45 |
| 1:A:1478:C:H2' | 1:A:1479:C:C6 | 2.52 | 0.45 |
| 1:A:1508:G:H2' | 1:A:1509:C:O4' | 2.16 | 0.45 |
| 20:T:63:ILE:HG23 | 20:T:77:ALA:HB1 | 1.97 | 0.45 |
| 1:A:187:C:N3 | 1:A:191:G:C2 | 2.84 | 0.45 |
| 1:A:571:U:C3' | 1:A:572:A:H5'' | 2.47 | 0.45 |
| 1:A:929:G:C2 | 1:A:930:C:C2 | 3.04 | 0.45 |
| 1:A:939:G:C2 | 1:A:940:C:N3 | 2.85 | 0.45 |
| 1:A:1390:U:H2' | 1:A:1391:U:C6 | 2.52 | 0.45 |
| 3:C:174:PRO:HD2 | 3:C:182:ILE:HD11 | 1.99 | 0.45 |
| 1:A:15:G:N2 | 5:E:17:ALA:O | 2.47 | 0.45 |
| 1:A:15:G:C5 | 1:A:16:A:N7 | 2.85 | 0.45 |
| 1:A:370:C:N3 | 1:A:392:G:C2 | 2.85 | 0.45 |
| 1:A:886:G:C2 | 1:A:912:C:O2 | 2.70 | 0.45 |
| 1:A:1120:G:H2' | 1:A:1121:U:C6 | 2.51 | 0.45 |
| 1:A:1488:G:H2' | 1:A:1489:G:H8 | 1.81 | 0.45 |
| 6:F:48:LEU:HD13 | 6:F:52:ILE:HB | 1.99 | 0.45 |
| 7:G:65:ALA:HB1 | 7:G:127:ALA:HB3 | 1.99 | 0.45 |
| 25:Z:70:G:C6 | 25:Z:71:C:N3 | 2.85 | 0.45 |
| 1:A:145:G:C2 | 1:A:178:C:N3 | 2.86 | 0.45 |
| 1:A:743:U:H2' | 1:A:744:C:H6 | 1.81 | 0.45 |
| 1:A:1171:G:C2 | 1:A:1172:C:C2 | 3.05 | 0.45 |
| 1:A:1343:G:C6 | 1:A:1344:C:N3 | 2.85 | 0.45 |
| 4:D:88:VAL:HG12 | 4:D:91:SER:H | 1.82 | 0.45 |
| 17:Q:29:HIS:CE1 | 17:Q:31:LEU:HB3 | 2.52 | 0.45 |
| 1:A:105:G:C2 | 1:A:106:C:C2 | 3.05 | 0.44 |
| 1:A:127:G:C2 | 1:A:235:C:N3 | 2.85 | 0.44 |
| 1:A:252:U:H2' | 1:A:253:U:C6 | 2.52 | 0.44 |
| 1:A:443:C:C2 | 1:A:492:G:N2 | 2.85 | 0.44 |
| 1:A:864:A:C2' | 1:A:865:A:C8 | 2.88 | 0.44 |
| 1:A:1086:U:O5' | 1:A:1086:U:H6 | 2.00 | 0.44 |
| 1:A:1327:C:H2' | 1:A:1328:C:C6 | 2.52 | 0.44 |
| 1:A:1526:G:H2' | 1:A:1527:C:C6 | 2.51 | 0.44 |
| 3:C:57:ILE:HG12 | 3:C:66:VAL:HG22 | 1.99 | 0.44 |
| 5:E:93:PRO:CB | 8:H:105:ARG:NH2 | 2.64 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:101:A:C4 | 1:A:102:G:C8 | 3.05 | 0.44 |
| 1:A:823:G:C2 | 1:A:824:C:C2 | 3.05 | 0.44 |
| 1:A:1222:G:C2 | 1:A:1223:C:N3 | 2.85 | 0.44 |
| 1:A:1225:A:H2' | 1:A:1225:A:N3 | 2.31 | 0.44 |
| 1:A:1252:A:H2' | 1:A:1253:G:O4' | 2.17 | 0.44 |
| 1:A:1371:G:H2' | 1:A:1372:U:C6 | 2.52 | 0.44 |
| 1:A:1478:C:H2' | 1:A:1479:C:H6 | 1.81 | 0.44 |
| 9:I:89:ASN:HB3 | 9:I:92:TYR:CE2 | 2.52 | 0.44 |
| 13:M:88:ARG:O | 13:M:92:HIS:HD2 | 2.00 | 0.44 |
| 1:A:514:C:H42 | 1:A:537:G:H1 | 1.65 | 0.44 |
| 1:A:518:C:H2' | 1:A:530:G:C8 | 2.52 | 0.44 |
| 1:A:914:A:C4 | 1:A:915:A:N7 | 2.86 | 0.44 |
| 1:A:1134:G:C2 | 1:A:1141:C:N3 | 2.85 | 0.44 |
| 4:D:57:ARG:HH11 | 4:D:57:ARG:HG3 | 1.82 | 0.44 |
| 17:Q:21:VAL:HG11 | 17:Q:59:ILE:HG13 | 1.99 | 0.44 |
| 25:Z:37:A:C5 | 25:Z:38:A:C5 | 3.06 | 0.44 |
| 1:A:255:G:C2 | 1:A:272:C:C2 | 3.06 | 0.44 |
| 1:A:262:A:H5'' | 20:T:76:ALA:HB2 | 2.00 | 0.44 |
| 1:A:748:C:H1' | 1:A:749:C:H5 | 1.82 | 0.44 |
| 1:A:982:U:H4' | 1:A:983:A:O4' | 2.18 | 0.44 |
| 1:A:1014:A:N1 | 19:S:34:TRP:CE2 | 2.86 | 0.44 |
| 1:A:1133:G:H1 | 1:A:1141:C:N4 | 2.15 | 0.44 |
| 1:A:1537:U:H3 | 24:Y:28:A:N6 | 2.15 | 0.44 |
| 2:B:126:GLU:HA | 2:B:129:GLU:HG3 | 1.99 | 0.44 |
| 3:C:24:ALA:HB3 | 3:C:29:TYR:CD2 | 2.53 | 0.44 |
| 5:E:18:ARG:HD3 | 5:E:20:GLN:NE2 | 2.32 | 0.44 |
| 23:X:4:GLU:HA | 23:X:66:ARG:NH1 | 2.32 | 0.44 |
| 1:A:109:A:C6 | 1:A:326:G:C6 | 3.06 | 0.44 |
| 1:A:138:G:H1 | 1:A:225:C:N4 | 2.15 | 0.44 |
| 1:A:256:U:H2' | 1:A:257:G:C8 | 2.52 | 0.44 |
| 1:A:354:G:N1 | 1:A:355:C:C4 | 2.86 | 0.44 |
| 1:A:577:G:C6 | 1:A:578:C:C4 | 3.05 | 0.44 |
| 1:A:590:C:C2 | 1:A:650:G:N2 | 2.85 | 0.44 |
| 1:A:932:C:C2 | 1:A:1386:G:N2 | 2.85 | 0.44 |
| 1:A:1220:G:H2' | 1:A:1221:G:O4' | 2.17 | 0.44 |
| 1:A:1464:G:C2 | 1:A:1465:C:N3 | 2.86 | 0.44 |
| 7:G:27:ILE:HA | 7:G:30:ILE:HD12 | 1.98 | 0.44 |
| 9:I:3:GLN:HA | 9:I:19:LEU:O | 2.18 | 0.44 |
| 15:O:85:LEU:HD12 | 15:O:87:ILE:HD11 | 1.98 | 0.44 |
| 1:A:1129:C:O5' | 1:A:1130:A:H8 | 2.00 | 0.44 |
| 1:A:1380:U:C5 | 7:G:3:ARG:HG3 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 5:E:76:ILE:HD12 | 5:E:118:ILE:HG21 | 2.00 | 0.44 |
| 1:A:230:G:H2' | 1:A:231:G:O4' | 2.18 | 0.44 |
| 1:A:372:C:H4' | 1:A:373:A:O5' | 2.17 | 0.44 |
| 1:A:701:C:H3' | 23:X:67:TYR:OH | 2.17 | 0.44 |
| 1:A:806:C:H2' | 1:A:807:A:H8 | 1.83 | 0.44 |
| 1:A:929:G:C6 | 1:A:930:C:C4 | 3.06 | 0.44 |
| 1:A:975:A:C5' | 1:A:975:A:H8 | 2.31 | 0.44 |
| 1:A:1004:A:H5'' | 1:A:1025:U:C4 | 2.52 | 0.44 |
| 1:A:1353:G:N1 | 1:A:1354:C:C4 | 2.86 | 0.44 |
| 1:A:1419:G:C6 | 1:A:1420:C:C4 | 3.05 | 0.44 |
| 3:C:79:ARG:HG3 | 3:C:82:GLU:HG2 | 1.99 | 0.44 |
| 3:C:150:LYS:HG3 | 3:C:169:ALA:HB2 | 1.99 | 0.44 |
| 4:D:107:ARG:HD3 | 4:D:173:TRP:HZ2 | 1.82 | 0.44 |
| 25:Z:49:G:O5' | 25:Z:49:G:H8 | 2.00 | 0.44 |
| 1:A:90:U:H2' | 1:A:91:C:C5 | 2.52 | 0.44 |
| 1:A:585:G:C6 | 1:A:586:C:C4 | 3.05 | 0.44 |
| 1:A:769:G:H4' | 1:A:1513:A:H4' | 2.00 | 0.44 |
| 1:A:823:G:C6 | 1:A:824:C:N4 | 2.85 | 0.44 |
| 1:A:947:G:C2 | 1:A:948:C:C2 | 3.06 | 0.44 |
| 1:A:956:U:O2 | 1:A:956:U:C2' | 2.66 | 0.44 |
| 19:S:34:TRP:HA | 19:S:52:TYR:CB | 2.43 | 0.44 |
| 25:Z:16:C:H2' | 25:Z:17:C:C5 | 2.53 | 0.44 |
| 25:Z:18:G:H21 | 25:Z:57:A:H2' | 1.83 | 0.44 |
| 1:A:105:G:C5 | 1:A:106:C:C4 | 3.05 | 0.44 |
| 1:A:223:U:H5' | 20:T:68:LYS:NZ | 2.33 | 0.44 |
| 1:A:524:G:N2 | 1:A:525:C:N3 | 2.66 | 0.44 |
| 1:A:874:G:N1 | 1:A:875:C:C4 | 2.85 | 0.44 |
| 1:A:1408:A:H2' | 1:A:1409:C:C6 | 2.53 | 0.44 |
| 1:A:1422:G:H1 | 1:A:1478:C:H42 | 1.66 | 0.44 |
| 1:A:1437:C:H2' | 1:A:1438:G:C8 | 2.53 | 0.44 |
| 1:A:1464:G:C6 | 1:A:1465:C:N4 | 2.86 | 0.44 |
| 6:F:50:TYR:CE1 | 18:R:77:GLY:HA2 | 2.52 | 0.44 |
| 25:Z:37:A:C3' | 25:Z:38:A:H8 | 2.31 | 0.44 |
| 25:Z:40:C:H2' | 25:Z:41:C:H6 | 1.80 | 0.44 |
| 25:Z:60:U:H2' | 25:Z:61:C:C5 | 2.53 | 0.44 |
| 25:Z:65:C:H2' | 25:Z:66:C:O4' | 2.18 | 0.44 |
| 1:A:819:A:H5' | 1:A:820:U:H5 | 1.82 | 0.43 |
| 1:A:1257:U:H4' | 1:A:1258:G:O5' | 2.18 | 0.43 |
| 1:A:1422:G:H1 | 1:A:1478:C:N4 | 2.16 | 0.43 |
| 1:A:1504:G:H4' | 1:A:1505:G:O5' | 2.17 | 0.43 |
| 1:A:1507:A:C2 | 1:A:1508:G:C4 | 3.06 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1534:A:N1 | 24:Y:31:U:O4 | 2.51 | 0.43 |
| 4:D:100:ARG:CZ | 4:D:137:SER:HA | 2.48 | 0.43 |
| 6:F:33:TYR:HB2 | 6:F:75:LEU:HD23 | 1.99 | 0.43 |
| 25:Z:19:G:H5' | 25:Z:60:U:O4 | 2.18 | 0.43 |
| 1:A:51:A:H4' | 1:A:52:G:C5' | 2.48 | 0.43 |
| 1:A:130:A:OP1 | 1:A:130:A:C8 | 2.71 | 0.43 |
| 1:A:825:G:C2 | 1:A:826:C:C2 | 3.06 | 0.43 |
| 1:A:1119:C:H2' | 1:A:1120:G:C8 | 2.53 | 0.43 |
| 1:A:1233:G:C2 | 1:A:1234:C:N3 | 2.87 | 0.43 |
| 1:A:1526:G:C2 | 1:A:1527:C:C2 | 3.06 | 0.43 |
| 4:D:31:CYS:C | 4:D:33:MET:H | 2.21 | 0.43 |
| 7:G:69:VAL:HG11 | 7:G:134:ALA:HB1 | 2.00 | 0.43 |
| 12:L:64:TYR:HB3 | 12:L:66:VAL:HG13 | 2.00 | 0.43 |
| 16:P:59:TRP:HA | 16:P:62:VAL:HG22 | 2.00 | 0.43 |
| 22:W:15:GLU:HB3 | 22:W:23:ARG:CB | 2.45 | 0.43 |
| 22:W:70:ARG:HB2 | 22:W:71:LYS:HD2 | 2.00 | 0.43 |
| 25:Z:52:G:N2 | 25:Z:63:G:N3 | 2.65 | 0.43 |
| 1:A:320:C:H2' | 1:A:321:A:C8 | 2.52 | 0.43 |
| 1:A:389:A:H3' | 1:A:390:C:H6 | 1.82 | 0.43 |
| 1:A:774:G:C2 | 1:A:806:C:C2 | 3.05 | 0.43 |
| 1:A:861:G:C2 | 1:A:862:C:C2 | 3.06 | 0.43 |
| 1:A:1014:A:C2 | 19:S:34:TRP:CD1 | 3.06 | 0.43 |
| 1:A:1096:C:H2' | 1:A:1097:C:H6 | 1.81 | 0.43 |
| 1:A:1425:U:H2' | 1:A:1426:C:C6 | 2.53 | 0.43 |
| 2:B:172:ILE:H | 2:B:172:ILE:HG13 | 1.43 | 0.43 |
| 1:A:25:C:H2' | 1:A:26:A:C8 | 2.53 | 0.43 |
| 1:A:198:G:H1 | 1:A:219:C:N4 | 2.16 | 0.43 |
| 1:A:352:C:H4' | 1:A:354:G:OP1 | 2.17 | 0.43 |
| 1:A:769:G:N1 | 1:A:770:C:C4 | 2.86 | 0.43 |
| 1:A:1050:G:C2 | 1:A:1209:C:O2 | 2.71 | 0.43 |
| 1:A:1356:G:C2 | 1:A:1367:C:C2 | 3.07 | 0.43 |
| 6:F:11:ASN:HB2 | 6:F:86:ARG:HH21 | 1.83 | 0.43 |
| 9:I:104:ARG:NH1 | 9:I:106:ALA:HA | 2.33 | 0.43 |
| 25:Z:67:C:H2' | 25:Z:68:C:C6 | 2.54 | 0.43 |
| 1:A:394:G:C2 | 1:A:395:C:C2 | 3.06 | 0.43 |
| 1:A:926:G:N2 | 24:Y:37:U:OP2 | 2.52 | 0.43 |
| 1:A:1063:C:H42 | 1:A:1193:G:H1 | 1.65 | 0.43 |
| 1:A:1241:G:N1 | 1:A:1242:C:C4 | 2.86 | 0.43 |
| 10:J:71:LEU:HD22 | 10:J:71:LEU:HA | 1.71 | 0.43 |
| 16:P:9:PHE:CD1 | 16:P:18:ARG:HG3 | 2.53 | 0.43 |
| 20:T:43:LEU:HD13 | 20:T:52:ALA:HA | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 25:Z:50:U:C2 | 25:Z:51:C:C4 | 3.07 | 0.43 |
| 1:A:34:C:H2' | 1:A:35:G:H8 | 1.83 | 0.43 |
| 1:A:456:C:C4 | 1:A:457:C:N4 | 2.87 | 0.43 |
| 1:A:1022:G:H2' | 1:A:1023:G:H8 | 1.79 | 0.43 |
| 1:A:1053:G:N7 | 1:A:1200:C:H5'' | 2.34 | 0.43 |
| 1:A:1249:C:H4' | 9:I:73:GLN:HE22 | 1.83 | 0.43 |
| 1:A:1286:A:H2' | 1:A:1287:A:H4' | 2.01 | 0.43 |
| 1:A:1365:G:C5 | 1:A:1366:C:C4 | 3.07 | 0.43 |
| 4:D:177:ASP:HB3 | 4:D:182:LYS:HB2 | 2.01 | 0.43 |
| 1:A:384:G:C2 | 1:A:385:C:C2 | 3.07 | 0.43 |
| 1:A:1149:C:H2' | 1:A:1150:U:O4' | 2.19 | 0.43 |
| 1:A:1431:C:H2' | 1:A:1432:G:O4' | 2.18 | 0.43 |
| 1:A:1505:G:H4' | 1:A:1506:U:H5'' | 2.01 | 0.43 |
| 2:B:142:LEU:O | 2:B:146:GLN:HB2 | 2.18 | 0.43 |
| 15:O:3:ILE:HA | 15:O:38:ARG:HH22 | 1.84 | 0.43 |
| 25:Z:37:A:C2' | 25:Z:38:A:C8 | 3.02 | 0.43 |
| 1:A:70:G:C6 | 1:A:100:C:N3 | 2.87 | 0.43 |
| 1:A:504:C:C2 | 1:A:542:G:C2 | 3.07 | 0.43 |
| 1:A:881:G:C6 | 1:A:882:C:C4 | 3.06 | 0.43 |
| 1:A:955:U:H1' | 1:A:1227:A:H61 | 1.84 | 0.43 |
| 1:A:1074:G:C2 | 1:A:1075:C:C2 | 3.07 | 0.43 |
| 1:A:1207:G:C6 | 1:A:1208:C:C4 | 3.07 | 0.43 |
| 3:C:32:LEU:HG | 3:C:32:LEU:H | 1.70 | 0.43 |
| 9:I:89:ASN:HA | 9:I:90:PRO:HD2 | 1.79 | 0.43 |
| 15:O:87:ILE:HG22 | 15:O:88:ARG:H | 1.82 | 0.43 |
| 19:S:11:VAL:HB | 19:S:16:LEU:HD22 | 2.00 | 0.43 |
| 23:X:20:GLY:HA2 | 23:X:59:ILE:HD12 | 2.00 | 0.43 |
| 1:A:235:C:OP1 | 17:Q:70:ARG:NH1 | 2.51 | 0.43 |
| 1:A:524:G:N2 | 1:A:525:C:C2 | 2.87 | 0.43 |
| 1:A:1250:A:H4' | 9:I:67:GLY:HA2 | 2.00 | 0.43 |
| 2:B:124:SER:O | 2:B:127:ILE:HG13 | 2.19 | 0.43 |
| 13:M:18:ALA:O | 13:M:21:TYR:HB2 | 2.19 | 0.43 |
| 25:Z:52:G:C6 | 25:Z:53:G:C5 | 3.07 | 0.43 |
| 1:A:17:U:O2' | 1:A:1079:G:H1' | 2.18 | 0.43 |
| 1:A:101:A:H2' | 1:A:102:G:C8 | 2.48 | 0.43 |
| 1:A:385:C:H2' | 1:A:386:C:O4' | 2.19 | 0.43 |
| 1:A:500:G:H1 | 1:A:545:C:H42 | 1.67 | 0.43 |
| 1:A:876:G:C2 | 1:A:877:C:N3 | 2.87 | 0.43 |
| 1:A:966:G:C2 | 1:A:967:C:C2 | 3.07 | 0.43 |
| 1:A:1077:G:C2 | 1:A:1079:G:H3' | 2.50 | 0.43 |
| 1:A:1135:U:H4' | 1:A:1136:U:H5 | 1.84 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:H:39:LEU:HB3 | 8:H:45:ILE:HG12 | 2.00 | 0.43 |
| 13:M:23:TYR:HB3 | 13:M:67:GLU:HA | 2.00 | 0.43 |
| 14:N:9:LYS:HG3 | 14:N:21:TYR:O | 2.19 | 0.43 |
| 25:Z:17:C:O2 | 25:Z:17:C:H2' | 2.18 | 0.43 |
| 1:A:79:G:C2' | 1:A:80:G:H8 | 2.32 | 0.42 |
| 1:A:102:G:C2 | 1:A:103:C:C2 | 3.07 | 0.42 |
| 1:A:216:G:H2' | 1:A:217:C:C6 | 2.53 | 0.42 |
| 1:A:685:G:H5' | 11:K:12:ARG:HH12 | 1.84 | 0.42 |
| 1:A:1163:C:C2 | 1:A:1174:G:N2 | 2.87 | 0.42 |
| 1:A:1524:C:H5'' | 11:K:120:ARG:NH2 | 2.34 | 0.42 |
| 2:B:18:GLY:HA3 | 2:B:41:ILE:HA | 2.00 | 0.42 |
| 17:Q:26:GLN:HE21 | 17:Q:26:GLN:HB2 | 1.74 | 0.42 |
| 1:A:91:C:C6 | 1:A:91:C:H3' | 2.54 | 0.42 |
| 1:A:164:U:H2' | 1:A:165:C:C6 | 2.53 | 0.42 |
| 1:A:374:A:C6 | 1:A:375:U:C4 | 3.08 | 0.42 |
| 1:A:402:G:C2 | 1:A:403:C:C2 | 3.07 | 0.42 |
| 1:A:550:G:H2' | 1:A:551:U:C6 | 2.54 | 0.42 |
| 1:A:855:G:C6 | 1:A:856:C:C4 | 3.07 | 0.42 |
| 1:A:867:G:N2 | 1:A:868:C:C2 | 2.87 | 0.42 |
| 1:A:903:G:C2 | 1:A:904:C:C2 | 3.07 | 0.42 |
| 1:A:1179:A:OP2 | 9:I:93:ARG:NH2 | 2.51 | 0.42 |
| 1:A:1207:G:C2 | 1:A:1208:C:C2 | 3.07 | 0.42 |
| 1:A:1489:G:C2 | 1:A:1490:C:C2 | 3.06 | 0.42 |
| 3:C:35:GLU:HB3 | 3:C:59:ARG:HH22 | 1.83 | 0.42 |
| 10:J:50:ILE:N | 10:J:60:ARG:HG3 | 2.34 | 0.42 |
| 19:S:5:LEU:HD13 | 19:S:9:VAL:HA | 2.01 | 0.42 |
| 25:Z:18:G:H8 | 25:Z:18:G:O5' | 2.01 | 0.42 |
| 25:Z:55:PSU:H2' | 25:Z:56:C:H3' | 2.00 | 0.42 |
| 1:A:110:C:H2' | 1:A:111:G:O4' | 2.20 | 0.42 |
| 1:A:728:A:H2' | 1:A:729:A:C8 | 2.54 | 0.42 |
| 1:A:926:G:C6 | 1:A:1505:G:C6 | 3.08 | 0.42 |
| 1:A:1151:A:O2' | 1:A:1152:A:H8 | 2.02 | 0.42 |
| 1:A:1231:G:H4' | 9:I:126:SER:HB3 | 2.01 | 0.42 |
| 3:C:150:LYS:HB3 | 3:C:201:TYR:HB2 | 2.01 | 0.42 |
| 1:A:64:G:H4' | 1:A:65:U:H5'' | 2.01 | 0.42 |
| 1:A:342:C:C2 | 1:A:348:G:N2 | 2.87 | 0.42 |
| 1:A:500:G:N2 | 1:A:501:C:C2 | 2.88 | 0.42 |
| 1:A:562:C:H1' | 12:L:15:ARG:HG3 | 2.01 | 0.42 |
| 1:A:682:G:H2' | 1:A:683:G:O4' | 2.19 | 0.42 |
| 1:A:872:A:H2' | 1:A:872:A:N3 | 2.35 | 0.42 |
| 1:A:918:A:H2 | 1:A:1079:G:H21 | 1.50 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:1050:G:C2 | 1:A:1051:C:C2 | 3.07 | 0.42 |
| 1:A:1078:U:O2' | 1:A:1079:G:O4' | 2.36 | 0.42 |
| 1:A:1097:C:H2' | 1:A:1098:C:C6 | 2.55 | 0.42 |
| 1:A:1165:C:H42 | 1:A:1171:G:H1 | 1.68 | 0.42 |
| 1:A:1363(A):A:H1' | 1:A:1365:G:N7 | 2.34 | 0.42 |
| 12:L:93:LEU:HA | 12:L:94:PRO:HD3 | 1.91 | 0.42 |
| 1:A:245:C:C2 | 1:A:284:G:C2 | 3.07 | 0.42 |
| 1:A:309:G:H2' | 1:A:310:G:C8 | 2.53 | 0.42 |
| 1:A:318:G:N2 | 1:A:336:C:C2 | 2.88 | 0.42 |
| 1:A:500:G:C2 | 1:A:501:C:C2 | 3.08 | 0.42 |
| 1:A:734:G:C2 | 1:A:735:C:C2 | 3.07 | 0.42 |
| 1:A:917:G:C6 | 1:A:918:A:C6 | 3.08 | 0.42 |
| 1:A:1088:G:H2' | 1:A:1089:G:O4' | 2.20 | 0.42 |
| 1:A:1220:G:H2' | 1:A:1221:G:H8 | 1.84 | 0.42 |
| 1:A:1230:C:H5' | 25:Z:30:G:H5'' | 2.01 | 0.42 |
| 1:A:1353:G:C6 | 1:A:1354:C:N4 | 2.88 | 0.42 |
| 1:A:1540:U:H3 | 24:Y:25:A:N6 | 2.17 | 0.42 |
| 3:C:177:THR:HG23 | 3:C:180:ALA:HB2 | 2.01 | 0.42 |
| 22:W:40:MET:HA | 22:W:45:ILE:HD12 | 2.01 | 0.42 |
| 25:Z:41:C:H2' | 25:Z:42:G:H8 | 1.82 | 0.42 |
| 1:A:1253:G:C2 | 1:A:1254:C:C2 | 3.08 | 0.42 |
| 1:A:1310:G:C2 | 1:A:1328:C:N3 | 2.88 | 0.42 |
| 10:J:24:VAL:HG12 | 10:J:28:ARG:HE | 1.83 | 0.42 |
| 1:A:198:G:OP2 | 1:A:198:G:C8 | 2.72 | 0.42 |
| 1:A:444:C:H42 | 1:A:490:G:H1 | 1.67 | 0.42 |
| 1:A:742:G:H2' | 1:A:743:U:O4' | 2.20 | 0.42 |
| 1:A:786:G:H2' | 1:A:787:A:O4' | 2.20 | 0.42 |
| 1:A:975:A:C8 | 1:A:975:A:C5' | 3.02 | 0.42 |
| 1:A:1116:C:H2' | 1:A:1117:G:O4' | 2.20 | 0.42 |
| 1:A:1305:G:N2 | 1:A:1331:G:H1' | 2.34 | 0.42 |
| 1:A:1445:C:O2 | 1:A:1458:G:C2 | 2.72 | 0.42 |
| 1:A:1526:G:C6 | 1:A:1527:C:N4 | 2.88 | 0.42 |
| 2:B:233:SER:HA | 2:B:234:PRO:HD3 | 1.77 | 0.42 |
| 9:I:13:ALA:HB2 | 9:I:68:GLY:HA3 | 2.00 | 0.42 |
| 13:M:102:ARG:NH1 | 13:M:104:ARG:HB3 | 2.34 | 0.42 |
| 18:R:47:THR:HG22 | 18:R:83:GLU:H | 1.84 | 0.42 |
| 1:A:42:G:C6 | 1:A:43:C:C4 | 3.07 | 0.42 |
| 1:A:147:G:C2 | 1:A:176:C:C2 | 3.07 | 0.42 |
| 1:A:321:A:H2' | 1:A:322:C:H6 | 1.85 | 0.42 |
| 1:A:416:G:C6 | 1:A:417:C:N3 | 2.88 | 0.42 |
| 1:A:553:A:H1' | 12:L:31:PRO:HG3 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:736:C:H2' | 1:A:737:A:H8 | 1.83 | 0.42 |
| 1:A:800:G:H2' | 1:A:801:U:C6 | 2.54 | 0.42 |
| 1:A:855:G:C2 | 1:A:856:C:C2 | 3.08 | 0.42 |
| 1:A:1074:G:N1 | 1:A:1075:C:C2 | 2.88 | 0.42 |
| 1:A:1084:G:H2' | 1:A:1085:U:C6 | 2.54 | 0.42 |
| 1:A:1144:G:N2 | 1:A:1146:A:H62 | 2.17 | 0.42 |
| 12:L:124:LYS:HA | 12:L:125:PRO:HD2 | 1.82 | 0.42 |
| 1:A:79:G:N1 | 1:A:91:C:C2 | 2.87 | 0.42 |
| 1:A:370:C:O2 | 1:A:482:A:O2' | 2.38 | 0.42 |
| 1:A:409:G:OP1 | 4:D:24:GLU:HB3 | 2.20 | 0.42 |
| 1:A:445:G:H2' | 1:A:446:G:O4' | 2.19 | 0.42 |
| 1:A:689:C:H42 | 1:A:698:G:H1 | 1.67 | 0.42 |
| 1:A:784:C:N3 | 1:A:799:G:C2 | 2.88 | 0.42 |
| 1:A:817:C:C2 | 1:A:819:A:O4' | 2.73 | 0.42 |
| 1:A:895:G:C2 | 1:A:896:C:C2 | 3.07 | 0.42 |
| 1:A:918:A:H2' | 1:A:919:A:O4' | 2.20 | 0.42 |
| 1:A:1080:A:H5'' | 5:E:16:THR:CB | 2.46 | 0.42 |
| 1:A:1371:G:OP1 | 9:I:68:GLY:HA2 | 2.20 | 0.42 |
| 1:A:1538:C:C5 | 18:R:16:PRO:HA | 2.55 | 0.42 |
| 2:B:28:PHE:HA | 2:B:194:PRO:HG3 | 2.02 | 0.42 |
| 3:C:46:GLU:HB2 | 3:C:47:LEU:HD12 | 2.02 | 0.42 |
| 4:D:185:PHE:HZ | 4:D:189:PRO:HD3 | 1.84 | 0.42 |
| 12:L:24:VAL:HG13 | 12:L:98:TYR:HE1 | 1.85 | 0.42 |
| 20:T:73:HIS:HB3 | 20:T:74:LYS:HG3 | 2.01 | 0.42 |
| 1:A:354:G:C6 | 1:A:355:C:N4 | 2.88 | 0.42 |
| 1:A:356:A:H2' | 1:A:357:G:O4' | 2.20 | 0.42 |
| 1:A:376:G:H2' | 1:A:377:G:C8 | 2.50 | 0.42 |
| 1:A:505:G:H2' | 1:A:506:G:C8 | 2.53 | 0.42 |
| 1:A:1064:G:N2 | 1:A:1190:G:C2' | 2.79 | 0.42 |
| 1:A:1106:G:C2 | 1:A:1107:C:N3 | 2.88 | 0.42 |
| 10:J:75:ILE:H | 10:J:75:ILE:HG13 | 1.55 | 0.42 |
| 15:O:35:ARG:HB3 | 15:O:59:MET:SD | 2.60 | 0.42 |
| 17:Q:29:HIS:HE1 | 17:Q:31:LEU:HB3 | 1.85 | 0.42 |
| 25:Z:60:U:H2' | 25:Z:61:C:H5 | 1.85 | 0.42 |
| 1:A:43:C:H2' | 1:A:44:G:C8 | 2.55 | 0.41 |
| 1:A:81:U:H1' | 1:A:88:A:H62 | 1.86 | 0.41 |
| 1:A:104:G:C2 | 1:A:105:G:C5 | 3.08 | 0.41 |
| 1:A:319:G:C2 | 1:A:320:C:C2 | 3.07 | 0.41 |
| 1:A:338:A:H2' | 1:A:339:C:O4' | 2.20 | 0.41 |
| 1:A:402:G:C6 | 1:A:403:C:C4 | 3.07 | 0.41 |
| 1:A:407:G:C2 | 1:A:436:C:C2 | 3.08 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:524:G:N1 | 1:A:525:C:N4 | 2.68 | 0.41 |
| 1:A:903:G:C6 | 1:A:904:C:C4 | 3.08 | 0.41 |
| 1:A:949:A:O2' | 1:A:971:G:O6 | 2.25 | 0.41 |
| 1:A:959:A:H1' | 1:A:985:C:H1' | 2.01 | 0.41 |
| 1:A:1116:C:H3' | 1:A:1117:G:H5'' | 2.02 | 0.41 |
| 1:A:1241:G:C6 | 1:A:1242:C:N4 | 2.88 | 0.41 |
| 1:A:1314:C:OP2 | 19:S:6:LYS:HB3 | 2.19 | 0.41 |
| 1:A:1387:G:C2 | 1:A:1388:C:C2 | 3.08 | 0.41 |
| 1:A:1423:G:C2 | 1:A:1424:C:C2 | 3.08 | 0.41 |
| 1:A:1488:G:H2' | 1:A:1489:G:C8 | 2.54 | 0.41 |
| 6:F:15:ASP:OD1 | 6:F:18:GLN:HB2 | 2.20 | 0.41 |
| 11:K:27:ASN:HB2 | 11:K:55:LYS:HB3 | 2.01 | 0.41 |
| 13:M:84:ILE:HG22 | 19:S:66:MET:HE3 | 2.02 | 0.41 |
| 19:S:12:ASP:OD1 | 19:S:37:ARG:HB2 | 2.20 | 0.41 |
| 25:Z:18:G:O5' | 25:Z:18:G:C8 | 2.73 | 0.41 |
| 1:A:28:G:H2' | 1:A:29:G:O4' | 2.20 | 0.41 |
| 1:A:258:G:C2 | 1:A:269:C:C2 | 3.09 | 0.41 |
| 1:A:295:C:C4 | 1:A:296:U:C4 | 3.08 | 0.41 |
| 1:A:333:G:C2 | 1:A:334:C:C2 | 3.08 | 0.41 |
| 1:A:344:A:H5'' | 1:A:345:C:H5 | 1.85 | 0.41 |
| 1:A:662:G:C6 | 1:A:744:C:N3 | 2.88 | 0.41 |
| 1:A:681:C:N4 | 1:A:709:G:H1 | 2.18 | 0.41 |
| 1:A:825:G:C6 | 1:A:826:C:C4 | 3.08 | 0.41 |
| 1:A:1040:U:H2' | 1:A:1041:A:C8 | 2.55 | 0.41 |
| 2:B:19:HIS:CD2 | 2:B:20:GLU:HG2 | 2.55 | 0.41 |
| 3:C:30:ARG:HB2 | 3:C:30:ARG:NH2 | 2.23 | 0.41 |
| 18:R:19:LYS:HB3 | 18:R:20:ALA:H | 1.69 | 0.41 |
| 25:Z:22:G:C2 | 25:Z:23:C:C2 | 3.08 | 0.41 |
| 1:A:310:G:H5' | 16:P:31:LYS:HB2 | 2.01 | 0.41 |
| 1:A:321:A:H2' | 1:A:322:C:C6 | 2.54 | 0.41 |
| 1:A:414:A:H2' | 1:A:415:A:O4' | 2.19 | 0.41 |
| 1:A:453:A:H2' | 1:A:454:C:C6 | 2.55 | 0.41 |
| 1:A:576:G:H3' | 1:A:577:G:C5' | 2.49 | 0.41 |
| 1:A:646:U:H2' | 1:A:647:C:C6 | 2.55 | 0.41 |
| 1:A:794:A:H2' | 1:A:795:C:C6 | 2.55 | 0.41 |
| 1:A:981:U:O4 | 1:A:1223:C:N4 | 2.53 | 0.41 |
| 1:A:1074:G:H1 | 1:A:1083:U:H3 | 1.69 | 0.41 |
| 1:A:1078:U:H5 | 1:A:1079:G:C6 | 2.39 | 0.41 |
| 1:A:1166:G:N2 | 1:A:1169:A:H3' | 2.35 | 0.41 |
| 1:A:1190:G:H5' | 3:C:176:HIS:HE1 | 1.84 | 0.41 |
| 1:A:1371:G:O3' | 9:I:69:GLY:HA3 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1375:A:N3 | 1:A:1375:A:H2' | 2.34 | 0.41 |
| 3:C:3:ASN:HB2 | 3:C:4:LYS:H | 1.72 | 0.41 |
| 4:D:3:ARG:HH21 | 4:D:71:SER:HB2 | 1.85 | 0.41 |
| 6:F:12:PRO:HG3 | 6:F:57:GLN:O | 2.20 | 0.41 |
| 8:H:82:HIS:CE1 | 8:H:84:ARG:HB2 | 2.55 | 0.41 |
| 25:Z:36:U:C2 | 25:Z:37:A:C8 | 3.09 | 0.41 |
| 1:A:77:G:H3' | 1:A:77:G:C8 | 2.56 | 0.41 |
| 1:A:157:G:C6 | 1:A:165:C:N3 | 2.89 | 0.41 |
| 1:A:446:G:N2 | 1:A:489:C:C2 | 2.88 | 0.41 |
| 1:A:519:C:H2' | 1:A:520:A:C8 | 2.54 | 0.41 |
| 1:A:660:G:H2' | 1:A:661:G:O4' | 2.20 | 0.41 |
| 1:A:876:G:C2 | 1:A:877:C:C2 | 3.08 | 0.41 |
| 1:A:1424:C:N4 | 1:A:1476:G:H1 | 2.18 | 0.41 |
| 2:B:54:THR:HG23 | 2:B:199:TYR:HB3 | 2.02 | 0.41 |
| 4:D:8:VAL:HG11 | 4:D:21:LEU:HB2 | 2.03 | 0.41 |
| 11:K:110:ASP:HB3 | 18:R:85:LEU:HB3 | 2.02 | 0.41 |
| 13:M:84:ILE:HG22 | 19:S:66:MET:CE | 2.50 | 0.41 |
| 16:P:59:TRP:CA | 16:P:62:VAL:HG22 | 2.50 | 0.41 |
| 20:T:36:LEU:HD23 | 20:T:36:LEU:HA | 1.90 | 0.41 |
| 25:Z:22:G:N1 | 25:Z:23:C:C4 | 2.89 | 0.41 |
| 1:A:15:G:O4' | 1:A:1396:A:O2' | 2.39 | 0.41 |
| 1:A:317:G:H2' | 1:A:318:G:O4' | 2.20 | 0.41 |
| 1:A:518:C:H4' | 1:A:519:C:O5' | 2.21 | 0.41 |
| 1:A:830:G:N2 | 1:A:857:C:C2 | 2.89 | 0.41 |
| 1:A:947:G:C6 | 1:A:948:C:C4 | 3.08 | 0.41 |
| 1:A:1157:A:H4' | 1:A:1158:C:O5' | 2.19 | 0.41 |
| 4:D:175:SER:HB3 | 4:D:186:LEU:HD11 | 2.02 | 0.41 |
| 8:H:119:LEU:HD13 | 8:H:124:ALA:HB2 | 2.03 | 0.41 |
| 1:A:41:G:H2' | 1:A:42:G:C8 | 2.56 | 0.41 |
| 1:A:42:G:C2 | 1:A:43:C:C2 | 3.08 | 0.41 |
| 1:A:289:G:C2 | 1:A:290:C:C2 | 3.08 | 0.41 |
| 1:A:363:A:C6 | 12:L:31:PRO:HD2 | 2.56 | 0.41 |
| 1:A:551:U:H2' | 1:A:552:U:H6 | 1.82 | 0.41 |
| 1:A:832:C:O2 | 1:A:855:G:C2 | 2.74 | 0.41 |
| 1:A:910:C:H5'' | 12:L:97:ARG:HH21 | 1.86 | 0.41 |
| 1:A:1171:G:N1 | 1:A:1172:C:C4 | 2.89 | 0.41 |
| 2:B:184:VAL:N | 2:B:198:ASP:HB2 | 2.30 | 0.41 |
| 3:C:108:ASN:HA | 3:C:109:PRO:HD2 | 1.77 | 0.41 |
| 8:H:29:SER:HB3 | 8:H:32:LYS:HB2 | 2.02 | 0.41 |
| 17:Q:62:SER:OG | 17:Q:72:ARG:HG3 | 2.20 | 0.41 |
| 21:V:10:ARG:HA | 21:V:13:ILE:HD12 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 23:X:100:GLN:HA | 23:X:103:LEU:HD23 | 2.02 | 0.41 |
| 1:A:299:G:C6 | 1:A:300:A:C6 | 3.09 | 0.41 |
| 1:A:336:C:H2' | 1:A:337:C:C6 | 2.56 | 0.41 |
| 1:A:456:C:C2 | 1:A:476:G:C2 | 3.09 | 0.41 |
| 1:A:671:G:C6 | 1:A:736:C:N4 | 2.88 | 0.41 |
| 1:A:763:G:C6 | 1:A:764:C:C4 | 3.09 | 0.41 |
| 1:A:872:A:C8 | 1:A:874:G:C8 | 3.09 | 0.41 |
| 1:A:1292:U:H2' | 1:A:1293:G:C8 | 2.56 | 0.41 |
| 1:A:1368:G:N1 | 1:A:1369:C:C4 | 2.88 | 0.41 |
| 3:C:6:HIS:CG | 14:N:49:HIS:HB3 | 2.56 | 0.41 |
| 8:H:83:ILE:HG13 | 8:H:137:VAL:HG22 | 2.03 | 0.41 |
| 9:I:74:ILE:HA | 9:I:77:ILE:HD12 | 2.02 | 0.41 |
| 1:A:146:G:C2 | 1:A:177:C:C2 | 3.09 | 0.41 |
| 1:A:217:C:H2' | 1:A:218:C:H6 | 1.85 | 0.41 |
| 1:A:319:G:C6 | 1:A:320:C:C4 | 3.09 | 0.41 |
| 1:A:741:G:H2' | 1:A:742:G:O4' | 2.21 | 0.41 |
| 1:A:863:U:H2' | 1:A:865:A:OP2 | 2.21 | 0.41 |
| 1:A:1068:G:C2 | 1:A:1069:C:C2 | 3.09 | 0.41 |
| 1:A:1235:U:H2' | 1:A:1236:A:O4' | 2.20 | 0.41 |
| 1:A:1253:G:C6 | 1:A:1254:C:C4 | 3.08 | 0.41 |
| 2:B:167:PRO:HG2 | 2:B:192:SER:OG | 2.20 | 0.41 |
| 4:D:50:ARG:HA | 4:D:51:PRO:HD3 | 1.87 | 0.41 |
| 4:D:135:LEU:HA | 4:D:136:PRO:HD3 | 1.92 | 0.41 |
| 4:D:196:LEU:HA | 4:D:197:PRO:HD3 | 1.89 | 0.41 |
| 5:E:69:VAL:HG21 | 5:E:113:ALA:HB1 | 2.02 | 0.41 |
| 10:J:50:ILE:HG13 | 10:J:60:ARG:CD | 2.35 | 0.41 |
| 11:K:18:ARG:HA | 11:K:81:ASP:H | 1.84 | 0.41 |
| 15:O:39:LEU:HD13 | 15:O:56:LEU:HA | 2.03 | 0.41 |
| 25:Z:60:U:H3' | 25:Z:61:C:C5 | 2.55 | 0.41 |
| 1:A:77:G:C8 | 1:A:77:G:C3' | 3.04 | 0.41 |
| 1:A:119:A:H2' | 1:A:240:C:H41 | 1.85 | 0.41 |
| 1:A:392:G:P | 16:P:8:ARG:HH22 | 2.44 | 0.41 |
| 1:A:433:C:H2' | 1:A:434:U:C6 | 2.56 | 0.41 |
| 1:A:542:G:C6 | 1:A:543:C:N4 | 2.89 | 0.41 |
| 1:A:544:G:C2 | 1:A:545:C:C2 | 3.09 | 0.41 |
| 1:A:579:G:H1 | 1:A:762:C:H42 | 1.68 | 0.41 |
| 1:A:643:C:H2' | 1:A:644:G:C8 | 2.55 | 0.41 |
| 1:A:691:G:H3' | 11:K:26:ASN:ND2 | 2.35 | 0.41 |
| 1:A:725:G:C2 | 1:A:726:C:C2 | 3.09 | 0.41 |
| 1:A:832:C:C2 | 1:A:855:G:C2 | 3.09 | 0.41 |
| 1:A:837:G:H2' | 1:A:838:G:O4' | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:862:C:H2' | 1:A:863:U:O4' | 2.20 | 0.41 |
| 1:A:895:G:C6 | 1:A:896:C:C4 | 3.09 | 0.41 |
| 1:A:918:A:C6 | 1:A:919:A:C6 | 3.09 | 0.41 |
| 1:A:999:C:H2' | 1:A:1000:U:H5' | 2.03 | 0.41 |
| 1:A:1000:U:C5 | 1:A:1001:A:C8 | 3.08 | 0.41 |
| 1:A:1028:C:H2' | 1:A:1029:C:C4' | 2.51 | 0.41 |
| 1:A:1075:C:H5' | 1:A:1101:A:N6 | 2.36 | 0.41 |
| 1:A:1076:C:H2' | 1:A:1077:G:H8 | 1.83 | 0.41 |
| 1:A:1080:A:P | 5:E:14:ARG:HH22 | 2.43 | 0.41 |
| 1:A:1255:G:O2' | 1:A:1258:G:H1' | 2.21 | 0.41 |
| 1:A:1292:U:H2' | 1:A:1293:G:H8 | 1.86 | 0.41 |
| 1:A:1307:U:H2' | 1:A:1308:U:C6 | 2.55 | 0.41 |
| 1:A:1369:C:OP1 | 14:N:61:TRP:NE1 | 2.51 | 0.41 |
| 2:B:12:GLU:HG3 | 2:B:15:VAL:HB | 2.02 | 0.41 |
| 4:D:98:GLU:HG3 | 4:D:103:ASN:ND2 | 2.36 | 0.41 |
| 6:F:69:GLU:H | 6:F:69:GLU:HG3 | 1.57 | 0.41 |
| 7:G:69:VAL:O | 7:G:71:PRO:HD3 | 2.21 | 0.41 |
| 7:G:149:ARG:HG2 | 7:G:152:ALA:HB2 | 2.03 | 0.41 |
| 11:K:121:PRO:HB2 | 11:K:125:PHE:HB2 | 2.02 | 0.41 |
| 17:Q:61:GLU:HA | 17:Q:71:PHE:CD1 | 2.56 | 0.41 |
| 18:R:44:LEU:HD12 | 18:R:79:LEU:HD22 | 2.03 | 0.41 |
| 20:T:53:LEU:HD22 | 20:T:102:GLY:HA3 | 2.01 | 0.41 |
| 20:T:89:ARG:HD2 | 20:T:104:LEU:HD22 | 2.03 | 0.41 |
| 1:A:13:U:H3' | 1:A:14:U:H6 | 1.86 | 0.41 |
| 1:A:324:G:N2 | 1:A:326:G:H3' | 2.36 | 0.41 |
| 1:A:625:G:H2' | 1:A:626:U:C6 | 2.56 | 0.41 |
| 1:A:896:C:H2' | 1:A:897:C:O4' | 2.21 | 0.41 |
| 1:A:919:A:N3 | 1:A:1080:A:C2 | 2.89 | 0.41 |
| 1:A:975:A:H5'' | 1:A:975:A:H8 | 1.85 | 0.41 |
| 1:A:1348:U:H2' | 1:A:1349:A:H8 | 1.86 | 0.41 |
| 1:A:1492:A:H2' | 22:W:19:ASN:HA | 2.02 | 0.41 |
| 7:G:113:GLU:HG2 | 7:G:119:ARG:HG2 | 2.03 | 0.41 |
| 25:Z:51:C:H42 | 25:Z:63:G:H1 | 1.68 | 0.41 |
| 1:A:44:G:OP2 | 16:P:12:LYS:HE3 | 2.20 | 0.40 |
| 1:A:527:G:N2 | 1:A:528:C:C2 | 2.89 | 0.40 |
| 1:A:942:G:C6 | 1:A:1342:C:N3 | 2.89 | 0.40 |
| 1:A:956:U:H2' | 1:A:957:U:O4' | 2.22 | 0.40 |
| 1:A:1050:G:N1 | 1:A:1051:C:C4 | 2.89 | 0.40 |
| 1:A:1314:C:N4 | 19:S:4:SER:HB2 | 2.35 | 0.40 |
| 1:A:1345:U:C4 | 1:A:1375:A:N6 | 2.60 | 0.40 |
| 1:A:1411:C:H4' | 12:L:43:VAL:HG11 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1423:G:C6 | 1:A:1424:C:C4 | 3.10 | 0.40 |
| 13:M:96:LEU:HD23 | 13:M:97:PRO:HD2 | 2.03 | 0.40 |
| 1:A:289:G:C6 | 1:A:290:C:C4 | 3.09 | 0.40 |
| 1:A:373:A:H2' | 1:A:374:A:H8 | 1.86 | 0.40 |
| 1:A:552:U:H2' | 1:A:553:A:H8 | 1.86 | 0.40 |
| 1:A:751:U:H2' | 1:A:752:G:O4' | 2.21 | 0.40 |
| 1:A:861:G:C6 | 1:A:862:C:C4 | 3.09 | 0.40 |
| 1:A:921:U:H2' | 1:A:922:G:O4' | 2.20 | 0.40 |
| 1:A:986:A:H2' | 1:A:987:G:O4' | 2.20 | 0.40 |
| 1:A:988:G:C2 | 1:A:989:C:C2 | 3.08 | 0.40 |
| 1:A:1060:C:P | 14:N:45:ARG:HH22 | 2.44 | 0.40 |
| 1:A:1077:G:N1 | 1:A:1080:A:OP2 | 2.51 | 0.40 |
| 1:A:1312:G:N2 | 1:A:1326:C:C2 | 2.89 | 0.40 |
| 1:A:1371:G:H2' | 1:A:1372:U:H6 | 1.85 | 0.40 |
| 1:A:1528:U:H1' | 1:A:1530:G:H5' | 2.03 | 0.40 |
| 7:G:106:GLN:O | 7:G:110:GLN:HG2 | 2.21 | 0.40 |
| 11:K:34:ASP:OD2 | 11:K:38:ASN:HB2 | 2.20 | 0.40 |
| 12:L:60:LEU:HD21 | 12:L:66:VAL:HG22 | 2.02 | 0.40 |
| 1:A:174:C:H2' | 1:A:175:C:C6 | 2.56 | 0.40 |
| 1:A:394:G:C6 | 1:A:395:C:C4 | 3.09 | 0.40 |
| 1:A:677:U:H3 | 1:A:713:G:H1 | 1.68 | 0.40 |
| 1:A:678:U:H2' | 1:A:679:C:H6 | 1.82 | 0.40 |
| 1:A:731:G:C6 | 1:A:732:C:C4 | 3.10 | 0.40 |
| 1:A:1129:C:H1' | 1:A:1132:C:H5 | 1.86 | 0.40 |
| 1:A:1409:C:H2' | 1:A:1410:G:C8 | 2.55 | 0.40 |
| 1:A:1431:C:H42 | 1:A:1469:G:H1 | 1.69 | 0.40 |
| 1:A:1512:U:H2' | 1:A:1513:A:C8 | 2.57 | 0.40 |
| 6:F:50:TYR:HE1 | 18:R:77:GLY:HA2 | 1.86 | 0.40 |
| 25:Z:2:G:C2 | 25:Z:3:C:C2 | 3.10 | 0.40 |
| 25:Z:31:G:H2' | 25:Z:32:OMC:C6 | 2.55 | 0.40 |
| 1:A:105:G:C6 | 1:A:106:C:C4 | 3.09 | 0.40 |
| 1:A:671:G:H2' | 1:A:672:U:O4' | 2.21 | 0.40 |
| 1:A:1351:U:H2' | 1:A:1352:C:H6 | 1.85 | 0.40 |
| 1:A:1361:G:C2 | 1:A:1362:C:O2 | 2.74 | 0.40 |
| 1:A:1440:C:N4 | 1:A:1461:G:H1 | 2.19 | 0.40 |
| 1:A:1461:G:H2' | 1:A:1462:G:C8 | 2.56 | 0.40 |
| 3:C:39:ILE:O | 3:C:43:LEU:HG | 2.21 | 0.40 |
| 3:C:82:GLU:O | 3:C:85:ARG:HB3 | 2.20 | 0.40 |
| 4:D:171:GLY:C | 4:D:173:TRP:H | 2.25 | 0.40 |
| 5:E:80:ILE:HD12 | 5:E:91:LEU:HB2 | 2.03 | 0.40 |
| 13:M:22:ILE:HG22 | 13:M:24:GLY:H | 1.86 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 25:Z:18:G:C4 | 25:Z:57:A:C6 | 3.09 | 0.40 |
| 1:A:16:A:C2 | 1:A:17:U:C6 | 3.09 | 0.40 |
| 1:A:123:C:H5'' | 1:A:311:C:O2' | 2.21 | 0.40 |
| 1:A:137:C:C2 | 1:A:227:G:C2 | 3.09 | 0.40 |
| 1:A:200:G:C6 | 1:A:201:C:N3 | 2.90 | 0.40 |
| 1:A:328:C:H4' | 1:A:329:A:H5' | 2.03 | 0.40 |
| 1:A:542:G:C2 | 1:A:543:C:C2 | 3.10 | 0.40 |
| 1:A:629:G:H2' | 1:A:630:G:O4' | 2.21 | 0.40 |
| 1:A:902:G:H2' | 1:A:903:G:H8 | 1.86 | 0.40 |
| 1:A:968:A:C8 | 1:A:1062:U:H4' | 2.56 | 0.40 |
| 7:G:96:GLN:HA | 7:G:99:LEU:HD12 | 2.03 | 0.40 |
| 11:K:123:LYS:HA | 11:K:126:ARG:HG3 | 2.03 | 0.40 |
| 13:M:45:VAL:HA | 13:M:48:LEU:HD12 | 2.04 | 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 PDB entries followed by that with respect to all EM entries.

