



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 12:01 pm GMT

PDB ID : 4DR5
Title : Crystal structure of the *Thermus thermophilus* (HB8) 30S ribosomal subunit with codon, crystallographically disordered cognate transfer RNA anticodon stem-loop and streptomycin bound
Authors : Demirci, H.; Murphy IV, F.; Murphy, E.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.
Deposited on : 2012-02-16
Resolution : 3.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

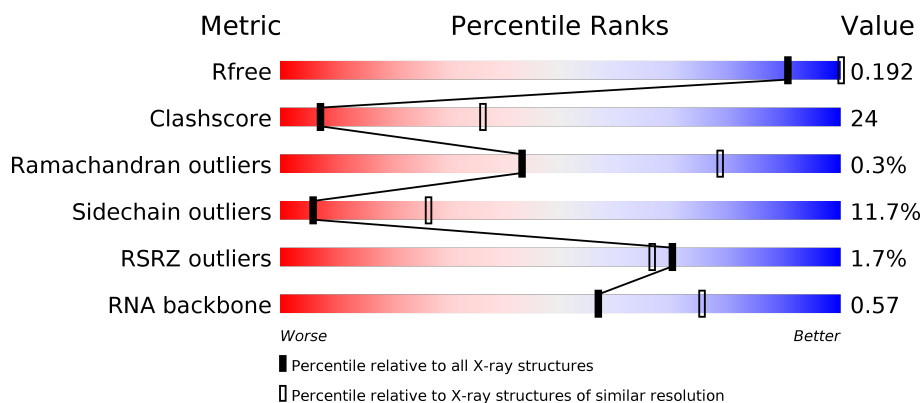
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






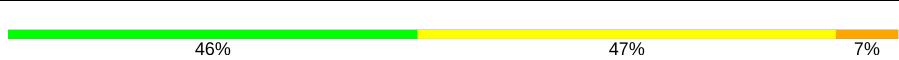
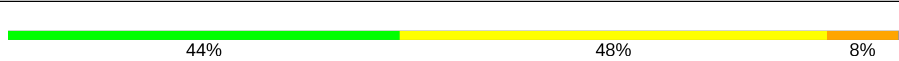
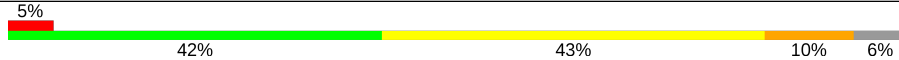
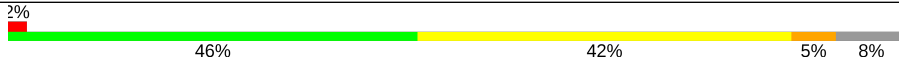
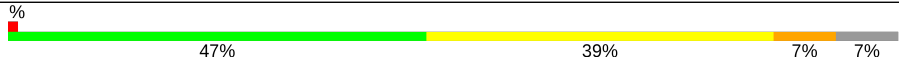
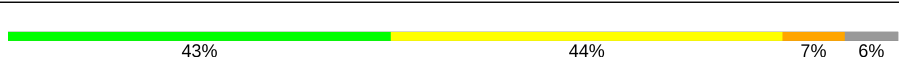
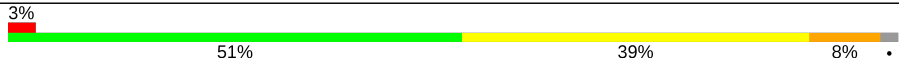
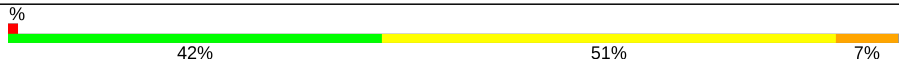
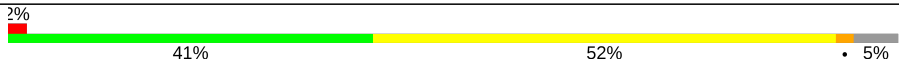
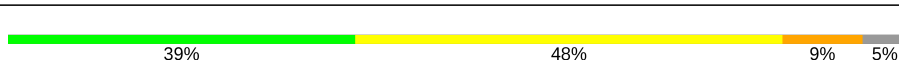
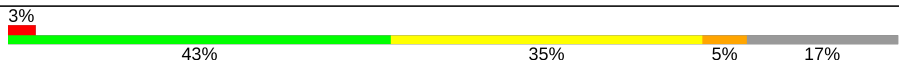
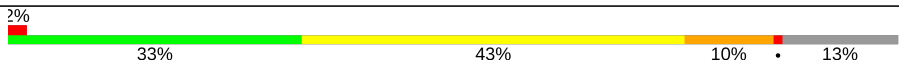
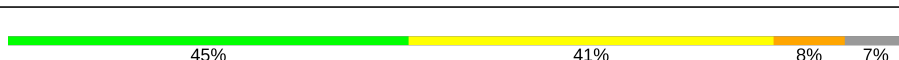
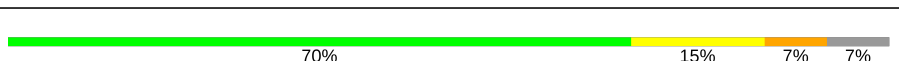


| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 111664 | 1091 (3.52-3.40) |
| Clashscore | 122126 | 1166 (3.52-3.40) |
| Ramachandran outliers | 120053 | 1135 (3.52-3.40) |
| Sidechain outliers | 120020 | 1136 (3.52-3.40) |
| RSRZ outliers | 108989 | 1015 (3.52-3.40) |
| RNA backbone | 2636 | 1048 (4.02-2.90) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 1522 | <div> <div>3%</div> <div>36% 50% 13% ..</div> </div> |
| 2 | B | 256 | <div> <div>37% 49% 6% 8%</div> </div> |
| 3 | C | 239 | <div> <div>43% 36% 8% 13%</div> </div> |
| 4 | D | 209 | <div> <div>3%</div> <div>54% 39% 7%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 5 | E | 162 |  |
| 6 | F | 101 |  |
| 7 | G | 156 |  |
| 8 | H | 138 |  |
| 9 | I | 128 |  |
| 10 | J | 105 |  |
| 11 | K | 129 |  |
| 12 | L | 135 |  |
| 13 | M | 126 |  |
| 14 | N | 61 |  |
| 15 | O | 89 |  |
| 16 | P | 88 |  |
| 17 | Q | 105 |  |
| 18 | R | 88 |  |
| 19 | S | 93 |  |
| 20 | T | 106 |  |
| 21 | U | 27 |  |
| 22 | V | 3 |  |
| 23 | W | 15 |  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|---------|-----------|----------|---------|------------------|
| 1 | UR3 | A | 1498 | - | - | X | - |
| 1 | MA6 | A | 1518[B] | - | - | X | - |
| 1 | PSU | A | 1540 | - | - | - | X |
| 1 | PSU | A | 1541 | - | - | - | X |
| 24 | MG | A | 1615 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 24 | MG | A | 1659 | - | - | - | X |
| 24 | MG | A | 1697 | - | - | - | X |
| 24 | MG | A | 1711 | - | - | - | X |
| 24 | MG | A | 1722 | - | - | - | X |
| 24 | MG | A | 1730 | - | - | - | X |
| 24 | MG | A | 1731 | - | - | - | X |
| 24 | MG | A | 1732 | - | - | - | X |
| 24 | MG | A | 1746 | - | - | - | X |
| 24 | MG | A | 1747 | - | - | - | X |
| 24 | MG | A | 1749 | - | - | - | X |
| 24 | MG | A | 1768 | - | - | - | X |
| 24 | MG | A | 1779 | - | - | - | X |
| 24 | MG | A | 1790 | - | - | - | X |
| 24 | MG | A | 1794 | - | - | - | X |
| 24 | MG | A | 1795 | - | - | - | X |
| 24 | MG | A | 1808 | - | - | - | X |
| 24 | MG | A | 1825 | - | - | - | X |
| 24 | MG | A | 1851 | - | - | - | X |
| 24 | MG | F | 201 | - | - | - | X |
| 24 | MG | N | 102 | - | - | - | X |

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 53065 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1 | A | 1512 | Total | C | N | O | P | 0 | 6 | 0 |
| | | | 32641 | 14540 | 6039 | 10545 | 1517 | | | |

There are 2 discrepancies between the modelled and reference sequences:

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2 | B | 236 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1896 | 1211 | 337 | 343 | 5 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | C | 207 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1613 | 1016 | 315 | 281 | 1 | | | |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | E | 151 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1147 | 724 | 218 | 201 | 4 | | | |

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | J | 99 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 793 | 498 | 157 | 137 | 1 | | | |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | L | 125 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 973 | 612 | 196 | 163 | 2 | | | |

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | P | 84 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 701 | 443 | 140 | 117 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17 | Q | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 834 | 534 | 156 | 142 | 2 | | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| Q | 96 | GLN | GLU | CONFLICT | UNP Q5SHP7 |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | S | 81 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 648 | 414 | 120 | 112 | 2 | | | |

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

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

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 21 | U | 25 | Total | C | N | O | 0 | 0 | 1 |
| | | | 209 | 128 | 51 | 30 | | | |

- Molecule 22 is a RNA chain called 5'-R(*UP*UP*U)-3'.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---|---------|---------|-------|
| 22 | V | 3 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 57 | 27 | 6 | 22 | 2 | | | |

- Molecule 23 is a RNA chain called 5'-R(*GP*GP*GP*AP*UP*UP*GP*AP*AP*AP*AP*UP*CP*CP*C)-3'.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 23 | W | 15 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 319 | 144 | 60 | 101 | 14 | | | |

- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

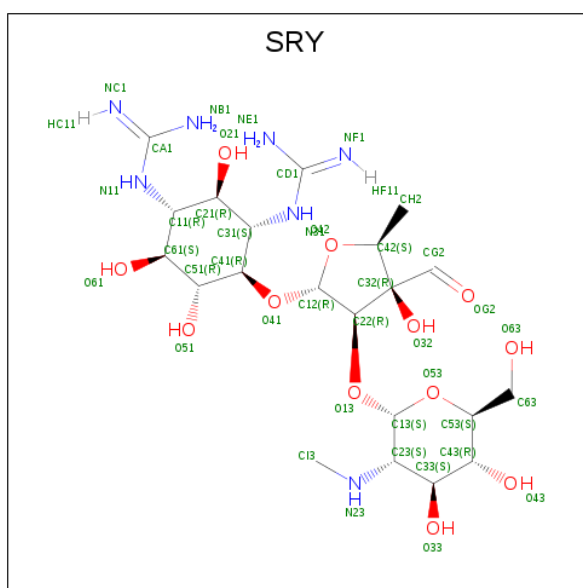
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 24 | P | 3 | Total | Mg | 0 | 0 |
| | | | 3 | 3 | | |
| 24 | G | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 24 | Q | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 24 | D | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 24 | E | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 24 | H | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 24 | A | 259 | Total | Mg | 0 | 0 |
| | | | 259 | 259 | | |
| 24 | N | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 24 | L | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 24 | S | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 24 | F | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 25 is STREPTOMYCIN (three-letter code: SRY) (formula: $C_{21}H_{39}N_7O_{12}$).

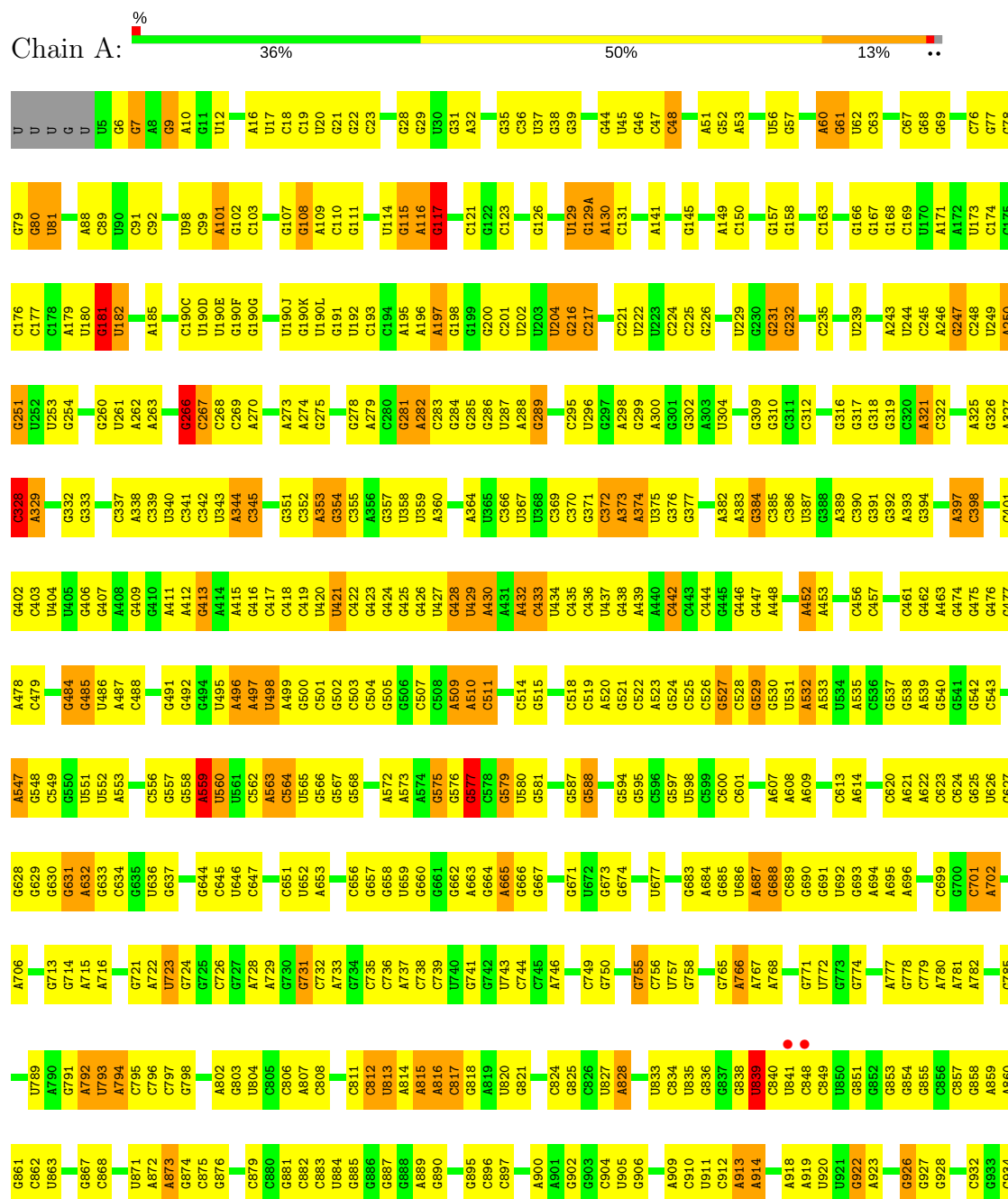


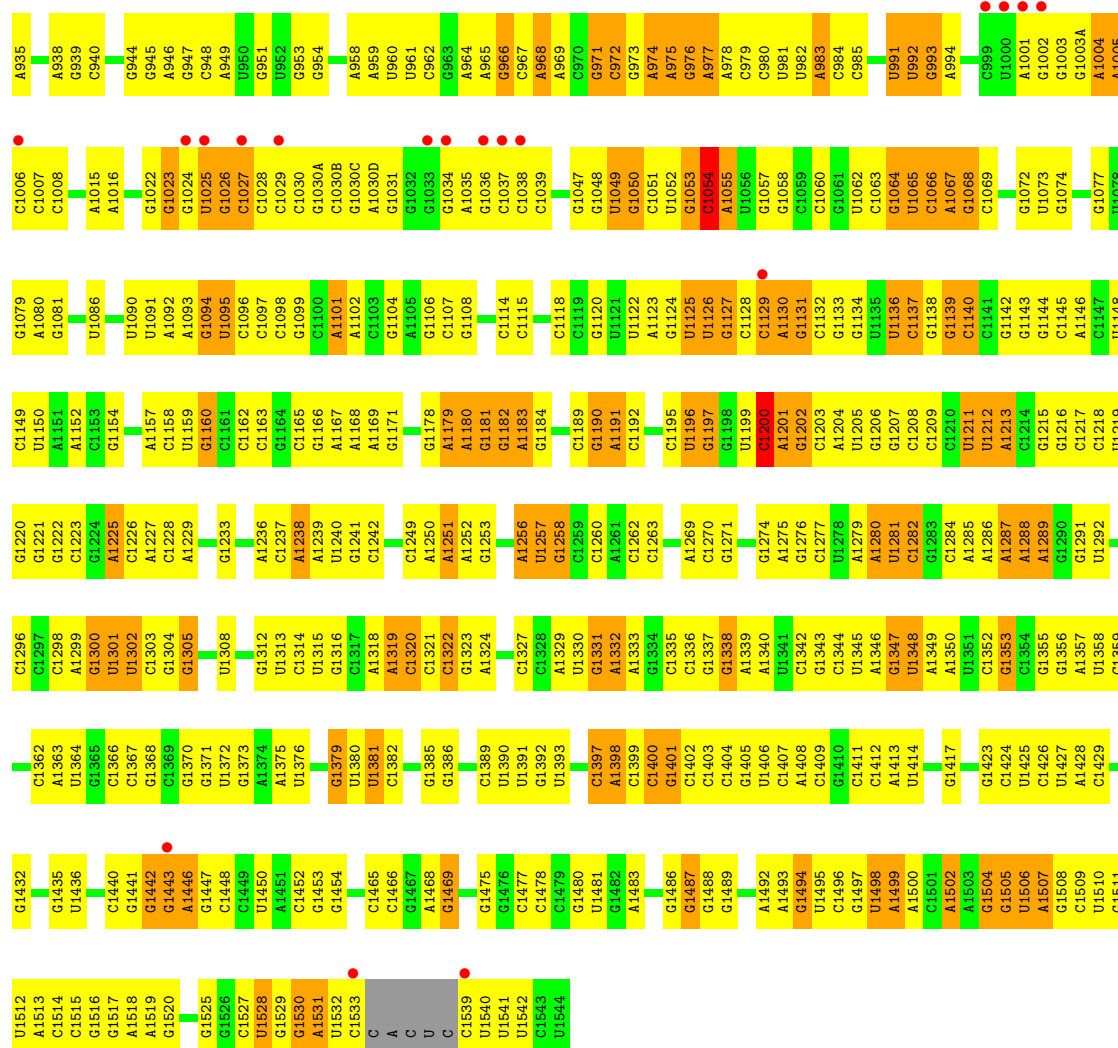
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 27 | A | 572 | Total 572 | O 572 | 0 | 0 |
| 27 | D | 2 | Total 2 | O 2 | 0 | 0 |
| 27 | E | 3 | Total 3 | O 3 | 0 | 0 |
| 27 | L | 1 | Total 1 | O 1 | 0 | 0 |
| 27 | O | 1 | Total 1 | O 1 | 0 | 0 |
| 27 | P | 1 | Total 1 | O 1 | 0 | 0 |
| 27 | Q | 1 | Total 1 | O 1 | 0 | 0 |
| 27 | T | 1 | Total 1 | O 1 | 0 | 0 |

3 Residue-property plots

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

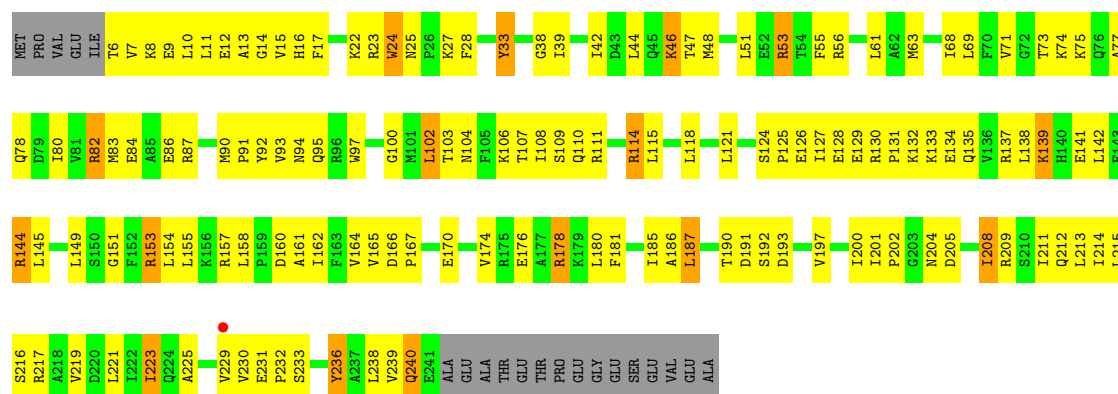
• Molecule 1: 16S rRNA





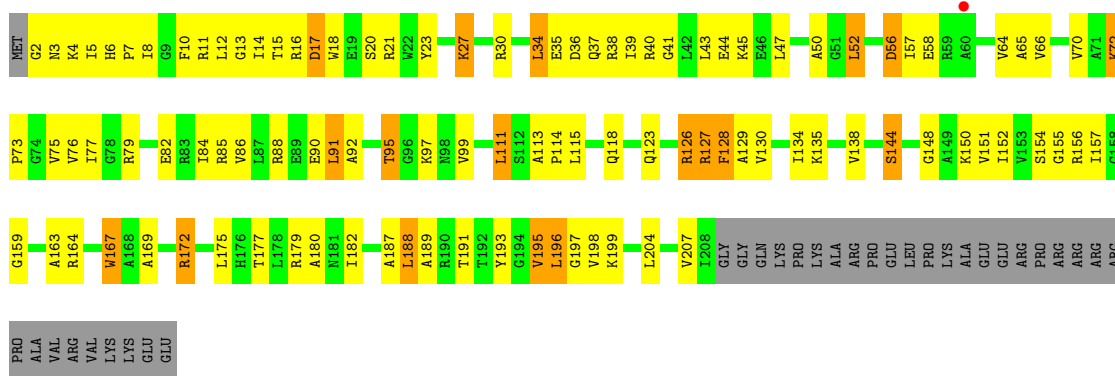
• Molecule 2: 30S ribosomal protein S2

Chain B: 37% 49% 6% 8%

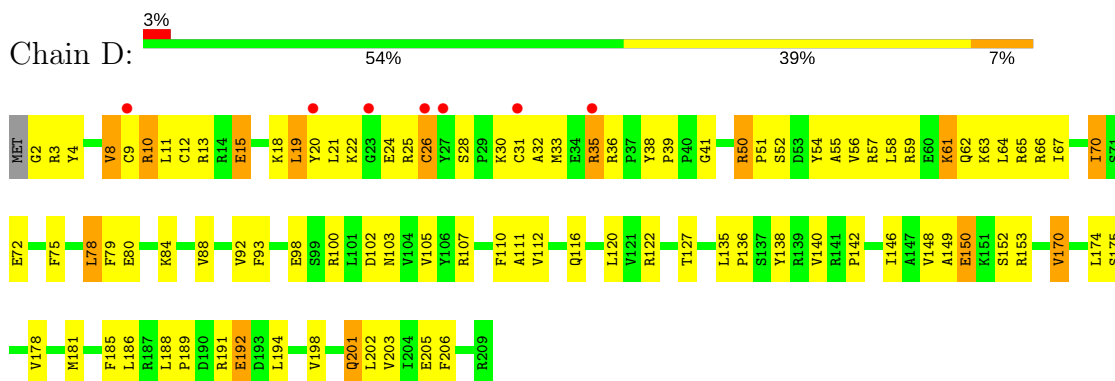


• Molecule 3: 30S ribosomal protein S3

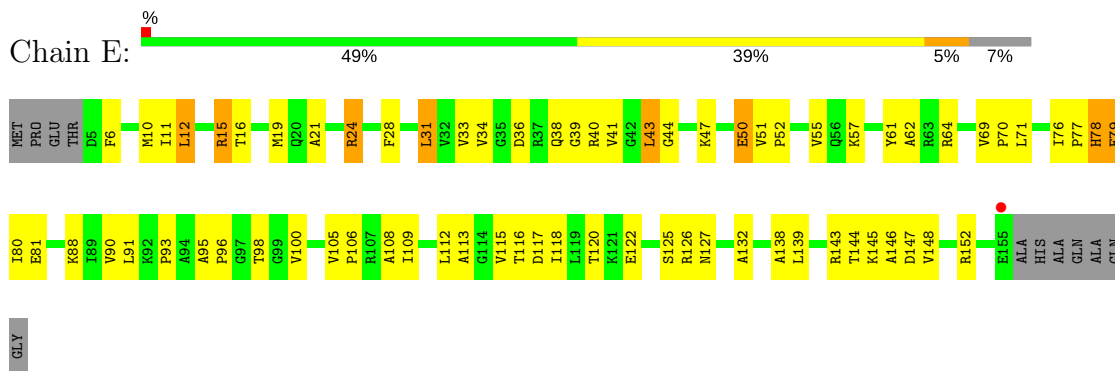
Chain C: 43% 36% 8% 13%



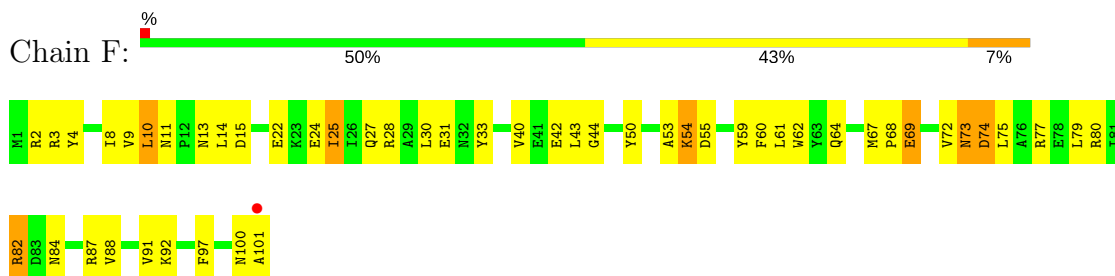
- Molecule 4: 30S ribosomal protein S4



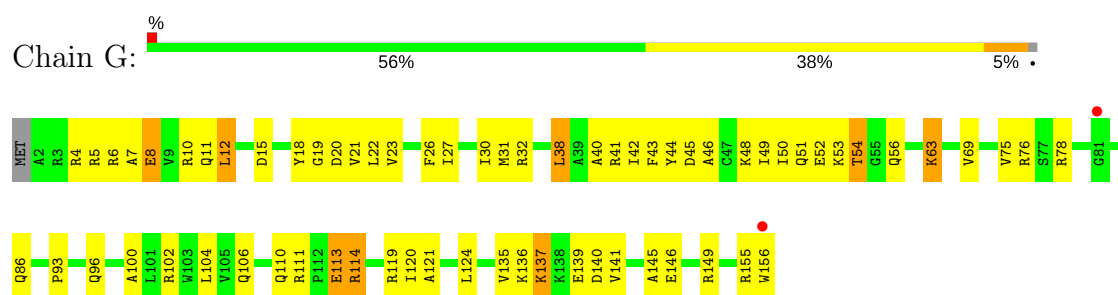
- Molecule 5: 30S ribosomal protein S5



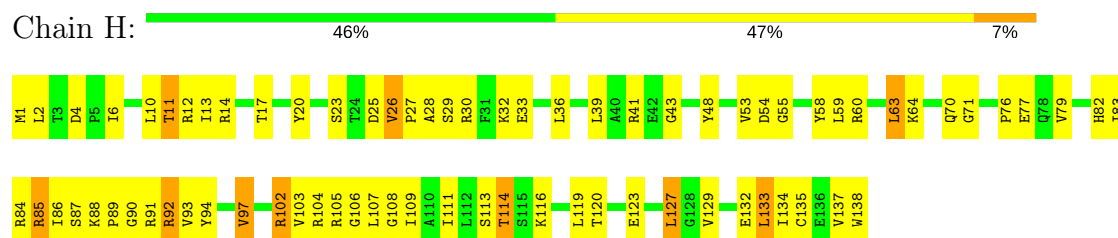
- Molecule 6: 30S ribosomal protein S6



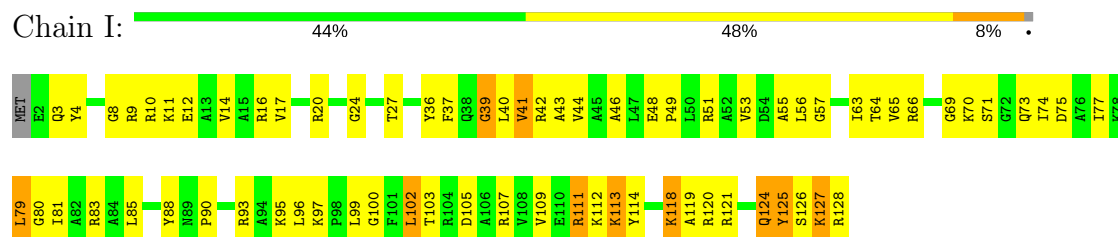
- Molecule 7: 30S ribosomal protein S7



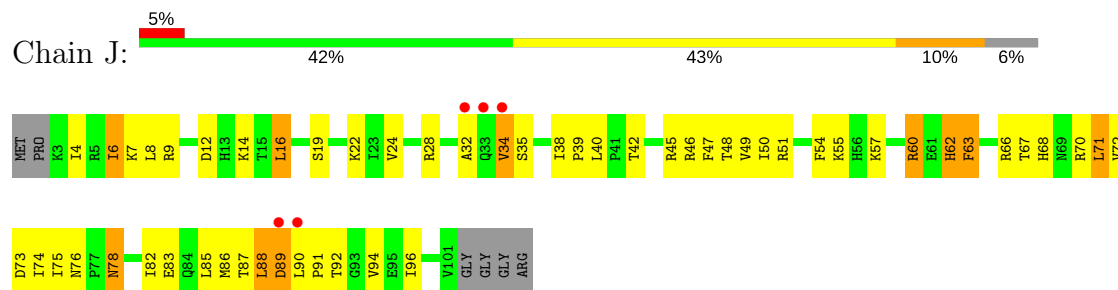
• Molecule 8: 30S ribosomal protein S8



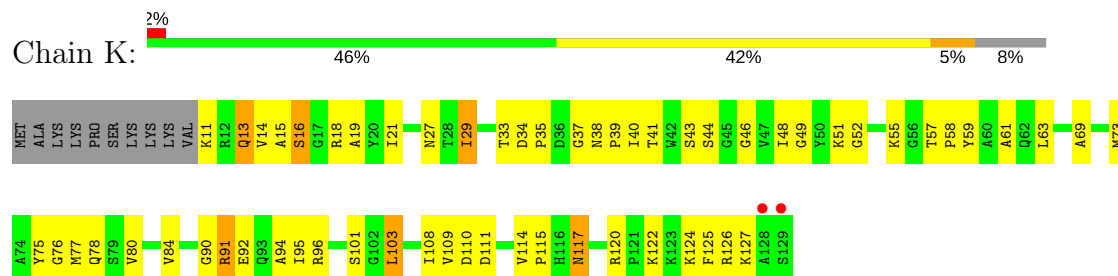
• Molecule 9: 30S ribosomal protein S9



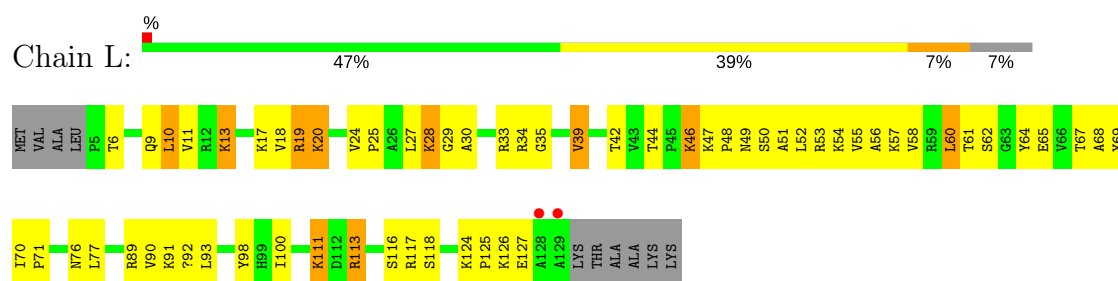
• Molecule 10: 30S ribosomal protein S10



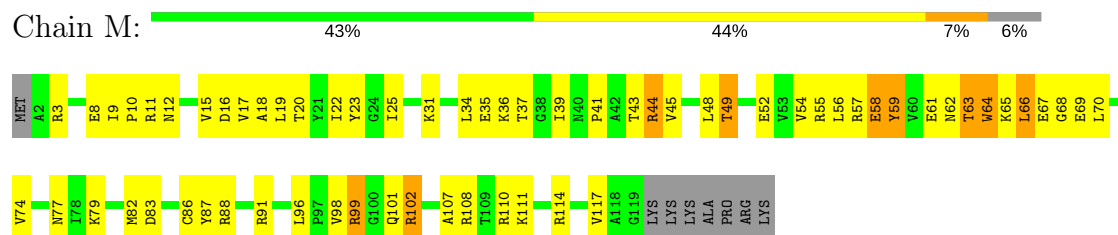
• Molecule 11: 30S ribosomal protein S11



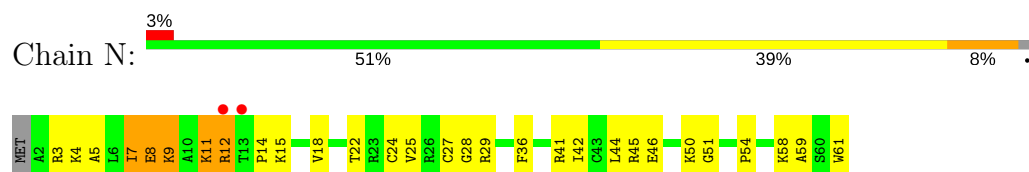
• Molecule 12: 30S ribosomal protein S12



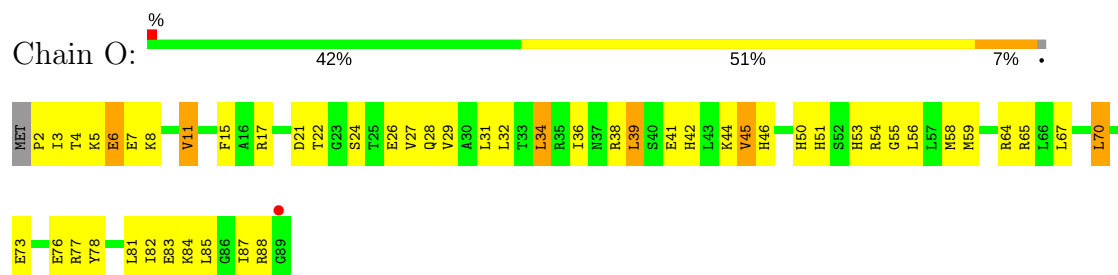
• Molecule 13: 30S ribosomal protein S13



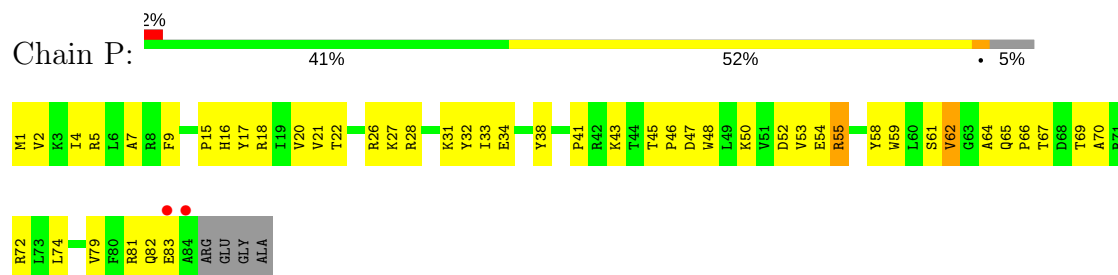
• Molecule 14: 30S ribosomal protein S14



• Molecule 15: 30S ribosomal protein S15

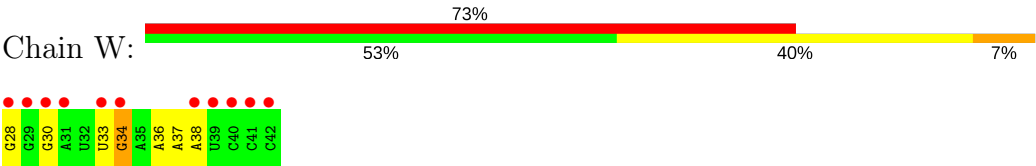


• Molecule 16: 30S ribosomal protein S16



• Molecule 17: 30S ribosomal protein S17





4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 41 21 2 | Depositor |
| Cell constants a, b, c, α , β , γ | 400.51Å 400.51Å 175.41Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 19.90 – 3.45 19.90 – 3.45 | Depositor EDS |
| % Data completeness (in resolution range) | 100.0 (19.90-3.45) 100.0 (19.90-3.45) | Depositor EDS |
| R_{merge} | 0.12 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.53 (at 3.44Å) | Xtriage |
| Refinement program | PHENIX dev_978 | Depositor |
| R, R_{free} | 0.152 , 0.192 0.152 , 0.192 | Depositor DCC |
| R_{free} test set | 9323 reflections (5.04%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 111.7 | Xtriage |
| Anisotropy | 0.223 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.28 , 83.4 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.96 | EDS |
| Total number of atoms | 53065 | wwPDB-VP |
| Average B, all atoms (Å ²) | 117.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, M2G, MA6, 0TD, MG, 2MG, 5MC, UR3, 4OC, SRY, 7MG, PSU

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------|-------------|-----------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | A | 0.49 | 0/36136 | 0.87 | 37/56392 (0.1%) |
| 2 | B | 0.31 | 0/1931 | 0.53 | 0/2607 |
| 3 | C | 0.31 | 0/1637 | 0.50 | 0/2207 |
| 4 | D | 0.34 | 0/1733 | 0.53 | 0/2318 |
| 5 | E | 0.43 | 0/1163 | 0.64 | 0/1566 |
| 6 | F | 0.31 | 0/856 | 0.51 | 0/1154 |
| 7 | G | 0.33 | 0/1276 | 0.52 | 0/1709 |
| 8 | H | 0.41 | 0/1136 | 0.62 | 0/1527 |
| 9 | I | 0.30 | 0/1029 | 0.56 | 1/1379 (0.1%) |
| 10 | J | 0.32 | 0/806 | 0.57 | 0/1084 |
| 11 | K | 0.38 | 0/900 | 0.65 | 0/1213 |
| 12 | L | 0.38 | 0/978 | 0.67 | 0/1308 |
| 13 | M | 0.31 | 0/947 | 0.52 | 0/1270 |
| 14 | N | 0.36 | 0/501 | 0.54 | 0/664 |
| 15 | O | 0.36 | 0/745 | 0.54 | 0/992 |
| 16 | P | 0.42 | 0/717 | 0.62 | 0/965 |
| 17 | Q | 0.45 | 0/847 | 0.66 | 0/1131 |
| 18 | R | 0.33 | 0/604 | 0.54 | 0/801 |
| 19 | S | 0.27 | 0/662 | 0.54 | 0/892 |
| 20 | T | 0.39 | 0/765 | 0.67 | 0/1007 |
| 21 | U | 0.34 | 0/213 | 0.57 | 0/279 |
| 22 | V | 0.23 | 0/62 | 0.67 | 0/94 |
| 23 | W | 0.18 | 0/357 | 0.47 | 0/555 |
| All | All | 0.45 | 0/56001 | 0.78 | 38/83114 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2 | B | 0 | 1 |
| 8 | H | 0 | 1 |
| 12 | L | 0 | 1 |
| All | All | 0 | 3 |

There are no bond length outliers.

