



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 10:15 AM UTC

PDB ID : 3JAM / pdb_00003jam
EMDB ID : EMD-3047
Title : CryoEM structure of 40S-eIF1A-eIF1 complex from yeast
Authors : Llacer, J.L.; Hussain, T.; Ramakrishnan, V.
Deposited on : 2015-06-17
Resolution : 3.46 Å (reported)
Based on initial model : 3J80

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:

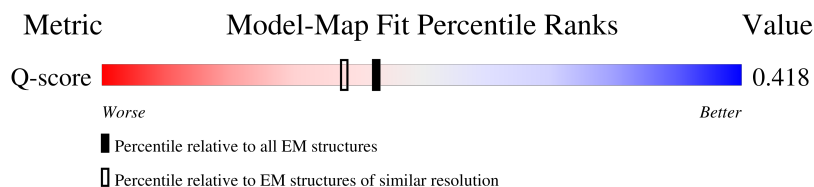
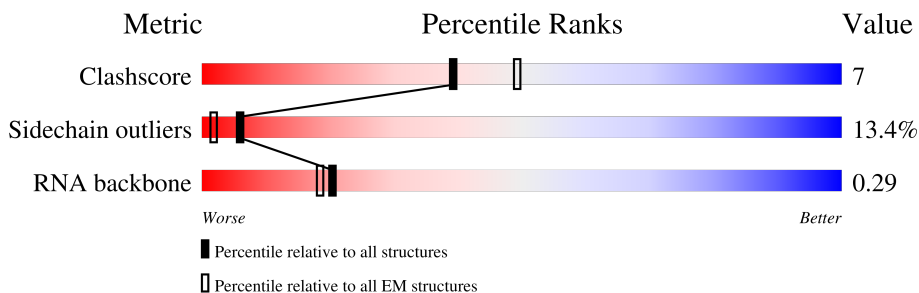
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.46 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) | Similar EM resolution (#Entries, resolution range(Å)) |
|--------------------|-----------------------------|-----------------------------|--|
| Clashscore | 229148 | 23984 | - |
| Sidechain outliers | 223484 | 23102 | - |
| RNA backbone | 8273 | 3508 | - |
| Q-score | - | 25397 | 13788 (2.96 - 3.96) |

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 | 2 | 1799 | |
| 2 | A | 254 | |
| 3 | B | 255 | |
| 4 | C | 259 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|-------------------------------|
| 5 | D | 237 | 9% 71% 19% 6% |
| 6 | E | 261 | 75% 21% |
| 7 | F | 227 | 15% 69% 21% 9% |
| 8 | G | 236 | 77% 18% |
| 9 | H | 190 | 5% 74% 21% |
| 10 | I | 201 | 6% 76% 14% 6% |
| 11 | J | 188 | 69% 24% |
| 12 | K | 106 | 14% 65% 23% 9% |
| 13 | L | 156 | 11% 81% 16% |
| 14 | M | 134 | 66% 70% 15% 6% 9% |
| 15 | N | 151 | 80% 19% |
| 16 | O | 137 | 73% 19% 7% |
| 17 | P | 142 | 30% 65% 20% 13% |
| 18 | Q | 143 | 70% 24% 5% |
| 19 | R | 136 | 68% 19% 8% |
| 20 | S | 146 | 39% 68% 28% |
| 21 | T | 144 | 9% 73% 24% |
| 22 | U | 117 | 16% 68% 21% 9% |
| 23 | V | 87 | 79% 18% |
| 24 | W | 130 | 71% 25% |
| 25 | X | 145 | 78% 16% 6% |
| 26 | Y | 135 | 76% 21% |
| 27 | Z | 108 | 60% 48% 17% 35% |
| 28 | a | 119 | 66% 14% 18% |
| 29 | b | 82 | 79% 18% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 30 | c | 67 | |
| 31 | d | 56 | |
| 32 | e | 63 | |
| 33 | f | 150 | |
| 34 | g | 326 | |
| 35 | h | 25 | |
| 36 | i | 153 | |
| 37 | j | 108 | |

2 Entry composition [i](#)

There are 39 unique types of molecules in this entry. The entry contains 77850 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 18S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| | | | Total | C | N | O | P | | |
| 1 | 2 | 1780 | 37797 | 16892 | 6658 | 12467 | 1780 | 0 | 0 |

- Molecule 2 is a protein called uS2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 2 | A | 208 | 1626 | 1040 | 286 | 298 | 2 | 0 | 0 |

- Molecule 3 is a protein called eS1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 3 | B | 223 | 1774 | 1120 | 325 | 326 | 3 | 0 | 0 |

- Molecule 4 is a protein called uS5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 4 | C | 217 | 1629 | 1041 | 287 | 297 | 4 | 0 | 0 |

- Molecule 5 is a protein called uS3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 5 | D | 223 | 1744 | 1108 | 313 | 318 | 5 | 0 | 0 |

- Molecule 6 is a protein called eS4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 6 | E | 260 | 2078 | 1322 | 393 | 359 | 4 | 0 | 0 |

- Molecule 7 is a protein called uS7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 7 | F | 206 | 1609 | 1008 | 298 | 300 | 3 | 0 | 0 |

- Molecule 8 is a protein called eS6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 8 | G | 226 | 1812 | 1134 | 348 | 326 | 4 | 0 | 0 |

- Molecule 9 is a protein called eS7.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| | | | Total | C | N | O | | |
| 9 | H | 184 | 1483 | 950 | 270 | 263 | 0 | 0 |

- Molecule 10 is a protein called eS8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 10 | I | 188 | 1489 | 923 | 300 | 265 | 1 | 0 | 0 |

- Molecule 11 is a protein called uS4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 11 | J | 182 | 1471 | 929 | 287 | 254 | 1 | 0 | 0 |

- Molecule 12 is a protein called eS10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 12 | K | 96 | 809 | 533 | 129 | 146 | 1 | 0 | 0 |

- Molecule 13 is a protein called uS17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 13 | L | 155 | 1248 | 798 | 237 | 210 | 3 | 0 | 0 |

- Molecule 14 is a protein called eS12.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 14 | M | 122 | Total | C | N | O | 0 | 0 |
| | | | 922 | 575 | 167 | 180 | | |

- Molecule 15 is a protein called uS15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15 | N | 150 | Total | C | N | O | S | 0 | 0 |
| | | | 1187 | 756 | 223 | 206 | 2 | | |

- Molecule 16 is a protein called uS11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16 | O | 127 | Total | C | N | O | S | 0 | 0 |
| | | | 942 | 578 | 188 | 173 | 3 | | |

- Molecule 17 is a protein called uS19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17 | P | 123 | Total | C | N | O | S | 0 | 0 |
| | | | 980 | 628 | 179 | 168 | 5 | | |

- Molecule 18 is a protein called uS9.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 18 | Q | 141 | Total | C | N | O | 0 | 0 |
| | | | 1105 | 709 | 204 | 192 | | |

- Molecule 19 is a protein called eS17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19 | R | 125 | Total | C | N | O | S | 0 | 0 |
| | | | 991 | 619 | 182 | 187 | 3 | | |

- Molecule 20 is a protein called uS13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20 | S | 145 | Total | C | N | O | S | 0 | 0 |
| | | | 1193 | 741 | 240 | 210 | 2 | | |

- Molecule 21 is a protein called eS19.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 21 | T | 143 | Total | C | N | O | 0 | 0 |
| | | | 1110 | 693 | 210 | 207 | | |

- Molecule 22 is a protein called uS10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22 | U | 106 | Total | C | N | O | S | 0 | 0 |
| | | | 845 | 540 | 152 | 152 | 1 | | |

- Molecule 23 is a protein called eS21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23 | V | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 687 | 424 | 126 | 135 | 2 | | |

- Molecule 24 is a protein called uS8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24 | W | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 1021 | 651 | 187 | 180 | 3 | | |

- Molecule 25 is a protein called uS12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25 | X | 144 | Total | C | N | O | S | 0 | 0 |
| | | | 1119 | 708 | 218 | 191 | 2 | | |

- Molecule 26 is a protein called eS24.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 26 | Y | 134 | Total | C | N | O | 0 | 0 |
| | | | 1061 | 665 | 207 | 189 | | |

- Molecule 27 is a protein called eS25.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 27 | Z | 70 | Total | C | N | O | S | 0 | 0 |
| | | | 558 | 355 | 104 | 98 | 1 | | |

- Molecule 28 is a protein called eS26.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28 | a | 98 | Total | C | N | O | S | 0 | 0 |
| | | | 779 | 480 | 165 | 129 | 5 | | |

- Molecule 29 is a protein called eS27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29 | b | 81 | Total | C | N | O | S | 0 | 0 |
| | | | 609 | 379 | 112 | 113 | 5 | | |

- Molecule 30 is a protein called eS28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 30 | c | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 494 | 305 | 98 | 90 | 1 | | |

- Molecule 31 is a protein called uS14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 31 | d | 53 | Total | C | N | O | S | 0 | 0 |
| | | | 446 | 280 | 89 | 76 | 1 | | |

- Molecule 32 is a protein called eS30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 32 | e | 53 | Total | C | N | O | S | 0 | 0 |
| | | | 428 | 268 | 87 | 72 | 1 | | |

- Molecule 33 is a protein called eS31.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 33 | f | 69 | Total | C | N | O | S | 0 | 0 |
| | | | 549 | 352 | 102 | 91 | 4 | | |

- Molecule 34 is a protein called RACK1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 34 | g | 318 | Total | C | N | O | S | 0 | 0 |
| | | | 2466 | 1561 | 430 | 470 | 5 | | |

- Molecule 35 is a protein called eL41.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 35 | h | 25 | 233 | 142 | 63 | 27 | 1 | 0 | 0 |

- Molecule 36 is a protein called eIF1A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 36 | i | 96 | 778 | 482 | 144 | 147 | 5 | 0 | 0 |

- Molecule 37 is a protein called eIF1.

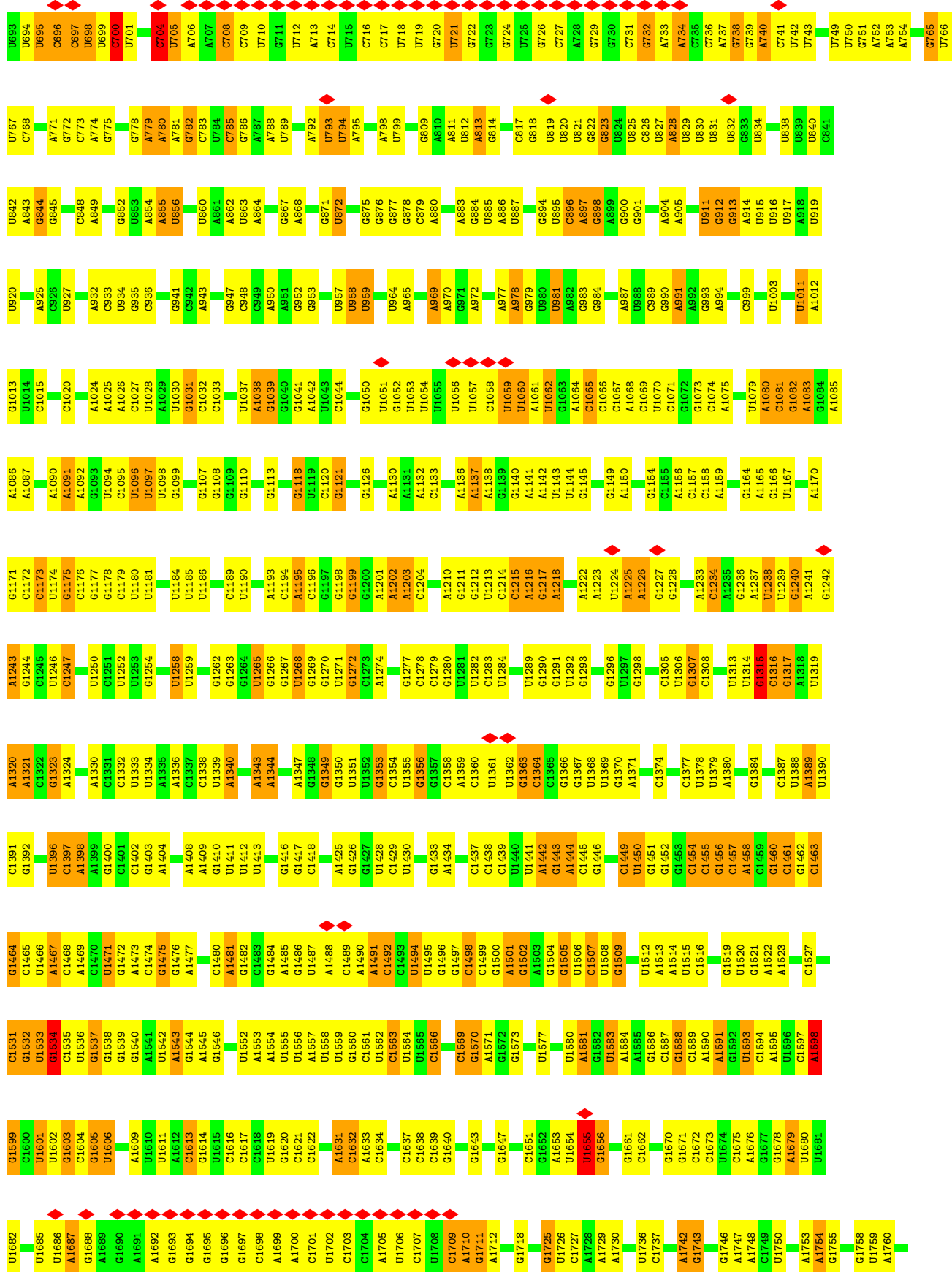
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 37 | j | 86 | 695 | 439 | 128 | 124 | 4 | 0 | 0 |

- Molecule 38 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| | | | Total | Mg | |
| 38 | 2 | 78 | 78 | 78 | 0 |
| 38 | J | 1 | 1 | 1 | 0 |
| 38 | f | 1 | 1 | 1 | 0 |

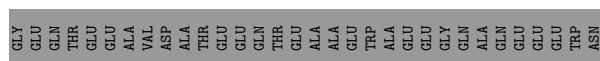
- Molecule 39 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| | | | Total | Zn | |
| 39 | a | 1 | 1 | 1 | 0 |
| 39 | b | 1 | 1 | 1 | 0 |
| 39 | f | 1 | 1 | 1 | 0 |

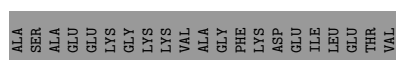




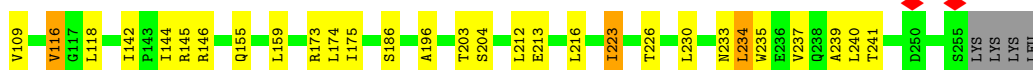
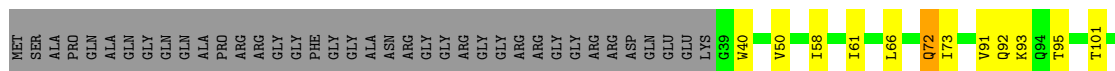
• Molecule 2: uS2



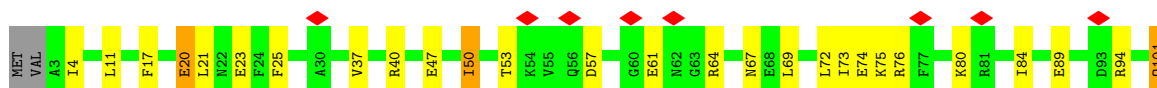
• Molecule 3: eS1

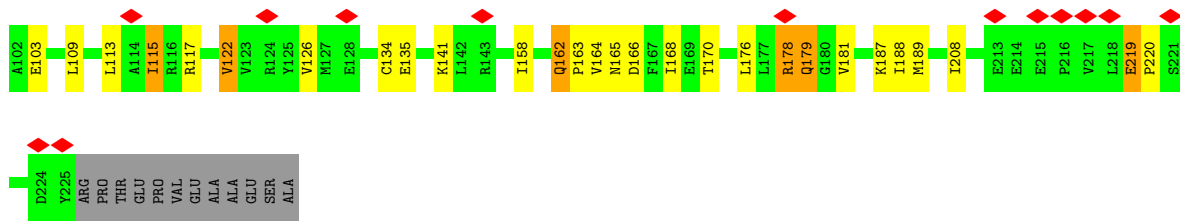


• Molecule 4: uS5

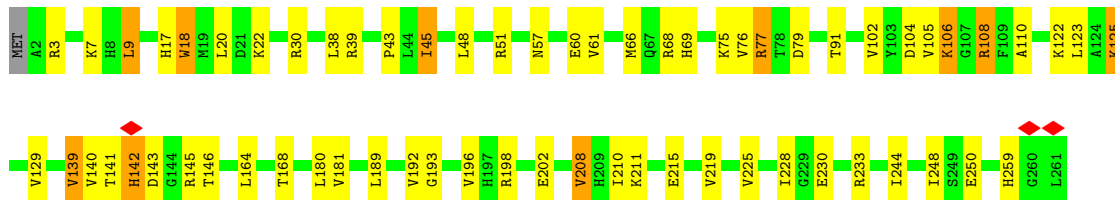
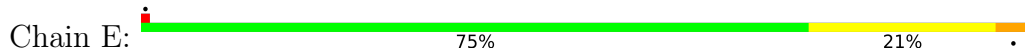


• Molecule 5: uS3

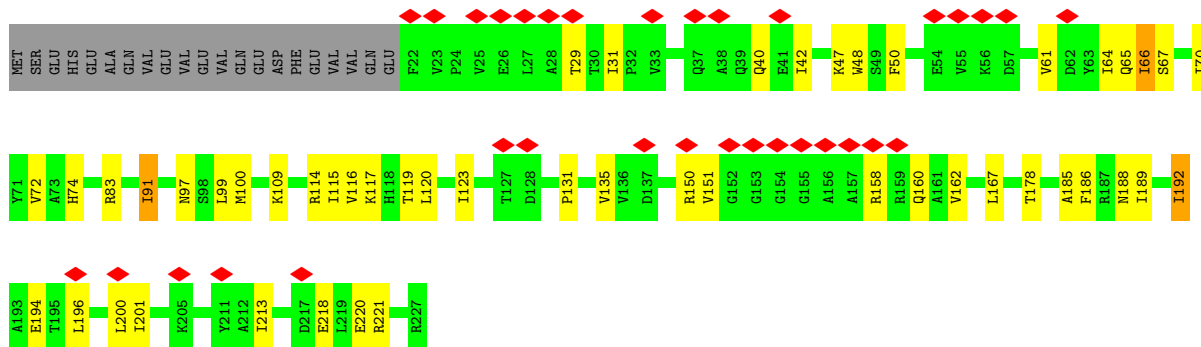




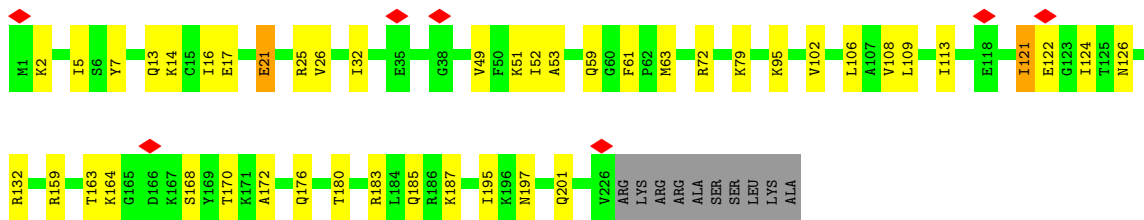
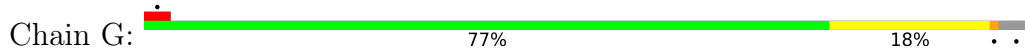
• Molecule 6: eS4



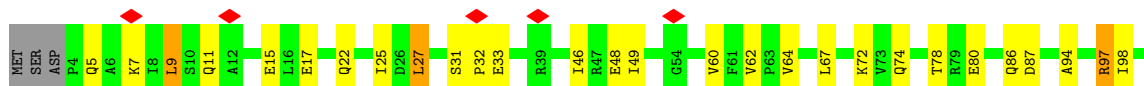
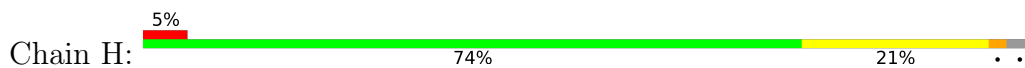
• Molecule 7: uS7



• Molecule 8: eS6

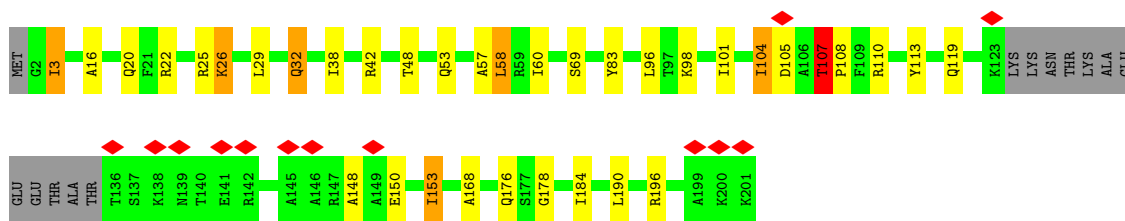
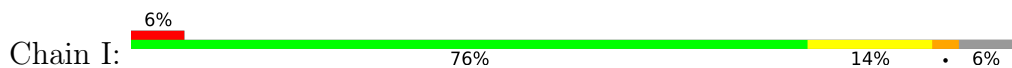


• Molecule 9: eS7

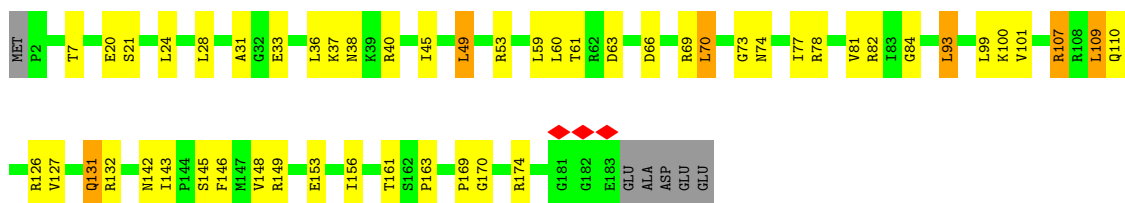




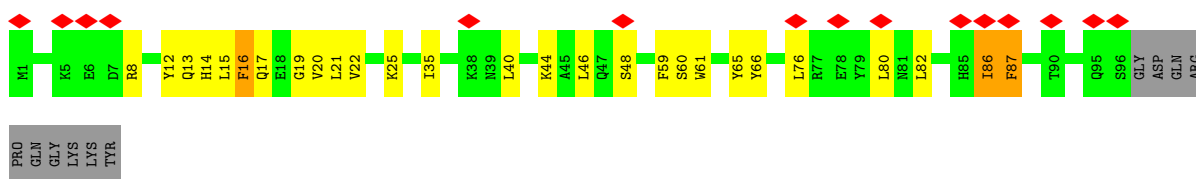
• Molecule 10: eS8



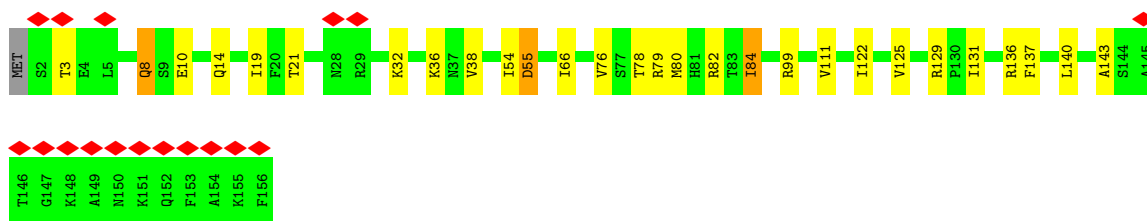
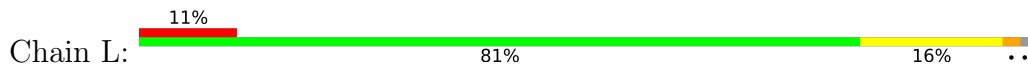
• Molecule 11: uS4



• Molecule 12: eS10

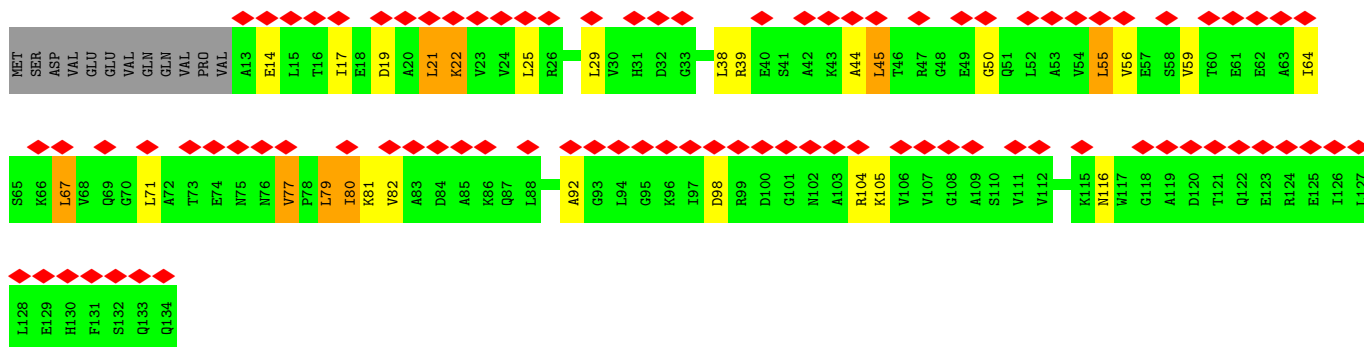


• Molecule 13: uS17

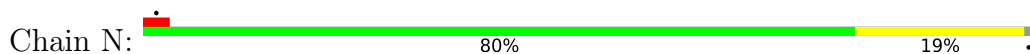


• Molecule 14: eS12





• Molecule 15: uS15



• Molecule 16: uS11



• Molecule 17: uS19

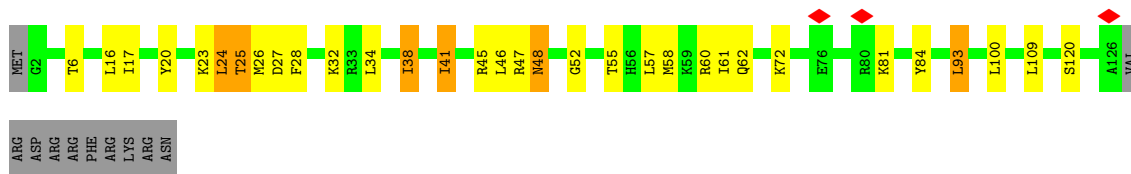


• Molecule 18: uS9

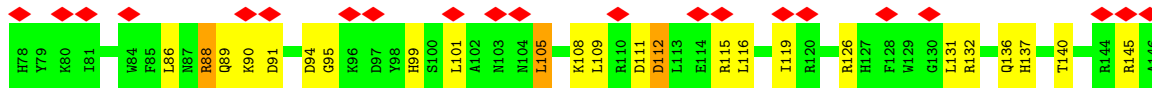
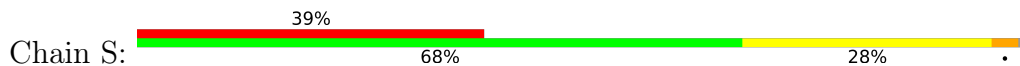


• Molecule 19: eS17

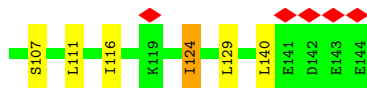
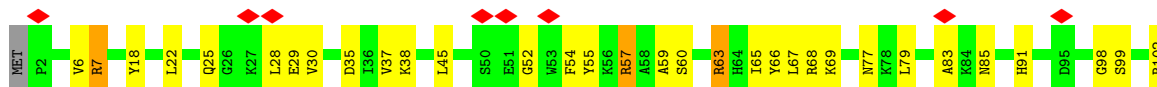




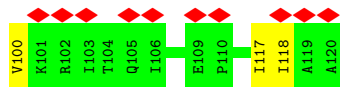
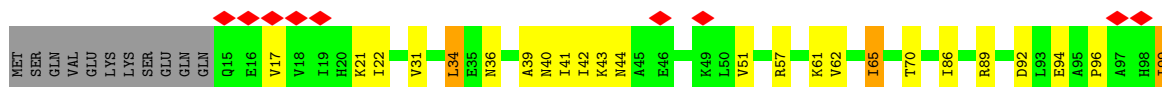
• Molecule 20: uS13



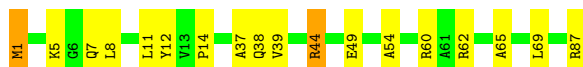
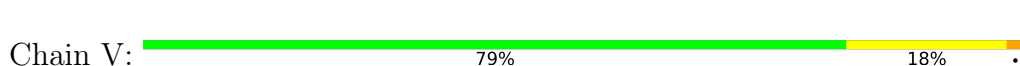
• Molecule 21: eS19



• Molecule 22: uS10

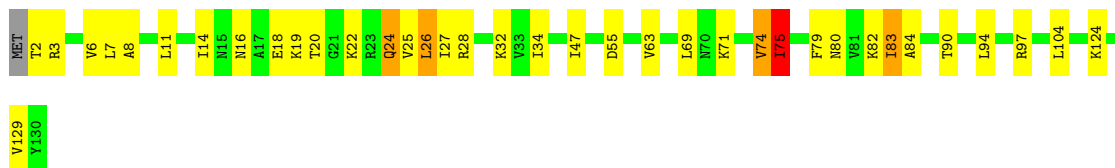


• Molecule 23: eS21

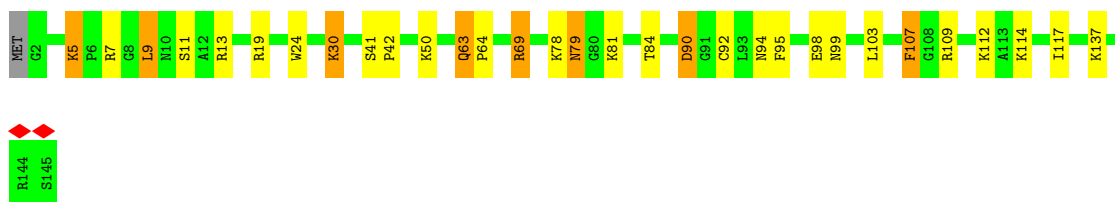
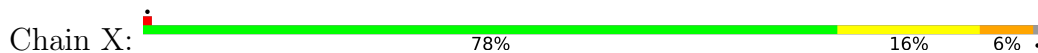


• Molecule 24: uS8

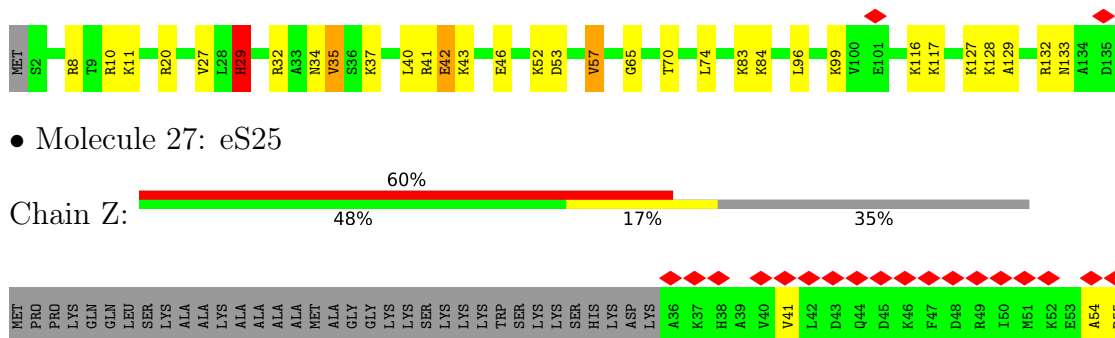
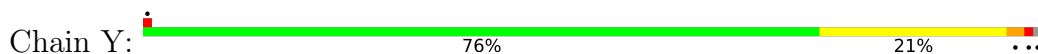