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%) | 195 (84%) | 24 (10%) | 13 (6%) | 1 | 15 |
| 3 | C | 204/239 (85%) | 177 (87%) | 18 (9%) | 9 (4%) | 2 | 18 |
| 4 | D | 206/209 (99%) | 191 (93%) | 12 (6%) | 3 (2%) | 8 | 39 |
| 5 | E | 148/162 (91%) | 140 (95%) | 8 (5%) | 0 | 100 | 100 |
| 6 | F | 99/101 (98%) | 94 (95%) | 5 (5%) | 0 | 100 | 100 |
| 7 | G | 153/156 (98%) | 144 (94%) | 7 (5%) | 2 (1%) | 10 | 42 |
| 8 | H | 136/138 (99%) | 129 (95%) | 6 (4%) | 1 (1%) | 19 | 56 |
| 9 | I | 125/128 (98%) | 107 (86%) | 15 (12%) | 3 (2%) | 5 | 28 |
| 10 | J | 96/105 (91%) | 72 (75%) | 16 (17%) | 8 (8%) | 0 | 10 |
| 11 | K | 117/129 (91%) | 99 (85%) | 13 (11%) | 5 (4%) | 2 | 18 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 12 | L | 122/132 (92%) | 101 (83%) | 17 (14%) | 4 (3%) | 3 | 21 |
| 13 | M | 119/126 (94%) | 102 (86%) | 16 (13%) | 1 (1%) | 16 | 54 |
| 14 | N | 58/61 (95%) | 51 (88%) | 5 (9%) | 2 (3%) | 3 | 21 |
| 15 | O | 86/89 (97%) | 84 (98%) | 1 (1%) | 1 (1%) | 11 | 44 |
| 16 | P | 81/88 (92%) | 73 (90%) | 7 (9%) | 1 (1%) | 11 | 44 |
| 17 | Q | 97/105 (92%) | 88 (91%) | 6 (6%) | 3 (3%) | 3 | 22 |
| 18 | R | 71/88 (81%) | 66 (93%) | 4 (6%) | 1 (1%) | 9 | 40 |
| 19 | S | 80/93 (86%) | 66 (82%) | 11 (14%) | 3 (4%) | 2 | 19 |
| 20 | T | 97/106 (92%) | 80 (82%) | 12 (12%) | 5 (5%) | 1 | 16 |
| 21 | V | 22/27 (82%) | 21 (96%) | 1 (4%) | 0 | 100 | 100 |
| 22 | W | 69/72 (96%) | 58 (84%) | 7 (10%) | 4 (6%) | 1 | 14 |
| 23 | X | 166/171 (97%) | 150 (90%) | 13 (8%) | 3 (2%) | 7 | 34 |
| All | All | 2584/2781 (93%) | 2288 (88%) | 224 (9%) | 72 (3%) | 6 | 24 |