All (38) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^{\circ}$) | Ideal($^{\circ}$) |
|-----|-------|------|------|-----------|-------|------------------------|---------------------|
| 1 | A | 108 | G | C4-C5-N7 | 7.91 | 113.97 | 110.80 |
| 1 | A | 108 | G | N7-C8-N9 | 7.26 | 116.73 | 113.10 |
| 1 | A | 108 | G | C5-N7-C8 | -7.26 | 100.67 | 104.30 |
| 1 | A | 108 | G | C6-C5-N7 | -7.07 | 126.16 | 130.40 |
| 1 | A | 108 | G | C4-N9-C1' | 7.03 | 135.64 | 126.50 |
| 1 | A | 266 | G | C6-C5-N7 | -6.49 | 126.51 | 130.40 |
| 1 | A | 1064 | G | N3-C4-N9 | -6.44 | 122.14 | 126.00 |
| 1 | A | 181 | G | N3-C4-C5 | -6.43 | 125.38 | 128.60 |
| 1 | A | 117 | G | N1-C6-O6 | 6.29 | 123.68 | 119.90 |
| 9 | I | 39 | GLY | N-CA-C | -6.15 | 97.73 | 113.10 |
| 1 | A | 1054 | C | C2-N1-C1' | 6.14 | 125.56 | 118.80 |
| 1 | A | 875 | C | C6-N1-C2 | 6.08 | 122.73 | 120.30 |
| 1 | A | 108 | G | N1-C6-O6 | 6.06 | 123.53 | 119.90 |
| 1 | A | 1528 | U | C2-N1-C1' | 5.83 | 124.69 | 117.70 |
| 1 | A | 624 | C | C6-N1-C2 | 5.80 | 122.62 | 120.30 |
| 1 | A | 108 | G | C8-N9-C1' | -5.76 | 119.51 | 127.00 |
| 1 | A | 129 | U | C2-N1-C1' | -5.56 | 111.03 | 117.70 |
| 1 | A | 577 | G | C8-N9-C4 | 5.52 | 108.61 | 106.40 |
| 1 | A | 1064 | G | N3-C2-N2 | -5.50 | 116.05 | 119.90 |
| 1 | A | 824 | C | C6-N1-C2 | 5.49 | 122.50 | 120.30 |
| 1 | A | 266 | G | C4-C5-N7 | 5.47 | 112.99 | 110.80 |
| 1 | A | 232 | G | N1-C6-O6 | 5.47 | 123.18 | 119.90 |
| 1 | A | 1054 | C | C6-N1-C1' | -5.42 | 114.30 | 120.80 |
| 1 | A | 529 | G | N1-C6-O6 | 5.42 | 123.15 | 119.90 |
| 1 | A | 839 | U | C2-N1-C1' | 5.34 | 124.11 | 117.70 |
| 1 | A | 266 | G | N1-C6-O6 | 5.33 | 123.10 | 119.90 |
| 1 | A | 181 | G | C4-N9-C1' | 5.25 | 133.33 | 126.50 |
| 1 | A | 1200 | C | N1-C2-O2 | 5.21 | 122.03 | 118.90 |
| 1 | A | 266 | G | C5-N7-C8 | -5.19 | 101.71 | 104.30 |
| 1 | A | 785 | G | C8-N9-C4 | 5.18 | 108.47 | 106.40 |
| 1 | A | 1079 | G | C5-C6-O6 | 5.14 | 131.69 | 128.60 |
| 1 | A | 1528 | U | P-O3'-C3' | 5.14 | 125.86 | 119.70 |
| 1 | A | 328 | C | C6-N1-C2 | -5.12 | 118.25 | 120.30 |
| 1 | A | 1305 | G | N3-C4-N9 | -5.09 | 122.95 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1 | A | 971 | G | C8-N9-C4 | 5.09 | 108.43 | 106.40 |
| 1 | A | 181 | G | N3-C4-N9 | 5.08 | 129.05 | 126.00 |
| 1 | A | 559 | A | C8-N9-C4 | -5.07 | 103.77 | 105.80 |
| 1 | A | 266 | G | N7-C8-N9 | 5.02 | 115.61 | 113.10 |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 2 | B | 14 | GLY | Peptide |
| 8 | H | 90 | GLY | Peptide |
| 12 | L | 46 | LYS | Peptide |

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 32641 | 0 | 16508 | 1073 | 1 |
| 2 | B | 1896 | 0 | 1936 | 125 | 0 |
| 3 | C | 1613 | 0 | 1677 | 108 | 0 |
| 4 | D | 1703 | 0 | 1763 | 85 | 0 |
| 5 | E | 1147 | 0 | 1207 | 73 | 0 |
| 6 | F | 843 | 0 | 857 | 45 | 0 |
| 7 | G | 1257 | 0 | 1296 | 64 | 0 |
| 8 | H | 1116 | 0 | 1177 | 69 | 0 |
| 9 | I | 1010 | 0 | 1037 | 77 | 0 |
| 10 | J | 793 | 0 | 835 | 68 | 0 |
| 11 | K | 885 | 0 | 904 | 48 | 0 |
| 12 | L | 973 | 0 | 1058 | 67 | 0 |
| 13 | M | 937 | 0 | 995 | 71 | 0 |
| 14 | N | 492 | 0 | 529 | 34 | 0 |
| 15 | O | 734 | 0 | 771 | 50 | 0 |
| 16 | P | 701 | 0 | 720 | 44 | 0 |
| 17 | Q | 834 | 0 | 906 | 69 | 0 |
| 18 | R | 598 | 0 | 670 | 38 | 0 |
| 19 | S | 648 | 0 | 673 | 59 | 0 |
| 20 | T | 763 | 0 | 861 | 64 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 21 | U | 209 | 0 | 221 | 10 | 0 |
| 22 | V | 57 | 0 | 32 | 0 | 0 |
| 23 | W | 319 | 0 | 164 | 8 | 0 |
| 24 | A | 259 | 0 | 0 | 0 | 0 |
| 24 | D | 2 | 0 | 0 | 0 | 0 |
| 24 | E | 1 | 0 | 0 | 0 | 0 |
| 24 | F | 1 | 0 | 0 | 0 | 0 |
| 24 | G | 1 | 0 | 0 | 0 | 0 |
| 24 | H | 1 | 0 | 0 | 0 | 0 |
| 24 | L | 1 | 0 | 0 | 0 | 0 |
| 24 | N | 1 | 0 | 0 | 0 | 0 |
| 24 | P | 3 | 0 | 0 | 0 | 0 |
| 24 | Q | 1 | 0 | 0 | 0 | 0 |
| 24 | S | 1 | 0 | 0 | 0 | 0 |
| 25 | A | 40 | 0 | 37 | 9 | 0 |
| 26 | D | 1 | 0 | 0 | 0 | 0 |
| 26 | N | 1 | 0 | 0 | 0 | 0 |
| 27 | A | 572 | 0 | 0 | 21 | 0 |
| 27 | D | 2 | 0 | 0 | 0 | 0 |
| 27 | E | 3 | 0 | 0 | 0 | 0 |
| 27 | L | 1 | 0 | 0 | 0 | 0 |
| 27 | O | 1 | 0 | 0 | 0 | 0 |
| 27 | P | 1 | 0 | 0 | 0 | 0 |
| 27 | Q | 1 | 0 | 0 | 0 | 0 |
| 27 | T | 1 | 0 | 0 | 0 | 0 |
| All | All | 53065 | 0 | 36834 | 2136 | 1 |

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 24.