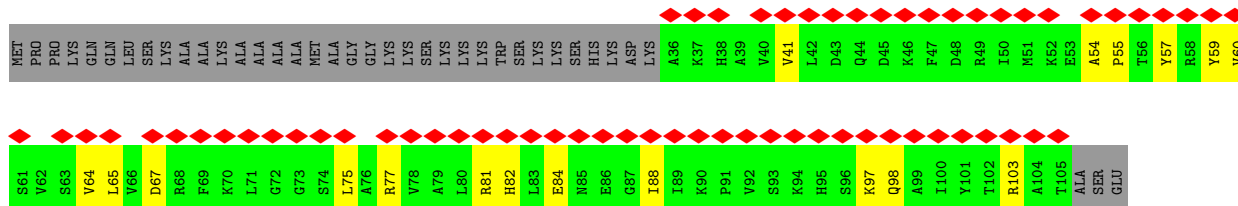
• Molecule 25: uS12



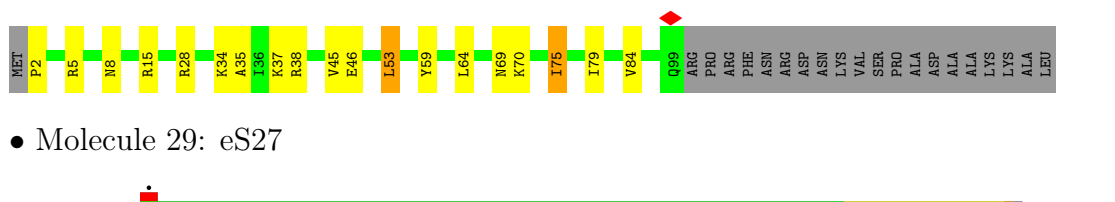
• Molecule 26: eS24



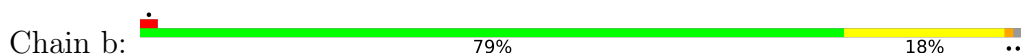
• Molecule 27: eS25



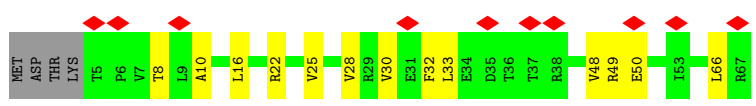
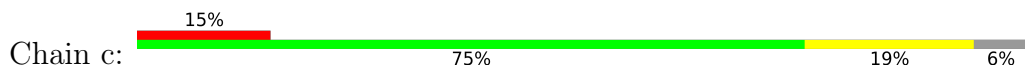
• Molecule 28: eS26



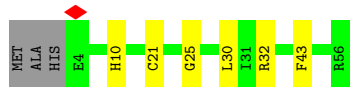
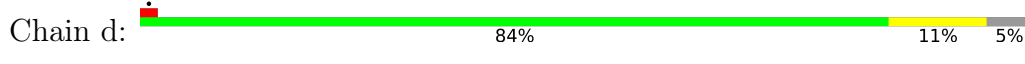
• Molecule 29: eS27



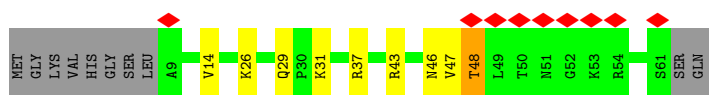
• Molecule 30: eS28



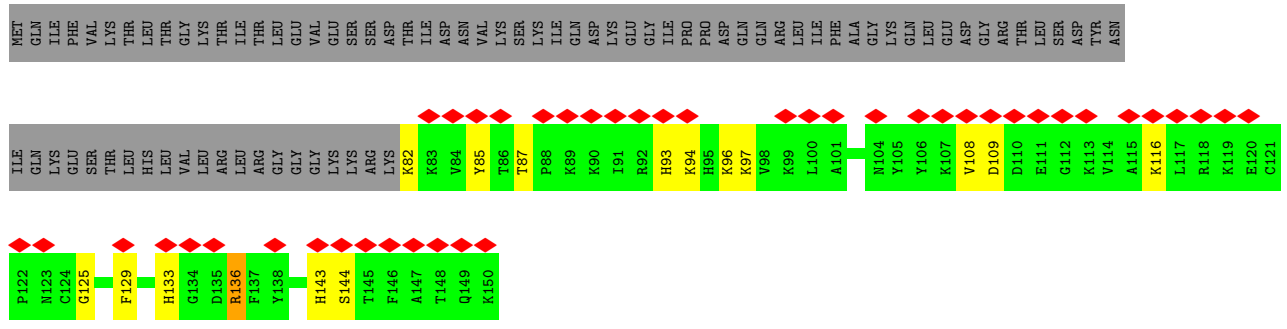
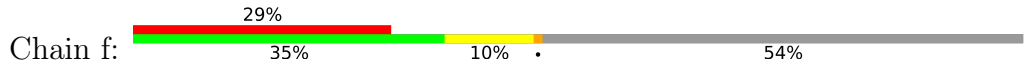
• Molecule 31: uS14



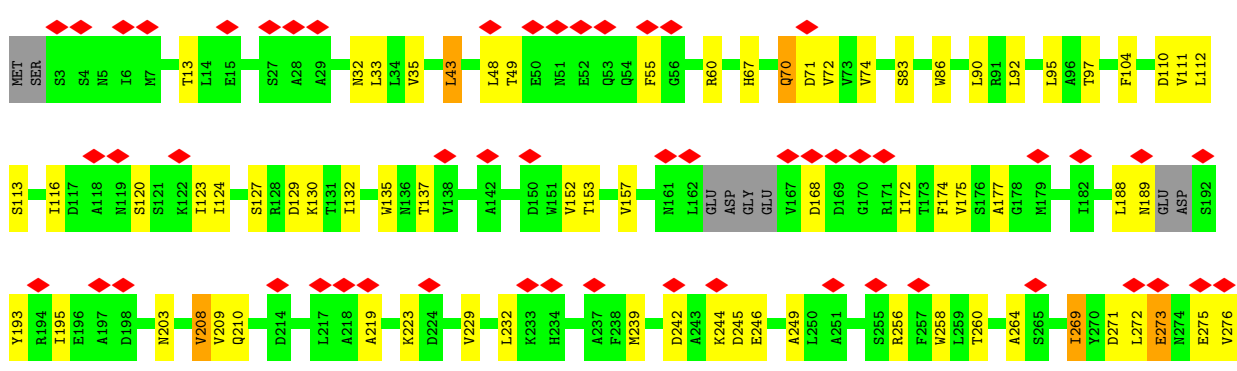
• Molecule 32: eS30

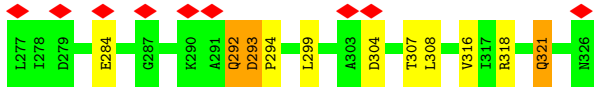


• Molecule 33: eS31

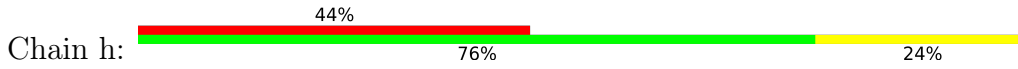


• Molecule 34: RACK1

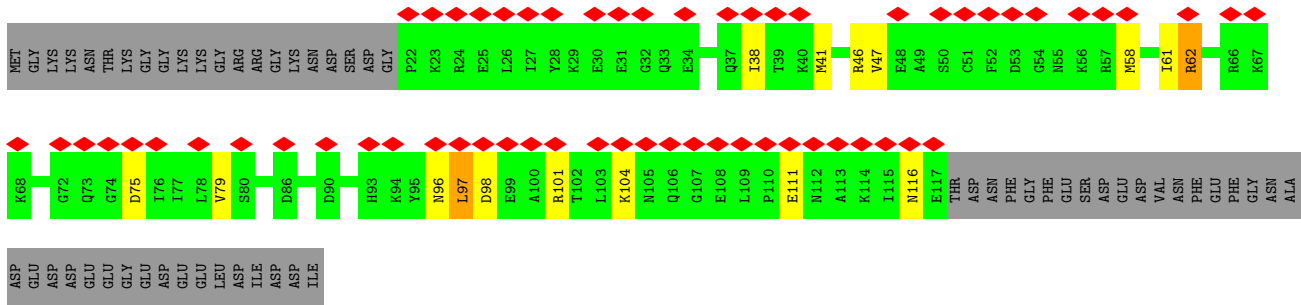




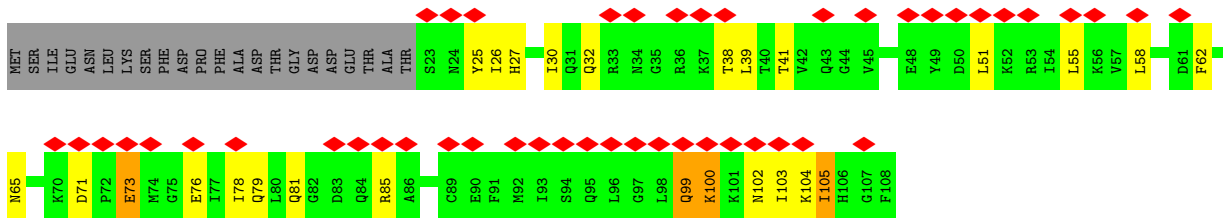
• Molecule 35: eL41



• Molecule 36: eIF1A



• Molecule 37: eIF1



4 Experimental information

| Property | Value | Source |
|--------------------------------------|-------------------------|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 86055 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | Not provided | |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 27 | Depositor |
| Minimum defocus (nm) | 1500 | Depositor |
| Maximum defocus (nm) | 4000 | Depositor |
| Magnification | 104478 | Depositor |
| Image detector | FEI FALCON II (4k x 4k) | Depositor |
| Maximum map value | 1.016 | Depositor |
| Minimum map value | -0.605 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.041 | Depositor |
| Recommended contour level | 0.1 | Depositor |
| Map size (\AA) | 402.0, 402.0, 402.0 | wwPDB |
| Map dimensions | 300, 300, 300 | wwPDB |
| Map angles ($^\circ$) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (\AA) | 1.34, 1.34, 1.34 | Depositor |

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN

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 | 2 | 0.39 | 0/42269 | 0.75 | 37/65862 (0.1%) |
| 2 | A | 0.59 | 0/1666 | 1.16 | 5/2279 (0.2%) |
| 3 | B | 0.56 | 1/1798 (0.1%) | 1.01 | 2/2421 (0.1%) |
| 4 | C | 0.57 | 0/1659 | 1.09 | 1/2252 (0.0%) |
| 5 | D | 0.60 | 0/1769 | 1.06 | 2/2378 (0.1%) |
| 6 | E | 0.53 | 0/2122 | 0.93 | 1/2861 (0.0%) |
| 7 | F | 0.61 | 0/1628 | 1.15 | 0/2198 |
| 8 | G | 0.57 | 0/1835 | 0.97 | 1/2451 (0.0%) |
| 9 | H | 0.63 | 0/1507 | 1.07 | 2/2028 (0.1%) |
| 10 | I | 0.53 | 0/1515 | 1.04 | 1/2029 (0.0%) |
| 11 | J | 0.57 | 0/1495 | 1.17 | 3/2001 (0.1%) |
| 12 | K | 0.60 | 0/831 | 1.15 | 2/1123 (0.2%) |
| 13 | L | 0.55 | 0/1276 | 0.92 | 1/1718 (0.1%) |
| 14 | M | 0.67 | 0/929 | 1.15 | 1/1255 (0.1%) |
| 15 | N | 0.56 | 0/1210 | 1.18 | 0/1628 |
| 16 | O | 0.58 | 0/953 | 1.06 | 2/1279 (0.2%) |
| 17 | P | 0.65 | 0/1000 | 1.14 | 2/1343 (0.1%) |
| 18 | Q | 0.60 | 0/1125 | 1.09 | 0/1510 |
| 19 | R | 0.59 | 0/1002 | 1.17 | 1/1346 (0.1%) |
| 20 | S | 0.58 | 0/1212 | 1.08 | 0/1629 |
| 21 | T | 0.61 | 0/1129 | 1.15 | 0/1520 |
| 22 | U | 0.58 | 0/857 | 1.00 | 0/1158 |
| 23 | V | 0.54 | 0/696 | 0.99 | 0/938 |
| 24 | W | 0.50 | 0/1039 | 1.10 | 4/1399 (0.3%) |
| 25 | X | 0.54 | 0/1137 | 1.01 | 2/1516 (0.1%) |
| 26 | Y | 0.51 | 0/1075 | 1.08 | 2/1433 (0.1%) |
| 27 | Z | 0.70 | 0/567 | 1.07 | 1/762 (0.1%) |
| 28 | a | 0.56 | 0/791 | 1.01 | 0/1059 |
| 29 | b | 0.54 | 0/619 | 0.90 | 0/837 |
| 30 | c | 0.65 | 0/496 | 0.92 | 1/666 (0.2%) |
| 31 | d | 0.53 | 0/457 | 0.94 | 0/607 |
| 32 | e | 0.54 | 0/435 | 1.03 | 1/579 (0.2%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 33 | f | 0.71 | 0/562 | 1.06 | 2/751 (0.3%) |
| 34 | g | 0.60 | 0/2521 | 0.86 | 2/3431 (0.1%) |
| 35 | h | 0.56 | 0/234 | 1.27 | 1/300 (0.3%) |
| 36 | i | 0.54 | 0/788 | 0.86 | 0/1051 |
| 37 | j | 0.58 | 0/703 | 1.01 | 3/938 (0.3%) |
| All | All | 0.49 | 1/82907 (0.0%) | 0.90 | 83/120536 (0.1%) |

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 |
|-----|-------|---------------------|---------------------|
| 12 | K | 0 | 1 |
| 17 | P | 0 | 1 |
| 18 | Q | 0 | 1 |
| 25 | X | 0 | 1 |
| 26 | Y | 0 | 1 |
| All | All | 0 | 5 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 3 | B | 189 | ILE | CA-CB | 5.98 | 1.57 | 1.54 |

All (83) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | 2 | 1534 | G | C2'-C3'-O3' | 9.36 | 123.53 | 109.50 |
| 1 | 2 | 828 | A | C2'-C3'-O3' | 8.69 | 122.53 | 109.50 |
| 1 | 2 | 277 | U | C2'-C3'-O3' | 8.30 | 121.96 | 109.50 |
| 5 | D | 219 | GLU | CA-C-N | 7.92 | 129.75 | 119.84 |
| 5 | D | 219 | GLU | C-N-CA | 7.92 | 129.75 | 119.84 |
| 1 | 2 | 1315 | G | C2'-C3'-O3' | 7.60 | 125.10 | 113.70 |
| 1 | 2 | 157 | U | C4'-C3'-O3' | 7.58 | 120.77 | 109.40 |
| 1 | 2 | 538 | G | C2'-C3'-O3' | 7.50 | 120.75 | 109.50 |
| 35 | h | 14 | LYS | CA-C-O | -7.45 | 112.66 | 120.55 |
| 1 | 2 | 1791 | G | C4'-C3'-O3' | 7.43 | 120.54 | 109.40 |
| 1 | 2 | 279 | U | C2'-C3'-O3' | 7.41 | 120.62 | 109.50 |
| 1 | 2 | 704 | C | C4'-C3'-O3' | 7.09 | 120.04 | 109.40 |
| 1 | 2 | 721 | U | C2'-C3'-O3' | 7.02 | 120.04 | 109.50 |
| 12 | K | 87 | PHE | CA-C-N | 6.93 | 128.50 | 119.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | K | 87 | PHE | C-N-CA | 6.93 | 128.50 | 119.84 |
| 1 | 2 | 912 | G | C2'-C3'-O3' | 6.92 | 119.88 | 109.50 |
| 1 | 2 | 1243 | A | C2'-C3'-O3' | 6.92 | 119.88 | 109.50 |
| 1 | 2 | 564 | C | C4'-C3'-O3' | 6.89 | 119.74 | 109.40 |
| 1 | 2 | 1598 | A | C4'-C3'-O3' | 6.85 | 119.67 | 109.40 |
| 1 | 2 | 421 | G | C4'-C3'-O3' | -6.59 | 103.11 | 113.00 |
| 33 | f | 125 | GLY | CA-C-N | 6.51 | 127.97 | 119.84 |
| 33 | f | 125 | GLY | C-N-CA | 6.51 | 127.97 | 119.84 |
| 1 | 2 | 299 | A | C4'-C3'-O3' | -6.30 | 103.55 | 113.00 |
| 24 | W | 28 | ARG | CA-C-N | -6.29 | 111.98 | 119.84 |
| 24 | W | 28 | ARG | C-N-CA | -6.29 | 111.98 | 119.84 |
| 9 | H | 74 | GLN | N-CA-C | 6.28 | 124.18 | 110.80 |
| 1 | 2 | 73 | U | C2'-C3'-O3' | 6.28 | 118.91 | 109.50 |
| 1 | 2 | 695 | U | C2'-C3'-O3' | 6.28 | 118.91 | 109.50 |
| 26 | Y | 29 | HIS | CA-C-N | 6.27 | 127.67 | 119.84 |
| 26 | Y | 29 | HIS | C-N-CA | 6.27 | 127.67 | 119.84 |
| 2 | A | 141 | ILE | N-CA-C | 6.23 | 114.75 | 107.77 |
| 1 | 2 | 557 | U | C2'-C3'-O3' | -6.21 | 104.39 | 113.70 |
| 1 | 2 | 1491 | A | C2'-C3'-O3' | 6.17 | 122.96 | 113.70 |
| 2 | A | 53 | THR | N-CA-CB | 6.16 | 119.17 | 110.12 |
| 37 | j | 71 | ASP | CA-C-N | 6.14 | 127.52 | 119.84 |
| 37 | j | 71 | ASP | C-N-CA | 6.14 | 127.52 | 119.84 |
| 2 | A | 69 | ASN | CA-C-N | 6.11 | 127.48 | 119.84 |
| 2 | A | 69 | ASN | C-N-CA | 6.11 | 127.48 | 119.84 |
| 11 | J | 99 | LEU | N-CA-C | 6.09 | 117.61 | 110.97 |
| 1 | 2 | 708 | C | C4'-C3'-O3' | 6.03 | 118.45 | 109.40 |
| 17 | P | 36 | LEU | N-CA-C | 5.88 | 117.77 | 111.36 |
| 1 | 2 | 1655 | U | C4'-C3'-O3' | 5.85 | 118.17 | 109.40 |
| 25 | X | 90 | ASP | N-CA-C | 5.85 | 117.33 | 111.07 |
| 24 | W | 75 | ILE | CB-CA-C | 5.83 | 118.96 | 110.98 |
| 4 | C | 239 | ALA | N-CA-C | 5.82 | 117.70 | 111.36 |
| 13 | L | 79 | ARG | N-CA-C | 5.78 | 118.05 | 111.11 |
| 30 | c | 33 | LEU | N-CA-C | 5.75 | 117.24 | 110.97 |
| 1 | 2 | 1501 | A | C2'-C3'-O3' | 5.74 | 122.31 | 113.70 |
| 3 | B | 205 | PHE | CA-C-N | 5.57 | 126.80 | 119.84 |
| 3 | B | 205 | PHE | C-N-CA | 5.57 | 126.80 | 119.84 |
| 1 | 2 | 1195 | A | C4'-C3'-O3' | 5.54 | 117.71 | 109.40 |
| 1 | 2 | 700 | C | C2'-C3'-O3' | 5.45 | 121.88 | 113.70 |
| 1 | 2 | 239 | C | C4'-C3'-O3' | 5.43 | 117.55 | 109.40 |
| 6 | E | 145 | ARG | N-CA-C | 5.42 | 117.68 | 110.53 |
| 19 | R | 25 | THR | N-CA-C | 5.41 | 117.55 | 108.73 |
| 1 | 2 | 1601 | U | C4'-C3'-O3' | -5.40 | 104.90 | 113.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | g | 95 | LEU | N-CA-C | 5.40 | 117.25 | 111.36 |
| 34 | g | 272 | LEU | N-CA-C | 5.33 | 116.95 | 111.03 |
| 27 | Z | 67 | ASP | N-CA-C | 5.32 | 117.50 | 111.11 |
| 1 | 2 | 542 | C | C2'-C3'-O3' | 5.30 | 117.46 | 109.50 |
| 16 | O | 56 | SER | CA-C-N | 5.30 | 125.36 | 119.32 |
| 16 | O | 56 | SER | C-N-CA | 5.30 | 125.36 | 119.32 |
| 32 | e | 43 | ARG | N-CA-C | 5.25 | 119.60 | 111.56 |
| 1 | 2 | 1765 | G | C2'-C3'-O3' | 5.25 | 117.37 | 109.50 |
| 25 | X | 78 | LYS | N-CA-C | 5.25 | 117.00 | 111.28 |
| 10 | I | 107 | THR | O-C-N | 5.21 | 125.61 | 120.71 |
| 1 | 2 | 1765 | G | C4'-C3'-O3' | 5.19 | 117.18 | 109.40 |
| 1 | 2 | 258 | U | C4'-C3'-O3' | 5.17 | 117.16 | 109.40 |
| 9 | H | 97 | ARG | N-CA-C | 5.16 | 116.76 | 111.03 |
| 14 | M | 45 | LEU | N-CA-C | 5.16 | 116.59 | 110.97 |
| 2 | A | 170 | ILE | CB-CA-C | -5.15 | 105.37 | 111.97 |
| 37 | j | 73 | GLU | N-CA-C | 5.13 | 118.28 | 111.30 |
| 1 | 2 | 73 | U | C4'-C3'-O3' | 5.12 | 117.08 | 109.40 |
| 1 | 2 | 700 | C | C3'-C2'-O2' | 5.11 | 118.36 | 110.70 |
| 17 | P | 88 | GLU | N-CA-C | -5.11 | 108.07 | 114.56 |
| 1 | 2 | 130 | C | C4'-C3'-O3' | 5.10 | 117.06 | 109.40 |
| 8 | G | 61 | PHE | N-CA-C | 5.09 | 115.83 | 109.57 |
| 1 | 2 | 1491 | A | C3'-C2'-O2' | 5.07 | 118.30 | 110.70 |
| 1 | 2 | 227 | G | C4'-C3'-O3' | -5.06 | 105.41 | 113.00 |
| 24 | W | 83 | ILE | N-CA-C | 5.05 | 119.85 | 109.34 |
| 11 | J | 101 | VAL | N-CA-C | 5.02 | 118.10 | 111.17 |
| 11 | J | 81 | VAL | N-CA-CB | 5.01 | 117.36 | 110.54 |
| 1 | 2 | 66 | U | C4'-C3'-O3' | 5.01 | 116.92 | 109.40 |

There are no chirality outliers.

All (5) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 12 | K | 87 | PHE | Peptide |
| 17 | P | 28 | MET | Peptide |
| 18 | Q | 40 | GLN | Peptide |
| 25 | X | 63 | GLN | Peptide |
| 26 | Y | 29 | HIS | Peptide |

5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | 2 | 37797 | 0 | 19016 | 584 | 0 |
| 2 | A | 1626 | 0 | 1633 | 26 | 0 |
| 3 | B | 1774 | 0 | 1834 | 19 | 0 |
| 4 | C | 1629 | 0 | 1710 | 18 | 0 |
| 5 | D | 1744 | 0 | 1826 | 18 | 0 |
| 6 | E | 2078 | 0 | 2157 | 21 | 0 |
| 7 | F | 1609 | 0 | 1679 | 23 | 0 |
| 8 | G | 1812 | 0 | 1911 | 21 | 0 |
| 9 | H | 1483 | 0 | 1579 | 16 | 0 |
| 10 | I | 1489 | 0 | 1504 | 17 | 0 |
| 11 | J | 1471 | 0 | 1554 | 22 | 0 |
| 12 | K | 809 | 0 | 810 | 12 | 0 |
| 13 | L | 1248 | 0 | 1311 | 15 | 0 |
| 14 | M | 922 | 0 | 953 | 10 | 0 |
| 15 | N | 1187 | 0 | 1251 | 6 | 0 |
| 16 | O | 942 | 0 | 979 | 11 | 0 |
| 17 | P | 980 | 0 | 1026 | 16 | 0 |
| 18 | Q | 1105 | 0 | 1170 | 23 | 0 |
| 19 | R | 991 | 0 | 1039 | 16 | 0 |
| 20 | S | 1193 | 0 | 1217 | 22 | 0 |
| 21 | T | 1110 | 0 | 1124 | 19 | 0 |
| 22 | U | 845 | 0 | 913 | 10 | 0 |
| 23 | V | 687 | 0 | 682 | 12 | 0 |
| 24 | W | 1021 | 0 | 1056 | 21 | 0 |
| 25 | X | 1119 | 0 | 1198 | 14 | 0 |
| 26 | Y | 1061 | 0 | 1111 | 11 | 0 |
| 27 | Z | 558 | 0 | 585 | 6 | 0 |
| 28 | a | 779 | 0 | 828 | 10 | 0 |
| 29 | b | 609 | 0 | 631 | 7 | 0 |
| 30 | c | 494 | 0 | 534 | 5 | 0 |
| 31 | d | 446 | 0 | 436 | 3 | 0 |
| 32 | e | 428 | 0 | 468 | 3 | 0 |
| 33 | f | 549 | 0 | 564 | 5 | 0 |
| 34 | g | 2466 | 0 | 2406 | 28 | 0 |
| 35 | h | 233 | 0 | 284 | 5 | 0 |
| 36 | i | 778 | 0 | 779 | 7 | 0 |
| 37 | j | 695 | 0 | 729 | 10 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 38 | 2 | 78 | 0 | 0 | 0 | 0 |
| 38 | J | 1 | 0 | 0 | 0 | 0 |
| 38 | f | 1 | 0 | 0 | 0 | 0 |
| 39 | a | 1 | 0 | 0 | 0 | 0 |
| 39 | b | 1 | 0 | 0 | 0 | 0 |
| 39 | f | 1 | 0 | 0 | 0 | 0 |
| All | All | 77850 | 0 | 60487 | 979 | 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 7.