All (72) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 21 | ARG |
| 2 | B | 24 | TRP |
| 9 | I | 119 | ALA |
| 11 | K | 101 | SER |
| 12 | L | 79 | GLU |
| 18 | R | 87 | ARG |
| 20 | T | 94 | ALA |
| 23 | X | 8 | ASN |
| 23 | X | 54 | PRO |
| 2 | B | 17 | PHE |
| 2 | B | 207 | ALA |
| 3 | C | 61 | ALA |
| 3 | C | 154 | SER |
| 3 | C | 179 | ARG |
| 7 | G | 7 | ALA |
| 9 | I | 56 | LEU |
| 10 | J | 55 | LYS |
| 16 | P | 81 | ARG |
| 19 | S | 30 | LEU |
| 20 | T | 13 | LEU |
| 20 | T | 49 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 20 | GLU |
| 2 | B | 99 | GLY |
| 2 | B | 204 | ASN |
| 2 | B | 228 | GLY |
| 3 | C | 14 | ILE |
| 10 | J | 30 | SER |
| 10 | J | 34 | VAL |
| 10 | J | 35 | SER |
| 10 | J | 90 | LEU |
| 11 | K | 126 | ARG |
| 12 | L | 27 | LEU |
| 14 | N | 31 | ARG |
| 15 | O | 88 | ARG |
| 17 | Q | 68 | ARG |
| 19 | S | 6 | LYS |
| 22 | W | 2 | LYS |
| 2 | B | 95 | GLN |
| 3 | C | 4 | LYS |
| 3 | C | 81 | GLY |
| 3 | C | 108 | ASN |
| 3 | C | 168 | ALA |
| 4 | D | 5 | ILE |
| 4 | D | 172 | PRO |
| 9 | I | 58 | HIS |
| 14 | N | 23 | ARG |
| 17 | Q | 99 | SER |
| 19 | S | 71 | LEU |
| 20 | T | 97 | ALA |
| 22 | W | 44 | TYR |
| 2 | B | 229 | VAL |
| 10 | J | 39 | PRO |
| 10 | J | 54 | PHE |
| 11 | K | 12 | ARG |
| 11 | K | 13 | GLN |
| 12 | L | 45 | PRO |
| 17 | Q | 80 | GLY |
| 20 | T | 9 | ASN |
| 23 | X | 73 | GLU |
| 2 | B | 130 | ARG |
| 7 | G | 55 | GLY |
| 10 | J | 40 | LEU |
| 12 | L | 51 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | M | 6 | GLY |
| 22 | W | 45 | ILE |
| 3 | C | 205 | GLY |
| 4 | D | 142 | PRO |
| 8 | H | 5 | PRO |
| 11 | K | 90 | GLY |
| 2 | B | 125 | PRO |
| 2 | B | 208 | ILE |
| 22 | W | 50 | GLY |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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%) | 166 (82%) | 36 (18%) | 1 | 9 |
| 3 | C | 160/188 (85%) | 142 (89%) | 18 (11%) | 4 | 18 |
| 4 | D | 180/181 (99%) | 148 (82%) | 32 (18%) | 1 | 9 |
| 5 | E | 115/123 (94%) | 93 (81%) | 22 (19%) | 1 | 7 |
| 6 | F | 90/90 (100%) | 75 (83%) | 15 (17%) | 2 | 10 |
| 7 | G | 126/127 (99%) | 121 (96%) | 5 (4%) | 27 | 48 |
| 8 | H | 119/119 (100%) | 98 (82%) | 21 (18%) | 1 | 9 |
| 9 | I | 98/99 (99%) | 84 (86%) | 14 (14%) | 2 | 14 |
| 10 | J | 87/92 (95%) | 76 (87%) | 11 (13%) | 3 | 16 |
| 11 | K | 90/99 (91%) | 73 (81%) | 17 (19%) | 1 | 7 |
| 12 | L | 104/109 (95%) | 89 (86%) | 15 (14%) | 2 | 13 |
| 13 | M | 97/101 (96%) | 84 (87%) | 13 (13%) | 3 | 15 |
| 14 | N | 49/50 (98%) | 43 (88%) | 6 (12%) | 4 | 17 |
| 15 | O | 79/80 (99%) | 64 (81%) | 15 (19%) | 1 | 7 |
| 16 | P | 72/74 (97%) | 59 (82%) | 13 (18%) | 1 | 9 |
| 17 | Q | 94/97 (97%) | 80 (85%) | 14 (15%) | 2 | 13 |
| 18 | R | 64/77 (83%) | 52 (81%) | 12 (19%) | 1 | 8 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|-----|
| 19 | S | 71/80 (89%) | 58 (82%) | 13 (18%) | 1 | 8 |
| 20 | T | 76/82 (93%) | 60 (79%) | 16 (21%) | 1 | 5 |
| 21 | V | 19/22 (86%) | 19 (100%) | 0 | 100 | 100 |
| 22 | W | 62/63 (98%) | 52 (84%) | 10 (16%) | 2 | 11 |
| 23 | X | 145/150 (97%) | 126 (87%) | 19 (13%) | 3 | 15 |
| All | All | 2199/2323 (95%) | 1862 (85%) | 337 (15%) | 4 | 12 |