All (2136) 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) |
|------------------|-----------------|--------------------------|-------------------|
| 11:K:15:ALA:HA | 11:K:77:MET:HA | 1.32 | 1.12 |
| 15:O:39:LEU:HD12 | 15:O:56:LEU:HB2 | 1.29 | 1.06 |
| 15:O:87:ILE:HG22 | 15:O:88:ARG:H | 1.18 | 1.06 |
| 1:A:1498:UR3:O2' | 1:A:1499:A:OP2 | 1.75 | 1.04 |
| 3:C:27:LYS:H | 3:C:27:LYS:HD3 | 1.19 | 1.04 |
| 1:A:1129:C:H4' | 1:A:1130:A:OP2 | 1.55 | 1.04 |
| 10:J:49:VAL:HG23 | 14:N:41:ARG:HB2 | 1.39 | 1.01 |
| 19:S:33:THR:HG22 | 19:S:35:SER:H | 1.26 | 1.01 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1540:PSU:H3' | 1:A:1540:PSU:H6 | 1.25 | 1.01 |
| 1:A:250:A:H4' | 1:A:251:G:O5' | 1.59 | 0.99 |
| 1:A:1005:A:N3 | 1:A:1026:G:N2 | 2.11 | 0.98 |
| 1:A:1057:G:H5'' | 3:C:154:SER:HB2 | 1.42 | 0.97 |
| 1:A:235:C:H5' | 17:Q:70:ARG:HG2 | 1.46 | 0.97 |
| 1:A:1399:C:H4' | 1:A:1400:5MC:H5'' | 1.47 | 0.97 |
| 1:A:1182:G:O2' | 1:A:1183:A:OP2 | 1.82 | 0.97 |
| 1:A:413:G:N2 | 1:A:429:U:OP2 | 1.99 | 0.96 |
| 3:C:127:ARG:HH12 | 3:C:193:TYR:HE2 | 1.10 | 0.95 |
| 1:A:1054:C:H42 | 23:W:34:G:C1' | 1.78 | 0.95 |
| 2:B:77:ALA:HB2 | 2:B:211:ILE:HD13 | 1.48 | 0.94 |
| 1:A:442:C:H42 | 1:A:492:G:H1 | 1.13 | 0.94 |
| 12:L:6:THR:OG1 | 12:L:9:GLN:HG3 | 1.67 | 0.93 |
| 15:O:17:ARG:HH11 | 15:O:17:ARG:HG3 | 1.33 | 0.93 |
| 1:A:664:G:H22 | 1:A:741:G:H1 | 1.12 | 0.92 |
| 1:A:1497:G:H2' | 1:A:1498:UR3:H5' | 1.52 | 0.91 |
| 1:A:609:A:N6 | 27:A:2206:HOH:O | 2.04 | 0.91 |
| 1:A:975:A:H5' | 1:A:975:A:H8 | 1.35 | 0.91 |
| 1:A:1443:G:H4' | 1:A:1446:A:O5' | 1.70 | 0.90 |
| 3:C:91:LEU:HD21 | 3:C:99:VAL:HG22 | 1.53 | 0.90 |
| 1:A:204:U:H5' | 1:A:216:G:OP1 | 1.72 | 0.89 |
| 1:A:344:A:H5' | 1:A:345:C:H5 | 1.37 | 0.89 |
| 1:A:975:A:H4' | 1:A:976:G:H5'' | 1.53 | 0.88 |
| 2:B:130:ARG:HB3 | 2:B:131:PRO:HD2 | 1.53 | 0.88 |
| 1:A:328:C:O2 | 1:A:328:C:H2' | 1.70 | 0.88 |
| 1:A:932:C:H4' | 7:G:4:ARG:HH21 | 1.39 | 0.87 |
| 13:M:49:THR:HG22 | 13:M:52:GLU:H | 1.38 | 0.87 |
| 1:A:974:A:OP2 | 14:N:41:ARG:NH1 | 2.06 | 0.87 |
| 1:A:279:A:OP2 | 17:Q:95:TYR:OH | 1.92 | 0.87 |
| 18:R:25:THR:HG21 | 18:R:42:ARG:NH2 | 1.89 | 0.87 |
| 1:A:1277:C:HO2' | 1:A:1279:A:H8 | 1.19 | 0.87 |
| 1:A:1412:C:H2' | 1:A:1413:A:C8 | 2.10 | 0.87 |
| 1:A:1086:U:H3 | 1:A:1099:G:H22 | 1.17 | 0.86 |
| 1:A:1331:G:O2' | 1:A:1332:A:OP2 | 1.91 | 0.86 |
| 3:C:14:ILE:HG22 | 3:C:15:THR:HG23 | 1.57 | 0.86 |
| 4:D:150:GLU:CD | 4:D:150:GLU:H | 1.76 | 0.86 |
| 12:L:27:LEU:O | 12:L:29:GLY:N | 2.07 | 0.86 |
| 17:Q:27:PHE:CE1 | 17:Q:36:ILE:HD11 | 2.09 | 0.86 |
| 9:I:24:GLY:HA3 | 9:I:57:GLY:HA2 | 1.57 | 0.86 |
| 11:K:40:ILE:HG22 | 11:K:41:THR:HG23 | 1.58 | 0.86 |
| 1:A:1053:G:HO2' | 1:A:1199:U:H5 | 1.24 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:A:1435:G:H2' | 1:A:1436:U:C6 | 2.12 | 0.85 |
| 3:C:156:ARG:H | 3:C:163:ALA:HA | 1.42 | 0.84 |
| 7:G:15:ASP:OD2 | 7:G:44:TYR:OH | 1.95 | 0.84 |
| 21:U:6:ARG:HD2 | 21:U:15:ARG:HH22 | 1.41 | 0.84 |
| 8:H:41:ARG:NH1 | 8:H:123:GLU:OE2 | 2.11 | 0.84 |
| 1:A:371:G:O2' | 1:A:372:C:H5' | 1.77 | 0.83 |
| 1:A:353:A:H5' | 1:A:353:A:H8 | 1.43 | 0.83 |
| 6:F:2:ARG:NE | 6:F:69:GLU:HG2 | 1.93 | 0.83 |
| 10:J:50:ILE:HG22 | 10:J:60:ARG:HD3 | 1.61 | 0.83 |
| 1:A:1212:U:O2' | 1:A:1213:A:O5' | 1.97 | 0.83 |
| 3:C:150:LYS:HG3 | 3:C:169:ALA:HB2 | 1.58 | 0.83 |
| 1:A:1285:A:H4' | 1:A:1286:A:O5' | 1.77 | 0.82 |
| 1:A:1095:U:H2' | 1:A:1096:C:C6 | 2.14 | 0.82 |
| 18:R:32:ARG:HA | 18:R:69:THR:HG21 | 1.61 | 0.82 |
| 6:F:97:PHE:HB2 | 18:R:32:ARG:NH1 | 1.94 | 0.82 |
| 10:J:91:PRO:HB2 | 10:J:94:VAL:HB | 1.62 | 0.82 |
| 1:A:1498:UR3:O4' | 1:A:1519[A]:MA6:H2 | 1.80 | 0.81 |
| 1:A:1136:U:H5'' | 1:A:1137:C:OP2 | 1.80 | 0.81 |
| 9:I:10:ARG:NH1 | 9:I:75:ASP:OD2 | 2.12 | 0.81 |
| 16:P:26:ARG:HD2 | 16:P:31:LYS:O | 1.80 | 0.81 |
| 17:Q:40:LYS:HD2 | 17:Q:42:TYR:CZ | 2.14 | 0.81 |
| 1:A:737:A:H1' | 6:F:73:ASN:ND2 | 1.95 | 0.81 |
| 10:J:63:PHE:HB3 | 14:N:58:LYS:HA | 1.63 | 0.81 |
| 18:R:25:THR:HG21 | 18:R:42:ARG:HH21 | 1.43 | 0.81 |
| 20:T:50:GLU:HB2 | 20:T:99:LEU:HD12 | 1.63 | 0.81 |
| 13:M:19:LEU:O | 13:M:22:ILE:HG12 | 1.81 | 0.81 |
| 3:C:64:VAL:HB | 3:C:99:VAL:HB | 1.62 | 0.81 |
| 1:A:266:G:H5' | 1:A:268:C:H41 | 1.44 | 0.80 |
| 6:F:25:ILE:HD13 | 6:F:82:ARG:HD2 | 1.64 | 0.80 |
| 1:A:372:C:H4' | 1:A:373:A:O5' | 1.80 | 0.80 |
| 7:G:146:GLU:HA | 7:G:149:ARG:HG2 | 1.62 | 0.80 |
| 1:A:1251:A:H4' | 9:I:12:GLU:OE1 | 1.82 | 0.80 |
| 8:H:28:ALA:HA | 8:H:59:LEU:HD11 | 1.64 | 0.80 |
| 10:J:50:ILE:HA | 10:J:60:ARG:HA | 1.63 | 0.80 |
| 1:A:1366:C:O2' | 10:J:60:ARG:NH1 | 2.13 | 0.80 |
| 1:A:932:C:H4' | 7:G:4:ARG:NH2 | 1.96 | 0.80 |
| 1:A:1406:U:O2' | 1:A:1517[B]:G:N2 | 2.15 | 0.79 |
| 1:A:975:A:H5' | 1:A:975:A:C8 | 2.18 | 0.79 |
| 1:A:983:A:OP1 | 14:N:3:ARG:NH2 | 2.15 | 0.79 |
| 2:B:197:VAL:HB | 2:B:200:ILE:HG12 | 1.64 | 0.79 |
| 1:A:537:G:OP1 | 12:L:113:ARG:NH2 | 2.16 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1035:A:H2' | 1:A:1036:G:H8 | 1.47 | 0.79 |
| 1:A:266:G:H5'' | 1:A:267:C:C5 | 2.16 | 0.79 |
| 12:L:19:ARG:H | 12:L:19:ARG:HD3 | 1.47 | 0.79 |
| 1:A:1200:C:O2' | 1:A:1205:U:O4 | 2.00 | 0.79 |
| 1:A:1540:PSU:H3' | 1:A:1540:PSU:C6 | 2.11 | 0.79 |
| 1:A:432:A:H2' | 1:A:433:C:O4' | 1.82 | 0.79 |
| 11:K:101:SER:OG | 11:K:103:LEU:HB2 | 1.82 | 0.79 |
| 21:U:10:ARG:HG3 | 21:U:10:ARG:HH11 | 1.46 | 0.79 |
| 1:A:673:G:H2' | 1:A:674:G:C8 | 2.19 | 0.78 |
| 10:J:82:ILE:HA | 10:J:85:LEU:HB2 | 1.62 | 0.78 |
| 1:A:946:A:H2' | 1:A:947:G:C8 | 2.18 | 0.78 |
| 1:A:737:A:H1' | 6:F:73:ASN:HD21 | 1.48 | 0.78 |
| 19:S:18:LYS:HG2 | 19:S:31:ILE:HD11 | 1.66 | 0.78 |
| 1:A:1054:C:H3' | 1:A:1054:C:O2 | 1.84 | 0.78 |
| 1:A:1054:C:H42 | 23:W:34:G:H1' | 1.48 | 0.78 |
| 1:A:1129:C:C4' | 1:A:1130:A:OP2 | 2.32 | 0.78 |
| 8:H:87:SER:HA | 8:H:93:VAL:HG23 | 1.66 | 0.77 |
| 1:A:103:C:OP1 | 20:T:17:ARG:NH1 | 2.18 | 0.77 |
| 1:A:1327:C:H5 | 21:U:6:ARG:HH22 | 1.32 | 0.77 |
| 1:A:1497:G:C2' | 1:A:1498:UR3:H5' | 2.15 | 0.77 |
| 1:A:677:U:H3 | 1:A:713:G:H22 | 1.30 | 0.77 |
| 2:B:124:SER:HB2 | 2:B:125:PRO:HD2 | 1.67 | 0.77 |
| 1:A:1028:C:N3 | 1:A:1034:G:N2 | 2.33 | 0.77 |
| 1:A:107:G:H2' | 1:A:108:G:H5' | 1.67 | 0.77 |
| 1:A:60:A:H4' | 1:A:61:G:O5' | 1.85 | 0.77 |
| 3:C:16:ARG:HD2 | 3:C:17:ASP:H | 1.47 | 0.77 |
| 1:A:427:U:OP1 | 4:D:13:ARG:NH2 | 2.17 | 0.77 |
| 13:M:10:PRO:HB2 | 13:M:18:ALA:HB1 | 1.67 | 0.76 |
| 1:A:939:G:H2' | 1:A:940:C:C6 | 2.20 | 0.76 |
| 1:A:390:C:O3' | 16:P:28:ARG:NH2 | 2.17 | 0.76 |
| 17:Q:66:SER:O | 17:Q:70:ARG:NH1 | 2.18 | 0.76 |
| 1:A:1397:C:H4' | 1:A:1398:A:OP2 | 1.86 | 0.76 |
| 1:A:1331:G:O2' | 1:A:1332:A:P | 2.44 | 0.75 |
| 1:A:1541:PSU:O4 | 1:A:1541:PSU:H2' | 1.86 | 0.75 |
| 15:O:87:ILE:HG22 | 15:O:88:ARG:N | 2.00 | 0.75 |
| 2:B:13:ALA:HB1 | 2:B:209:ARG:HB3 | 1.68 | 0.75 |
| 21:U:6:ARG:HD2 | 21:U:15:ARG:NH2 | 2.01 | 0.75 |
| 7:G:46:ALA:O | 7:G:50:ILE:HG12 | 1.87 | 0.75 |
| 1:A:1128:C:H42 | 1:A:1143:G:H1 | 1.34 | 0.74 |
| 1:A:1281:U:O2' | 1:A:1282:C:OP1 | 2.04 | 0.74 |
| 1:A:923:A:OP1 | 5:E:21:ALA:HB2 | 1.86 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 15:O:70:LEU:HD13 | 15:O:78:TYR:HA | 1.69 | 0.74 |
| 20:T:57:ARG:HE | 20:T:102:GLY:HA2 | 1.51 | 0.74 |
| 1:A:216:G:O2' | 1:A:217:C:O5' | 2.05 | 0.74 |
| 14:N:27:CYS:SG | 14:N:29:ARG:HB2 | 2.27 | 0.74 |
| 3:C:5:ILE:HD13 | 3:C:10:PHE:HB2 | 1.69 | 0.74 |
| 7:G:38:LEU:O | 7:G:42:ILE:HG13 | 1.87 | 0.74 |
| 1:A:656:C:O2' | 15:O:28:GLN:OE1 | 2.04 | 0.74 |
| 1:A:699:C:N4 | 27:A:2306:HOH:O | 2.19 | 0.74 |
| 2:B:97:TRP:HH2 | 2:B:176:GLU:CD | 1.90 | 0.74 |
| 15:O:87:ILE:O | 15:O:88:ARG:HB2 | 1.86 | 0.74 |
| 3:C:27:LYS:HD3 | 3:C:27:LYS:N | 2.00 | 0.74 |
| 9:I:90:PRO:O | 9:I:93:ARG:HG3 | 1.87 | 0.74 |
| 1:A:1101:A:H4' | 1:A:1102:A:O5' | 1.87 | 0.74 |
| 1:A:1313:U:O4 | 19:S:4:SER:OG | 2.03 | 0.74 |
| 1:A:21:G:H2' | 1:A:22:G:C8 | 2.23 | 0.74 |
| 1:A:631:G:O2' | 27:A:2340:HOH:O | 2.05 | 0.74 |
| 7:G:12:LEU:H | 7:G:12:LEU:HD12 | 1.52 | 0.74 |
| 1:A:1532:U:H2' | 1:A:1533:C:H5'' | 1.71 | 0.73 |
| 1:A:1148:U:H2' | 1:A:1149:C:O4' | 1.88 | 0.73 |
| 11:K:69:ALA:O | 11:K:73:MET:HG2 | 1.88 | 0.73 |
| 4:D:20:TYR:HD2 | 4:D:26:CYS:HB3 | 1.53 | 0.73 |
| 1:A:107:G:C2' | 1:A:108:G:H5' | 2.18 | 0.73 |
| 1:A:1291:G:H4' | 9:I:39:GLY:HA3 | 1.69 | 0.73 |
| 1:A:1352:C:H2' | 1:A:1353:G:C8 | 2.23 | 0.73 |
| 1:A:1530:G:OP1 | 1:A:1530:G:H4' | 1.89 | 0.73 |
| 20:T:14:LYS:HA | 20:T:17:ARG:HG3 | 1.70 | 0.73 |
| 20:T:75:ASN:OD1 | 20:T:75:ASN:N | 2.21 | 0.73 |
| 1:A:299:G:H2' | 1:A:300:A:C8 | 2.24 | 0.73 |
| 12:L:111:LYS:HA | 12:L:111:LYS:NZ | 2.04 | 0.73 |
| 2:B:16:HIS:HB3 | 2:B:44:LEU:HD11 | 1.69 | 0.73 |
| 9:I:43:ALA:HA | 9:I:74:ILE:HD13 | 1.68 | 0.73 |
| 1:A:1366:C:HO2' | 10:J:60:ARG:HH12 | 1.36 | 0.73 |
| 1:A:370:C:C2' | 1:A:371:G:H5' | 2.19 | 0.73 |
| 4:D:102:ASP:OD1 | 4:D:103:ASN:N | 2.21 | 0.73 |
| 20:T:82:SER:O | 20:T:86:ARG:HG3 | 1.87 | 0.73 |
| 1:A:509:A:O2' | 1:A:510:A:OP1 | 2.06 | 0.73 |
| 1:A:812:C:H4' | 1:A:813:U:O5' | 1.89 | 0.72 |
| 2:B:47:THR:HA | 2:B:202:PRO:HG2 | 1.71 | 0.72 |
| 1:A:1347:G:O2' | 1:A:1348:U:P | 2.47 | 0.72 |
| 10:J:48:THR:HA | 10:J:62:HIS:CB | 2.20 | 0.72 |
| 16:P:22:THR:HA | 16:P:33:ILE:HG13 | 1.69 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1504:G:OP1 | 1:A:1507:A:H4' | 1.90 | 0.72 |
| 1:A:328:C:O2' | 1:A:329:A:OP2 | 2.08 | 0.72 |
| 3:C:34:LEU:HD21 | 3:C:38:ARG:NH2 | 2.04 | 0.72 |
| 5:E:144:THR:O | 5:E:148:VAL:HG23 | 1.88 | 0.72 |
| 1:A:1131:G:H8 | 1:A:1131:G:OP2 | 1.72 | 0.72 |
| 1:A:1242:C:O2' | 27:A:2149:HOH:O | 2.08 | 0.72 |
| 1:A:370:C:O2' | 1:A:371:G:H5' | 1.88 | 0.72 |
| 1:A:1003(A):G:N2 | 1:A:1038:C:O2 | 2.23 | 0.72 |
| 3:C:138:VAL:HG23 | 3:C:151:VAL:HG23 | 1.71 | 0.72 |
| 4:D:98:GLU:OE2 | 4:D:107:ARG:NE | 2.23 | 0.72 |
| 12:L:20:LYS:HD2 | 12:L:20:LYS:H | 1.53 | 0.72 |
| 18:R:74:ARG:HB3 | 18:R:81:PHE:CE1 | 2.25 | 0.72 |
| 4:D:70:ILE:HD11 | 4:D:100:ARG:CZ | 2.19 | 0.72 |
| 1:A:1180:A:H5'' | 1:A:1181:G:OP2 | 1.90 | 0.71 |
| 3:C:6:HIS:CD2 | 3:C:7:PRO:HD2 | 2.25 | 0.71 |
| 13:M:11:ARG:HG2 | 13:M:12:ASN:N | 2.04 | 0.71 |
| 16:P:74:LEU:O | 16:P:79:VAL:HG23 | 1.90 | 0.71 |
| 1:A:7:G:H5' | 1:A:298:A:O4' | 1.90 | 0.71 |
| 5:E:15:ARG:HB2 | 5:E:28:PHE:CE2 | 2.24 | 0.71 |
| 1:A:689:C:OP1 | 11:K:27:ASN:ND2 | 2.23 | 0.71 |
| 1:A:428:G:H1' | 1:A:429:U:OP2 | 1.89 | 0.71 |
| 17:Q:67:LYS:HA | 17:Q:70:ARG:HH12 | 1.53 | 0.71 |
| 19:S:11:VAL:HG13 | 19:S:38:SER:HB2 | 1.71 | 0.71 |
| 1:A:839:U:O2 | 1:A:839:U:H2' | 1.89 | 0.71 |
| 1:A:660:G:OP2 | 15:O:5:LYS:HE2 | 1.90 | 0.71 |
| 20:T:13:LEU:HD12 | 20:T:14:LYS:N | 2.05 | 0.71 |
| 1:A:1392:G:H21 | 1:A:1502:A:H8 | 1.36 | 0.71 |
| 1:A:1508:G:OP1 | 27:A:1927:HOH:O | 2.07 | 0.71 |
| 12:L:33:ARG:HG2 | 12:L:62:SER:HB2 | 1.72 | 0.71 |
| 2:B:91:PRO:HG2 | 2:B:155:LEU:HD23 | 1.71 | 0.71 |
| 18:R:47:THR:HG22 | 18:R:48:GLY:H | 1.56 | 0.71 |
| 12:L:24:VAL:HG13 | 12:L:98:TYR:HE2 | 1.55 | 0.71 |
| 19:S:40:ILE:HG23 | 19:S:62:ILE:HD11 | 1.73 | 0.71 |
| 1:A:397:A:H5' | 1:A:398:C:OP1 | 1.91 | 0.70 |
| 1:A:344:A:H5' | 1:A:345:C:C5 | 2.25 | 0.70 |
| 1:A:1240:U:H1' | 7:G:38:LEU:HD21 | 1.73 | 0.70 |
| 1:A:792:A:H4' | 1:A:793:U:O5' | 1.90 | 0.70 |
| 2:B:118:LEU:HB3 | 2:B:142:LEU:HD12 | 1.73 | 0.70 |
| 1:A:542:G:OP1 | 4:D:10:ARG:NH2 | 2.19 | 0.70 |
| 1:A:1095:U:H2' | 1:A:1096:C:H6 | 1.56 | 0.70 |
| 1:A:1392:G:N2 | 1:A:1502:A:H8 | 1.89 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:231:G:O2' | 1:A:232:G:H5' | 1.91 | 0.70 |
| 7:G:50:ILE:HD11 | 7:G:121:ALA:HA | 1.74 | 0.70 |
| 1:A:1160:G:O6 | 1:A:1181:G:O6 | 2.10 | 0.70 |
| 1:A:141:A:H1' | 1:A:182:U:O2 | 1.91 | 0.70 |
| 17:Q:66:SER:HB3 | 17:Q:69:LYS:HB2 | 1.73 | 0.69 |
| 3:C:155:GLY:HA2 | 3:C:164:ARG:O | 1.92 | 0.69 |
| 5:E:144:THR:HG22 | 5:E:146:ALA:H | 1.57 | 0.69 |
| 15:O:39:LEU:CD1 | 15:O:56:LEU:HB2 | 2.17 | 0.69 |
| 14:N:41:ARG:HG3 | 14:N:42:ILE:N | 2.05 | 0.69 |
| 16:P:26:ARG:CD | 16:P:31:LYS:O | 2.41 | 0.69 |
| 9:I:3:GLN:HG3 | 9:I:20:ARG:HG2 | 1.75 | 0.69 |
| 1:A:1314:C:OP2 | 19:S:6:LYS:HD3 | 1.92 | 0.69 |
| 13:M:88:ARG:HG3 | 19:S:3:ARG:HH22 | 1.58 | 0.69 |
| 1:A:254:G:OP1 | 17:Q:67:LYS:O | 2.09 | 0.69 |
| 1:A:1191:A:H5'' | 3:C:4:LYS:NZ | 2.08 | 0.69 |
| 1:A:1442:G:C6 | 1:A:1446:A:N6 | 2.60 | 0.69 |
| 1:A:1207:2MG:HM23 | 1:A:1208:C:H1' | 1.75 | 0.68 |
| 1:A:1286:A:H2' | 1:A:1287:A:H4' | 1.74 | 0.68 |
| 1:A:1371:G:O3' | 9:I:69:GLY:HA3 | 1.93 | 0.68 |
| 1:A:204:U:O2 | 1:A:204:U:H2' | 1.93 | 0.68 |
| 10:J:49:VAL:CG2 | 14:N:41:ARG:HB2 | 2.20 | 0.68 |
| 1:A:1054:C:H5 | 1:A:1196:U:C5 | 2.12 | 0.68 |
| 2:B:10:LEU:HD22 | 2:B:15:VAL:HG21 | 1.75 | 0.68 |
| 3:C:58:GLU:HB3 | 10:J:92:THR:HG21 | 1.74 | 0.68 |
| 19:S:40:ILE:HG22 | 19:S:67:VAL:HA | 1.75 | 0.68 |
| 20:T:57:ARG:HE | 20:T:102:GLY:CA | 2.07 | 0.68 |
| 1:A:1435:G:H2' | 1:A:1436:U:H6 | 1.58 | 0.68 |
| 3:C:180:ALA:HB1 | 3:C:182:ILE:HG13 | 1.76 | 0.68 |
| 15:O:78:TYR:CZ | 15:O:82:ILE:HD11 | 2.27 | 0.68 |
| 4:D:111:ALA:HB2 | 4:D:120:LEU:HD12 | 1.76 | 0.68 |
| 5:E:76:ILE:HG12 | 5:E:118:ILE:HD12 | 1.76 | 0.68 |
| 10:J:63:PHE:HA | 14:N:59:ALA:H | 1.58 | 0.68 |
| 10:J:87:THR:O | 10:J:88:LEU:HD23 | 1.94 | 0.68 |
| 1:A:835:U:OP1 | 18:R:64:ARG:NH2 | 2.26 | 0.68 |
| 1:A:1347:G:O2' | 1:A:1348:U:OP2 | 2.12 | 0.68 |
| 1:A:560:U:H6 | 1:A:560:U:H5' | 1.59 | 0.68 |
| 1:A:983:A:O2' | 1:A:1050:G:OP2 | 2.12 | 0.68 |
| 7:G:93:PRO:HA | 7:G:96:GLN:HG3 | 1.74 | 0.68 |
| 1:A:1256:A:H5' | 1:A:1258:G:H1' | 1.75 | 0.68 |
| 2:B:53:ARG:HA | 2:B:56:ARG:NH1 | 2.09 | 0.68 |
| 1:A:1212:U:HO2' | 1:A:1213:A:P | 2.17 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:A:499:A:H4' | 1:A:500:G:OP1 | 1.94 | 0.67 |
| 4:D:189:PRO:HB2 | 4:D:194:LEU:HD21 | 1.76 | 0.67 |
| 12:L:24:VAL:HG13 | 12:L:98:TYR:CE2 | 2.28 | 0.67 |
| 1:A:795:C:H5'' | 1:A:796:C:OP2 | 1.95 | 0.67 |
| 6:F:9:VAL:HB | 6:F:87:ARG:HB2 | 1.76 | 0.67 |
| 16:P:38:TYR:OH | 16:P:47:ASP:OD1 | 2.10 | 0.67 |
| 1:A:1300:G:O2' | 1:A:1301:U:P | 2.52 | 0.67 |
| 1:A:196:A:OP1 | 20:T:68:LYS:NZ | 2.19 | 0.67 |
| 20:T:65:LYS:HA | 20:T:68:LYS:HG3 | 1.76 | 0.67 |
| 1:A:1366:C:H2' | 1:A:1367:C:C6 | 2.30 | 0.67 |
| 20:T:81:LYS:O | 20:T:85:MET:HG3 | 1.94 | 0.67 |
| 1:A:1279:A:H5'' | 1:A:1280:A:OP1 | 1.94 | 0.67 |
| 1:A:1305:G:H22 | 1:A:1331:G:C2' | 2.08 | 0.67 |
| 6:F:30:LEU:HD23 | 6:F:75:LEU:HD11 | 1.74 | 0.67 |
| 1:A:965:A:H4' | 1:A:966:M2G:O5' | 1.95 | 0.67 |
| 3:C:111:LEU:HD21 | 3:C:144:SER:O | 1.94 | 0.67 |
| 1:A:304:U:O4 | 27:A:2271:HOH:O | 2.13 | 0.67 |
| 1:A:976:G:H5' | 1:A:1358:U:O2' | 1.95 | 0.67 |
| 1:A:1366:C:H2' | 1:A:1367:C:H6 | 1.59 | 0.67 |
| 1:A:1065:U:H4' | 1:A:1066:C:O5' | 1.95 | 0.67 |
| 1:A:527:7MG:OP2 | 25:A:1860:SRY:O32 | 2.07 | 0.67 |
| 3:C:43:LEU:O | 3:C:47:LEU:HB2 | 1.95 | 0.67 |
| 1:A:61:G:O2' | 27:A:1902:HOH:O | 2.13 | 0.66 |
| 2:B:11:LEU:H | 2:B:11:LEU:HD12 | 1.58 | 0.66 |
| 8:H:28:ALA:HA | 8:H:59:LEU:CD1 | 2.25 | 0.66 |
| 21:U:5:ASP:O | 21:U:11:GLY:HA3 | 1.94 | 0.66 |
| 1:A:1540:PSU:C3' | 1:A:1540:PSU:C6 | 2.75 | 0.66 |
| 1:A:833:U:H2' | 1:A:834:C:C6 | 2.30 | 0.66 |
| 8:H:116:LYS:HG3 | 8:H:127:LEU:HD12 | 1.77 | 0.66 |
| 5:E:152:ARG:O | 8:H:64:LYS:NZ | 2.29 | 0.66 |
| 12:L:113:ARG:NH1 | 12:L:116:SER:H | 1.93 | 0.66 |
| 1:A:560:U:H5'' | 1:A:566:G:N2 | 2.11 | 0.66 |
| 1:A:914:A:P | 25:A:1860:SRY:HI33 | 2.36 | 0.66 |
| 11:K:78:GLN:O | 11:K:103:LEU:HD23 | 1.96 | 0.66 |
| 7:G:75:VAL:HG21 | 7:G:86:GLN:HB3 | 1.76 | 0.66 |
| 1:A:91:C:H2' | 1:A:92:C:H6 | 1.61 | 0.66 |
| 18:R:88:LYS:HD3 | 18:R:88:LYS:OXT | 1.94 | 0.66 |
| 1:A:1190:G:O2' | 1:A:1191:A:P | 2.54 | 0.66 |
| 9:I:81:ILE:O | 9:I:85:LEU:HB2 | 1.95 | 0.66 |
| 1:A:1442:G:H5'' | 1:A:1443:G:OP1 | 1.96 | 0.66 |
| 3:C:128:PHE:HD2 | 3:C:129:ALA:N | 1.93 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:266:G:H5'' | 1:A:267:C:H5 | 1.59 | 0.66 |
| 1:A:547:A:H4' | 1:A:548:G:O5' | 1.96 | 0.66 |
| 1:A:687:A:H4' | 1:A:688:G:O5' | 1.95 | 0.66 |
| 1:A:1006:C:H42 | 1:A:1024:G:H22 | 1.44 | 0.65 |
| 1:A:1054:C:N4 | 23:W:34:G:H1' | 2.11 | 0.65 |
| 1:A:1229:A:OP2 | 13:M:114:ARG:HD3 | 1.95 | 0.65 |
| 1:A:646:U:H2' | 1:A:647:C:C6 | 2.31 | 0.65 |
| 1:A:731:G:OP1 | 1:A:766:A:H1' | 1.96 | 0.65 |
| 2:B:114:ARG:NH1 | 2:B:118:LEU:HD21 | 2.11 | 0.65 |
| 1:A:825:G:H21 | 8:H:11:THR:HG21 | 1.61 | 0.65 |
| 1:A:1331:G:HO2' | 1:A:1332:A:P | 2.18 | 0.65 |
| 1:A:1139:G:N2 | 1:A:1142:G:O6 | 2.29 | 0.65 |
| 1:A:560:U:H5' | 1:A:560:U:C6 | 2.31 | 0.65 |
| 1:A:765:G:H5'' | 1:A:766:A:OP1 | 1.95 | 0.65 |
| 3:C:34:LEU:HD13 | 14:N:25:VAL:HG21 | 1.78 | 0.65 |
| 7:G:45:ASP:O | 7:G:49:ILE:HG13 | 1.96 | 0.65 |
| 10:J:16:LEU:HD13 | 10:J:70:ARG:HG2 | 1.79 | 0.65 |
| 1:A:1212:U:O2' | 1:A:1213:A:P | 2.54 | 0.65 |
| 10:J:39:PRO:HB3 | 10:J:70:ARG:NH1 | 2.10 | 0.65 |
| 17:Q:40:LYS:HD2 | 17:Q:42:TYR:CE1 | 2.32 | 0.65 |
| 1:A:1168:A:H2' | 1:A:1169:A:C8 | 2.32 | 0.65 |
| 1:A:651:C:O2' | 1:A:652:U:H5' | 1.97 | 0.65 |
| 10:J:32:ALA:O | 10:J:34:VAL:HG23 | 1.97 | 0.65 |
| 1:A:1515[B]:C:N4 | 1:A:1520[B]:G:O6 | 2.29 | 0.65 |
| 4:D:64:LEU:HD12 | 4:D:75:PHE:HZ | 1.62 | 0.65 |
| 20:T:74:LYS:HB3 | 20:T:74:LYS:NZ | 2.11 | 0.65 |
| 1:A:1005:A:C2 | 1:A:1026:G:N2 | 2.65 | 0.65 |
| 14:N:4:LYS:O | 14:N:7:ILE:HG12 | 1.97 | 0.65 |
| 15:O:56:LEU:HA | 15:O:59:MET:HE2 | 1.78 | 0.65 |
| 1:A:1350:A:OP2 | 9:I:118:LYS:HE2 | 1.96 | 0.65 |
| 2:B:174:VAL:O | 2:B:178:ARG:HG2 | 1.97 | 0.65 |
| 8:H:82:HIS:ND1 | 8:H:138:TRP:NE1 | 2.44 | 0.65 |
| 10:J:63:PHE:HZ | 14:N:45:ARG:HA | 1.62 | 0.65 |
| 1:A:1314:C:C5 | 19:S:6:LYS:HE2 | 2.33 | 0.64 |
| 3:C:72:LYS:HD3 | 3:C:75:VAL:HG21 | 1.79 | 0.64 |
| 1:A:1047:G:H2' | 1:A:1048:G:H5' | 1.79 | 0.64 |
| 1:A:983:A:H5'' | 1:A:984:C:OP2 | 1.96 | 0.64 |
| 8:H:86:ILE:HD12 | 8:H:133:LEU:HD22 | 1.79 | 0.64 |
| 10:J:32:ALA:HB3 | 10:J:75:ILE:O | 1.98 | 0.64 |
| 1:A:1182:G:O2' | 1:A:1183:A:P | 2.55 | 0.64 |
| 1:A:262:A:H5' | 20:T:74:LYS:HG3 | 1.80 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:918:A:H2' | 1:A:919:A:C8 | 2.32 | 0.64 |
| 3:C:130:VAL:O | 3:C:134:ILE:HG13 | 1.98 | 0.64 |
| 11:K:126:ARG:O | 11:K:127:LYS:HE2 | 1.97 | 0.64 |
| 12:L:53:ARG:HH12 | 12:L:92:OTD:CG | 2.10 | 0.64 |
| 21:U:10:ARG:HH11 | 21:U:10:ARG:CG | 2.11 | 0.64 |
| 1:A:99:C:H2' | 1:A:101:A:C8 | 2.33 | 0.64 |
| 7:G:51:GLN:O | 7:G:52:GLU:HG2 | 1.98 | 0.64 |
| 17:Q:63:ARG:HG2 | 17:Q:64:PRO:HD2 | 1.79 | 0.64 |
| 18:R:36:ASN:OD1 | 18:R:39:VAL:HG12 | 1.96 | 0.64 |
| 1:A:281:G:O2' | 1:A:282:A:OP2 | 2.15 | 0.64 |
| 13:M:88:ARG:HG2 | 13:M:98:VAL:CG1 | 2.28 | 0.64 |
| 1:A:1347:G:C2' | 1:A:1348:U:OP2 | 2.45 | 0.64 |
| 1:A:928:G:O2' | 1:A:1533:C:OP1 | 2.16 | 0.64 |
| 1:A:353:A:H5' | 1:A:353:A:C8 | 2.29 | 0.64 |
| 1:A:580:U:H2' | 1:A:581:G:O4' | 1.98 | 0.64 |
| 1:A:620:C:H2' | 1:A:621:A:O4' | 1.97 | 0.64 |
| 4:D:36:ARG:HB3 | 4:D:38:TYR:CE2 | 2.33 | 0.64 |
| 8:H:82:HIS:NE2 | 8:H:84:ARG:HB2 | 2.13 | 0.64 |
| 1:A:1399:C:O2 | 1:A:1401:G:C5 | 2.51 | 0.64 |
| 1:A:1443:G:H4' | 1:A:1446:A:C5' | 2.27 | 0.64 |
| 20:T:13:LEU:C | 20:T:13:LEU:HD12 | 2.17 | 0.64 |
| 1:A:1003(A):G:N2 | 1:A:1038:C:C2 | 2.66 | 0.64 |
| 1:A:966:M2G:HM22 | 1:A:967:5MC:O2 | 1.98 | 0.64 |
| 5:E:71:LEU:HD21 | 5:E:115:VAL:HG22 | 1.79 | 0.64 |
| 5:E:51:VAL:O | 5:E:55:VAL:HG23 | 1.98 | 0.64 |
| 20:T:74:LYS:HZ3 | 20:T:74:LYS:HA | 1.61 | 0.64 |
| 1:A:1510:U:H2' | 1:A:1511:G:C8 | 2.32 | 0.64 |
| 1:A:630:G:H5' | 1:A:631:G:OP2 | 1.98 | 0.64 |
| 3:C:5:ILE:O | 3:C:5:ILE:HD12 | 1.98 | 0.64 |
| 12:L:42:THR:OG1 | 12:L:52:LEU:HB3 | 1.98 | 0.64 |
| 13:M:37:THR:HG23 | 13:M:55:ARG:HD2 | 1.79 | 0.64 |
| 17:Q:65:ILE:N | 17:Q:65:ILE:HD12 | 2.13 | 0.64 |
| 6:F:50:TYR:CE1 | 18:R:77:GLY:HA2 | 2.33 | 0.64 |
| 18:R:46:GLU:OE2 | 18:R:46:GLU:N | 2.23 | 0.63 |
| 1:A:1443:G:C4' | 1:A:1446:A:O5' | 2.45 | 0.63 |
| 1:A:45:U:H2' | 1:A:46:G:C8 | 2.33 | 0.63 |
| 2:B:69:LEU:HD22 | 2:B:71:VAL:HG23 | 1.80 | 0.63 |
| 3:C:6:HIS:HD2 | 3:C:7:PRO:HD2 | 1.61 | 0.63 |
| 6:F:4:TYR:CE1 | 6:F:92:LYS:HG2 | 2.33 | 0.63 |
| 13:M:34:LEU:HD13 | 13:M:41:PRO:HA | 1.79 | 0.63 |
| 20:T:67:ALA:HA | 20:T:73:HIS:H | 1.62 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:130:VAL:HG21 | 3:C:157:ILE:HG23 | 1.80 | 0.63 |
| 1:A:192:U:H1' | 20:T:103:GLY:HA2 | 1.80 | 0.63 |
| 1:A:972:C:OP1 | 10:J:57:LYS:NZ | 2.19 | 0.63 |
| 4:D:32:ALA:HA | 4:D:35:ARG:HG3 | 1.81 | 0.63 |
| 1:A:598:U:H4' | 8:H:94:TYR:CD1 | 2.34 | 0.63 |
| 19:S:31:ILE:HG21 | 19:S:49:ILE:HG23 | 1.79 | 0.63 |
| 4:D:188:LEU:HD23 | 4:D:189:PRO:HD2 | 1.80 | 0.63 |
| 1:A:359:U:H2' | 1:A:360:A:C8 | 2.33 | 0.63 |
| 1:A:1493:A:N1 | 23:W:36:A:O2' | 2.26 | 0.62 |
| 2:B:44:LEU:H | 2:B:44:LEU:HD22 | 1.64 | 0.62 |
| 14:N:9:LYS:C | 14:N:9:LYS:HD2 | 2.19 | 0.62 |
| 8:H:86:ILE:HG13 | 8:H:135:CYS:HA | 1.79 | 0.62 |
| 18:R:46:GLU:CD | 18:R:46:GLU:H | 2.02 | 0.62 |
| 1:A:359:U:H2' | 1:A:360:A:H8 | 1.64 | 0.62 |
| 1:A:882:C:O2' | 1:A:883:C:H5' | 2.00 | 0.62 |
| 12:L:60:LEU:HB2 | 12:L:64:TYR:O | 1.98 | 0.62 |
| 1:A:1296:C:H4' | 1:A:1302:U:C5 | 2.34 | 0.62 |
| 4:D:22:LYS:HB2 | 4:D:26:CYS:SG | 2.39 | 0.62 |
| 3:C:151:VAL:O | 3:C:167:TRP:O | 2.16 | 0.62 |
| 6:F:22:GLU:OE2 | 6:F:82:ARG:HD3 | 1.98 | 0.62 |
| 2:B:74:LYS:HD2 | 2:B:166:ASP:HB2 | 1.82 | 0.62 |
| 7:G:111:ARG:HB3 | 7:G:113:GLU:HG2 | 1.81 | 0.62 |
| 15:O:87:ILE:CG2 | 15:O:88:ARG:H | 2.01 | 0.62 |
| 1:A:1047:G:C2' | 1:A:1048:G:H5' | 2.29 | 0.62 |
| 1:A:1304:G:C6 | 1:A:1305:G:N1 | 2.67 | 0.62 |
| 1:A:376:G:H2' | 1:A:377:G:H8 | 1.64 | 0.62 |
| 1:A:814:A:H2' | 1:A:816:A:C5' | 2.29 | 0.62 |
| 2:B:144:ARG:HD2 | 2:B:145:LEU:HD23 | 1.82 | 0.62 |
| 9:I:70:LYS:O | 9:I:74:ILE:HG13 | 1.99 | 0.62 |
| 13:M:63:THR:HG23 | 13:M:64:TRP:H | 1.63 | 0.62 |
| 13:M:66:LEU:O | 13:M:69:GLU:HB2 | 1.99 | 0.62 |
| 1:A:1502:A:H2 | 1:A:1505:G:H1 | 1.48 | 0.62 |
| 6:F:10:LEU:CD1 | 6:F:59:TYR:HB3 | 2.29 | 0.62 |
| 18:R:38:GLU:CD | 18:R:38:GLU:H | 2.01 | 0.62 |
| 8:H:54:ASP:CG | 8:H:55:GLY:H | 2.03 | 0.62 |
| 19:S:70:LYS:N | 19:S:73:GLU:OE2 | 2.32 | 0.62 |
| 1:A:1342:C:O2' | 9:I:124:GLN:HB2 | 1.99 | 0.62 |
| 2:B:82:ARG:O | 2:B:86:GLU:HG3 | 2.00 | 0.62 |
| 2:B:91:PRO:HG2 | 2:B:155:LEU:CD2 | 2.30 | 0.62 |
| 3:C:167:TRP:HZ3 | 3:C:169:ALA:HB3 | 1.64 | 0.62 |
| 3:C:35:GLU:OE1 | 3:C:95:THR:HB | 2.00 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 9:I:97:LYS:HA | 9:I:102:LEU:HD11 | 1.82 | 0.62 |
| 9:I:93:ARG:HB3 | 9:I:93:ARG:NH1 | 2.14 | 0.62 |
| 3:C:5:ILE:CG2 | 10:J:51:ARG:HH12 | 2.12 | 0.62 |
| 12:L:10:LEU:HB3 | 17:Q:32:TYR:CE1 | 2.35 | 0.62 |
| 19:S:33:THR:HG22 | 19:S:35:SER:N | 2.06 | 0.62 |
| 1:A:116:A:H2' | 1:A:117:G:H8 | 1.65 | 0.61 |
| 11:K:57:THR:HG22 | 11:K:59:TYR:H | 1.64 | 0.61 |
| 12:L:25:PRO:C | 12:L:27:LEU:H | 2.03 | 0.61 |
| 16:P:52:ASP:OD1 | 16:P:54:GLU:HG3 | 1.99 | 0.61 |
| 19:S:17:GLU:O | 19:S:21:GLU:HB2 | 2.00 | 0.61 |
| 1:A:130:A:OP2 | 1:A:190(E):U:O2' | 2.10 | 0.61 |
| 1:A:665:A:H2' | 1:A:732:C:O2 | 2.00 | 0.61 |
| 2:B:128:GLU:HA | 2:B:135:GLN:NE2 | 2.14 | 0.61 |
| 1:A:972:C:P | 10:J:57:LYS:HD3 | 2.40 | 0.61 |
| 9:I:126:SER:C | 9:I:128:ARG:H | 2.03 | 0.61 |
| 2:B:71:VAL:HG22 | 2:B:93:VAL:HB | 1.83 | 0.61 |
| 1:A:667:G:H4' | 15:O:51:HIS:CE1 | 2.34 | 0.61 |
| 1:A:913:A:H1' | 1:A:914:A:OP2 | 2.00 | 0.61 |
| 1:A:1343:G:H2' | 1:A:1344:C:C6 | 2.36 | 0.61 |
| 1:A:974:A:P | 14:N:41:ARG:HH12 | 2.24 | 0.61 |
| 4:D:62:GLN:OE1 | 4:D:65:ARG:NH1 | 2.33 | 0.61 |
| 10:J:48:THR:HA | 10:J:62:HIS:HB3 | 1.81 | 0.61 |
| 9:I:55:ALA:O | 9:I:56:LEU:HD23 | 2.01 | 0.61 |
| 1:A:192:U:C1' | 20:T:103:GLY:HA2 | 2.30 | 0.61 |
| 1:A:1402:4OC:HM22 | 1:A:1403:C:H5' | 1.82 | 0.61 |
| 1:A:1518[B]:MA6:H102 | 1:A:1519[B]:MA6:H103 | 1.83 | 0.61 |
| 1:A:108:G:H2' | 1:A:109:A:OP1 | 2.01 | 0.61 |
| 12:L:113:ARG:HH11 | 12:L:116:SER:H | 1.48 | 0.61 |
| 1:A:262:A:C6 | 1:A:263:A:C6 | 2.89 | 0.61 |
| 10:J:46:ARG:HG3 | 10:J:46:ARG:HH11 | 1.66 | 0.61 |
| 1:A:938:A:N6 | 1:A:939:G:C6 | 2.69 | 0.60 |
| 1:A:706:A:O4' | 11:K:29:ILE:HD11 | 2.00 | 0.60 |
| 14:N:8:GLU:O | 14:N:11:LYS:HE3 | 2.00 | 0.60 |
| 1:A:1178:G:N7 | 9:I:97:LYS:NZ | 2.47 | 0.60 |
| 1:A:1190:G:O2' | 1:A:1191:A:OP2 | 2.19 | 0.60 |
| 3:C:188:LEU:HD11 | 3:C:195:VAL:HG22 | 1.83 | 0.60 |
| 7:G:78:ARG:HD2 | 7:G:156:TRP:HE3 | 1.65 | 0.60 |
| 1:A:1026:G:O2' | 1:A:1027:C:OP1 | 2.18 | 0.60 |
| 1:A:1195:C:H5'' | 1:A:1196:U:OP2 | 2.01 | 0.60 |
| 2:B:219:VAL:O | 2:B:223:ILE:HG12 | 2.00 | 0.60 |
| 2:B:80:ILE:HD11 | 2:B:208:ILE:HG22 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:24:GLU:O | 4:D:25:ARG:HB3 | 2.01 | 0.60 |
| 7:G:12:LEU:N | 7:G:12:LEU:HD12 | 2.16 | 0.60 |
| 20:T:10:LEU:HD12 | 20:T:10:LEU:C | 2.22 | 0.60 |
| 1:A:109:A:H2' | 1:A:326:G:N2 | 2.15 | 0.60 |
| 1:A:281:G:O2' | 1:A:282:A:P | 2.59 | 0.60 |
| 1:A:983:A:H1' | 1:A:1049:U:O2 | 2.01 | 0.60 |
| 4:D:170:VAL:CG1 | 4:D:174:LEU:HB2 | 2.31 | 0.60 |
| 8:H:27:PRO:HA | 8:H:58:TYR:CD2 | 2.37 | 0.60 |
| 13:M:57:ARG:HG2 | 13:M:61:GLU:HG3 | 1.84 | 0.60 |
| 3:C:30:ARG:HB3 | 14:N:36:PHE:O | 2.01 | 0.60 |
| 1:A:1391:U:H2' | 1:A:1392:G:C8 | 2.36 | 0.60 |
| 1:A:579:G:H5' | 1:A:728:A:H1' | 1.84 | 0.60 |
| 2:B:130:ARG:HB3 | 2:B:131:PRO:CD | 2.28 | 0.60 |
| 2:B:158:LEU:H | 2:B:158:LEU:HD12 | 1.67 | 0.60 |
| 5:E:76:ILE:HG23 | 5:E:77:PRO:HD2 | 1.83 | 0.60 |
| 10:J:32:ALA:CB | 10:J:76:ASN:HB2 | 2.31 | 0.60 |
| 1:A:631:G:O3' | 1:A:632:A:H8 | 1.84 | 0.60 |
| 3:C:155:GLY:HA3 | 3:C:163:ALA:HB1 | 1.83 | 0.60 |
| 10:J:8:LEU:CD2 | 10:J:96:ILE:HG12 | 2.31 | 0.60 |
| 12:L:47:LYS:N | 12:L:48:PRO:HD2 | 2.15 | 0.60 |
| 1:A:1349:A:OP1 | 9:I:118:LYS:HD2 | 2.02 | 0.60 |
| 1:A:190(F):G:H4' | 1:A:190(G):G:OP2 | 2.00 | 0.60 |
| 1:A:328:C:O2 | 1:A:328:C:C2' | 2.44 | 0.60 |
| 1:A:524:G:H2' | 1:A:525:C:C6 | 2.36 | 0.60 |
| 1:A:1097:C:H2' | 1:A:1098:C:C6 | 2.37 | 0.60 |
| 1:A:1128:C:O2' | 1:A:1130:A:C8 | 2.51 | 0.60 |
| 4:D:28:SER:O | 4:D:30:LYS:N | 2.33 | 0.60 |
| 5:E:24:ARG:HH11 | 5:E:24:ARG:HB3 | 1.66 | 0.60 |
| 1:A:633:G:H2' | 1:A:634:C:C6 | 2.37 | 0.60 |
| 10:J:50:ILE:HA | 10:J:60:ARG:CA | 2.30 | 0.60 |
| 10:J:38:ILE:HB | 10:J:71:LEU:HB3 | 1.83 | 0.60 |
| 17:Q:3:LYS:HD3 | 17:Q:61:GLU:O | 2.02 | 0.60 |
| 1:A:337:C:H2' | 1:A:338:A:C8 | 2.37 | 0.60 |
| 1:A:371:G:C2' | 1:A:372:C:H5' | 2.31 | 0.60 |
| 7:G:5:ARG:NE | 7:G:7:ALA:HA | 2.17 | 0.60 |
| 9:I:39:GLY:O | 9:I:40:LEU:HD23 | 2.02 | 0.60 |
| 13:M:65:LYS:CG | 13:M:69:GLU:HB3 | 2.31 | 0.60 |
| 1:A:889:A:H4' | 1:A:890:G:OP1 | 2.00 | 0.59 |
| 16:P:34:GLU:OE2 | 16:P:55:ARG:HD2 | 2.02 | 0.59 |
| 20:T:39:LYS:HD3 | 20:T:55:ILE:HD13 | 1.83 | 0.59 |
| 1:A:1004:A:O2' | 1:A:1005:A:OP1 | 2.15 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:A:1052:U:H2' | 1:A:1055:A:OP1 | 2.02 | 0.59 |
| 1:A:1399:C:C2 | 1:A:1502:A:N6 | 2.71 | 0.59 |
| 5:E:12:LEU:HD13 | 5:E:31:LEU:HB2 | 1.85 | 0.59 |
| 6:F:33:TYR:CE2 | 6:F:74:ASP:HB3 | 2.36 | 0.59 |
| 1:A:1540:PSU:H2' | 1:A:1541:PSU:H5'' | 1.84 | 0.59 |
| 1:A:284:G:H2' | 1:A:285:G:H8 | 1.67 | 0.59 |
| 1:A:814:A:H2' | 1:A:816:A:H5' | 1.84 | 0.59 |
| 5:E:11:ILE:HG23 | 5:E:105:VAL:HG22 | 1.84 | 0.59 |
| 19:S:80:TYR:CE1 | 19:S:81:ARG:HD3 | 2.37 | 0.59 |
| 1:A:1498:UR3:C4' | 1:A:1519[A]:MA6:H2 | 2.33 | 0.59 |
| 4:D:148:VAL:HG12 | 4:D:149:ALA:N | 2.17 | 0.59 |
| 19:S:40:ILE:CG2 | 19:S:62:ILE:HD11 | 2.31 | 0.59 |
| 1:A:328:C:H1' | 1:A:329:A:OP2 | 2.03 | 0.59 |
| 1:A:664:G:OP1 | 18:R:64:ARG:HD2 | 2.02 | 0.59 |
| 10:J:48:THR:HA | 10:J:62:HIS:HB2 | 1.85 | 0.59 |
| 1:A:1381:U:C5 | 1:A:1382:C:C5 | 2.90 | 0.59 |
| 1:A:631:G:H2' | 27:A:2342:HOH:O | 2.02 | 0.59 |
| 1:A:1249:C:O2' | 9:I:73:GLN:NE2 | 2.35 | 0.59 |
| 1:A:110:C:H2' | 1:A:111:G:O4' | 2.03 | 0.59 |
| 1:A:1157:A:C2 | 1:A:1181:G:H1' | 2.37 | 0.59 |
| 1:A:959:A:C2 | 1:A:1222:G:O4' | 2.55 | 0.59 |
| 1:A:1356:G:H2' | 1:A:1357:A:C8 | 2.37 | 0.59 |
| 1:A:1425:U:H3 | 1:A:1475:G:H1 | 1.49 | 0.59 |
| 1:A:501:C:H2' | 1:A:502:G:C8 | 2.37 | 0.59 |
| 19:S:15:LEU:O | 19:S:19:VAL:HG12 | 2.03 | 0.59 |
| 20:T:74:LYS:HB3 | 20:T:74:LYS:HZ2 | 1.65 | 0.59 |
| 1:A:1499:A:H1' | 1:A:1520[A]:G:H5' | 1.84 | 0.59 |
| 2:B:78:GLN:O | 2:B:94:ASN:ND2 | 2.22 | 0.59 |
| 12:L:28:LYS:C | 12:L:30:ALA:N | 2.55 | 0.59 |
| 1:A:509:A:N3 | 1:A:543:C:O2' | 2.29 | 0.59 |
| 3:C:150:LYS:HD3 | 3:C:152:ILE:HD11 | 1.84 | 0.59 |