All (979) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:2:51:A:N6 | 1:2:439:U:H3 | 1.05 | 1.41 |
| 1:2:1593:U:H3 | 1:2:1598:A:N6 | 1.13 | 1.40 |
| 1:2:480:A:N1 | 1:2:506:U:O4 | 1.62 | 1.33 |
| 1:2:628:U:N3 | 1:2:969:A:N6 | 1.77 | 1.32 |
| 1:2:1079:U:O4 | 1:2:1090:A:N1 | 1.66 | 1.25 |
| 1:2:480:A:N1 | 1:2:506:U:C4 | 2.13 | 1.17 |
| 1:2:864:A:N1 | 1:2:964:U:O4 | 1.83 | 1.11 |
| 1:2:51:A:N1 | 1:2:439:U:O4 | 1.87 | 1.08 |
| 1:2:1292:U:C4 | 1:2:1321:A:N1 | 2.22 | 1.08 |
| 1:2:1292:U:O4 | 1:2:1321:A:N1 | 1.86 | 1.07 |
| 1:2:299:A:H2' | 1:2:300:A:C8 | 1.91 | 1.06 |
| 1:2:1037:U:H3 | 1:2:1091:A:N6 | 1.54 | 1.05 |
| 1:2:1593:U:O4 | 1:2:1598:A:N1 | 1.90 | 1.04 |
| 1:2:864:A:N1 | 1:2:964:U:C4 | 2.28 | 1.01 |
| 1:2:628:U:N3 | 1:2:969:A:C6 | 2.26 | 1.01 |
| 1:2:628:U:C2 | 1:2:969:A:N6 | 2.28 | 1.00 |
| 1:2:480:A:C2 | 1:2:506:U:O4 | 2.16 | 0.98 |
| 1:2:1037:U:O4 | 1:2:1091:A:N1 | 1.98 | 0.97 |
| 1:2:51:A:N6 | 1:2:439:U:N3 | 1.83 | 0.95 |
| 1:2:989:C:H5 | 1:2:1013:G:H1 | 1.08 | 0.95 |
| 1:2:1590:A:H2' | 1:2:1591:A:C8 | 2.02 | 0.94 |
| 1:2:548:G:H1 | 1:2:588:C:H5 | 1.15 | 0.94 |
| 1:2:1238:U:H1' | 1:2:1247:C:H42 | 1.32 | 0.94 |
| 1:2:1037:U:H3 | 1:2:1091:A:H61 | 0.98 | 0.93 |
| 1:2:239:C:H4' | 1:2:240:U:OP2 | 1.69 | 0.92 |
| 1:2:628:U:C4 | 1:2:969:A:N6 | 2.37 | 0.91 |
| 1:2:8:U:N3 | 1:2:1138:A:N6 | 2.18 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:2:1079:U:H3 | 1:2:1090:A:N6 | 1.70 | 0.90 |
| 24:W:8:ALA:HA | 24:W:74:VAL:HG21 | 1.54 | 0.89 |
| 24:W:6:VAL:HG12 | 24:W:34:ILE:HD11 | 1.57 | 0.87 |
| 1:2:894:G:H1 | 1:2:916:U:H3 | 1.22 | 0.86 |
| 1:2:1540:G:H22 | 1:2:1566:C:H2' | 1.39 | 0.86 |
| 1:2:1290:G:N2 | 1:2:1323:G:H22 | 1.73 | 0.86 |
| 1:2:1601:U:H2' | 1:2:1602:U:C6 | 2.12 | 0.84 |
| 2:A:62:ARG:HG2 | 2:A:62:ARG:HH11 | 1.44 | 0.82 |
| 1:2:1292:U:C4 | 1:2:1321:A:C2 | 2.67 | 0.82 |
| 1:2:1450:U:H2' | 1:2:1451:G:C8 | 2.16 | 0.81 |
| 1:2:480:A:C6 | 1:2:506:U:O4 | 2.34 | 0.81 |
| 1:2:991:A:N6 | 1:2:1011:U:H3 | 1.76 | 0.81 |
| 1:2:1170:A:H2' | 1:2:1171:G:C8 | 2.17 | 0.80 |
| 1:2:61:A:H8 | 1:2:268:G:HO2' | 1.29 | 0.80 |
| 1:2:867:G:H1 | 1:2:959:U:H3 | 1.29 | 0.80 |
| 1:2:1292:U:O4 | 1:2:1321:A:C6 | 2.35 | 0.79 |
| 1:2:1450:U:H2' | 1:2:1451:G:H8 | 1.48 | 0.78 |
| 1:2:864:A:C2 | 1:2:964:U:C4 | 2.71 | 0.78 |
| 1:2:1593:U:N3 | 1:2:1598:A:N6 | 1.90 | 0.78 |
| 1:2:1137:A:H2' | 1:2:1138:A:C8 | 2.19 | 0.77 |
| 1:2:168:A:H5' | 8:G:176:GLN:HG2 | 1.66 | 0.77 |
| 1:2:1319:U:O2' | 1:2:1321:A:OP1 | 2.04 | 0.76 |
| 1:2:157:U:H4' | 1:2:158:U:OP1 | 1.85 | 0.76 |
| 2:A:70:PRO:HB3 | 2:A:94:GLY:HA3 | 1.66 | 0.74 |
| 1:2:291:U:H2' | 1:2:292:U:C6 | 2.23 | 0.74 |
| 1:2:1079:U:N3 | 1:2:1090:A:N6 | 2.33 | 0.74 |
| 1:2:1173:C:N3 | 1:2:1464:G:C2 | 2.56 | 0.74 |
| 1:2:793:U:H3' | 1:2:794:U:C5' | 2.18 | 0.73 |
| 2:A:124:THR:HG22 | 2:A:174:TRP:HE1 | 1.52 | 0.73 |
| 11:J:109:LEU:HB2 | 11:J:146:PHE:HB3 | 1.69 | 0.73 |
| 1:2:749:U:H2' | 1:2:750:U:C6 | 2.23 | 0.73 |
| 1:2:1378:U:H2' | 1:2:1379:U:C6 | 2.23 | 0.73 |
| 26:Y:129:ALA:O | 26:Y:133:ASN:HB2 | 1.89 | 0.73 |
| 1:2:864:A:C6 | 1:2:964:U:O4 | 2.40 | 0.73 |
| 4:C:144:ILE:HD13 | 4:C:196:ALA:HB1 | 1.70 | 0.72 |
| 1:2:150:G:H21 | 8:G:13:GLN:HE22 | 1.37 | 0.72 |
| 1:2:1079:U:C4 | 1:2:1090:A:N1 | 2.57 | 0.72 |
| 1:2:255:A:H2' | 1:2:256:A:O4' | 1.90 | 0.72 |
| 1:2:590:A:H2' | 1:2:591:G:C8 | 2.25 | 0.71 |
| 1:2:298:A:H2' | 1:2:299:A:H5' | 1.71 | 0.70 |
| 1:2:991:A:H61 | 1:2:1011:U:H3 | 1.34 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:65:A:H2 | 1:2:84:A:H62 | 1.39 | 0.70 |
| 1:2:1670:G:H2' | 1:2:1671:G:H8 | 1.56 | 0.70 |
| 7:F:48:TRP:HZ2 | 7:F:120:LEU:HB3 | 1.57 | 0.70 |
| 1:2:1670:G:H2' | 1:2:1671:G:C8 | 2.26 | 0.70 |
| 1:2:121:U:H2' | 1:2:122:U:C6 | 2.27 | 0.70 |
| 5:D:25:PHE:HE2 | 5:D:50:ILE:HG12 | 1.57 | 0.70 |
| 26:Y:41:ARG:HG2 | 26:Y:57:VAL:HG23 | 1.74 | 0.69 |
| 1:2:140:A:H2 | 1:2:265:A:H4' | 1.57 | 0.69 |
| 21:T:7:ARG:HH11 | 21:T:7:ARG:HG2 | 1.57 | 0.69 |
| 1:2:1033:C:HO2' | 24:W:2:THR:N | 1.89 | 0.69 |
| 1:2:793:U:H3' | 1:2:794:U:H5'' | 1.75 | 0.69 |
| 1:2:1143:U:H2' | 1:2:1144:U:C6 | 2.27 | 0.69 |
| 1:2:1477:A:OP1 | 21:T:57:ARG:HG2 | 1.91 | 0.69 |
| 2:A:50:VAL:HA | 2:A:53:THR:HG23 | 1.73 | 0.69 |
| 1:2:1292:U:O4 | 1:2:1321:A:C2 | 2.46 | 0.69 |
| 1:2:1343:A:H2' | 1:2:1344:A:C8 | 2.27 | 0.69 |
| 19:R:34:LEU:O | 19:R:38:ILE:HG12 | 1.93 | 0.67 |
| 1:2:1290:G:N2 | 1:2:1323:G:N2 | 2.42 | 0.67 |
| 1:2:1455:C:O2' | 1:2:1456:G:H5' | 1.95 | 0.67 |
| 11:J:49:LEU:HD13 | 11:J:53:ARG:HH12 | 1.58 | 0.67 |
| 11:J:77:ILE:HD11 | 11:J:93:LEU:HB2 | 1.75 | 0.67 |
| 1:2:71:A:H3' | 1:2:72:A:H5'' | 1.76 | 0.67 |
| 1:2:984:G:H1 | 1:2:1015:C:H5 | 1.43 | 0.67 |
| 1:2:8:U:C4 | 1:2:1138:A:N6 | 2.63 | 0.66 |
| 1:2:51:A:N1 | 1:2:439:U:C4 | 2.64 | 0.66 |
| 16:O:81:ILE:HB | 16:O:115:ILE:HG22 | 1.77 | 0.66 |
| 1:2:991:A:N6 | 1:2:1011:U:N3 | 2.37 | 0.66 |
| 1:2:1289:U:H2' | 1:2:1290:G:C8 | 2.30 | 0.66 |
| 24:W:11:LEU:HD12 | 24:W:74:VAL:HG22 | 1.77 | 0.66 |
| 1:2:1316:C:H2' | 1:2:1317:G:O4' | 1.94 | 0.66 |
| 1:2:1778:G:O2' | 1:2:1779:A:C8 | 2.48 | 0.66 |
| 1:2:1292:U:C5 | 1:2:1321:A:C2 | 2.84 | 0.66 |
| 29:b:21:LEU:HA | 29:b:26:GLN:HG2 | 1.78 | 0.65 |
| 1:2:1290:G:H22 | 1:2:1323:G:H22 | 1.45 | 0.65 |
| 1:2:1290:G:H22 | 1:2:1323:G:N2 | 1.95 | 0.65 |
| 1:2:45:U:O2' | 1:2:46:A:H2' | 1.97 | 0.65 |
| 1:2:868:A:H61 | 1:2:957:U:H5 | 1.42 | 0.65 |
| 1:2:1679:A:H2 | 1:2:1718:G:H21 | 1.44 | 0.65 |
| 1:2:1570:G:H5'' | 1:2:1570:G:N3 | 2.12 | 0.65 |
| 1:2:979:G:H4' | 1:2:1774:A:H4' | 1.78 | 0.65 |
| 1:2:61:A:H8 | 1:2:268:G:O2' | 1.78 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:512:U:H2' | 1:2:513:G:C8 | 2.33 | 0.64 |
| 1:2:1174:U:H2' | 1:2:1175:G:H8 | 1.62 | 0.64 |
| 7:F:115:ILE:O | 7:F:119:THR:HG23 | 1.97 | 0.64 |
| 18:Q:55:VAL:HG21 | 18:Q:105:LEU:HG | 1.80 | 0.64 |
| 9:H:98:ILE:HD11 | 9:H:121:VAL:HG11 | 1.79 | 0.64 |
| 1:2:1320:A:H4' | 1:2:1321:A:OP1 | 1.98 | 0.64 |
| 1:2:537:A:C8 | 1:2:542:C:N4 | 2.66 | 0.63 |
| 1:2:700:C:H42 | 1:2:738:G:H1 | 1.45 | 0.63 |
| 21:T:60:SER:O | 21:T:63:ARG:HG3 | 1.99 | 0.63 |
| 7:F:123:ILE:HB | 7:F:131:PRO:HB3 | 1.80 | 0.63 |
| 1:2:1363:G:N2 | 1:2:1364:C:C2 | 2.66 | 0.63 |
| 7:F:115:ILE:HG12 | 7:F:192:ILE:HD13 | 1.81 | 0.63 |
| 20:S:57:ARG:HH22 | 27:Z:75:LEU:HD11 | 1.62 | 0.63 |
| 1:2:8:U:H3 | 1:2:1138:A:N6 | 1.95 | 0.63 |
| 1:2:991:A:N3 | 1:2:991:A:H5' | 2.14 | 0.62 |
| 1:2:1417:G:C6 | 1:2:1418:C:N3 | 2.67 | 0.62 |
| 37:j:99:GLN:HG3 | 37:j:102:ASN:H | 1.62 | 0.62 |
| 1:2:221:A:H61 | 1:2:838:U:H3 | 1.48 | 0.62 |
| 1:2:1279:C:H2' | 1:2:1280:G:H8 | 1.64 | 0.62 |
| 1:2:1754:A:H62 | 36:i:61:ILE:HG21 | 1.63 | 0.62 |
| 17:P:30:THR:O | 17:P:34:VAL:HG23 | 1.99 | 0.62 |
| 24:W:8:ALA:HA | 24:W:74:VAL:CG2 | 2.27 | 0.62 |
| 1:2:68:A:H2 | 8:G:132:ARG:NH2 | 1.97 | 0.62 |
| 1:2:1583:U:H3 | 1:2:1609:A:H2 | 1.47 | 0.62 |
| 1:2:17:C:O2' | 1:2:1136:A:N1 | 2.28 | 0.62 |
| 1:2:1462:G:N1 | 1:2:1463:C:C4 | 2.68 | 0.62 |
| 5:D:219:GLU:HG2 | 5:D:220:PRO:HD2 | 1.80 | 0.62 |
| 18:Q:77:GLN:O | 18:Q:81:ILE:HG13 | 2.00 | 0.62 |
| 1:2:1452:G:H4' | 17:P:122:THR:HG21 | 1.82 | 0.61 |
| 1:2:539:G:N2 | 1:2:541:A:N7 | 2.46 | 0.61 |
| 3:B:54:LEU:O | 3:B:55:LYS:HB2 | 2.00 | 0.61 |
| 13:L:54:ILE:HG23 | 13:L:55:ASP:H | 1.66 | 0.61 |
| 20:S:37:GLY:HA2 | 20:S:105:LEU:HD21 | 1.82 | 0.61 |
| 24:W:90:THR:HG23 | 24:W:94:LEU:HD12 | 1.82 | 0.61 |
| 14:M:67:LEU:HA | 33:f:108:VAL:HG21 | 1.82 | 0.61 |
| 3:B:176:VAL:HG12 | 3:B:177:GLN:H | 1.66 | 0.61 |
| 1:2:1462:G:N2 | 1:2:1463:C:C2 | 2.69 | 0.61 |
| 13:L:66:ILE:HG13 | 13:L:140:LEU:HD21 | 1.83 | 0.61 |
| 1:2:1349:G:N1 | 1:2:1374:C:C2 | 2.69 | 0.61 |
| 1:2:1240:G:H1' | 17:P:79:HIS:HB2 | 1.82 | 0.60 |
| 1:2:61:A:C8 | 1:2:268:G:O2' | 2.52 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:516:U:H3 | 1:2:534:A:H61 | 1.48 | 0.60 |
| 1:2:1217:G:H5'' | 1:2:1442:A:N6 | 2.16 | 0.60 |
| 9:H:31:SER:HB2 | 9:H:32:PRO:HD3 | 1.84 | 0.60 |
| 6:E:9:LEU:HB2 | 6:E:30:ARG:HB2 | 1.83 | 0.60 |
| 10:I:57:ALA:HB2 | 10:I:178:GLY:HA2 | 1.83 | 0.60 |
| 34:g:43:LEU:HD21 | 34:g:72:VAL:HG21 | 1.84 | 0.60 |
| 1:2:512:U:H4' | 11:J:131:GLN:HG3 | 1.84 | 0.60 |
| 4:C:116:VAL:HG22 | 4:C:144:ILE:HD11 | 1.83 | 0.60 |
| 1:2:1277:G:C6 | 1:2:1278:C:N3 | 2.70 | 0.59 |
| 11:J:38:ASN:HB3 | 11:J:40:ARG:H | 1.65 | 0.59 |
| 1:2:1079:U:O4 | 1:2:1090:A:C2 | 2.52 | 0.59 |
| 7:F:66:ILE:HD12 | 7:F:67:SER:H | 1.67 | 0.59 |
| 7:F:114:ARG:HH22 | 18:Q:43:ILE:HB | 1.68 | 0.59 |
| 5:D:69:LEU:HA | 5:D:72:LEU:HD12 | 1.85 | 0.59 |
| 1:2:124:A:H2' | 1:2:125:U:O4' | 2.03 | 0.59 |
| 1:2:732:G:H1' | 1:2:734:A:N6 | 2.18 | 0.58 |
| 34:g:111:VAL:HA | 34:g:127:SER:HB3 | 1.85 | 0.58 |
| 4:C:233:ASN:HB2 | 23:V:1:MET:HG3 | 1.84 | 0.58 |
| 25:X:79:ASN:HD22 | 25:X:81:LYS:H | 1.52 | 0.58 |
| 1:2:406:A:H2' | 1:2:407:C:C6 | 2.39 | 0.58 |
| 1:2:911:U:C2 | 1:2:913:G:N2 | 2.72 | 0.58 |
| 1:2:1349:G:C6 | 1:2:1374:C:N3 | 2.72 | 0.58 |
| 34:g:112:LEU:HD12 | 34:g:153:THR:HA | 1.86 | 0.58 |
| 1:2:1349:G:C2 | 1:2:1374:C:O2 | 2.56 | 0.58 |
| 1:2:1085:A:H2' | 1:2:1086:A:C8 | 2.38 | 0.58 |
| 34:g:13:THR:HG22 | 34:g:318:ARG:HG2 | 1.86 | 0.58 |
| 4:C:50:VAL:HG21 | 4:C:73:ILE:HG23 | 1.85 | 0.58 |
| 1:2:1562:U:H2' | 1:2:1563:C:C6 | 2.38 | 0.58 |
| 1:2:1265:U:H2' | 1:2:1266:G:C8 | 2.39 | 0.58 |
| 1:2:1602:U:H5' | 18:Q:129:PHE:HB3 | 1.86 | 0.58 |
| 1:2:1177:G:H3' | 1:2:1178:G:H8 | 1.68 | 0.57 |
| 1:2:1598:A:H2' | 1:2:1598:A:N3 | 2.19 | 0.57 |
| 10:I:107:THR:N | 10:I:108:PRO:HD2 | 2.18 | 0.57 |
| 1:2:1581:A:H5'' | 18:Q:135:ARG:HH21 | 1.69 | 0.57 |
| 21:T:22:LEU:HB3 | 21:T:55:TYR:HD2 | 1.68 | 0.57 |
| 1:2:299:A:H2' | 1:2:300:A:H8 | 1.63 | 0.57 |
| 1:2:1754:A:H5' | 1:2:1754:A:H8 | 1.69 | 0.57 |
| 5:D:40:ARG:HB2 | 5:D:47:GLU:HB2 | 1.85 | 0.57 |
| 1:2:704:C:H4' | 1:2:705:U:OP1 | 2.04 | 0.57 |
| 1:2:1061:A:H2' | 1:2:1062:U:O4' | 2.04 | 0.57 |
| 1:2:1584:A:H5'' | 18:Q:136:SER:HB3 | 1.87 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:G:7:TYR:HD1 | 8:G:113:ILE:HG23 | 1.68 | 0.57 |
| 9:H:46:ILE:HG12 | 9:H:60:VAL:HG12 | 1.86 | 0.57 |
| 1:2:1442:A:H4' | 1:2:1443:G:H5' | 1.85 | 0.57 |
| 5:D:170:THR:HG22 | 5:D:187:LYS:HG2 | 1.86 | 0.57 |
| 9:H:101:LYS:HA | 9:H:112:ARG:NH2 | 2.18 | 0.57 |
| 1:2:1387:C:O2' | 19:R:52:GLY:HA3 | 2.04 | 0.57 |
| 1:2:1781:C:H2' | 1:2:1782:C:C6 | 2.39 | 0.57 |
| 1:2:813:A:N1 | 1:2:856:U:O4 | 2.38 | 0.56 |
| 7:F:120:LEU:HD23 | 7:F:131:PRO:HB2 | 1.86 | 0.56 |
| 14:M:98:ASP:HB2 | 14:M:104:ARG:HG3 | 1.86 | 0.56 |
| 1:2:1584:A:H1' | 1:2:1609:A:N6 | 2.20 | 0.56 |
| 1:2:363:G:N2 | 1:2:380:C:C2 | 2.72 | 0.56 |
| 2:A:205:ARG:HH22 | 19:R:84:TYR:HB3 | 1.71 | 0.56 |
| 5:D:162:GLN:N | 5:D:163:PRO:HD2 | 2.21 | 0.56 |
| 1:2:1593:U:C4 | 1:2:1598:A:N1 | 2.71 | 0.56 |
| 15:N:114:ARG:HG2 | 15:N:114:ARG:HH11 | 1.70 | 0.56 |
| 1:2:1237:A:N6 | 1:2:1247:C:H41 | 2.04 | 0.56 |
| 1:2:1267:G:H1 | 1:2:1439:C:H42 | 1.51 | 0.56 |
| 1:2:1653:A:N6 | 1:2:1743:G:H1' | 2.21 | 0.56 |
| 37:j:99:GLN:O | 37:j:100:LYS:HB2 | 2.05 | 0.56 |
| 1:2:10:G:C6 | 1:2:1631:A:C2 | 2.94 | 0.56 |
| 34:g:208:VAL:HG21 | 34:g:249:ALA:HA | 1.87 | 0.56 |
| 1:2:5:U:H2' | 1:2:6:G:H8 | 1.71 | 0.56 |
| 1:2:207:U:H2' | 1:2:208:U:C6 | 2.40 | 0.56 |
| 1:2:813:A:N6 | 1:2:856:U:N3 | 2.52 | 0.56 |
| 1:2:140:A:H61 | 8:G:187:LYS:HB2 | 1.71 | 0.56 |
| 1:2:925:A:H5'' | 1:2:925:A:H8 | 1.71 | 0.56 |
| 4:C:144:ILE:HG12 | 4:C:223:ILE:HG23 | 1.87 | 0.56 |
| 8:G:32:ILE:HG23 | 8:G:53:ALA:HA | 1.88 | 0.56 |
| 1:2:353:C:H5'' | 10:I:16:ALA:HB2 | 1.87 | 0.55 |
| 1:2:1531:C:H2' | 1:2:1532:G:O4' | 2.06 | 0.55 |
| 19:R:28:PHE:HA | 19:R:55:THR:HG21 | 1.88 | 0.55 |
| 1:2:1778:G:O2' | 1:2:1779:A:H8 | 1.86 | 0.55 |
| 23:V:5:LYS:HB2 | 23:V:7:GLN:HE21 | 1.70 | 0.55 |
| 1:2:798:A:C2 | 1:2:799:U:C2 | 2.94 | 0.55 |
| 1:2:1619:U:H2' | 1:2:1620:G:C8 | 2.42 | 0.55 |
| 18:Q:78:VAL:HA | 18:Q:81:ILE:HD12 | 1.87 | 0.55 |
| 1:2:1671:G:C2 | 1:2:1672:C:C2 | 2.95 | 0.55 |
| 1:2:1710:A:H2' | 1:2:1711:G:H4' | 1.87 | 0.55 |
| 27:Z:59:TYR:HB3 | 27:Z:64:VAL:HG11 | 1.87 | 0.55 |
| 14:M:21:LEU:HD21 | 14:M:80:ILE:HG21 | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:69:G:H1 | 1:2:82:U:H3 | 1.54 | 0.55 |
| 22:U:57:ARG:HG2 | 22:U:89:ARG:HD2 | 1.88 | 0.55 |
| 1:2:1086:A:H2' | 1:2:1087:A:C8 | 2.41 | 0.55 |
| 1:2:1559:U:H2' | 1:2:1560:G:H8 | 1.71 | 0.55 |
| 11:J:132:ARG:HH22 | 26:Y:65:GLY:HA2 | 1.72 | 0.54 |
| 19:R:93:LEU:HD12 | 19:R:100:LEU:HB3 | 1.89 | 0.54 |
| 1:2:216:A:H2' | 1:2:217:A:C8 | 2.42 | 0.54 |
| 15:N:114:ARG:O | 15:N:118:ILE:HG12 | 2.07 | 0.54 |
| 24:W:18:GLU:HG2 | 24:W:69:LEU:O | 2.06 | 0.54 |
| 1:2:864:A:C2 | 1:2:964:U:O4 | 2.55 | 0.54 |
| 1:2:1772:G:H2' | 1:2:1773:U:O4' | 2.07 | 0.54 |
| 7:F:160:GLN:HG2 | 30:c:66:LEU:HD22 | 1.89 | 0.54 |
| 1:2:240:U:C6 | 1:2:240:U:H5'' | 2.42 | 0.54 |
| 1:2:561:G:C2 | 1:2:583:C:C2 | 2.95 | 0.54 |
| 1:2:1173:C:C2 | 1:2:1464:G:N2 | 2.75 | 0.54 |
| 34:g:245:ASP:HB3 | 34:g:264:ALA:HB3 | 1.90 | 0.54 |
| 1:2:360:C:C2 | 1:2:383:G:N2 | 2.76 | 0.54 |
| 1:2:428:G:H1' | 1:2:439:U:O2 | 2.08 | 0.54 |
| 1:2:1037:U:C4 | 1:2:1091:A:N1 | 2.74 | 0.54 |
| 1:2:1654:U:H3 | 1:2:1742:A:H61 | 1.55 | 0.54 |
| 4:C:61:ILE:HA | 4:C:66:LEU:HD12 | 1.88 | 0.54 |
| 1:2:1333:U:H2' | 1:2:1334:U:O4' | 2.07 | 0.54 |
| 1:2:1771:C:H2' | 1:2:1772:G:C8 | 2.42 | 0.54 |
| 4:C:234:LEU:HD11 | 23:V:14:PRO:HD2 | 1.89 | 0.54 |
| 6:E:211:LYS:HD3 | 6:E:215:GLU:HG2 | 1.90 | 0.54 |
| 1:2:123:G:H3' | 1:2:124:A:H5'' | 1.90 | 0.54 |
| 1:2:363:G:C2 | 1:2:380:C:C2 | 2.96 | 0.54 |
| 1:2:1137:A:H2' | 1:2:1138:A:N7 | 2.22 | 0.54 |
| 11:J:82:ARG:HH21 | 11:J:149:ARG:HD3 | 1.71 | 0.54 |
| 34:g:177:ALA:HB2 | 34:g:209:VAL:HG23 | 1.87 | 0.54 |
| 1:2:1279:C:H2' | 1:2:1280:G:C8 | 2.41 | 0.54 |
| 1:2:1343:A:H4' | 1:2:1344:A:OP1 | 2.08 | 0.54 |
| 9:H:126:LEU:HG | 9:H:173:TYR:CE1 | 2.43 | 0.54 |
| 1:2:542:C:O2 | 1:2:542:C:O4' | 2.24 | 0.54 |
| 1:2:1085:A:C2 | 1:2:1086:A:C2 | 2.95 | 0.54 |
| 1:2:628:U:C4 | 1:2:969:A:C6 | 2.93 | 0.53 |
| 4:C:240:LEU:HD21 | 23:V:54:ALA:HB2 | 1.89 | 0.53 |
| 1:2:283:G:O6 | 8:G:185:GLN:HG3 | 2.08 | 0.53 |
| 1:2:989:C:H5 | 1:2:1013:G:N1 | 1.91 | 0.53 |
| 1:2:1096:U:H1' | 4:C:173:ARG:HD2 | 1.89 | 0.53 |
| 14:M:22:LYS:HA | 14:M:25:LEU:HD12 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 21:T:65:ILE:HG22 | 21:T:124:ILE:HG13 | 1.88 | 0.53 |
| 1:2:273:G:C6 | 1:2:274:C:N4 | 2.77 | 0.53 |
| 1:2:328:G:H5'' | 10:I:98:LYS:HB3 | 1.90 | 0.53 |
| 6:E:193:GLY:HA3 | 6:E:210:ILE:CG2 | 2.37 | 0.53 |
| 12:K:8:ARG:O | 12:K:12:TYR:HD1 | 1.92 | 0.53 |
| 28:a:75:ILE:O | 28:a:79:ILE:HG12 | 2.09 | 0.53 |
| 37:j:51:LEU:HD13 | 37:j:76:GLU:HG2 | 1.91 | 0.53 |
| 1:2:294:A:H2' | 1:2:295:U:O4' | 2.08 | 0.53 |
| 1:2:647:G:N3 | 1:2:647:G:H2' | 2.23 | 0.53 |
| 1:2:1185:U:O4 | 1:2:1199:G:N2 | 2.39 | 0.53 |
| 1:2:698:U:H2' | 1:2:699:U:C6 | 2.44 | 0.53 |
| 1:2:1239:U:H2' | 1:2:1240:G:H5'' | 1.90 | 0.53 |
| 1:2:256:A:C2 | 1:2:257:C:C2 | 2.96 | 0.53 |
| 1:2:1474:C:H2' | 1:2:1475:G:H8 | 1.74 | 0.53 |
| 1:2:1589:C:H2' | 1:2:1590:A:H8 | 1.72 | 0.53 |
| 1:2:1770:C:C6 | 1:2:1770:C:H5'' | 2.44 | 0.53 |
| 12:K:16:PHE:HE2 | 12:K:86:ILE:HD13 | 1.73 | 0.53 |
| 1:2:883:A:H2' | 1:2:884:G:C8 | 2.44 | 0.53 |
| 2:A:155:TYR:HB3 | 23:V:60:ARG:HH21 | 1.74 | 0.53 |
| 18:Q:39:VAL:HG21 | 18:Q:48:VAL:HG21 | 1.91 | 0.53 |
| 1:2:14:C:O2 | 1:2:1140:G:C2 | 2.62 | 0.53 |
| 1:2:1272:G:N7 | 1:2:1428:U:H3' | 2.23 | 0.53 |
| 1:2:1771:C:C2 | 1:2:1787:G:C2 | 2.97 | 0.53 |
| 4:C:118:LEU:HD11 | 4:C:216:LEU:HB3 | 1.91 | 0.53 |
| 1:2:1583:U:OP1 | 18:Q:124:PRO:HA | 2.08 | 0.53 |
| 2:A:179:ARG:HD3 | 2:A:183:ARG:CZ | 2.39 | 0.53 |
| 3:B:138:PHE:HB2 | 3:B:213:ARG:O | 2.08 | 0.53 |
| 8:G:2:LYS:HG3 | 8:G:17:GLU:HG3 | 1.91 | 0.53 |
| 1:2:486:G:H1 | 1:2:499:C:H42 | 1.57 | 0.52 |
| 1:2:1449:C:O2' | 1:2:1450:U:H5' | 2.08 | 0.52 |
| 19:R:25:THR:HA | 19:R:58:MET:HE2 | 1.91 | 0.52 |
| 34:g:256:ARG:HB2 | 34:g:258:TRP:CD1 | 2.44 | 0.52 |
| 1:2:490:C:H2' | 1:2:491:A:H4' | 1.91 | 0.52 |
| 1:2:700:C:C2 | 1:2:739:G:N1 | 2.77 | 0.52 |
| 1:2:1455:C:O3' | 20:S:137:HIS:HB2 | 2.10 | 0.52 |
| 1:2:50:C:O2 | 1:2:429:G:C2 | 2.62 | 0.52 |
| 1:2:1053:U:H2' | 1:2:1054:U:O4' | 2.09 | 0.52 |
| 1:2:1173:C:N4 | 1:2:1464:G:C6 | 2.77 | 0.52 |
| 8:G:159:ARG:HE | 8:G:172:ALA:HB2 | 1.75 | 0.52 |
| 27:Z:81:ARG:HA | 27:Z:84:GLU:HB3 | 1.91 | 0.52 |
| 1:2:294:A:C2 | 1:2:295:U:C2 | 2.97 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 26:Y:43:LYS:O | 26:Y:46:GLU:HG2 | 2.10 | 0.52 |
| 1:2:12:U:H2' | 1:2:13:C:C6 | 2.45 | 0.52 |
| 1:2:239:C:C4' | 1:2:240:U:OP2 | 2.49 | 0.52 |
| 1:2:1015:C:O4' | 1:2:1015:C:O2 | 2.26 | 0.52 |
| 1:2:1097:U:H1' | 24:W:71:LYS:HD2 | 1.91 | 0.52 |
| 1:2:1214:C:H2' | 1:2:1215:C:C6 | 2.45 | 0.52 |
| 1:2:1789:A:H5' | 28:a:8:ASN:HB3 | 1.90 | 0.52 |
| 1:2:142:G:H2' | 1:2:143:G:C8 | 2.44 | 0.52 |
| 12:K:15:LEU:O | 12:K:19:GLY:N | 2.42 | 0.52 |
| 13:L:3:THR:HA | 13:L:82:ARG:HH21 | 1.74 | 0.52 |
| 1:2:1223:A:H61 | 1:2:1258:U:H3 | 1.56 | 0.52 |
| 2:A:35:PRO:HG3 | 23:V:87:ARG:HH21 | 1.75 | 0.52 |
| 12:K:13:GLN:HA | 12:K:80:LEU:HD11 | 1.91 | 0.52 |
| 1:2:487:G:H1 | 1:2:498:U:H5 | 1.58 | 0.52 |
| 1:2:653:C:N4 | 1:2:679:U:H3 | 2.08 | 0.52 |
| 1:2:916:U:O2' | 16:O:29:HIS:HD2 | 1.92 | 0.52 |
| 1:2:1566:C:OP1 | 20:S:36:ARG:HG3 | 2.10 | 0.52 |
| 23:V:60:ARG:HA | 23:V:65:ALA:HB2 | 1.91 | 0.52 |
| 1:2:1604:C:H2' | 1:2:1605:G:C8 | 2.44 | 0.51 |
| 7:F:29:THR:HG23 | 18:Q:28:LEU:HD23 | 1.92 | 0.51 |
| 9:H:98:ILE:HG13 | 9:H:121:VAL:HG21 | 1.93 | 0.51 |
| 19:R:57:LEU:O | 19:R:60:ARG:HG2 | 2.10 | 0.51 |
| 24:W:20:THR:HG23 | 24:W:22:LYS:HG2 | 1.92 | 0.51 |
| 24:W:24:GLN:HE22 | 29:b:4:VAL:HA | 1.73 | 0.51 |
| 34:g:86:TRP:HA | 34:g:110:ASP:HB2 | 1.93 | 0.51 |
| 1:2:511:A:H5'' | 11:J:163:PRO:HG2 | 1.91 | 0.51 |
| 1:2:813:A:N3 | 1:2:813:A:H2' | 2.25 | 0.51 |
| 1:2:1210:A:H1' | 17:P:99:GLY:O | 2.10 | 0.51 |
| 1:2:958:U:H2' | 1:2:958:U:O2 | 2.09 | 0.51 |
| 1:2:1217:G:H5'' | 1:2:1442:A:H61 | 1.74 | 0.51 |
| 1:2:1771:C:H2' | 1:2:1772:G:H8 | 1.73 | 0.51 |
| 7:F:48:TRP:CZ2 | 7:F:120:LEU:HB3 | 2.42 | 0.51 |
| 13:L:122:ILE:HG13 | 13:L:143:ALA:HB3 | 1.92 | 0.51 |
| 34:g:70:GLN:HG3 | 34:g:86:TRP:HE1 | 1.75 | 0.51 |
| 1:2:813:A:N6 | 1:2:856:U:H3 | 2.08 | 0.51 |
| 1:2:864:A:C2 | 1:2:964:U:C5 | 2.97 | 0.51 |
| 1:2:1639:C:H4' | 35:h:1:MET:N | 2.26 | 0.51 |
| 7:F:150:ARG:HH21 | 30:c:22:ARG:HH21 | 1.58 | 0.51 |
| 1:2:487:G:C2 | 1:2:499:C:C2 | 2.99 | 0.51 |
| 34:g:43:LEU:HD11 | 34:g:83:SER:HB3 | 1.93 | 0.51 |
| 1:2:1121:G:H5'' | 1:2:1121:G:H8 | 1.76 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:D:126:VAL:HG11 | 5:D:134:CYS:HB2 | 1.93 | 0.51 |
| 16:O:99:GLN:HE22 | 28:a:45:VAL:HA | 1.76 | 0.51 |
| 24:W:82:LYS:O | 24:W:84:ALA:N | 2.44 | 0.51 |
| 1:2:5:U:H2' | 1:2:6:G:C8 | 2.45 | 0.51 |
| 1:2:538:G:O5' | 1:2:538:G:H8 | 1.94 | 0.51 |
| 1:2:1611:U:O2 | 1:2:1611:U:O4' | 2.29 | 0.51 |
| 13:L:21:THR:HG22 | 13:L:32:LYS:H | 1.75 | 0.51 |
| 1:2:452:U:O2 | 1:2:452:U:H3' | 2.11 | 0.50 |
| 1:2:868:A:N6 | 1:2:957:U:H5 | 2.08 | 0.50 |
| 1:2:1137:A:C5 | 1:2:1138:A:N6 | 2.79 | 0.50 |
| 15:N:54:LEU:HB3 | 15:N:60:VAL:HB | 1.92 | 0.50 |
| 17:P:17:TYR:HB2 | 17:P:25:LEU:HD21 | 1.93 | 0.50 |
| 22:U:65:ILE:HG21 | 31:d:43:PHE:CE2 | 2.46 | 0.50 |
| 1:2:1398:A:H5' | 19:R:60:ARG:HH12 | 1.77 | 0.50 |
| 1:2:1540:G:N2 | 1:2:1566:C:H2' | 2.19 | 0.50 |
| 1:2:653:C:H42 | 1:2:679:U:H3 | 1.60 | 0.50 |
| 12:K:82:LEU:HD22 | 12:K:86:ILE:HG21 | 1.93 | 0.50 |
| 13:L:125:VAL:HG22 | 13:L:137:PHE:HB3 | 1.93 | 0.50 |
| 25:X:63:GLN:HB3 | 25:X:64:PRO:CD | 2.42 | 0.50 |
| 1:2:1542:U:H3' | 1:2:1543:A:H5'' | 1.94 | 0.50 |
| 1:2:1586:G:N1 | 1:2:1587:C:C2 | 2.79 | 0.50 |
| 18:Q:7:VAL:HG23 | 18:Q:22:VAL:HG23 | 1.92 | 0.50 |
| 1:2:228:U:H3 | 1:2:235:A:H61 | 1.58 | 0.50 |
| 1:2:385:G:H2' | 1:2:386:A:C8 | 2.46 | 0.50 |
| 1:2:1038:A:H4' | 23:V:62:ARG:HH12 | 1.76 | 0.50 |
| 1:2:1671:G:C6 | 1:2:1672:C:C4 | 3.00 | 0.50 |
| 2:A:50:VAL:HA | 2:A:53:THR:CG2 | 2.40 | 0.50 |
| 20:S:37:GLY:CA | 20:S:105:LEU:HD21 | 2.42 | 0.50 |
| 1:2:51:A:N6 | 1:2:439:U:C2 | 2.64 | 0.50 |
| 37:j:41:THR:HG22 | 37:j:79:GLN:HG2 | 1.94 | 0.50 |
| 1:2:1783:U:H2' | 1:2:1784:G:H8 | 1.76 | 0.50 |
| 19:R:20:TYR:O | 19:R:24:LEU:HB2 | 2.12 | 0.50 |
| 34:g:32:ASN:HA | 34:g:48:LEU:HD12 | 1.94 | 0.50 |
| 3:B:43:VAL:HG11 | 3:B:68:VAL:HG11 | 1.93 | 0.50 |
| 5:D:178:ARG:HH21 | 5:D:179:GLN:HE22 | 1.60 | 0.50 |
| 19:R:23:LYS:HG2 | 19:R:23:LYS:O | 2.10 | 0.50 |
| 1:2:1588:G:OP1 | 21:T:91:HIS:HB2 | 2.11 | 0.50 |
| 33:f:133:HIS:HB2 | 33:f:136:ARG:HB2 | 1.93 | 0.50 |
| 1:2:141:U:H2' | 1:2:142:G:H8 | 1.77 | 0.49 |
| 4:C:173:ARG:HB3 | 4:C:204:SER:HB2 | 1.94 | 0.49 |
| 5:D:20:GLU:HG2 | 12:K:61:TRP:CE3 | 2.47 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:P:100:LYS:HG2 | 17:P:101:VAL:HG23 | 1.93 | 0.49 |
| 19:R:41:ILE:HD13 | 19:R:47:ARG:HG3 | 1.93 | 0.49 |
| 1:2:1069:C:H4' | 29:b:17:ARG:HD2 | 1.94 | 0.49 |
| 16:O:99:GLN:HG2 | 28:a:46:GLU:HB2 | 1.94 | 0.49 |
| 1:2:388:G:C2 | 1:2:408:C:C2 | 3.01 | 0.49 |
| 1:2:454:C:H3' | 1:2:455:A:H8 | 1.77 | 0.49 |
| 1:2:1389:A:H2' | 1:2:1390:U:C6 | 2.48 | 0.49 |
| 34:g:189:ASN:HB2 | 34:g:193:TYR:CZ | 2.47 | 0.49 |
| 34:g:260:THR:HG23 | 34:g:269:ILE:HG12 | 1.94 | 0.49 |
| 1:2:567:G:H4' | 25:X:90:ASP:HA | 1.93 | 0.49 |
| 1:2:768:C:H1' | 11:J:143:ILE:HG21 | 1.94 | 0.49 |
| 1:2:900:G:H2' | 1:2:901:G:O4' | 2.12 | 0.49 |
| 1:2:969:A:N6 | 1:2:970:A:C4 | 2.80 | 0.49 |
| 17:P:62:ALA:HA | 17:P:65:LEU:HD12 | 1.94 | 0.49 |
| 21:T:18:TYR:HB3 | 21:T:59:ALA:HB1 | 1.94 | 0.49 |
| 1:2:71:A:H3' | 1:2:72:A:C5' | 2.41 | 0.49 |
| 1:2:1330:A:OP1 | 19:R:45:ARG:NH2 | 2.42 | 0.49 |
| 6:E:198:ARG:HG2 | 6:E:208:VAL:HG12 | 1.95 | 0.49 |
| 13:L:8:GLN:NE2 | 13:L:14:GLN:H | 2.10 | 0.49 |
| 24:W:8:ALA:CA | 24:W:74:VAL:HG21 | 2.34 | 0.49 |
| 1:2:883:A:H2' | 1:2:884:G:H8 | 1.77 | 0.49 |
| 1:2:1066:C:H5'' | 3:B:150:VAL:HG23 | 1.94 | 0.49 |
| 1:2:1170:A:H2' | 1:2:1171:G:H8 | 1.74 | 0.49 |
| 1:2:1651:C:C2 | 1:2:1746:G:C2 | 3.01 | 0.49 |
| 1:2:1671:G:H2' | 1:2:1672:C:C6 | 2.48 | 0.49 |
| 2:A:120:LEU:HD11 | 2:A:144:ILE:HD12 | 1.94 | 0.49 |
| 9:H:134:GLU:HB2 | 9:H:155:ASN:HD21 | 1.77 | 0.49 |
| 37:j:85:ARG:HD2 | 37:j:105:ILE:HG22 | 1.93 | 0.49 |
| 1:2:1538:G:H1 | 1:2:1569:C:H42 | 1.60 | 0.49 |
| 22:U:51:VAL:HB | 22:U:94:GLU:HB2 | 1.94 | 0.49 |
| 26:Y:53:ASP:HB3 | 26:Y:96:LEU:HD21 | 1.94 | 0.49 |
| 1:2:698:U:H3 | 1:2:740:A:H61 | 1.60 | 0.49 |
| 5:D:72:LEU:HD22 | 12:K:65:TYR:HB3 | 1.94 | 0.49 |
| 6:E:106:LYS:HB3 | 6:E:108:ARG:HE | 1.78 | 0.49 |
| 26:Y:29:HIS:HB3 | 26:Y:32:ARG:O | 2.12 | 0.49 |
| 36:i:38:ILE:HG21 | 36:i:41:MET:HE2 | 1.94 | 0.49 |
| 1:2:590:A:H2' | 1:2:591:G:H8 | 1.75 | 0.49 |
| 1:2:1355:U:H2' | 1:2:1356:G:H8 | 1.77 | 0.49 |
| 1:2:1464:G:N2 | 1:2:1465:C:C2 | 2.81 | 0.49 |
| 1:2:1471:U:H5' | 7:F:192:ILE:HD11 | 1.93 | 0.49 |
| 1:2:782:G:N2 | 1:2:783:C:C2 | 2.81 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:B:176:VAL:C | 3:B:178:ASN:H | 2.21 | 0.49 |
| 10:I:148:ALA:C | 10:I:150:GLU:H | 2.21 | 0.49 |
| 1:2:473:A:H5'' | 1:2:473:A:H8 | 1.78 | 0.48 |
| 1:2:1292:U:O4 | 1:2:1293:G:C5 | 2.66 | 0.48 |
| 1:2:1472:G:H2' | 1:2:1473:A:C8 | 2.48 | 0.48 |
| 3:B:121:ILE:HG12 | 3:B:161:ILE:HG23 | 1.95 | 0.48 |
| 1:2:871:G:H2' | 1:2:872:U:O4' | 2.13 | 0.48 |
| 1:2:999:C:O2 | 1:2:999:C:O4' | 2.29 | 0.48 |
| 1:2:1499:C:C2 | 1:2:1505:G:C2 | 3.01 | 0.48 |
| 1:2:1586:G:H1 | 1:2:1606:U:H3 | 1.60 | 0.48 |
| 1:2:1653:A:H61 | 1:2:1743:G:H1' | 1.75 | 0.48 |
| 1:2:293:C:H2' | 1:2:294:A:H5'' | 1.95 | 0.48 |
| 1:2:60:U:H5' | 1:2:454:C:N4 | 2.28 | 0.48 |
| 1:2:228:U:H2' | 1:2:229:C:C6 | 2.48 | 0.48 |
| 1:2:298:A:C2' | 1:2:299:A:H5' | 2.42 | 0.48 |
| 1:2:609:G:N3 | 1:2:609:G:H2' | 2.27 | 0.48 |
| 8:G:32:ILE:HD11 | 8:G:63:MET:HB3 | 1.95 | 0.48 |
| 17:P:22:LEU:HD23 | 17:P:109:PRO:HG2 | 1.96 | 0.48 |
| 26:Y:27:VAL:HG11 | 26:Y:35:VAL:HG21 | 1.95 | 0.48 |
| 1:2:281:C:H2' | 1:2:282:U:O4' | 2.14 | 0.48 |
| 3:B:168:ILE:O | 3:B:172:LEU:HG | 2.12 | 0.48 |
| 10:I:104:ILE:HD13 | 10:I:168:ALA:HB3 | 1.94 | 0.48 |
| 1:2:1164:G:H2' | 1:2:1165:A:C8 | 2.48 | 0.48 |
| 6:E:140:VAL:HG22 | 6:E:146:THR:HG22 | 1.96 | 0.48 |
| 19:R:26:MET:HG2 | 19:R:62:GLN:HE22 | 1.78 | 0.48 |
| 22:U:34:LEU:HD11 | 22:U:89:ARG:HG3 | 1.96 | 0.48 |
| 25:X:11:SER:O | 25:X:13:ARG:N | 2.47 | 0.48 |
| 34:g:123:ILE:HB | 34:g:135:TRP:HB2 | 1.96 | 0.48 |
| 1:2:823:G:N2 | 1:2:848:C:C2 | 2.82 | 0.48 |
| 1:2:1267:G:H1 | 1:2:1439:C:N4 | 2.11 | 0.48 |
| 34:g:223:LYS:HA | 34:g:246:GLU:HG3 | 1.94 | 0.48 |
| 1:2:879:C:H2' | 1:2:880:A:O4' | 2.14 | 0.48 |
| 1:2:977:A:H2' | 1:2:978:A:O4' | 2.13 | 0.48 |
| 1:2:1174:U:H2' | 1:2:1175:G:C8 | 2.47 | 0.48 |
| 1:2:1502:G:OP2 | 21:T:99:SER:HB3 | 2.12 | 0.48 |
| 1:2:1577:U:O2' | 18:Q:139:GLN:HA | 2.13 | 0.48 |
| 1:2:1173:C:C2 | 1:2:1464:G:C2 | 3.02 | 0.48 |
| 1:2:1225:A:H5'' | 1:2:1226:A:O5' | 2.14 | 0.48 |
| 6:E:76:VAL:O | 6:E:77:ARG:HB2 | 2.13 | 0.48 |
| 21:T:83:ALA:HB1 | 21:T:91:HIS:HB3 | 1.94 | 0.48 |
| 1:2:542:C:H4' | 1:2:543:A:OP2 | 2.13 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:1252:U:H5'' | 14:M:39:ARG:HH22 | 1.79 | 0.47 |
| 2:A:3:LEU:HD13 | 23:V:39:VAL:HG11 | 1.95 | 0.47 |
| 21:T:6:VAL:HB | 21:T:66:TYR:CE1 | 2.49 | 0.47 |
| 29:b:50:ALA:O | 29:b:51:GLN:HB2 | 2.13 | 0.47 |
| 30:c:49:ARG:HG2 | 30:c:50:GLU:N | 2.29 | 0.47 |
| 1:2:480:A:C6 | 1:2:506:U:C4 | 2.95 | 0.47 |
| 1:2:700:C:N3 | 1:2:739:G:C6 | 2.83 | 0.47 |
| 1:2:732:G:H1' | 1:2:734:A:H61 | 1.78 | 0.47 |
| 1:2:989:C:H2' | 1:2:990:G:O4' | 2.14 | 0.47 |
| 1:2:1073:G:N2 | 1:2:1074:C:C2 | 2.82 | 0.47 |
| 1:2:1593:U:C2 | 1:2:1598:A:N6 | 2.73 | 0.47 |
| 2:A:189:PRO:HA | 23:V:44:ARG:HH22 | 1.78 | 0.47 |
| 13:L:99:ARG:NH1 | 25:X:7:ARG:O | 2.45 | 0.47 |
| 1:2:896:C:N4 | 1:2:913:G:C6 | 2.82 | 0.47 |
| 20:S:91:ASP:HB3 | 20:S:95:GLY:H | 1.79 | 0.47 |
| 34:g:157:VAL:HA | 34:g:174:PHE:HB3 | 1.95 | 0.47 |
| 1:2:1044:C:C2 | 1:2:1073:G:C2 | 3.01 | 0.47 |
| 5:D:61:GLU:H | 5:D:64:ARG:HB3 | 1.79 | 0.47 |
| 1:2:116:U:H3 | 1:2:299:A:H2 | 1.56 | 0.47 |
| 19:R:28:PHE:HZ | 19:R:48:ASN:ND2 | 2.12 | 0.47 |
| 20:S:48:LYS:HD3 | 21:T:35:ASP:HB3 | 1.95 | 0.47 |
| 37:j:30:ILE:HD11 | 37:j:85:ARG:HE | 1.78 | 0.47 |
| 4:C:144:ILE:CD1 | 4:C:196:ALA:HB1 | 2.40 | 0.47 |
| 11:J:170:GLY:HA2 | 11:J:174:ARG:HD3 | 1.96 | 0.47 |
| 26:Y:42:GLU:HG3 | 26:Y:52:LYS:HD2 | 1.97 | 0.47 |
| 1:2:18:C:H2' | 1:2:19:A:H8 | 1.78 | 0.47 |
| 1:2:588:C:O2 | 1:2:588:C:O4' | 2.32 | 0.47 |
| 1:2:1558:U:H2' | 1:2:1559:U:O4' | 2.15 | 0.47 |
| 1:2:1782:C:H2' | 1:2:1783:U:C6 | 2.49 | 0.47 |
| 5:D:53:THR:HA | 5:D:94:ARG:HH21 | 1.80 | 0.47 |
| 5:D:164:VAL:HA | 5:D:168:ILE:HD12 | 1.96 | 0.47 |
| 6:E:105:VAL:HG12 | 6:E:244:ILE:H | 1.80 | 0.47 |
| 7:F:74:HIS:CD2 | 7:F:109:LYS:HD2 | 2.49 | 0.47 |