All (337) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 11 | LEU |
| 2 | B | 21 | ARG |
| 2 | B | 23 | ARG |
| 2 | B | 24 | TRP |
| 2 | B | 25 | ASN |
| 2 | B | 44 | LEU |
| 2 | B | 48 | MET |
| 2 | B | 51 | LEU |
| 2 | B | 59 | GLU |
| 2 | B | 61 | LEU |
| 2 | B | 67 | THR |
| 2 | B | 96 | ARG |
| 2 | B | 97 | TRP |
| 2 | B | 103 | THR |
| 2 | B | 107 | THR |
| 2 | B | 108 | ILE |
| 2 | B | 111 | ARG |
| 2 | B | 136 | VAL |
| 2 | B | 137 | ARG |
| 2 | B | 144 | ARG |
| 2 | B | 154 | LEU |
| 2 | B | 163 | PHE |
| 2 | B | 165 | VAL |
| 2 | B | 172 | ILE |
| 2 | B | 178 | ARG |
| 2 | B | 179 | LYS |
| 2 | B | 187 | LEU |
| 2 | B | 198 | ASP |
| 2 | B | 204 | ASN |
| 2 | B | 208 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 213 | LEU |
| 2 | B | 215 | LEU |
| 2 | B | 216 | SER |
| 2 | B | 236 | TYR |
| 2 | B | 238 | LEU |
| 2 | B | 240 | GLN |
| 3 | C | 3 | ASN |
| 3 | C | 14 | ILE |
| 3 | C | 17 | ASP |
| 3 | C | 26 | LYS |
| 3 | C | 30 | ARG |
| 3 | C | 37 | GLN |
| 3 | C | 56 | ASP |
| 3 | C | 79 | ARG |
| 3 | C | 88 | ARG |
| 3 | C | 90 | GLU |
| 3 | C | 91 | LEU |
| 3 | C | 99 | VAL |
| 3 | C | 162 | GLN |
| 3 | C | 167 | TRP |
| 3 | C | 172 | ARG |
| 3 | C | 188 | LEU |
| 3 | C | 191 | THR |
| 3 | C | 204 | LEU |
| 4 | D | 3 | ARG |
| 4 | D | 14 | ARG |
| 4 | D | 34 | GLU |
| 4 | D | 35 | ARG |
| 4 | D | 42 | GLN |
| 4 | D | 50 | ARG |
| 4 | D | 53 | ASP |
| 4 | D | 59 | ARG |
| 4 | D | 64 | LEU |
| 4 | D | 66 | ARG |
| 4 | D | 73 | ARG |
| 4 | D | 76 | ARG |
| 4 | D | 81 | GLU |
| 4 | D | 83 | SER |
| 4 | D | 118 | ARG |
| 4 | D | 122 | ARG |
| 4 | D | 131 | ARG |
| 4 | D | 132 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | D | 134 | ASP |
| 4 | D | 135 | LEU |
| 4 | D | 141 | ARG |
| 4 | D | 150 | GLU |
| 4 | D | 152 | SER |
| 4 | D | 159 | ARG |
| 4 | D | 162 | LEU |
| 4 | D | 176 | LEU |
| 4 | D | 186 | LEU |
| 4 | D | 187 | ARG |
| 4 | D | 190 | ASP |
| 4 | D | 192 | GLU |
| 4 | D | 194 | LEU |
| 4 | D | 207 | TYR |
| 5 | E | 6 | PHE |
| 5 | E | 12 | LEU |
| 5 | E | 13 | ILE |
| 5 | E | 15 | ARG |
| 5 | E | 24 | ARG |
| 5 | E | 41 | VAL |
| 5 | E | 43 | LEU |
| 5 | E | 53 | LEU |
| 5 | E | 56 | GLN |
| 5 | E | 76 | ILE |
| 5 | E | 80 | ILE |
| 5 | E | 87 | SER |
| 5 | E | 98 | THR |
| 5 | E | 112 | LEU |
| 5 | E | 118 | ILE |
| 5 | E | 119 | LEU |
| 5 | E | 137 | GLU |
| 5 | E | 141 | GLN |
| 5 | E | 144 | THR |
| 5 | E | 147 | ASP |
| 5 | E | 148 | VAL |
| 5 | E | 150 | ARG |
| 6 | F | 2 | ARG |
| 6 | F | 21 | LEU |
| 6 | F | 36 | ARG |
| 6 | F | 45 | LEU |
| 6 | F | 46 | ARG |
| 6 | F | 47 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | F | 54 | LYS |
| 6 | F | 65 | VAL |
| 6 | F | 69 | GLU |
| 6 | F | 71 | ARG |
| 6 | F | 73 | ASN |
| 6 | F | 75 | LEU |
| 6 | F | 78 | GLU |
| 6 | F | 89 | MET |
| 6 | F | 98 | LEU |
| 7 | G | 8 | GLU |
| 7 | G | 11 | GLN |
| 7 | G | 38 | LEU |
| 7 | G | 72 | ARG |
| 7 | G | 126 | ASP |
| 8 | H | 11 | THR |
| 8 | H | 18 | ARG |
| 8 | H | 21 | LYS |
| 8 | H | 22 | GLU |
| 8 | H | 24 | THR |
| 8 | H | 36 | LEU |
| 8 | H | 39 | LEU |
| 8 | H | 50 | ARG |
| 8 | H | 52 | ASP |
| 8 | H | 54 | ASP |
| 8 | H | 59 | LEU |
| 8 | H | 69 | ARG |
| 8 | H | 85 | ARG |
| 8 | H | 99 | GLU |
| 8 | H | 102 | ARG |
| 8 | H | 105 | ARG |
| 8 | H | 112 | LEU |
| 8 | H | 115 | SER |
| 8 | H | 127 | LEU |
| 8 | H | 135 | CYS |
| 8 | H | 136 | GLU |
| 9 | I | 2 | GLU |
| 9 | I | 3 | GLN |
| 9 | I | 12 | GLU |
| 9 | I | 14 | VAL |
| 9 | I | 34 | ASN |
| 9 | I | 35 | GLU |
| 9 | I | 38 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | I | 71 | SER |
| 9 | I | 79 | LEU |
| 9 | I | 102 | LEU |
| 9 | I | 111 | ARG |
| 9 | I | 112 | LYS |
| 9 | I | 118 | LYS |
| 9 | I | 121 | ARG |
| 10 | J | 17 | ASP |
| 10 | J | 49 | VAL |
| 10 | J | 60 | ARG |
| 10 | J | 71 | LEU |
| 10 | J | 75 | ILE |
| 10 | J | 79 | ARG |
| 10 | J | 82 | ILE |
| 10 | J | 86 | MET |
| 10 | J | 87 | THR |
| 10 | J | 89 | ASP |
| 10 | J | 92 | THR |
| 11 | K | 11 | LYS |
| 11 | K | 14 | VAL |
| 11 | K | 16 | SER |
| 11 | K | 18 | ARG |
| 11 | K | 41 | THR |
| 11 | K | 57 | THR |
| 11 | K | 62 | GLN |
| 11 | K | 84 | VAL |
| 11 | K | 91 | ARG |
| 11 | K | 92 | GLU |
| 11 | K | 93 | GLN |
| 11 | K | 96 | ARG |
| 11 | K | 98 | LEU |
| 11 | K | 108 | ILE |
| 11 | K | 120 | ARG |
| 11 | K | 126 | ARG |
| 11 | K | 129 | SER |
| 12 | L | 6 | THR |
| 12 | L | 13 | LYS |
| 12 | L | 15 | ARG |
| 12 | L | 33 | ARG |
| 12 | L | 37 | CYS |
| 12 | L | 41 | ARG |
| 12 | L | 42 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | L | 53 | ARG |
| 12 | L | 59 | ARG |
| 12 | L | 77 | LEU |
| 12 | L | 78 | GLN |
| 12 | L | 97 | ARG |
| 12 | L | 104 | VAL |
| 12 | L | 111 | LYS |
| 12 | L | 126 | LYS |
| 13 | M | 12 | ASN |
| 13 | M | 16 | ASP |
| 13 | M | 31 | LYS |
| 13 | M | 32 | GLU |
| 13 | M | 35 | GLU |
| 13 | M | 44 | ARG |
| 13 | M | 56 | LEU |
| 13 | M | 80 | ARG |
| 13 | M | 81 | LEU |
| 13 | M | 84 | ILE |
| 13 | M | 96 | LEU |
| 13 | M | 102 | ARG |
| 13 | M | 121 | LYS |
| 14 | N | 16 | PHE |
| 14 | N | 17 | LYS |
| 14 | N | 22 | THR |
| 14 | N | 41 | ARG |
| 14 | N | 44 | LEU |
| 14 | N | 61 | TRP |
| 15 | O | 3 | ILE |
| 15 | O | 5 | LYS |
| 15 | O | 8 | LYS |
| 15 | O | 25 | THR |
| 15 | O | 31 | LEU |
| 15 | O | 39 | LEU |
| 15 | O | 41 | GLU |
| 15 | O | 43 | LEU |
| 15 | O | 52 | SER |
| 15 | O | 54 | ARG |
| 15 | O | 56 | LEU |
| 15 | O | 63 | ARG |
| 15 | O | 64 | ARG |
| 15 | O | 70 | LEU |
| 15 | O | 81 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16 | P | 8 | ARG |
| 16 | P | 26 | ARG |
| 16 | P | 28 | ARG |
| 16 | P | 44 | THR |
| 16 | P | 53 | VAL |
| 16 | P | 60 | LEU |
| 16 | P | 67 | THR |
| 16 | P | 68 | ASP |
| 16 | P | 69 | THR |
| 16 | P | 71 | ARG |
| 16 | P | 72 | ARG |
| 16 | P | 79 | VAL |
| 16 | P | 83 | GLU |
| 17 | Q | 24 | GLU |
| 17 | Q | 26 | GLN |
| 17 | Q | 34 | LYS |
| 17 | Q | 53 | LEU |
| 17 | Q | 57 | VAL |
| 17 | Q | 58 | GLU |
| 17 | Q | 68 | ARG |
| 17 | Q | 70 | ARG |
| 17 | Q | 72 | ARG |
| 17 | Q | 81 | ARG |
| 17 | Q | 91 | ARG |
| 17 | Q | 92 | ARG |
| 17 | Q | 98 | LEU |
| 17 | Q | 100 | LYS |
| 18 | R | 17 | SER |
| 18 | R | 21 | LYS |
| 18 | R | 23 | LYS |
| 18 | R | 25 | THR |
| 18 | R | 39 | VAL |
| 18 | R | 47 | THR |
| 18 | R | 53 | ARG |
| 18 | R | 55 | ARG |
| 18 | R | 75 | ILE |
| 18 | R | 81 | PHE |
| 18 | R | 82 | THR |
| 18 | R | 87 | ARG |
| 19 | S | 6 | LYS |
| 19 | S | 7 | LYS |
| 19 | S | 29 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19 | S | 30 | LEU |
| 19 | S | 37 | ARG |
| 19 | S | 39 | THR |
| 19 | S | 41 | VAL |
| 19 | S | 49 | ILE |
| 19 | S | 53 | ASN |
| 19 | S | 63 | THR |
| 19 | S | 66 | MET |
| 19 | S | 79 | THR |
| 19 | S | 80 | TYR |
| 20 | T | 8 | ARG |
| 20 | T | 10 | LEU |
| 20 | T | 13 | LEU |
| 20 | T | 17 | ARG |
| 20 | T | 19 | SER |
| 20 | T | 25 | ARG |
| 20 | T | 39 | LYS |
| 20 | T | 42 | GLN |
| 20 | T | 45 | GLN |
| 20 | T | 53 | LEU |
| 20 | T | 55 | ILE |
| 20 | T | 56 | MET |
| 20 | T | 64 | ASP |
| 20 | T | 68 | LYS |
| 20 | T | 73 | HIS |
| 20 | T | 84 | LEU |
| 22 | W | 2 | LYS |
| 22 | W | 6 | THR |
| 22 | W | 14 | THR |
| 22 | W | 21 | THR |
| 22 | W | 32 | ILE |
| 22 | W | 33 | LEU |
| 22 | W | 46 | ARG |
| 22 | W | 58 | THR |
| 22 | W | 63 | THR |
| 22 | W | 71 | LYS |
| 23 | X | 7 | THR |
| 23 | X | 12 | ARG |
| 23 | X | 31 | THR |
| 23 | X | 35 | LEU |
| 23 | X | 64 | LYS |
| 23 | X | 67 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23 | X | 87 | SER |
| 23 | X | 91 | ARG |
| 23 | X | 92 | VAL |
| 23 | X | 95 | ASP |
| 23 | X | 98 | ASP |
| 23 | X | 103 | LEU |
| 23 | X | 118 | VAL |
| 23 | X | 125 | ARG |
| 23 | X | 147 | LEU |
| 23 | X | 151 | GLU |
| 23 | X | 162 | ASN |
| 23 | X | 164 | LEU |
| 23 | X | 168 | VAL |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 19 | HIS |
| 2 | B | 104 | ASN |
| 3 | C | 6 | HIS |
| 3 | C | 69 | HIS |
| 3 | C | 108 | ASN |
| 3 | C | 136 | GLN |
| 3 | C | 176 | HIS |
| 4 | D | 45 | GLN |
| 4 | D | 62 | GLN |
| 4 | D | 161 | ASN |
| 5 | E | 20 | GLN |
| 7 | G | 28 | ASN |
| 7 | G | 37 | ASN |
| 9 | I | 73 | GLN |
| 9 | I | 124 | GLN |
| 10 | J | 76 | ASN |
| 10 | J | 78 | ASN |
| 11 | K | 26 | ASN |
| 11 | K | 38 | ASN |
| 12 | L | 75 | HIS |
| 13 | M | 92 | HIS |
| 17 | Q | 26 | GLN |
| 19 | S | 53 | ASN |
| 19 | S | 56 | GLN |
| 19 | S | 83 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23 | X | 100 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | A | 1505/1522 (98%) | 420 (27%) | 103 (6%) |
| 24 | Y | 15/42 (35%) | 7 (46%) | 0 |
| 25 | Z | 74/77 (96%) | 33 (44%) | 9 (12%) |
| All | All | 1594/1641 (97%) | 460 (28%) | 112 (7%) |