| 4:D:64:LEU:HD12 | 4:D:75:PHE:CZ | 2.38 | 0.59 |
| 1:A:1127:G:N2 | 1:A:1145:C:C2 | 2.71 | 0.58 |
| 1:A:976:G:OP2 | 1:A:1358:U:O2' | 2.20 | 0.58 |
| 1:A:914:A:OP1 | 25:A:1860:SRV:HI33 | 2.02 | 0.58 |
| 2:B:63:MET:HB3 | 2:B:225:ALA:HB1 | 1.84 | 0.58 |
| 4:D:25:ARG:HA | 4:D:28:SER:HB2 | 1.85 | 0.58 |
| 1:A:600:C:OP1 | 8:H:97:VAL:HG12 | 2.03 | 0.58 |
| 1:A:689:C:P | 11:K:46:GLY:HA3 | 2.43 | 0.58 |
| 17:Q:31:LEU:HG | 17:Q:32:TYR:CE2 | 2.37 | 0.58 |
| 1:A:1226:C:H4' | 1:A:1227:A:OP1 | 2.01 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|----------------------|--------------------------|-------------------|
| 1:A:1498:UR3:C2' | 1:A:1499:A:OP2 | 2.51 | 0.58 |
| 1:A:474:G:O2' | 1:A:475:G:H5' | 2.04 | 0.58 |
| 1:A:991:U:O2' | 1:A:992:U:O5' | 2.17 | 0.58 |
| 5:E:79:GLU:HA | 5:E:91:LEU:O | 2.03 | 0.58 |
| 8:H:64:LYS:HG2 | 8:H:79:VAL:HG21 | 1.85 | 0.58 |
| 3:C:23:TYR:OH | 10:J:9:ARG:HD3 | 2.03 | 0.58 |
| 1:A:1320:C:H2' | 1:A:1321:C:O4' | 2.04 | 0.58 |
| 1:A:179:A:H2' | 1:A:180:U:C6 | 2.38 | 0.58 |
| 7:G:20:ASP:OD2 | 7:G:63:LYS:HE2 | 2.04 | 0.58 |
| 1:A:1022:G:H2' | 1:A:1023:G:C8 | 2.38 | 0.58 |
| 1:A:1305:G:N2 | 1:A:1331:G:O2' | 2.36 | 0.58 |
| 1:A:35:G:H2' | 1:A:36:C:C6 | 2.39 | 0.58 |
| 4:D:63:LYS:HD2 | 4:D:198:VAL:HG22 | 1.85 | 0.58 |
| 7:G:5:ARG:HG3 | 7:G:7:ALA:H | 1.67 | 0.58 |
| 1:A:1157:A:H4' | 1:A:1158:C:O5' | 2.03 | 0.58 |
| 2:B:27:LYS:HD2 | 2:B:193:ASP:OD1 | 2.04 | 0.58 |
| 2:B:22:LYS:HG3 | 2:B:23:ARG:N | 2.19 | 0.58 |
| 4:D:24:GLU:HG2 | 4:D:25:ARG:N | 2.17 | 0.58 |
| 6:F:91:VAL:HG12 | 6:F:92:LYS:O | 2.04 | 0.58 |
| 7:G:69:VAL:HG12 | 7:G:100:ALA:HA | 1.86 | 0.58 |
| 8:H:20:TYR:CE1 | 8:H:76:PRO:HG2 | 2.39 | 0.58 |
| 1:A:1057:G:H5'' | 3:C:154:SER:CB | 2.25 | 0.58 |
| 4:D:150:GLU:N | 4:D:150:GLU:OE2 | 2.28 | 0.58 |
| 8:H:102:ARG:H | 8:H:102:ARG:CD | 2.15 | 0.58 |
| 19:S:15:LEU:HA | 19:S:18:LYS:HB2 | 1.85 | 0.58 |
| 1:A:117:G:OP2 | 27:A:1918:HOH:O | 2.17 | 0.58 |
| 1:A:1405:G:HO2' | 1:A:1518[B]:MA6:HO2' | 1.50 | 0.58 |
| 2:B:161:ALA:HB1 | 2:B:185:ILE:HD11 | 1.85 | 0.58 |
| 3:C:126:ARG:O | 3:C:127:ARG:HB2 | 2.03 | 0.58 |
| 5:E:144:THR:HG22 | 5:E:146:ALA:N | 2.19 | 0.58 |
| 12:L:69:TYR:CD1 | 12:L:90:VAL:HG21 | 2.39 | 0.58 |
| 15:O:3:ILE:HD13 | 15:O:34:LEU:HD13 | 1.85 | 0.58 |
| 19:S:27:GLU:HG2 | 19:S:28:LYS:H | 1.69 | 0.58 |
| 10:J:62:HIS:O | 10:J:62:HIS:ND1 | 2.32 | 0.58 |
| 19:S:41:VAL:HG23 | 19:S:43:GLU:HG2 | 1.85 | 0.58 |
| 20:T:10:LEU:CD1 | 20:T:12:ALA:H | 2.17 | 0.58 |
| 1:A:1054:C:N4 | 23:W:34:G:C1' | 2.59 | 0.58 |
| 1:A:975:A:H4' | 1:A:976:G:C5' | 2.30 | 0.58 |
| 2:B:17:PHE:O | 2:B:204:ASN:HB2 | 2.04 | 0.58 |
| 9:I:79:LEU:HD22 | 9:I:83:ARG:HG3 | 1.86 | 0.58 |
| 13:M:16:ASP:OD2 | 13:M:16:ASP:N | 2.37 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 13:M:88:ARG:HG2 | 13:M:98:VAL:HG12 | 1.86 | 0.57 |
| 17:Q:22:LEU:HD12 | 17:Q:23:VAL:N | 2.18 | 0.57 |
| 1:A:1189:C:OP1 | 10:J:51:ARG:NH2 | 2.30 | 0.57 |
| 1:A:1513:A:H2' | 1:A:1514:C:C6 | 2.39 | 0.57 |
| 1:A:945:G:C2 | 1:A:946:A:C8 | 2.92 | 0.57 |
| 1:A:116:A:H2' | 1:A:117:G:C8 | 2.39 | 0.57 |
| 2:B:130:ARG:HH21 | 3:C:207:VAL:HG21 | 1.69 | 0.57 |
| 1:A:954:G:H21 | 1:A:1227:A:H62 | 1.52 | 0.57 |
| 1:A:200:G:H2' | 1:A:201:C:O4' | 2.04 | 0.57 |
| 1:A:337:C:H2' | 1:A:338:A:H8 | 1.68 | 0.57 |
| 5:E:24:ARG:HB3 | 5:E:24:ARG:NH1 | 2.19 | 0.57 |
| 5:E:95:ALA:O | 5:E:98:THR:OG1 | 2.16 | 0.57 |
| 12:L:28:LYS:HB3 | 12:L:30:ALA:HB2 | 1.86 | 0.57 |
| 1:A:1208:C:H2' | 1:A:1209:C:H6 | 1.69 | 0.57 |
| 1:A:372:C:H1' | 1:A:373:A:OP2 | 2.04 | 0.57 |
| 13:M:23:TYR:HB3 | 13:M:67:GLU:H | 1.69 | 0.57 |
| 17:Q:48:GLU:HB2 | 17:Q:50:LYS:HG3 | 1.85 | 0.57 |
| 1:A:1069:C:O2' | 1:A:1192:C:H1' | 2.05 | 0.57 |
| 1:A:1208:C:H2' | 1:A:1209:C:C6 | 2.39 | 0.57 |
| 1:A:77:G:O2' | 1:A:78:G:H5' | 2.04 | 0.57 |
| 1:A:833:U:H2' | 1:A:834:C:H6 | 1.68 | 0.57 |
| 2:B:167:PRO:HG2 | 2:B:192:SER:CB | 2.34 | 0.57 |
| 7:G:15:ASP:HB3 | 7:G:20:ASP:H | 1.69 | 0.57 |
| 8:H:84:ARG:O | 8:H:135:CYS:HB2 | 2.04 | 0.57 |
| 1:A:739:C:O2' | 15:O:42:HIS:ND1 | 2.33 | 0.57 |
| 17:Q:18:THR:HG23 | 17:Q:69:LYS:HE3 | 1.86 | 0.57 |
| 1:A:1026:G:O6 | 1:A:1027:C:N4 | 2.37 | 0.57 |
| 1:A:1091:U:O2 | 1:A:1093:A:C8 | 2.58 | 0.57 |
| 1:A:1197:G:OP1 | 27:A:2127:HOH:O | 2.18 | 0.57 |
| 1:A:393:A:C2' | 1:A:394:G:H5' | 2.35 | 0.57 |
| 1:A:811:C:H4' | 1:A:900:A:N6 | 2.19 | 0.57 |
| 5:E:36:ASP:OD2 | 5:E:38:GLN:HB2 | 2.04 | 0.57 |
| 15:O:70:LEU:HD13 | 15:O:78:TYR:CA | 2.35 | 0.57 |
| 1:A:376:G:H5'' | 16:P:5:ARG:HD2 | 1.86 | 0.57 |
| 1:A:1053:G:C4 | 1:A:1199:U:C5 | 2.93 | 0.57 |
| 2:B:126:GLU:O | 2:B:129:GLU:HG2 | 2.05 | 0.57 |
| 3:C:11:ARG:O | 3:C:14:ILE:O | 2.22 | 0.57 |
| 1:A:1003(A):G:H2' | 1:A:1004:A:H4' | 1.85 | 0.57 |
| 1:A:1035:A:H2' | 1:A:1036:G:C8 | 2.35 | 0.57 |
| 1:A:982:U:H4' | 1:A:983:A:O5' | 2.05 | 0.57 |
| 8:H:102:ARG:N | 8:H:102:ARG:CD | 2.67 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 13:M:96:LEU:O | 13:M:110:ARG:NH1 | 2.38 | 0.57 |
| 17:Q:31:LEU:HG | 17:Q:32:TYR:CD2 | 2.40 | 0.57 |
| 17:Q:83:ASP:N | 17:Q:83:ASP:OD1 | 2.37 | 0.57 |
| 1:A:1114:C:H2' | 1:A:1115:C:H6 | 1.70 | 0.56 |
| 2:B:170:GLU:HA | 2:B:170:GLU:OE2 | 2.05 | 0.56 |
| 12:L:111:LYS:HA | 12:L:111:LYS:HZ2 | 1.69 | 0.56 |
| 1:A:310:G:OP2 | 16:P:27:LYS:HE2 | 2.05 | 0.56 |
| 1:A:509:A:HO2' | 1:A:510:A:P | 2.25 | 0.56 |
| 2:B:25:ASN:ND2 | 2:B:193:ASP:HB2 | 2.20 | 0.56 |
| 6:F:42:GLU:HG3 | 6:F:61:LEU:CD2 | 2.35 | 0.56 |
| 11:K:91:ARG:HG2 | 11:K:92:GLU:N | 2.18 | 0.56 |
| 17:Q:27:PHE:CD1 | 17:Q:36:ILE:HD11 | 2.40 | 0.56 |
| 1:A:1054:C:O2' | 1:A:1055:A:O5' | 2.22 | 0.56 |
| 1:A:386:C:H1' | 27:A:1902:HOH:O | 2.06 | 0.56 |
| 15:O:50:HIS:O | 15:O:53:HIS:HB3 | 2.05 | 0.56 |
| 1:A:559:A:H4' | 1:A:560:U:O5' | 2.04 | 0.56 |
| 13:M:65:LYS:C | 13:M:66:LEU:HD23 | 2.25 | 0.56 |
| 1:A:1338:G:H2' | 1:A:1339:A:C8 | 2.41 | 0.56 |
| 1:A:1392:G:O2' | 1:A:1393:U:H5' | 2.06 | 0.56 |
| 1:A:289:G:OP2 | 27:A:1917:HOH:O | 2.17 | 0.56 |
| 20:T:8:ARG:HD2 | 20:T:8:ARG:N | 2.21 | 0.56 |
| 1:A:1238:A:OP1 | 1:A:1336:C:H5 | 1.89 | 0.56 |
| 1:A:559:A:OP1 | 5:E:126:ARG:NH2 | 2.29 | 0.56 |
| 1:A:794:A:OP1 | 27:A:2172:HOH:O | 2.17 | 0.56 |
| 1:A:946:A:H2' | 1:A:947:G:H8 | 1.70 | 0.56 |
| 8:H:113:SER:HB2 | 8:H:134:ILE:HD11 | 1.88 | 0.56 |
| 1:A:1505:G:H4' | 1:A:1506:U:O5' | 2.06 | 0.56 |
| 1:A:216:G:O2' | 1:A:217:C:O4' | 2.13 | 0.56 |
| 1:A:539:A:H2' | 1:A:540:G:C8 | 2.40 | 0.56 |
| 1:A:807:A:H2' | 1:A:808:C:C6 | 2.41 | 0.56 |
| 1:A:827:U:H5'' | 1:A:828:A:OP2 | 2.04 | 0.56 |
| 12:L:35:GLY:HA3 | 12:L:60:LEU:HD13 | 1.87 | 0.56 |
| 12:L:58:VAL:O | 12:L:65:GLU:HA | 2.05 | 0.56 |
| 17:Q:24:GLU:OE1 | 17:Q:37:LYS:HD3 | 2.05 | 0.56 |
| 1:A:714:G:H2' | 1:A:715:A:C8 | 2.40 | 0.56 |
| 12:L:126:LYS:O | 12:L:127:GLU:HG3 | 2.06 | 0.56 |
| 1:A:1211:U:H2' | 1:A:1212:U:OP2 | 2.06 | 0.56 |
| 1:A:1427:U:H2' | 1:A:1428:A:C8 | 2.41 | 0.56 |
| 1:A:1402:4OC:O2 | 1:A:1500:A:N1 | 2.39 | 0.56 |
| 1:A:872:A:H4' | 1:A:873:A:OP1 | 2.04 | 0.56 |
| 1:A:384:G:H2' | 1:A:385:C:C6 | 2.41 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:134:GLU:O | 2:B:138:LEU:HG | 2.06 | 0.56 |
| 4:D:146:ILE:HD12 | 4:D:146:ILE:N | 2.21 | 0.56 |
| 4:D:175:SER:HB3 | 4:D:186:LEU:HD21 | 1.88 | 0.56 |
| 4:D:20:TYR:CD2 | 4:D:26:CYS:HB3 | 2.39 | 0.56 |
| 1:A:1086:U:H3 | 1:A:1099:G:N2 | 1.98 | 0.56 |
| 3:C:73:PRO:O | 3:C:77:ILE:HG12 | 2.06 | 0.56 |
| 2:B:178:ARG:O | 8:H:71:GLY:HA2 | 2.05 | 0.56 |
| 1:A:1006:C:H42 | 1:A:1024:G:N2 | 2.04 | 0.55 |
| 1:A:1157:A:H2 | 1:A:1181:G:H1' | 1.72 | 0.55 |
| 1:A:327:A:H4' | 1:A:328:C:OP2 | 2.06 | 0.55 |
| 1:A:721:G:H4' | 1:A:722:A:O4' | 2.05 | 0.55 |
| 13:M:22:ILE:HB | 13:M:25:ILE:HD12 | 1.88 | 0.55 |
| 20:T:92:LEU:O | 20:T:96:GLY:N | 2.39 | 0.55 |
| 1:A:267:C:H2' | 1:A:268:C:C6 | 2.41 | 0.55 |
| 1:A:838:G:H2' | 1:A:839:U:H5'' | 1.87 | 0.55 |
| 4:D:18:LYS:HD3 | 4:D:20:TYR:CE2 | 2.41 | 0.55 |
| 15:O:55:GLY:HA2 | 15:O:58:MET:HE2 | 1.88 | 0.55 |
| 16:P:45:THR:HB | 16:P:46:PRO:HD2 | 1.88 | 0.55 |
| 1:A:1118:C:H1' | 1:A:1179:A:C5 | 2.41 | 0.55 |
| 1:A:426:G:OP1 | 4:D:36:ARG:NH2 | 2.38 | 0.55 |
| 3:C:72:LYS:HD3 | 3:C:75:VAL:CG2 | 2.37 | 0.55 |
| 4:D:25:ARG:O | 4:D:25:ARG:HG2 | 2.06 | 0.55 |
| 5:E:143:ARG:NH1 | 8:H:77:GLU:OE2 | 2.39 | 0.55 |
| 13:M:79:LYS:HE2 | 13:M:83:ASP:OD1 | 2.06 | 0.55 |
| 19:S:31:ILE:HG22 | 19:S:49:ILE:HA | 1.89 | 0.55 |
| 1:A:267:C:H2' | 1:A:268:C:H6 | 1.71 | 0.55 |
| 5:E:98:THR:HB | 5:E:117:ASP:HB3 | 1.89 | 0.55 |
| 11:K:126:ARG:O | 11:K:127:LYS:HB2 | 2.06 | 0.55 |
| 25:A:1860:SRY:O51 | 12:L:46:LYS:HE3 | 2.05 | 0.55 |
| 19:S:58:VAL:HG23 | 19:S:60:VAL:HG23 | 1.89 | 0.55 |
| 1:A:1499:A:C1' | 1:A:1520[A]:G:H5' | 2.37 | 0.55 |
| 1:A:35:G:H2' | 1:A:36:C:H6 | 1.72 | 0.55 |
| 2:B:130:ARG:HH21 | 3:C:207:VAL:CG2 | 2.20 | 0.55 |
| 3:C:86:VAL:O | 3:C:90:GLU:HG3 | 2.06 | 0.55 |
| 9:I:53:VAL:HG21 | 9:I:85:LEU:HD21 | 1.89 | 0.55 |
| 10:J:8:LEU:HD23 | 10:J:96:ILE:HG12 | 1.88 | 0.55 |
| 13:M:11:ARG:HG2 | 13:M:12:ASN:HB2 | 1.89 | 0.55 |
| 1:A:1330:U:OP1 | 13:M:23:TYR:O | 2.24 | 0.55 |
| 1:A:109:A:C6 | 1:A:326:G:C6 | 2.94 | 0.55 |
| 1:A:1065:U:H1' | 1:A:1066:C:OP2 | 2.06 | 0.55 |
| 1:A:1131:G:H2' | 1:A:1132:C:C6 | 2.41 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1319:A:H5' | 19:S:5:LEU:CD2 | 2.37 | 0.55 |
| 2:B:187:LEU:HD23 | 2:B:205:ASP:HB3 | 1.89 | 0.55 |
| 4:D:19:LEU:H | 4:D:19:LEU:HD23 | 1.72 | 0.55 |
| 20:T:10:LEU:HD12 | 20:T:10:LEU:O | 2.07 | 0.55 |
| 1:A:1178:G:N2 | 1:A:1180:A:H3' | 2.21 | 0.55 |
| 1:A:1329:A:C2' | 1:A:1330:U:H5' | 2.36 | 0.55 |
| 2:B:51:LEU:O | 2:B:55:PHE:HB2 | 2.07 | 0.55 |
| 8:H:104:ARG:O | 8:H:105:ARG:C | 2.45 | 0.55 |
| 1:A:1131:G:H3' | 1:A:1131:G:OP2 | 2.06 | 0.55 |
| 1:A:1236:A:H4' | 1:A:1304:G:H4' | 1.88 | 0.55 |
| 1:A:197:A:C6 | 1:A:221:C:H5' | 2.42 | 0.55 |
| 1:A:247:G:OP2 | 17:Q:100:LYS:HB2 | 2.07 | 0.55 |
| 1:A:424:G:H2' | 1:A:425:G:H8 | 1.71 | 0.55 |
| 2:B:167:PRO:HG2 | 2:B:192:SER:HB2 | 1.88 | 0.55 |
| 2:B:53:ARG:HA | 2:B:56:ARG:HH12 | 1.70 | 0.55 |
| 4:D:24:GLU:HG2 | 4:D:25:ARG:H | 1.72 | 0.55 |
| 1:A:1319:A:H5' | 19:S:5:LEU:HD22 | 1.88 | 0.55 |
| 1:A:1145:C:H4' | 1:A:1146:A:OP1 | 2.06 | 0.54 |
| 1:A:115:G:H4' | 1:A:116:A:O5' | 2.06 | 0.54 |
| 1:A:1180:A:OP1 | 9:I:103:THR:HG23 | 2.08 | 0.54 |
| 1:A:393:A:O2' | 1:A:394:G:H5' | 2.07 | 0.54 |
| 1:A:448:A:C4 | 1:A:487:A:C2 | 2.95 | 0.54 |
| 7:G:75:VAL:O | 7:G:75:VAL:HG13 | 2.06 | 0.54 |
| 17:Q:53:LEU:HD21 | 17:Q:85:VAL:HG11 | 1.89 | 0.54 |
| 20:T:56:MET:HE3 | 20:T:88:VAL:HG11 | 1.88 | 0.54 |
| 1:A:17:U:H2' | 1:A:18:C:C6 | 2.42 | 0.54 |
| 1:A:243:A:C2 | 1:A:246:A:C8 | 2.94 | 0.54 |
| 1:A:328:C:C2' | 1:A:329:A:OP2 | 2.55 | 0.54 |
| 1:A:972:C:O5' | 10:J:57:LYS:HD3 | 2.07 | 0.54 |
| 3:C:41:GLY:O | 3:C:45:LYS:HG3 | 2.08 | 0.54 |
| 2:B:181:PHE:CD2 | 8:H:70:GLN:HB3 | 2.42 | 0.54 |
| 13:M:3:ARG:HA | 13:M:9:ILE:HG12 | 1.88 | 0.54 |
| 13:M:65:LYS:HG3 | 13:M:69:GLU:HB3 | 1.88 | 0.54 |
| 19:S:62:ILE:HG13 | 19:S:66:MET:HE2 | 1.89 | 0.54 |
| 20:T:74:LYS:CB | 20:T:74:LYS:NZ | 2.70 | 0.54 |
| 1:A:1236:A:H2' | 1:A:1237:C:C6 | 2.43 | 0.54 |
| 1:A:239:U:O4 | 27:A:2450:HOH:O | 2.17 | 0.54 |
| 1:A:37:U:O2' | 1:A:500:G:H4' | 2.07 | 0.54 |
| 9:I:65:VAL:HG11 | 9:I:73:GLN:HB3 | 1.90 | 0.54 |
| 11:K:59:TYR:CE2 | 11:K:63:LEU:HD11 | 2.42 | 0.54 |
| 13:M:59:TYR:O | 13:M:63:THR:HG22 | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:728:A:C8 | 15:O:54:ARG:NH1 | 2.76 | 0.54 |
| 20:T:16:HIS:CE1 | 20:T:20:LEU:HD11 | 2.42 | 0.54 |
| 1:A:1004:A:O2' | 1:A:1038:C:O2 | 2.26 | 0.54 |
| 1:A:1260:C:O5' | 1:A:1284:C:H4' | 2.07 | 0.54 |
| 1:A:1465:C:H2' | 1:A:1466:C:O4' | 2.07 | 0.54 |
| 2:B:84:GLU:OE1 | 2:B:216:SER:HA | 2.07 | 0.54 |
| 3:C:134:ILE:HG22 | 3:C:151:VAL:HB | 1.88 | 0.54 |
| 8:H:53:VAL:HB | 8:H:58:TYR:CD1 | 2.41 | 0.54 |
| 18:R:53:ARG:HD3 | 18:R:63:GLN:HB2 | 1.88 | 0.54 |
| 1:A:1239:A:C4 | 1:A:1298:C:N4 | 2.76 | 0.54 |
| 1:A:390:C:H2' | 1:A:391:G:C8 | 2.42 | 0.54 |
| 13:M:88:ARG:HG3 | 19:S:3:ARG:NH2 | 2.22 | 0.54 |
| 15:O:4:THR:OG1 | 15:O:7:GLU:OE2 | 2.19 | 0.54 |
| 1:A:235:C:C5' | 17:Q:70:ARG:HG2 | 2.30 | 0.54 |
| 18:R:36:ASN:CG | 18:R:39:VAL:HG12 | 2.28 | 0.54 |
| 1:A:1005:A:C4 | 1:A:1026:G:N2 | 2.75 | 0.54 |
| 1:A:1220:G:H2' | 1:A:1221:G:C8 | 2.43 | 0.54 |
| 1:A:1486:G:H2' | 1:A:1487:G:O4' | 2.07 | 0.54 |
| 1:A:355:C:H5' | 1:A:389:A:OP2 | 2.07 | 0.54 |
| 1:A:46:G:H2' | 1:A:366:C:C5 | 2.42 | 0.54 |
| 1:A:628:G:O2' | 1:A:629:G:H5' | 2.07 | 0.54 |
| 7:G:75:VAL:CG2 | 7:G:86:GLN:HB3 | 2.36 | 0.54 |
| 1:A:1300:G:C2' | 1:A:1301:U:OP2 | 2.55 | 0.54 |
| 1:A:173:U:H6 | 1:A:198:G:HO2' | 1.56 | 0.54 |
| 1:A:563:A:H2' | 1:A:567:G:C8 | 2.43 | 0.54 |
| 2:B:165:VAL:O | 2:B:187:LEU:O | 2.26 | 0.54 |
| 8:H:102:ARG:H | 8:H:102:ARG:HD2 | 1.71 | 0.54 |
| 8:H:53:VAL:HB | 8:H:58:TYR:CE1 | 2.43 | 0.54 |
| 9:I:69:GLY:O | 9:I:73:GLN:HG3 | 2.08 | 0.54 |
| 11:K:14:VAL:O | 11:K:15:ALA:HB3 | 2.07 | 0.54 |
| 11:K:13:GLN:HA | 11:K:75:TYR:O | 2.07 | 0.54 |
| 1:A:275:G:H5' | 17:Q:14:LYS:HB3 | 1.89 | 0.54 |
| 1:A:1023:G:O6 | 1:A:1024:G:C2 | 2.61 | 0.54 |
| 1:A:1049:U:H4' | 1:A:1050:G:O5' | 2.08 | 0.54 |
| 1:A:501:C:H2' | 1:A:502:G:H8 | 1.72 | 0.54 |
| 1:A:685:G:O2' | 1:A:686:U:H5' | 2.08 | 0.54 |
| 2:B:74:LYS:O | 2:B:75:LYS:HB2 | 2.06 | 0.54 |
| 4:D:201:GLN:NE2 | 5:E:116:THR:HG23 | 2.22 | 0.54 |
| 8:H:26:VAL:HG23 | 8:H:27:PRO:HD2 | 1.90 | 0.54 |
| 12:L:53:ARG:HG3 | 12:L:93:LEU:HD21 | 1.90 | 0.54 |
| 17:Q:34:LYS:HG3 | 17:Q:35:VAL:N | 2.23 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 18:R:47:THR:HG22 | 18:R:48:GLY:N | 2.21 | 0.54 |
| 1:A:190(L):U:O2 | 20:T:105:SER:HB2 | 2.07 | 0.54 |
| 20:T:45:GLN:HB2 | 20:T:91:LEU:HD13 | 1.90 | 0.54 |
| 1:A:229:U:H5' | 16:P:33:ILE:HD13 | 1.89 | 0.54 |
| 3:C:130:VAL:HG12 | 3:C:134:ILE:HD11 | 1.89 | 0.54 |
| 10:J:90:LEU:N | 10:J:91:PRO:HD2 | 2.22 | 0.54 |
| 11:K:14:VAL:HG21 | 11:K:40:ILE:HD11 | 1.89 | 0.54 |
| 1:A:1124:G:N7 | 1:A:1145:C:O2' | 2.34 | 0.54 |
| 1:A:1277:C:O2' | 1:A:1279:A:H1' | 2.08 | 0.54 |
| 1:A:322:C:H4' | 20:T:23:ARG:HD2 | 1.89 | 0.54 |
| 7:G:78:ARG:HD2 | 7:G:156:TRP:CE3 | 2.43 | 0.54 |
| 1:A:262:A:N6 | 1:A:263:A:N6 | 2.56 | 0.53 |
| 1:A:737:A:H2' | 1:A:738:C:C6 | 2.42 | 0.53 |
| 17:Q:84:LEU:HD23 | 17:Q:84:LEU:N | 2.23 | 0.53 |
| 1:A:1515[B]:C:H2' | 1:A:1516[B]:G:H5' | 1.91 | 0.53 |
| 1:A:755:G:OP2 | 15:O:65:ARG:HD2 | 2.09 | 0.53 |
| 1:A:951:G:OP2 | 13:M:102:ARG:NH2 | 2.41 | 0.53 |
| 2:B:75:LYS:HA | 2:B:78:GLN:HB2 | 1.91 | 0.53 |
| 8:H:25:ASP:OD1 | 8:H:60:ARG:HD3 | 2.08 | 0.53 |
| 19:S:50:ALA:HA | 19:S:58:VAL:O | 2.09 | 0.53 |
| 1:A:532:A:H61 | 3:C:193:TYR:HA | 1.74 | 0.53 |
| 1:A:958:A:N3 | 1:A:985:C:O2' | 2.33 | 0.53 |
| 1:A:1349:A:OP1 | 9:I:120:ARG:HB2 | 2.08 | 0.53 |
| 1:A:1064:G:H22 | 1:A:1190:G:C2' | 2.21 | 0.53 |
| 1:A:428:G:H4' | 1:A:429:U:O5' | 2.08 | 0.53 |
| 1:A:688:G:H2' | 1:A:689:C:H6 | 1.72 | 0.53 |
| 1:A:984:C:H42 | 1:A:1221:G:H1 | 1.56 | 0.53 |
| 15:O:17:ARG:HG3 | 15:O:17:ARG:NH1 | 2.10 | 0.53 |
| 16:P:74:LEU:HB3 | 16:P:79:VAL:HG21 | 1.90 | 0.53 |
| 1:A:1124:G:H4' | 10:J:38:ILE:HD11 | 1.90 | 0.53 |
| 1:A:1399:C:C2 | 1:A:1401:G:C5 | 2.96 | 0.53 |
| 1:A:1516[A]:G:H2' | 1:A:1518[A]:MA6:OP2 | 2.09 | 0.53 |
| 1:A:537:G:H2' | 1:A:538:G:C8 | 2.43 | 0.53 |
| 1:A:556:C:C2' | 1:A:557:G:H5' | 2.38 | 0.53 |
| 8:H:103:VAL:HG21 | 8:H:109:ILE:O | 2.07 | 0.53 |
| 10:J:35:SER:HB3 | 10:J:73:ASP:O | 2.09 | 0.53 |
| 17:Q:100:LYS:HB3 | 17:Q:101:ARG:CZ | 2.38 | 0.53 |
| 1:A:1372:U:H2' | 1:A:1373:G:O4' | 2.08 | 0.53 |
| 1:A:701:C:H4' | 1:A:702:A:O5' | 2.08 | 0.53 |
| 2:B:97:TRP:CH2 | 2:B:176:GLU:CD | 2.77 | 0.53 |
| 3:C:113:ALA:N | 3:C:114:PRO:HD2 | 2.23 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:115:LEU:HD23 | 3:C:118:GLN:OE1 | 2.09 | 0.53 |
| 5:E:76:ILE:HG22 | 5:E:78:HIS:H | 1.74 | 0.53 |
| 7:G:38:LEU:HD11 | 7:G:42:ILE:HD11 | 1.90 | 0.53 |
| 8:H:111:ILE:O | 8:H:134:ILE:HB | 2.09 | 0.53 |
| 10:J:63:PHE:CZ | 14:N:45:ARG:HA | 2.43 | 0.53 |
| 1:A:1211:U:C2' | 1:A:1212:U:OP2 | 2.56 | 0.53 |
| 1:A:836:G:C6 | 1:A:851:G:C6 | 2.96 | 0.53 |
| 3:C:148:GLY:HA3 | 3:C:172:ARG:O | 2.09 | 0.53 |
| 1:A:302:G:H5'' | 12:L:17:LYS:HE2 | 1.91 | 0.53 |
| 12:L:56:ALA:HB2 | 12:L:70:ILE:HD11 | 1.91 | 0.53 |
| 1:A:432:A:O2' | 1:A:433:C:P | 2.66 | 0.53 |
| 1:A:853:G:C2' | 1:A:854:G:H5' | 2.39 | 0.53 |
| 1:A:620:C:N1 | 4:D:135:LEU:HD13 | 2.23 | 0.53 |
| 15:O:4:THR:HB | 15:O:6:GLU:HG2 | 1.90 | 0.53 |
| 1:A:1034:G:N2 | 1:A:1035:A:N6 | 2.57 | 0.53 |
| 1:A:1049:U:H4' | 1:A:1050:G:C5' | 2.39 | 0.53 |
| 1:A:797:C:OP1 | 11:K:124:LYS:HE2 | 2.09 | 0.53 |
| 4:D:201:GLN:O | 4:D:205:GLU:HG3 | 2.09 | 0.53 |
| 6:F:101:ALA:HB2 | 18:R:28:GLU:HB2 | 1.91 | 0.53 |
| 1:A:1054:C:OP1 | 1:A:1197:G:OP2 | 2.26 | 0.53 |
| 1:A:1502:A:N1 | 1:A:1504:G:C2 | 2.76 | 0.53 |
| 1:A:176:C:H2' | 1:A:177:C:H6 | 1.73 | 0.53 |
| 3:C:50:ALA:HB1 | 3:C:70:VAL:HG11 | 1.89 | 0.53 |
| 5:E:39:GLY:O | 5:E:69:VAL:N | 2.33 | 0.53 |
| 6:F:69:GLU:CD | 6:F:69:GLU:H | 2.11 | 0.53 |
| 8:H:4:ASP:OD2 | 8:H:89:PRO:HD3 | 2.08 | 0.53 |
| 9:I:111:ARG:O | 9:I:113:LYS:HD2 | 2.08 | 0.53 |
| 9:I:24:GLY:CA | 9:I:57:GLY:HA2 | 2.35 | 0.53 |
| 1:A:1003:G:C6 | 1:A:1003(A):G:C6 | 2.97 | 0.52 |
| 1:A:1253:G:H1' | 1:A:1355:G:O2' | 2.10 | 0.52 |
| 1:A:1357:A:H5'' | 1:A:1358:U:OP2 | 2.10 | 0.52 |
| 1:A:627:G:O2' | 1:A:628:G:H5' | 2.09 | 0.52 |
| 1:A:938:A:C6 | 1:A:939:G:C5 | 2.97 | 0.52 |
| 1:A:939:G:H2' | 1:A:940:C:H6 | 1.68 | 0.52 |
| 1:A:993:G:H4' | 1:A:994:A:OP2 | 2.10 | 0.52 |
| 3:C:128:PHE:CD2 | 3:C:129:ALA:N | 2.75 | 0.52 |
| 3:C:6:HIS:HD2 | 3:C:7:PRO:CD | 2.21 | 0.52 |
| 5:E:11:ILE:HB | 5:E:31:LEU:HB3 | 1.90 | 0.52 |
| 10:J:71:LEU:HD13 | 10:J:72:VAL:N | 2.25 | 0.52 |
| 13:M:102:ARG:HG3 | 13:M:102:ARG:O | 2.09 | 0.52 |
| 18:R:53:ARG:NE | 18:R:58:LEU:O | 2.41 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:117:G:P | 27:A:1918:HOH:O | 2.67 | 0.52 |
| 5:E:90:VAL:O | 5:E:91:LEU:HD23 | 2.08 | 0.52 |
| 1:A:1379:G:OP1 | 7:G:6:ARG:NH2 | 2.42 | 0.52 |
| 17:Q:20:THR:HG21 | 17:Q:41:LYS:HD2 | 1.91 | 0.52 |
| 1:A:1028:C:N3 | 1:A:1034:G:C2 | 2.76 | 0.52 |
| 1:A:1049:U:H1' | 1:A:1050:G:OP2 | 2.09 | 0.52 |
| 1:A:1120:G:N2 | 1:A:1154:G:H1' | 2.24 | 0.52 |
| 1:A:1269:A:N1 | 1:A:1312:G:O2' | 2.38 | 0.52 |
| 1:A:961:U:H2' | 1:A:962:C:H5' | 1.90 | 0.52 |
| 4:D:15:GLU:OE2 | 4:D:59:ARG:NE | 2.40 | 0.52 |
| 5:E:90:VAL:O | 5:E:120:THR:HA | 2.09 | 0.52 |
| 12:L:76:ASN:O | 12:L:77:LEU:HD23 | 2.09 | 0.52 |
| 13:M:79:LYS:HA | 13:M:82:MET:HE2 | 1.91 | 0.52 |
| 18:R:52:PRO:O | 18:R:56:THR:HG23 | 2.09 | 0.52 |
| 1:A:1104:G:O5' | 2:B:111:ARG:HD2 | 2.08 | 0.52 |
| 19:S:14:HIS:O | 19:S:18:LYS:HE3 | 2.09 | 0.52 |
| 19:S:44:MET:O | 19:S:62:ILE:HG21 | 2.09 | 0.52 |
| 1:A:1525:G:P | 11:K:120:ARG:HH22 | 2.33 | 0.52 |
| 1:A:266:G:C5' | 1:A:268:C:H41 | 2.19 | 0.52 |
| 1:A:478:A:O2' | 1:A:479:C:H5' | 2.10 | 0.52 |
| 2:B:187:LEU:CD1 | 2:B:214:ILE:HG13 | 2.40 | 0.52 |
| 2:B:68:ILE:O | 2:B:90:MET:HB3 | 2.09 | 0.52 |
| 8:H:54:ASP:CG | 8:H:55:GLY:N | 2.63 | 0.52 |
| 19:S:53:ASN:OD1 | 19:S:56:GLN:N | 2.39 | 0.52 |
| 1:A:192:U:H2' | 1:A:193:C:H6 | 1.74 | 0.52 |
| 1:A:409:G:OP1 | 4:D:24:GLU:O | 2.27 | 0.52 |
| 5:E:71:LEU:HD11 | 5:E:113:ALA:O | 2.09 | 0.52 |
| 12:L:27:LEU:C | 12:L:29:GLY:N | 2.63 | 0.52 |
| 12:L:55:VAL:HG12 | 12:L:56:ALA:N | 2.24 | 0.52 |
| 12:L:6:THR:O | 12:L:9:GLN:HB2 | 2.10 | 0.52 |
| 1:A:1241:G:H2' | 1:A:1242:C:C6 | 2.44 | 0.52 |
| 1:A:204:U:O2 | 1:A:204:U:C2' | 2.57 | 0.52 |
| 1:A:476:G:O2' | 1:A:477:G:H5' | 2.10 | 0.52 |
| 1:A:537:G:H2' | 1:A:538:G:H8 | 1.74 | 0.52 |
| 5:E:11:ILE:HG12 | 5:E:33:VAL:HG23 | 1.91 | 0.52 |
| 1:A:1300:G:O2' | 1:A:1301:U:OP2 | 2.28 | 0.52 |
| 8:H:103:VAL:HG21 | 8:H:109:ILE:C | 2.30 | 0.52 |
| 10:J:24:VAL:O | 10:J:28:ARG:HG3 | 2.10 | 0.52 |
| 17:Q:100:LYS:HD2 | 17:Q:101:ARG:NH2 | 2.25 | 0.52 |
| 1:A:109:A:H4' | 1:A:110:C:OP2 | 2.09 | 0.52 |
| 1:A:129:U:O3' | 1:A:129(A):G:H3' | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:A:1397:C:C4' | 1:A:1398:A:OP2 | 2.58 | 0.52 |
| 1:A:289:G:P | 27:A:1915:HOH:O | 2.67 | 0.52 |
| 6:F:10:LEU:HD12 | 6:F:59:TYR:HB3 | 1.92 | 0.52 |
| 17:Q:4:LYS:HD2 | 17:Q:6:LEU:HD21 | 1.92 | 0.52 |
| 17:Q:59:ILE:HG23 | 17:Q:71:PHE:CD1 | 2.44 | 0.52 |
| 1:A:364:A:N6 | 12:L:28:LYS:HE2 | 2.25 | 0.52 |
| 1:A:62:U:OP1 | 1:A:385:C:O2' | 2.27 | 0.52 |
| 19:S:31:ILE:HD13 | 19:S:32:LYS:H | 1.74 | 0.52 |
| 20:T:61:SER:O | 20:T:65:LYS:HG3 | 2.09 | 0.52 |
| 1:A:500:G:H2' | 1:A:501:C:C6 | 2.45 | 0.51 |
| 9:I:39:GLY:C | 9:I:40:LEU:HD23 | 2.30 | 0.51 |
| 12:L:20:LYS:HD2 | 12:L:20:LYS:N | 2.25 | 0.51 |
| 1:A:1054:C:C3' | 1:A:1054:C:O2 | 2.55 | 0.51 |
| 1:A:1404:5MC:HM51 | 1:A:1404:5MC:OP2 | 2.10 | 0.51 |
| 25:A:1860:SRV:HH23 | 12:L:48:PRO:HG3 | 1.92 | 0.51 |
| 2:B:80:ILE:HD13 | 2:B:212:GLN:HB2 | 1.92 | 0.51 |
| 9:I:48:GLU:CD | 9:I:51:ARG:HH21 | 2.13 | 0.51 |
| 15:O:73:GLU:HA | 15:O:73:GLU:OE1 | 2.10 | 0.51 |
| 1:A:1003:G:N2 | 1:A:1039:C:O2 | 2.43 | 0.51 |
| 1:A:1342:C:H2' | 1:A:1343:G:C8 | 2.46 | 0.51 |
| 1:A:421:U:H4' | 1:A:422:C:OP2 | 2.08 | 0.51 |
| 4:D:8:VAL:O | 4:D:11:LEU:N | 2.40 | 0.51 |
| 10:J:42:THR:HG23 | 10:J:67:THR:O | 2.09 | 0.51 |
| 3:C:12:LEU:HD11 | 14:N:51:GLY:HA2 | 1.92 | 0.51 |
| 1:A:1104:G:P | 2:B:111:ARG:HD2 | 2.51 | 0.51 |
| 1:A:1502:A:H2 | 1:A:1505:G:N1 | 2.09 | 0.51 |
| 1:A:631:G:H5' | 1:A:632:A:P | 2.51 | 0.51 |
| 1:A:633:G:H2' | 1:A:634:C:H6 | 1.75 | 0.51 |
| 4:D:191:ARG:HG3 | 4:D:192:GLU:OE2 | 2.10 | 0.51 |
| 12:L:28:LYS:O | 12:L:28:LYS:HG3 | 2.09 | 0.51 |
| 1:A:1005:A:H8 | 1:A:1005:A:OP2 | 1.92 | 0.51 |
| 1:A:1368:G:H5'' | 9:I:112:LYS:HB3 | 1.92 | 0.51 |
| 1:A:325:A:H2' | 1:A:326:G:O4' | 2.10 | 0.51 |
| 5:E:76:ILE:O | 5:E:93:PRO:HB3 | 2.11 | 0.51 |
| 7:G:26:PHE:O | 7:G:30:ILE:HG13 | 2.10 | 0.51 |
| 11:K:34:ASP:HB2 | 11:K:35:PRO:CD | 2.41 | 0.51 |
| 16:P:58:TYR:CE1 | 16:P:62:VAL:HG21 | 2.45 | 0.51 |
| 1:A:1035:A:C4 | 1:A:1036:G:C8 | 2.98 | 0.51 |
| 1:A:1095:U:H2' | 1:A:1096:C:O4' | 2.09 | 0.51 |
| 1:A:563:A:H5'' | 1:A:564:C:OP1 | 2.09 | 0.51 |
| 1:A:731:G:H5' | 1:A:766:A:H4' | 1.91 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:K:48:ILE:HG22 | 11:K:49:GLY:H | 1.75 | 0.51 |
| 12:L:28:LYS:O | 12:L:30:ALA:N | 2.43 | 0.51 |
| 17:Q:68:ARG:H | 17:Q:70:ARG:NH1 | 2.08 | 0.51 |
| 1:A:62:U:H2' | 1:A:63:C:C6 | 2.46 | 0.51 |
| 1:A:945:G:H2' | 1:A:945:G:N3 | 2.25 | 0.51 |
| 2:B:53:ARG:HH11 | 2:B:53:ARG:HB3 | 1.75 | 0.51 |
| 5:E:96:PRO:HA | 5:E:117:ASP:OD2 | 2.11 | 0.51 |
| 13:M:15:VAL:HG23 | 13:M:43:THR:O | 2.11 | 0.51 |
| 17:Q:65:ILE:H | 17:Q:65:ILE:HD12 | 1.76 | 0.51 |
| 17:Q:67:LYS:O | 17:Q:68:ARG:HB2 | 2.10 | 0.51 |
| 2:B:213:LEU:O | 2:B:217:ARG:HG2 | 2.11 | 0.51 |
| 1:A:1190:G:HO2' | 1:A:1191:A:P | 2.34 | 0.51 |
| 1:A:1054:C:H5 | 1:A:1196:U:C6 | 2.29 | 0.51 |
| 1:A:1300:G:O2' | 1:A:1301:U:H6 | 1.93 | 0.51 |
| 1:A:76:C:O2' | 1:A:77:G:H5' | 2.10 | 0.51 |
| 2:B:103:THR:HA | 2:B:180:LEU:HD11 | 1.92 | 0.51 |
| 9:I:36:TYR:HD2 | 9:I:37:PHE:CE2 | 2.29 | 0.51 |
| 7:G:40:ALA:HB3 | 9:I:41:VAL:HG21 | 1.91 | 0.51 |
| 15:O:7:GLU:O | 15:O:11:VAL:HG13 | 2.11 | 0.51 |
| 1:A:1068:G:H8 | 1:A:1068:G:OP2 | 1.93 | 0.51 |
| 1:A:905:U:H2' | 1:A:906:G:H5' | 1.93 | 0.51 |
| 4:D:61:LYS:HA | 4:D:203:VAL:HG22 | 1.92 | 0.51 |
| 11:K:14:VAL:HG12 | 11:K:16:SER:H | 1.75 | 0.51 |
| 20:T:70:SER:HA | 20:T:73:HIS:CD2 | 2.46 | 0.51 |
| 1:A:1024:G:N7 | 1:A:1025:U:C4 | 2.79 | 0.50 |
| 1:A:1030(B):C:H2' | 1:A:1030(C):G:O4' | 2.11 | 0.50 |
| 1:A:327:A:O3' | 1:A:328:C:C4' | 2.59 | 0.50 |
| 1:A:456:C:H2' | 1:A:457:C:C6 | 2.46 | 0.50 |
| 1:A:867:G:C2' | 1:A:868:C:H5' | 2.41 | 0.50 |
| 9:I:95:LYS:HD2 | 9:I:95:LYS:N | 2.25 | 0.50 |
| 3:C:18:TRP:CD1 | 14:N:54:PRO:HA | 2.46 | 0.50 |
| 16:P:81:ARG:HG3 | 16:P:83:GLU:HG2 | 1.92 | 0.50 |
| 19:S:31:ILE:CG2 | 19:S:49:ILE:HG23 | 2.41 | 0.50 |
| 20:T:56:MET:HG3 | 20:T:84:LEU:HD22 | 1.93 | 0.50 |
| 1:A:1026:G:C2' | 1:A:1027:C:OP1 | 2.59 | 0.50 |
| 1:A:1368:G:OP2 | 9:I:112:LYS:HD3 | 2.10 | 0.50 |
| 1:A:502:G:H2' | 1:A:503:C:O4' | 2.12 | 0.50 |
| 1:A:728:A:H2' | 1:A:729:A:O4' | 2.11 | 0.50 |
| 2:B:7:VAL:HG13 | 2:B:48:MET:CE | 2.41 | 0.50 |
| 9:I:46:ALA:HB2 | 9:I:74:ILE:HG23 | 1.92 | 0.50 |
| 12:L:28:LYS:O | 12:L:29:GLY:C | 2.49 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 12:L:50:SER:O | 12:L:51:ALA:HB2 | 2.10 | 0.50 |
| 1:A:1298:C:H4' | 1:A:1299:A:O4' | 2.11 | 0.50 |
| 1:A:1327:C:H5 | 21:U:6:ARG:NH2 | 2.06 | 0.50 |
| 1:A:428:G:C1' | 1:A:429:U:OP2 | 2.59 | 0.50 |
| 8:H:83:ILE:O | 8:H:83:ILE:HG23 | 2.11 | 0.50 |
| 9:I:4:TYR:CE2 | 9:I:88:TYR:HD1 | 2.28 | 0.50 |
| 15:O:17:ARG:HH11 | 15:O:17:ARG:CG | 2.13 | 0.50 |
| 1:A:895:G:H2' | 1:A:896:C:C6 | 2.46 | 0.50 |
| 2:B:185:ILE:H | 2:B:185:ILE:HD12 | 1.77 | 0.50 |
| 3:C:52:LEU:O | 3:C:52:LEU:HD23 | 2.11 | 0.50 |
| 12:L:117:ARG:HH22 | 12:L:124:LYS:HD3 | 1.76 | 0.50 |
| 17:Q:100:LYS:HB3 | 17:Q:101:ARG:NH2 | 2.27 | 0.50 |
| 1:A:357:G:C2 | 1:A:358:U:C5 | 2.99 | 0.50 |
| 4:D:88:VAL:O | 4:D:92:VAL:HG23 | 2.11 | 0.50 |
| 12:L:19:ARG:CD | 12:L:19:ARG:H | 2.14 | 0.50 |
| 15:O:17:ARG:NH1 | 15:O:77:ARG:NH1 | 2.58 | 0.50 |
| 23:W:28:G:H2' | 23:W:28:G:N3 | 2.27 | 0.50 |
| 1:A:1053:G:O2' | 1:A:1199:U:H5 | 1.91 | 0.50 |
| 1:A:828:A:H4' | 1:A:828:A:OP1 | 2.10 | 0.50 |
| 5:E:71:LEU:CD2 | 5:E:115:VAL:HG22 | 2.41 | 0.50 |
| 1:A:1256:A:H4' | 1:A:1257:U:OP2 | 2.10 | 0.50 |
| 1:A:149:A:H2' | 1:A:150:C:C6 | 2.47 | 0.50 |
| 1:A:181:G:C4' | 1:A:182:U:OP2 | 2.60 | 0.50 |
| 1:A:529:G:O6 | 12:L:49:ASN:OD1 | 2.30 | 0.50 |
| 1:A:922:G:C6 | 1:A:923:A:C6 | 3.00 | 0.50 |
| 5:E:43:LEU:O | 5:E:62:ALA:HA | 2.12 | 0.50 |
| 1:A:1385:G:H2' | 1:A:1386:G:O4' | 2.11 | 0.50 |
| 1:A:657:G:H4' | 15:O:28:GLN:HG2 | 1.94 | 0.50 |
| 6:F:42:GLU:HG3 | 6:F:61:LEU:HD23 | 1.92 | 0.50 |
| 18:R:47:THR:HA | 18:R:83:GLU:HB2 | 1.93 | 0.50 |
| 1:A:1300:G:C6 | 1:A:1335:C:C5 | 2.99 | 0.50 |
| 1:A:196:A:HO2' | 1:A:221:C:HO2' | 1.59 | 0.50 |
| 1:A:427:U:OP2 | 1:A:428:G:O2' | 2.29 | 0.50 |
| 2:B:141:GLU:O | 2:B:145:LEU:HG | 2.12 | 0.50 |
| 4:D:8:VAL:HG12 | 4:D:21:LEU:HD13 | 1.93 | 0.50 |
| 10:J:48:THR:HG23 | 10:J:62:HIS:HB3 | 1.94 | 0.50 |
| 13:M:11:ARG:CG | 13:M:12:ASN:N | 2.74 | 0.50 |
| 14:N:42:ILE:O | 14:N:46:GLU:HG3 | 2.11 | 0.50 |
| 17:Q:76:LEU:HD12 | 17:Q:77:VAL:N | 2.27 | 0.50 |
| 1:A:1106:G:H5'' | 3:C:172:ARG:HG2 | 1.94 | 0.49 |
| 1:A:1401:G:C2 | 1:A:1402:4OC:H1' | 2.47 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1511:G:H2' | 1:A:1512:U:O4' | 2.11 | 0.49 |
| 1:A:281:G:H8 | 1:A:281:G:O5' | 1.93 | 0.49 |
| 1:A:806:C:O2' | 1:A:807:A:H5' | 2.12 | 0.49 |
| 1:A:961:U:C2' | 1:A:962:C:H5' | 2.42 | 0.49 |
| 2:B:24:TRP:HA | 2:B:190:THR:HG22 | 1.94 | 0.49 |
| 1:A:1162:C:H2' | 1:A:1163:C:C6 | 2.47 | 0.49 |
| 1:A:1515[B]:C:C2' | 1:A:1516[B]:G:H5' | 2.42 | 0.49 |
| 1:A:192:U:H2' | 1:A:193:C:C6 | 2.46 | 0.49 |
| 1:A:587:G:O2' | 1:A:588:G:OP2 | 2.22 | 0.49 |
| 1:A:814:A:H2' | 1:A:816:A:H5'' | 1.93 | 0.49 |
| 1:A:88:A:H2' | 1:A:89:C:O4' | 2.12 | 0.49 |
| 3:C:6:HIS:O | 3:C:10:PHE:N | 2.46 | 0.49 |
| 1:A:1292:U:P | 7:G:41:ARG:HH22 | 2.35 | 0.49 |
| 10:J:45:ARG:HG2 | 10:J:47:PHE:CZ | 2.47 | 0.49 |
| 11:K:108:ILE:N | 11:K:108:ILE:HD12 | 2.27 | 0.49 |
| 13:M:8:GLU:HG3 | 13:M:22:ILE:HG23 | 1.94 | 0.49 |
| 19:S:10:PHE:CD2 | 19:S:10:PHE:C | 2.86 | 0.49 |
| 21:U:10:ARG:NH1 | 21:U:10:ARG:CG | 2.71 | 0.49 |
| 1:A:1057:G:H2' | 1:A:1058:G:O4' | 2.11 | 0.49 |
| 1:A:1207:2MG:H2' | 1:A:1208:C:H6 | 1.77 | 0.49 |
| 1:A:645:C:O2' | 1:A:646:U:H5' | 2.13 | 0.49 |
| 1:A:771:G:O2' | 1:A:772:U:H5' | 2.12 | 0.49 |
| 3:C:20:SER:HB3 | 3:C:40:ARG:HH22 | 1.77 | 0.49 |
| 4:D:10:ARG:HG2 | 4:D:11:LEU:HD23 | 1.93 | 0.49 |
| 4:D:52:SER:O | 4:D:56:VAL:HG23 | 2.12 | 0.49 |
| 6:F:24:GLU:OE2 | 6:F:28:ARG:NH1 | 2.45 | 0.49 |
| 10:J:12:ASP:OD1 | 10:J:14:LYS:N | 2.43 | 0.49 |
| 13:M:36:LYS:HB2 | 13:M:59:TYR:HE2 | 1.77 | 0.49 |
| 1:A:1062:U:H2' | 1:A:1063:C:C6 | 2.47 | 0.49 |
| 1:A:1406:U:HO2' | 1:A:1517[B]:G:N2 | 2.11 | 0.49 |
| 1:A:384:G:H2' | 1:A:385:C:H6 | 1.77 | 0.49 |
| 1:A:484:G:H5' | 1:A:486:U:O4' | 2.13 | 0.49 |
| 1:A:838:G:N2 | 1:A:849:C:C2 | 2.81 | 0.49 |
| 1:A:973:G:H3' | 1:A:974:A:H5'' | 1.94 | 0.49 |