| 1:2:218:A:H2' | 1:2:219:A:H8 | 1.79 | 0.47 |
| 1:2:690:A:H2' | 1:2:691:U:O4' | 2.15 | 0.47 |
| 1:2:1794:C:H5' | 1:2:1795:A:C2 | 2.50 | 0.47 |
| 1:2:1262:G:C2 | 1:2:1263:G:H1' | 2.50 | 0.47 |
| 1:2:1363:G:N1 | 1:2:1364:C:C4 | 2.83 | 0.47 |
| 3:B:119:THR:HG23 | 3:B:155:TYR:HD1 | 1.79 | 0.47 |
| 1:2:147:U:H5'' | 1:2:148:C:H5 | 1.78 | 0.47 |
| 11:J:148:VAL:HG11 | 11:J:156:ILE:HD11 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:89:G:C6 | 1:2:90:C:C4 | 3.02 | 0.46 |
| 1:2:767:U:O2 | 1:2:767:U:O4' | 2.32 | 0.46 |
| 1:2:1450:U:O2' | 17:P:79:HIS:HD2 | 1.97 | 0.46 |
| 2:A:66:ALA:HB2 | 23:V:37:ALA:HB2 | 1.96 | 0.46 |
| 21:T:37:VAL:HG22 | 21:T:38:LYS:H | 1.79 | 0.46 |
| 34:g:239:MET:HE3 | 34:g:273:GLU:HG3 | 1.97 | 0.46 |
| 1:2:140:A:C2 | 1:2:265:A:H4' | 2.45 | 0.46 |
| 1:2:209:A:H5'' | 1:2:209:A:H8 | 1.80 | 0.46 |
| 1:2:384:A:H5' | 10:I:25:ARG:HH22 | 1.79 | 0.46 |
| 1:2:557:U:H5' | 1:2:558:C:OP1 | 2.14 | 0.46 |
| 1:2:798:A:H2' | 1:2:799:U:C6 | 2.50 | 0.46 |
| 4:C:92:GLN:HG2 | 4:C:101:THR:HG22 | 1.97 | 0.46 |
| 7:F:40:GLN:HE22 | 18:Q:56:GLY:HA2 | 1.80 | 0.46 |
| 11:J:84:GLY:HA3 | 11:J:107:ARG:HH11 | 1.80 | 0.46 |
| 37:j:55:LEU:HA | 37:j:58:LEU:HD12 | 1.96 | 0.46 |
| 13:L:54:ILE:HG23 | 13:L:55:ASP:N | 2.30 | 0.46 |
| 16:O:99:GLN:NE2 | 28:a:45:VAL:HA | 2.30 | 0.46 |
| 22:U:17:VAL:HG13 | 22:U:96:PRO:HG3 | 1.98 | 0.46 |
| 1:2:10:G:C5 | 1:2:1631:A:C2 | 3.03 | 0.46 |
| 1:2:274:C:N4 | 1:2:275:C:N4 | 2.64 | 0.46 |
| 1:2:360:C:C2 | 1:2:383:G:C2 | 3.03 | 0.46 |
| 1:2:843:A:H2' | 1:2:844:G:C8 | 2.50 | 0.46 |
| 1:2:1179:C:H1' | 1:2:1458:A:H61 | 1.81 | 0.46 |
| 1:2:1437:C:N4 | 1:2:1438:C:N4 | 2.63 | 0.46 |
| 5:D:101:GLN:HG3 | 5:D:122:VAL:HG22 | 1.97 | 0.46 |
| 14:M:77:VAL:HG12 | 14:M:79:LEU:HB2 | 1.97 | 0.46 |
| 20:S:38:VAL:HG22 | 20:S:101:LEU:HD22 | 1.97 | 0.46 |
| 1:2:254:U:H2' | 1:2:255:A:H5' | 1.98 | 0.46 |
| 1:2:700:C:N4 | 1:2:738:G:H1 | 2.12 | 0.46 |
| 1:2:1353:G:C2 | 1:2:1354:C:C2 | 3.03 | 0.46 |
| 1:2:1466:U:H2' | 1:2:1467:A:O4' | 2.16 | 0.46 |
| 11:J:63:ASP:O | 11:J:66:ASP:HB3 | 2.15 | 0.46 |
| 15:N:35:GLU:HA | 15:N:38:ILE:HG12 | 1.98 | 0.46 |
| 18:Q:69:VAL:HG21 | 18:Q:81:ILE:HG12 | 1.96 | 0.46 |
| 20:S:88:ARG:HH22 | 20:S:108:LYS:HB3 | 1.81 | 0.46 |
| 20:S:112:ASP:HA | 20:S:115:ARG:HD2 | 1.98 | 0.46 |
| 1:2:52:U:H2' | 1:2:53:G:C8 | 2.50 | 0.46 |
| 1:2:75:U:H4' | 1:2:76:A:OP1 | 2.15 | 0.46 |
| 1:2:565:C:OP1 | 36:i:62:ARG:HG2 | 2.15 | 0.46 |
| 1:2:1120:C:O2 | 1:2:1126:G:C2 | 2.69 | 0.46 |
| 1:2:1655:U:H4' | 1:2:1656:G:O5' | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 22:U:22:ILE:HG21 | 22:U:100:VAL:HG11 | 1.97 | 0.46 |
| 28:a:45:VAL:HG21 | 28:a:53:LEU:HD22 | 1.97 | 0.46 |
| 1:2:160:U:O2' | 1:2:161:A:OP2 | 2.29 | 0.46 |
| 1:2:1590:A:C2 | 1:2:1591:A:C6 | 3.04 | 0.46 |
| 1:2:521:U:H5' | 1:2:522:G:OP2 | 2.16 | 0.46 |
| 11:J:61:THR:HA | 24:W:97:ARG:HH12 | 1.80 | 0.46 |
| 34:g:71:ASP:HB3 | 34:g:113:SER:HA | 1.98 | 0.46 |
| 1:2:89:G:N1 | 1:2:90:C:C2 | 2.84 | 0.46 |
| 1:2:544:A:H2' | 32:e:31:LYS:HD2 | 1.98 | 0.46 |
| 1:2:642:G:C2 | 1:2:692:C:C2 | 3.04 | 0.46 |
| 1:2:1082:G:H3' | 1:2:1083:A:H5'' | 1.98 | 0.46 |
| 1:2:1367:G:H5'' | 21:T:69:LYS:HG2 | 1.97 | 0.46 |
| 1:2:1754:A:H8 | 1:2:1754:A:C5' | 2.29 | 0.46 |
| 1:2:1038:A:O2' | 1:2:1039:G:O5' | 2.30 | 0.45 |
| 1:2:1177:G:H3' | 1:2:1178:G:C8 | 2.50 | 0.45 |
| 6:E:45:ILE:HA | 6:E:61:VAL:HG11 | 1.98 | 0.45 |
| 6:E:68:ARG:HH12 | 6:E:76:VAL:HG21 | 1.81 | 0.45 |
| 11:J:59:LEU:HD13 | 11:J:73:GLY:HA2 | 1.98 | 0.45 |
| 20:S:63:GLN:HA | 20:S:66:LEU:HD12 | 1.98 | 0.45 |
| 34:g:111:VAL:HA | 34:g:127:SER:CB | 2.45 | 0.45 |
| 1:2:981:U:H5'' | 1:2:981:U:H6 | 1.82 | 0.45 |
| 13:L:78:THR:HG22 | 13:L:84:ILE:HD11 | 1.97 | 0.45 |
| 22:U:34:LEU:CD1 | 22:U:89:ARG:HG3 | 2.46 | 0.45 |
| 24:W:6:VAL:HG12 | 24:W:34:ILE:CD1 | 2.38 | 0.45 |
| 1:2:1349:G:C2 | 1:2:1374:C:C2 | 3.04 | 0.45 |
| 8:G:2:LYS:HB3 | 8:G:108:VAL:HG22 | 1.98 | 0.45 |
| 10:I:113:TYR:CE1 | 10:I:153:ILE:HD11 | 2.51 | 0.45 |
| 1:2:45:U:HO2' | 1:2:46:A:H2' | 1.82 | 0.45 |
| 1:2:326:U:H2' | 1:2:327:A:C8 | 2.51 | 0.45 |
| 1:2:1671:G:C5 | 1:2:1672:C:C4 | 3.04 | 0.45 |
| 7:F:114:ARG:NH2 | 18:Q:43:ILE:HB | 2.29 | 0.45 |
| 15:N:40:TYR:HB3 | 15:N:50:ILE:HG12 | 1.98 | 0.45 |
| 1:2:637:U:O2 | 1:2:637:U:O4' | 2.34 | 0.45 |
| 1:2:1238:U:C1' | 1:2:1247:C:H42 | 2.16 | 0.45 |
| 1:2:1472:G:H2' | 1:2:1473:A:H8 | 1.81 | 0.45 |
| 3:B:48:VAL:HG21 | 3:B:61:LEU:HD11 | 1.98 | 0.45 |
| 22:U:96:PRO:HG2 | 22:U:99:ILE:HD13 | 1.97 | 0.45 |
| 32:e:46:ASN:HB3 | 32:e:48:THR:HG23 | 1.99 | 0.45 |
| 1:2:28:A:H2' | 1:2:29:U:O4' | 2.17 | 0.45 |
| 1:2:1091:A:O2' | 1:2:1092:A:H3' | 2.17 | 0.45 |
| 1:2:1180:U:H2' | 1:2:1181:U:O4' | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:1240:G:C1' | 17:P:79:HIS:HB2 | 2.45 | 0.45 |
| 1:2:1687:A:H2 | 1:2:1709:C:H42 | 1.64 | 0.45 |
| 17:P:17:TYR:HB3 | 17:P:18:LYS:H | 1.66 | 0.45 |
| 21:T:77:ASN:OD1 | 21:T:98:GLY:HA2 | 2.17 | 0.45 |
| 1:2:17:C:H2' | 1:2:18:C:C6 | 2.52 | 0.45 |
| 1:2:648:U:O2' | 1:2:649:U:C6 | 2.68 | 0.45 |
| 1:2:1588:G:C2 | 1:2:1589:C:C2 | 3.04 | 0.45 |
| 5:D:74:GLU:HG3 | 5:D:84:ILE:HD12 | 1.99 | 0.45 |
| 7:F:97:ASN:O | 7:F:100:MET:HB2 | 2.16 | 0.45 |
| 11:J:21:SER:HA | 11:J:24:LEU:HD12 | 1.98 | 0.45 |
| 1:2:414:C:O2 | 1:2:418:G:C2 | 2.70 | 0.45 |
| 1:2:556:G:C6 | 1:2:558:C:N4 | 2.84 | 0.45 |
| 1:2:637:U:OP2 | 24:W:32:LYS:HD2 | 2.17 | 0.45 |
| 1:2:969:A:C8 | 1:2:969:A:H3' | 2.52 | 0.45 |
| 1:2:1323:G:H4' | 2:A:113:ARG:HH21 | 1.81 | 0.45 |
| 1:2:1332:C:H2' | 1:2:1333:U:C6 | 2.51 | 0.45 |
| 1:2:1171:G:C2 | 1:2:1172:C:C2 | 3.05 | 0.45 |
| 1:2:1277:G:C6 | 1:2:1278:C:C4 | 3.05 | 0.45 |
| 1:2:1338:C:O2' | 1:2:1340:A:N7 | 2.44 | 0.45 |
| 1:2:1640:G:H5' | 35:h:1:MET:HB2 | 1.98 | 0.45 |
| 37:j:27:HIS:HB3 | 37:j:104:LYS:HG3 | 1.97 | 0.45 |
| 1:2:1171:G:C6 | 1:2:1172:C:C4 | 3.05 | 0.45 |
| 1:2:1537:G:O6 | 20:S:27:ASN:HB2 | 2.16 | 0.45 |
| 1:2:1637:C:H2' | 1:2:1638:C:O4' | 2.17 | 0.45 |
| 13:L:66:ILE:HG21 | 13:L:140:LEU:HD11 | 1.99 | 0.45 |
| 24:W:75:ILE:HD11 | 24:W:79:PHE:HD2 | 1.82 | 0.45 |
| 1:2:222:U:H2' | 1:2:223:C:C6 | 2.52 | 0.44 |
| 1:2:1073:G:N1 | 1:2:1074:C:C4 | 2.85 | 0.44 |
| 1:2:1402:C:H2' | 1:2:1403:G:H8 | 1.82 | 0.44 |
| 1:2:334:U:H4' | 13:L:129:ARG:HD3 | 1.98 | 0.44 |
| 1:2:1353:G:C6 | 1:2:1354:C:C4 | 3.05 | 0.44 |
| 4:C:159:LEU:HD22 | 4:C:226:THR:HG21 | 2.00 | 0.44 |
| 12:K:25:LYS:HD2 | 12:K:59:PHE:HZ | 1.82 | 0.44 |
| 17:P:124:THR:HA | 17:P:125:PRO:HD3 | 1.87 | 0.44 |
| 19:R:24:LEU:HA | 19:R:34:LEU:HD13 | 1.99 | 0.44 |
| 1:2:280:G:C2 | 1:2:281:C:C2 | 3.06 | 0.44 |
| 1:2:462:U:H2' | 1:2:463:A:C8 | 2.53 | 0.44 |
| 1:2:504:A:H5'' | 1:2:504:A:H8 | 1.82 | 0.44 |
| 1:2:947:G:C2 | 1:2:948:C:C2 | 3.05 | 0.44 |
| 1:2:1141:A:H5'' | 28:a:2:PRO:HB3 | 1.98 | 0.44 |
| 1:2:1494:U:O2 | 1:2:1509:G:O6 | 2.35 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:E:104:ASP:HB3 | 6:E:110:ALA:HB2 | 1.98 | 0.44 |
| 1:2:561:G:N2 | 1:2:583:C:C2 | 2.85 | 0.44 |
| 1:2:1064:A:H2' | 1:2:1065:C:O4' | 2.17 | 0.44 |
| 1:2:1268:U:O2 | 1:2:1268:U:H5' | 2.17 | 0.44 |
| 1:2:1290:G:H2' | 1:2:1291:G:H8 | 1.81 | 0.44 |
| 1:2:1291:G:C4 | 1:2:1292:U:O2 | 2.71 | 0.44 |
| 1:2:1441:U:H4' | 1:2:1444:A:N3 | 2.32 | 0.44 |
| 4:C:40:TRP:CE2 | 4:C:72:GLN:HG3 | 2.53 | 0.44 |
| 11:J:31:ALA:HA | 11:J:36:LEU:HD12 | 1.98 | 0.44 |
| 11:J:127:VAL:O | 11:J:131:GLN:HB2 | 2.18 | 0.44 |
| 12:K:60:SER:HB2 | 12:K:65:TYR:HE2 | 1.83 | 0.44 |
| 25:X:41:SER:HA | 25:X:42:PRO:HD3 | 1.87 | 0.44 |
| 1:2:186:G:H22 | 1:2:196:A:H2' | 1.82 | 0.44 |
| 1:2:775:G:C6 | 1:2:785:C:N4 | 2.86 | 0.44 |
| 1:2:1175:G:C2 | 1:2:1176:C:C2 | 3.05 | 0.44 |
| 1:2:1279:C:O2' | 22:U:70:THR:HG22 | 2.17 | 0.44 |
| 35:h:5:TRP:HA | 35:h:5:TRP:CE3 | 2.52 | 0.44 |
| 1:2:93:A:H1' | 6:E:3:ARG:HB3 | 1.99 | 0.44 |
| 1:2:1396:U:H3' | 1:2:1397:C:H5' | 2.00 | 0.44 |
| 1:2:1613:C:C5 | 7:F:83:ARG:HA | 2.52 | 0.44 |
| 1:2:1673:C:C2 | 1:2:1725:G:C2 | 3.06 | 0.44 |
| 5:D:109:LEU:HD21 | 5:D:115:ILE:HG23 | 1.99 | 0.44 |
| 10:I:42:ARG:HB3 | 10:I:58:LEU:O | 2.18 | 0.44 |
| 25:X:50:LYS:HG3 | 25:X:103:LEU:HD23 | 2.00 | 0.44 |
| 26:Y:128:LYS:O | 26:Y:132:ARG:HB2 | 2.17 | 0.44 |
| 30:c:10:ALA:HA | 30:c:32:PHE:HA | 2.00 | 0.44 |
| 1:2:14:C:C2 | 1:2:1140:G:C2 | 3.05 | 0.44 |
| 1:2:72:A:H4' | 1:2:73:U:OP1 | 2.16 | 0.44 |
| 1:2:480:A:H61 | 1:2:506:U:H3 | 1.66 | 0.44 |
| 1:2:772:G:C6 | 1:2:773:C:N3 | 2.86 | 0.44 |
| 1:2:897:A:N3 | 1:2:898:G:H1' | 2.32 | 0.44 |
| 1:2:89:G:C2 | 1:2:90:C:C2 | 3.06 | 0.44 |
| 1:2:221:A:N6 | 1:2:838:U:H3 | 2.12 | 0.44 |
| 1:2:279:U:H4' | 1:2:280:G:O5' | 2.18 | 0.44 |
| 1:2:389:G:N3 | 1:2:389:G:H5'' | 2.33 | 0.44 |
| 1:2:417:G:C8 | 8:G:59:GLN:HG2 | 2.53 | 0.44 |
| 1:2:566:A:N1 | 1:2:582:C:H1' | 2.33 | 0.44 |
| 1:2:1402:C:H2' | 1:2:1403:G:C8 | 2.52 | 0.44 |
| 16:O:24:ASN:HA | 16:O:55:SER:HB3 | 1.99 | 0.44 |
| 18:Q:48:VAL:HG22 | 18:Q:78:VAL:HG13 | 2.00 | 0.44 |
| 20:S:25:ASN:HD21 | 27:Z:41:VAL:HG13 | 1.82 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:2:51:A:C6 | 1:2:439:U:N3 | 2.68 | 0.44 |
| 1:2:592:U:H4' | 1:2:594:G:H4' | 1.98 | 0.44 |
| 1:2:765:G:C6 | 11:J:149:ARG:HB2 | 2.52 | 0.44 |
| 1:2:842:U:H2' | 1:2:843:A:C8 | 2.52 | 0.44 |
| 1:2:1137:A:H2' | 1:2:1138:A:H8 | 1.80 | 0.44 |
| 1:2:1178:G:C6 | 1:2:1179:C:N3 | 2.86 | 0.44 |
| 1:2:1290:G:O5' | 1:2:1290:G:H8 | 2.01 | 0.44 |
| 1:2:1603:G:C6 | 1:2:1604:C:C4 | 3.05 | 0.44 |
| 3:B:103:MET:HE1 | 3:B:212:ILE:O | 2.18 | 0.44 |
| 12:K:46:LEU:HD13 | 12:K:66:TYR:CD2 | 2.53 | 0.44 |
| 13:L:14:GLN:HB3 | 13:L:54:ILE:HG21 | 1.98 | 0.44 |
| 17:P:21:ASP:H | 17:P:24:LYS:HD2 | 1.82 | 0.44 |
| 25:X:5:LYS:H | 25:X:5:LYS:HG3 | 1.62 | 0.44 |
| 25:X:109:ARG:HB3 | 25:X:112:LYS:HB2 | 2.00 | 0.44 |
| 1:2:151:U:H3 | 1:2:161:A:H61 | 1.66 | 0.43 |
| 1:2:309:C:C2 | 1:2:356:G:C2 | 3.06 | 0.43 |
| 1:2:885:U:H2' | 1:2:886:A:O4' | 2.18 | 0.43 |
| 1:2:1178:G:C2 | 1:2:1179:C:C2 | 3.06 | 0.43 |
| 1:2:1277:G:C2 | 1:2:1278:C:C2 | 3.06 | 0.43 |
| 8:G:14:LYS:HZ1 | 8:G:122:GLU:HB2 | 1.83 | 0.43 |
| 18:Q:51:PRO:HA | 18:Q:109:PHE:HE1 | 1.83 | 0.43 |
| 26:Y:37:LYS:HA | 26:Y:40:LEU:HD12 | 2.00 | 0.43 |
| 37:j:55:LEU:HD12 | 37:j:78:ILE:HG23 | 1.99 | 0.43 |
| 1:2:1270:G:H2' | 1:2:1271:U:C6 | 2.53 | 0.43 |
| 1:2:1481:A:H2' | 1:2:1482:G:C8 | 2.52 | 0.43 |
| 1:2:1486:G:H3' | 1:2:1513:A:H61 | 1.82 | 0.43 |
| 1:2:1589:C:C2 | 1:2:1590:A:C8 | 3.07 | 0.43 |
| 20:S:38:VAL:HG11 | 20:S:73:MET:HE1 | 2.00 | 0.43 |
| 1:2:10:G:C6 | 1:2:11:A:C5 | 3.06 | 0.43 |
| 1:2:1059:U:H2' | 1:2:1060:U:H4' | 2.00 | 0.43 |
| 1:2:1178:G:C6 | 1:2:1179:C:C4 | 3.05 | 0.43 |
| 1:2:1315:G:C2 | 1:2:1316:C:C2 | 3.07 | 0.43 |
| 1:2:1774:A:H2' | 1:2:1775:G:C8 | 2.54 | 0.43 |
| 9:H:22:GLN:HA | 9:H:25:ILE:HD12 | 2.00 | 0.43 |
| 9:H:102:PRO:HD2 | 9:H:112:ARG:HH21 | 1.84 | 0.43 |
| 24:W:16:ASN:O | 24:W:20:THR:HG22 | 2.18 | 0.43 |
| 1:2:516:U:H3 | 1:2:534:A:N6 | 2.13 | 0.43 |
| 1:2:585:G:C2 | 1:2:586:C:C2 | 3.07 | 0.43 |
| 1:2:1736:U:H2' | 1:2:1737:C:C6 | 2.53 | 0.43 |
| 1:2:1754:A:H5' | 1:2:1754:A:C8 | 2.52 | 0.43 |
| 3:B:137:ILE:HG22 | 3:B:215:VAL:HG13 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:F:135:VAL:HA | 7:F:200:LEU:HD22 | 2.01 | 0.43 |
| 23:V:38:GLN:HG3 | 23:V:49:GLU:HG2 | 1.99 | 0.43 |
| 1:2:1233:A:H4' | 33:f:143:HIS:ND1 | 2.33 | 0.43 |
| 1:2:1234:C:H1' | 33:f:144:SER:HB2 | 2.00 | 0.43 |
| 1:2:1603:G:C2 | 1:2:1604:C:C2 | 3.07 | 0.43 |
| 3:B:110:LEU:HD13 | 3:B:213:ARG:HD2 | 2.00 | 0.43 |
| 1:2:1118:G:H5'' | 1:2:1118:G:H8 | 1.83 | 0.43 |
| 2:A:68:PRO:HD2 | 2:A:119:ARG:HH12 | 1.84 | 0.43 |
| 14:M:44:ALA:HB1 | 14:M:50:GLY:HA3 | 2.00 | 0.43 |
| 16:O:64:ALA:HB3 | 16:O:104:ALA:HB3 | 2.00 | 0.43 |
| 20:S:116:LEU:HA | 20:S:119:ILE:HG12 | 2.01 | 0.43 |
| 1:2:392:C:H2' | 1:2:393:C:C6 | 2.53 | 0.43 |
| 1:2:1154:G:C2 | 1:2:1622:C:C2 | 3.07 | 0.43 |
| 1:2:1156:A:H2' | 1:2:1159:A:N7 | 2.33 | 0.43 |
| 1:2:1457:C:H5' | 20:S:131:LEU:HD22 | 2.01 | 0.43 |
| 1:2:1675:C:H2' | 1:2:1676:A:O4' | 2.19 | 0.43 |
| 3:B:208:GLN:HG2 | 3:B:209:ASN:N | 2.34 | 0.43 |
| 9:H:31:SER:CB | 9:H:32:PRO:HD3 | 2.49 | 0.43 |
| 18:Q:6:SER:HA | 18:Q:22:VAL:O | 2.18 | 0.43 |
| 27:Z:54:ALA:H | 27:Z:55:PRO:HD2 | 1.82 | 0.43 |
| 36:i:104:LYS:HD2 | 36:i:111:GLU:HG2 | 2.01 | 0.43 |
| 1:2:537:A:H2 | 1:2:539:G:H22 | 1.60 | 0.43 |
| 1:2:1454:C:O2 | 1:2:1454:C:O4' | 2.34 | 0.43 |
| 1:2:1486:G:O2' | 1:2:1492:C:O2 | 2.35 | 0.43 |
| 2:A:193:GLN:HA | 2:A:194:PRO:HD3 | 1.81 | 0.43 |
| 1:2:155:A:H2' | 1:2:156:A:O4' | 2.19 | 0.43 |
| 1:2:1497:G:C2 | 1:2:1498:C:C2 | 3.07 | 0.43 |
| 1:2:1791:G:O2' | 28:a:5:ARG:NH2 | 2.52 | 0.43 |
| 10:I:83:TYR:HD2 | 10:I:101:ILE:HD13 | 1.82 | 0.43 |
| 1:2:612:G:H4' | 1:2:613:C:OP1 | 2.19 | 0.43 |
| 1:2:1408:A:H2' | 1:2:1409:A:C8 | 2.54 | 0.43 |
| 1:2:1590:A:C2 | 1:2:1602:U:N3 | 2.84 | 0.43 |
| 8:G:163:THR:HG22 | 8:G:168:SER:HA | 2.01 | 0.43 |
| 17:P:20:VAL:HG21 | 17:P:28:MET:HE1 | 2.00 | 0.43 |
| 21:T:28:LEU:O | 21:T:29:GLU:HB2 | 2.17 | 0.43 |
| 24:W:24:GLN:HA | 24:W:63:VAL:O | 2.19 | 0.43 |
| 29:b:20:LYS:O | 29:b:21:LEU:HB2 | 2.19 | 0.43 |
| 36:i:38:ILE:HD12 | 36:i:75:ASP:HB2 | 2.00 | 0.43 |
| 1:2:452:U:O2 | 1:2:452:U:C2' | 2.66 | 0.42 |
| 1:2:1216:A:H4' | 12:K:44:LYS:HD3 | 2.01 | 0.42 |
| 6:E:17:HIS:HB3 | 6:E:108:ARG:HA | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 34:g:90:LEU:HB2 | 34:g:104:PHE:HB2 | 2.01 | 0.42 |
| 1:2:1203:A:N3 | 1:2:1203:A:H2' | 2.35 | 0.42 |
| 1:2:1542:U:H4' | 20:S:132:ARG:HH11 | 1.84 | 0.42 |
| 1:2:1620:G:C2 | 1:2:1621:C:C2 | 3.07 | 0.42 |
| 1:2:1661:G:C6 | 1:2:1662:C:C4 | 3.07 | 0.42 |
| 1:2:1671:G:C6 | 1:2:1672:C:N4 | 2.87 | 0.42 |
| 6:E:18:TRP:CZ2 | 6:E:43:PRO:HD3 | 2.54 | 0.42 |
| 14:M:25:LEU:HD13 | 14:M:92:ALA:HB2 | 2.02 | 0.42 |
| 15:N:55:ARG:HA | 15:N:60:VAL:O | 2.19 | 0.42 |
| 28:a:35:ALA:HB3 | 28:a:37:LYS:HE2 | 2.01 | 0.42 |
| 28:a:37:LYS:HB3 | 28:a:70:LYS:HE2 | 2.00 | 0.42 |
| 36:i:96:ASN:HB3 | 36:i:97:LEU:H | 1.65 | 0.42 |
| 1:2:779:A:H3' | 1:2:780:A:H4' | 2.01 | 0.42 |
| 10:I:107:THR:N | 10:I:108:PRO:CD | 2.83 | 0.42 |
| 16:O:121:VAL:HA | 16:O:122:PRO:HD3 | 1.93 | 0.42 |
| 1:2:50:C:N3 | 1:2:429:G:C6 | 2.88 | 0.42 |
| 1:2:696:C:H4' | 1:2:697:C:OP1 | 2.19 | 0.42 |
| 1:2:1175:G:C6 | 1:2:1176:C:C4 | 3.08 | 0.42 |
| 1:2:1343:A:C2 | 1:2:1344:A:C6 | 3.07 | 0.42 |
| 1:2:1391:C:H2' | 1:2:1392:G:H8 | 1.84 | 0.42 |
| 1:2:1496:G:O6 | 1:2:1507:C:N4 | 2.52 | 0.42 |
| 1:2:1542:U:H5' | 20:S:136:GLN:HE22 | 1.85 | 0.42 |
| 2:A:50:VAL:HG22 | 19:R:109:LEU:HD21 | 2.01 | 0.42 |
| 3:B:70:LEU:HD13 | 3:B:82:ARG:HG2 | 2.01 | 0.42 |
| 7:F:151:VAL:HG11 | 30:c:66:LEU:HB3 | 2.01 | 0.42 |
| 9:H:67:LEU:HD13 | 9:H:94:ALA:HB2 | 2.01 | 0.42 |
| 21:T:28:LEU:HD21 | 21:T:30:VAL:HG23 | 2.01 | 0.42 |
| 25:X:24:TRP:HE3 | 25:X:30:LYS:HG2 | 1.85 | 0.42 |
| 1:2:240:U:H5'' | 1:2:240:U:H6 | 1.84 | 0.42 |
| 1:2:699:U:H2' | 1:2:700:C:C6 | 2.54 | 0.42 |
| 1:2:1073:G:C6 | 1:2:1074:C:N4 | 2.88 | 0.42 |
| 1:2:1377:C:H1' | 18:Q:19:VAL:HG11 | 2.00 | 0.42 |
| 3:B:92:GLN:HB2 | 3:B:95:ASN:HB2 | 2.00 | 0.42 |
| 1:2:15:U:H2' | 1:2:16:G:O4' | 2.19 | 0.42 |
| 1:2:52:U:H2' | 1:2:53:G:H8 | 1.84 | 0.42 |
| 1:2:121:U:O2 | 1:2:122:U:C2 | 2.73 | 0.42 |
| 1:2:520:A:H2' | 1:2:521:U:O4' | 2.19 | 0.42 |
| 1:2:878:G:C2 | 1:2:879:C:C2 | 3.07 | 0.42 |
| 1:2:1500:G:N7 | 21:T:102:ARG:NH2 | 2.66 | 0.42 |
| 8:G:14:LYS:NZ | 8:G:122:GLU:HB2 | 2.35 | 0.42 |
| 24:W:26:LEU:HB2 | 29:b:7:LEU:HD13 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:53:G:C2 | 1:2:54:C:C2 | 3.07 | 0.42 |
| 1:2:737:A:O2' | 1:2:738:G:H8 | 2.02 | 0.42 |
| 1:2:782:G:C2 | 1:2:783:C:C2 | 3.08 | 0.42 |
| 1:2:917:U:H4' | 16:O:18:ARG:HD3 | 2.02 | 0.42 |
| 1:2:1292:U:O4 | 1:2:1293:G:C4 | 2.72 | 0.42 |
| 1:2:1497:G:C6 | 1:2:1498:C:C4 | 3.08 | 0.42 |
| 1:2:1770:C:H5'' | 1:2:1770:C:H6 | 1.83 | 0.42 |
| 14:M:55:LEU:HB3 | 14:M:81:LYS:HG2 | 2.01 | 0.42 |
| 34:g:219:ALA:HA | 34:g:229:VAL:HA | 2.02 | 0.42 |
| 35:h:2:ARG:HB2 | 35:h:5:TRP:CD1 | 2.55 | 0.42 |
| 1:2:454:C:H3' | 1:2:455:A:C8 | 2.52 | 0.42 |
| 1:2:1443:G:C2 | 33:f:87:THR:HB | 2.54 | 0.42 |
| 1:2:1527:C:O5' | 1:2:1527:C:H6 | 2.03 | 0.42 |
| 1:2:1533:U:H4' | 1:2:1534:G:C2 | 2.54 | 0.42 |
| 1:2:1560:G:C2 | 1:2:1561:C:C2 | 3.08 | 0.42 |
| 1:2:1586:G:C6 | 1:2:1587:C:C4 | 3.07 | 0.42 |
| 2:A:21:ARG:HD2 | 2:A:24:LEU:HD13 | 2.01 | 0.42 |
| 2:A:131:GLN:HE21 | 2:A:135:GLU:HG3 | 1.84 | 0.42 |
| 10:I:107:THR:HG22 | 10:I:110:ARG:HH21 | 1.85 | 0.42 |
| 1:2:473:A:H5'' | 1:2:473:A:C8 | 2.55 | 0.42 |
| 1:2:1132:A:H2' | 1:2:1133:C:O4' | 2.19 | 0.42 |
| 1:2:1307:G:C2 | 1:2:1308:C:C2 | 3.08 | 0.42 |
| 1:2:1654:U:H3 | 1:2:1742:A:N6 | 2.18 | 0.42 |
| 1:2:1661:G:C2 | 1:2:1662:C:C2 | 3.08 | 0.42 |
| 1:2:1679:A:H2 | 1:2:1718:G:N2 | 2.16 | 0.42 |
| 2:A:176:LEU:O | 2:A:180:GLU:HG2 | 2.20 | 0.42 |
| 3:B:36:SER:HA | 3:B:41:ARG:HD2 | 2.02 | 0.42 |
| 9:H:9:LEU:HD21 | 9:H:17:GLU:HB3 | 2.00 | 0.42 |
| 11:J:110:GLN:HE22 | 11:J:126:ARG:HD3 | 1.84 | 0.42 |
| 1:2:896:C:C4 | 1:2:913:G:C6 | 3.07 | 0.42 |
| 1:2:935:G:C2 | 1:2:936:C:C2 | 3.08 | 0.42 |
| 1:2:1070:U:O3' | 29:b:19:HIS:HB2 | 2.19 | 0.42 |
| 1:2:1203:A:C2 | 31:d:10:HIS:HE1 | 2.38 | 0.42 |
| 1:2:1544:G:H2' | 1:2:1545:A:O4' | 2.19 | 0.42 |
| 1:2:1564:U:H5'' | 20:S:39:GLY:H | 1.84 | 0.42 |
| 1:2:1598:A:H1' | 1:2:1599:G:H5' | 2.02 | 0.42 |
| 2:A:37:VAL:HG13 | 2:A:149:LEU:HD23 | 2.01 | 0.42 |
| 2:A:90:ALA:HA | 2:A:95:ALA:HB3 | 2.02 | 0.42 |
| 10:I:58:LEU:H | 10:I:58:LEU:HG | 1.69 | 0.42 |
| 22:U:39:ALA:HA | 22:U:42:ILE:HG12 | 2.02 | 0.42 |
| 36:i:98:ASP:O | 36:i:101:ARG:HG2 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:53:G:C6 | 1:2:54:C:C4 | 3.07 | 0.41 |
| 1:2:147:U:H3' | 1:2:148:C:H6 | 1.83 | 0.41 |
| 1:2:623:G:C2 | 1:2:624:C:C2 | 3.08 | 0.41 |
| 6:E:18:TRP:HB3 | 6:E:20:LEU:HG | 2.02 | 0.41 |
| 6:E:141:THR:C | 6:E:143:ASP:H | 2.27 | 0.41 |
| 8:G:21:GLU:HB2 | 8:G:25:ARG:HH12 | 1.84 | 0.41 |
| 8:G:102:VAL:HG13 | 8:G:106:LEU:HD22 | 2.01 | 0.41 |
| 9:H:46:ILE:CG1 | 9:H:60:VAL:HG12 | 2.49 | 0.41 |
| 11:J:163:PRO:HG3 | 11:J:169:PRO:O | 2.20 | 0.41 |
| 13:L:84:ILE:HD13 | 13:L:111:VAL:HG21 | 2.02 | 0.41 |
| 34:g:129:ASP:O | 34:g:130:LYS:HB2 | 2.19 | 0.41 |
| 1:2:886:A:C6 | 1:2:887:U:C4 | 3.08 | 0.41 |
| 1:2:1094:U:H4' | 24:W:19:LYS:NZ | 2.34 | 0.41 |
| 1:2:1213:U:H2' | 1:2:1214:C:C6 | 2.55 | 0.41 |
| 1:2:1673:C:C2 | 1:2:1725:G:N2 | 2.89 | 0.41 |
| 6:E:66:MET:C | 6:E:68:ARG:H | 2.28 | 0.41 |
| 10:I:38:ILE:HA | 10:I:60:ILE:O | 2.20 | 0.41 |
| 18:Q:18:ALA:HB2 | 18:Q:69:VAL:HG13 | 2.01 | 0.41 |
| 25:X:107:PHE:CE1 | 25:X:114:LYS:HD2 | 2.55 | 0.41 |
| 1:2:44:U:H3' | 1:2:45:U:H5' | 2.02 | 0.41 |
| 1:2:431:G:C6 | 1:2:432:C:N3 | 2.88 | 0.41 |
| 1:2:568:C:H41 | 25:X:69:ARG:HH12 | 1.68 | 0.41 |
| 1:2:751:G:H2' | 1:2:752:A:C8 | 2.56 | 0.41 |
| 1:2:1397:C:H4' | 1:2:1398:A:O5' | 2.20 | 0.41 |
| 3:B:149:GLN:HE22 | 3:B:154:SER:HB3 | 1.86 | 0.41 |
| 5:D:75:LYS:HB3 | 12:K:22:VAL:HB | 2.02 | 0.41 |
| 18:Q:54:LEU:HD11 | 18:Q:112:TYR:HB3 | 2.02 | 0.41 |
| 34:g:292:GLN:HB2 | 34:g:293:ASP:H | 1.57 | 0.41 |
| 1:2:16:G:C6 | 1:2:17:C:N4 | 2.89 | 0.41 |
| 1:2:69:G:C2 | 1:2:70:C:C2 | 3.08 | 0.41 |
| 1:2:73:U:H4' | 1:2:74:U:OP1 | 2.21 | 0.41 |
| 1:2:86:A:H2' | 1:2:87:C:H6 | 1.85 | 0.41 |
| 1:2:624:C:H2' | 1:2:625:U:C6 | 2.55 | 0.41 |
| 1:2:1278:C:H2' | 1:2:1279:C:O4' | 2.20 | 0.41 |
| 1:2:1332:C:H2' | 1:2:1333:U:H6 | 1.86 | 0.41 |
| 1:2:1726:U:H2' | 1:2:1727:C:C6 | 2.55 | 0.41 |
| 17:P:17:TYR:HA | 17:P:112:VAL:HG11 | 2.02 | 0.41 |
| 21:T:7:ARG:HE | 21:T:67:LEU:HD22 | 1.85 | 0.41 |
| 25:X:92:CYS:HA | 25:X:95:PHE:HD2 | 1.85 | 0.41 |
| 34:g:35:VAL:HG22 | 34:g:43:LEU:HD22 | 2.02 | 0.41 |
| 1:2:4:C:H4' | 4:C:186:SER:HB3 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:2:268:G:C2 | 1:2:269:C:C2 | 3.08 | 0.41 |
| 1:2:556:G:N2 | 1:2:558:C:C2 | 2.88 | 0.41 |
| 1:2:628:U:O4 | 1:2:969:A:N7 | 2.54 | 0.41 |
| 1:2:884:G:H2' | 1:2:885:U:O4' | 2.20 | 0.41 |
| 1:2:886:A:H5'' | 16:O:120:PRO:HB3 | 2.03 | 0.41 |
| 1:2:1460:G:C6 | 1:2:1461:C:C4 | 3.09 | 0.41 |
| 2:A:170:ILE:H | 2:A:170:ILE:HG12 | 1.57 | 0.41 |
| 4:C:174:LEU:HD23 | 4:C:203:THR:HG22 | 2.01 | 0.41 |
| 20:S:89:GLN:C | 20:S:91:ASP:H | 2.28 | 0.41 |
| 1:2:93:A:C6 | 1:2:397:G:C6 | 3.09 | 0.41 |
| 1:2:280:G:C6 | 1:2:281:C:C4 | 3.09 | 0.41 |
| 1:2:328:G:H2' | 1:2:329:G:H8 | 1.85 | 0.41 |
| 1:2:504:A:H8 | 1:2:504:A:C5' | 2.33 | 0.41 |
| 1:2:609:G:H5'' | 1:2:610:U:C5 | 2.56 | 0.41 |
| 1:2:1080:A:O2' | 1:2:1081:C:H2' | 2.20 | 0.41 |
| 1:2:1202:A:H3' | 1:2:1203:A:H8 | 1.85 | 0.41 |
| 1:2:1474:C:H2' | 1:2:1475:G:C8 | 2.54 | 0.41 |
| 1:2:1480:C:H5 | 1:2:1523:A:H62 | 1.66 | 0.41 |
| 1:2:1560:G:C6 | 1:2:1561:C:C4 | 3.09 | 0.41 |
| 2:A:157:ASP:O | 2:A:158:VAL:HB | 2.20 | 0.41 |
| 9:H:27:LEU:HD11 | 9:H:80:GLU:HB3 | 2.02 | 0.41 |
| 24:W:14:ILE:HD11 | 24:W:27:ILE:HD11 | 2.03 | 0.41 |
| 32:e:29:GLN:O | 32:e:31:LYS:HE2 | 2.20 | 0.41 |
| 1:2:69:G:C6 | 1:2:70:C:C4 | 3.09 | 0.41 |
| 1:2:886:A:C2 | 1:2:925:A:C2 | 3.08 | 0.41 |
| 1:2:952:G:H2' | 1:2:953:G:C8 | 2.56 | 0.41 |
| 1:2:1218:A:N6 | 1:2:1263:G:O2' | 2.53 | 0.41 |
| 1:2:1632:C:H2' | 1:2:1632:C:O2 | 2.21 | 0.41 |
| 20:S:86:LEU:HA | 20:S:99:HIS:HD2 | 1.85 | 0.41 |
| 34:g:307:THR:HG22 | 34:g:321:GLN:HG2 | 2.03 | 0.41 |
| 1:2:10:G:C6 | 1:2:1631:A:H2 | 2.37 | 0.41 |
| 1:2:399:A:C2 | 10:I:26:LYS:HG3 | 2.55 | 0.41 |
| 1:2:1679:A:H5' | 1:2:1680:U:C6 | 2.55 | 0.41 |
| 5:D:73:ILE:HG22 | 5:D:84:ILE:HD13 | 2.03 | 0.41 |
| 14:M:45:LEU:HD13 | 14:M:71:LEU:HB3 | 2.02 | 0.41 |
| 20:S:88:ARG:HG3 | 20:S:91:ASP:HA | 2.02 | 0.41 |
| 34:g:116:ILE:HG12 | 34:g:120:SER:HA | 2.03 | 0.41 |
| 1:2:67:A:N6 | 1:2:83:G:O2' | 2.54 | 0.41 |
| 1:2:360:C:N3 | 1:2:383:G:C2 | 2.88 | 0.41 |
| 1:2:362:G:C2 | 1:2:381:C:C2 | 3.09 | 0.41 |
| 1:2:367:U:C2' | 1:2:368:A:H5' | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:2:1012:A:H2' | 1:2:1013:G:O4' | 2.21 | 0.41 |
| 1:2:1144:U:C4 | 1:2:1145:G:N7 | 2.89 | 0.41 |
| 1:2:1746:G:H2' | 1:2:1747:A:C8 | 2.55 | 0.41 |
| 1:2:1796:U:H4' | 1:2:1797:U:O5' | 2.21 | 0.41 |
| 3:B:23:PRO:HB3 | 3:B:26:ARG:NH2 | 2.36 | 0.41 |
| 9:H:114:ARG:HA | 9:H:117:THR:HG23 | 2.02 | 0.41 |
| 10:I:3:ILE:HD11 | 10:I:32:GLN:HE21 | 1.86 | 0.41 |
| 13:L:99:ARG:HG2 | 25:X:9:LEU:HA | 2.02 | 0.41 |
| 16:O:87:GLY:HA3 | 16:O:120:PRO:HD2 | 2.01 | 0.41 |
| 17:P:30:THR:HA | 17:P:33:PHE:CD2 | 2.55 | 0.41 |
| 18:Q:38:LEU:O | 18:Q:40:GLN:N | 2.53 | 0.41 |
| 21:T:52:GLY:C | 21:T:54:PHE:H | 2.29 | 0.41 |
| 35:h:5:TRP:HA | 35:h:5:TRP:HE3 | 1.86 | 0.41 |
| 1:2:158:U:H6 | 26:Y:117:LYS:HA | 1.85 | 0.41 |
| 1:2:1031:G:C6 | 1:2:1032:C:C4 | 3.09 | 0.41 |
| 1:2:1067:C:H2' | 1:2:1068:A:H8 | 1.86 | 0.41 |
| 1:2:1118:G:H5'' | 1:2:1118:G:C8 | 2.56 | 0.41 |
| 6:E:57:ASN:O | 6:E:61:VAL:HG23 | 2.21 | 0.41 |
| 6:E:125:LYS:HB3 | 6:E:142:HIS:HB2 | 2.03 | 0.41 |
| 8:G:5:ILE:HD13 | 8:G:16:ILE:HD12 | 2.02 | 0.41 |
| 37:j:32:GLN:HA | 37:j:38:THR:HG22 | 2.02 | 0.41 |
| 1:2:1143:U:O2 | 1:2:1144:U:C2 | 2.74 | 0.40 |
| 8:G:14:LYS:HD3 | 8:G:16:ILE:HD11 | 2.04 | 0.40 |
| 11:J:70:LEU:O | 11:J:74:ASN:HB2 | 2.20 | 0.40 |
| 31:d:21:CYS:HB3 | 31:d:25:GLY:H | 1.86 | 0.40 |
| 1:2:284:G:C2 | 1:2:285:C:C2 | 3.09 | 0.40 |
| 1:2:1588:G:C6 | 1:2:1589:C:C4 | 3.09 | 0.40 |
| 2:A:62:ARG:HG2 | 2:A:62:ARG:NH1 | 2.19 | 0.40 |
| 6:E:129:VAL:HG22 | 6:E:139:VAL:HG23 | 2.03 | 0.40 |
| 7:F:64:ILE:HG23 | 7:F:91:ILE:HG21 | 2.03 | 0.40 |
| 7:F:91:ILE:H | 7:F:91:ILE:HG13 | 1.58 | 0.40 |
| 7:F:218:GLU:O | 7:F:221:ARG:HG2 | 2.21 | 0.40 |
| 18:Q:52:LEU:HA | 18:Q:60:PHE:CE1 | 2.56 | 0.40 |
| 1:2:403:G:C2 | 1:2:404:C:C2 | 3.09 | 0.40 |
| 6:E:122:LYS:HB2 | 6:E:164:LEU:HD12 | 2.03 | 0.40 |
| 7:F:185:ALA:HB2 | 7:F:192:ILE:HG23 | 2.01 | 0.40 |
| 27:Z:57:TYR:H | 27:Z:103:ARG:HG2 | 1.86 | 0.40 |
| 1:2:108:A:H2' | 1:2:109:G:C8 | 2.56 | 0.40 |
| 1:2:332:A:H5' | 10:I:48:THR:HB | 2.04 | 0.40 |
| 1:2:855:A:H62 | 9:H:97:ARG:H | 1.69 | 0.40 |
| 2:A:122:ILE:HA | 2:A:144:ILE:O | 2.22 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 8:G:121:ILE:HB | 8:G:124:ILE:HG22 | 2.03 | 0.40 |
| 8:G:197:ASN:O | 8:G:201:GLN:HG2 | 2.22 | 0.40 |
| 1:2:2:A:C2 | 4:C:175:ILE:HD13 | 2.56 | 0.40 |
| 1:2:225:A:H2' | 1:2:225:A:N3 | 2.36 | 0.40 |
| 1:2:366:A:H2' | 1:2:367:U:O4' | 2.21 | 0.40 |
| 1:2:585:G:C6 | 1:2:586:C:C4 | 3.09 | 0.40 |
| 1:2:1185:U:H2' | 1:2:1186:U:O4' | 2.22 | 0.40 |
| 1:2:1711:G:H2' | 1:2:1711:G:N3 | 2.36 | 0.40 |
| 34:g:293:ASP:HA | 34:g:294:PRO:HD3 | 1.94 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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 | A | 174/211 (82%) | 139 (80%) | 35 (20%) | 1 7 |
| 3 | B | 198/228 (87%) | 169 (85%) | 29 (15%) | 3 17 |
| 4 | C | 176/203 (87%) | 157 (89%) | 19 (11%) | 6 27 |
| 5 | D | 185/196 (94%) | 153 (83%) | 32 (17%) | 2 12 |
| 6 | E | 223/224 (100%) | 185 (83%) | 38 (17%) | 2 12 |
| 7 | F | 174/194 (90%) | 148 (85%) | 26 (15%) | 3 17 |
| 8 | G | 192/200 (96%) | 176 (92%) | 16 (8%) | 10 35 |
| 9 | H | 164/170 (96%) | 142 (87%) | 22 (13%) | 4 20 |
| 10 | I | 147/159 (92%) | 128 (87%) | 19 (13%) | 4 21 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 11 | J | 153/158 (97%) | 133 (87%) | 20 (13%) | 4 | 21 |
| 12 | K | 88/96 (92%) | 78 (89%) | 10 (11%) | 5 | 25 |
| 13 | L | 136/137 (99%) | 125 (92%) | 11 (8%) | 11 | 36 |
| 14 | M | 97/109 (89%) | 79 (81%) | 18 (19%) | 1 | 9 |
| 15 | N | 127/128 (99%) | 107 (84%) | 20 (16%) | 2 | 15 |
| 16 | O | 96/104 (92%) | 82 (85%) | 14 (15%) | 3 | 17 |
| 17 | P | 105/119 (88%) | 96 (91%) | 9 (9%) | 10 | 34 |
| 18 | Q | 117/119 (98%) | 99 (85%) | 18 (15%) | 2 | 16 |
| 19 | R | 112/124 (90%) | 97 (87%) | 15 (13%) | 4 | 20 |
| 20 | S | 128/129 (99%) | 107 (84%) | 21 (16%) | 2 | 14 |
| 21 | T | 117/118 (99%) | 103 (88%) | 14 (12%) | 5 | 23 |
| 22 | U | 96/107 (90%) | 80 (83%) | 16 (17%) | 2 | 13 |
| 23 | V | 73/73 (100%) | 67 (92%) | 6 (8%) | 10 | 35 |
| 24 | W | 110/111 (99%) | 96 (87%) | 14 (13%) | 4 | 22 |
| 25 | X | 119/120 (99%) | 106 (89%) | 13 (11%) | 6 | 27 |
| 26 | Y | 108/109 (99%) | 93 (86%) | 15 (14%) | 3 | 19 |
| 27 | Z | 60/88 (68%) | 53 (88%) | 7 (12%) | 5 | 25 |
| 28 | a | 83/100 (83%) | 73 (88%) | 10 (12%) | 5 | 23 |
| 29 | b | 71/72 (99%) | 63 (89%) | 8 (11%) | 5 | 25 |
| 30 | c | 55/59 (93%) | 49 (89%) | 6 (11%) | 6 | 27 |
| 31 | d | 46/48 (96%) | 44 (96%) | 2 (4%) | 26 | 52 |
| 32 | e | 47/55 (86%) | 42 (89%) | 5 (11%) | 6 | 27 |
| 33 | f | 58/133 (44%) | 48 (83%) | 10 (17%) | 2 | 12 |
| 34 | g | 265/272 (97%) | 227 (86%) | 38 (14%) | 3 | 18 |
| 35 | h | 23/23 (100%) | 21 (91%) | 2 (9%) | 9 | 34 |
| 36 | i | 83/130 (64%) | 76 (92%) | 7 (8%) | 10 | 35 |
| 37 | j | 77/96 (80%) | 66 (86%) | 11 (14%) | 3 | 18 |
| All | All | 4283/4722 (91%) | 3707 (87%) | 576 (13%) | 6 | 20 |