All (460) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 8 | A |
| 1 | A | 9 | G |
| 1 | A | 13 | U |
| 1 | A | 19 | C |
| 1 | A | 22 | G |
| 1 | A | 29 | G |
| 1 | A | 31 | G |
| 1 | A | 32 | A |
| 1 | A | 39 | G |
| 1 | A | 43 | C |
| 1 | A | 44 | G |
| 1 | A | 47 | C |
| 1 | A | 48 | C |
| 1 | A | 49 | U |
| 1 | A | 50 | A |
| 1 | A | 51 | A |
| 1 | A | 52 | G |
| 1 | A | 54 | C |
| 1 | A | 58 | C |
| 1 | A | 60 | A |
| 1 | A | 61 | G |
| 1 | A | 66 | G |
| 1 | A | 68 | G |
| 1 | A | 72 | C |
| 1 | A | 76 | C |
| 1 | A | 77 | G |
| 1 | A | 78 | G |
| 1 | A | 79 | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | A | 81 | U |
| 1 | A | 91 | C |
| 1 | A | 97 | G |
| 1 | A | 100 | C |
| 1 | A | 108 | G |
| 1 | A | 115 | G |
| 1 | A | 116 | A |
| 1 | A | 120 | A |
| 1 | A | 121 | C |
| 1 | A | 122 | G |
| 1 | A | 129(A) | G |
| 1 | A | 130 | A |
| 1 | A | 131 | C |
| 1 | A | 144 | G |
| 1 | A | 151 | A |
| 1 | A | 157 | G |
| 1 | A | 163 | C |
| 1 | A | 181 | G |
| 1 | A | 182 | U |
| 1 | A | 189(E) | U |
| 1 | A | 189(F) | U |
| 1 | A | 189(G) | G |
| 1 | A | 189(H) | G |
| 1 | A | 195 | A |
| 1 | A | 197 | A |
| 1 | A | 198 | G |
| 1 | A | 199 | G |
| 1 | A | 201 | C |
| 1 | A | 203 | U |
| 1 | A | 217 | C |
| 1 | A | 220 | G |
| 1 | A | 244 | U |
| 1 | A | 247 | G |
| 1 | A | 251 | G |
| 1 | A | 253 | U |
| 1 | A | 266 | G |
| 1 | A | 267 | C |
| 1 | A | 280 | C |
| 1 | A | 281 | G |
| 1 | A | 282 | A |
| 1 | A | 283 | C |
| 1 | A | 288 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 289 | G |
| 1 | A | 291 | C |
| 1 | A | 298 | A |
| 1 | A | 301 | G |
| 1 | A | 306 | G |
| 1 | A | 313 | A |
| 1 | A | 315 | A |
| 1 | A | 316 | G |
| 1 | A | 325 | A |
| 1 | A | 328 | C |
| 1 | A | 329 | A |
| 1 | A | 330 | C |
| 1 | A | 332 | G |
| 1 | A | 342 | C |
| 1 | A | 344 | A |
| 1 | A | 345 | C |
| 1 | A | 347 | G |
| 1 | A | 350 | G |
| 1 | A | 351 | G |
| 1 | A | 352 | C |
| 1 | A | 353 | A |
| 1 | A | 354 | G |
| 1 | A | 366 | C |
| 1 | A | 367 | U |
| 1 | A | 372 | C |
| 1 | A | 373 | A |
| 1 | A | 375 | U |
| 1 | A | 378 | G |
| 1 | A | 384 | G |
| 1 | A | 388 | G |
| 1 | A | 390 | C |
| 1 | A | 392 | G |
| 1 | A | 393 | A |
| 1 | A | 397 | A |
| 1 | A | 398 | C |
| 1 | A | 406 | G |
| 1 | A | 409 | G |
| 1 | A | 412 | A |
| 1 | A | 413 | G |
| 1 | A | 414 | A |
| 1 | A | 419 | C |
| 1 | A | 421 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 422 | C |
| 1 | A | 423 | G |
| 1 | A | 428 | G |
| 1 | A | 429 | U |
| 1 | A | 430 | A |
| 1 | A | 439 | A |
| 1 | A | 441 | A |
| 1 | A | 450 | G |
| 1 | A | 452 | A |
| 1 | A | 453 | A |
| 1 | A | 454 | C |
| 1 | A | 455 | C |
| 1 | A | 470 | C |
| 1 | A | 481 | G |
| 1 | A | 484 | G |
| 1 | A | 485 | G |
| 1 | A | 495 | A |
| 1 | A | 496 | A |
| 1 | A | 498 | U |
| 1 | A | 509 | A |
| 1 | A | 510 | A |
| 1 | A | 511 | C |
| 1 | A | 518 | C |
| 1 | A | 519 | C |
| 1 | A | 521 | G |
| 1 | A | 524 | G |
| 1 | A | 527 | G |
| 1 | A | 528 | C |
| 1 | A | 529 | G |
| 1 | A | 531 | U |
| 1 | A | 532 | A |
| 1 | A | 534 | U |
| 1 | A | 535 | A |
| 1 | A | 540 | G |
| 1 | A | 543 | C |
| 1 | A | 545 | C |
| 1 | A | 547 | A |
| 1 | A | 550 | G |
| 1 | A | 559 | A |
| 1 | A | 560 | U |
| 1 | A | 561 | U |
| 1 | A | 562 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 564 | C |
| 1 | A | 568 | G |
| 1 | A | 572 | A |
| 1 | A | 573 | A |
| 1 | A | 574 | A |
| 1 | A | 575 | G |
| 1 | A | 576 | G |
| 1 | A | 577 | G |
| 1 | A | 596 | C |
| 1 | A | 607 | A |
| 1 | A | 619 | U |
| 1 | A | 641 | U |
| 1 | A | 642 | A |
| 1 | A | 653 | A |
| 1 | A | 665 | A |
| 1 | A | 666 | G |
| 1 | A | 671 | G |
| 1 | A | 687 | A |
| 1 | A | 688 | G |
| 1 | A | 693 | G |
| 1 | A | 701 | C |
| 1 | A | 702 | A |
| 1 | A | 703 | G |
| 1 | A | 713 | G |
| 1 | A | 716 | A |
| 1 | A | 717 | C |
| 1 | A | 721 | G |
| 1 | A | 723 | U |
| 1 | A | 724 | G |
| 1 | A | 728 | A |
| 1 | A | 731 | G |
| 1 | A | 744 | C |
| 1 | A | 748 | C |
| 1 | A | 749 | C |
| 1 | A | 755 | G |
| 1 | A | 760 | G |
| 1 | A | 774 | G |
| 1 | A | 785 | G |
| 1 | A | 787 | A |
| 1 | A | 789 | U |
| 1 | A | 792 | A |
| 1 | A | 793 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 794 | A |
| 1 | A | 796 | C |
| 1 | A | 799 | G |
| 1 | A | 804 | U |
| 1 | A | 809 | G |
| 1 | A | 811 | C |
| 1 | A | 812 | C |
| 1 | A | 815 | A |
| 1 | A | 817 | C |
| 1 | A | 818 | G |
| 1 | A | 819 | A |
| 1 | A | 821 | G |
| 1 | A | 828 | A |
| 1 | A | 839 | U |
| 1 | A | 841 | U |
| 1 | A | 853 | G |
| 1 | A | 855 | G |
| 1 | A | 864 | A |
| 1 | A | 870 | U |
| 1 | A | 871 | U |
| 1 | A | 873 | A |
| 1 | A | 876 | G |
| 1 | A | 882 | C |
| 1 | A | 885 | G |
| 1 | A | 900 | A |
| 1 | A | 902 | G |
| 1 | A | 919 | A |
| 1 | A | 922 | G |
| 1 | A | 926 | G |
| 1 | A | 927 | G |
| 1 | A | 931 | C |
| 1 | A | 932 | C |
| 1 | A | 933 | G |
| 1 | A | 934 | C |
| 1 | A | 935 | A |
| 1 | A | 938 | A |
| 1 | A | 945 | G |
| 1 | A | 951 | G |
| 1 | A | 955 | U |
| 1 | A | 956 | U |
| 1 | A | 957 | U |
| 1 | A | 958 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 959 | A |
| 1 | A | 961 | U |
| 1 | A | 965 | A |
| 1 | A | 966 | G |
| 1 | A | 969 | A |
| 1 | A | 971 | G |
| 1 | A | 974 | A |
| 1 | A | 975 | A |
| 1 | A | 976 | G |
| 1 | A | 977 | A |
| 1 | A | 985 | C |
| 1 | A | 986 | A |
| 1 | A | 991 | U |
| 1 | A | 992 | U |
| 1 | A | 993 | G |
| 1 | A | 994 | A |
| 1 | A | 998 | G |
| 1 | A | 1000 | U |
| 1 | A | 1001 | A |
| 1 | A | 1002 | G |
| 1 | A | 1005 | A |
| 1 | A | 1014 | A |
| 1 | A | 1015 | A |
| 1 | A | 1016 | A |
| 1 | A | 1017 | G |
| 1 | A | 1023 | G |
| 1 | A | 1025 | U |
| 1 | A | 1026 | G |
| 1 | A | 1028 | C |
| 1 | A | 1029 | C |
| 1 | A | 1030 | C |
| 1 | A | 1031 | G |
| 1 | A | 1036 | G |
| 1 | A | 1045 | C |
| 1 | A | 1050 | G |
| 1 | A | 1051 | C |
| 1 | A | 1053 | G |
| 1 | A | 1054 | C |
| 1 | A | 1056 | U |
| 1 | A | 1060 | C |
| 1 | A | 1064 | G |
| 1 | A | 1065 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1066 | C |
| 1 | A | 1067 | A |
| 1 | A | 1075 | C |
| 1 | A | 1076 | C |
| 1 | A | 1078 | U |
| 1 | A | 1079 | G |
| 1 | A | 1085 | U |
| 1 | A | 1086 | U |
| 1 | A | 1094 | G |
| 1 | A | 1095 | U |
| 1 | A | 1101 | A |
| 1 | A | 1102 | A |
| 1 | A | 1104 | G |
| 1 | A | 1117 | G |
| 1 | A | 1124 | G |
| 1 | A | 1125 | U |
| 1 | A | 1127 | G |
| 1 | A | 1128 | C |
| 1 | A | 1129 | C |
| 1 | A | 1130 | A |
| 1 | A | 1131 | G |
| 1 | A | 1134 | G |
| 1 | A | 1135 | U |
| 1 | A | 1136 | U |
| 1 | A | 1137 | C |
| 1 | A | 1138 | G |
| 1 | A | 1139 | G |
| 1 | A | 1140 | C |
| 1 | A | 1145 | C |
| 1 | A | 1146 | A |
| 1 | A | 1152 | A |
| 1 | A | 1157 | A |
| 1 | A | 1159 | U |
| 1 | A | 1160 | G |
| 1 | A | 1171 | G |
| 1 | A | 1183 | A |
| 1 | A | 1184 | G |
| 1 | A | 1187 | G |
| 1 | A | 1190 | G |
| 1 | A | 1191 | A |
| 1 | A | 1195 | C |
| 1 | A | 1196 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1197 | G |
| 1 | A | 1200 | C |
| 1 | A | 1201 | A |
| 1 | A | 1202 | G |
| 1 | A | 1210 | C |
| 1 | A | 1212 | U |
| 1 | A | 1213 | A |
| 1 | A | 1215 | G |
| 1 | A | 1222 | G |
| 1 | A | 1223 | C |
| 1 | A | 1224 | G |
| 1 | A | 1225 | A |
| 1 | A | 1226 | C |
| 1 | A | 1227 | A |
| 1 | A | 1236 | A |
| 1 | A | 1238 | A |
| 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 | 1282 | C |
| 1 | A | 1285 | A |
| 1 | A | 1286 | A |
| 1 | A | 1287 | A |
| 1 | A | 1290 | G |
| 1 | A | 1299 | A |
| 1 | A | 1300 | G |
| 1 | A | 1301 | U |
| 1 | A | 1302 | U |
| 1 | A | 1303 | C |
| 1 | A | 1305 | G |
| 1 | A | 1312 | G |
| 1 | A | 1315 | U |
| 1 | A | 1317 | C |
| 1 | A | 1318 | A |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | A | 1319 | A |
| 1 | A | 1320 | C |
| 1 | A | 1322 | C |
| 1 | A | 1323 | G |
| 1 | A | 1328 | C |
| 1 | A | 1336 | C |
| 1 | A | 1346 | A |
| 1 | A | 1347 | G |
| 1 | A | 1353 | G |
| 1 | A | 1357 | A |
| 1 | A | 1363 | C |
| 1 | A | 1363(A) | A |
| 1 | A | 1364 | U |
| 1 | A | 1367 | C |
| 1 | A | 1370 | G |
| 1 | A | 1379 | G |
| 1 | A | 1380 | U |
| 1 | A | 1381 | U |
| 1 | A | 1394 | A |
| 1 | A | 1398 | A |
| 1 | A | 1412 | C |
| 1 | A | 1419 | G |
| 1 | A | 1423 | G |
| 1 | A | 1440 | C |
| 1 | A | 1442 | G |
| 1 | A | 1443 | G |
| 1 | A | 1447 | A |
| 1 | A | 1452 | C |
| 1 | A | 1456 | G |
| 1 | A | 1457 | G |
| 1 | A | 1488 | G |
| 1 | A | 1492 | A |
| 1 | A | 1493 | A |
| 1 | A | 1494 | G |
| 1 | A | 1499 | A |
| 1 | A | 1502 | A |
| 1 | A | 1503 | A |
| 1 | A | 1504 | G |
| 1 | A | 1505 | G |
| 1 | A | 1506 | U |
| 1 | A | 1507 | A |
| 1 | A | 1517 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 1 | A | 1520 | G |
| 1 | A | 1528 | U |
| 1 | A | 1529 | G |
| 1 | A | 1530 | G |
| 1 | A | 1531 | A |
| 1 | A | 1532 | U |
| 1 | A | 1533 | C |
| 1 | A | 1534 | A |
| 1 | A | 1535 | C |
| 1 | A | 1536 | C |
| 1 | A | 1537 | U |
| 1 | A | 1539 | C |
| 1 | A | 1540 | U |
| 1 | A | 1541 | U |
| 24 | Y | 28 | A |
| 24 | Y | 30 | G |
| 24 | Y | 31 | U |
| 24 | Y | 32 | A |
| 24 | Y | 37 | U |
| 24 | Y | 38 | G |
| 24 | Y | 39 | U |
| 25 | Z | 3 | C |
| 25 | Z | 6 | G |
| 25 | Z | 7 | G |
| 25 | Z | 8 | 4SU |
| 25 | Z | 9 | G |
| 25 | Z | 13 | C |
| 25 | Z | 16 | C |
| 25 | Z | 17 | C |
| 25 | Z | 17(A) | U |
| 25 | Z | 18 | G |
| 25 | Z | 19 | G |
| 25 | Z | 20 | U |
| 25 | Z | 26 | G |
| 25 | Z | 34 | C |
| 25 | Z | 36 | U |
| 25 | Z | 37 | A |
| 25 | Z | 40 | C |
| 25 | Z | 42 | G |
| 25 | Z | 43 | A |
| 25 | Z | 47 | U |
| 25 | Z | 48 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | Z | 50 | U |
| 25 | Z | 51 | C |
| 25 | Z | 53 | G |
| 25 | Z | 55 | PSU |
| 25 | Z | 56 | C |
| 25 | Z | 59 | A |
| 25 | Z | 66 | C |
| 25 | Z | 67 | C |
| 25 | Z | 68 | C |
| 25 | Z | 69 | C |
| 25 | Z | 70 | G |
| 25 | Z | 76 | A |