| 6:F:100:ASN:OD1 | 18:R:23:LYS:HE2 | 2.12 | 0.49 |
| 6:F:10:LEU:HD12 | 6:F:10:LEU:H | 1.77 | 0.49 |
| 9:I:53:VAL:CG2 | 9:I:85:LEU:HD21 | 2.42 | 0.49 |
| 13:M:49:THR:HG22 | 13:M:52:GLU:N | 2.19 | 0.49 |
| 16:P:38:TYR:HE2 | 16:P:50:LYS:HE2 | 1.77 | 0.49 |
| 19:S:22:LEU:O | 19:S:26:GLY:O | 2.30 | 0.49 |
| 1:A:1203:C:H2' | 1:A:1204:A:O4' | 2.11 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 1:A:1216:G:H2' | 1:A:1217:C:H6 | 1.78 | 0.49 |
| 1:A:1423:G:H2' | 1:A:1424:C:H6 | 1.77 | 0.49 |
| 1:A:295:C:H2' | 1:A:296:U:O4' | 2.12 | 0.49 |
| 1:A:477:G:H2' | 1:A:478:A:H8 | 1.77 | 0.49 |
| 2:B:8:LYS:O | 2:B:12:GLU:HG3 | 2.12 | 0.49 |
| 2:B:69:LEU:HB3 | 2:B:162:ILE:HG22 | 1.94 | 0.49 |
| 4:D:54:TYR:CE2 | 4:D:58:LEU:HD12 | 2.48 | 0.49 |
| 4:D:58:LEU:C | 4:D:58:LEU:HD23 | 2.32 | 0.49 |
| 10:J:19:SER:HB2 | 10:J:91:PRO:HG3 | 1.95 | 0.49 |
| 18:R:87:ARG:O | 18:R:88:LYS:CB | 2.60 | 0.49 |
| 1:A:1318:A:O2' | 19:S:37:ARG:HD2 | 2.12 | 0.49 |
| 1:A:370:C:H2' | 1:A:371:G:H5' | 1.93 | 0.49 |
| 1:A:421:U:H5' | 1:A:422:C:C5 | 2.47 | 0.49 |
| 1:A:452:A:OP1 | 16:P:43:LYS:NZ | 2.37 | 0.49 |
| 1:A:577:G:H1' | 1:A:816:A:C4 | 2.48 | 0.49 |
| 2:B:107:THR:O | 2:B:110:GLN:HB2 | 2.13 | 0.49 |
| 2:B:16:HIS:HB3 | 2:B:44:LEU:CD1 | 2.40 | 0.49 |
| 3:C:20:SER:CB | 3:C:40:ARG:HH22 | 2.24 | 0.49 |
| 4:D:105:VAL:HG13 | 4:D:110:PHE:HB2 | 1.93 | 0.49 |
| 4:D:12:CYS:HA | 4:D:19:LEU:CD2 | 2.42 | 0.49 |
| 19:S:31:ILE:HG22 | 19:S:50:ALA:H | 1.78 | 0.49 |
| 1:A:1300:G:O2' | 1:A:1301:U:O5' | 2.31 | 0.49 |
| 1:A:1300:G:HO2' | 1:A:1301:U:P | 2.32 | 0.49 |
| 1:A:1518[B]:MA6:H102 | 1:A:1519[B]:MA6:C10 | 2.43 | 0.49 |
| 1:A:728:A:O5' | 1:A:728:A:H8 | 1.96 | 0.49 |
| 4:D:150:GLU:HA | 4:D:153:ARG:CZ | 2.42 | 0.49 |
| 5:E:81:GLU:HG2 | 5:E:90:VAL:HG13 | 1.94 | 0.49 |
| 11:K:58:PRO:HA | 11:K:90:GLY:HA3 | 1.93 | 0.49 |
| 16:P:55:ARG:O | 16:P:58:TYR:HB3 | 2.13 | 0.49 |
| 23:W:37:A:N6 | 23:W:38:A:C2 | 2.81 | 0.49 |
| 1:A:1220:G:H2' | 1:A:1221:G:H8 | 1.77 | 0.49 |
| 1:A:328:C:HO2' | 1:A:329:A:P | 2.32 | 0.49 |
| 1:A:397:A:C6 | 1:A:548:G:N7 | 2.81 | 0.49 |
| 1:A:78:G:C2' | 1:A:79:G:O5' | 2.60 | 0.49 |
| 7:G:23:VAL:O | 7:G:27:ILE:HG12 | 2.12 | 0.49 |
| 1:A:1275:A:H2' | 1:A:1276:G:C8 | 2.48 | 0.49 |
| 1:A:1292:U:P | 7:G:41:ARG:NH2 | 2.85 | 0.49 |
| 1:A:1497:G:O2' | 1:A:1518[A]:MA6:N1 | 2.45 | 0.49 |
| 1:A:16:A:O2' | 5:E:16:THR:HB | 2.13 | 0.49 |
| 1:A:269:C:H2' | 1:A:270:A:C8 | 2.47 | 0.49 |
| 1:A:114:U:H1' | 1:A:353:A:H1' | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:803:G:C5 | 1:A:804:U:C4 | 3.00 | 0.49 |
| 1:A:818:G:HO2' | 1:A:820:U:H6 | 1.61 | 0.49 |
| 5:E:127:ASN:OD1 | 5:E:127:ASN:C | 2.51 | 0.49 |
| 1:A:939:G:H5'' | 7:G:102:ARG:NH2 | 2.27 | 0.49 |
| 9:I:11:LYS:O | 9:I:12:GLU:HB2 | 2.13 | 0.49 |
| 10:J:6:ILE:HD12 | 10:J:72:VAL:HG11 | 1.94 | 0.49 |
| 18:R:40:LEU:HB3 | 18:R:79:LEU:HD11 | 1.95 | 0.49 |
| 1:A:1406:U:H3' | 1:A:1407:5MC:HM51 | 1.95 | 0.49 |
| 1:A:129(A):G:H1' | 1:A:190(E):U:H2' | 1.94 | 0.49 |
| 1:A:539:A:H2' | 1:A:540:G:H8 | 1.77 | 0.49 |
| 1:A:80:G:C5' | 1:A:81:U:OP2 | 2.61 | 0.49 |
| 3:C:95:THR:C | 3:C:97:LYS:H | 2.14 | 0.49 |
| 4:D:4:TYR:CE2 | 4:D:11:LEU:HD11 | 2.48 | 0.49 |
| 9:I:51:ARG:HG2 | 9:I:56:LEU:HD13 | 1.95 | 0.49 |
| 13:M:37:THR:HG22 | 13:M:39:ILE:HG13 | 1.95 | 0.49 |
| 1:A:1308:U:C5 | 13:M:99:ARG:NH1 | 2.81 | 0.49 |
| 20:T:53:LEU:HB2 | 20:T:100:ILE:CG2 | 2.43 | 0.49 |
| 1:A:1127:G:N2 | 1:A:1145:C:N3 | 2.55 | 0.48 |
| 1:A:1191:A:H5'' | 3:C:4:LYS:HZ3 | 1.77 | 0.48 |
| 1:A:1274:G:O5' | 1:A:1274:G:H8 | 1.96 | 0.48 |
| 1:A:1516[A]:G:C6 | 1:A:1520[A]:G:C2 | 3.01 | 0.48 |
| 1:A:386:C:C2' | 1:A:387:U:H5' | 2.43 | 0.48 |
| 1:A:723:U:O2 | 1:A:723:U:H2' | 2.12 | 0.48 |
| 1:A:743:U:H2' | 1:A:744:C:C6 | 2.48 | 0.48 |
| 2:B:22:LYS:CG | 2:B:23:ARG:N | 2.76 | 0.48 |
| 3:C:79:ARG:O | 3:C:82:GLU:HG3 | 2.12 | 0.48 |
| 19:S:51:VAL:O | 19:S:58:VAL:HG22 | 2.13 | 0.48 |
| 1:A:1139:G:H4' | 1:A:1140:C:OP1 | 2.13 | 0.48 |
| 1:A:1130:A:C2 | 1:A:1146:A:C4 | 3.00 | 0.48 |
| 1:A:432:A:O2' | 1:A:433:C:OP1 | 2.30 | 0.48 |
| 1:A:857:C:H2' | 1:A:858:G:O4' | 2.14 | 0.48 |
| 4:D:148:VAL:HG12 | 4:D:149:ALA:H | 1.78 | 0.48 |
| 8:H:11:THR:HG22 | 8:H:12:ARG:N | 2.28 | 0.48 |
| 13:M:17:VAL:O | 13:M:20:THR:HB | 2.13 | 0.48 |
| 17:Q:75:ARG:HG3 | 17:Q:75:ARG:NH1 | 2.27 | 0.48 |
| 1:A:1053:G:C3' | 1:A:1054:C:H5' | 2.43 | 0.48 |
| 1:A:1502:A:C2 | 1:A:1504:G:C2 | 3.01 | 0.48 |
| 1:A:522:C:C2' | 1:A:523:A:H5' | 2.43 | 0.48 |
| 1:A:683:G:H2' | 1:A:684:A:C8 | 2.49 | 0.48 |
| 7:G:54:THR:CG2 | 7:G:56:GLN:HB2 | 2.44 | 0.48 |
| 11:K:57:THR:CG2 | 11:K:58:PRO:HD2 | 2.44 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 13:M:107:ALA:O | 13:M:111:LYS:HB2 | 2.13 | 0.48 |
| 17:Q:4:LYS:HD2 | 17:Q:6:LEU:CD2 | 2.42 | 0.48 |
| 19:S:80:TYR:CZ | 19:S:81:ARG:HD3 | 2.48 | 0.48 |
| 20:T:43:LEU:HD12 | 20:T:52:ALA:HA | 1.95 | 0.48 |
| 1:A:1007:C:H42 | 1:A:1022:G:H1 | 1.60 | 0.48 |
| 1:A:179:A:H2' | 1:A:180:U:H6 | 1.78 | 0.48 |
| 1:A:738:C:OP1 | 6:F:2:ARG:NH1 | 2.47 | 0.48 |
| 1:A:923:A:O4' | 1:A:1398:A:C2 | 2.67 | 0.48 |
| 13:M:91:ARG:NH1 | 13:M:96:LEU:HD13 | 2.29 | 0.48 |
| 19:S:31:ILE:HG21 | 19:S:49:ILE:HD12 | 1.94 | 0.48 |
| 1:A:1316:G:H4' | 14:N:18:VAL:CG1 | 2.43 | 0.48 |
| 1:A:1423:G:H2' | 1:A:1424:C:C6 | 2.49 | 0.48 |
| 1:A:1427:U:H2' | 1:A:1428:A:H8 | 1.78 | 0.48 |
| 1:A:182:U:OP2 | 1:A:182:U:H6 | 1.96 | 0.48 |
| 1:A:442:C:N4 | 1:A:492:G:H1 | 1.96 | 0.48 |
| 1:A:690:G:H2' | 1:A:691:G:O4' | 2.14 | 0.48 |
| 4:D:61:LYS:HD2 | 4:D:61:LYS:C | 2.33 | 0.48 |
| 11:K:73:MET:O | 11:K:76:GLY:N | 2.40 | 0.48 |
| 1:A:1541:PSU:O4 | 1:A:1541:PSU:C2' | 2.57 | 0.48 |
| 1:A:353:A:H2' | 1:A:354:G:OP2 | 2.14 | 0.48 |
| 1:A:905:U:C2' | 1:A:906:G:H5' | 2.43 | 0.48 |
| 4:D:38:TYR:HB2 | 4:D:39:PRO:HD2 | 1.96 | 0.48 |
| 1:A:542:G:H5' | 4:D:41:GLY:HA3 | 1.95 | 0.48 |
| 6:F:10:LEU:HD11 | 6:F:59:TYR:CD2 | 2.49 | 0.48 |
| 12:L:13:LYS:HB2 | 12:L:13:LYS:HE3 | 1.70 | 0.48 |
| 19:S:36:ARG:HH21 | 19:S:53:ASN:HA | 1.78 | 0.48 |
| 20:T:53:LEU:HD13 | 20:T:100:ILE:HG22 | 1.94 | 0.48 |
| 1:A:1051:C:H2' | 1:A:1052:U:C6 | 2.49 | 0.48 |
| 1:A:1092:A:H5'' | 7:G:4:ARG:NH1 | 2.28 | 0.48 |
| 3:C:123:GLN:O | 3:C:128:PHE:HB2 | 2.14 | 0.48 |
| 4:D:112:VAL:HG22 | 4:D:116:GLN:OE1 | 2.13 | 0.48 |
| 4:D:112:VAL:N | 4:D:116:GLN:OE1 | 2.42 | 0.48 |
| 1:A:547:A:OP2 | 4:D:2:GLY:HA3 | 2.14 | 0.48 |
| 4:D:9:CYS:O | 4:D:12:CYS:HB2 | 2.14 | 0.48 |
| 16:P:20:VAL:HG11 | 16:P:32:TYR:CB | 2.43 | 0.48 |
| 1:A:1002:G:H2' | 1:A:1003:G:C8 | 2.48 | 0.48 |
| 1:A:1048:G:O3' | 1:A:1049:U:H3' | 2.14 | 0.48 |
| 1:A:1318:A:H4' | 19:S:10:PHE:CE1 | 2.49 | 0.48 |
| 1:A:793:U:O4 | 1:A:1517[A]:G:H5' | 2.14 | 0.48 |
| 1:A:353:A:H8 | 1:A:353:A:C5' | 2.21 | 0.48 |
| 1:A:397:A:N3 | 1:A:397:A:H3' | 2.29 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 1:A:56:U:H2' | 1:A:57:G:C8 | 2.48 | 0.48 |
| 2:B:121:LEU:C | 2:B:121:LEU:HD23 | 2.34 | 0.48 |
| 5:E:40:ARG:HH11 | 5:E:40:ARG:HG2 | 1.79 | 0.48 |
| 9:I:97:LYS:HB2 | 9:I:102:LEU:HD21 | 1.95 | 0.48 |
| 10:J:78:ASN:N | 10:J:78:ASN:OD1 | 2.46 | 0.48 |
| 15:O:8:LYS:O | 15:O:11:VAL:HG22 | 2.14 | 0.48 |
| 16:P:9:PHE:CE2 | 16:P:18:ARG:HD2 | 2.49 | 0.48 |
| 19:S:7:LYS:HD2 | 19:S:7:LYS:C | 2.34 | 0.48 |
| 20:T:13:LEU:C | 20:T:13:LEU:CD1 | 2.82 | 0.48 |
| 1:A:78:G:H2' | 1:A:79:G:O5' | 2.14 | 0.48 |
| 1:A:977:A:H2' | 1:A:978:A:H5'' | 1.96 | 0.48 |
| 5:E:11:ILE:HD11 | 5:E:108:ALA:HB3 | 1.95 | 0.48 |
| 5:E:36:ASP:CG | 5:E:38:GLN:HB2 | 2.35 | 0.48 |
| 7:G:155:ARG:O | 7:G:156:TRP:CG | 2.67 | 0.48 |
| 8:H:86:ILE:HG21 | 8:H:133:LEU:HD13 | 1.96 | 0.48 |
| 9:I:118:LYS:O | 9:I:120:ARG:N | 2.42 | 0.48 |
| 1:A:1345:U:OP1 | 9:I:120:ARG:NH1 | 2.47 | 0.48 |
| 10:J:50:ILE:HG22 | 10:J:60:ARG:CD | 2.39 | 0.48 |
| 1:A:1308:U:OP2 | 13:M:99:ARG:HG3 | 2.14 | 0.48 |
| 15:O:15:PHE:CE2 | 15:O:84:LYS:HD2 | 2.49 | 0.48 |
| 19:S:40:ILE:CG2 | 19:S:67:VAL:HA | 2.43 | 0.48 |
| 1:A:191:G:O2' | 20:T:102:GLY:O | 2.29 | 0.48 |
| 1:A:108:G:C2' | 1:A:109:A:OP1 | 2.62 | 0.48 |
| 1:A:19:C:O2' | 1:A:20:U:H5' | 2.13 | 0.48 |
| 1:A:716:A:H1' | 11:K:117:ASN:O | 2.13 | 0.48 |
| 8:H:36:LEU:HD12 | 8:H:59:LEU:HD22 | 1.96 | 0.48 |
| 11:K:108:ILE:HG22 | 11:K:109:VAL:N | 2.29 | 0.48 |
| 1:A:1091:U:O2 | 1:A:1093:A:H8 | 1.97 | 0.47 |
| 1:A:1179:A:C2' | 1:A:1180:A:O5' | 2.62 | 0.47 |
| 1:A:1358:U:H3' | 1:A:1359:C:H6 | 1.79 | 0.47 |
| 1:A:376:G:P | 16:P:67:THR:HG21 | 2.54 | 0.47 |
| 1:A:502:G:P | 12:L:118:SER:HG | 2.36 | 0.47 |
| 5:E:81:GLU:OE2 | 5:E:88:LYS:HE2 | 2.13 | 0.47 |
| 1:A:1149:C:OP1 | 9:I:9:ARG:NH1 | 2.47 | 0.47 |
| 15:O:26:GLU:HA | 15:O:81:LEU:HD22 | 1.95 | 0.47 |
| 12:L:10:LEU:HB3 | 17:Q:32:TYR:CD1 | 2.49 | 0.47 |
| 17:Q:35:VAL:HG12 | 17:Q:35:VAL:O | 2.14 | 0.47 |
| 1:A:1023:G:C6 | 1:A:1024:G:C2 | 3.02 | 0.47 |
| 1:A:1074:G:O6 | 27:A:2019:HOH:O | 2.20 | 0.47 |
| 1:A:1408:A:H2' | 1:A:1409:C:H6 | 1.79 | 0.47 |
| 1:A:1516[B]:G:N2 | 1:A:1519[B]:MA6:OP2 | 2.46 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|---------------------|--------------------------|-------------------|
| 1:A:6:G:H4' | 1:A:298:A:H4' | 1.96 | 0.47 |
| 1:A:403:C:OP1 | 4:D:136:PRO:HD2 | 2.13 | 0.47 |
| 1:A:658:G:OP1 | 15:O:8:LYS:NZ | 2.43 | 0.47 |
| 1:A:665:A:N3 | 1:A:732:C:H2' | 2.28 | 0.47 |
| 1:A:80:G:H5'' | 1:A:81:U:OP2 | 2.13 | 0.47 |
| 1:A:817:C:H4' | 1:A:818:G:OP1 | 2.14 | 0.47 |
| 2:B:142:LEU:HD23 | 2:B:142:LEU:O | 2.14 | 0.47 |
| 3:C:64:VAL:CB | 3:C:99:VAL:HB | 2.41 | 0.47 |
| 1:A:620:C:C1' | 4:D:135:LEU:HD13 | 2.44 | 0.47 |
| 8:H:123:GLU:O | 8:H:127:LEU:HB2 | 2.15 | 0.47 |
| 2:B:181:PHE:HD2 | 8:H:70:GLN:HB3 | 1.79 | 0.47 |
| 11:K:19:ALA:HB2 | 11:K:80:VAL:HG21 | 1.95 | 0.47 |
| 13:M:108:ARG:NH2 | 13:M:111:LYS:HE2 | 2.29 | 0.47 |
| 1:A:1216:G:H5'' | 14:N:5:ALA:CB | 2.44 | 0.47 |
| 2:B:161:ALA:HB1 | 2:B:185:ILE:CD1 | 2.44 | 0.47 |
| 2:B:33:TYR:C | 2:B:33:TYR:CD2 | 2.87 | 0.47 |
| 3:C:13:GLY:O | 3:C:14:ILE:HD13 | 2.14 | 0.47 |
| 5:E:12:LEU:C | 5:E:12:LEU:HD22 | 2.35 | 0.47 |
| 6:F:53:ALA:C | 6:F:54:LYS:HG2 | 2.35 | 0.47 |
| 8:H:83:ILE:HG13 | 8:H:137:VAL:HG22 | 1.96 | 0.47 |
| 10:J:19:SER:O | 10:J:22:LYS:HB2 | 2.15 | 0.47 |
| 13:M:65:LYS:O | 13:M:70:LEU:HG | 2.13 | 0.47 |
| 14:N:5:ALA:O | 14:N:8:GLU:CG | 2.62 | 0.47 |
| 1:A:1143:G:C6 | 1:A:1144:G:C6 | 3.02 | 0.47 |
| 1:A:1406:U:H4' | 1:A:1518[B]:MA6:H1' | 1.95 | 0.47 |
| 1:A:664:G:N2 | 1:A:741:G:H1 | 1.95 | 0.47 |
| 1:A:977:A:O2' | 1:A:979:C:OP2 | 2.30 | 0.47 |
| 2:B:114:ARG:NH1 | 2:B:141:GLU:OE1 | 2.47 | 0.47 |
| 4:D:142:PRO:HA | 4:D:185:PHE:O | 2.14 | 0.47 |
| 4:D:70:ILE:HD11 | 4:D:100:ARG:NE | 2.29 | 0.47 |
| 20:T:53:LEU:O | 20:T:57:ARG:HD3 | 2.14 | 0.47 |
| 1:A:1114:C:H2' | 1:A:1115:C:C6 | 2.50 | 0.47 |
| 1:A:1316:G:N1 | 1:A:1319:A:OP2 | 2.48 | 0.47 |
| 1:A:273:A:N6 | 1:A:274:A:C6 | 2.83 | 0.47 |
| 1:A:340:U:H2' | 1:A:341:C:C6 | 2.49 | 0.47 |
| 1:A:913:A:C1' | 1:A:914:A:OP2 | 2.63 | 0.47 |
| 1:A:983:A:H3' | 1:A:983:A:N3 | 2.29 | 0.47 |
| 2:B:133:LYS:O | 2:B:137:ARG:HG3 | 2.15 | 0.47 |
| 2:B:61:LEU:HD21 | 2:B:160:ASP:CB | 2.44 | 0.47 |
| 9:I:17:VAL:HG21 | 9:I:80:GLY:HA3 | 1.97 | 0.47 |
| 12:L:54:LYS:N | 12:L:54:LYS:HD2 | 2.29 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 16:P:9:PHE:CD2 | 16:P:18:ARG:HG3 | 2.49 | 0.47 |
| 20:T:84:LEU:HD23 | 20:T:84:LEU:C | 2.35 | 0.47 |
| 1:A:1038:C:H2' | 1:A:1039:C:H6 | 1.79 | 0.47 |
| 1:A:1440:C:H2' | 1:A:1441:G:O4' | 2.14 | 0.47 |
| 1:A:17:U:H4' | 1:A:1080:A:O4' | 2.14 | 0.47 |
| 2:B:8:LYS:HA | 2:B:11:LEU:HD13 | 1.95 | 0.47 |
| 4:D:31:CYS:C | 4:D:33:MET:H | 2.16 | 0.47 |
| 8:H:23:SER:HA | 8:H:63:LEU:HD22 | 1.97 | 0.47 |
| 15:O:22:THR:O | 15:O:27:VAL:HG11 | 2.13 | 0.47 |
| 1:A:1179:A:HO2' | 1:A:1180:A:P | 2.37 | 0.47 |
| 1:A:1468:A:H2' | 1:A:1469:G:O4' | 2.14 | 0.47 |
| 2:B:87:ARG:CZ | 2:B:233:SER:HB2 | 2.45 | 0.47 |
| 4:D:31:CYS:O | 4:D:32:ALA:HB3 | 2.15 | 0.47 |
| 17:Q:63:ARG:HG2 | 17:Q:64:PRO:CD | 2.45 | 0.47 |
| 1:A:1201:A:H4' | 1:A:1202:G:O5' | 2.15 | 0.47 |
| 1:A:344:A:H4' | 1:A:345:C:OP2 | 2.14 | 0.47 |
| 3:C:5:ILE:C | 3:C:5:ILE:HD12 | 2.35 | 0.47 |
| 7:G:145:ALA:O | 7:G:146:GLU:CB | 2.62 | 0.47 |
| 11:K:110:ASP:HB2 | 18:R:88:LYS:HG3 | 1.96 | 0.47 |
| 13:M:44:ARG:N | 13:M:44:ARG:HD2 | 2.30 | 0.47 |
| 16:P:20:VAL:CG1 | 16:P:32:TYR:HB2 | 2.44 | 0.47 |
| 17:Q:54:GLY:O | 17:Q:80:GLY:HA2 | 2.15 | 0.47 |
| 18:R:59:SER:H | 18:R:62:GLU:HB2 | 1.80 | 0.47 |
| 1:A:103:C:P | 20:T:17:ARG:HH12 | 2.37 | 0.47 |
| 1:A:17:U:H1' | 1:A:1080:A:N3 | 2.30 | 0.47 |
| 1:A:1412:C:H2' | 1:A:1413:A:H8 | 1.69 | 0.47 |
| 1:A:325:A:OP2 | 20:T:70:SER:HB2 | 2.15 | 0.47 |
| 2:B:6:THR:HA | 2:B:9:GLU:OE1 | 2.14 | 0.47 |
| 8:H:48:TYR:HA | 8:H:60:ARG:O | 2.14 | 0.47 |
| 12:L:124:LYS:HD2 | 12:L:125:PRO:HD2 | 1.97 | 0.47 |
| 13:M:22:ILE:CB | 13:M:25:ILE:HD12 | 2.45 | 0.47 |
| 13:M:37:THR:HG22 | 13:M:37:THR:O | 2.15 | 0.47 |
| 1:A:1124:G:H2' | 1:A:1145:C:H5 | 1.79 | 0.47 |
| 1:A:1179:A:O2' | 1:A:1180:A:P | 2.72 | 0.47 |
| 1:A:31:G:O2' | 1:A:48:C:N4 | 2.47 | 0.47 |
| 1:A:452:A:HO2' | 1:A:453:A:H8 | 1.59 | 0.47 |
| 1:A:860:A:H2' | 1:A:861:G:O4' | 2.14 | 0.47 |
| 19:S:22:LEU:HD23 | 19:S:25:LYS:NZ | 2.29 | 0.47 |
| 20:T:35:THR:HA | 20:T:38:LYS:HE3 | 1.96 | 0.47 |
| 1:A:1179:A:O2' | 1:A:1180:A:OP1 | 2.29 | 0.47 |
| 1:A:1400:5MC:H3' | 1:A:1401:G:H5' | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:A:1411:C:H2' | 1:A:1412:C:C6 | 2.50 | 0.47 |
| 2:B:106:LYS:O | 2:B:109:SER:OG | 2.21 | 0.47 |
| 2:B:100:GLY:N | 2:B:176:GLU:OE2 | 2.44 | 0.47 |
| 3:C:128:PHE:HD2 | 3:C:129:ALA:H | 1.63 | 0.47 |
| 3:C:36:ASP:O | 3:C:39:ILE:HB | 2.15 | 0.47 |
| 4:D:148:VAL:CG1 | 4:D:149:ALA:N | 2.77 | 0.47 |
| 4:D:62:GLN:O | 4:D:66:ARG:HB2 | 2.14 | 0.47 |
| 1:A:1321:C:H4' | 13:M:87:TYR:CE2 | 2.50 | 0.47 |
| 19:S:43:GLU:OE2 | 19:S:43:GLU:N | 2.46 | 0.47 |
| 20:T:105:SER:O | 20:T:106:ALA:C | 2.53 | 0.47 |
| 1:A:1304:G:H1' | 1:A:1333:A:H61 | 1.80 | 0.46 |
| 1:A:1322:C:H4' | 1:A:1323:G:OP1 | 2.14 | 0.46 |
| 1:A:1498:UR3:H4' | 1:A:1519[A]:MA6:N1 | 2.29 | 0.46 |
| 1:A:9:G:OP1 | 5:E:122:GLU:HG3 | 2.16 | 0.46 |
| 7:G:113:GLU:CG | 7:G:119:ARG:HG2 | 2.45 | 0.46 |
| 8:H:119:LEU:HA | 8:H:123:GLU:OE1 | 2.15 | 0.46 |
| 17:Q:22:LEU:HD12 | 17:Q:23:VAL:H | 1.80 | 0.46 |
| 18:R:59:SER:N | 18:R:62:GLU:OE1 | 2.46 | 0.46 |
| 1:A:1001:A:H2' | 1:A:1002:G:C8 | 2.50 | 0.46 |
| 1:A:1023:G:O6 | 1:A:1024:G:N2 | 2.47 | 0.46 |
| 1:A:1480:G:C6 | 1:A:1481:U:C4 | 3.04 | 0.46 |
| 1:A:1518[B]:MA6:O2' | 1:A:1519[B]:MA6:O5' | 2.34 | 0.46 |
| 1:A:21:G:OP1 | 27:A:1942:HOH:O | 2.19 | 0.46 |
| 1:A:253:U:OP1 | 17:Q:67:LYS:HE2 | 2.15 | 0.46 |
| 1:A:283:C:C2 | 1:A:284:G:C8 | 3.03 | 0.46 |
| 1:A:421:U:O2 | 1:A:421:U:H2' | 2.15 | 0.46 |
| 1:A:854:G:H3' | 1:A:871:U:O4 | 2.15 | 0.46 |
| 2:B:97:TRP:CH2 | 2:B:176:GLU:OE2 | 2.68 | 0.46 |
| 5:E:33:VAL:HG11 | 5:E:109:ILE:HA | 1.97 | 0.46 |
| 17:Q:5:VAL:O | 17:Q:6:LEU:HD23 | 2.16 | 0.46 |
| 6:F:91:VAL:HG11 | 18:R:72:ARG:NH1 | 2.29 | 0.46 |
| 19:S:27:GLU:HG2 | 19:S:28:LYS:N | 2.30 | 0.46 |
| 1:A:1225:A:N3 | 1:A:1225:A:H2' | 2.30 | 0.46 |
| 1:A:1450:U:H2' | 1:A:1452:C:C5 | 2.50 | 0.46 |
| 1:A:370:C:HO2' | 1:A:371:G:H5' | 1.80 | 0.46 |
| 1:A:966:M2G:HM22 | 1:A:967:5MC:C2 | 2.50 | 0.46 |
| 4:D:191:ARG:O | 4:D:191:ARG:HD2 | 2.15 | 0.46 |
| 7:G:113:GLU:HB2 | 7:G:119:ARG:HG2 | 1.97 | 0.46 |
| 8:H:104:ARG:CZ | 8:H:138:TRP:CH2 | 2.98 | 0.46 |
| 1:A:1072:G:H2' | 1:A:1073:U:C6 | 2.49 | 0.46 |
| 1:A:1281:U:HO2' | 1:A:1282:C:P | 2.34 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1339:A:H2' | 1:A:1340:A:O4' | 2.16 | 0.46 |
| 1:A:166:G:O2' | 1:A:167:G:H5' | 2.15 | 0.46 |
| 1:A:28:G:O2' | 1:A:296:U:OP1 | 2.32 | 0.46 |
| 1:A:557:G:C6 | 1:A:558:G:C6 | 3.03 | 0.46 |
| 1:A:60:A:H5' | 27:A:1901:HOH:O | 2.16 | 0.46 |
| 1:A:909:A:H2' | 1:A:910:C:O4' | 2.13 | 0.46 |
| 1:A:973:G:H2' | 1:A:974:A:OP1 | 2.15 | 0.46 |
| 6:F:54:LYS:HE3 | 6:F:54:LYS:HA | 1.97 | 0.46 |
| 1:A:1150:U:O2 | 10:J:39:PRO:HG2 | 2.16 | 0.46 |
| 13:M:59:TYR:CE1 | 13:M:63:THR:HG21 | 2.50 | 0.46 |
| 15:O:3:ILE:HG12 | 15:O:38:ARG:NH1 | 2.30 | 0.46 |
| 1:A:1158:C:O2 | 1:A:1158:C:C2' | 2.64 | 0.46 |
| 1:A:1118:C:H1' | 1:A:1179:A:C4 | 2.51 | 0.46 |
| 1:A:248:C:C2' | 1:A:249:U:H5' | 2.46 | 0.46 |
| 1:A:434:U:H2' | 1:A:435:C:C6 | 2.50 | 0.46 |
| 1:A:437:U:C2' | 1:A:438:G:H5' | 2.45 | 0.46 |
| 1:A:594:G:C2' | 1:A:595:G:H5' | 2.45 | 0.46 |
| 3:C:64:VAL:HG12 | 3:C:66:VAL:HG23 | 1.96 | 0.46 |
| 4:D:138:TYR:C | 4:D:138:TYR:CD2 | 2.88 | 0.46 |
| 6:F:8:ILE:HD11 | 6:F:79:LEU:HD13 | 1.97 | 0.46 |
| 1:A:1332:A:C2 | 1:A:1333:A:C4 | 3.02 | 0.46 |
| 1:A:1531:A:O5' | 1:A:1531:A:H8 | 1.98 | 0.46 |
| 1:A:157:G:H2' | 1:A:158:G:H8 | 1.81 | 0.46 |
| 1:A:245:C:O2 | 1:A:283:C:N3 | 2.49 | 0.46 |
| 1:A:491:G:C4 | 1:A:492:G:C8 | 3.03 | 0.46 |
| 1:A:559:A:H2' | 1:A:559:A:N3 | 2.29 | 0.46 |
| 1:A:757:U:O2' | 1:A:879:C:H1' | 2.15 | 0.46 |
| 9:I:118:LYS:C | 9:I:120:ARG:H | 2.18 | 0.46 |
| 9:I:71:SER:O | 9:I:74:ILE:HB | 2.16 | 0.46 |
| 10:J:60:ARG:H | 10:J:60:ARG:HG2 | 1.32 | 0.46 |
| 11:K:21:ILE:HD13 | 11:K:94:ALA:CB | 2.45 | 0.46 |
| 12:L:126:LYS:C | 12:L:127:GLU:HG3 | 2.35 | 0.46 |
| 1:A:376:G:OP2 | 16:P:67:THR:HG21 | 2.15 | 0.46 |
| 17:Q:19:VAL:HG23 | 17:Q:44:ALA:HB3 | 1.97 | 0.46 |
| 1:A:1149:C:H2' | 1:A:1150:U:C6 | 2.51 | 0.46 |
| 1:A:1532:U:C2' | 1:A:1533:C:H5'' | 2.44 | 0.46 |
| 1:A:496:A:H4' | 1:A:497:A:OP1 | 2.12 | 0.46 |
| 2:B:164:VAL:HB | 2:B:186:ALA:HB2 | 1.97 | 0.46 |
| 4:D:146:ILE:N | 4:D:146:ILE:CD1 | 2.79 | 0.46 |
| 1:A:689:C:OP2 | 11:K:46:GLY:HA3 | 2.16 | 0.46 |
| 19:S:5:LEU:O | 19:S:6:LYS:HB2 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:A:309:G:H1' | 1:A:608:A:C2 | 2.51 | 0.46 |
| 1:A:437:U:H2' | 1:A:438:G:H5' | 1.96 | 0.46 |
| 1:A:487:A:H2' | 1:A:488:C:O4' | 2.15 | 0.46 |
| 1:A:739:C:HO2' | 15:O:42:HIS:CE1 | 2.27 | 0.46 |
| 8:H:108:GLY:HA3 | 8:H:138:TRP:HB3 | 1.97 | 0.46 |
| 18:R:55:ARG:HB3 | 18:R:55:ARG:NH1 | 2.31 | 0.46 |
| 1:A:1038:C:H2' | 1:A:1039:C:C6 | 2.51 | 0.46 |
| 1:A:1331:G:C2' | 1:A:1332:A:OP2 | 2.64 | 0.46 |
| 1:A:1238:A:H5' | 1:A:1336:C:H41 | 1.81 | 0.46 |
| 1:A:1413:A:H2' | 1:A:1414:U:O4' | 2.16 | 0.46 |
| 1:A:926:G:H3' | 1:A:1505:G:H21 | 1.80 | 0.46 |
| 1:A:321:A:C2 | 1:A:333:G:C2 | 3.03 | 0.46 |
| 1:A:766:A:C8 | 1:A:814:A:C6 | 3.04 | 0.46 |
| 7:G:15:ASP:O | 7:G:19:GLY:HA2 | 2.15 | 0.46 |
| 16:P:4:ILE:O | 16:P:66:PRO:HA | 2.16 | 0.46 |
| 17:Q:59:ILE:HG23 | 17:Q:71:PHE:HD1 | 1.80 | 0.46 |
| 20:T:33:ILE:HD12 | 20:T:63:ILE:HG12 | 1.97 | 0.46 |
| 1:A:1007:C:H2' | 1:A:1008:C:C6 | 2.51 | 0.46 |
| 1:A:114:U:O2' | 1:A:115:G:H5' | 2.16 | 0.46 |
| 1:A:1223:C:P | 19:S:78:ARG:HH12 | 2.39 | 0.46 |
| 1:A:197:A:N6 | 1:A:221:C:H5' | 2.31 | 0.46 |
| 1:A:328:C:H4' | 1:A:329:A:H5'' | 1.98 | 0.46 |
| 1:A:376:G:H2' | 1:A:377:G:C8 | 2.47 | 0.46 |
| 1:A:390:C:O5' | 1:A:390:C:H6 | 1.98 | 0.46 |
| 1:A:474:G:H4' | 16:P:81:ARG:NH2 | 2.30 | 0.46 |
| 1:A:497:A:H4' | 1:A:498:U:OP2 | 2.15 | 0.46 |
| 1:A:820:U:H4' | 1:A:821:G:OP2 | 2.16 | 0.46 |
| 12:L:69:TYR:HE2 | 12:L:71:PRO:HA | 1.81 | 0.46 |
| 15:O:78:TYR:CZ | 15:O:82:ILE:CD1 | 2.98 | 0.46 |
| 20:T:10:LEU:HD13 | 20:T:12:ALA:H | 1.81 | 0.46 |
| 20:T:74:LYS:HZ3 | 20:T:74:LYS:CA | 2.26 | 0.46 |
| 1:A:1165:C:C2' | 1:A:1166:G:H5' | 2.47 | 0.45 |
| 1:A:1251:A:H2' | 1:A:1252:A:O4' | 2.16 | 0.45 |
| 1:A:1518[B]:MA6:C2' | 1:A:1519[B]:MA6:O5' | 2.64 | 0.45 |
| 25:A:1860:SRY:C22 | 25:A:1860:SRY:HI32 | 2.46 | 0.45 |
| 1:A:390:C:H2' | 1:A:391:G:H8 | 1.80 | 0.45 |
| 1:A:646:U:H2' | 1:A:647:C:H6 | 1.80 | 0.45 |
| 1:A:797:C:O2' | 1:A:798:G:H5' | 2.16 | 0.45 |
| 1:A:815:A:O2' | 1:A:1527:C:H1' | 2.15 | 0.45 |
| 1:A:979:C:OP2 | 1:A:980:C:H5 | 1.99 | 0.45 |
| 2:B:46:LYS:CA | 2:B:46:LYS:HE3 | 2.45 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:33:TYR:HE2 | 6:F:74:ASP:HB3 | 1.78 | 0.45 |
| 8:H:11:THR:O | 8:H:14:ARG:N | 2.49 | 0.45 |
| 8:H:94:TYR:HE2 | 8:H:132:GLU:OE1 | 1.99 | 0.45 |
| 10:J:38:ILE:O | 10:J:71:LEU:N | 2.39 | 0.45 |
| 11:K:33:THR:HG22 | 11:K:39:PRO:HA | 1.98 | 0.45 |
| 13:M:45:VAL:HG13 | 13:M:48:LEU:HD12 | 1.98 | 0.45 |
| 13:M:54:VAL:O | 13:M:58:GLU:HB2 | 2.16 | 0.45 |
| 14:N:50:LYS:HB3 | 14:N:50:LYS:HE3 | 1.65 | 0.45 |
| 1:A:1127:G:N2 | 1:A:1145:C:O2 | 2.50 | 0.45 |
| 1:A:1281:U:O3' | 1:A:1282:C:H6 | 1.99 | 0.45 |
| 1:A:1292:U:OP1 | 7:G:41:ARG:NH2 | 2.40 | 0.45 |
| 1:A:975:A:N6 | 1:A:1366:C:O2' | 2.47 | 0.45 |
| 1:A:407:G:C2 | 1:A:436:C:C2 | 3.04 | 0.45 |
| 1:A:556:C:H2' | 1:A:557:G:O4' | 2.16 | 0.45 |
| 1:A:737:A:H2' | 1:A:738:C:H6 | 1.81 | 0.45 |
| 6:F:4:TYR:CZ | 6:F:72:VAL:HG21 | 2.52 | 0.45 |
| 9:I:126:SER:C | 9:I:128:ARG:N | 2.68 | 0.45 |
| 1:A:1122:U:C2' | 1:A:1123:A:H5' | 2.47 | 0.45 |
| 1:A:126:G:H4' | 1:A:634:C:O2 | 2.17 | 0.45 |
| 1:A:664:G:O2' | 1:A:666:G:OP2 | 2.29 | 0.45 |
| 1:A:695:A:H2' | 1:A:696:A:C8 | 2.51 | 0.45 |
| 4:D:148:VAL:CG1 | 4:D:149:ALA:H | 2.29 | 0.45 |
| 4:D:79:PHE:HA | 4:D:93:PHE:CD2 | 2.52 | 0.45 |
| 5:E:57:LYS:HG2 | 5:E:61:TYR:CE2 | 2.51 | 0.45 |
| 6:F:4:TYR:HE1 | 6:F:92:LYS:HG2 | 1.80 | 0.45 |
| 9:I:105:ASP:OD1 | 9:I:107:ARG:HG3 | 2.16 | 0.45 |
| 9:I:16:ARG:HD2 | 9:I:64:THR:HB | 1.97 | 0.45 |
| 17:Q:68:ARG:N | 17:Q:70:ARG:NH1 | 2.64 | 0.45 |
| 1:A:1366:C:O2' | 1:A:1367:C:H5' | 2.16 | 0.45 |
| 1:A:666:G:H5' | 1:A:726:C:H1' | 1.97 | 0.45 |
| 1:A:911:U:H2' | 1:A:912:C:C6 | 2.51 | 0.45 |
| 3:C:15:THR:HG21 | 3:C:179:ARG:HA | 1.99 | 0.45 |
| 3:C:154:SER:CB | 3:C:197:GLY:H | 2.30 | 0.45 |
| 3:C:64:VAL:HB | 3:C:99:VAL:CB | 2.38 | 0.45 |
| 7:G:8:GLU:HG3 | 7:G:8:GLU:H | 1.61 | 0.45 |
| 11:K:43:SER:O | 11:K:44:SER:HB3 | 2.16 | 0.45 |
| 16:P:7:ALA:O | 16:P:17:TYR:HA | 2.17 | 0.45 |
| 20:T:33:ILE:HD13 | 20:T:62:LEU:HB3 | 1.98 | 0.45 |
| 1:A:1120:G:C2 | 1:A:1154:G:N3 | 2.84 | 0.45 |
| 1:A:1256:A:H5' | 1:A:1258:G:C1' | 2.43 | 0.45 |
| 1:A:281:G:C2' | 1:A:282:A:OP2 | 2.64 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:A:782:A:H4' | 1:A:1514:C:O2' | 2.15 | 0.45 |
| 2:B:215:LEU:HD23 | 2:B:215:LEU:HA | 1.69 | 0.45 |
| 9:I:42:ARG:HB2 | 9:I:42:ARG:NH1 | 2.32 | 0.45 |
| 9:I:99:LEU:N | 9:I:99:LEU:HD22 | 2.30 | 0.45 |
| 15:O:36:ILE:HG12 | 15:O:59:MET:HE3 | 1.98 | 0.45 |
| 19:S:13:ASP:O | 19:S:17:GLU:HG2 | 2.17 | 0.45 |
| 1:A:1285:A:O4' | 1:A:1286:A:N7 | 2.50 | 0.45 |
| 1:A:52:G:O2' | 1:A:53:A:H5' | 2.16 | 0.45 |
| 1:A:757:U:H2' | 1:A:758:G:O4' | 2.16 | 0.45 |
| 1:A:897:C:H5' | 17:Q:101:ARG:O | 2.16 | 0.45 |
| 5:E:51:VAL:N | 5:E:52:PRO:HD2 | 2.32 | 0.45 |
| 11:K:51:LYS:O | 11:K:55:LYS:HE2 | 2.17 | 0.45 |
| 1:A:1327:C:OP2 | 21:U:12:LYS:NZ | 2.50 | 0.45 |
| 1:A:1024:G:N7 | 1:A:1025:U:C5 | 2.85 | 0.45 |
| 1:A:1067:A:H4' | 1:A:1068:G:O5' | 2.17 | 0.45 |
| 1:A:1072:G:C5 | 1:A:1073:U:C4 | 3.04 | 0.45 |
| 1:A:949:A:C2 | 1:A:1233:G:N3 | 2.85 | 0.45 |
| 1:A:1287:A:H2' | 1:A:1288:A:C8 | 2.52 | 0.45 |
| 1:A:1337:G:H5'' | 1:A:1338:G:OP1 | 2.17 | 0.45 |
| 1:A:328:C:C1' | 1:A:329:A:OP2 | 2.64 | 0.45 |
| 1:A:382:A:H2' | 1:A:383:A:C8 | 2.51 | 0.45 |
| 1:A:403:C:O2' | 1:A:404:U:H5' | 2.17 | 0.45 |
| 1:A:629:G:H2' | 1:A:630:G:O4' | 2.16 | 0.45 |
| 7:G:43:PHE:O | 7:G:46:ALA:HB3 | 2.16 | 0.45 |
| 8:H:11:THR:O | 8:H:12:ARG:C | 2.55 | 0.45 |
| 14:N:11:LYS:HA | 14:N:11:LYS:HD3 | 1.72 | 0.45 |
| 15:O:26:GLU:OE2 | 15:O:77:ARG:NH1 | 2.50 | 0.45 |
| 20:T:14:LYS:O | 20:T:18:GLN:HG3 | 2.16 | 0.45 |
| 1:A:389:A:C6 | 1:A:390:C:H1' | 2.52 | 0.45 |
| 1:A:446:G:H2' | 1:A:447:G:O4' | 2.16 | 0.45 |
| 3:C:34:LEU:HD21 | 3:C:38:ARG:HH22 | 1.79 | 0.45 |
| 5:E:28:PHE:O | 5:E:47:LYS:HA | 2.16 | 0.45 |
| 6:F:2:ARG:CD | 6:F:69:GLU:HG2 | 2.46 | 0.45 |
| 8:H:88:LYS:O | 8:H:92:ARG:HG2 | 2.15 | 0.45 |
| 9:I:125:TYR:HD2 | 9:I:125:TYR:H | 1.64 | 0.45 |
| 12:L:100:ILE:N | 12:L:100:ILE:HD12 | 2.32 | 0.45 |
| 13:M:37:THR:HG23 | 13:M:55:ARG:CG | 2.47 | 0.45 |
| 1:A:1371:G:OP1 | 9:I:11:LYS:O | 2.34 | 0.45 |
| 1:A:1375:A:H2' | 1:A:1376:U:O4' | 2.16 | 0.45 |
| 25:A:1860:SRY:O13 | 25:A:1860:SRY:HI32 | 2.15 | 0.45 |
| 1:A:577:G:H1' | 1:A:816:A:N3 | 2.32 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:68:G:C2' | 1:A:69:G:O5' | 2.65 | 0.45 |
| 2:B:103:THR:N | 2:B:176:GLU:OE1 | 2.30 | 0.45 |
| 3:C:135:LYS:HE3 | 5:E:50:GLU:HG2 | 1.99 | 0.45 |
| 1:A:376:G:H5'' | 16:P:5:ARG:CD | 2.47 | 0.45 |
| 1:A:477:G:H2' | 1:A:478:A:C8 | 2.51 | 0.45 |
| 1:A:778:G:O2' | 1:A:779:C:H5' | 2.17 | 0.45 |
| 4:D:57:ARG:HB3 | 4:D:206:PHE:HB2 | 1.99 | 0.45 |
| 9:I:48:GLU:N | 9:I:49:PRO:CD | 2.79 | 0.45 |
| 9:I:8:GLY:HA2 | 9:I:79:LEU:HD13 | 1.99 | 0.45 |
| 12:L:34:ARG:O | 12:L:61:THR:HG23 | 2.17 | 0.45 |
| 17:Q:56:VAL:HG21 | 17:Q:81:ARG:HD3 | 1.98 | 0.45 |
| 1:A:1152:A:OP1 | 10:J:68:HIS:ND1 | 2.50 | 0.44 |
| 1:A:1240:U:H3' | 1:A:1241:G:H5' | 1.99 | 0.44 |
| 1:A:1323:G:H2' | 1:A:1324:A:C8 | 2.52 | 0.44 |
| 1:A:519:C:H2' | 1:A:520:A:C8 | 2.52 | 0.44 |
| 1:A:862:C:O2' | 1:A:863:U:H5' | 2.17 | 0.44 |
| 5:E:80:ILE:HD11 | 5:E:138:ALA:HB1 | 1.98 | 0.44 |
| 9:I:127:LYS:O | 9:I:128:ARG:HB2 | 2.16 | 0.44 |
| 10:J:86:MET:HA | 10:J:86:MET:CE | 2.47 | 0.44 |
| 1:A:1428:A:H2' | 1:A:1429:C:C6 | 2.52 | 0.44 |
| 1:A:1508:G:H2' | 1:A:1509:C:O4' | 2.17 | 0.44 |
| 1:A:224:C:O2' | 1:A:225:C:H5' | 2.17 | 0.44 |
| 1:A:369:C:H2' | 1:A:369:C:O2 | 2.17 | 0.44 |
| 1:A:527:7MG:C2' | 1:A:528:C:H5' | 2.47 | 0.44 |
| 1:A:660:G:C2 | 1:A:746:A:C2 | 3.06 | 0.44 |
| 1:A:1104:G:OP1 | 2:B:111:ARG:HD2 | 2.18 | 0.44 |
| 2:B:92:TYR:O | 2:B:151:GLY:HA3 | 2.17 | 0.44 |
| 7:G:5:ARG:CZ | 7:G:7:ALA:HA | 2.48 | 0.44 |
| 8:H:127:LEU:HA | 8:H:127:LEU:HD22 | 1.70 | 0.44 |
| 10:J:90:LEU:N | 10:J:91:PRO:CD | 2.80 | 0.44 |
| 11:K:111:ASP:OD2 | 11:K:111:ASP:O | 2.35 | 0.44 |
| 11:K:84:VAL:HG21 | 11:K:95:ILE:HD11 | 1.98 | 0.44 |
| 12:L:39:VAL:HG23 | 12:L:57:LYS:HB2 | 1.98 | 0.44 |
| 18:R:42:ARG:NH1 | 18:R:42:ARG:HB3 | 2.32 | 0.44 |
| 1:A:1358:U:H3' | 1:A:1359:C:C6 | 2.51 | 0.44 |
| 1:A:1443:G:H5'' | 1:A:1443:G:N3 | 2.33 | 0.44 |
| 1:A:19:C:H2' | 1:A:20:U:H6 | 1.83 | 0.44 |
| 1:A:357:G:O2' | 1:A:358:U:H5' | 2.16 | 0.44 |
| 1:A:782:A:O3' | 1:A:1515[A]:C:H4' | 2.18 | 0.44 |
| 1:A:526:C:OP1 | 1:A:913:A:H3' | 2.16 | 0.44 |
| 3:C:91:LEU:HD23 | 3:C:92:ALA:N | 2.31 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:43:LEU:HD11 | 5:E:132:ALA:HB1 | 1.99 | 0.44 |
| 7:G:102:ARG:O | 7:G:106:GLN:HG3 | 2.16 | 0.44 |
| 7:G:38:LEU:HD12 | 7:G:38:LEU:O | 2.17 | 0.44 |
| 12:L:92:0TD:C | 12:L:92:0TD:OD1 | 2.65 | 0.44 |
| 13:M:37:THR:HG23 | 13:M:55:ARG:CD | 2.46 | 0.44 |
| 15:O:76:GLU:OE1 | 15:O:76:GLU:HA | 2.16 | 0.44 |
| 1:A:1320:C:N3 | 19:S:36:ARG:HD3 | 2.32 | 0.44 |
| 1:A:1077:G:C6 | 1:A:1081:G:C6 | 3.05 | 0.44 |
| 1:A:1064:G:N2 | 1:A:1190:G:C2' | 2.81 | 0.44 |
| 1:A:1477:C:H2' | 1:A:1478:C:H6 | 1.82 | 0.44 |
| 1:A:1505:G:H3' | 1:A:1505:G:C8 | 2.52 | 0.44 |
| 1:A:190(D):U:O2' | 1:A:190(E):U:H5' | 2.18 | 0.44 |
| 1:A:342:C:H2' | 1:A:343:U:H5' | 1.99 | 0.44 |
| 1:A:509:A:H3' | 1:A:509:A:C8 | 2.52 | 0.44 |
| 1:A:631:G:O3' | 1:A:632:A:C8 | 2.69 | 0.44 |
| 3:C:50:ALA:HB1 | 3:C:70:VAL:CG1 | 2.47 | 0.44 |
| 7:G:12:LEU:CD1 | 7:G:12:LEU:H | 2.26 | 0.44 |
| 12:L:28:LYS:HG2 | 12:L:33:ARG:HH12 | 1.82 | 0.44 |
| 15:O:29:VAL:HG12 | 15:O:85:LEU:CD1 | 2.48 | 0.44 |
| 16:P:43:LYS:HA | 16:P:48:TRP:HB3 | 1.99 | 0.44 |
| 6:F:100:ASN:HD21 | 18:R:23:LYS:HG2 | 1.82 | 0.44 |
| 1:A:1054:C:C5 | 1:A:1196:U:C6 | 3.06 | 0.44 |
| 1:A:984:C:N4 | 1:A:1221:G:H1 | 2.15 | 0.44 |
| 1:A:1532:U:H2' | 1:A:1533:C:C5' | 2.46 | 0.44 |
| 1:A:22:G:H2' | 1:A:23:C:H6 | 1.82 | 0.44 |
| 1:A:287:U:O2' | 1:A:288:A:H5' | 2.17 | 0.44 |
| 1:A:401:C:H2' | 1:A:402:G:H8 | 1.82 | 0.44 |
| 1:A:484:G:H1' | 1:A:485:G:OP2 | 2.16 | 0.44 |
| 1:A:505:G:C6 | 1:A:535:A:C2 | 3.06 | 0.44 |
| 1:A:551:U:H2' | 1:A:552:U:C6 | 2.52 | 0.44 |
| 1:A:558:G:H3' | 1:A:559:A:H3' | 1.99 | 0.44 |
| 1:A:651:C:H2' | 1:A:652:U:C6 | 2.52 | 0.44 |
| 1:A:81:U:H3' | 1:A:81:U:H6 | 1.83 | 0.44 |
| 4:D:78:LEU:HA | 4:D:78:LEU:HD23 | 1.45 | 0.44 |
| 6:F:67:MET:HB2 | 6:F:68:PRO:HD2 | 2.00 | 0.44 |
| 7:G:51:GLN:C | 7:G:53:LYS:N | 2.71 | 0.44 |
| 12:L:69:TYR:CE2 | 12:L:71:PRO:HA | 2.53 | 0.44 |
| 13:M:79:LYS:HA | 13:M:82:MET:CE | 2.46 | 0.44 |
| 17:Q:45:HIS:CD2 | 17:Q:47:PRO:HG3 | 2.53 | 0.44 |