All (576) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | A | 9 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | A | 15 | GLN |
| 2 | A | 16 | LEU |
| 2 | A | 31 | VAL |
| 2 | A | 32 | HIS |
| 2 | A | 33 | GLN |
| 2 | A | 37 | VAL |
| 2 | A | 50 | VAL |
| 2 | A | 53 | THR |
| 2 | A | 56 | LYS |
| 2 | A | 58 | VAL |
| 2 | A | 59 | LEU |
| 2 | A | 62 | ARG |
| 2 | A | 88 | LYS |
| 2 | A | 93 | THR |
| 2 | A | 108 | THR |
| 2 | A | 111 | ILE |
| 2 | A | 112 | THR |
| 2 | A | 120 | LEU |
| 2 | A | 122 | ILE |
| 2 | A | 123 | VAL |
| 2 | A | 133 | ILE |
| 2 | A | 134 | LYS |
| 2 | A | 157 | ASP |
| 2 | A | 165 | ARG |
| 2 | A | 167 | LYS |
| 2 | A | 170 | ILE |
| 2 | A | 172 | LEU |
| 2 | A | 173 | ILE |
| 2 | A | 177 | LEU |
| 2 | A | 193 | GLN |
| 2 | A | 197 | ILE |
| 2 | A | 198 | MET |
| 2 | A | 201 | LEU |
| 2 | A | 205 | ARG |
| 3 | B | 20 | VAL |
| 3 | B | 37 | THR |
| 3 | B | 47 | LEU |
| 3 | B | 48 | VAL |
| 3 | B | 64 | ARG |
| 3 | B | 70 | LEU |
| 3 | B | 82 | ARG |
| 3 | B | 83 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 3 | B | 84 | VAL |
| 3 | B | 96 | LEU |
| 3 | B | 104 | ASP |
| 3 | B | 118 | GLN |
| 3 | B | 120 | LEU |
| 3 | B | 127 | VAL |
| 3 | B | 131 | ASP |
| 3 | B | 132 | ASP |
| 3 | B | 140 | ILE |
| 3 | B | 166 | LYS |
| 3 | B | 171 | ILE |
| 3 | B | 181 | LEU |
| 3 | B | 183 | GLN |
| 3 | B | 189 | ILE |
| 3 | B | 191 | GLU |
| 3 | B | 196 | GLU |
| 3 | B | 207 | LEU |
| 3 | B | 208 | GLN |
| 3 | B | 213 | ARG |
| 3 | B | 220 | GLN |
| 3 | B | 228 | LEU |
| 4 | C | 58 | ILE |
| 4 | C | 72 | GLN |
| 4 | C | 91 | VAL |
| 4 | C | 93 | LYS |
| 4 | C | 95 | THR |
| 4 | C | 109 | VAL |
| 4 | C | 116 | VAL |
| 4 | C | 142 | ILE |
| 4 | C | 145 | ARG |
| 4 | C | 146 | ARG |
| 4 | C | 155 | GLN |
| 4 | C | 212 | LEU |
| 4 | C | 213 | GLU |
| 4 | C | 223 | ILE |
| 4 | C | 230 | LEU |
| 4 | C | 234 | LEU |
| 4 | C | 235 | TRP |
| 4 | C | 237 | VAL |
| 4 | C | 241 | THR |
| 5 | D | 4 | ILE |
| 5 | D | 11 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 5 | D | 17 | PHE |
| 5 | D | 20 | GLU |
| 5 | D | 21 | LEU |
| 5 | D | 23 | GLU |
| 5 | D | 37 | VAL |
| 5 | D | 50 | ILE |
| 5 | D | 57 | ASP |
| 5 | D | 67 | ASN |
| 5 | D | 76 | ARG |
| 5 | D | 80 | LYS |
| 5 | D | 89 | GLU |
| 5 | D | 101 | GLN |
| 5 | D | 103 | GLU |
| 5 | D | 113 | LEU |
| 5 | D | 115 | ILE |
| 5 | D | 117 | ARG |
| 5 | D | 122 | VAL |
| 5 | D | 135 | GLU |
| 5 | D | 141 | LYS |
| 5 | D | 158 | ILE |
| 5 | D | 162 | GLN |
| 5 | D | 165 | ASN |
| 5 | D | 166 | ASP |
| 5 | D | 176 | LEU |
| 5 | D | 178 | ARG |
| 5 | D | 179 | GLN |
| 5 | D | 181 | VAL |
| 5 | D | 188 | ILE |
| 5 | D | 189 | MET |
| 5 | D | 208 | ILE |
| 6 | E | 7 | LYS |
| 6 | E | 9 | LEU |
| 6 | E | 18 | TRP |
| 6 | E | 22 | LYS |
| 6 | E | 38 | LEU |
| 6 | E | 39 | ARG |
| 6 | E | 45 | ILE |
| 6 | E | 48 | LEU |
| 6 | E | 51 | ARG |
| 6 | E | 60 | GLU |
| 6 | E | 69 | HIS |
| 6 | E | 75 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 6 | E | 77 | ARG |
| 6 | E | 79 | ASP |
| 6 | E | 91 | THR |
| 6 | E | 102 | VAL |
| 6 | E | 106 | LYS |
| 6 | E | 108 | ARG |
| 6 | E | 123 | LEU |
| 6 | E | 125 | LYS |
| 6 | E | 139 | VAL |
| 6 | E | 142 | HIS |
| 6 | E | 168 | THR |
| 6 | E | 180 | LEU |
| 6 | E | 181 | VAL |
| 6 | E | 189 | LEU |
| 6 | E | 192 | VAL |
| 6 | E | 196 | VAL |
| 6 | E | 202 | GLU |
| 6 | E | 208 | VAL |
| 6 | E | 219 | VAL |
| 6 | E | 225 | VAL |
| 6 | E | 228 | ILE |
| 6 | E | 230 | GLU |
| 6 | E | 233 | ARG |
| 6 | E | 248 | ILE |
| 6 | E | 250 | GLU |
| 6 | E | 259 | HIS |
| 7 | F | 31 | ILE |
| 7 | F | 42 | ILE |
| 7 | F | 47 | LYS |
| 7 | F | 50 | PHE |
| 7 | F | 61 | VAL |
| 7 | F | 65 | GLN |
| 7 | F | 66 | ILE |
| 7 | F | 70 | ILE |
| 7 | F | 72 | VAL |
| 7 | F | 91 | ILE |
| 7 | F | 99 | LEU |
| 7 | F | 116 | VAL |
| 7 | F | 117 | LYS |
| 7 | F | 158 | ARG |
| 7 | F | 162 | VAL |
| 7 | F | 167 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 7 | F | 178 | THR |
| 7 | F | 186 | PHE |
| 7 | F | 188 | ASN |
| 7 | F | 189 | ILE |
| 7 | F | 192 | ILE |
| 7 | F | 194 | GLU |
| 7 | F | 196 | LEU |
| 7 | F | 201 | ILE |
| 7 | F | 213 | ILE |
| 7 | F | 220 | GLU |
| 8 | G | 21 | GLU |
| 8 | G | 26 | VAL |
| 8 | G | 49 | VAL |
| 8 | G | 51 | LYS |
| 8 | G | 52 | ILE |
| 8 | G | 72 | ARG |
| 8 | G | 79 | LYS |
| 8 | G | 95 | LYS |
| 8 | G | 109 | LEU |
| 8 | G | 121 | ILE |
| 8 | G | 126 | ASN |
| 8 | G | 164 | LYS |
| 8 | G | 170 | THR |
| 8 | G | 180 | THR |
| 8 | G | 183 | ARG |
| 8 | G | 195 | ILE |
| 9 | H | 5 | GLN |
| 9 | H | 7 | LYS |
| 9 | H | 9 | LEU |
| 9 | H | 11 | GLN |
| 9 | H | 15 | GLU |
| 9 | H | 27 | LEU |
| 9 | H | 33 | GLU |
| 9 | H | 48 | GLU |
| 9 | H | 49 | ILE |
| 9 | H | 62 | VAL |
| 9 | H | 64 | VAL |
| 9 | H | 72 | LYS |
| 9 | H | 78 | THR |
| 9 | H | 86 | GLN |
| 9 | H | 87 | ASP |
| 9 | H | 114 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 9 | H | 129 | LEU |
| 9 | H | 130 | VAL |
| 9 | H | 136 | VAL |
| 9 | H | 139 | ARG |
| 9 | H | 152 | ILE |
| 9 | H | 162 | ILE |
| 10 | I | 3 | ILE |
| 10 | I | 20 | GLN |
| 10 | I | 22 | ARG |
| 10 | I | 26 | LYS |
| 10 | I | 29 | LEU |
| 10 | I | 32 | GLN |
| 10 | I | 53 | GLN |
| 10 | I | 58 | LEU |
| 10 | I | 69 | SER |
| 10 | I | 96 | LEU |
| 10 | I | 104 | ILE |
| 10 | I | 105 | ASP |
| 10 | I | 107 | THR |
| 10 | I | 119 | GLN |
| 10 | I | 153 | ILE |
| 10 | I | 176 | GLN |
| 10 | I | 184 | ILE |
| 10 | I | 190 | LEU |
| 10 | I | 196 | ARG |
| 11 | J | 7 | THR |
| 11 | J | 20 | GLU |
| 11 | J | 28 | LEU |
| 11 | J | 33 | GLU |
| 11 | J | 37 | LYS |
| 11 | J | 45 | ILE |
| 11 | J | 49 | LEU |
| 11 | J | 60 | LEU |
| 11 | J | 69 | ARG |
| 11 | J | 70 | LEU |
| 11 | J | 78 | ARG |
| 11 | J | 93 | LEU |
| 11 | J | 100 | LYS |
| 11 | J | 107 | ARG |
| 11 | J | 109 | LEU |
| 11 | J | 131 | GLN |
| 11 | J | 142 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 11 | J | 145 | SER |
| 11 | J | 153 | GLU |
| 11 | J | 161 | THR |
| 12 | K | 14 | HIS |
| 12 | K | 16 | PHE |
| 12 | K | 17 | GLN |
| 12 | K | 20 | VAL |
| 12 | K | 21 | LEU |
| 12 | K | 35 | ILE |
| 12 | K | 40 | LEU |
| 12 | K | 48 | SER |
| 12 | K | 76 | LEU |
| 12 | K | 86 | ILE |
| 13 | L | 8 | GLN |
| 13 | L | 10 | GLU |
| 13 | L | 19 | ILE |
| 13 | L | 36 | LYS |
| 13 | L | 38 | VAL |
| 13 | L | 55 | ASP |
| 13 | L | 76 | VAL |
| 13 | L | 80 | MET |
| 13 | L | 84 | ILE |
| 13 | L | 131 | ILE |
| 13 | L | 136 | ARG |
| 14 | M | 14 | GLU |
| 14 | M | 17 | ILE |
| 14 | M | 19 | ASP |
| 14 | M | 21 | LEU |
| 14 | M | 22 | LYS |
| 14 | M | 29 | LEU |
| 14 | M | 38 | LEU |
| 14 | M | 55 | LEU |
| 14 | M | 56 | VAL |
| 14 | M | 59 | VAL |
| 14 | M | 64 | ILE |
| 14 | M | 67 | LEU |
| 14 | M | 77 | VAL |
| 14 | M | 79 | LEU |
| 14 | M | 80 | ILE |
| 14 | M | 82 | VAL |
| 14 | M | 105 | LYS |
| 14 | M | 116 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 15 | N | 3 | ARG |
| 15 | N | 4 | MET |
| 15 | N | 9 | LYS |
| 15 | N | 27 | LYS |
| 15 | N | 39 | LYS |
| 15 | N | 42 | ARG |
| 15 | N | 53 | LEU |
| 15 | N | 64 | LYS |
| 15 | N | 72 | LEU |
| 15 | N | 73 | ARG |
| 15 | N | 88 | LEU |
| 15 | N | 96 | VAL |
| 15 | N | 99 | ARG |
| 15 | N | 100 | LYS |
| 15 | N | 102 | LEU |
| 15 | N | 104 | ARG |
| 15 | N | 106 | ARG |
| 15 | N | 107 | LYS |
| 15 | N | 121 | ARG |
| 15 | N | 125 | LEU |
| 16 | O | 19 | ILE |
| 16 | O | 24 | ASN |
| 16 | O | 37 | GLU |
| 16 | O | 49 | LYS |
| 16 | O | 65 | GLN |
| 16 | O | 86 | THR |
| 16 | O | 92 | LYS |
| 16 | O | 102 | LEU |
| 16 | O | 110 | LEU |
| 16 | O | 112 | ILE |
| 16 | O | 114 | ARG |
| 16 | O | 116 | GLU |
| 16 | O | 124 | ASP |
| 16 | O | 129 | LYS |
| 17 | P | 20 | VAL |
| 17 | P | 35 | LYS |
| 17 | P | 40 | ARG |
| 17 | P | 57 | MET |
| 17 | P | 79 | HIS |
| 17 | P | 81 | ARG |
| 17 | P | 84 | ILE |
| 17 | P | 126 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 17 | P | 127 | ARG |
| 18 | Q | 7 | VAL |
| 18 | Q | 9 | THR |
| 18 | Q | 19 | VAL |
| 18 | Q | 29 | ILE |
| 18 | Q | 45 | ARG |
| 18 | Q | 48 | VAL |
| 18 | Q | 52 | LEU |
| 18 | Q | 53 | LEU |
| 18 | Q | 54 | LEU |
| 18 | Q | 94 | GLN |
| 18 | Q | 105 | LEU |
| 18 | Q | 113 | ASP |
| 18 | Q | 114 | ARG |
| 18 | Q | 121 | SER |
| 18 | Q | 127 | LYS |
| 18 | Q | 128 | LYS |
| 18 | Q | 137 | ARG |
| 18 | Q | 142 | TYR |
| 19 | R | 6 | THR |
| 19 | R | 16 | LEU |
| 19 | R | 17 | ILE |
| 19 | R | 24 | LEU |
| 19 | R | 27 | ASP |
| 19 | R | 32 | LYS |
| 19 | R | 38 | ILE |
| 19 | R | 41 | ILE |
| 19 | R | 46 | LEU |
| 19 | R | 48 | ASN |
| 19 | R | 61 | ILE |
| 19 | R | 72 | LYS |
| 19 | R | 81 | LYS |
| 19 | R | 93 | LEU |
| 19 | R | 120 | SER |
| 20 | S | 14 | ILE |
| 20 | S | 15 | LEU |
| 20 | S | 16 | ARG |
| 20 | S | 17 | LEU |
| 20 | S | 18 | LEU |
| 20 | S | 20 | THR |
| 20 | S | 26 | ILE |
| 20 | S | 38 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 20 | S | 45 | LEU |
| 20 | S | 49 | LYS |
| 20 | S | 77 | THR |
| 20 | S | 88 | ARG |
| 20 | S | 90 | LYS |
| 20 | S | 94 | ASP |
| 20 | S | 105 | LEU |
| 20 | S | 109 | LEU |
| 20 | S | 111 | ASP |
| 20 | S | 112 | ASP |
| 20 | S | 126 | ARG |
| 20 | S | 140 | THR |
| 20 | S | 145 | ARG |
| 21 | T | 7 | ARG |
| 21 | T | 25 | GLN |
| 21 | T | 45 | LEU |
| 21 | T | 57 | ARG |
| 21 | T | 63 | ARG |
| 21 | T | 68 | ARG |
| 21 | T | 79 | LEU |
| 21 | T | 85 | ASN |
| 21 | T | 107 | SER |
| 21 | T | 111 | LEU |
| 21 | T | 116 | ILE |
| 21 | T | 124 | ILE |
| 21 | T | 129 | LEU |
| 21 | T | 140 | LEU |
| 22 | U | 21 | LYS |
| 22 | U | 31 | VAL |
| 22 | U | 34 | LEU |
| 22 | U | 36 | ASN |
| 22 | U | 40 | ASN |
| 22 | U | 41 | ILE |
| 22 | U | 43 | LYS |
| 22 | U | 44 | ASN |
| 22 | U | 61 | LYS |
| 22 | U | 62 | VAL |
| 22 | U | 65 | ILE |
| 22 | U | 86 | ILE |
| 22 | U | 92 | ASP |
| 22 | U | 99 | ILE |
| 22 | U | 117 | ILE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 22 | U | 118 | ILE |
| 23 | V | 1 | MET |
| 23 | V | 8 | LEU |
| 23 | V | 11 | LEU |
| 23 | V | 12 | TYR |
| 23 | V | 44 | ARG |
| 23 | V | 69 | LEU |
| 24 | W | 3 | ARG |
| 24 | W | 7 | LEU |
| 24 | W | 24 | GLN |
| 24 | W | 25 | VAL |
| 24 | W | 26 | LEU |
| 24 | W | 47 | ILE |
| 24 | W | 55 | ASP |
| 24 | W | 74 | VAL |
| 24 | W | 75 | ILE |
| 24 | W | 80 | ASN |
| 24 | W | 83 | ILE |
| 24 | W | 104 | LEU |
| 24 | W | 124 | LYS |
| 24 | W | 129 | VAL |
| 25 | X | 5 | LYS |
| 25 | X | 9 | LEU |
| 25 | X | 19 | ARG |
| 25 | X | 30 | LYS |
| 25 | X | 69 | ARG |
| 25 | X | 79 | ASN |
| 25 | X | 84 | THR |
| 25 | X | 94 | ASN |
| 25 | X | 98 | GLU |
| 25 | X | 99 | ASN |
| 25 | X | 107 | PHE |
| 25 | X | 117 | ILE |
| 25 | X | 137 | LYS |
| 26 | Y | 8 | ARG |
| 26 | Y | 10 | ARG |
| 26 | Y | 11 | LYS |
| 26 | Y | 20 | ARG |
| 26 | Y | 34 | ASN |
| 26 | Y | 35 | VAL |
| 26 | Y | 42 | GLU |
| 26 | Y | 57 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 26 | Y | 70 | THR |
| 26 | Y | 74 | LEU |
| 26 | Y | 83 | LYS |
| 26 | Y | 84 | LYS |
| 26 | Y | 99 | LYS |
| 26 | Y | 116 | LYS |
| 26 | Y | 127 | LYS |
| 27 | Z | 60 | VAL |
| 27 | Z | 65 | LEU |
| 27 | Z | 77 | ARG |
| 27 | Z | 82 | HIS |
| 27 | Z | 88 | ILE |
| 27 | Z | 97 | LYS |
| 27 | Z | 98 | GLN |
| 28 | a | 15 | ARG |
| 28 | a | 28 | ARG |
| 28 | a | 34 | LYS |
| 28 | a | 38 | ARG |
| 28 | a | 53 | LEU |
| 28 | a | 59 | TYR |
| 28 | a | 64 | LEU |
| 28 | a | 69 | ASN |
| 28 | a | 75 | ILE |
| 28 | a | 84 | VAL |
| 29 | b | 3 | LEU |
| 29 | b | 9 | HIS |
| 29 | b | 20 | LYS |
| 29 | b | 23 | THR |
| 29 | b | 24 | LEU |
| 29 | b | 54 | VAL |
| 29 | b | 57 | GLU |
| 29 | b | 67 | THR |
| 30 | c | 8 | THR |
| 30 | c | 16 | LEU |
| 30 | c | 25 | VAL |
| 30 | c | 28 | VAL |
| 30 | c | 30 | VAL |
| 30 | c | 48 | VAL |
| 31 | d | 30 | LEU |
| 31 | d | 32 | ARG |
| 32 | e | 14 | VAL |
| 32 | e | 26 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 32 | e | 37 | ARG |
| 32 | e | 47 | VAL |
| 32 | e | 48 | THR |
| 33 | f | 82 | LYS |
| 33 | f | 85 | TYR |
| 33 | f | 93 | HIS |
| 33 | f | 94 | LYS |
| 33 | f | 96 | LYS |
| 33 | f | 97 | LYS |
| 33 | f | 109 | ASP |
| 33 | f | 116 | LYS |
| 33 | f | 129 | PHE |
| 33 | f | 136 | ARG |
| 34 | g | 33 | LEU |
| 34 | g | 43 | LEU |
| 34 | g | 49 | THR |
| 34 | g | 55 | PHE |
| 34 | g | 60 | ARG |
| 34 | g | 67 | HIS |
| 34 | g | 70 | GLN |
| 34 | g | 74 | VAL |
| 34 | g | 92 | LEU |
| 34 | g | 97 | THR |
| 34 | g | 124 | ILE |
| 34 | g | 132 | ILE |
| 34 | g | 137 | THR |
| 34 | g | 152 | VAL |
| 34 | g | 168 | ASP |
| 34 | g | 172 | ILE |
| 34 | g | 175 | VAL |
| 34 | g | 188 | LEU |
| 34 | g | 195 | ILE |
| 34 | g | 203 | ASN |
| 34 | g | 208 | VAL |
| 34 | g | 210 | GLN |
| 34 | g | 232 | LEU |
| 34 | g | 242 | ASP |
| 34 | g | 244 | LYS |
| 34 | g | 269 | ILE |
| 34 | g | 271 | ASP |
| 34 | g | 273 | GLU |
| 34 | g | 275 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | g | 276 | VAL |
| 34 | g | 284 | GLU |
| 34 | g | 292 | GLN |
| 34 | g | 293 | ASP |
| 34 | g | 299 | LEU |
| 34 | g | 304 | ASP |
| 34 | g | 308 | LEU |
| 34 | g | 316 | VAL |
| 34 | g | 321 | GLN |
| 35 | h | 12 | ARG |
| 35 | h | 16 | LYS |
| 36 | i | 46 | ARG |
| 36 | i | 47 | VAL |
| 36 | i | 58 | MET |
| 36 | i | 62 | ARG |
| 36 | i | 79 | VAL |
| 36 | i | 97 | LEU |
| 36 | i | 116 | ASN |
| 37 | j | 25 | TYR |
| 37 | j | 26 | ILE |
| 37 | j | 39 | LEU |
| 37 | j | 62 | PHE |
| 37 | j | 65 | ASN |
| 37 | j | 73 | GLU |
| 37 | j | 81 | GLN |
| 37 | j | 99 | GLN |
| 37 | j | 100 | LYS |
| 37 | j | 103 | ILE |
| 37 | j | 105 | ILE |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | A | 109 | ASN |
| 2 | A | 131 | GLN |
| 2 | A | 193 | GLN |
| 3 | B | 74 | GLN |
| 3 | B | 99 | ASN |
| 3 | B | 101 | HIS |
| 3 | B | 118 | GLN |
| 3 | B | 163 | GLN |
| 3 | B | 177 | GLN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 3 | B | 220 | GLN |
| 4 | C | 87 | ASN |
| 4 | C | 94 | GLN |
| 4 | C | 99 | GLN |
| 4 | C | 155 | GLN |
| 4 | C | 214 | ASN |
| 5 | D | 67 | ASN |
| 5 | D | 159 | HIS |
| 5 | D | 162 | GLN |
| 5 | D | 165 | ASN |
| 5 | D | 179 | GLN |
| 5 | D | 195 | ASN |
| 6 | E | 67 | GLN |
| 6 | E | 130 | GLN |
| 6 | E | 224 | ASN |
| 7 | F | 36 | GLN |
| 7 | F | 39 | GLN |
| 7 | F | 40 | GLN |
| 7 | F | 81 | ASN |
| 7 | F | 97 | ASN |
| 7 | F | 105 | ASN |
| 7 | F | 188 | ASN |
| 8 | G | 10 | ASN |
| 8 | G | 13 | GLN |
| 8 | G | 139 | ASN |
| 8 | G | 182 | GLN |
| 8 | G | 185 | GLN |
| 8 | G | 199 | GLN |
| 9 | H | 19 | GLN |
| 9 | H | 155 | ASN |
| 10 | I | 20 | GLN |
| 10 | I | 116 | HIS |
| 11 | J | 142 | ASN |
| 12 | K | 17 | GLN |
| 12 | K | 39 | ASN |
| 12 | K | 58 | GLN |
| 13 | L | 8 | GLN |
| 13 | L | 22 | ASN |
| 13 | L | 106 | ASN |
| 13 | L | 152 | GLN |
| 14 | M | 51 | GLN |
| 14 | M | 102 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 15 | N | 36 | GLN |
| 15 | N | 49 | GLN |
| 15 | N | 62 | GLN |
| 15 | N | 78 | ASN |
| 15 | N | 151 | ASN |
| 16 | O | 12 | GLN |
| 16 | O | 29 | HIS |
| 16 | O | 80 | HIS |
| 16 | O | 99 | GLN |
| 17 | P | 70 | ASN |
| 17 | P | 79 | HIS |
| 18 | Q | 8 | GLN |
| 18 | Q | 40 | GLN |
| 19 | R | 31 | ASN |
| 19 | R | 48 | ASN |
| 19 | R | 62 | GLN |
| 19 | R | 83 | GLN |
| 19 | R | 105 | GLN |
| 20 | S | 25 | ASN |
| 20 | S | 74 | GLN |
| 20 | S | 89 | GLN |
| 20 | S | 99 | HIS |
| 20 | S | 136 | GLN |
| 21 | T | 25 | GLN |
| 21 | T | 70 | GLN |
| 21 | T | 85 | ASN |
| 21 | T | 101 | ASN |
| 21 | T | 106 | GLN |
| 22 | U | 40 | ASN |
| 22 | U | 44 | ASN |
| 23 | V | 7 | GLN |
| 23 | V | 21 | ASN |
| 23 | V | 29 | HIS |
| 23 | V | 38 | GLN |
| 23 | V | 81 | ASN |
| 24 | W | 24 | GLN |
| 24 | W | 92 | ASN |
| 25 | X | 18 | HIS |
| 25 | X | 22 | ASN |
| 25 | X | 79 | ASN |
| 26 | Y | 15 | ASN |
| 26 | Y | 106 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26 | Y | 110 | GLN |
| 27 | Z | 44 | GLN |
| 27 | Z | 82 | HIS |
| 28 | a | 8 | ASN |
| 28 | a | 17 | HIS |
| 29 | b | 26 | GLN |
| 29 | b | 42 | ASN |
| 30 | c | 27 | GLN |
| 31 | d | 10 | HIS |
| 31 | d | 37 | ASN |
| 31 | d | 48 | ASN |
| 33 | f | 93 | HIS |
| 33 | f | 132 | ASN |
| 34 | g | 70 | GLN |
| 34 | g | 119 | ASN |
| 34 | g | 231 | ASN |
| 34 | g | 234 | HIS |
| 34 | g | 292 | GLN |
| 34 | g | 315 | ASN |
| 36 | i | 33 | GLN |
| 36 | i | 44 | ASN |
| 36 | i | 60 | HIS |
| 36 | i | 85 | GLN |
| 36 | i | 93 | HIS |
| 36 | i | 106 | GLN |
| 36 | i | 112 | ASN |
| 37 | j | 99 | GLN |