All (112) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | A | 7 | G |
| 1 | A | 30 | U |
| 1 | A | 31 | G |
| 1 | A | 48 | C |
| 1 | A | 49 | U |
| 1 | A | 51 | A |
| 1 | A | 60 | A |
| 1 | A | 115 | G |
| 1 | A | 119 | A |
| 1 | A | 129(A) | G |
| 1 | A | 181 | G |
| 1 | A | 189(F) | U |
| 1 | A | 197 | A |
| 1 | A | 202 | U |
| 1 | A | 243 | A |
| 1 | A | 250 | A |
| 1 | A | 266 | G |
| 1 | A | 279 | A |
| 1 | A | 281 | G |
| 1 | A | 305 | G |
| 1 | A | 315 | A |
| 1 | A | 328 | C |
| 1 | A | 329 | A |
| 1 | A | 344 | A |
| 1 | A | 351 | G |
| 1 | A | 372 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 389 | A |
| 1 | A | 428 | G |
| 1 | A | 429 | U |
| 1 | A | 484 | G |
| 1 | A | 495 | A |
| 1 | A | 496 | A |
| 1 | A | 508 | C |
| 1 | A | 509 | A |
| 1 | A | 518 | C |
| 1 | A | 531 | U |
| 1 | A | 535 | A |
| 1 | A | 559 | A |
| 1 | A | 560 | U |
| 1 | A | 561 | U |
| 1 | A | 575 | G |
| 1 | A | 576 | G |
| 1 | A | 595 | G |
| 1 | A | 641 | U |
| 1 | A | 687 | A |
| 1 | A | 701 | C |
| 1 | A | 703 | G |
| 1 | A | 717 | C |
| 1 | A | 748 | C |
| 1 | A | 792 | A |
| 1 | A | 864 | A |
| 1 | A | 872 | A |
| 1 | A | 884 | U |
| 1 | A | 931 | C |
| 1 | A | 933 | G |
| 1 | A | 934 | C |
| 1 | A | 956 | U |
| 1 | A | 958 | A |
| 1 | A | 960 | U |
| 1 | A | 965 | A |
| 1 | A | 968 | A |
| 1 | A | 975 | A |
| 1 | A | 992 | U |
| 1 | A | 993 | G |
| 1 | A | 1000 | U |
| 1 | A | 1065 | U |
| 1 | A | 1078 | U |
| 1 | A | 1101 | A |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | A | 1139 | G |
| 1 | A | 1145 | C |
| 1 | A | 1182 | G |
| 1 | A | 1190 | G |
| 1 | A | 1196 | U |
| 1 | A | 1201 | A |
| 1 | A | 1212 | U |
| 1 | A | 1214 | C |
| 1 | A | 1222 | G |
| 1 | A | 1224 | G |
| 1 | A | 1225 | A |
| 1 | A | 1226 | C |
| 1 | A | 1239 | A |
| 1 | A | 1257 | U |
| 1 | A | 1278 | U |
| 1 | A | 1279 | A |
| 1 | A | 1285 | A |
| 1 | A | 1299 | A |
| 1 | A | 1300 | G |
| 1 | A | 1301 | U |
| 1 | A | 1318 | A |
| 1 | A | 1331 | G |
| 1 | A | 1346 | A |
| 1 | A | 1363(A) | A |
| 1 | A | 1380 | U |
| 1 | A | 1415 | G |
| 1 | A | 1442(B) | A |
| 1 | A | 1447 | A |
| 1 | A | 1493 | A |
| 1 | A | 1498 | U |
| 1 | A | 1504 | G |
| 1 | A | 1531 | A |
| 1 | A | 1533 | C |
| 1 | A | 1534 | A |
| 1 | A | 1536 | C |
| 25 | Z | 17 | C |
| 25 | Z | 36 | U |
| 25 | Z | 47 | U |
| 25 | Z | 50 | U |
| 25 | Z | 51 | C |
| 25 | Z | 55 | PSU |
| 25 | Z | 58 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | Z | 60 | U |
| 25 | Z | 71 | C |

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | # $ Z > 2$ | Counts | RMSZ | # $ Z > 2$ |
| 25 | PSU | Z | 55 | 25 | 18,21,22 | 1.49 | 1 (5%) | 22,30,33 | 1.92 | 5 (22%) |
| 25 | OMC | Z | 32 | 25 | 19,22,23 | 0.94 | 1 (5%) | 26,31,34 | 1.27 | 3 (11%) |
| 25 | 5MU | Z | 54 | 25 | 19,22,23 | 1.57 | 3 (15%) | 28,32,35 | 1.96 | 7 (25%) |
| 25 | G7M | Z | 46 | 25 | 20,26,27 | 2.82 | 4 (20%) | 17,39,42 | 1.31 | 2 (11%) |
| 25 | 4SU | Z | 8 | 25 | 18,21,22 | 1.76 | 4 (22%) | 26,30,33 | 1.96 | 6 (23%) |

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 |
|-----|------|-------|-----|------|---------|-----------|---------|
| 25 | PSU | Z | 55 | 25 | - | 2/7/25/26 | 0/2/2/2 |
| 25 | OMC | Z | 32 | 25 | - | 0/9/27/28 | 0/2/2/2 |
| 25 | 5MU | Z | 54 | 25 | - | 0/7/25/26 | 0/2/2/2 |
| 25 | G7M | Z | 46 | 25 | - | 0/3/25/26 | 0/3/3/3 |
| 25 | 4SU | Z | 8 | 25 | - | 0/7/25/26 | 0/2/2/2 |

All (13) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 25 | Z | 46 | G7M | C8-N9 | 8.16 | 1.48 | 1.33 |
| 25 | Z | 46 | G7M | C8-N7 | 7.36 | 1.46 | 1.33 |
| 25 | Z | 55 | PSU | C6-C5 | 4.89 | 1.41 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25 | Z | 46 | G7M | C5-C4 | 4.87 | 1.48 | 1.39 |
| 25 | Z | 8 | 4SU | C4-S4 | -4.41 | 1.60 | 1.68 |
| 25 | Z | 54 | 5MU | C6-C5 | 4.30 | 1.41 | 1.34 |
| 25 | Z | 8 | 4SU | C4-N3 | -3.23 | 1.34 | 1.37 |
| 25 | Z | 54 | 5MU | C4-C5 | 3.08 | 1.49 | 1.44 |
| 25 | Z | 8 | 4SU | C2-N1 | 2.85 | 1.43 | 1.38 |
| 25 | Z | 54 | 5MU | C4-N3 | -2.50 | 1.34 | 1.38 |
| 25 | Z | 8 | 4SU | C6-C5 | 2.29 | 1.40 | 1.35 |
| 25 | Z | 46 | G7M | O4'-C1' | 2.19 | 1.44 | 1.41 |
| 25 | Z | 32 | OMC | C6-C5 | 2.17 | 1.40 | 1.35 |

All (23) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25 | Z | 54 | 5MU | N3-C2-N1 | 5.86 | 122.67 | 114.89 |
| 25 | Z | 55 | PSU | N1-C2-N3 | 5.52 | 121.38 | 115.13 |
| 25 | Z | 8 | 4SU | C4-N3-C2 | -5.07 | 122.42 | 127.34 |
| 25 | Z | 8 | 4SU | C5-C4-N3 | 4.93 | 119.27 | 114.69 |
| 25 | Z | 8 | 4SU | N3-C2-N1 | 4.07 | 120.30 | 114.89 |
| 25 | Z | 55 | PSU | O2-C2-N1 | -3.74 | 118.68 | 122.79 |
| 25 | Z | 54 | 5MU | C4-N3-C2 | -3.67 | 122.60 | 127.35 |
| 25 | Z | 54 | 5MU | O2-C2-N1 | -3.65 | 117.93 | 122.79 |
| 25 | Z | 54 | 5MU | C6-N1-C2 | -3.18 | 118.08 | 121.30 |
| 25 | Z | 32 | OMC | O2-C2-N3 | -3.17 | 117.17 | 122.33 |
| 25 | Z | 55 | PSU | C6-C5-C4 | -3.16 | 115.99 | 118.20 |
| 25 | Z | 55 | PSU | C4-N3-C2 | -3.04 | 121.96 | 126.34 |
| 25 | Z | 54 | 5MU | C1'-N1-C6 | 2.60 | 125.45 | 121.12 |
| 25 | Z | 46 | G7M | CN7-N7-C8 | -2.60 | 112.94 | 125.43 |
| 25 | Z | 8 | 4SU | C6-N1-C2 | -2.57 | 117.70 | 120.99 |
| 25 | Z | 32 | OMC | O4'-C1'-N1 | 2.39 | 113.83 | 108.36 |
| 25 | Z | 54 | 5MU | C5-C4-N3 | 2.32 | 117.29 | 115.31 |
| 25 | Z | 8 | 4SU | C5-C4-S4 | -2.31 | 121.49 | 124.47 |
| 25 | Z | 8 | 4SU | O2-C2-N3 | -2.11 | 117.58 | 121.50 |
| 25 | Z | 55 | PSU | O2'-C2'-C1' | -2.09 | 106.26 | 111.23 |
| 25 | Z | 54 | 5MU | C5-C6-N1 | -2.09 | 121.19 | 123.34 |
| 25 | Z | 46 | G7M | O4'-C1'-C2' | -2.07 | 103.90 | 106.93 |
| 25 | Z | 32 | OMC | O3'-C3'-C2' | 2.04 | 116.96 | 111.17 |

There are no chirality outliers.

All (2) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|---------------|
| 25 | Z | 55 | PSU | C4'-C5'-O5'-P |
| 25 | Z | 55 | PSU | O4'-C1'-C5-C4 |

There are no ring outliers.

3 monomers are involved in 8 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 25 | Z | 55 | PSU | 5 | 0 |
| 25 | Z | 32 | OMC | 2 | 0 |
| 25 | Z | 54 | 5MU | 2 | 0 |

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1 | A | 7 |
| 25 | Z | 2 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | A | 841:U | O3' | 848:C | P | 5.77 |
| 1 | A | 84:U | O3' | 88:A | P | 5.45 |
| 1 | A | 93:G | O3' | 96:U | P | 5.02 |
| 1 | A | 204:U | O3' | 216:G | P | 3.93 |
| 1 | A | 1442(A):G | O3' | 1442(B):A | P | 3.82 |
| 1 | Z | 21:A | O3' | 22:G | P | 3.81 |
| 1 | A | 1389:C | O3' | 1390:U | P | 3.33 |
| 1 | Z | 14:A | O3' | 15:G | P | 3.31 |
| 1 | A | 927:G | O3' | 928:G | P | 3.06 |

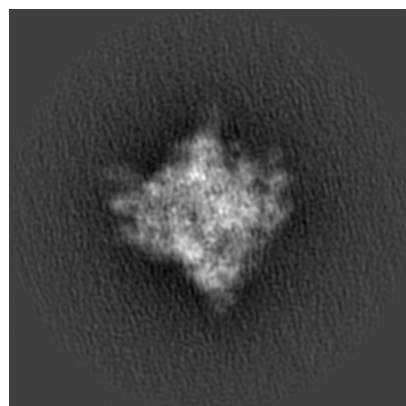
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4077. These allow visual inspection of the internal detail of the map and identification of artifacts.

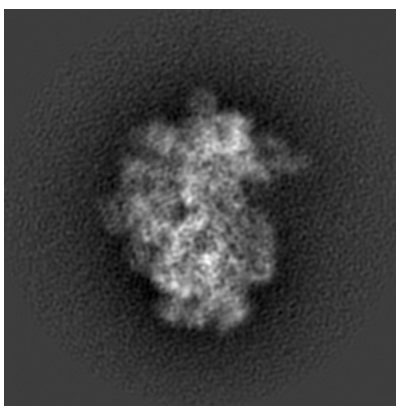
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

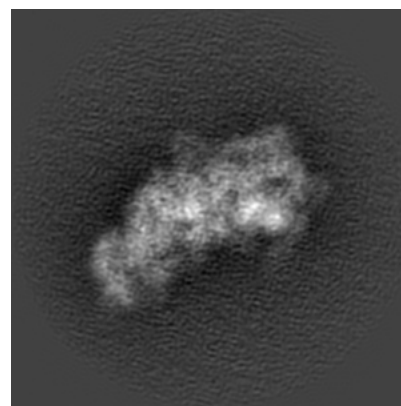
6.1.1 Primary map



X

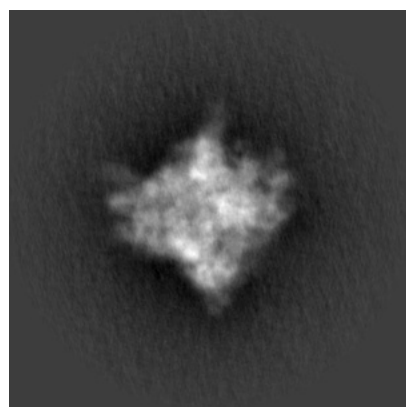


Y

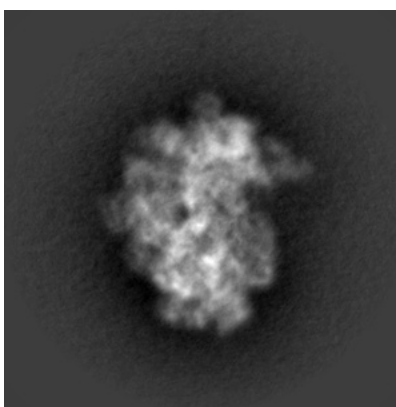


Z

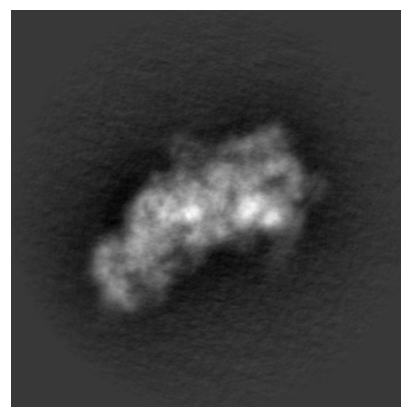
6.1.2 Raw map



X



Y

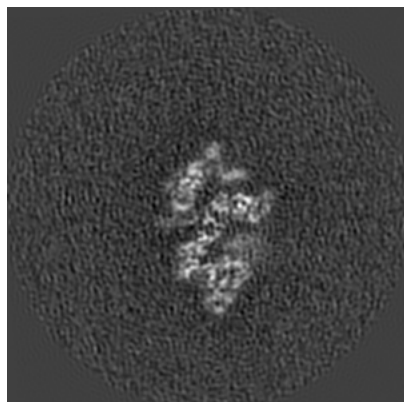


Z

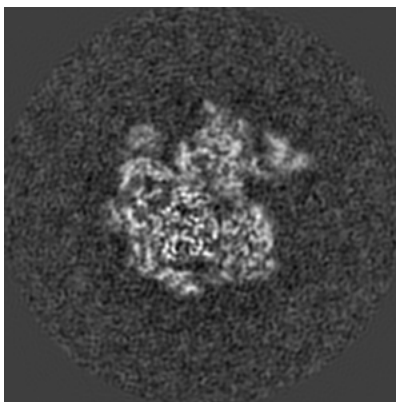
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

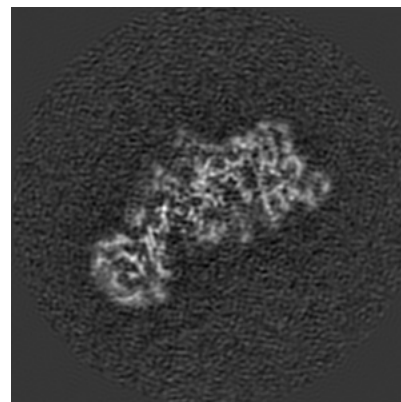
6.2.1 Primary map



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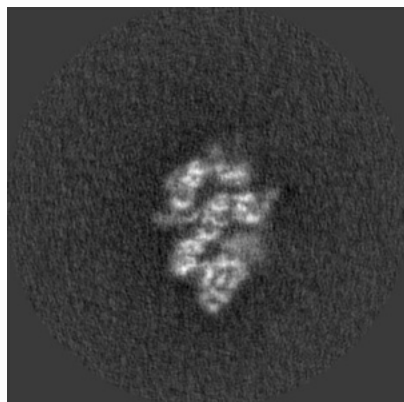