| 17:Q:48:GLU:OE1 | 17:Q:50:LYS:HD2 | 2.18 | 0.44 |
| 1:A:1030(C):G:C6 | 1:A:1030(D):A:C6 | 3.06 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1379:G:C6 | 1:A:1380:U:C4 | 3.06 | 0.44 |
| 1:A:1540:PSU:H6 | 1:A:1540:PSU:C3' | 2.06 | 0.44 |
| 1:A:168:G:C2 | 1:A:169:C:C5 | 3.06 | 0.44 |
| 1:A:284:G:H2' | 1:A:285:G:C8 | 2.50 | 0.44 |
| 1:A:452:A:N3 | 16:P:72:ARG:NH1 | 2.66 | 0.44 |
| 1:A:594:G:H2' | 1:A:595:G:H5' | 1.98 | 0.44 |
| 2:B:239:VAL:O | 2:B:240:GLN:CB | 2.64 | 0.44 |
| 3:C:20:SER:HB3 | 3:C:57:ILE:HB | 1.99 | 0.44 |
| 3:C:73:PRO:O | 3:C:76:VAL:HG22 | 2.17 | 0.44 |
| 4:D:149:ALA:HB3 | 4:D:152:SER:HB2 | 1.99 | 0.44 |
| 5:E:31:LEU:HD23 | 5:E:31:LEU:HA | 1.49 | 0.44 |
| 5:E:80:ILE:HD11 | 5:E:138:ALA:CA | 2.47 | 0.44 |
| 7:G:15:ASP:OD1 | 7:G:18:TYR:N | 2.40 | 0.44 |
| 11:K:34:ASP:HB2 | 11:K:35:PRO:HD2 | 2.00 | 0.44 |
| 1:A:1028:C:C5 | 1:A:1029:C:C5 | 3.06 | 0.44 |
| 1:A:1426:C:H2' | 1:A:1427:U:H6 | 1.83 | 0.44 |
| 1:A:221:C:O2' | 1:A:222:U:H5' | 2.17 | 0.44 |
| 1:A:243:A:H4' | 1:A:244:U:H5'' | 2.00 | 0.44 |
| 1:A:316:G:H4' | 27:A:2121:HOH:O | 2.18 | 0.44 |
| 1:A:328:C:O2' | 1:A:329:A:P | 2.75 | 0.44 |
| 1:A:403:C:H2' | 1:A:404:U:H6 | 1.83 | 0.44 |
| 1:A:485:G:O2' | 1:A:486:U:OP2 | 2.32 | 0.44 |
| 2:B:91:PRO:HG3 | 2:B:154:LEU:HB2 | 1.99 | 0.44 |
| 3:C:187:ALA:HB3 | 3:C:198:VAL:HB | 2.00 | 0.44 |
| 3:C:56:ASP:O | 3:C:66:VAL:HA | 2.17 | 0.44 |
| 3:C:70:VAL:HG12 | 3:C:72:LYS:H | 1.83 | 0.44 |
| 5:E:76:ILE:CG2 | 5:E:77:PRO:HD2 | 2.47 | 0.44 |
| 7:G:137:LYS:O | 7:G:141:VAL:HG23 | 2.18 | 0.44 |
| 11:K:124:LYS:HD2 | 11:K:125:PHE:CE2 | 2.53 | 0.44 |
| 15:O:41:GLU:OE1 | 15:O:44:LYS:HD2 | 2.17 | 0.44 |
| 17:Q:60:ILE:HD13 | 17:Q:61:GLU:O | 2.17 | 0.44 |
| 18:R:45:SER:O | 18:R:47:THR:O | 2.36 | 0.44 |
| 1:A:1496:C:H2' | 1:A:1497:G:O4' | 2.17 | 0.44 |
| 1:A:429:U:H1' | 1:A:430:A:H5'' | 1.99 | 0.44 |
| 1:A:564:C:H2' | 1:A:565:U:O4' | 2.18 | 0.44 |
| 1:A:948:C:O2' | 1:A:949:A:H5' | 2.17 | 0.44 |
| 2:B:125:PRO:HG2 | 2:B:126:GLU:OE1 | 2.17 | 0.44 |
| 3:C:134:ILE:CG2 | 3:C:151:VAL:HB | 2.48 | 0.44 |
| 5:E:116:THR:HG22 | 5:E:117:ASP:OD2 | 2.17 | 0.44 |
| 7:G:78:ARG:NH1 | 7:G:156:TRP:HB3 | 2.33 | 0.44 |
| 12:L:68:ALA:HB3 | 12:L:100:ILE:HD11 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 13:M:8:GLU:OE1 | 13:M:23:TYR:N | 2.48 | 0.44 |
| 19:S:13:ASP:HA | 19:S:16:LEU:HB3 | 1.99 | 0.44 |
| 1:A:1271:G:H5' | 1:A:1314:C:OP1 | 2.18 | 0.44 |
| 1:A:1347:G:H2' | 1:A:1373:G:H1 | 1.82 | 0.44 |
| 1:A:564:C:C5 | 17:Q:31:LEU:HD11 | 2.53 | 0.44 |
| 7:G:21:VAL:HG23 | 7:G:22:LEU:N | 2.33 | 0.44 |
| 8:H:10:LEU:HD22 | 8:H:83:ILE:HD11 | 1.99 | 0.44 |
| 9:I:10:ARG:CZ | 9:I:105:ASP:OD2 | 2.66 | 0.44 |
| 10:J:4:ILE:HD12 | 10:J:4:ILE:O | 2.18 | 0.44 |
| 10:J:89:ASP:OD2 | 10:J:91:PRO:HG2 | 2.17 | 0.44 |
| 16:P:9:PHE:N | 16:P:16:HIS:O | 2.49 | 0.44 |
| 1:A:1519[B]:MA6:H5' | 1:A:1520[B]:G:OP2 | 2.17 | 0.43 |
| 1:A:342:C:C2' | 1:A:343:U:H5' | 2.47 | 0.43 |
| 1:A:417:C:H2' | 1:A:418:C:H6 | 1.82 | 0.43 |
| 1:A:522:C:OP2 | 12:L:69:TYR:OH | 2.24 | 0.43 |
| 1:A:789:U:H2' | 1:A:791:G:OP2 | 2.18 | 0.43 |
| 1:A:79:G:C2 | 1:A:91:C:C2 | 3.06 | 0.43 |
| 5:E:12:LEU:HD13 | 5:E:31:LEU:CB | 2.48 | 0.43 |
| 5:E:144:THR:H | 5:E:147:ASP:HB2 | 1.83 | 0.43 |
| 10:J:74:ILE:O | 10:J:74:ILE:HG13 | 2.17 | 0.43 |
| 11:K:21:ILE:HD13 | 11:K:94:ALA:HB1 | 2.00 | 0.43 |
| 13:M:70:LEU:HD23 | 13:M:70:LEU:HA | 1.73 | 0.43 |
| 15:O:85:LEU:HB2 | 15:O:87:ILE:HG13 | 1.99 | 0.43 |
| 16:P:38:TYR:CE2 | 16:P:50:LYS:HB3 | 2.53 | 0.43 |
| 1:A:1402:4OC:H2' | 1:A:1403:C:O4' | 2.18 | 0.43 |
| 1:A:317:G:C6 | 1:A:318:G:N7 | 2.86 | 0.43 |
| 1:A:854:G:C6 | 1:A:855:G:N7 | 2.86 | 0.43 |
| 2:B:239:VAL:O | 2:B:240:GLN:HB3 | 2.17 | 0.43 |
| 3:C:152:ILE:HB | 3:C:199:LYS:HB2 | 1.99 | 0.43 |
| 4:D:188:LEU:HD23 | 4:D:188:LEU:HA | 1.90 | 0.43 |
| 4:D:28:SER:C | 4:D:30:LYS:H | 2.21 | 0.43 |
| 7:G:104:LEU:HA | 7:G:104:LEU:HD23 | 1.81 | 0.43 |
| 8:H:59:LEU:N | 8:H:59:LEU:HD12 | 2.33 | 0.43 |
| 12:L:60:LEU:HB3 | 12:L:62:SER:HB3 | 2.00 | 0.43 |
| 1:A:1450:U:H2' | 1:A:1452:C:C4 | 2.54 | 0.43 |
| 1:A:298:A:H2' | 1:A:299:G:O4' | 2.18 | 0.43 |
| 1:A:1308:U:P | 13:M:99:ARG:HG3 | 2.58 | 0.43 |
| 20:T:87:LYS:HE2 | 20:T:87:LYS:HB2 | 1.80 | 0.43 |
| 1:A:1030(A):G:N2 | 1:A:1030(C):G:O5' | 2.51 | 0.43 |
| 1:A:1190:G:C2' | 1:A:1191:A:OP2 | 2.66 | 0.43 |
| 1:A:1426:C:C2 | 1:A:1427:U:C5 | 3.06 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|---------------------|--------------------------|-------------------|
| 1:A:327:A:O2' | 1:A:328:C:H6 | 2.02 | 0.43 |
| 1:A:420:U:H1' | 1:A:424:G:N2 | 2.34 | 0.43 |
| 1:A:644:G:C5 | 1:A:645:C:C5 | 3.06 | 0.43 |
| 1:A:803:G:C6 | 1:A:804:U:C4 | 3.06 | 0.43 |
| 1:A:838:G:C2' | 1:A:839:U:H5'' | 2.48 | 0.43 |
| 2:B:38:GLY:C | 2:B:39:ILE:HG13 | 2.38 | 0.43 |
| 2:B:73:THR:O | 2:B:73:THR:HG22 | 2.19 | 0.43 |
| 3:C:6:HIS:HE2 | 3:C:8:ILE:HD12 | 1.84 | 0.43 |
| 4:D:80:GLU:O | 4:D:84:LYS:HG3 | 2.18 | 0.43 |
| 8:H:29:SER:OG | 8:H:32:LYS:HG3 | 2.18 | 0.43 |
| 13:M:31:LYS:O | 13:M:35:GLU:HG3 | 2.18 | 0.43 |
| 16:P:58:TYR:O | 16:P:61:SER:N | 2.51 | 0.43 |
| 19:S:12:ASP:H | 19:S:38:SER:HB3 | 1.83 | 0.43 |
| 1:A:532:A:N6 | 3:C:193:TYR:HA | 2.33 | 0.43 |
| 1:A:781:A:C5 | 1:A:802:A:C2 | 3.07 | 0.43 |
| 2:B:208:ILE:HD13 | 2:B:208:ILE:N | 2.33 | 0.43 |
| 3:C:34:LEU:HD21 | 3:C:38:ARG:CZ | 2.49 | 0.43 |
| 6:F:14:LEU:HD21 | 6:F:84:ASN:OD1 | 2.18 | 0.43 |
| 10:J:24:VAL:HG13 | 10:J:34:VAL:HG11 | 2.00 | 0.43 |
| 1:A:1229:A:P | 13:M:114:ARG:HD3 | 2.59 | 0.43 |
| 1:A:1106:G:O2' | 1:A:1107:C:H5' | 2.18 | 0.43 |
| 1:A:1190:G:OP1 | 3:C:4:LYS:HA | 2.17 | 0.43 |
| 1:A:181:G:H4' | 1:A:182:U:OP2 | 2.17 | 0.43 |
| 1:A:185:A:N3 | 20:T:81:LYS:NZ | 2.59 | 0.43 |
| 1:A:321:A:H2' | 1:A:322:C:C6 | 2.53 | 0.43 |
| 1:A:977:A:C2' | 1:A:978:A:H5'' | 2.49 | 0.43 |
| 13:M:74:VAL:O | 13:M:77:ASN:N | 2.52 | 0.43 |
| 15:O:17:ARG:CG | 15:O:17:ARG:NH1 | 2.77 | 0.43 |
| 1:A:1262:C:H2' | 1:A:1263:C:C6 | 2.53 | 0.43 |
| 1:A:1347:G:C6 | 9:I:107:ARG:NH2 | 2.87 | 0.43 |
| 1:A:1406:U:C4' | 1:A:1518[B]:MA6:H1' | 2.48 | 0.43 |
| 13:M:34:LEU:HD13 | 13:M:41:PRO:CA | 2.48 | 0.43 |
| 17:Q:75:ARG:HG3 | 17:Q:75:ARG:HH11 | 1.84 | 0.43 |
| 17:Q:76:LEU:HD12 | 17:Q:76:LEU:C | 2.39 | 0.43 |
| 1:A:1004:A:N7 | 1:A:1036:G:O6 | 2.52 | 0.43 |
| 1:A:1221:G:C4 | 1:A:1222:G:C8 | 3.06 | 0.43 |
| 1:A:1223:C:P | 19:S:78:ARG:NH1 | 2.92 | 0.43 |
| 1:A:190(C):C:H2' | 1:A:190(D):U:O4' | 2.19 | 0.43 |
| 1:A:353:A:C2' | 1:A:354:G:OP2 | 2.67 | 0.43 |
| 1:A:373:A:C2' | 1:A:374:A:O5' | 2.66 | 0.43 |
| 1:A:377:G:C2 | 1:A:387:U:O2 | 2.72 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:B:135:GLN:O | 2:B:139:LYS:HB2 | 2.19 | 0.43 |
| 9:I:102:LEU:H | 9:I:102:LEU:HD12 | 1.84 | 0.43 |
| 9:I:55:ALA:C | 9:I:56:LEU:HD23 | 2.37 | 0.43 |
| 13:M:10:PRO:CB | 13:M:18:ALA:HB1 | 2.42 | 0.43 |
| 18:R:82:THR:HG23 | 18:R:83:GLU:N | 2.34 | 0.43 |
| 19:S:27:GLU:OE1 | 19:S:27:GLU:N | 2.52 | 0.43 |
| 1:A:1127:G:O2' | 9:I:16:ARG:NH2 | 2.44 | 0.43 |
| 1:A:1055:A:N7 | 1:A:1200:C:N4 | 2.66 | 0.43 |
| 1:A:1347:G:H1' | 1:A:1348:U:H5 | 1.82 | 0.43 |
| 1:A:1497:G:HO2' | 1:A:1518[A]:MA6:C2 | 2.31 | 0.43 |
| 1:A:427:U:H3' | 1:A:428:G:H2' | 2.00 | 0.43 |
| 1:A:600:C:H2' | 1:A:601:C:H6 | 1.83 | 0.43 |
| 1:A:659:U:O2' | 1:A:660:G:H5' | 2.18 | 0.43 |
| 1:A:895:G:H2' | 1:A:896:C:H6 | 1.84 | 0.43 |
| 5:E:12:LEU:C | 5:E:12:LEU:CD2 | 2.87 | 0.43 |
| 8:H:116:LYS:HD3 | 8:H:116:LYS:HA | 1.88 | 0.43 |
| 10:J:39:PRO:HB3 | 10:J:70:ARG:HH11 | 1.79 | 0.43 |
| 12:L:126:LYS:HD2 | 12:L:126:LYS:N | 2.34 | 0.43 |
| 14:N:7:ILE:C | 14:N:9:LYS:N | 2.72 | 0.43 |
| 19:S:19:VAL:HG13 | 19:S:20:LEU:N | 2.34 | 0.43 |
| 1:A:1206:G:C4 | 1:A:1207:2MG:C8 | 3.07 | 0.43 |
| 1:A:201:C:H42 | 1:A:216:G:H1 | 1.67 | 0.43 |
| 2:B:100:GLY:O | 2:B:104:ASN:N | 2.51 | 0.43 |
| 2:B:28:PHE:CD2 | 2:B:190:THR:HA | 2.54 | 0.43 |
| 2:B:187:LEU:HA | 2:B:201:ILE:HB | 2.01 | 0.43 |
| 2:B:92:TYR:CD1 | 2:B:151:GLY:HA3 | 2.54 | 0.43 |
| 7:G:114:ARG:O | 7:G:119:ARG:NH1 | 2.51 | 0.43 |
| 7:G:51:GLN:C | 7:G:53:LYS:H | 2.22 | 0.43 |
| 12:L:60:LEU:HB3 | 12:L:62:SER:H | 1.83 | 0.43 |
| 16:P:2:VAL:HG13 | 16:P:64:ALA:HA | 2.01 | 0.43 |
| 16:P:41:PRO:O | 16:P:43:LYS:HD2 | 2.19 | 0.43 |
| 20:T:91:LEU:HD23 | 20:T:91:LEU:HA | 1.70 | 0.43 |
| 1:A:101:A:O2' | 1:A:102:G:H5' | 2.18 | 0.42 |
| 1:A:1299:A:C5 | 1:A:1301:U:O2 | 2.72 | 0.42 |
| 1:A:1497:G:C3' | 1:A:1498:UR3:H5' | 2.48 | 0.42 |
| 1:A:181:G:H4' | 1:A:182:U:H5' | 2.01 | 0.42 |
| 25:A:1860:SRY:OG2 | 12:L:91:LYS:NZ | 2.33 | 0.42 |
| 1:A:22:G:C6 | 1:A:23:C:C4 | 3.07 | 0.42 |
| 1:A:123:C:OP1 | 1:A:312:C:H5' | 2.19 | 0.42 |
| 1:A:327:A:HO2' | 1:A:328:C:H6 | 1.66 | 0.42 |
| 1:A:622:A:C8 | 1:A:623:C:C6 | 3.07 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:132:LYS:HD3 | 2:B:135:GLN:HB2 | 2.01 | 0.42 |
| 4:D:142:PRO:HA | 4:D:185:PHE:HD2 | 1.84 | 0.42 |
| 1:A:1346:A:C4 | 7:G:10:ARG:NH2 | 2.87 | 0.42 |
| 9:I:112:LYS:NZ | 9:I:113:LYS:O | 2.52 | 0.42 |
| 12:L:27:LEU:HG | 12:L:28:LYS:H | 1.84 | 0.42 |
| 1:A:530:G:N7 | 23:W:34:G:N2 | 2.66 | 0.42 |
| 1:A:1054:C:HO2' | 1:A:1055:A:P | 2.40 | 0.42 |
| 1:A:1080:A:H5'' | 5:E:16:THR:HG21 | 2.01 | 0.42 |
| 1:A:1300:G:C5 | 1:A:1335:C:C5 | 3.07 | 0.42 |
| 1:A:1347:G:HO2' | 1:A:1348:U:H6 | 1.62 | 0.42 |
| 1:A:1389:C:H2' | 1:A:1390:U:O4' | 2.18 | 0.42 |
| 1:A:285:G:O2' | 1:A:286:G:H5' | 2.19 | 0.42 |
| 1:A:392:G:C2 | 1:A:393:A:C4 | 3.06 | 0.42 |
| 1:A:436:C:H2' | 1:A:437:U:C6 | 2.54 | 0.42 |
| 1:A:779:C:H2' | 1:A:780:A:O4' | 2.19 | 0.42 |
| 1:A:12:U:O2' | 1:A:914:A:OP1 | 2.31 | 0.42 |
| 2:B:47:THR:HG23 | 2:B:202:PRO:O | 2.19 | 0.42 |
| 3:C:84:ILE:HG13 | 3:C:88:ARG:NH1 | 2.35 | 0.42 |
| 6:F:97:PHE:HB2 | 18:R:32:ARG:HH11 | 1.75 | 0.42 |
| 8:H:104:ARG:O | 8:H:106:GLY:N | 2.51 | 0.42 |
| 12:L:27:LEU:C | 12:L:29:GLY:H | 2.20 | 0.42 |
| 17:Q:100:LYS:O | 17:Q:101:ARG:C | 2.56 | 0.42 |
| 19:S:36:ARG:NH2 | 19:S:53:ASN:HA | 2.34 | 0.42 |
| 1:A:1189:C:H5'' | 3:C:5:ILE:HG12 | 2.00 | 0.42 |
| 1:A:1368:G:OP2 | 9:I:114:TYR:N | 2.52 | 0.42 |
| 1:A:67:C:O2' | 1:A:171:A:H1' | 2.19 | 0.42 |
| 1:A:321:A:H2' | 1:A:322:C:H6 | 1.83 | 0.42 |
| 3:C:154:SER:OG | 3:C:197:GLY:N | 2.42 | 0.42 |
| 7:G:135:VAL:O | 7:G:139:GLU:HG3 | 2.19 | 0.42 |
| 7:G:41:ARG:O | 7:G:42:ILE:C | 2.58 | 0.42 |
| 9:I:48:GLU:OE1 | 9:I:48:GLU:HA | 2.19 | 0.42 |
| 9:I:8:GLY:HA3 | 9:I:79:LEU:HB3 | 2.01 | 0.42 |
| 1:A:1321:C:C5' | 13:M:87:TYR:HE2 | 2.31 | 0.42 |
| 1:A:1400:5MC:H3' | 1:A:1401:G:C5' | 2.48 | 0.42 |
| 1:A:1406:U:C5 | 1:A:1407:5MC:HM52 | 2.55 | 0.42 |
| 1:A:1417:G:H1' | 1:A:1483:A:N6 | 2.34 | 0.42 |
| 1:A:260:G:H2' | 1:A:261:U:C6 | 2.54 | 0.42 |
| 1:A:273:A:N6 | 1:A:274:A:N6 | 2.68 | 0.42 |
| 1:A:338:A:C6 | 1:A:339:C:C4 | 3.07 | 0.42 |
| 1:A:625:G:H2' | 1:A:626:U:C6 | 2.55 | 0.42 |
| 1:A:693:G:C6 | 1:A:694:A:C5 | 3.07 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:767:A:H2' | 1:A:768:A:O4' | 2.19 | 0.42 |
| 1:A:890:G:O2' | 1:A:906:G:O6 | 2.30 | 0.42 |
| 1:A:993:G:N3 | 1:A:993:G:H2' | 2.35 | 0.42 |
| 2:B:69:LEU:HD12 | 2:B:155:LEU:HD11 | 2.01 | 0.42 |
| 2:B:93:VAL:HG11 | 2:B:97:TRP:HD1 | 1.84 | 0.42 |
| 3:C:127:ARG:HH22 | 3:C:191:THR:HB | 1.83 | 0.42 |
| 3:C:189:ALA:HB3 | 3:C:196:LEU:HB2 | 2.00 | 0.42 |
| 4:D:153:ARG:HG2 | 4:D:181:MET:SD | 2.60 | 0.42 |
| 17:Q:27:PHE:O | 17:Q:36:ILE:HD13 | 2.18 | 0.42 |
| 6:F:91:VAL:HG13 | 18:R:72:ARG:NH2 | 2.33 | 0.42 |
| 1:A:1003(A):G:C6 | 1:A:1004:A:N3 | 2.87 | 0.42 |
| 1:A:1015:A:H2' | 1:A:1016:A:O4' | 2.18 | 0.42 |
| 1:A:1060:C:C5 | 3:C:2:GLY:HA2 | 2.54 | 0.42 |
| 1:A:10:A:HO2' | 1:A:507:C:HO2' | 1.63 | 0.42 |
| 1:A:1500:A:OP1 | 27:A:1927:HOH:O | 2.22 | 0.42 |
| 1:A:919:A:O2' | 1:A:920:U:H5' | 2.20 | 0.42 |
| 3:C:39:ILE:O | 3:C:43:LEU:HD23 | 2.19 | 0.42 |
| 5:E:43:LEU:HD23 | 5:E:43:LEU:HA | 1.82 | 0.42 |
| 9:I:17:VAL:HG11 | 9:I:81:ILE:HA | 2.00 | 0.42 |
| 10:J:82:ILE:O | 10:J:82:ILE:HG22 | 2.18 | 0.42 |
| 13:M:49:THR:HB | 13:M:52:GLU:OE1 | 2.18 | 0.42 |
| 1:A:1090:U:O2' | 1:A:1091:U:H5' | 2.20 | 0.42 |
| 1:A:232:G:H1' | 1:A:262:A:N1 | 2.35 | 0.42 |
| 2:B:100:GLY:HA3 | 2:B:104:ASN:HB2 | 2.01 | 0.42 |
| 3:C:40:ARG:O | 3:C:44:GLU:HG3 | 2.19 | 0.42 |
| 5:E:112:LEU:HA | 5:E:112:LEU:HD23 | 1.76 | 0.42 |
| 5:E:24:ARG:HH11 | 5:E:24:ARG:CB | 2.31 | 0.42 |
| 9:I:102:LEU:HD12 | 9:I:102:LEU:N | 2.34 | 0.42 |
| 9:I:100:GLY:O | 9:I:103:THR:HB | 2.20 | 0.42 |
| 10:J:54:PHE:HD2 | 10:J:55:LYS:HG2 | 1.84 | 0.42 |
| 11:K:57:THR:HG23 | 11:K:58:PRO:HD2 | 2.02 | 0.42 |
| 14:N:14:PRO:O | 14:N:15:LYS:HB3 | 2.20 | 0.42 |
| 15:O:27:VAL:O | 15:O:31:LEU:HD13 | 2.19 | 0.42 |
| 1:A:1094:G:O5' | 1:A:1095:U:H5 | 2.03 | 0.42 |
| 1:A:1216:G:H5'' | 14:N:5:ALA:HB2 | 2.00 | 0.42 |
| 1:A:575:G:O2' | 1:A:821:G:H5' | 2.20 | 0.42 |
| 1:A:948:C:OP2 | 13:M:108:ARG:HB2 | 2.19 | 0.42 |
| 2:B:158:LEU:N | 2:B:158:LEU:HD12 | 2.33 | 0.42 |
| 6:F:10:LEU:HD11 | 6:F:59:TYR:HD2 | 1.83 | 0.42 |
| 11:K:69:ALA:HB1 | 11:K:103:LEU:HD12 | 2.02 | 0.42 |
| 10:J:62:HIS:O | 14:N:59:ALA:HB3 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 19:S:22:LEU:HA | 19:S:22:LEU:HD23 | 1.90 | 0.42 |
| 1:A:1498:UR3:OP2 | 1:A:1542:U:O2' | 2.32 | 0.42 |
| 25:A:1860:SRV:H22 | 25:A:1860:SRV:HI32 | 2.01 | 0.42 |
| 5:E:11:ILE:HG22 | 5:E:12:LEU:N | 2.35 | 0.42 |
| 5:E:43:LEU:HD22 | 5:E:44:GLY:N | 2.35 | 0.42 |
| 8:H:13:ILE:O | 8:H:17:THR:HG23 | 2.19 | 0.42 |
| 11:K:114:VAL:HG22 | 11:K:115:PRO:O | 2.20 | 0.42 |
| 13:M:64:TRP:HB2 | 13:M:66:LEU:HD21 | 2.02 | 0.42 |
| 15:O:45:VAL:HB | 15:O:46:HIS:CD2 | 2.55 | 0.42 |
| 16:P:52:ASP:OD1 | 16:P:52:ASP:C | 2.58 | 0.42 |
| 17:Q:59:ILE:HD12 | 17:Q:73:VAL:HA | 2.02 | 0.42 |
| 18:R:31:LEU:HD23 | 18:R:31:LEU:HA | 1.91 | 0.42 |
| 1:A:1077:G:N2 | 1:A:1080:A:OP2 | 2.51 | 0.42 |
| 1:A:1240:U:H3' | 1:A:1241:G:C5' | 2.50 | 0.42 |
| 1:A:1488:G:H2' | 1:A:1489:G:H8 | 1.83 | 0.42 |
| 1:A:190(L):U:C2 | 20:T:105:SER:HB2 | 2.54 | 0.42 |
| 1:A:28:G:H2' | 1:A:29:G:O4' | 2.20 | 0.42 |
| 3:C:114:PRO:O | 3:C:118:GLN:HG3 | 2.20 | 0.42 |
| 5:E:105:VAL:N | 5:E:106:PRO:HD2 | 2.35 | 0.42 |
| 5:E:145:LYS:HE3 | 8:H:107:LEU:HD23 | 2.01 | 0.42 |
| 8:H:1:MET:HG3 | 8:H:2:LEU:O | 2.19 | 0.42 |
| 16:P:38:TYR:CE2 | 16:P:50:LYS:HE2 | 2.55 | 0.42 |
| 17:Q:34:LYS:CG | 17:Q:35:VAL:N | 2.83 | 0.42 |
| 1:A:1516[B]:G:C4 | 1:A:1518[B]:MA6:OP2 | 2.72 | 0.42 |
| 1:A:327:A:O2' | 1:A:328:C:O4' | 2.38 | 0.42 |
| 1:A:552:U:O2' | 1:A:553:A:H5' | 2.19 | 0.42 |
| 1:A:981:U:H2' | 1:A:982:U:C5 | 2.55 | 0.42 |
| 3:C:58:GLU:HB2 | 3:C:65:ALA:HB2 | 2.02 | 0.42 |
| 4:D:140:VAL:CG1 | 4:D:146:ILE:HD11 | 2.50 | 0.42 |
| 10:J:28:ARG:HA | 10:J:34:VAL:HG21 | 2.02 | 0.42 |
| 14:N:4:LYS:N | 14:N:4:LYS:HD2 | 2.34 | 0.42 |
| 15:O:21:ASP:OD2 | 15:O:24:SER:HB3 | 2.20 | 0.42 |
| 1:A:1167:A:C6 | 1:A:1168:A:C6 | 3.07 | 0.41 |
| 1:A:243:A:N6 | 1:A:281:G:H1' | 2.35 | 0.41 |
| 1:A:922:G:H4' | 5:E:19:MET:O | 2.19 | 0.41 |
| 1:A:944:G:H5'' | 1:A:945:G:OP2 | 2.20 | 0.41 |
| 1:A:967:5MC:H5'' | 1:A:968:A:OP2 | 2.19 | 0.41 |
| 2:B:73:THR:HG23 | 2:B:95:GLN:O | 2.20 | 0.41 |
| 8:H:82:HIS:C | 8:H:82:HIS:CD2 | 2.93 | 0.41 |
| 1:A:581:G:O3' | 15:O:64:ARG:NH2 | 2.53 | 0.41 |
| 1:A:130:A:C8 | 17:Q:63:ARG:HG3 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:991:U:O4 | 1:A:1212:U:H1' | 2.19 | 0.41 |
| 1:A:1228:C:O2' | 13:M:117:VAL:HG22 | 2.19 | 0.41 |
| 1:A:1281:U:H5'' | 1:A:1282:C:H5 | 1.85 | 0.41 |
| 1:A:22:G:H2' | 1:A:23:C:C6 | 2.55 | 0.41 |
| 1:A:364:A:H61 | 12:L:28:LYS:HE2 | 1.84 | 0.41 |
| 1:A:413:G:O2' | 1:A:428:G:N2 | 2.53 | 0.41 |
| 1:A:485:G:HO2' | 1:A:486:U:P | 2.41 | 0.41 |
| 1:A:510:A:H5'' | 1:A:511:C:P | 2.60 | 0.41 |
| 1:A:542:G:O2' | 1:A:543:C:H5' | 2.20 | 0.41 |
| 1:A:556:C:H2' | 1:A:557:G:C5' | 2.49 | 0.41 |
| 1:A:688:G:H2' | 1:A:689:C:C6 | 2.53 | 0.41 |
| 1:A:991:U:HO2' | 1:A:992:U:P | 2.43 | 0.41 |
| 3:C:15:THR:O | 3:C:16:ARG:HB2 | 2.19 | 0.41 |
| 10:J:7:LYS:HE3 | 10:J:40:LEU:CD1 | 2.50 | 0.41 |
| 17:Q:29:HIS:HE1 | 17:Q:31:LEU:HB3 | 1.85 | 0.41 |
| 1:A:1315:U:H2' | 1:A:1316:G:O4' | 2.21 | 0.41 |
| 1:A:1432:G:O5' | 1:A:1432:G:H8 | 2.02 | 0.41 |
| 1:A:926:G:C6 | 1:A:1505:G:C5 | 3.09 | 0.41 |
| 1:A:1539:C:OP1 | 1:A:1540:PSU:OP2 | 2.38 | 0.41 |
| 1:A:302:G:O2' | 1:A:556:C:H5'' | 2.21 | 0.41 |
| 1:A:597:G:H2' | 1:A:598:U:H5' | 2.03 | 0.41 |
| 1:A:645:C:H2' | 1:A:646:U:C6 | 2.55 | 0.41 |
| 1:A:781:A:H5' | 1:A:782:A:OP2 | 2.21 | 0.41 |
| 2:B:61:LEU:HD21 | 2:B:160:ASP:HB3 | 2.02 | 0.41 |
| 3:C:115:LEU:HA | 3:C:115:LEU:HD23 | 1.82 | 0.41 |
| 6:F:44:GLY:HA2 | 6:F:59:TYR:CZ | 2.55 | 0.41 |
| 7:G:26:PHE:CE2 | 7:G:30:ILE:HD11 | 2.55 | 0.41 |
| 8:H:104:ARG:NH2 | 8:H:138:TRP:CH2 | 2.88 | 0.41 |
| 13:M:36:LYS:HD2 | 13:M:59:TYR:OH | 2.20 | 0.41 |
| 14:N:24:CYS:O | 14:N:28:GLY:HA2 | 2.20 | 0.41 |
| 20:T:10:LEU:HD12 | 20:T:12:ALA:H | 1.83 | 0.41 |
| 1:A:1124:G:H2' | 1:A:1145:C:C5 | 2.55 | 0.41 |
| 1:A:1130:A:OP1 | 1:A:1131:G:P | 2.78 | 0.41 |
| 1:A:115:G:H1' | 1:A:116:A:N7 | 2.35 | 0.41 |
| 1:A:1502:A:C2' | 1:A:1502:A:N3 | 2.83 | 0.41 |
| 1:A:462:G:C6 | 1:A:463:A:C5 | 3.08 | 0.41 |
| 1:A:636:U:H2' | 1:A:637:G:C8 | 2.56 | 0.41 |
| 2:B:83:MET:HA | 2:B:86:GLU:HB2 | 2.03 | 0.41 |
| 3:C:180:ALA:HB1 | 3:C:182:ILE:CG1 | 2.48 | 0.41 |
| 6:F:11:ASN:OD1 | 6:F:13:ASN:N | 2.45 | 0.41 |
| 9:I:44:VAL:HG12 | 9:I:51:ARG:HH22 | 1.86 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 16:P:15:PRO:HG2 | 16:P:41:PRO:HG2 | 2.03 | 0.41 |
| 20:T:50:GLU:CB | 20:T:99:LEU:HD12 | 2.41 | 0.41 |
| 1:A:1026:G:C6 | 1:A:1027:C:N4 | 2.89 | 0.41 |
| 1:A:1107:C:C4 | 1:A:1108:G:C8 | 3.08 | 0.41 |
| 1:A:1494:G:O2' | 1:A:1495:U:H5' | 2.20 | 0.41 |
| 1:A:397:A:C6 | 1:A:548:G:C8 | 3.08 | 0.41 |
| 1:A:662:G:H2' | 1:A:663:A:C8 | 2.55 | 0.41 |
| 1:A:867:G:O2' | 1:A:868:C:H5' | 2.20 | 0.41 |
| 5:E:69:VAL:HA | 5:E:70:PRO:HD3 | 1.77 | 0.41 |
| 8:H:30:ARG:O | 8:H:33:GLU:HB3 | 2.21 | 0.41 |
| 9:I:17:VAL:CG2 | 9:I:80:GLY:HA3 | 2.50 | 0.41 |
| 13:M:67:GLU:HB3 | 13:M:68:GLY:H | 1.52 | 0.41 |
| 15:O:32:LEU:HD23 | 15:O:32:LEU:HA | 1.76 | 0.41 |
| 17:Q:98:LEU:HG | 17:Q:98:LEU:H | 1.79 | 0.41 |
| 1:A:1035:A:C4 | 1:A:1036:G:N7 | 2.88 | 0.41 |
| 1:A:1287:A:C6 | 1:A:1288:A:C6 | 3.09 | 0.41 |
| 1:A:1288:A:C6 | 1:A:1289:A:C5 | 3.09 | 0.41 |
| 1:A:1288:A:C6 | 1:A:1289:A:C6 | 3.09 | 0.41 |
| 1:A:1347:G:O2' | 1:A:1348:U:O5' | 2.37 | 0.41 |
| 1:A:1406:U:C6 | 1:A:1407:5MC:HM52 | 2.56 | 0.41 |
| 1:A:556:C:H2' | 1:A:557:G:H5' | 2.02 | 0.41 |
| 2:B:191:ASP:N | 2:B:191:ASP:OD1 | 2.52 | 0.41 |
| 2:B:230:VAL:HG12 | 2:B:231:GLU:O | 2.20 | 0.41 |
| 5:E:11:ILE:HA | 5:E:11:ILE:HD13 | 1.69 | 0.41 |
| 11:K:33:THR:HB | 11:K:38:ASN:O | 2.20 | 0.41 |
| 16:P:70:ALA:O | 16:P:74:LEU:HG | 2.20 | 0.41 |
| 19:S:18:LYS:HE3 | 19:S:18:LYS:HB2 | 1.87 | 0.41 |
| 1:A:1090:U:H2' | 1:A:1091:U:H6 | 1.85 | 0.41 |
| 1:A:1064:G:N2 | 1:A:1190:G:H2' | 2.36 | 0.41 |
| 1:A:1342:C:H2' | 1:A:1343:G:H8 | 1.84 | 0.41 |
| 1:A:1426:C:H2' | 1:A:1427:U:C6 | 2.55 | 0.41 |
| 1:A:1494:G:C2' | 1:A:1495:U:H5' | 2.51 | 0.41 |
| 1:A:415:A:H2' | 1:A:416:G:C8 | 2.56 | 0.41 |
| 1:A:575:G:C8 | 1:A:881:G:N2 | 2.88 | 0.41 |
| 1:A:939:G:C6 | 1:A:940:C:N4 | 2.88 | 0.41 |
| 1:A:973:G:C2' | 1:A:974:A:OP1 | 2.69 | 0.41 |
| 2:B:236:TYR:O | 2:B:239:VAL:HG23 | 2.20 | 0.41 |
| 4:D:61:LYS:NZ | 4:D:72:GLU:OE2 | 2.53 | 0.41 |
| 5:E:78:HIS:CE1 | 8:H:104:ARG:HH21 | 2.37 | 0.41 |
| 6:F:9:VAL:HG22 | 6:F:60:PHE:CE2 | 2.56 | 0.41 |
| 13:M:59:TYR:CD1 | 13:M:63:THR:HG21 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 13:M:86:CYS:SG | 13:M:87:TYR:N | 2.94 | 0.41 |
| 15:O:2:PRO:HB2 | 15:O:3:ILE:H | 1.76 | 0.41 |
| 16:P:65:GLN:HA | 16:P:66:PRO:HD3 | 1.80 | 0.41 |
| 16:P:74:LEU:HD22 | 16:P:79:VAL:HG21 | 2.02 | 0.41 |
| 1:A:1028:C:C6 | 1:A:1029:C:C5 | 3.09 | 0.41 |
| 1:A:1179:A:H2' | 1:A:1180:A:O5' | 2.20 | 0.41 |
| 1:A:1218:C:H2' | 1:A:1219:U:C6 | 2.55 | 0.41 |
| 1:A:190(J):U:H2' | 1:A:190(K):G:C8 | 2.56 | 0.41 |
| 1:A:564:C:C6 | 17:Q:31:LEU:HD11 | 2.56 | 0.41 |
| 1:A:904:C:C2' | 1:A:905:U:H5' | 2.51 | 0.41 |
| 1:A:978:A:C6 | 1:A:1318:A:C6 | 3.09 | 0.41 |
| 2:B:130:ARG:HA | 2:B:130:ARG:HD3 | 1.63 | 0.41 |
| 2:B:149:LEU:O | 2:B:153:ARG:HB3 | 2.20 | 0.41 |
| 2:B:90:MET:HA | 2:B:91:PRO:HD3 | 1.85 | 0.41 |
| 4:D:140:VAL:HG11 | 4:D:146:ILE:HD11 | 2.01 | 0.41 |
| 6:F:27:GLN:O | 6:F:31:GLU:HG3 | 2.20 | 0.41 |
| 6:F:40:VAL:HG23 | 6:F:62:TRP:O | 2.21 | 0.41 |
| 1:A:825:G:N2 | 8:H:11:THR:HG21 | 2.33 | 0.41 |
| 8:H:82:HIS:ND1 | 8:H:138:TRP:CE2 | 2.88 | 0.41 |
| 1:A:1002:G:C6 | 1:A:1003:G:C6 | 3.09 | 0.41 |
| 1:A:1004:A:C6 | 1:A:1037:C:N4 | 2.88 | 0.41 |
| 1:A:1241:G:H2' | 1:A:1242:C:H6 | 1.85 | 0.41 |
| 1:A:1399:C:O2 | 1:A:1401:G:N7 | 2.54 | 0.41 |
| 1:A:149:A:O2' | 1:A:150:C:H5' | 2.21 | 0.41 |
| 1:A:692:U:H2' | 1:A:694:A:OP2 | 2.20 | 0.41 |
| 1:A:791:G:C6 | 1:A:792:A:N7 | 2.89 | 0.41 |
| 1:A:812:C:H1' | 1:A:813:U:OP2 | 2.21 | 0.41 |
| 1:A:98:U:O2' | 1:A:99:C:H5' | 2.21 | 0.41 |
| 2:B:180:LEU:HD23 | 2:B:180:LEU:HA | 1.91 | 0.41 |
| 4:D:50:ARG:HA | 4:D:51:PRO:HD3 | 1.81 | 0.41 |
| 4:D:52:SER:O | 4:D:55:ALA:HB3 | 2.21 | 0.41 |
| 8:H:114:THR:OG1 | 8:H:116:LYS:N | 2.51 | 0.41 |
| 18:R:45:SER:HB2 | 18:R:46:GLU:OE2 | 2.21 | 0.41 |
| 19:S:31:ILE:HG23 | 19:S:32:LYS:N | 2.35 | 0.41 |
| 1:A:37:U:H2' | 1:A:38:G:O4' | 2.20 | 0.41 |
| 1:A:392:G:C6 | 1:A:393:A:C5 | 3.09 | 0.41 |
| 1:A:504:C:C2 | 1:A:542:G:N2 | 2.89 | 0.41 |
| 2:B:124:SER:HB2 | 2:B:125:PRO:CD | 2.45 | 0.41 |
| 2:B:167:PRO:HG2 | 2:B:192:SER:HB3 | 2.03 | 0.41 |
| 2:B:231:GLU:HB3 | 2:B:232:PRO:HD2 | 2.02 | 0.41 |
| 2:B:238:LEU:HD23 | 2:B:238:LEU:HA | 1.89 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|--------------------|--------------------------|-------------------|
| 3:C:152:ILE:HD12 | 3:C:152:ILE:N | 2.36 | 0.41 |
| 3:C:150:LYS:CG | 3:C:169:ALA:HB2 | 2.40 | 0.41 |
| 4:D:63:LYS:O | 4:D:67:ILE:HG13 | 2.21 | 0.41 |
| 5:E:80:ILE:HD11 | 5:E:138:ALA:HA | 2.02 | 0.41 |
| 1:A:738:C:OP1 | 6:F:92:LYS:HD3 | 2.21 | 0.41 |
| 12:L:76:ASN:O | 12:L:76:ASN:CG | 2.59 | 0.41 |
| 16:P:21:VAL:HG11 | 16:P:59:TRP:CD2 | 2.56 | 0.41 |
| 17:Q:59:ILE:CG2 | 17:Q:71:PHE:CD1 | 3.03 | 0.41 |
| 1:A:192:U:O4' | 20:T:103:GLY:HA2 | 2.21 | 0.41 |
| 1:A:1137:C:OP2 | 1:A:1137:C:H6 | 2.04 | 0.41 |
| 1:A:1408:A:H2' | 1:A:1409:C:C6 | 2.55 | 0.41 |
| 1:A:166:G:H2' | 1:A:167:G:H8 | 1.86 | 0.41 |
| 1:A:216:G:O2' | 1:A:217:C:C5' | 2.68 | 0.41 |
| 1:A:514:C:H2' | 1:A:515:G:H8 | 1.85 | 0.41 |
| 1:A:567:G:H2' | 1:A:568:G:O4' | 2.21 | 0.41 |
| 1:A:645:C:H2' | 1:A:646:U:O4' | 2.21 | 0.41 |
| 1:A:658:G:H2' | 1:A:659:U:C6 | 2.56 | 0.41 |
| 2:B:102:LEU:HD12 | 2:B:102:LEU:HA | 1.81 | 0.41 |
| 2:B:115:LEU:HD21 | 2:B:153:ARG:HH21 | 1.85 | 0.41 |
| 3:C:50:ALA:HB2 | 3:C:75:VAL:HB | 2.02 | 0.41 |
| 5:E:100:VAL:HG13 | 5:E:118:ILE:HG22 | 2.02 | 0.41 |
| 8:H:6:ILE:HB | 8:H:85:ARG:NH2 | 2.36 | 0.41 |
| 9:I:8:GLY:CA | 9:I:79:LEU:HB3 | 2.51 | 0.41 |
| 12:L:111:LYS:HA | 12:L:111:LYS:HZ1 | 1.83 | 0.41 |
| 16:P:20:VAL:CG1 | 16:P:32:TYR:CB | 2.99 | 0.41 |
| 20:T:8:ARG:CD | 20:T:8:ARG:N | 2.82 | 0.41 |
| 21:U:10:ARG:HA | 21:U:10:ARG:HD3 | 1.69 | 0.41 |
| 1:A:1125:U:O2' | 1:A:1126:U:P | 2.79 | 0.40 |
| 1:A:1133:G:C2 | 1:A:1134:G:C8 | 3.09 | 0.40 |
| 1:A:1165:C:H2' | 1:A:1166:G:H5' | 2.03 | 0.40 |
| 1:A:1403:C:H2' | 1:A:1403:C:O2 | 2.20 | 0.40 |
| 1:A:1518[B]:MA6:H102 | 1:A:1519[B]:MA6:N6 | 2.36 | 0.40 |
| 1:A:538:G:C2 | 1:A:539:A:C4 | 3.09 | 0.40 |
| 1:A:663:A:O2' | 1:A:664:G:H5' | 2.20 | 0.40 |
| 2:B:130:ARG:CB | 2:B:131:PRO:HD2 | 2.37 | 0.40 |
| 5:E:139:LEU:HA | 5:E:139:LEU:HD23 | 1.87 | 0.40 |
| 7:G:120:ILE:N | 7:G:120:ILE:HD12 | 2.36 | 0.40 |
| 7:G:31:MET:CG | 7:G:32:ARG:N | 2.84 | 0.40 |
| 9:I:46:ALA:O | 9:I:81:ILE:HD12 | 2.20 | 0.40 |
| 9:I:93:ARG:HB3 | 9:I:93:ARG:CZ | 2.51 | 0.40 |
| 1:A:1124:G:O5' | 10:J:35:SER:O | 2.39 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 14:N:12:ARG:NH1 | 14:N:12:ARG:N | 2.69 | 0.40 |
| 16:P:69:THR:O | 16:P:72:ARG:HB3 | 2.20 | 0.40 |
| 17:Q:29:HIS:CE1 | 17:Q:32:TYR:H | 2.39 | 0.40 |
| 20:T:50:GLU:HB2 | 20:T:99:LEU:CD1 | 2.43 | 0.40 |
| 1:A:1300:G:H1' | 1:A:1301:U:H5 | 1.87 | 0.40 |
| 1:A:1453:G:N2 | 1:A:1454:G:N7 | 2.70 | 0.40 |
| 1:A:173:U:H4' | 1:A:174:C:OP2 | 2.21 | 0.40 |
| 1:A:384:G:O2' | 1:A:385:C:H5' | 2.21 | 0.40 |
| 1:A:665:A:H1' | 1:A:733:A:O4' | 2.22 | 0.40 |
| 2:B:239:VAL:HG12 | 2:B:239:VAL:O | 2.21 | 0.40 |
| 3:C:159:GLY:HA2 | 3:C:193:TYR:CD1 | 2.55 | 0.40 |
| 3:C:11:ARG:NH1 | 3:C:177:THR:O | 2.54 | 0.40 |
| 5:E:96:PRO:HA | 5:E:117:ASP:CG | 2.41 | 0.40 |
| 6:F:62:TRP:CH2 | 6:F:64:GLN:HB2 | 2.56 | 0.40 |
| 7:G:110:GLN:OE1 | 7:G:110:GLN:HA | 2.21 | 0.40 |
| 9:I:10:ARG:O | 9:I:11:LYS:C | 2.60 | 0.40 |
| 9:I:125:TYR:N | 9:I:125:TYR:CD2 | 2.89 | 0.40 |
| 10:J:63:PHE:HA | 14:N:59:ALA:N | 2.30 | 0.40 |
| 1:A:695:A:OP1 | 11:K:52:GLY:HA3 | 2.20 | 0.40 |
| 13:M:63:THR:HG23 | 13:M:64:TRP:N | 2.32 | 0.40 |
| 17:Q:24:GLU:HG2 | 17:Q:39:SER:HB3 | 2.03 | 0.40 |
| 18:R:36:ASN:O | 18:R:40:LEU:HG | 2.21 | 0.40 |
| 20:T:10:LEU:C | 20:T:10:LEU:CD1 | 2.89 | 0.40 |
| 20:T:73:HIS:HB3 | 20:T:74:LYS:H | 1.62 | 0.40 |
| 20:T:50:GLU:H | 20:T:99:LEU:HD12 | 1.85 | 0.40 |
| 1:A:1029:C:O2' | 1:A:1030:C:H5' | 2.21 | 0.40 |
| 1:A:1035:A:C5 | 1:A:1036:G:N7 | 2.89 | 0.40 |
| 1:A:1098:C:H2' | 1:A:1099:G:O4' | 2.22 | 0.40 |
| 1:A:1276:G:H8 | 1:A:1276:G:O5' | 2.05 | 0.40 |
| 1:A:1488:G:H2' | 1:A:1489:G:C8 | 2.57 | 0.40 |
| 1:A:247:G:C6 | 1:A:278:G:C2 | 3.09 | 0.40 |
| 1:A:501:C:H1' | 1:A:549:C:H1' | 2.03 | 0.40 |
| 1:A:519:C:H2' | 1:A:520:A:O4' | 2.20 | 0.40 |
| 1:A:556:C:O2' | 1:A:557:G:H5' | 2.20 | 0.40 |
| 2:B:108:ILE:O | 2:B:111:ARG:HB2 | 2.21 | 0.40 |
| 3:C:177:THR:O | 3:C:180:ALA:HB2 | 2.21 | 0.40 |
| 6:F:80:ARG:NH1 | 6:F:88:VAL:HB | 2.35 | 0.40 |
| 7:G:136:LYS:NZ | 7:G:140:ASP:OD2 | 2.38 | 0.40 |
| 11:K:34:ASP:O | 11:K:37:GLY:N | 2.41 | 0.40 |
| 11:K:43:SER:OG | 11:K:44:SER:N | 2.54 | 0.40 |
| 12:L:53:ARG:NH1 | 12:L:92:0TD:OD1 | 2.54 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-------------------|--------------------------|-------------------|
| 13:M:99:ARG:HB2 | 13:M:101:GLN:OE1 | 2.22 | 0.40 |
| 20:T:53:LEU:HB2 | 20:T:100:ILE:HG22 | 2.03 | 0.40 |
| 1:A:1073:U:OP2 | 5:E:57:LYS:NZ | 2.29 | 0.40 |
| 1:A:1160:G:H2' | 1:A:1160:G:N3 | 2.36 | 0.40 |
| 1:A:1211:U:H2' | 1:A:1211:U:O2 | 2.21 | 0.40 |
| 1:A:1316:G:N2 | 1:A:1319:A:OP2 | 2.54 | 0.40 |
| 1:A:522:C:O2' | 1:A:523:A:H5' | 2.21 | 0.40 |
| 1:A:613:C:H2' | 1:A:614:A:H8 | 1.87 | 0.40 |
| 1:A:664:G:H2' | 1:A:666:G:OP1 | 2.22 | 0.40 |
| 1:A:735:C:H2' | 1:A:736:C:H6 | 1.86 | 0.40 |
| 1:A:749:C:H2' | 1:A:750:G:H8 | 1.87 | 0.40 |
| 1:A:756:C:H2' | 1:A:757:U:O4' | 2.20 | 0.40 |
| 1:A:771:G:C2' | 1:A:772:U:H5' | 2.51 | 0.40 |
| 7:G:120:ILE:N | 7:G:120:ILE:CD1 | 2.85 | 0.40 |
| 7:G:54:THR:HB | 7:G:56:GLN:H | 1.86 | 0.40 |
| 10:J:62:HIS:CE1 | 14:N:61:TRP:CH2 | 3.09 | 0.40 |
| 15:O:67:LEU:HA | 15:O:67:LEU:HD23 | 1.91 | 0.40 |
| 17:Q:43:LEU:HG | 17:Q:68:ARG:HH12 | 1.86 | 0.40 |
| 19:S:9:VAL:HG12 | 19:S:10:PHE:N | 2.36 | 0.40 |
| 1:A:1053:G:C3' | 1:A:1054:C:C5' | 3.00 | 0.40 |
| 1:A:1092:A:C6 | 1:A:1093:A:C6 | 3.09 | 0.40 |
| 1:A:1447:G:H2' | 1:A:1448:C:H6 | 1.86 | 0.40 |
| 1:A:1447:G:H2' | 1:A:1448:C:C6 | 2.56 | 0.40 |
| 1:A:1509:C:H2' | 1:A:1510:U:O4' | 2.22 | 0.40 |
| 1:A:1525:G:OP1 | 11:K:120:ARG:NH2 | 2.55 | 0.40 |
| 1:A:375:U:C4 | 1:A:376:G:N7 | 2.90 | 0.40 |
| 1:A:393:A:H2' | 1:A:394:G:H5' | 2.03 | 0.40 |
| 1:A:401:C:H2' | 1:A:402:G:C8 | 2.55 | 0.40 |
| 1:A:428:G:O4' | 1:A:430:A:C8 | 2.74 | 0.40 |
| 1:A:429:U:H4' | 1:A:430:A:O5' | 2.22 | 0.40 |
| 1:A:884:U:H4' | 1:A:885:G:H5'' | 2.03 | 0.40 |
| 1:A:953:G:H2' | 1:A:954:G:O4' | 2.21 | 0.40 |
| 5:E:152:ARG:HB3 | 8:H:43:GLY:HA3 | 2.03 | 0.40 |
| 9:I:63:ILE:HD13 | 9:I:77:ILE:HG23 | 2.03 | 0.40 |
| 11:K:58:PRO:O | 11:K:61:ALA:HB3 | 2.21 | 0.40 |
| 10:J:62:HIS:HE1 | 14:N:61:TRP:CZ3 | 2.38 | 0.40 |
| 20:T:53:LEU:HB2 | 20:T:100:ILE:HG21 | 2.03 | 0.40 |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------|-----------------------|--------------------------|-------------------|
| 1:A:702:A:N6 | 1:A:1447:G:OP1[4_554] | 2.18 | 0.02 |