5.3.3 RNA [i](#)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | 2 | 1778/1799 (98%) | 684 (38%) | 113 (6%) |

All (684) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 2 | 2 | A |
| 1 | 2 | 4 | C |
| 1 | 2 | 17 | C |
| 1 | 2 | 25 | C |
| 1 | 2 | 26 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 2 | 32 | U |
| 1 | 2 | 34 | G |
| 1 | 2 | 39 | A |
| 1 | 2 | 40 | A |
| 1 | 2 | 42 | G |
| 1 | 2 | 45 | U |
| 1 | 2 | 47 | A |
| 1 | 2 | 51 | A |
| 1 | 2 | 57 | G |
| 1 | 2 | 59 | C |
| 1 | 2 | 60 | U |
| 1 | 2 | 61 | A |
| 1 | 2 | 65 | A |
| 1 | 2 | 67 | A |
| 1 | 2 | 68 | A |
| 1 | 2 | 69 | G |
| 1 | 2 | 71 | A |
| 1 | 2 | 72 | A |
| 1 | 2 | 73 | U |
| 1 | 2 | 74 | U |
| 1 | 2 | 75 | U |
| 1 | 2 | 76 | A |
| 1 | 2 | 77 | U |
| 1 | 2 | 78 | A |
| 1 | 2 | 80 | A |
| 1 | 2 | 82 | U |
| 1 | 2 | 93 | A |
| 1 | 2 | 100 | A |
| 1 | 2 | 104 | A |
| 1 | 2 | 111 | U |
| 1 | 2 | 114 | C |
| 1 | 2 | 115 | G |
| 1 | 2 | 123 | G |
| 1 | 2 | 124 | A |
| 1 | 2 | 127 | G |
| 1 | 2 | 129 | U |
| 1 | 2 | 130 | C |
| 1 | 2 | 131 | C |
| 1 | 2 | 132 | U |
| 1 | 2 | 133 | U |
| 1 | 2 | 134 | U |
| 1 | 2 | 136 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 2 | 137 | U |
| 1 | 2 | 138 | A |
| 1 | 2 | 139 | C |
| 1 | 2 | 140 | A |
| 1 | 2 | 141 | U |
| 1 | 2 | 144 | A |
| 1 | 2 | 146 | A |
| 1 | 2 | 147 | U |
| 1 | 2 | 149 | U |
| 1 | 2 | 157 | U |
| 1 | 2 | 158 | U |
| 1 | 2 | 159 | C |
| 1 | 2 | 160 | U |
| 1 | 2 | 161 | A |
| 1 | 2 | 167 | A |
| 1 | 2 | 173 | U |
| 1 | 2 | 176 | U |
| 1 | 2 | 178 | A |
| 1 | 2 | 183 | C |
| 1 | 2 | 190 | C |
| 1 | 2 | 191 | U |
| 1 | 2 | 192 | U |
| 1 | 2 | 193 | U |
| 1 | 2 | 194 | G |
| 1 | 2 | 195 | G |
| 1 | 2 | 198 | G |
| 1 | 2 | 203 | G |
| 1 | 2 | 209 | A |
| 1 | 2 | 214 | A |
| 1 | 2 | 217 | A |
| 1 | 2 | 218 | A |
| 1 | 2 | 220 | A |
| 1 | 2 | 224 | A |
| 1 | 2 | 225 | A |
| 1 | 2 | 226 | U |
| 1 | 2 | 227 | G |
| 1 | 2 | 228 | U |
| 1 | 2 | 230 | U |
| 1 | 2 | 231 | U |
| 1 | 2 | 232 | C |
| 1 | 2 | 233 | G |
| 1 | 2 | 237 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 2 | 239 | C |
| 1 | 2 | 240 | U |
| 1 | 2 | 241 | U |
| 1 | 2 | 248 | U |
| 1 | 2 | 249 | C |
| 1 | 2 | 256 | A |
| 1 | 2 | 259 | U |
| 1 | 2 | 264 | A |
| 1 | 2 | 265 | A |
| 1 | 2 | 266 | U |
| 1 | 2 | 267 | C |
| 1 | 2 | 268 | G |
| 1 | 2 | 270 | A |
| 1 | 2 | 271 | U |
| 1 | 2 | 274 | C |
| 1 | 2 | 275 | C |
| 1 | 2 | 276 | U |
| 1 | 2 | 277 | U |
| 1 | 2 | 278 | G |
| 1 | 2 | 279 | U |
| 1 | 2 | 280 | G |
| 1 | 2 | 286 | G |
| 1 | 2 | 287 | A |
| 1 | 2 | 288 | U |
| 1 | 2 | 289 | G |
| 1 | 2 | 294 | A |
| 1 | 2 | 298 | A |
| 1 | 2 | 301 | U |
| 1 | 2 | 307 | C |
| 1 | 2 | 308 | C |
| 1 | 2 | 309 | C |
| 1 | 2 | 311 | A |
| 1 | 2 | 312 | U |
| 1 | 2 | 313 | C |
| 1 | 2 | 314 | A |
| 1 | 2 | 315 | A |
| 1 | 2 | 320 | C |
| 1 | 2 | 321 | G |
| 1 | 2 | 336 | G |
| 1 | 2 | 337 | C |
| 1 | 2 | 350 | C |
| 1 | 2 | 351 | A |