Y Index: 130

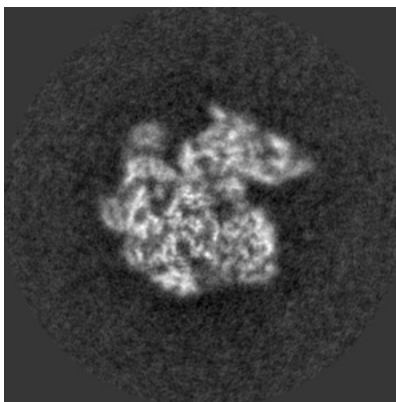


Z Index: 130

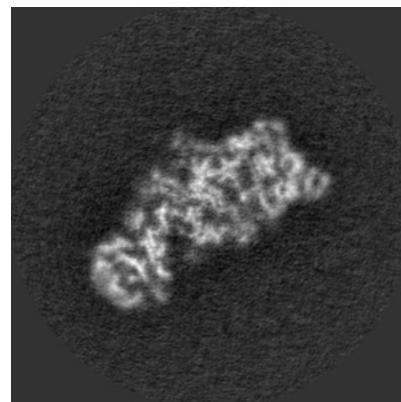
6.2.2 Raw map



X Index: 130



Y Index: 130

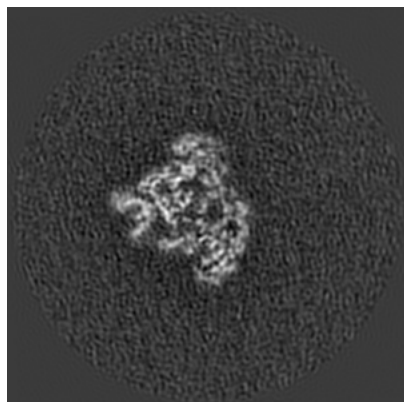


Z Index: 130

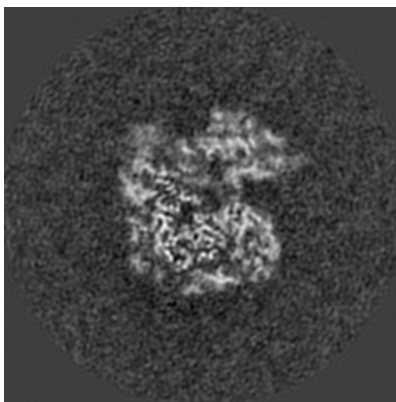
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

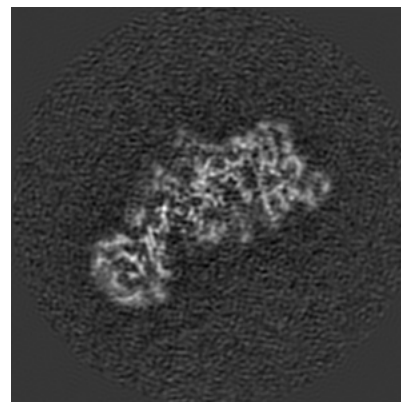
6.3.1 Primary map



X Index: 95

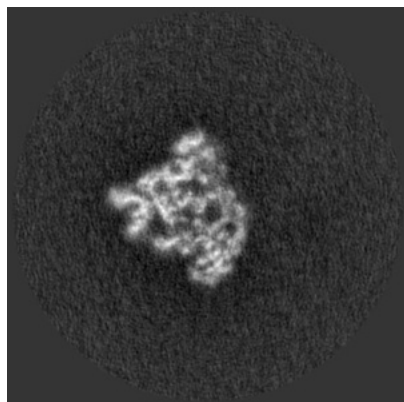


Y Index: 125

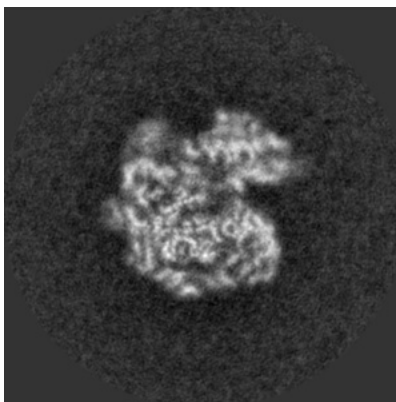


Z Index: 130

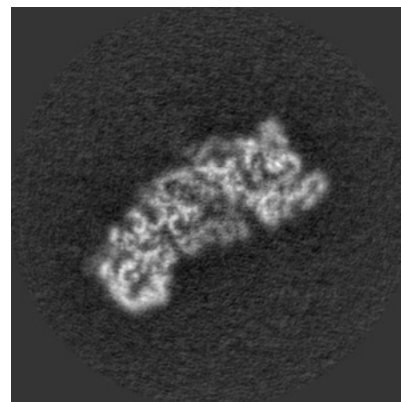
6.3.2 Raw map



X Index: 95



Y Index: 127

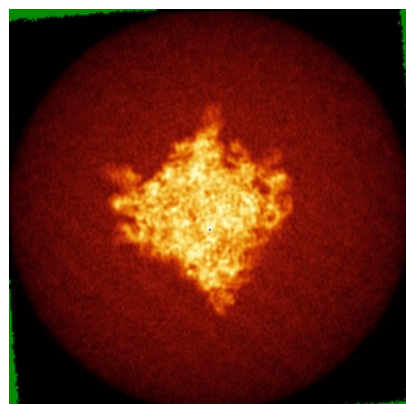


Z Index: 136

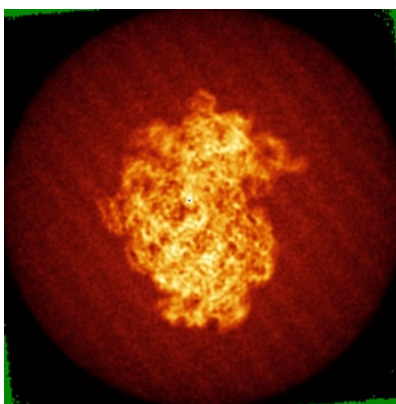
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

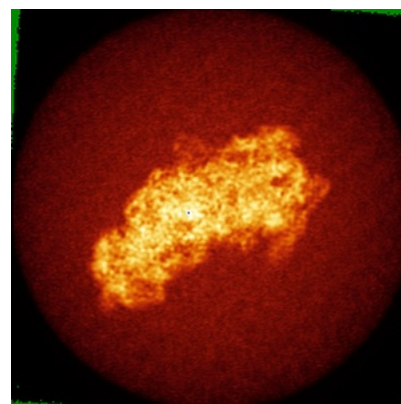
6.4.1 Primary map



X

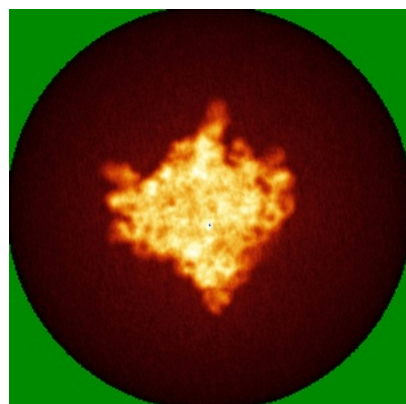


Y

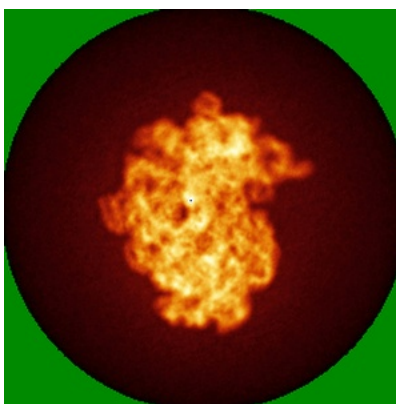


Z

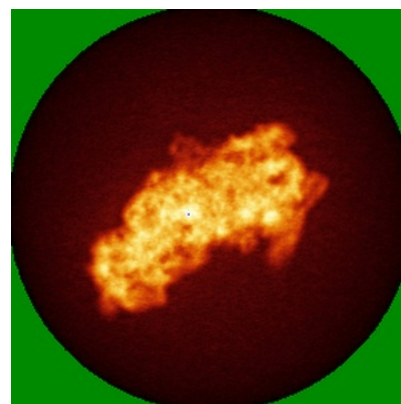
6.4.2 Raw map



X



Y

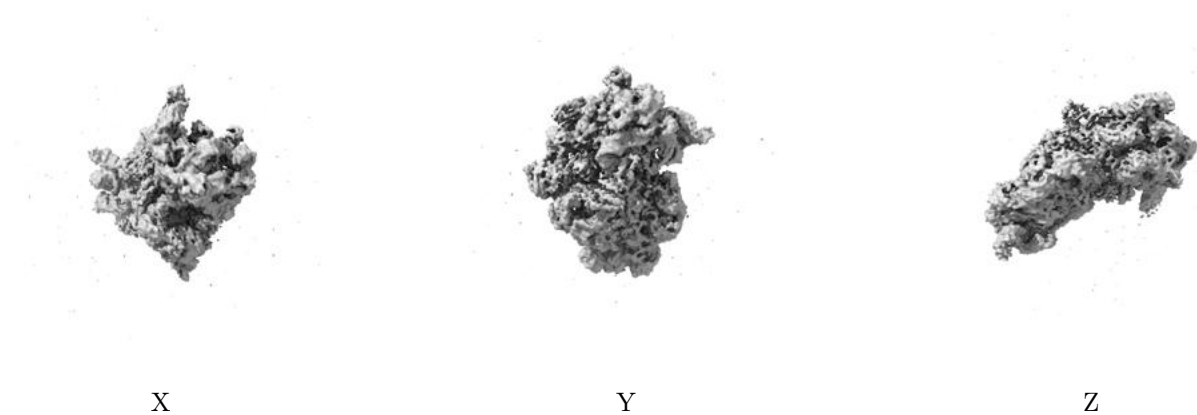


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

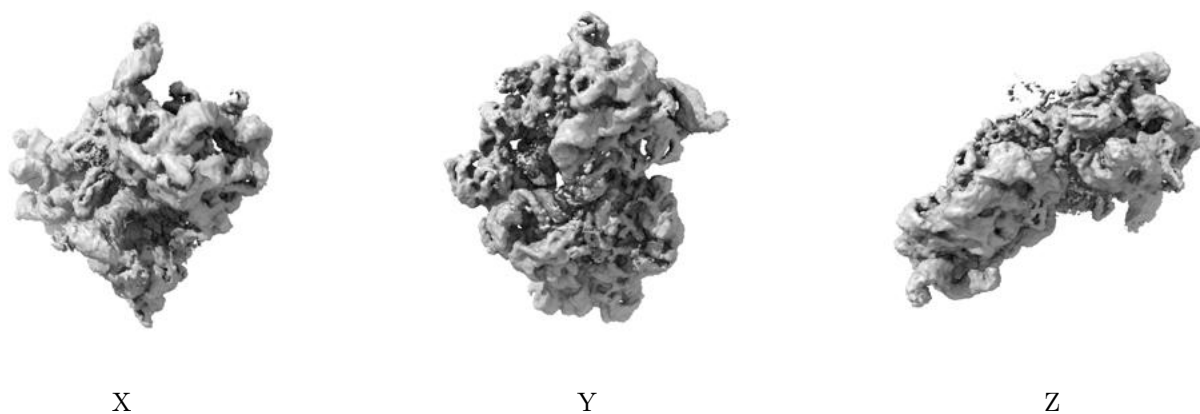
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.075. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

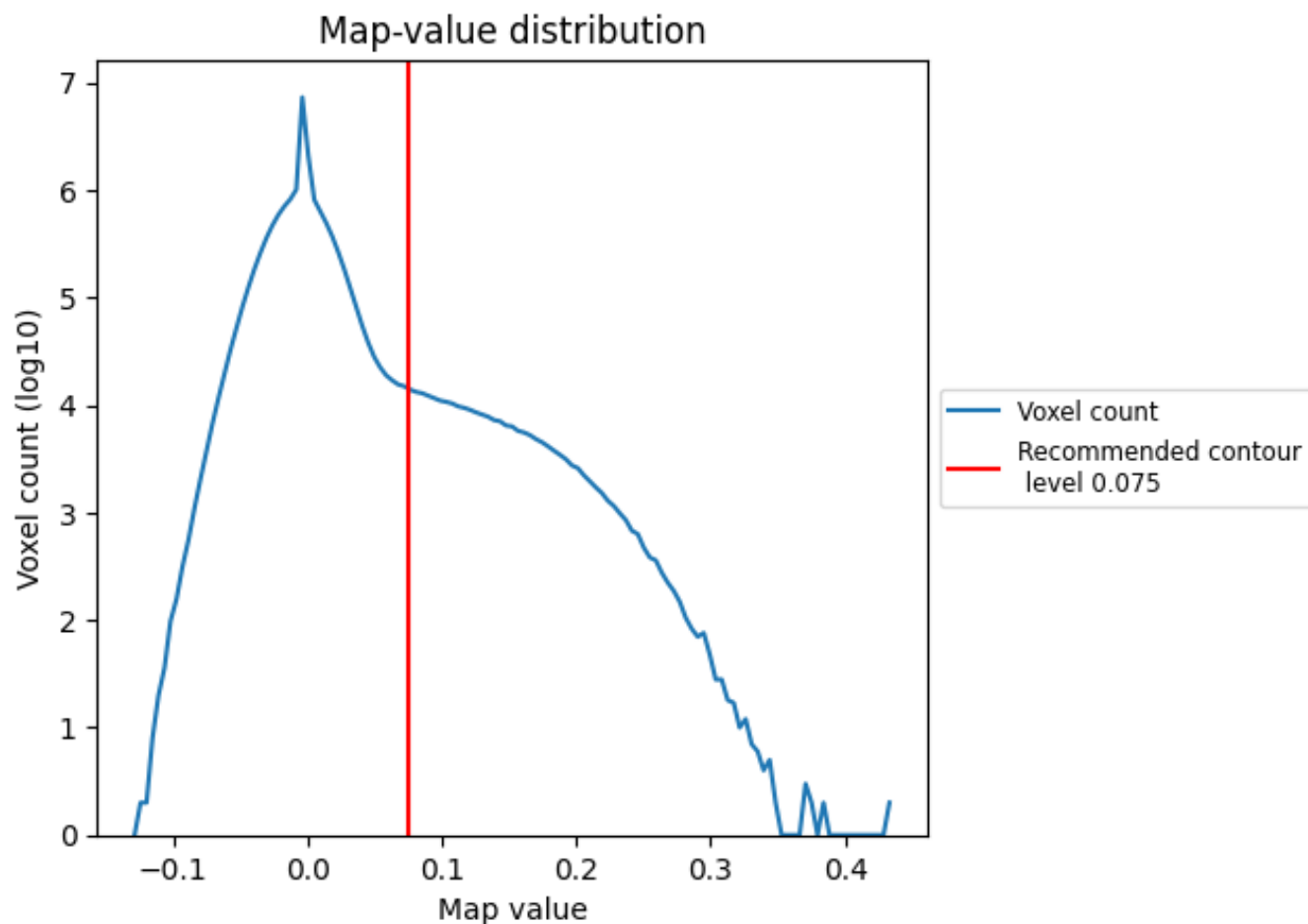
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

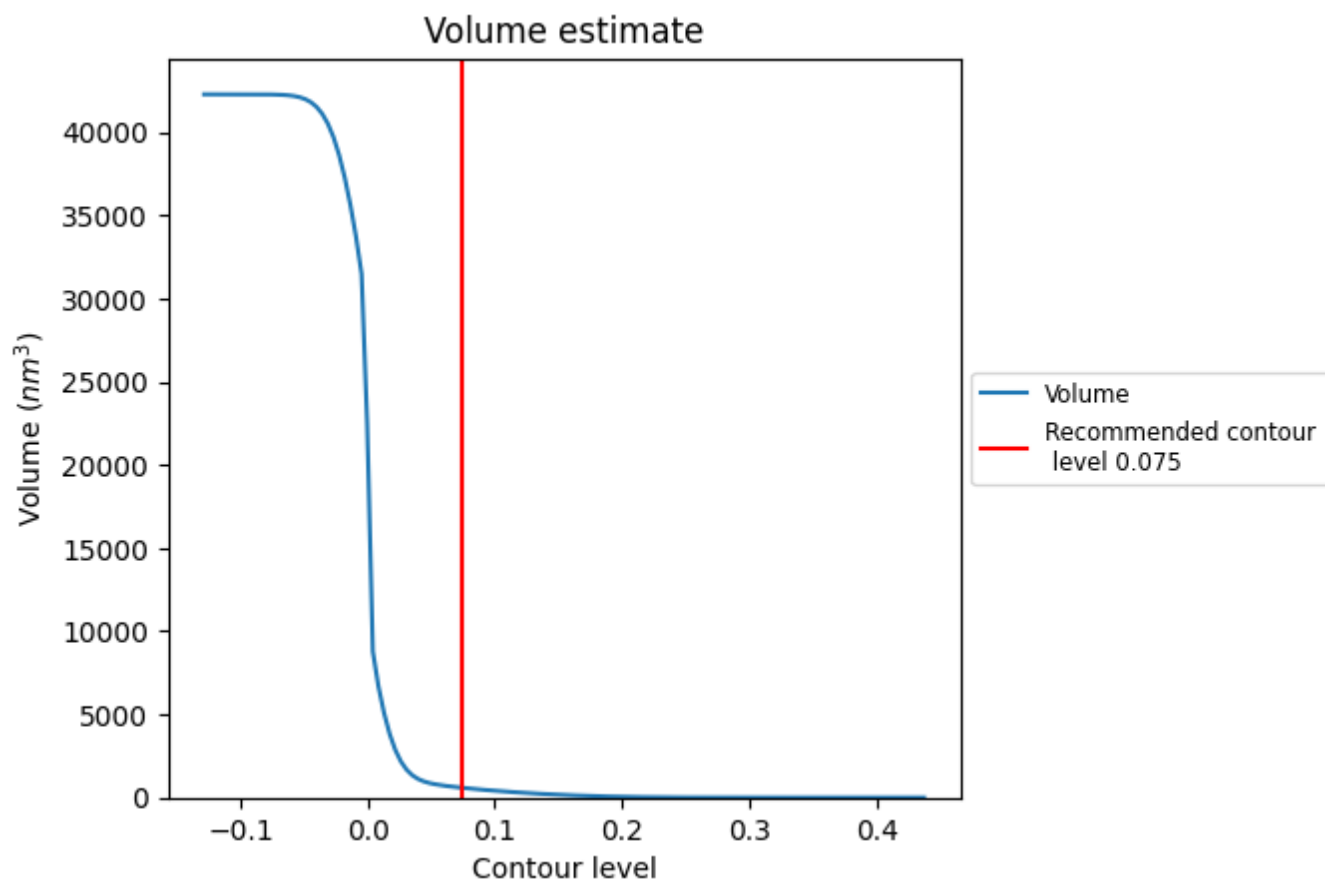
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