5.3 Torsion angles

5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 2 | B | 234/256 (91%) | 209 (89%) | 24 (10%) | 1 (0%) | 36 | 75 |
| 3 | C | 205/239 (86%) | 183 (89%) | 22 (11%) | 0 | 100 | 100 |
| 4 | D | 206/209 (99%) | 197 (96%) | 9 (4%) | 0 | 100 | 100 |
| 5 | E | 149/162 (92%) | 141 (95%) | 8 (5%) | 0 | 100 | 100 |
| 6 | F | 99/101 (98%) | 96 (97%) | 3 (3%) | 0 | 100 | 100 |
| 7 | G | 153/156 (98%) | 139 (91%) | 14 (9%) | 0 | 100 | 100 |
| 8 | H | 136/138 (99%) | 130 (96%) | 6 (4%) | 0 | 100 | 100 |
| 9 | I | 125/128 (98%) | 113 (90%) | 11 (9%) | 1 (1%) | 21 | 62 |
| 10 | J | 97/105 (92%) | 80 (82%) | 16 (16%) | 1 (1%) | 17 | 57 |
| 11 | K | 117/129 (91%) | 102 (87%) | 14 (12%) | 1 (1%) | 19 | 60 |
| 12 | L | 122/135 (90%) | 109 (89%) | 12 (10%) | 1 (1%) | 21 | 62 |
| 13 | M | 116/126 (92%) | 105 (90%) | 11 (10%) | 0 | 100 | 100 |
| 14 | N | 58/61 (95%) | 54 (93%) | 4 (7%) | 0 | 100 | 100 |
| 15 | O | 86/89 (97%) | 80 (93%) | 6 (7%) | 0 | 100 | 100 |
| 16 | P | 82/88 (93%) | 78 (95%) | 4 (5%) | 0 | 100 | 100 |
| 17 | Q | 98/105 (93%) | 93 (95%) | 5 (5%) | 0 | 100 | 100 |
| 18 | R | 71/88 (81%) | 68 (96%) | 3 (4%) | 0 | 100 | 100 |
| 19 | S | 79/93 (85%) | 69 (87%) | 8 (10%) | 2 (2%) | 6 | 37 |
| 20 | T | 97/106 (92%) | 84 (87%) | 13 (13%) | 0 | 100 | 100 |
| 21 | U | 23/27 (85%) | 22 (96%) | 1 (4%) | 0 | 100 | 100 |
| All | All | 2353/2541 (93%) | 2152 (92%) | 194 (8%) | 7 (0%) | 43 | 78 |

All (7) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | L | 28 | LYS |
| 19 | S | 31 | ILE |
| 19 | S | 6 | LYS |
| 11 | K | 117 | ASN |
| 9 | I | 119 | ALA |
| 2 | B | 229 | VAL |
| 10 | J | 34 | VAL |

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 X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2 | B | 201/220 (91%) | 181 (90%) | 20 (10%) | 8 | 34 |
| 3 | C | 160/188 (85%) | 136 (85%) | 24 (15%) | 3 | 17 |
| 4 | D | 180/181 (99%) | 161 (89%) | 19 (11%) | 7 | 31 |
| 5 | E | 115/123 (94%) | 101 (88%) | 14 (12%) | 5 | 25 |
| 6 | F | 90/90 (100%) | 78 (87%) | 12 (13%) | 4 | 22 |
| 7 | G | 126/127 (99%) | 114 (90%) | 12 (10%) | 9 | 36 |
| 8 | H | 119/119 (100%) | 105 (88%) | 14 (12%) | 6 | 26 |
| 9 | I | 98/99 (99%) | 83 (85%) | 15 (15%) | 3 | 17 |
| 10 | J | 87/92 (95%) | 76 (87%) | 11 (13%) | 5 | 23 |
| 11 | K | 90/99 (91%) | 81 (90%) | 9 (10%) | 8 | 34 |
| 12 | L | 103/110 (94%) | 90 (87%) | 13 (13%) | 5 | 23 |
| 13 | M | 94/101 (93%) | 83 (88%) | 11 (12%) | 6 | 26 |
| 14 | N | 49/50 (98%) | 42 (86%) | 7 (14%) | 3 | 19 |
| 15 | O | 79/80 (99%) | 72 (91%) | 7 (9%) | 11 | 39 |
| 16 | P | 72/74 (97%) | 67 (93%) | 5 (7%) | 17 | 51 |
| 17 | Q | 95/97 (98%) | 84 (88%) | 11 (12%) | 6 | 27 |
| 18 | R | 64/77 (83%) | 58 (91%) | 6 (9%) | 9 | 36 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 19 | S | 71/80 (89%) | 61 (86%) | 10 (14%) | 4 | 20 |
| 20 | T | 76/82 (93%) | 65 (86%) | 11 (14%) | 3 | 19 |
| 21 | U | 19/22 (86%) | 17 (90%) | 2 (10%) | 7 | 32 |
| All | All | 1988/2111 (94%) | 1755 (88%) | 233 (12%) | 6 | 26 |

All (233) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 24 | TRP |
| 2 | B | 33 | TYR |
| 2 | B | 42 | ILE |
| 2 | B | 46 | LYS |
| 2 | B | 53 | ARG |
| 2 | B | 82 | ARG |
| 2 | B | 102 | LEU |
| 2 | B | 114 | ARG |
| 2 | B | 127 | ILE |
| 2 | B | 139 | LYS |
| 2 | B | 144 | ARG |
| 2 | B | 153 | ARG |
| 2 | B | 157 | ARG |
| 2 | B | 178 | ARG |
| 2 | B | 187 | LEU |
| 2 | B | 208 | ILE |
| 2 | B | 221 | LEU |
| 2 | B | 223 | ILE |
| 2 | B | 236 | TYR |
| 2 | B | 240 | GLN |
| 3 | C | 3 | ASN |
| 3 | C | 17 | ASP |
| 3 | C | 21 | ARG |
| 3 | C | 27 | LYS |
| 3 | C | 34 | LEU |
| 3 | C | 37 | GLN |
| 3 | C | 52 | LEU |
| 3 | C | 56 | ASP |
| 3 | C | 72 | LYS |
| 3 | C | 85 | ARG |
| 3 | C | 91 | LEU |
| 3 | C | 95 | THR |
| 3 | C | 111 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 126 | ARG |
| 3 | C | 127 | ARG |
| 3 | C | 128 | PHE |
| 3 | C | 144 | SER |
| 3 | C | 167 | TRP |
| 3 | C | 172 | ARG |
| 3 | C | 175 | LEU |
| 3 | C | 188 | LEU |
| 3 | C | 195 | VAL |
| 3 | C | 196 | LEU |
| 3 | C | 204 | LEU |
| 4 | D | 3 | ARG |
| 4 | D | 8 | VAL |
| 4 | D | 10 | ARG |
| 4 | D | 15 | GLU |
| 4 | D | 19 | LEU |
| 4 | D | 26 | CYS |
| 4 | D | 35 | ARG |
| 4 | D | 50 | ARG |
| 4 | D | 61 | LYS |
| 4 | D | 70 | ILE |
| 4 | D | 78 | LEU |
| 4 | D | 122 | ARG |
| 4 | D | 127 | THR |
| 4 | D | 150 | GLU |
| 4 | D | 170 | VAL |
| 4 | D | 178 | VAL |
| 4 | D | 192 | GLU |
| 4 | D | 201 | GLN |
| 4 | D | 202 | LEU |
| 5 | E | 6 | PHE |
| 5 | E | 10 | MET |
| 5 | E | 12 | LEU |
| 5 | E | 15 | ARG |
| 5 | E | 24 | ARG |
| 5 | E | 31 | LEU |
| 5 | E | 34 | VAL |
| 5 | E | 41 | VAL |
| 5 | E | 43 | LEU |
| 5 | E | 50 | GLU |
| 5 | E | 64 | ARG |
| 5 | E | 78 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | E | 79 | GLU |
| 5 | E | 125 | SER |
| 6 | F | 3 | ARG |
| 6 | F | 10 | LEU |
| 6 | F | 15 | ASP |
| 6 | F | 25 | ILE |
| 6 | F | 43 | LEU |
| 6 | F | 54 | LYS |
| 6 | F | 55 | ASP |
| 6 | F | 69 | GLU |
| 6 | F | 73 | ASN |
| 6 | F | 74 | ASP |
| 6 | F | 77 | ARG |
| 6 | F | 82 | ARG |
| 7 | G | 8 | GLU |
| 7 | G | 11 | GLN |
| 7 | G | 12 | LEU |
| 7 | G | 38 | LEU |
| 7 | G | 48 | LYS |
| 7 | G | 54 | THR |
| 7 | G | 63 | LYS |
| 7 | G | 76 | ARG |
| 7 | G | 113 | GLU |
| 7 | G | 114 | ARG |
| 7 | G | 124 | LEU |
| 7 | G | 137 | LYS |
| 8 | H | 11 | THR |
| 8 | H | 26 | VAL |
| 8 | H | 39 | LEU |
| 8 | H | 63 | LEU |
| 8 | H | 85 | ARG |
| 8 | H | 91 | ARG |
| 8 | H | 92 | ARG |
| 8 | H | 97 | VAL |
| 8 | H | 102 | ARG |
| 8 | H | 114 | THR |
| 8 | H | 120 | THR |
| 8 | H | 127 | LEU |
| 8 | H | 129 | VAL |
| 8 | H | 133 | LEU |
| 9 | I | 14 | VAL |
| 9 | I | 27 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | I | 41 | VAL |
| 9 | I | 66 | ARG |
| 9 | I | 79 | LEU |
| 9 | I | 96 | LEU |
| 9 | I | 102 | LEU |
| 9 | I | 109 | VAL |
| 9 | I | 111 | ARG |
| 9 | I | 113 | LYS |
| 9 | I | 118 | LYS |
| 9 | I | 121 | ARG |
| 9 | I | 124 | GLN |
| 9 | I | 125 | TYR |
| 9 | I | 127 | LYS |
| 10 | J | 6 | ILE |
| 10 | J | 16 | LEU |
| 10 | J | 60 | ARG |
| 10 | J | 62 | HIS |
| 10 | J | 63 | PHE |
| 10 | J | 66 | ARG |
| 10 | J | 71 | LEU |
| 10 | J | 78 | ASN |
| 10 | J | 83 | GLU |
| 10 | J | 88 | LEU |
| 10 | J | 89 | ASP |
| 11 | K | 11 | LYS |
| 11 | K | 13 | GLN |
| 11 | K | 16 | SER |
| 11 | K | 18 | ARG |
| 11 | K | 29 | ILE |
| 11 | K | 91 | ARG |
| 11 | K | 96 | ARG |
| 11 | K | 103 | LEU |
| 11 | K | 122 | LYS |
| 12 | L | 10 | LEU |
| 12 | L | 11 | VAL |
| 12 | L | 13 | LYS |
| 12 | L | 18 | VAL |
| 12 | L | 19 | ARG |
| 12 | L | 20 | LYS |
| 12 | L | 39 | VAL |
| 12 | L | 44 | THR |
| 12 | L | 60 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | L | 67 | THR |
| 12 | L | 89 | ARG |
| 12 | L | 111 | LYS |
| 12 | L | 113 | ARG |
| 13 | M | 44 | ARG |
| 13 | M | 49 | THR |
| 13 | M | 56 | LEU |
| 13 | M | 58 | GLU |
| 13 | M | 59 | TYR |
| 13 | M | 62 | ASN |
| 13 | M | 63 | THR |
| 13 | M | 64 | TRP |
| 13 | M | 66 | LEU |
| 13 | M | 99 | ARG |
| 13 | M | 102 | ARG |
| 14 | N | 7 | ILE |
| 14 | N | 8 | GLU |
| 14 | N | 9 | LYS |
| 14 | N | 11 | LYS |
| 14 | N | 12 | ARG |
| 14 | N | 22 | THR |
| 14 | N | 44 | LEU |
| 15 | O | 6 | GLU |
| 15 | O | 11 | VAL |
| 15 | O | 34 | LEU |
| 15 | O | 39 | LEU |
| 15 | O | 45 | VAL |
| 15 | O | 70 | LEU |
| 15 | O | 83 | GLU |
| 16 | P | 1 | MET |
| 16 | P | 53 | VAL |
| 16 | P | 55 | ARG |
| 16 | P | 62 | VAL |
| 16 | P | 82 | GLN |
| 17 | Q | 9 | VAL |
| 17 | Q | 19 | VAL |
| 17 | Q | 22 | LEU |
| 17 | Q | 34 | LYS |
| 17 | Q | 36 | ILE |
| 17 | Q | 38 | ARG |
| 17 | Q | 59 | ILE |
| 17 | Q | 60 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17 | Q | 63 | ARG |
| 17 | Q | 68 | ARG |
| 17 | Q | 98 | LEU |
| 18 | R | 38 | GLU |
| 18 | R | 46 | GLU |
| 18 | R | 76 | LEU |
| 18 | R | 82 | THR |
| 18 | R | 86 | VAL |
| 18 | R | 88 | LYS |
| 19 | S | 7 | LYS |
| 19 | S | 13 | ASP |
| 19 | S | 14 | HIS |
| 19 | S | 15 | LEU |
| 19 | S | 18 | LYS |
| 19 | S | 30 | LEU |
| 19 | S | 31 | ILE |
| 19 | S | 36 | ARG |
| 19 | S | 43 | GLU |
| 19 | S | 81 | ARG |
| 20 | T | 8 | ARG |
| 20 | T | 9 | ASN |
| 20 | T | 10 | LEU |
| 20 | T | 19 | SER |
| 20 | T | 35 | THR |
| 20 | T | 57 | ARG |
| 20 | T | 62 | LEU |
| 20 | T | 72 | LEU |
| 20 | T | 74 | LYS |
| 20 | T | 75 | ASN |
| 20 | T | 87 | LYS |
| 21 | U | 10 | ARG |
| 21 | U | 15 | ARG |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 135 | GLN |
| 9 | I | 73 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | A | 1503/1522 (98%) | 248 (16%) | 43 (2%) |
| 22 | V | 2/3 (66%) | 0 | 0 |
| 23 | W | 14/15 (93%) | 3 (21%) | 0 |
| All | All | 1519/1540 (98%) | 251 (16%) | 43 (2%) |

All (251) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | A | 7 | G |
| 1 | A | 9 | G |
| 1 | A | 32 | A |
| 1 | A | 39 | G |
| 1 | A | 44 | G |
| 1 | A | 47 | C |
| 1 | A | 48 | C |
| 1 | A | 51 | A |
| 1 | A | 60 | A |
| 1 | A | 61 | G |
| 1 | A | 80 | G |
| 1 | A | 81 | U |
| 1 | A | 101 | A |
| 1 | A | 116 | A |
| 1 | A | 117 | G |
| 1 | A | 121 | C |
| 1 | A | 129(A) | G |
| 1 | A | 130 | A |
| 1 | A | 131 | C |
| 1 | A | 145 | G |
| 1 | A | 163 | C |
| 1 | A | 182 | U |
| 1 | A | 195 | A |
| 1 | A | 197 | A |
| 1 | A | 202 | U |
| 1 | A | 204 | U |
| 1 | A | 216 | G |
| 1 | A | 217 | C |
| 1 | A | 226 | G |
| 1 | A | 231 | G |
| 1 | A | 247 | G |
| 1 | A | 251 | G |
| 1 | A | 266 | G |
| 1 | A | 267 | C |
| 1 | A | 282 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 289 | G |
| 1 | A | 319 | G |
| 1 | A | 321 | A |
| 1 | A | 328 | C |
| 1 | A | 329 | A |
| 1 | A | 332 | G |
| 1 | A | 344 | A |
| 1 | A | 345 | C |
| 1 | A | 351 | G |
| 1 | A | 352 | C |
| 1 | A | 353 | A |
| 1 | A | 354 | G |
| 1 | A | 367 | U |
| 1 | A | 373 | A |
| 1 | A | 374 | A |
| 1 | A | 384 | G |
| 1 | A | 397 | A |
| 1 | A | 398 | C |
| 1 | A | 406 | G |
| 1 | A | 411 | A |
| 1 | A | 412 | A |
| 1 | A | 413 | G |
| 1 | A | 419 | C |
| 1 | A | 421 | U |
| 1 | A | 423 | G |
| 1 | A | 428 | G |
| 1 | A | 429 | U |
| 1 | A | 430 | A |
| 1 | A | 433 | C |
| 1 | A | 439 | A |
| 1 | A | 442 | C |
| 1 | A | 444 | C |
| 1 | A | 452 | A |
| 1 | A | 461 | C |
| 1 | A | 485 | G |
| 1 | A | 495 | U |
| 1 | A | 497 | A |
| 1 | A | 498 | U |
| 1 | A | 509 | A |
| 1 | A | 510 | A |
| 1 | A | 511 | C |
| 1 | A | 518 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 521 | G |
| 1 | A | 527 | 7MG |
| 1 | A | 531 | U |
| 1 | A | 532 | A |
| 1 | A | 533 | A |
| 1 | A | 547 | A |
| 1 | A | 559 | A |
| 1 | A | 560 | U |
| 1 | A | 562 | C |
| 1 | A | 563 | A |
| 1 | A | 564 | C |
| 1 | A | 572 | A |
| 1 | A | 573 | A |
| 1 | A | 576 | G |
| 1 | A | 577 | G |
| 1 | A | 579 | G |
| 1 | A | 588 | G |
| 1 | A | 607 | A |
| 1 | A | 631 | G |
| 1 | A | 632 | A |
| 1 | A | 653 | A |
| 1 | A | 665 | A |
| 1 | A | 671 | G |
| 1 | A | 687 | A |
| 1 | A | 688 | G |
| 1 | A | 701 | C |
| 1 | A | 702 | A |
| 1 | A | 723 | U |
| 1 | A | 724 | G |
| 1 | A | 731 | G |
| 1 | A | 755 | G |
| 1 | A | 766 | A |
| 1 | A | 774 | G |
| 1 | A | 777 | A |
| 1 | A | 792 | A |
| 1 | A | 793 | U |
| 1 | A | 794 | A |
| 1 | A | 813 | U |
| 1 | A | 815 | A |
| 1 | A | 816 | A |
| 1 | A | 817 | C |
| 1 | A | 828 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 839 | U |
| 1 | A | 840 | C |
| 1 | A | 841 | U |
| 1 | A | 848 | C |
| 1 | A | 859 | A |
| 1 | A | 873 | A |
| 1 | A | 874 | G |
| 1 | A | 876 | G |
| 1 | A | 887 | G |
| 1 | A | 902 | G |
| 1 | A | 914 | A |
| 1 | A | 922 | G |
| 1 | A | 926 | G |
| 1 | A | 927 | G |
| 1 | A | 934 | C |
| 1 | A | 935 | A |
| 1 | A | 960 | U |
| 1 | A | 964 | A |
| 1 | A | 966 | M2G |
| 1 | A | 968 | A |
| 1 | A | 969 | A |
| 1 | A | 971 | G |
| 1 | A | 972 | C |
| 1 | A | 974 | A |
| 1 | A | 975 | A |
| 1 | A | 976 | G |
| 1 | A | 977 | A |
| 1 | A | 983 | A |
| 1 | A | 991 | U |
| 1 | A | 992 | U |
| 1 | A | 993 | G |
| 1 | A | 1004 | A |
| 1 | A | 1005 | A |
| 1 | A | 1023 | G |
| 1 | A | 1025 | U |
| 1 | A | 1026 | G |
| 1 | A | 1027 | C |
| 1 | A | 1031 | G |
| 1 | A | 1050 | G |
| 1 | A | 1053 | G |
| 1 | A | 1054 | C |
| 1 | A | 1055 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1065 | U |
| 1 | A | 1066 | C |
| 1 | A | 1068 | G |
| 1 | A | 1094 | G |
| 1 | A | 1095 | U |
| 1 | A | 1101 | A |
| 1 | A | 1125 | U |
| 1 | A | 1126 | U |
| 1 | A | 1127 | G |
| 1 | A | 1129 | C |
| 1 | A | 1130 | A |
| 1 | A | 1131 | G |
| 1 | A | 1136 | U |
| 1 | A | 1137 | C |
| 1 | A | 1138 | G |
| 1 | A | 1139 | G |
| 1 | A | 1140 | C |
| 1 | A | 1159 | U |
| 1 | A | 1160 | G |
| 1 | A | 1171 | G |
| 1 | A | 1180 | A |
| 1 | A | 1181 | G |
| 1 | A | 1183 | A |
| 1 | A | 1184 | G |
| 1 | A | 1191 | A |
| 1 | A | 1196 | U |
| 1 | A | 1197 | G |
| 1 | A | 1200 | C |
| 1 | A | 1201 | A |
| 1 | A | 1202 | G |
| 1 | A | 1211 | U |
| 1 | A | 1212 | U |
| 1 | A | 1213 | A |
| 1 | A | 1215 | G |
| 1 | A | 1225 | A |
| 1 | A | 1238 | A |
| 1 | A | 1250 | A |
| 1 | A | 1251 | A |
| 1 | A | 1256 | A |
| 1 | A | 1257 | U |
| 1 | A | 1258 | G |
| 1 | A | 1270 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1280 | A |
| 1 | A | 1281 | U |
| 1 | A | 1282 | C |
| 1 | A | 1287 | A |
| 1 | A | 1288 | A |
| 1 | A | 1289 | A |
| 1 | A | 1300 | G |
| 1 | A | 1301 | U |
| 1 | A | 1302 | U |
| 1 | A | 1303 | C |
| 1 | A | 1319 | A |
| 1 | A | 1320 | C |
| 1 | A | 1322 | C |
| 1 | A | 1332 | A |
| 1 | A | 1338 | G |
| 1 | A | 1348 | U |
| 1 | A | 1353 | G |
| 1 | A | 1362 | C |
| 1 | A | 1363 | A |
| 1 | A | 1364 | U |
| 1 | A | 1370 | G |
| 1 | A | 1379 | G |
| 1 | A | 1381 | U |
| 1 | A | 1397 | C |
| 1 | A | 1398 | A |
| 1 | A | 1400 | 5MC |
| 1 | A | 1401 | G |
| 1 | A | 1442 | G |
| 1 | A | 1443 | G |
| 1 | A | 1446 | A |
| 1 | A | 1469 | G |
| 1 | A | 1487 | G |
| 1 | A | 1492 | A |
| 1 | A | 1494 | G |
| 1 | A | 1498 | UR3 |
| 1 | A | 1499 | A |
| 1 | A | 1502 | A |
| 1 | A | 1504 | G |
| 1 | A | 1505 | G |
| 1 | A | 1506 | U |
| 1 | A | 1507 | A |
| 1 | A | 1528 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1529 | G |
| 1 | A | 1530 | G |
| 1 | A | 1531 | A |
| 23 | W | 30 | G |
| 23 | W | 33 | U |
| 23 | W | 34 | G |