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Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 2 | 358 | A |
| 1 | 2 | 359 | A |
| 1 | 2 | 360 | C |
| 1 | 2 | 361 | G |
| 1 | 2 | 368 | A |
| 1 | 2 | 369 | A |
| 1 | 2 | 377 | A |
| 1 | 2 | 379 | U |
| 1 | 2 | 382 | G |
| 1 | 2 | 384 | A |
| 1 | 2 | 387 | G |
| 1 | 2 | 389 | G |
| 1 | 2 | 392 | C |
| 1 | 2 | 399 | A |
| 1 | 2 | 400 | A |
| 1 | 2 | 401 | C |
| 1 | 2 | 403 | G |
| 1 | 2 | 412 | U |
| 1 | 2 | 415 | A |
| 1 | 2 | 416 | A |
| 1 | 2 | 417 | G |
| 1 | 2 | 418 | G |
| 1 | 2 | 421 | G |
| 1 | 2 | 422 | G |
| 1 | 2 | 423 | C |
| 1 | 2 | 424 | A |
| 1 | 2 | 425 | G |
| 1 | 2 | 427 | A |
| 1 | 2 | 433 | G |
| 1 | 2 | 438 | U |
| 1 | 2 | 439 | U |
| 1 | 2 | 443 | C |
| 1 | 2 | 444 | A |
| 1 | 2 | 447 | C |
| 1 | 2 | 452 | U |
| 1 | 2 | 458 | G |
| 1 | 2 | 459 | A |
| 1 | 2 | 460 | G |
| 1 | 2 | 463 | A |
| 1 | 2 | 467 | A |
| 1 | 2 | 473 | A |
| 1 | 2 | 474 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 2 | 476 | A |
| 1 | 2 | 479 | G |
| 1 | 2 | 480 | A |
| 1 | 2 | 481 | U |
| 1 | 2 | 488 | C |
| 1 | 2 | 491 | A |
| 1 | 2 | 492 | U |
| 1 | 2 | 493 | U |
| 1 | 2 | 494 | C |
| 1 | 2 | 495 | G |
| 1 | 2 | 496 | G |
| 1 | 2 | 497 | G |
| 1 | 2 | 499 | C |
| 1 | 2 | 500 | U |
| 1 | 2 | 501 | U |
| 1 | 2 | 502 | G |
| 1 | 2 | 504 | A |
| 1 | 2 | 505 | A |
| 1 | 2 | 506 | U |
| 1 | 2 | 507 | U |
| 1 | 2 | 509 | G |
| 1 | 2 | 510 | A |
| 1 | 2 | 513 | G |
| 1 | 2 | 514 | A |
| 1 | 2 | 516 | U |
| 1 | 2 | 518 | C |
| 1 | 2 | 523 | U |
| 1 | 2 | 526 | A |
| 1 | 2 | 527 | U |
| 1 | 2 | 533 | A |
| 1 | 2 | 534 | A |
| 1 | 2 | 535 | C |
| 1 | 2 | 536 | G |
| 1 | 2 | 539 | G |
| 1 | 2 | 540 | A |
| 1 | 2 | 542 | C |
| 1 | 2 | 543 | A |
| 1 | 2 | 544 | A |
| 1 | 2 | 545 | C |
| 1 | 2 | 547 | G |
| 1 | 2 | 548 | G |
| 1 | 2 | 554 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 2 | 557 | U |
| 1 | 2 | 558 | C |
| 1 | 2 | 564 | C |
| 1 | 2 | 565 | C |
| 1 | 2 | 566 | A |
| 1 | 2 | 567 | G |
| 1 | 2 | 573 | G |
| 1 | 2 | 577 | U |
| 1 | 2 | 579 | A |
| 1 | 2 | 581 | U |
| 1 | 2 | 582 | C |
| 1 | 2 | 584 | A |
| 1 | 2 | 593 | A |
| 1 | 2 | 594 | G |
| 1 | 2 | 610 | U |
| 1 | 2 | 618 | A |
| 1 | 2 | 619 | A |
| 1 | 2 | 620 | A |
| 1 | 2 | 622 | A |
| 1 | 2 | 634 | A |
| 1 | 2 | 637 | U |
| 1 | 2 | 638 | U |
| 1 | 2 | 639 | U |
| 1 | 2 | 641 | G |
| 1 | 2 | 646 | G |
| 1 | 2 | 647 | G |
| 1 | 2 | 648 | U |
| 1 | 2 | 649 | U |
| 1 | 2 | 650 | G |
| 1 | 2 | 652 | C |
| 1 | 2 | 653 | C |
| 1 | 2 | 654 | G |
| 1 | 2 | 655 | G |
| 1 | 2 | 678 | U |
| 1 | 2 | 679 | U |
| 1 | 2 | 683 | C |
| 1 | 2 | 684 | A |
| 1 | 2 | 691 | U |
| 1 | 2 | 694 | U |
| 1 | 2 | 695 | U |
| 1 | 2 | 696 | C |
| 1 | 2 | 697 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 2 | 698 | U |
| 1 | 2 | 700 | C |
| 1 | 2 | 701 | U |
| 1 | 2 | 704 | C |
| 1 | 2 | 705 | U |
| 1 | 2 | 706 | A |
| 1 | 2 | 708 | C |
| 1 | 2 | 709 | C |
| 1 | 2 | 710 | U |
| 1 | 2 | 712 | U |
| 1 | 2 | 713 | A |
| 1 | 2 | 714 | C |
| 1 | 2 | 716 | C |
| 1 | 2 | 717 | C |
| 1 | 2 | 718 | U |
| 1 | 2 | 719 | U |
| 1 | 2 | 721 | U |
| 1 | 2 | 722 | G |
| 1 | 2 | 724 | G |
| 1 | 2 | 726 | G |
| 1 | 2 | 727 | C |
| 1 | 2 | 729 | G |
| 1 | 2 | 731 | C |
| 1 | 2 | 732 | G |
| 1 | 2 | 733 | A |
| 1 | 2 | 734 | A |
| 1 | 2 | 736 | C |
| 1 | 2 | 738 | G |
| 1 | 2 | 740 | A |
| 1 | 2 | 741 | C |
| 1 | 2 | 742 | U |
| 1 | 2 | 743 | U |
| 1 | 2 | 753 | A |
| 1 | 2 | 754 | A |
| 1 | 2 | 765 | G |
| 1 | 2 | 766 | U |
| 1 | 2 | 771 | A |
| 1 | 2 | 774 | A |
| 1 | 2 | 778 | G |
| 1 | 2 | 779 | A |
| 1 | 2 | 780 | A |
| 1 | 2 | 781 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 2 | 782 | G |
| 1 | 2 | 785 | C |
| 1 | 2 | 786 | G |
| 1 | 2 | 788 | A |
| 1 | 2 | 789 | U |
| 1 | 2 | 792 | A |
| 1 | 2 | 793 | U |
| 1 | 2 | 794 | U |
| 1 | 2 | 795 | A |
| 1 | 2 | 811 | A |
| 1 | 2 | 812 | U |
| 1 | 2 | 813 | A |
| 1 | 2 | 814 | G |
| 1 | 2 | 817 | C |
| 1 | 2 | 818 | G |
| 1 | 2 | 819 | U |
| 1 | 2 | 820 | U |
| 1 | 2 | 821 | U |
| 1 | 2 | 822 | G |
| 1 | 2 | 823 | G |
| 1 | 2 | 825 | U |
| 1 | 2 | 826 | C |
| 1 | 2 | 827 | U |
| 1 | 2 | 828 | A |
| 1 | 2 | 829 | U |
| 1 | 2 | 830 | U |
| 1 | 2 | 831 | U |
| 1 | 2 | 832 | U |
| 1 | 2 | 834 | U |
| 1 | 2 | 840 | U |
| 1 | 2 | 844 | G |
| 1 | 2 | 845 | G |
| 1 | 2 | 849 | A |
| 1 | 2 | 852 | G |
| 1 | 2 | 854 | A |
| 1 | 2 | 855 | A |
| 1 | 2 | 856 | U |
| 1 | 2 | 860 | U |
| 1 | 2 | 862 | A |
| 1 | 2 | 863 | U |
| 1 | 2 | 872 | U |
| 1 | 2 | 875 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 2 | 876 | G |
| 1 | 2 | 877 | G |
| 1 | 2 | 895 | U |
| 1 | 2 | 896 | C |
| 1 | 2 | 897 | A |
| 1 | 2 | 898 | G |
| 1 | 2 | 904 | A |
| 1 | 2 | 905 | A |
| 1 | 2 | 911 | U |
| 1 | 2 | 913 | G |
| 1 | 2 | 914 | A |
| 1 | 2 | 915 | U |
| 1 | 2 | 919 | U |
| 1 | 2 | 920 | U |
| 1 | 2 | 927 | U |
| 1 | 2 | 932 | A |
| 1 | 2 | 933 | C |
| 1 | 2 | 934 | U |
| 1 | 2 | 941 | G |
| 1 | 2 | 943 | A |
| 1 | 2 | 950 | A |
| 1 | 2 | 958 | U |
| 1 | 2 | 959 | U |
| 1 | 2 | 965 | A |
| 1 | 2 | 969 | A |
| 1 | 2 | 972 | A |
| 1 | 2 | 978 | A |
| 1 | 2 | 981 | U |
| 1 | 2 | 983 | G |
| 1 | 2 | 987 | A |
| 1 | 2 | 991 | A |
| 1 | 2 | 993 | G |
| 1 | 2 | 994 | A |
| 1 | 2 | 1003 | U |
| 1 | 2 | 1011 | U |
| 1 | 2 | 1020 | C |
| 1 | 2 | 1024 | A |
| 1 | 2 | 1025 | A |
| 1 | 2 | 1026 | A |
| 1 | 2 | 1027 | C |
| 1 | 2 | 1028 | U |
| 1 | 2 | 1030 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 2 | 1031 | G |
| 1 | 2 | 1038 | A |
| 1 | 2 | 1039 | G |
| 1 | 2 | 1041 | G |
| 1 | 2 | 1042 | A |
| 1 | 2 | 1050 | G |
| 1 | 2 | 1051 | U |
| 1 | 2 | 1052 | G |
| 1 | 2 | 1056 | U |
| 1 | 2 | 1057 | U |
| 1 | 2 | 1058 | C |
| 1 | 2 | 1059 | U |
| 1 | 2 | 1060 | U |
| 1 | 2 | 1062 | U |
| 1 | 2 | 1065 | C |
| 1 | 2 | 1071 | C |
| 1 | 2 | 1075 | A |
| 1 | 2 | 1080 | A |
| 1 | 2 | 1081 | C |
| 1 | 2 | 1082 | G |
| 1 | 2 | 1083 | A |
| 1 | 2 | 1091 | A |
| 1 | 2 | 1095 | C |
| 1 | 2 | 1096 | U |
| 1 | 2 | 1097 | U |
| 1 | 2 | 1098 | U |
| 1 | 2 | 1099 | G |
| 1 | 2 | 1107 | G |
| 1 | 2 | 1108 | G |
| 1 | 2 | 1110 | G |
| 1 | 2 | 1113 | G |
| 1 | 2 | 1118 | G |
| 1 | 2 | 1121 | G |
| 1 | 2 | 1130 | A |
| 1 | 2 | 1137 | A |
| 1 | 2 | 1142 | A |
| 1 | 2 | 1149 | G |
| 1 | 2 | 1150 | A |
| 1 | 2 | 1157 | C |
| 1 | 2 | 1158 | C |
| 1 | 2 | 1166 | G |
| 1 | 2 | 1167 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 2 | 1173 | C |
| 1 | 2 | 1175 | G |
| 1 | 2 | 1184 | U |
| 1 | 2 | 1189 | C |
| 1 | 2 | 1190 | U |
| 1 | 2 | 1193 | A |
| 1 | 2 | 1194 | C |
| 1 | 2 | 1195 | A |
| 1 | 2 | 1196 | C |
| 1 | 2 | 1198 | G |
| 1 | 2 | 1199 | G |
| 1 | 2 | 1201 | A |
| 1 | 2 | 1202 | A |
| 1 | 2 | 1203 | A |
| 1 | 2 | 1204 | C |
| 1 | 2 | 1211 | G |
| 1 | 2 | 1212 | G |
| 1 | 2 | 1215 | C |
| 1 | 2 | 1216 | A |
| 1 | 2 | 1217 | G |
| 1 | 2 | 1218 | A |
| 1 | 2 | 1222 | A |
| 1 | 2 | 1224 | U |
| 1 | 2 | 1225 | A |
| 1 | 2 | 1226 | A |
| 1 | 2 | 1227 | G |
| 1 | 2 | 1228 | G |
| 1 | 2 | 1234 | C |
| 1 | 2 | 1236 | G |
| 1 | 2 | 1238 | U |
| 1 | 2 | 1240 | G |
| 1 | 2 | 1241 | A |
| 1 | 2 | 1242 | G |
| 1 | 2 | 1243 | A |
| 1 | 2 | 1244 | G |
| 1 | 2 | 1246 | U |
| 1 | 2 | 1247 | C |
| 1 | 2 | 1250 | U |
| 1 | 2 | 1254 | G |
| 1 | 2 | 1258 | U |
| 1 | 2 | 1259 | U |
| 1 | 2 | 1265 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 2 | 1268 | U |
| 1 | 2 | 1269 | G |
| 1 | 2 | 1272 | G |
| 1 | 2 | 1274 | A |
| 1 | 2 | 1282 | U |
| 1 | 2 | 1283 | C |
| 1 | 2 | 1284 | U |
| 1 | 2 | 1296 | G |
| 1 | 2 | 1298 | G |
| 1 | 2 | 1305 | C |
| 1 | 2 | 1306 | U |
| 1 | 2 | 1307 | G |
| 1 | 2 | 1313 | U |
| 1 | 2 | 1314 | U |
| 1 | 2 | 1316 | C |
| 1 | 2 | 1317 | G |
| 1 | 2 | 1320 | A |
| 1 | 2 | 1321 | A |
| 1 | 2 | 1323 | G |
| 1 | 2 | 1324 | A |
| 1 | 2 | 1336 | A |
| 1 | 2 | 1339 | U |
| 1 | 2 | 1340 | A |
| 1 | 2 | 1343 | A |
| 1 | 2 | 1344 | A |
| 1 | 2 | 1347 | A |
| 1 | 2 | 1349 | G |
| 1 | 2 | 1350 | G |
| 1 | 2 | 1351 | U |
| 1 | 2 | 1353 | G |
| 1 | 2 | 1356 | G |
| 1 | 2 | 1358 | C |
| 1 | 2 | 1359 | A |
| 1 | 2 | 1360 | C |
| 1 | 2 | 1361 | U |
| 1 | 2 | 1362 | U |
| 1 | 2 | 1363 | G |
| 1 | 2 | 1364 | C |
| 1 | 2 | 1366 | G |
| 1 | 2 | 1368 | U |
| 1 | 2 | 1369 | U |
| 1 | 2 | 1370 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 2 | 1371 | A |
| 1 | 2 | 1380 | A |
| 1 | 2 | 1384 | G |
| 1 | 2 | 1388 | U |
| 1 | 2 | 1389 | A |
| 1 | 2 | 1396 | U |
| 1 | 2 | 1397 | C |
| 1 | 2 | 1398 | A |
| 1 | 2 | 1400 | G |
| 1 | 2 | 1404 | A |
| 1 | 2 | 1410 | G |
| 1 | 2 | 1411 | U |
| 1 | 2 | 1412 | U |
| 1 | 2 | 1413 | U |
| 1 | 2 | 1416 | G |
| 1 | 2 | 1425 | A |
| 1 | 2 | 1426 | G |
| 1 | 2 | 1429 | C |
| 1 | 2 | 1430 | U |
| 1 | 2 | 1433 | G |
| 1 | 2 | 1434 | A |
| 1 | 2 | 1442 | A |
| 1 | 2 | 1443 | G |
| 1 | 2 | 1444 | A |
| 1 | 2 | 1445 | C |
| 1 | 2 | 1446 | G |
| 1 | 2 | 1449 | C |
| 1 | 2 | 1450 | U |
| 1 | 2 | 1454 | C |
| 1 | 2 | 1456 | G |
| 1 | 2 | 1457 | C |
| 1 | 2 | 1458 | A |
| 1 | 2 | 1460 | G |
| 1 | 2 | 1461 | C |
| 1 | 2 | 1463 | C |
| 1 | 2 | 1464 | G |
| 1 | 2 | 1467 | A |
| 1 | 2 | 1468 | C |
| 1 | 2 | 1469 | A |
| 1 | 2 | 1471 | U |
| 1 | 2 | 1475 | G |
| 1 | 2 | 1476 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 2 | 1481 | A |
| 1 | 2 | 1484 | G |
| 1 | 2 | 1485 | A |
| 1 | 2 | 1487 | U |
| 1 | 2 | 1488 | A |
| 1 | 2 | 1489 | C |
| 1 | 2 | 1490 | A |
| 1 | 2 | 1491 | A |
| 1 | 2 | 1492 | C |
| 1 | 2 | 1494 | U |
| 1 | 2 | 1495 | U |
| 1 | 2 | 1498 | C |
| 1 | 2 | 1501 | A |
| 1 | 2 | 1502 | G |
| 1 | 2 | 1504 | G |
| 1 | 2 | 1505 | G |
| 1 | 2 | 1506 | U |
| 1 | 2 | 1507 | C |
| 1 | 2 | 1508 | U |
| 1 | 2 | 1509 | G |
| 1 | 2 | 1512 | U |
| 1 | 2 | 1514 | A |
| 1 | 2 | 1515 | U |
| 1 | 2 | 1516 | C |
| 1 | 2 | 1519 | G |
| 1 | 2 | 1520 | U |
| 1 | 2 | 1521 | G |
| 1 | 2 | 1522 | A |
| 1 | 2 | 1531 | C |
| 1 | 2 | 1532 | G |
| 1 | 2 | 1533 | U |
| 1 | 2 | 1534 | G |
| 1 | 2 | 1535 | C |
| 1 | 2 | 1536 | U |
| 1 | 2 | 1537 | G |
| 1 | 2 | 1539 | G |
| 1 | 2 | 1543 | A |
| 1 | 2 | 1546 | G |
| 1 | 2 | 1552 | U |
| 1 | 2 | 1553 | A |
| 1 | 2 | 1554 | A |
| 1 | 2 | 1555 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 2 | 1556 | U |
| 1 | 2 | 1557 | A |
| 1 | 2 | 1563 | C |
| 1 | 2 | 1566 | C |
| 1 | 2 | 1569 | C |
| 1 | 2 | 1570 | G |
| 1 | 2 | 1571 | A |
| 1 | 2 | 1573 | G |
| 1 | 2 | 1580 | U |
| 1 | 2 | 1581 | A |
| 1 | 2 | 1583 | U |
| 1 | 2 | 1588 | G |
| 1 | 2 | 1591 | A |
| 1 | 2 | 1593 | U |
| 1 | 2 | 1594 | C |
| 1 | 2 | 1595 | A |
| 1 | 2 | 1597 | C |
| 1 | 2 | 1598 | A |
| 1 | 2 | 1599 | G |
| 1 | 2 | 1603 | G |
| 1 | 2 | 1605 | G |
| 1 | 2 | 1606 | U |
| 1 | 2 | 1613 | C |
| 1 | 2 | 1614 | G |
| 1 | 2 | 1616 | C |
| 1 | 2 | 1617 | C |
| 1 | 2 | 1631 | A |
| 1 | 2 | 1632 | C |
| 1 | 2 | 1633 | A |
| 1 | 2 | 1634 | C |
| 1 | 2 | 1643 | G |
| 1 | 2 | 1647 | G |
| 1 | 2 | 1655 | U |
| 1 | 2 | 1656 | G |
| 1 | 2 | 1678 | G |
| 1 | 2 | 1679 | A |
| 1 | 2 | 1682 | U |
| 1 | 2 | 1685 | U |
| 1 | 2 | 1686 | U |
| 1 | 2 | 1687 | A |
| 1 | 2 | 1688 | G |
| 1 | 2 | 1692 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 2 | 1693 | G |
| 1 | 2 | 1694 | G |
| 1 | 2 | 1695 | G |
| 1 | 2 | 1696 | G |
| 1 | 2 | 1697 | G |
| 1 | 2 | 1698 | C |
| 1 | 2 | 1699 | A |
| 1 | 2 | 1700 | A |
| 1 | 2 | 1701 | C |
| 1 | 2 | 1702 | U |
| 1 | 2 | 1703 | C |
| 1 | 2 | 1705 | A |
| 1 | 2 | 1706 | U |
| 1 | 2 | 1707 | C |
| 1 | 2 | 1709 | C |
| 1 | 2 | 1710 | A |
| 1 | 2 | 1711 | G |
| 1 | 2 | 1712 | A |
| 1 | 2 | 1725 | G |
| 1 | 2 | 1729 | A |
| 1 | 2 | 1730 | A |
| 1 | 2 | 1742 | A |
| 1 | 2 | 1743 | G |
| 1 | 2 | 1748 | A |
| 1 | 2 | 1750 | U |
| 1 | 2 | 1753 | A |
| 1 | 2 | 1754 | A |
| 1 | 2 | 1755 | G |
| 1 | 2 | 1758 | G |
| 1 | 2 | 1760 | A |
| 1 | 2 | 1763 | A |
| 1 | 2 | 1764 | A |
| 1 | 2 | 1766 | G |
| 1 | 2 | 1767 | U |
| 1 | 2 | 1770 | C |
| 1 | 2 | 1777 | U |
| 1 | 2 | 1778 | G |
| 1 | 2 | 1779 | A |
| 1 | 2 | 1780 | A |
| 1 | 2 | 1781 | C |
| 1 | 2 | 1784 | G |
| 1 | 2 | 1790 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 2 | 1791 | G |
| 1 | 2 | 1792 | A |
| 1 | 2 | 1794 | C |
| 1 | 2 | 1795 | A |
| 1 | 2 | 1796 | U |
| 1 | 2 | 1797 | U |
| 1 | 2 | 1798 | A |

All (113) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 2 | 44 | U |
| 1 | 2 | 66 | U |
| 1 | 2 | 71 | A |
| 1 | 2 | 72 | A |
| 1 | 2 | 73 | U |
| 1 | 2 | 80 | A |
| 1 | 2 | 99 | C |
| 1 | 2 | 129 | U |
| 1 | 2 | 130 | C |
| 1 | 2 | 131 | C |
| 1 | 2 | 133 | U |
| 1 | 2 | 134 | U |
| 1 | 2 | 137 | U |
| 1 | 2 | 140 | A |
| 1 | 2 | 157 | U |
| 1 | 2 | 177 | U |
| 1 | 2 | 190 | C |
| 1 | 2 | 193 | U |
| 1 | 2 | 216 | A |
| 1 | 2 | 217 | A |
| 1 | 2 | 226 | U |
| 1 | 2 | 227 | G |
| 1 | 2 | 239 | C |
| 1 | 2 | 240 | U |
| 1 | 2 | 258 | U |
| 1 | 2 | 271 | U |
| 1 | 2 | 277 | U |
| 1 | 2 | 279 | U |
| 1 | 2 | 368 | A |
| 1 | 2 | 398 | A |
| 1 | 2 | 399 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 2 | 416 | A |
| 1 | 2 | 422 | G |
| 1 | 2 | 424 | A |
| 1 | 2 | 427 | A |
| 1 | 2 | 451 | A |
| 1 | 2 | 467 | A |
| 1 | 2 | 497 | G |
| 1 | 2 | 504 | A |
| 1 | 2 | 538 | G |
| 1 | 2 | 542 | C |
| 1 | 2 | 557 | U |
| 1 | 2 | 564 | C |
| 1 | 2 | 577 | U |
| 1 | 2 | 619 | A |
| 1 | 2 | 638 | U |
| 1 | 2 | 694 | U |
| 1 | 2 | 695 | U |
| 1 | 2 | 697 | C |
| 1 | 2 | 700 | C |
| 1 | 2 | 704 | C |
| 1 | 2 | 708 | C |
| 1 | 2 | 710 | U |
| 1 | 2 | 720 | G |
| 1 | 2 | 721 | U |
| 1 | 2 | 742 | U |
| 1 | 2 | 765 | G |
| 1 | 2 | 779 | A |
| 1 | 2 | 792 | A |
| 1 | 2 | 794 | U |
| 1 | 2 | 809 | G |
| 1 | 2 | 818 | G |
| 1 | 2 | 828 | A |
| 1 | 2 | 854 | A |
| 1 | 2 | 911 | U |
| 1 | 2 | 912 | G |
| 1 | 2 | 914 | A |
| 1 | 2 | 1051 | U |
| 1 | 2 | 1056 | U |
| 1 | 2 | 1080 | A |
| 1 | 2 | 1095 | C |
| 1 | 2 | 1098 | U |
| 1 | 2 | 1107 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 2 | 1189 | C |
| 1 | 2 | 1195 | A |
| 1 | 2 | 1216 | A |
| 1 | 2 | 1226 | A |
| 1 | 2 | 1241 | A |
| 1 | 2 | 1242 | G |
| 1 | 2 | 1243 | A |
| 1 | 2 | 1283 | C |
| 1 | 2 | 1313 | U |
| 1 | 2 | 1315 | G |
| 1 | 2 | 1320 | A |
| 1 | 2 | 1343 | A |
| 1 | 2 | 1397 | C |
| 1 | 2 | 1412 | U |
| 1 | 2 | 1429 | C |
| 1 | 2 | 1433 | G |
| 1 | 2 | 1443 | G |
| 1 | 2 | 1455 | C |
| 1 | 2 | 1491 | A |
| 1 | 2 | 1501 | A |
| 1 | 2 | 1505 | G |
| 1 | 2 | 1515 | U |
| 1 | 2 | 1534 | G |
| 1 | 2 | 1535 | C |
| 1 | 2 | 1554 | A |
| 1 | 2 | 1555 | U |
| 1 | 2 | 1580 | U |
| 1 | 2 | 1598 | A |
| 1 | 2 | 1613 | C |
| 1 | 2 | 1631 | A |
| 1 | 2 | 1632 | C |
| 1 | 2 | 1655 | U |
| 1 | 2 | 1678 | G |
| 1 | 2 | 1754 | A |
| 1 | 2 | 1759 | U |
| 1 | 2 | 1765 | G |
| 1 | 2 | 1766 | G |
| 1 | 2 | 1778 | G |
| 1 | 2 | 1791 | G |
| 1 | 2 | 1795 | A |

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 83 ligands modelled in this entry, 83 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

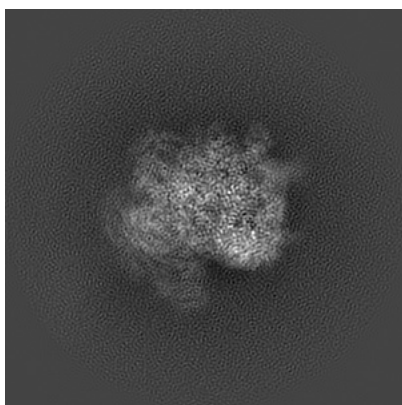
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3047. These allow visual inspection of the internal detail of the map and identification of artifacts.