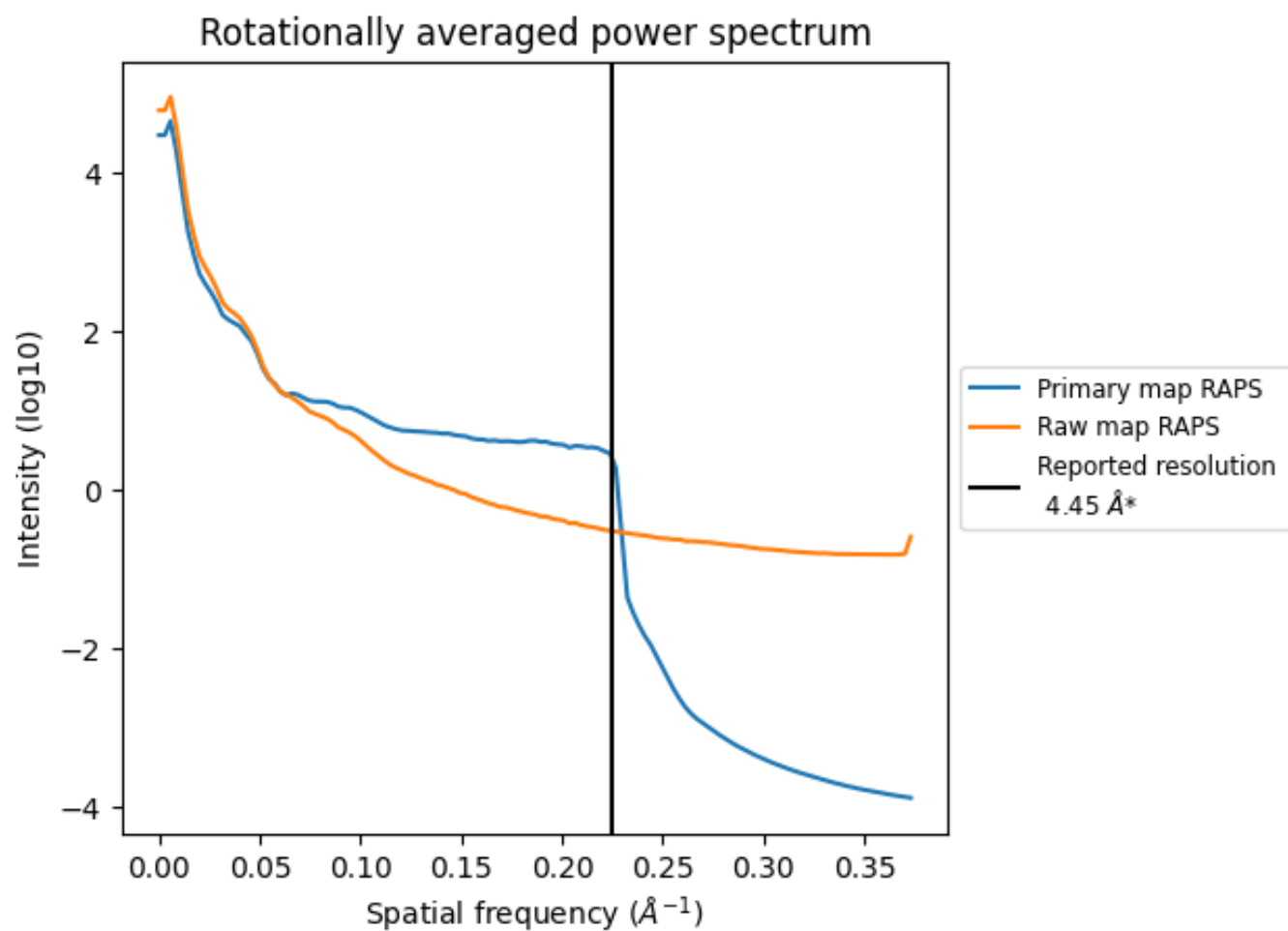
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 583 nm^3 ; this corresponds to an approximate mass of 527 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

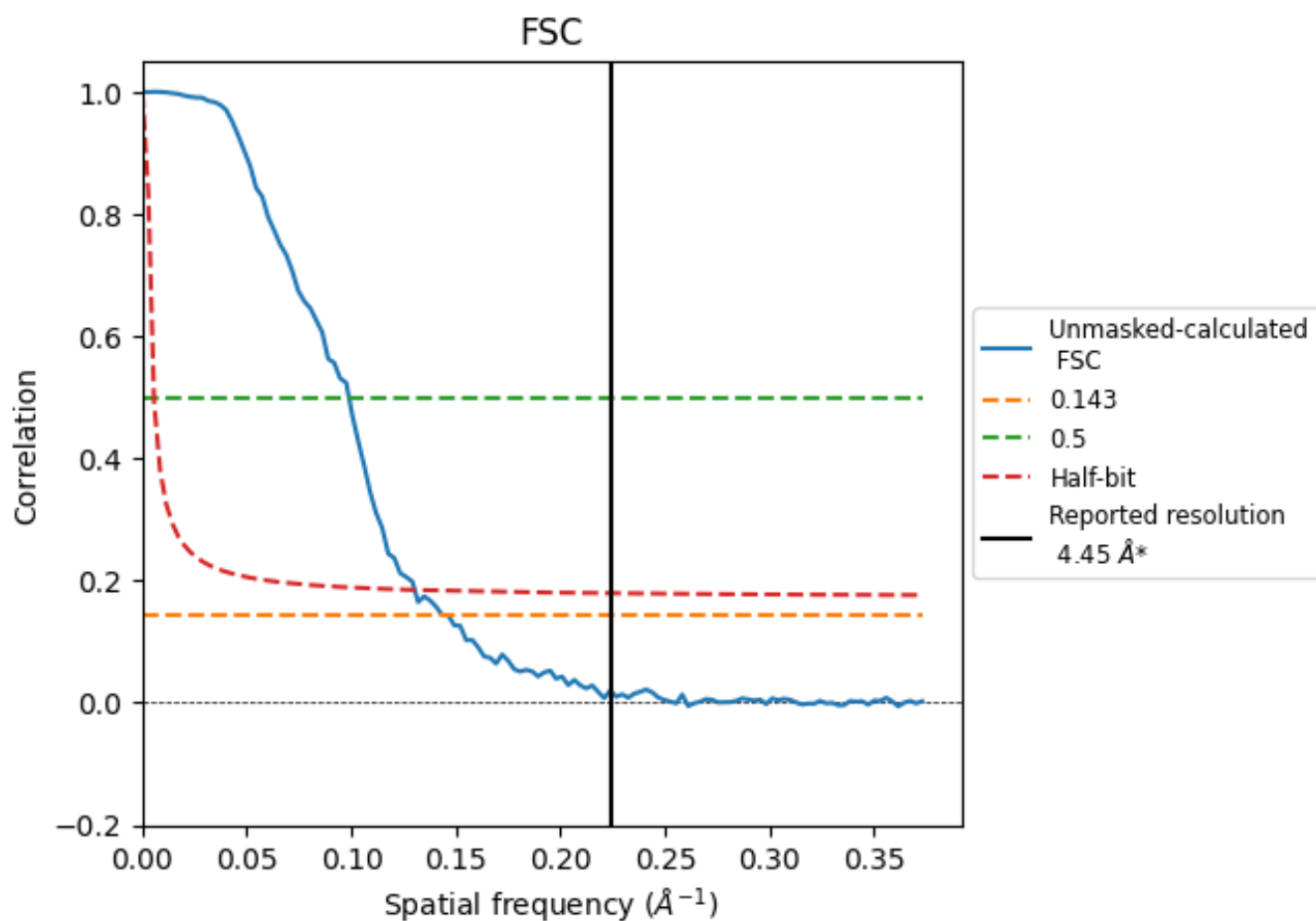


*Reported resolution corresponds to spatial frequency of 0.225 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.225 Å⁻¹

8.2 Resolution estimates [i](#)

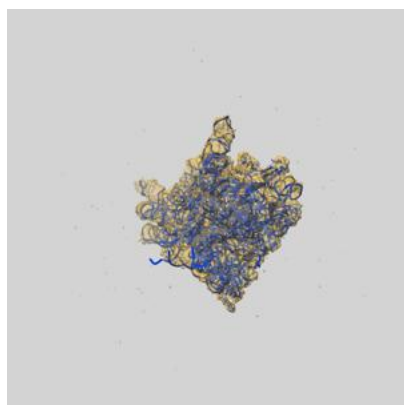
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|-------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 4.45 | - | - |
| Author-provided FSC curve | - | - | - |
| Unmasked-calculated* | 6.84 | 10.11 | 7.67 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.84 differs from the reported value 4.45 by more than 10 %

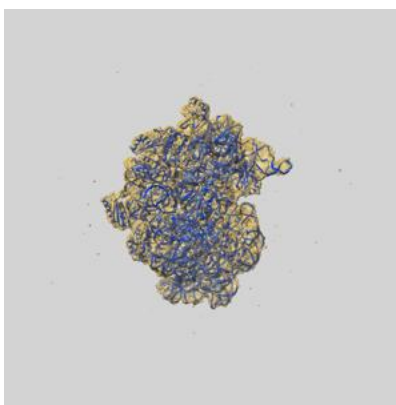
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4077 and PDB model 5LMR. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

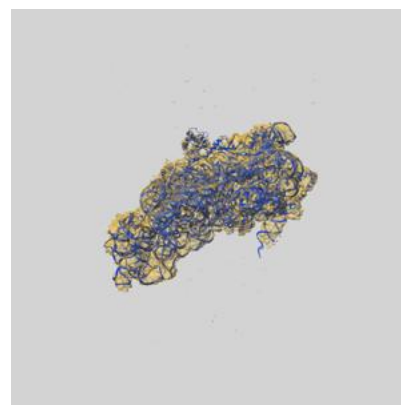
9.1 Map-model overlay [i](#)



X



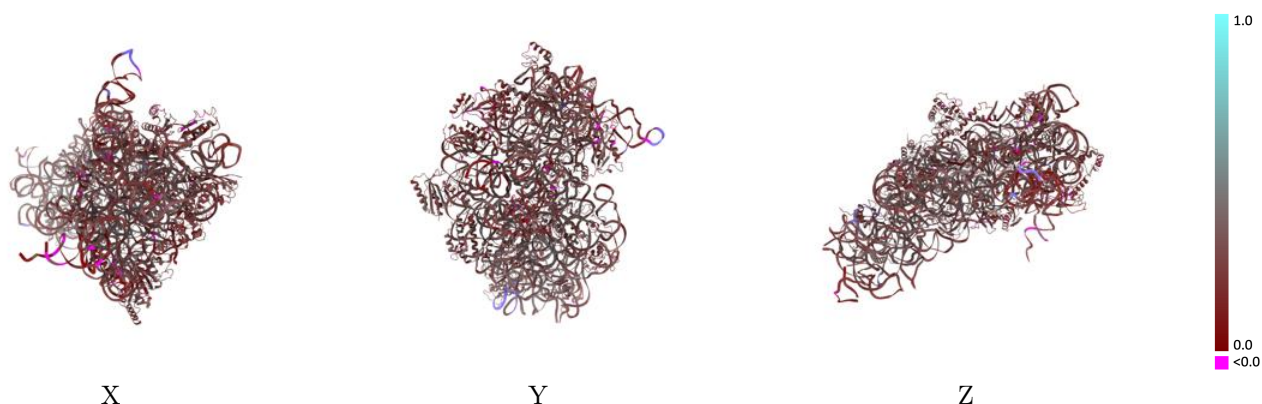
Y



Z

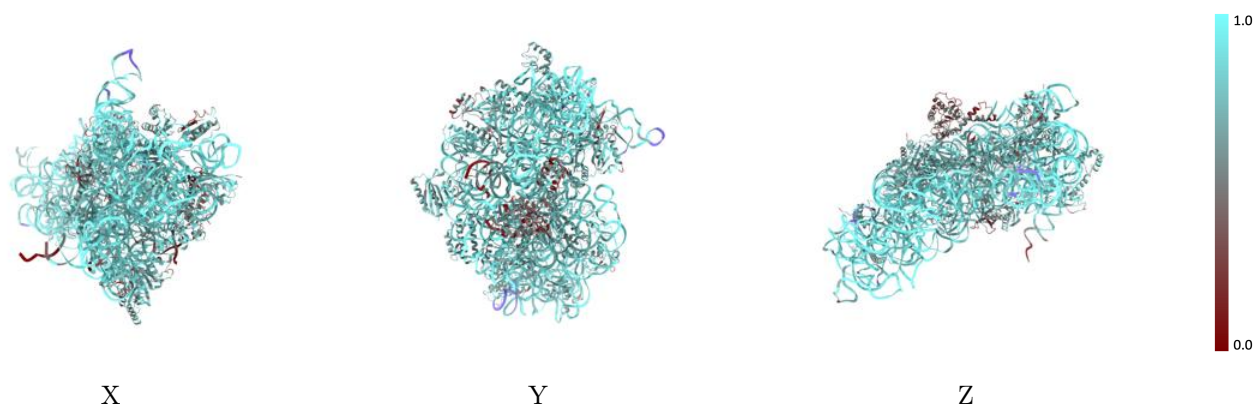
The images above show the 3D surface view of the map at the recommended contour level 0.075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



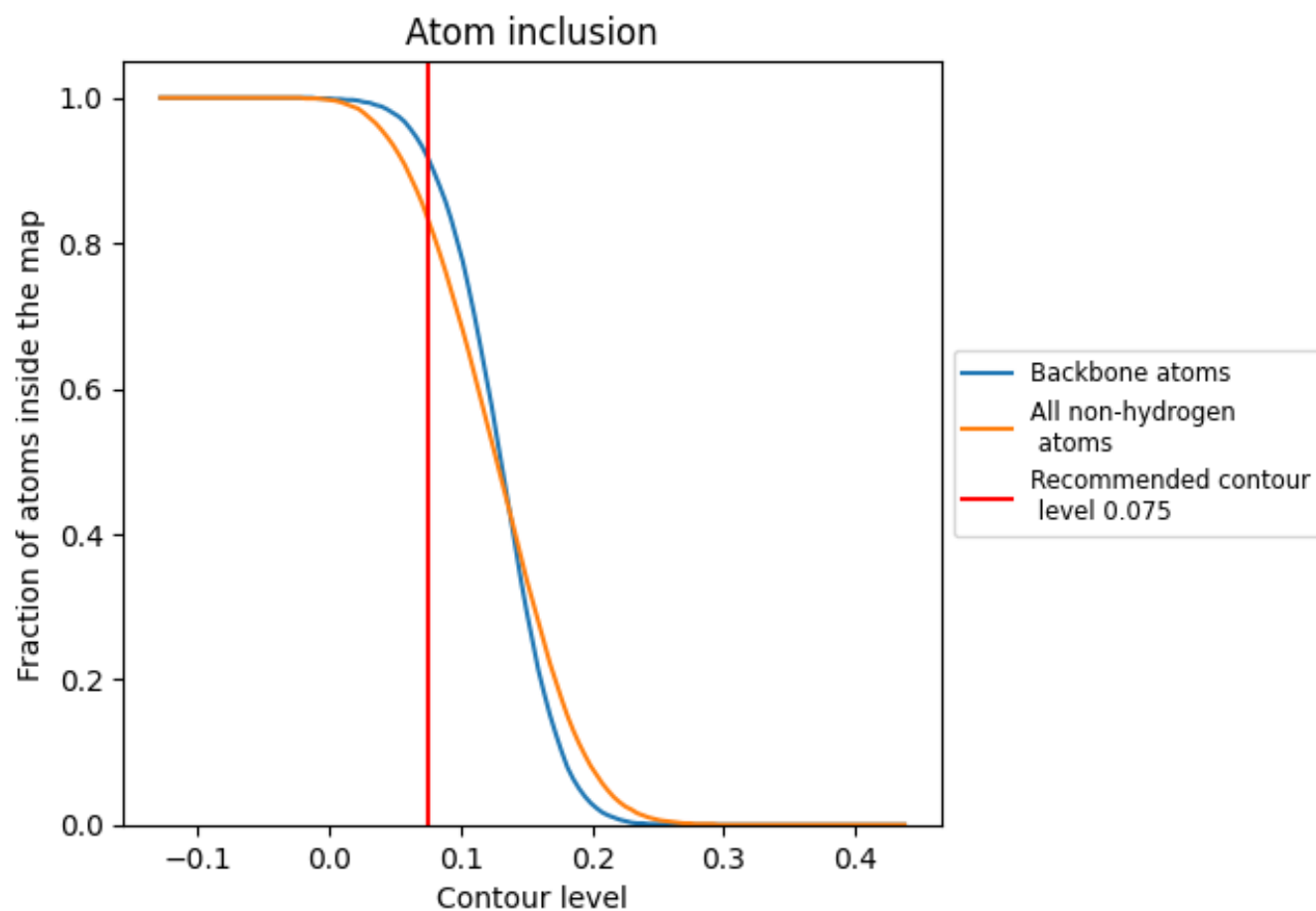
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.075).





















































9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.075) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.8330 |  0.2940 |
| A |  0.9430 |  0.3120 |
| B |  0.3130 |  0.2260 |
| C |  0.7170 |  0.2930 |
| D |  0.7150 |  0.2800 |
| E |  0.7230 |  0.3300 |
| F |  0.7210 |  0.2950 |
| G |  0.6980 |  0.2660 |
| H |  0.7320 |  0.3230 |
| I |  0.7440 |  0.2770 |
| J |  0.6070 |  0.2560 |
| K |  0.7540 |  0.2800 |
| L |  0.7290 |  0.3350 |
| M |  0.7100 |  0.2440 |
| N |  0.7240 |  0.3030 |
| O |  0.7350 |  0.2900 |
| P |  0.7650 |  0.3080 |
| Q |  0.7330 |  0.3140 |
| R |  0.7130 |  0.2900 |
| S |  0.7180 |  0.1960 |
| T |  0.7130 |  0.2700 |
| V |  0.7440 |  0.2620 |
| W |  0.4100 |  0.2570 |
| X |  0.6090 |  0.2370 |
| Y |  0.5150 |  0.1950 |
| Z |  0.7830 |  0.1610 |