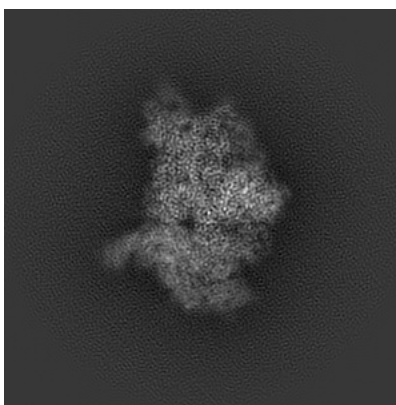
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

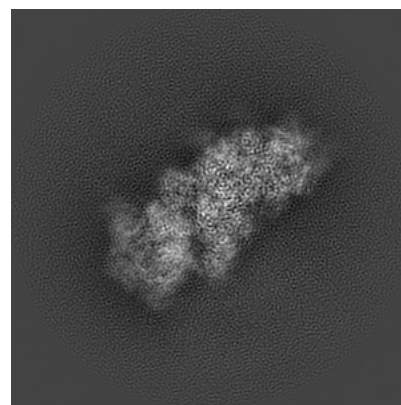
6.1.1 Primary map



X



Y

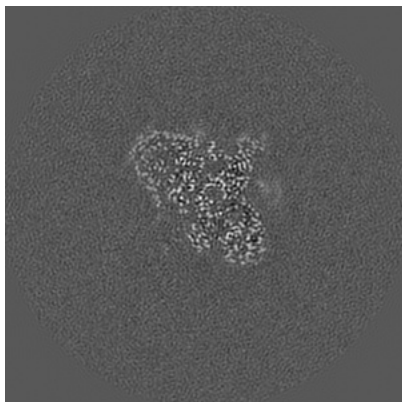


Z

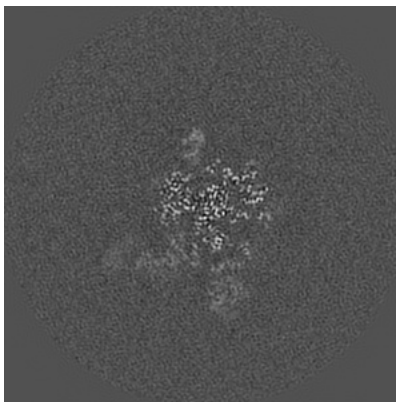
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

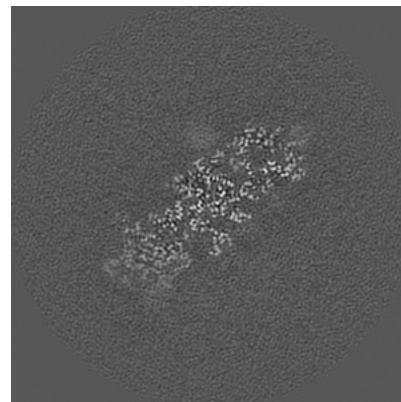
6.2.1 Primary map



X Index: 150



Y Index: 150

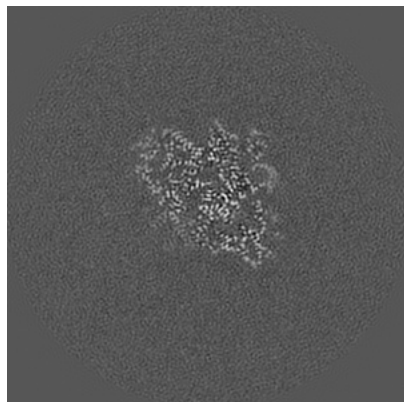


Z Index: 150

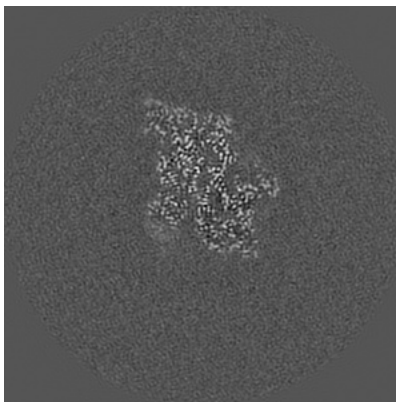
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

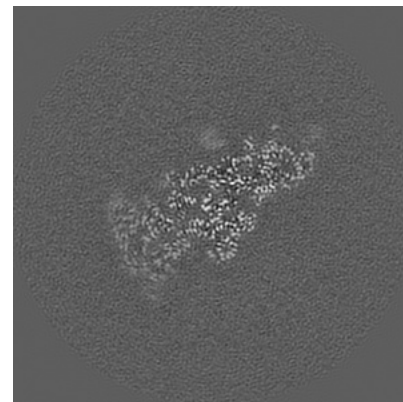
6.3.1 Primary map



X Index: 157



Y Index: 170

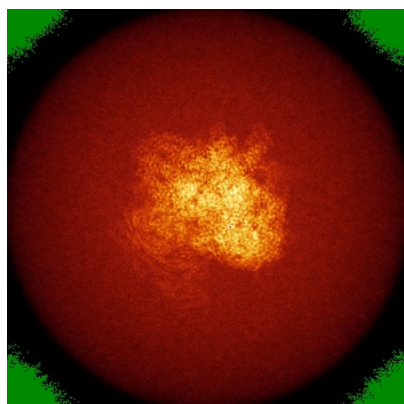


Z Index: 161

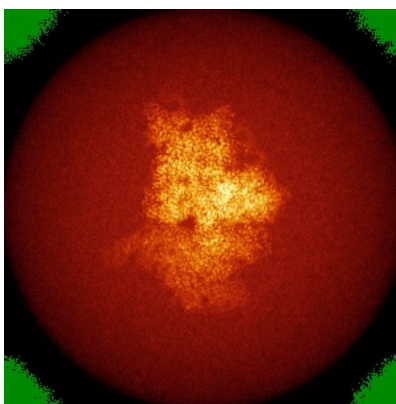
The images above show the largest variance slices of the map in three orthogonal directions.

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

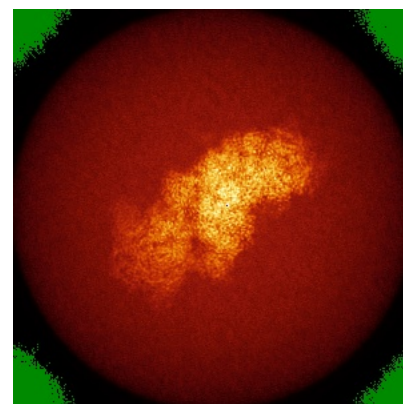
6.4.1 Primary map



X



Y

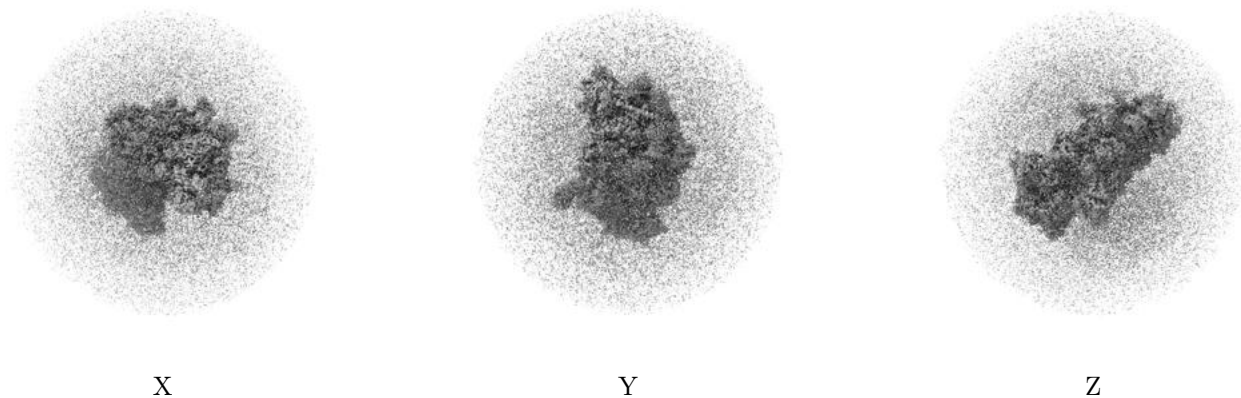


Z

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 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

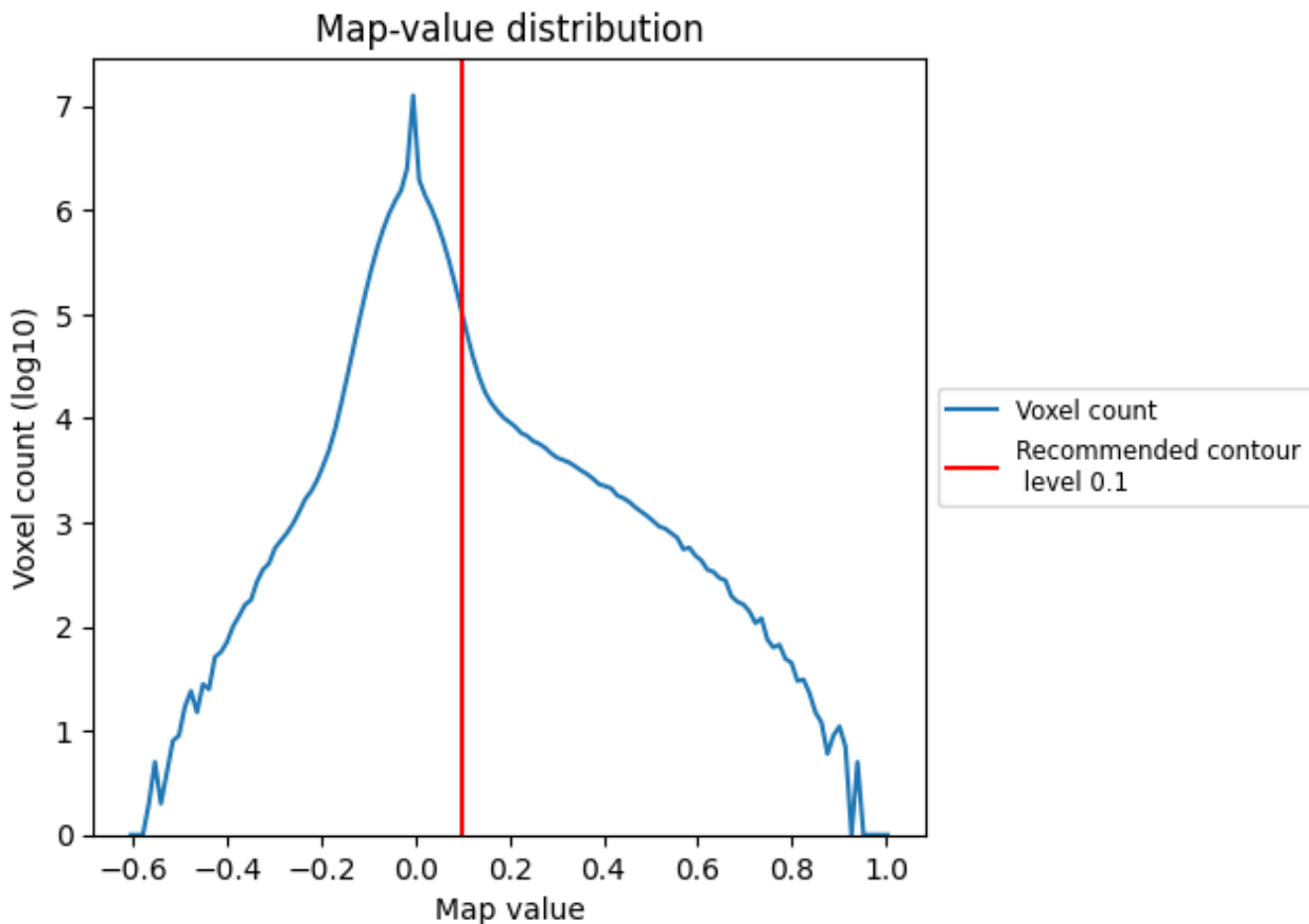
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

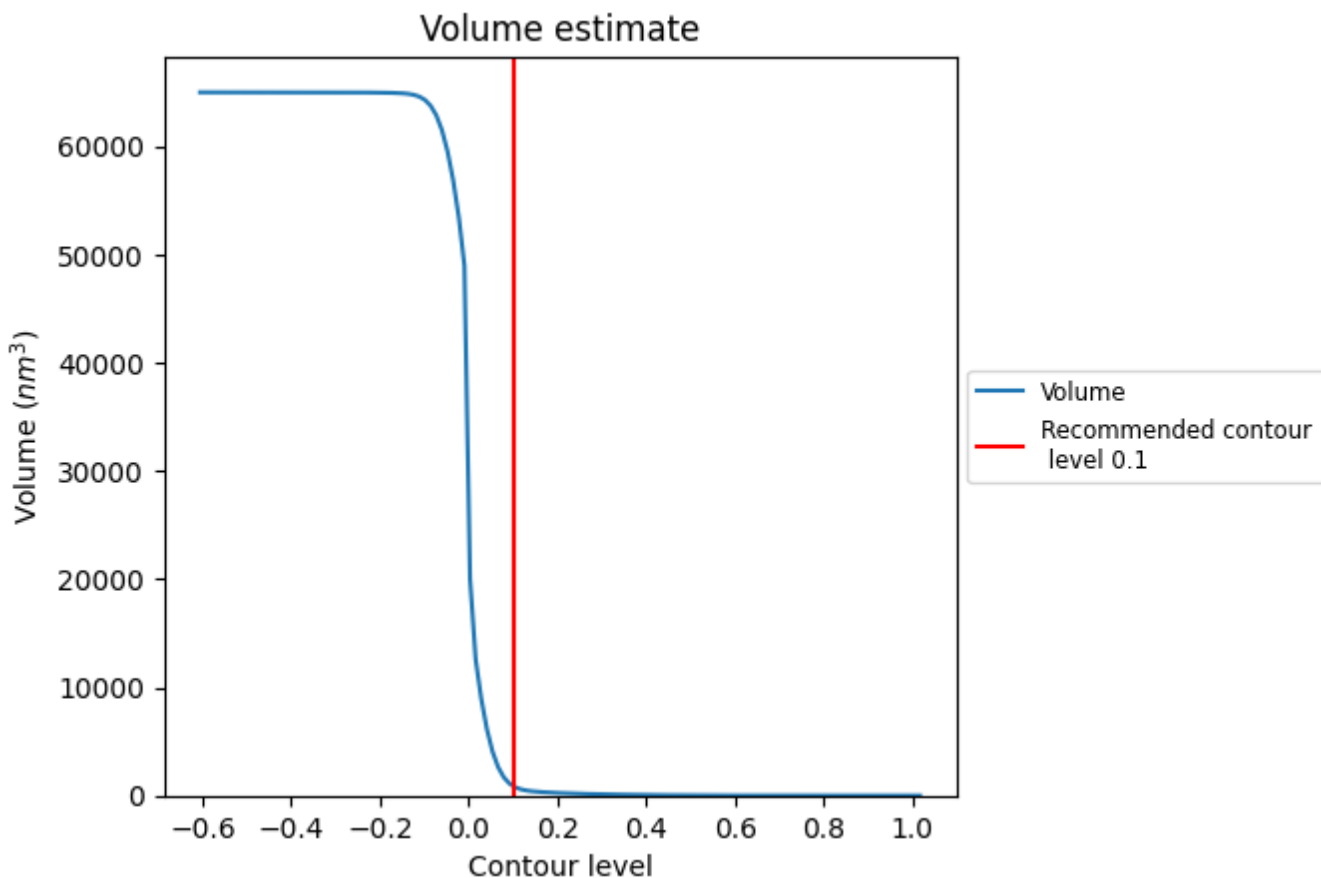
This section contains the results of statistical analysis of the map.

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.

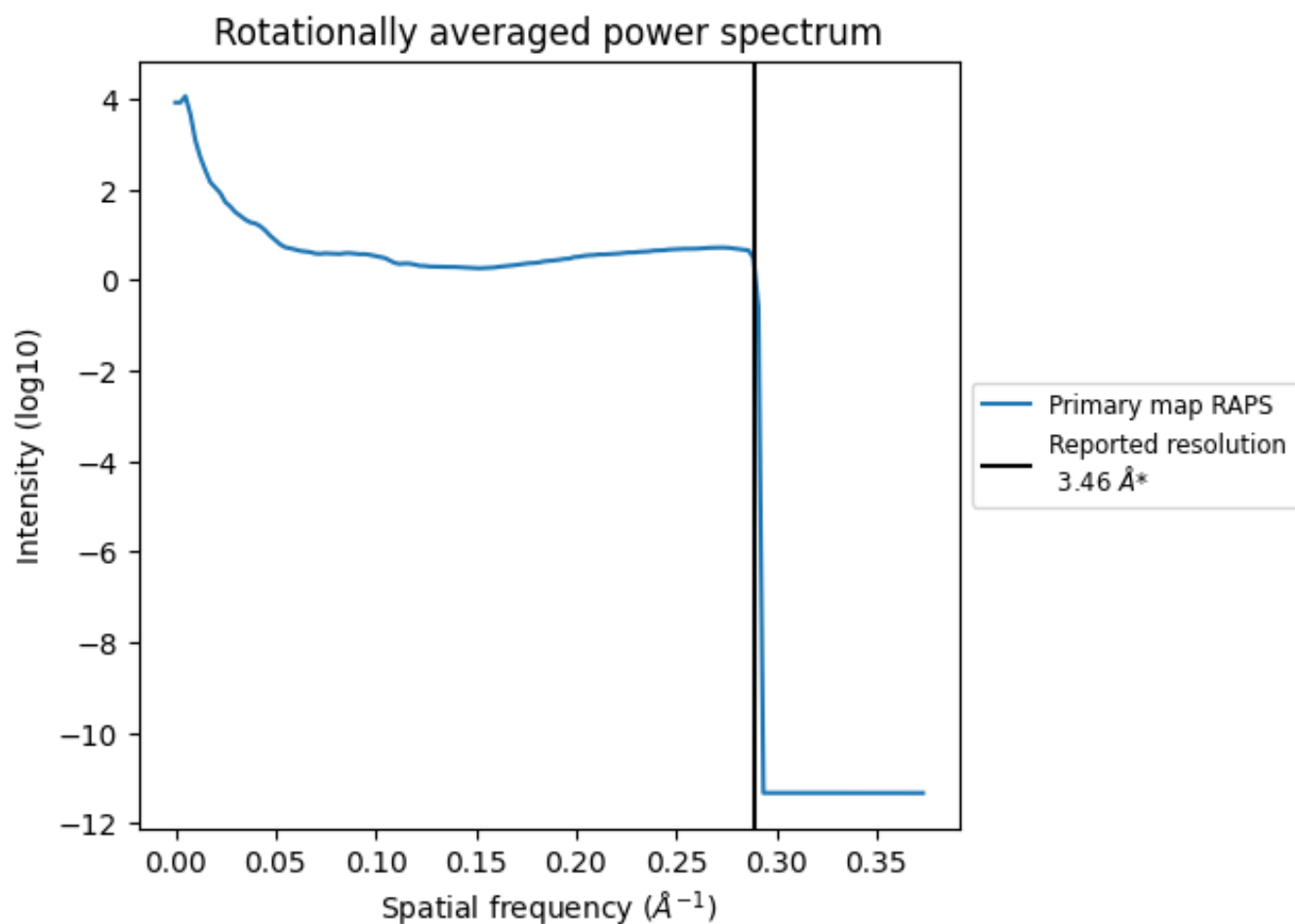
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 894 nm³; this corresponds to an approximate mass of 808 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 [\(i\)](#)

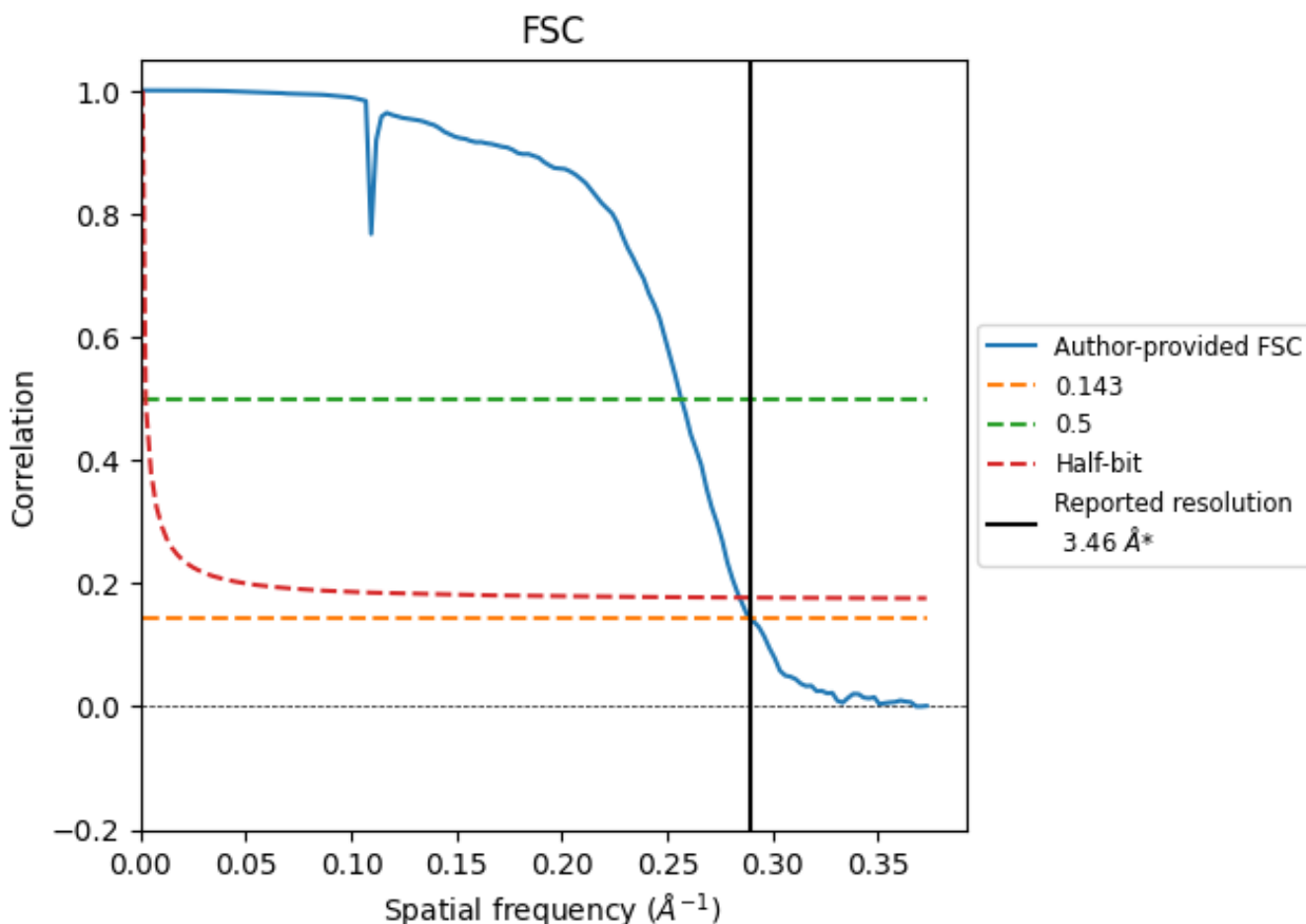


*Reported resolution corresponds to spatial frequency of 0.289 Å⁻¹

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 0.289\AA^{-1}

8.2 Resolution estimates [i](#)

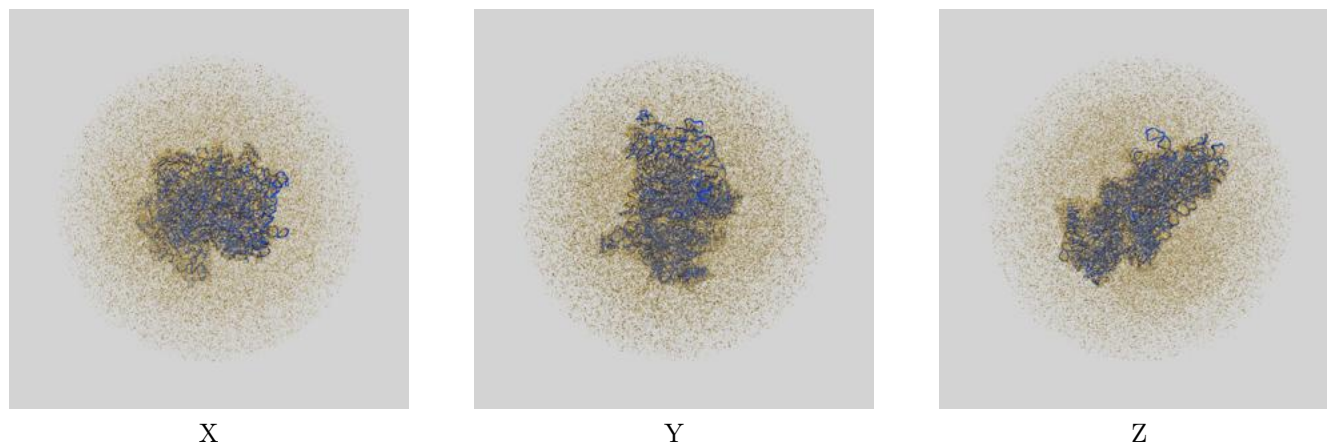
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.46 | - | - |
| Author-provided FSC curve | 3.46 | 3.90 | 3.52 |
| Unmasked-calculated* | - | - | - |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

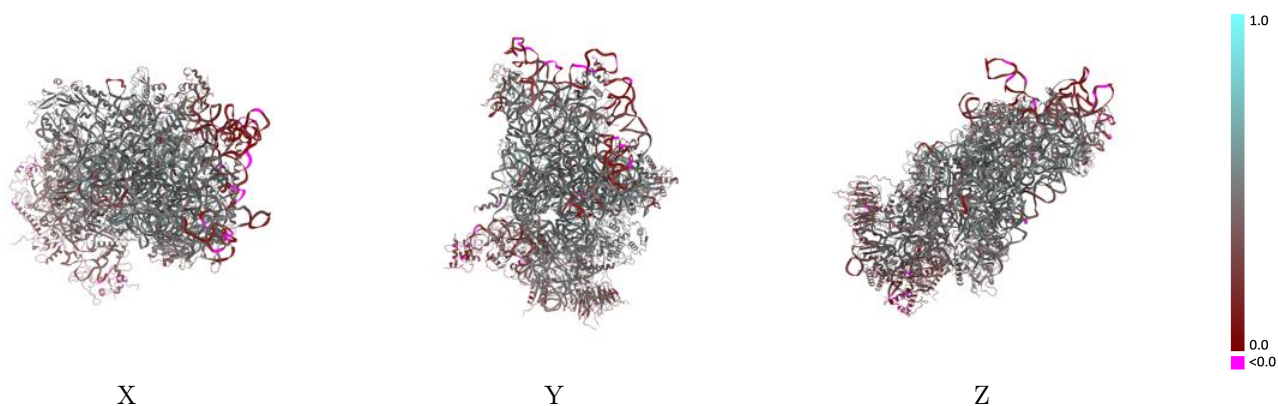
This section contains information regarding the fit between EMDB map EMD-3047 and PDB model 3JAM. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.1 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](#)

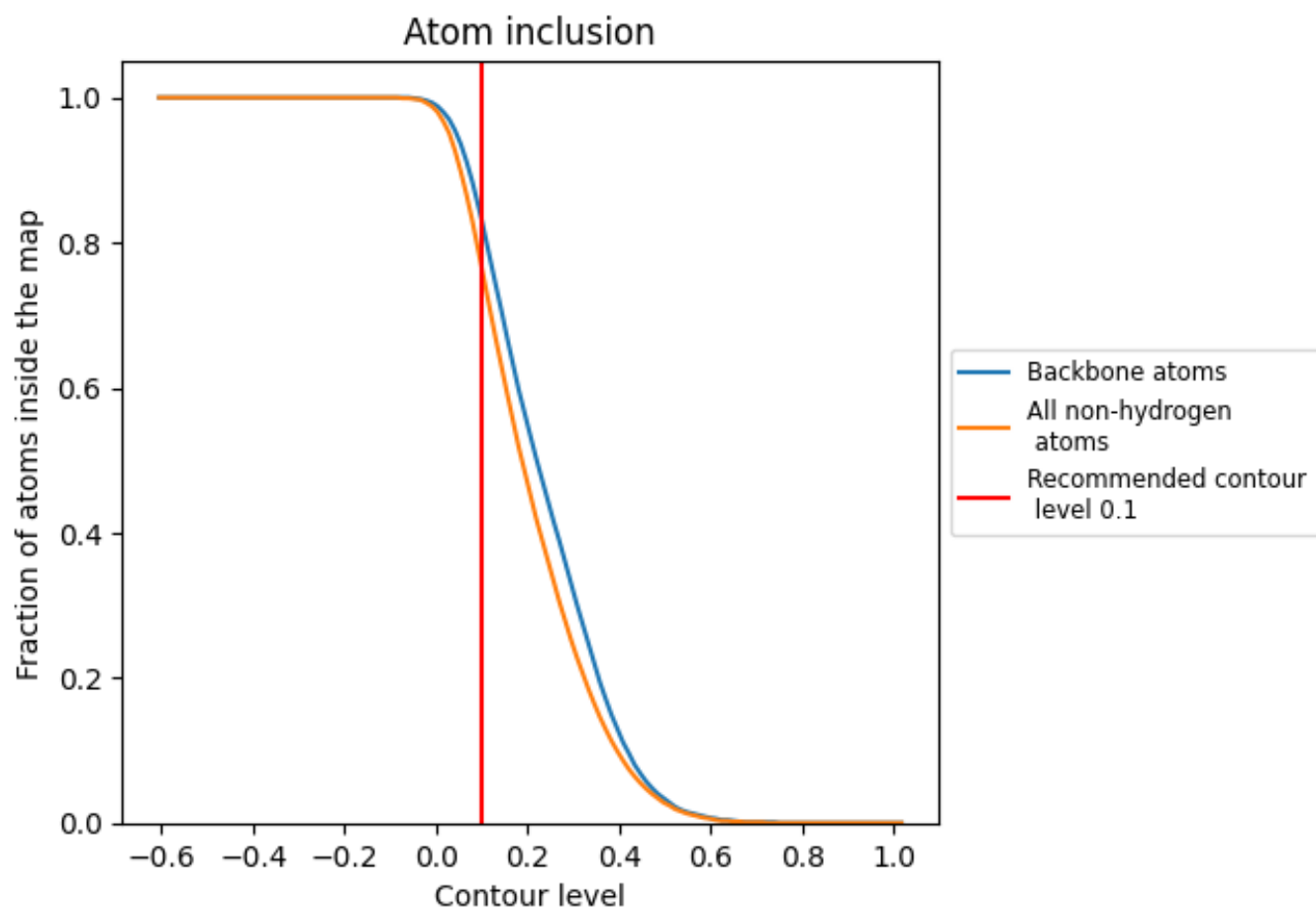


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)

This section was not generated.







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 76% 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 (0.1) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.7650 |  0.4180 |
| 2 |  0.8310 |  0.4190 |
| A |  0.8380 |  0.4840 |
| B |  0.7800 |  0.4680 |
| C |  0.8130 |  0.4990 |
| D |  0.6630 |  0.3870 |
| E |  0.8270 |  0.4990 |
| F |  0.6190 |  0.3510 |
| G |  0.7540 |  0.4320 |
| H |  0.7480 |  0.4370 |
| I |  0.7940 |  0.4730 |
| J |  0.8190 |  0.4900 |
| K |  0.6360 |  0.3370 |
| L |  0.7630 |  0.4730 |
| M |  0.2560 |  0.1520 |
| N |  0.8160 |  0.4800 |
| O |  0.8270 |  0.4730 |
| P |  0.4830 |  0.2740 |
| Q |  0.7460 |  0.4350 |
| R |  0.7500 |  0.4360 |
| S |  0.4800 |  0.2520 |
| T |  0.6870 |  0.3690 |
| U |  0.6370 |  0.3810 |
| V |  0.8320 |  0.4880 |
| W |  0.8560 |  0.5210 |
| X |  0.8530 |  0.5200 |
| Y |  0.8240 |  0.4810 |
| Z |  0.1160 |  0.1420 |
| a |  0.8530 |  0.5060 |
| b |  0.8160 |  0.4720 |
| c |  0.5950 |  0.3680 |
| d |  0.7960 |  0.4530 |
| e |  0.7100 |  0.4570 |
| f |  0.3350 |  0.2010 |
| g |  0.6200 |  0.3420 |



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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| h |  0.4620 |  0.3630 |
| i |  0.3580 |  0.3720 |
| j |  0.3810 |  0.3470 |