All (43) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | A | 60 | A |
| 1 | A | 115 | G |
| 1 | A | 129(A) | G |
| 1 | A | 181 | G |
| 1 | A | 216 | G |
| 1 | A | 250 | A |
| 1 | A | 266 | G |
| 1 | A | 281 | G |
| 1 | A | 328 | C |
| 1 | A | 372 | C |
| 1 | A | 428 | G |
| 1 | A | 429 | U |
| 1 | A | 432 | A |
| 1 | A | 484 | G |
| 1 | A | 496 | A |
| 1 | A | 509 | A |
| 1 | A | 559 | A |
| 1 | A | 575 | G |
| 1 | A | 687 | A |
| 1 | A | 701 | C |
| 1 | A | 812 | C |
| 1 | A | 913 | A |
| 1 | A | 991 | U |
| 1 | A | 1004 | A |
| 1 | A | 1026 | G |
| 1 | A | 1049 | U |
| 1 | A | 1065 | U |
| 1 | A | 1067 | A |
| 1 | A | 1129 | C |
| 1 | A | 1179 | A |
| 1 | A | 1182 | G |
| 1 | A | 1190 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1201 | A |
| 1 | A | 1211 | U |
| 1 | A | 1212 | U |
| 1 | A | 1281 | U |
| 1 | A | 1300 | G |
| 1 | A | 1331 | G |
| 1 | A | 1347 | G |
| 1 | A | 1397 | C |
| 1 | A | 1443 | G |
| 1 | A | 1505 | G |
| 1 | A | 1528 | U |

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|---------|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | # $ Z > 2$ | Counts | RMSZ | # $ Z > 2$ |
| 1 | 2MG | A | 1207 | 1 | 19,26,27 | 2.41 | 4 (21%) | 19,38,41 | 2.11 | 4 (21%) |
| 1 | 5MC | A | 1400 | 1 | 14,22,23 | 0.98 | 0 | 16,32,35 | 0.97 | 1 (6%) |
| 1 | 4OC | A | 1402 | 1 | 16,23,24 | 0.92 | 1 (6%) | 20,32,35 | 0.69 | 0 |
| 1 | 5MC | A | 1404 | 1 | 14,22,23 | 1.64 | 1 (7%) | 16,32,35 | 1.03 | 1 (6%) |
| 1 | 5MC | A | 1407 | 1 | 14,22,23 | 1.34 | 1 (7%) | 16,32,35 | 0.99 | 1 (6%) |
| 1 | UR3 | A | 1498 | 1 | 13,22,23 | 0.75 | 0 | 15,32,35 | 0.95 | 0 |
| 1 | MA6 | A | 1518[A] | 1 | 16,26,27 | 1.41 | 2 (12%) | 17,38,41 | 0.92 | 1 (5%) |
| 1 | MA6 | A | 1518[B] | 1 | 16,26,27 | 1.46 | 3 (18%) | 17,38,41 | 0.91 | 1 (5%) |
| 1 | MA6 | A | 1519[A] | 1 | 16,26,27 | 1.14 | 1 (6%) | 17,38,41 | 1.06 | 2 (11%) |
| 1 | MA6 | A | 1519[B] | 1 | 16,26,27 | 1.43 | 3 (18%) | 17,38,41 | 0.85 | 1 (5%) |
| 1 | PSU | A | 1540 | 1 | 16,21,22 | 1.21 | 1 (6%) | 20,30,33 | 3.55 | 6 (30%) |
| 1 | PSU | A | 1541 | 1 | 16,21,22 | 0.99 | 1 (6%) | 20,30,33 | 3.60 | 7 (35%) |
| 1 | PSU | A | 516 | 1,24 | 16,21,22 | 1.02 | 1 (6%) | 20,30,33 | 3.20 | 6 (30%) |
| 1 | 7MG | A | 527 | 1 | 20,26,27 | 2.22 | 7 (35%) | 23,39,42 | 1.61 | 6 (26%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | M2G | A | 966 | 1 | 20,27,28 | 1.79 | 5 (25%) | 20,40,43 | 2.50 | 4 (20%) |
| 1 | 5MC | A | 967 | 1 | 14,22,23 | 1.19 | 1 (7%) | 16,32,35 | 0.91 | 1 (6%) |
| 12 | 0TD | L | 92 | 12 | 5,9,10 | 2.91 | 1 (20%) | 3,11,13 | 3.04 | 3 (100%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|---------|------|---------|-----------|---------|
| 1 | 2MG | A | 1207 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | 5MC | A | 1400 | 1 | - | 0/3/25/26 | 0/2/2/2 |
| 1 | 4OC | A | 1402 | 1 | - | 0/7/29/30 | 0/2/2/2 |
| 1 | 5MC | A | 1404 | 1 | - | 0/3/25/26 | 0/2/2/2 |
| 1 | 5MC | A | 1407 | 1 | - | 0/3/25/26 | 0/2/2/2 |
| 1 | UR3 | A | 1498 | 1 | - | 0/3/25/26 | 0/2/2/2 |
| 1 | MA6 | A | 1518[A] | 1 | - | 0/7/29/30 | 0/3/3/3 |
| 1 | MA6 | A | 1518[B] | 1 | - | 0/7/29/30 | 0/3/3/3 |
| 1 | MA6 | A | 1519[A] | 1 | - | 0/7/29/30 | 0/3/3/3 |
| 1 | MA6 | A | 1519[B] | 1 | - | 0/7/29/30 | 0/3/3/3 |
| 1 | PSU | A | 1540 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | A | 1541 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | A | 516 | 1,24 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 7MG | A | 527 | 1 | - | 0/7/37/38 | 0/3/3/3 |
| 1 | M2G | A | 966 | 1 | - | 0/7/29/30 | 0/3/3/3 |
| 1 | 5MC | A | 967 | 1 | - | 0/3/25/26 | 0/2/2/2 |
| 12 | 0TD | L | 92 | 12 | - | 0/2/12/14 | 0/0/0/0 |

All (33) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|---------|-------|-------------|----------|
| 1 | A | 527 | 7MG | C8-N9 | -5.04 | 1.33 | 1.45 |
| 1 | A | 527 | 7MG | O5'-C5' | -2.55 | 1.41 | 1.44 |
| 1 | A | 527 | 7MG | CM7-N7 | -2.39 | 1.41 | 1.46 |
| 1 | A | 1402 | 4OC | O5'-C5' | -2.10 | 1.41 | 1.44 |
| 1 | A | 1518[B] | MA6 | C2-N3 | 2.14 | 1.35 | 1.32 |
| 1 | A | 1519[B] | MA6 | C2-N3 | 2.22 | 1.35 | 1.32 |
| 1 | A | 527 | 7MG | C6-C5 | 2.22 | 1.44 | 1.41 |
| 1 | A | 1518[A] | MA6 | C2-N1 | 2.26 | 1.38 | 1.33 |
| 1 | A | 966 | M2G | C2-N1 | 2.32 | 1.38 | 1.34 |
| 1 | A | 1518[B] | MA6 | C2-N1 | 2.34 | 1.38 | 1.33 |
| 1 | A | 527 | 7MG | C6-N1 | 2.34 | 1.37 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|-------|------|-------------|----------|
| 1 | A | 966 | M2G | C2-N2 | 2.42 | 1.38 | 1.34 |
| 1 | A | 966 | M2G | C4-N3 | 2.51 | 1.39 | 1.35 |
| 1 | A | 1519[B] | MA6 | C2-N1 | 2.58 | 1.38 | 1.33 |
| 1 | A | 1207 | 2MG | C4-N3 | 2.72 | 1.40 | 1.35 |
| 1 | A | 967 | 5MC | C5-C4 | 2.86 | 1.45 | 1.41 |
| 1 | A | 516 | PSU | C4-N3 | 2.90 | 1.38 | 1.33 |
| 1 | A | 1541 | PSU | C4-N3 | 3.07 | 1.38 | 1.33 |
| 1 | A | 1407 | 5MC | C5-C4 | 3.52 | 1.46 | 1.41 |
| 1 | A | 1540 | PSU | C4-N3 | 3.74 | 1.39 | 1.33 |
| 1 | A | 1519[B] | MA6 | C8-N9 | 3.83 | 1.41 | 1.36 |
| 1 | A | 1519[A] | MA6 | C8-N9 | 3.91 | 1.41 | 1.36 |
| 1 | A | 966 | M2G | C8-N9 | 3.94 | 1.41 | 1.36 |
| 1 | A | 1207 | 2MG | C8-N9 | 4.17 | 1.42 | 1.36 |
| 1 | A | 527 | 7MG | C4-N3 | 4.18 | 1.39 | 1.34 |
| 1 | A | 1518[B] | MA6 | C8-N9 | 4.27 | 1.42 | 1.36 |
| 1 | A | 1518[A] | MA6 | C8-N9 | 4.45 | 1.42 | 1.36 |
| 1 | A | 966 | M2G | C6-N1 | 4.70 | 1.41 | 1.33 |
| 1 | A | 1404 | 5MC | C5-C4 | 4.80 | 1.48 | 1.41 |
| 1 | A | 527 | 7MG | C2-N2 | 5.05 | 1.44 | 1.33 |
| 1 | A | 1207 | 2MG | C6-N1 | 5.29 | 1.42 | 1.33 |
| 12 | L | 92 | 0TD | CA-C | 6.09 | 1.58 | 1.50 |
| 1 | A | 1207 | 2MG | C2-N2 | 6.98 | 1.40 | 1.34 |

All (45) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1 | A | 1540 | PSU | N1-C2-N3 | -11.15 | 119.45 | 128.41 |
| 1 | A | 516 | PSU | N1-C2-N3 | -10.89 | 119.65 | 128.41 |
| 1 | A | 1541 | PSU | N1-C2-N3 | -10.69 | 119.82 | 128.41 |
| 1 | A | 966 | M2G | C5-C6-N1 | -7.86 | 112.29 | 123.47 |
| 1 | A | 1207 | 2MG | C5-C6-N1 | -7.17 | 113.28 | 123.47 |
| 1 | A | 1541 | PSU | C5-C1'-C2' | -6.94 | 102.94 | 115.32 |
| 1 | A | 1540 | PSU | C5-C1'-C2' | -6.03 | 104.57 | 115.32 |
| 1 | A | 1540 | PSU | C5-C4-N3 | -4.61 | 119.42 | 125.36 |
| 1 | A | 516 | PSU | C5-C4-N3 | -4.40 | 119.70 | 125.36 |
| 12 | L | 92 | 0TD | CSB-SB-CB | -4.07 | 93.84 | 101.85 |
| 1 | A | 1541 | PSU | C5-C4-N3 | -3.86 | 120.39 | 125.36 |
| 1 | A | 527 | 7MG | C5-C4-N3 | -3.72 | 120.26 | 126.47 |
| 1 | A | 1541 | PSU | C5-C6-N1 | -3.39 | 120.10 | 124.42 |
| 1 | A | 966 | M2G | N1-C2-N2 | -3.16 | 113.99 | 117.16 |
| 1 | A | 1404 | 5MC | N4-C4-N3 | -3.00 | 112.71 | 117.01 |
| 1 | A | 516 | PSU | C5-C6-N1 | -2.93 | 120.68 | 124.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-------------|-------|-------------|----------|
| 1 | A | 1407 | 5MC | N4-C4-N3 | -2.60 | 113.29 | 117.01 |
| 12 | L | 92 | 0TD | C-CA-N | -2.52 | 104.78 | 109.86 |
| 1 | A | 1540 | PSU | C3'-C2'-C1' | -2.31 | 99.27 | 101.93 |
| 1 | A | 967 | 5MC | N4-C4-N3 | -2.21 | 113.83 | 117.01 |
| 1 | A | 527 | 7MG | N1-C2-N3 | -2.20 | 121.93 | 125.43 |
| 1 | A | 527 | 7MG | C5-C6-N1 | -2.19 | 119.92 | 123.34 |
| 12 | L | 92 | 0TD | O-C-CA | -2.18 | 120.00 | 125.09 |
| 1 | A | 1400 | 5MC | CM5-C5-C6 | 2.09 | 122.99 | 118.66 |
| 1 | A | 1519[A] | MA6 | C2-N1-C6 | 2.12 | 116.96 | 111.81 |
| 1 | A | 516 | PSU | O4'-C1'-C2' | 2.13 | 108.11 | 104.66 |
| 1 | A | 1519[B] | MA6 | N3-C2-N1 | 2.13 | 130.69 | 128.86 |
| 1 | A | 1518[A] | MA6 | C2-N1-C6 | 2.23 | 117.22 | 111.81 |
| 1 | A | 1518[B] | MA6 | N3-C2-N1 | 2.23 | 130.78 | 128.86 |
| 1 | A | 1207 | 2MG | C4-C5-N7 | 2.30 | 111.64 | 109.41 |
| 1 | A | 1207 | 2MG | N2-C2-N3 | 2.31 | 119.17 | 116.96 |
| 1 | A | 1519[A] | MA6 | N3-C2-N1 | 2.31 | 130.84 | 128.86 |
| 1 | A | 1540 | PSU | C6-N1-C2 | 2.39 | 119.18 | 115.36 |
| 1 | A | 527 | 7MG | C2-N3-C4 | 2.40 | 120.68 | 113.95 |
| 1 | A | 527 | 7MG | C6-N1-C2 | 2.58 | 119.77 | 116.06 |
| 1 | A | 966 | M2G | N3-C2-N2 | 2.83 | 120.00 | 117.15 |
| 1 | A | 516 | PSU | C6-N1-C2 | 3.31 | 120.65 | 115.36 |
| 1 | A | 1541 | PSU | C6-N1-C2 | 3.67 | 121.23 | 115.36 |
| 1 | A | 1207 | 2MG | C6-N1-C2 | 3.86 | 122.09 | 115.18 |
| 1 | A | 1541 | PSU | O4'-C1'-C5 | 3.90 | 115.97 | 109.93 |
| 1 | A | 527 | 7MG | N3-C4-N9 | 4.12 | 132.24 | 126.98 |
| 1 | A | 1541 | PSU | C4-N3-C2 | 5.50 | 119.83 | 115.14 |
| 1 | A | 966 | M2G | C6-N1-C2 | 5.64 | 122.89 | 116.18 |
| 1 | A | 516 | PSU | C4-N3-C2 | 6.12 | 120.35 | 115.14 |
| 1 | A | 1540 | PSU | C4-N3-C2 | 7.09 | 121.18 | 115.14 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 54 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1 | A | 1207 | 2MG | 3 | 0 |
| 1 | A | 1400 | 5MC | 3 | 0 |
| 1 | A | 1402 | 4OC | 4 | 0 |
| 1 | A | 1404 | 5MC | 1 | 0 |
| 1 | A | 1407 | 5MC | 3 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|---------|------|---------|--------------|
| 1 | A | 1498 | UR3 | 9 | 0 |
| 1 | A | 1518[A] | MA6 | 3 | 0 |
| 1 | A | 1518[B] | MA6 | 9 | 0 |
| 1 | A | 1519[A] | MA6 | 3 | 0 |
| 1 | A | 1519[B] | MA6 | 7 | 0 |
| 1 | A | 1540 | PSU | 6 | 0 |
| 1 | A | 1541 | PSU | 3 | 0 |
| 1 | A | 527 | 7MG | 2 | 0 |
| 1 | A | 966 | M2G | 3 | 0 |
| 1 | A | 967 | 5MC | 3 | 0 |
| 12 | L | 92 | 0TD | 3 | 0 |

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 275 ligands modelled in this entry, 274 are monoatomic - leaving 1 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 25 | SRY | A | 1860 | - | 39,42,42 | 2.32 | 9 (23%) | 47,63,63 | 1.95 | 9 (19%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 25 | SRY | A | 1860 | - | - | 0/20/87/87 | 0/3/3/3 |

All (9) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 25 | A | 1860 | SRY | O53-C53 | -3.45 | 1.35 | 1.44 |
| 25 | A | 1860 | SRY | C23-N23 | -2.97 | 1.42 | 1.47 |
| 25 | A | 1860 | SRY | O32-C32 | -2.50 | 1.40 | 1.44 |
| 25 | A | 1860 | SRY | O51-C51 | -2.38 | 1.37 | 1.43 |
| 25 | A | 1860 | SRY | C21-C11 | -2.33 | 1.48 | 1.53 |
| 25 | A | 1860 | SRY | CD1-NE1 | 2.28 | 1.44 | 1.34 |
| 25 | A | 1860 | SRY | CA1-NB1 | 2.54 | 1.45 | 1.34 |
| 25 | A | 1860 | SRY | CA1-N11 | 7.10 | 1.45 | 1.33 |
| 25 | A | 1860 | SRY | CD1-N31 | 9.04 | 1.49 | 1.33 |

All (9) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25 | A | 1860 | SRY | C13-O13-C22 | -7.47 | 103.22 | 116.28 |
| 25 | A | 1860 | SRY | CI3-N23-C23 | -4.77 | 107.43 | 114.38 |
| 25 | A | 1860 | SRY | C12-O42-C42 | -4.64 | 101.02 | 108.42 |
| 25 | A | 1860 | SRY | C61-C11-N11 | -3.90 | 103.10 | 110.58 |
| 25 | A | 1860 | SRY | C43-C33-C23 | -3.46 | 105.21 | 110.33 |
| 25 | A | 1860 | SRY | C63-C53-C43 | -2.48 | 107.12 | 112.99 |
| 25 | A | 1860 | SRY | O41-C41-C51 | 2.55 | 114.11 | 107.27 |
| 25 | A | 1860 | SRY | O53-C53-C43 | 2.61 | 114.47 | 109.69 |
| 25 | A | 1860 | SRY | O13-C13-C23 | 3.18 | 114.01 | 108.28 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 9 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 25 | A | 1860 | SRY | 9 | 0 |

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|----------|
| 1 | A | 1498/1522 (98%) | -0.24 | 20 (1%) 77 72 | 63, 101, 189, 333 | 0 |
| 2 | B | 236/256 (92%) | -0.33 | 1 (0%) 92 90 | 93, 136, 194, 231 | 0 |
| 3 | C | 207/239 (86%) | -0.35 | 1 (0%) 90 88 | 106, 142, 183, 216 | 0 |
| 4 | D | 208/209 (99%) | -0.29 | 7 (3%) 45 42 | 77, 113, 175, 202 | 0 |
| 5 | E | 151/162 (93%) | -0.44 | 1 (0%) 87 84 | 68, 95, 131, 177 | 0 |
| 6 | F | 101/101 (100%) | -0.44 | 1 (0%) 82 78 | 93, 133, 164, 185 | 0 |
| 7 | G | 155/156 (99%) | -0.34 | 2 (1%) 77 72 | 90, 120, 183, 219 | 0 |
| 8 | H | 138/138 (100%) | -0.55 | 0 100 100 | 62, 85, 115, 146 | 0 |
| 9 | I | 127/128 (99%) | -0.29 | 0 100 100 | 95, 144, 180, 216 | 0 |
| 10 | J | 99/105 (94%) | -0.01 | 5 (5%) 28 27 | 105, 165, 237, 271 | 0 |
| 11 | K | 119/129 (92%) | -0.26 | 2 (1%) 70 66 | 72, 101, 148, 212 | 0 |
| 12 | L | 124/135 (91%) | -0.33 | 2 (1%) 72 68 | 64, 110, 146, 220 | 0 |
| 13 | M | 118/126 (93%) | -0.59 | 0 100 100 | 92, 124, 162, 204 | 0 |
| 14 | N | 60/61 (98%) | -0.28 | 2 (3%) 46 43 | 107, 133, 172, 248 | 0 |
| 15 | O | 88/89 (98%) | -0.45 | 1 (1%) 80 76 | 68, 102, 144, 210 | 0 |
| 16 | P | 84/88 (95%) | -0.45 | 2 (2%) 59 55 | 75, 96, 122, 171 | 0 |
| 17 | Q | 100/105 (95%) | -0.34 | 0 100 100 | 63, 89, 126, 182 | 0 |
| 18 | R | 73/88 (82%) | -0.27 | 3 (4%) 37 35 | 86, 109, 197, 245 | 0 |
| 19 | S | 81/93 (87%) | -0.27 | 2 (2%) 57 53 | 120, 154, 199, 254 | 0 |
| 20 | T | 99/106 (93%) | -0.61 | 0 100 100 | 73, 96, 140, 176 | 0 |
| 21 | U | 25/27 (92%) | -0.37 | 0 100 100 | 101, 121, 153, 171 | 0 |
| 22 | V | 3/3 (100%) | 2.48 | 2 (66%) 0 0 | 191, 191, 198, 226 | 3 (100%) |
| 23 | W | 15/15 (100%) | 3.28 | 11 (73%) 0 0 | 194, 222, 273, 301 | 8 (53%) |
| All | All | 3909/4081 (95%) | -0.30 | 65 (1%) 70 66 | 62, 112, 188, 333 | 11 (0%) |

All (65) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 12 | L | 129 | ALA | 7.4 |
| 11 | K | 129 | SER | 6.8 |
| 23 | W | 28 | G | 6.6 |
| 18 | R | 17 | SER | 6.1 |
| 23 | W | 42 | C | 5.6 |
| 18 | R | 16 | PRO | 5.1 |
| 10 | J | 33 | GLN | 5.1 |
| 11 | K | 128 | ALA | 4.8 |
| 23 | W | 41 | C | 4.4 |
| 23 | W | 29 | G | 4.2 |
| 12 | L | 128 | ALA | 3.8 |
| 10 | J | 90 | LEU | 3.7 |
| 23 | W | 30 | G | 3.7 |
| 1 | A | 1539 | C | 3.7 |
| 4 | D | 31 | CYS | 3.6 |
| 23 | W | 38 | A | 3.6 |
| 23 | W | 40 | C | 3.6 |
| 16 | P | 84 | ALA | 3.5 |
| 1 | A | 1129 | C | 3.4 |
| 18 | R | 18 | ARG | 3.3 |
| 23 | W | 39 | U | 3.3 |
| 4 | D | 23 | GLY | 3.3 |
| 22 | V | 3 | U | 3.2 |
| 15 | O | 89 | GLY | 3.2 |
| 23 | W | 34 | G | 3.1 |
| 19 | S | 27 | GLU | 3.1 |
| 1 | A | 1029 | C | 3.1 |
| 5 | E | 155 | GLU | 3.1 |
| 1 | A | 1024 | G | 3.1 |
| 4 | D | 27 | TYR | 3.0 |
| 1 | A | 1002 | G | 3.0 |
| 10 | J | 32 | ALA | 3.0 |
| 1 | A | 841 | U | 2.8 |
| 1 | A | 1037 | C | 2.8 |
| 1 | A | 1038 | C | 2.8 |
| 1 | A | 1036 | G | 2.8 |
| 4 | D | 9 | CYS | 2.8 |
| 6 | F | 101 | ALA | 2.7 |
| 1 | A | 1034 | G | 2.7 |
| 22 | V | 2 | U | 2.6 |
| 1 | A | 1000 | U | 2.5 |
| 1 | A | 1001 | A | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 23 | W | 31 | A | 2.5 |
| 7 | G | 156 | TRP | 2.5 |
| 3 | C | 60 | ALA | 2.4 |
| 4 | D | 20 | TYR | 2.4 |
| 4 | D | 26 | CYS | 2.4 |
| 16 | P | 83 | GLU | 2.4 |
| 19 | S | 28 | LYS | 2.4 |
| 14 | N | 12 | ARG | 2.3 |
| 1 | A | 1025 | U | 2.3 |
| 1 | A | 848 | C | 2.3 |
| 23 | W | 33 | U | 2.3 |
| 1 | A | 1027 | C | 2.3 |
| 1 | A | 1006 | C | 2.3 |
| 4 | D | 35 | ARG | 2.3 |
| 14 | N | 13 | THR | 2.2 |
| 1 | A | 1443 | G | 2.1 |
| 1 | A | 1533 | C | 2.1 |
| 10 | J | 34 | VAL | 2.1 |
| 10 | J | 89 | ASP | 2.1 |
| 1 | A | 1033 | G | 2.1 |
| 7 | G | 81 | GLY | 2.1 |
| 2 | B | 229 | VAL | 2.0 |
| 1 | A | 999 | C | 2.0 |

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|---------|-------|------|------|----------------------------|-------|
| 1 | PSU | A | 1541 | 20/21 | 0.71 | 0.47 | 188,196,202,203 | 0 |
| 1 | PSU | A | 1540 | 20/21 | 0.72 | 0.47 | 193,205,213,214 | 0 |
| 1 | 5MC | A | 1400 | 21/22 | 0.92 | 0.23 | 71,102,119,121 | 0 |
| 1 | M2G | A | 966 | 25/26 | 0.95 | 0.15 | 88,105,117,123 | 0 |
| 1 | MA6 | A | 1518[B] | 24/25 | 0.95 | 0.19 | 79,88,110,112 | 24 |
| 1 | MA6 | A | 1518[A] | 24/25 | 0.95 | 0.19 | 81,85,92,101 | 24 |
| 1 | UR3 | A | 1498 | 21/22 | 0.96 | 0.21 | 87,96,109,112 | 0 |
| 1 | 5MC | A | 1407 | 21/22 | 0.96 | 0.23 | 107,119,130,134 | 0 |
| 1 | 4OC | A | 1402 | 22/23 | 0.97 | 0.18 | 89,101,107,111 | 0 |
| 1 | MA6 | A | 1519[A] | 24/25 | 0.97 | 0.17 | 77,81,91,95 | 24 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|---------|-------|------|------|-----------------------------|-------|
| 12 | 0TD | L | 92 | 10/11 | 0.97 | 0.15 | 83,93,97,207 | 0 |
| 1 | 2MG | A | 1207 | 24/25 | 0.97 | 0.15 | 120,123,131,135 | 0 |
| 1 | MA6 | A | 1519[B] | 24/25 | 0.97 | 0.17 | 76,83,90,91 | 24 |
| 1 | 5MC | A | 1404 | 21/22 | 0.98 | 0.15 | 84,88,103,117 | 0 |
| 1 | 5MC | A | 967 | 21/22 | 0.98 | 0.13 | 90,98,107,115 | 0 |
| 1 | 7MG | A | 527 | 24/25 | 0.98 | 0.13 | 66,86,94,104 | 0 |
| 1 | PSU | A | 516 | 20/21 | 0.98 | 0.15 | 120,125,133,136 | 0 |

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 24 | MG | A | 1853 | 1/1 | 0.32 | 0.23 | 96,96,96,96 | 0 |
| 24 | MG | A | 1746 | 1/1 | 0.42 | 0.48 | 99,99,99,99 | 0 |
| 24 | MG | A | 1779 | 1/1 | 0.56 | 1.20 | 94,94,94,94 | 0 |
| 24 | MG | A | 1825 | 1/1 | 0.62 | 0.41 | 401,401,401,401 | 0 |
| 24 | MG | A | 1659 | 1/1 | 0.65 | 0.51 | 121,121,121,121 | 0 |
| 24 | MG | A | 1794 | 1/1 | 0.66 | 0.47 | 120,120,120,120 | 0 |
| 24 | MG | A | 1790 | 1/1 | 0.67 | 0.61 | 88,88,88,88 | 0 |
| 24 | MG | A | 1731 | 1/1 | 0.69 | 0.67 | 114,114,114,114 | 0 |
| 24 | MG | A | 1722 | 1/1 | 0.70 | 0.43 | 118,118,118,118 | 0 |
| 24 | MG | A | 1711 | 1/1 | 0.70 | 0.52 | 109,109,109,109 | 0 |
| 24 | MG | A | 1808 | 1/1 | 0.70 | 0.44 | 377,377,377,377 | 0 |
| 24 | MG | A | 1749 | 1/1 | 0.71 | 0.63 | 98,98,98,98 | 0 |
| 24 | MG | A | 1851 | 1/1 | 0.72 | 0.68 | 92,92,92,92 | 0 |
| 24 | MG | A | 1762 | 1/1 | 0.73 | 0.27 | 83,83,83,83 | 0 |
| 24 | MG | A | 1812 | 1/1 | 0.73 | 0.23 | 290,290,290,290 | 0 |
| 24 | MG | A | 1768 | 1/1 | 0.73 | 0.51 | 99,99,99,99 | 0 |
| 24 | MG | A | 1697 | 1/1 | 0.74 | 1.14 | 102,102,102,102 | 0 |
| 24 | MG | F | 201 | 1/1 | 0.74 | 0.45 | 79,79,79,79 | 0 |
| 24 | MG | A | 1732 | 1/1 | 0.75 | 0.71 | 97,97,97,97 | 0 |
| 24 | MG | A | 1633 | 1/1 | 0.75 | 0.15 | 85,85,85,85 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 24 | MG | A | 1795 | 1/1 | 0.76 | 0.41 | 85,85,85,85 | 0 |
| 24 | MG | A | 1646 | 1/1 | 0.76 | 0.37 | 79,79,79,79 | 0 |
| 24 | MG | A | 1765 | 1/1 | 0.77 | 0.11 | 93,93,93,93 | 0 |
| 24 | MG | A | 1777 | 1/1 | 0.78 | 0.39 | 100,100,100,100 | 0 |
| 24 | MG | N | 102 | 1/1 | 0.78 | 0.63 | 99,99,99,99 | 0 |
| 24 | MG | A | 1856 | 1/1 | 0.78 | 0.15 | 104,104,104,104 | 0 |
| 24 | MG | A | 1747 | 1/1 | 0.79 | 0.46 | 111,111,111,111 | 0 |
| 24 | MG | A | 1615 | 1/1 | 0.79 | 0.44 | 72,72,72,72 | 0 |
| 24 | MG | A | 1730 | 1/1 | 0.80 | 0.42 | 90,90,90,90 | 0 |
| 24 | MG | A | 1673 | 1/1 | 0.80 | 0.36 | 102,102,102,102 | 0 |
| 24 | MG | A | 1781 | 1/1 | 0.80 | 0.42 | 75,75,75,75 | 0 |
| 24 | MG | A | 1815 | 1/1 | 0.81 | 0.29 | 309,309,309,309 | 0 |
| 24 | MG | A | 1727 | 1/1 | 0.81 | 0.29 | 79,79,79,79 | 0 |
| 24 | MG | A | 1683 | 1/1 | 0.81 | 0.60 | 110,110,110,110 | 0 |
| 24 | MG | L | 201 | 1/1 | 0.81 | 0.14 | 81,81,81,81 | 0 |
| 24 | MG | A | 1848 | 1/1 | 0.81 | 0.37 | 87,87,87,87 | 0 |
| 24 | MG | A | 1724 | 1/1 | 0.82 | 0.23 | 99,99,99,99 | 0 |
| 24 | MG | A | 1773 | 1/1 | 0.82 | 0.78 | 88,88,88,88 | 0 |
| 24 | MG | A | 1740 | 1/1 | 0.82 | 0.32 | 89,89,89,89 | 0 |
| 24 | MG | G | 201 | 1/1 | 0.82 | 0.64 | 116,116,116,116 | 0 |
| 24 | MG | A | 1827 | 1/1 | 0.82 | 0.27 | 244,244,244,244 | 0 |
| 24 | MG | A | 1687 | 1/1 | 0.82 | 0.28 | 116,116,116,116 | 0 |
| 24 | MG | A | 1761 | 1/1 | 0.82 | 0.24 | 107,107,107,107 | 0 |
| 24 | MG | A | 1852 | 1/1 | 0.82 | 0.39 | 84,84,84,84 | 0 |
| 24 | MG | A | 1789 | 1/1 | 0.83 | 0.50 | 92,92,92,92 | 0 |
| 24 | MG | A | 1855 | 1/1 | 0.83 | 0.37 | 115,115,115,115 | 0 |
| 24 | MG | A | 1767 | 1/1 | 0.83 | 0.57 | 64,64,64,64 | 0 |
| 24 | MG | A | 1857 | 1/1 | 0.83 | 0.29 | 89,89,89,89 | 0 |
| 24 | MG | A | 1655 | 1/1 | 0.83 | 0.35 | 210,210,210,210 | 0 |
| 24 | MG | A | 1858 | 1/1 | 0.83 | 0.32 | 98,98,98,98 | 0 |
| 24 | MG | A | 1672 | 1/1 | 0.84 | 0.89 | 92,92,92,92 | 0 |
| 24 | MG | A | 1771 | 1/1 | 0.84 | 0.41 | 82,82,82,82 | 0 |
| 24 | MG | A | 1709 | 1/1 | 0.84 | 0.35 | 250,250,250,250 | 0 |
| 24 | MG | A | 1816 | 1/1 | 0.84 | 0.28 | 318,318,318,318 | 0 |
| 24 | MG | A | 1609 | 1/1 | 0.84 | 0.16 | 74,74,74,74 | 0 |
| 24 | MG | A | 1757 | 1/1 | 0.84 | 0.37 | 83,83,83,83 | 0 |
| 24 | MG | A | 1784 | 1/1 | 0.84 | 0.78 | 92,92,92,92 | 0 |
| 24 | MG | A | 1809 | 1/1 | 0.84 | 0.21 | 355,355,355,355 | 0 |
| 24 | MG | D | 303 | 1/1 | 0.85 | 0.94 | 97,97,97,97 | 0 |
| 24 | MG | A | 1634 | 1/1 | 0.85 | 0.27 | 243,243,243,243 | 0 |
| 24 | MG | P | 103 | 1/1 | 0.85 | 0.16 | 93,93,93,93 | 0 |
| 24 | MG | A | 1801 | 1/1 | 0.85 | 0.25 | 248,248,248,248 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 24 | MG | A | 1819 | 1/1 | 0.85 | 0.78 | 371,371,371,371 | 0 |
| 24 | MG | A | 1725 | 1/1 | 0.85 | 0.59 | 109,109,109,109 | 0 |
| 24 | MG | A | 1755 | 1/1 | 0.86 | 0.13 | 131,131,131,131 | 0 |
| 24 | MG | A | 1850 | 1/1 | 0.86 | 0.59 | 117,117,117,117 | 0 |
| 24 | MG | A | 1753 | 1/1 | 0.86 | 0.81 | 110,110,110,110 | 0 |
| 24 | MG | A | 1772 | 1/1 | 0.86 | 0.37 | 78,78,78,78 | 0 |
| 24 | MG | A | 1744 | 1/1 | 0.86 | 0.29 | 109,109,109,109 | 0 |
| 24 | MG | A | 1726 | 1/1 | 0.87 | 0.28 | 86,86,86,86 | 0 |
| 24 | MG | A | 1807 | 1/1 | 0.87 | 0.31 | 397,397,397,397 | 0 |
| 24 | MG | A | 1800 | 1/1 | 0.87 | 0.32 | 203,203,203,203 | 0 |
| 24 | MG | A | 1656 | 1/1 | 0.87 | 0.28 | 177,177,177,177 | 0 |
| 24 | MG | A | 1770 | 1/1 | 0.87 | 0.78 | 98,98,98,98 | 0 |
| 24 | MG | H | 201 | 1/1 | 0.87 | 0.26 | 63,63,63,63 | 0 |
| 24 | MG | A | 1682 | 1/1 | 0.87 | 0.28 | 228,228,228,228 | 0 |
| 24 | MG | A | 1791 | 1/1 | 0.87 | 0.20 | 109,109,109,109 | 0 |
| 24 | MG | A | 1766 | 1/1 | 0.87 | 0.27 | 95,95,95,95 | 0 |
| 24 | MG | A | 1622 | 1/1 | 0.88 | 0.78 | 75,75,75,75 | 0 |
| 24 | MG | A | 1657 | 1/1 | 0.88 | 0.31 | 189,189,189,189 | 0 |
| 24 | MG | A | 1641 | 1/1 | 0.88 | 0.42 | 92,92,92,92 | 0 |
| 24 | MG | A | 1718 | 1/1 | 0.89 | 0.24 | 220,220,220,220 | 0 |
| 24 | MG | A | 1818 | 1/1 | 0.89 | 0.25 | 249,249,249,249 | 0 |
| 24 | MG | P | 102 | 1/1 | 0.89 | 0.73 | 96,96,96,96 | 0 |
| 24 | MG | A | 1836 | 1/1 | 0.89 | 0.32 | 300,300,300,300 | 0 |
| 24 | MG | A | 1666 | 1/1 | 0.89 | 0.19 | 103,103,103,103 | 0 |
| 24 | MG | A | 1792 | 1/1 | 0.89 | 0.23 | 91,91,91,91 | 0 |
| 24 | MG | A | 1798 | 1/1 | 0.89 | 0.20 | 115,115,115,115 | 0 |
| 24 | MG | A | 1739 | 1/1 | 0.89 | 0.65 | 103,103,103,103 | 0 |
| 24 | MG | A | 1769 | 1/1 | 0.89 | 0.27 | 92,92,92,92 | 0 |
| 24 | MG | A | 1625 | 1/1 | 0.89 | 0.25 | 194,194,194,194 | 0 |
| 24 | MG | A | 1676 | 1/1 | 0.89 | 0.21 | 138,138,138,138 | 0 |
| 24 | MG | A | 1859 | 1/1 | 0.89 | 0.54 | 94,94,94,94 | 0 |
| 24 | MG | A | 1774 | 1/1 | 0.90 | 0.66 | 61,61,61,61 | 0 |
| 24 | MG | A | 1750 | 1/1 | 0.90 | 0.59 | 92,92,92,92 | 0 |
| 24 | MG | A | 1667 | 1/1 | 0.90 | 0.64 | 168,168,168,168 | 0 |
| 24 | MG | A | 1719 | 1/1 | 0.90 | 0.32 | 88,88,88,88 | 0 |
| 24 | MG | A | 1720 | 1/1 | 0.90 | 0.20 | 64,64,64,64 | 0 |
| 24 | MG | A | 1679 | 1/1 | 0.90 | 0.24 | 168,168,168,168 | 0 |
| 24 | MG | A | 1847 | 1/1 | 0.90 | 0.35 | 334,334,334,334 | 0 |
| 24 | MG | A | 1652 | 1/1 | 0.90 | 0.32 | 96,96,96,96 | 0 |
| 24 | MG | A | 1644 | 1/1 | 0.90 | 0.51 | 95,95,95,95 | 0 |
| 24 | MG | A | 1695 | 1/1 | 0.91 | 0.44 | 88,88,88,88 | 0 |
| 24 | MG | A | 1603 | 1/1 | 0.91 | 0.23 | 97,97,97,97 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 24 | MG | A | 1658 | 1/1 | 0.91 | 0.18 | 102,102,102,102 | 0 |
| 24 | MG | A | 1689 | 1/1 | 0.91 | 0.16 | 132,132,132,132 | 0 |
| 24 | MG | A | 1803 | 1/1 | 0.91 | 0.54 | 324,324,324,324 | 0 |
| 24 | MG | A | 1752 | 1/1 | 0.91 | 0.24 | 90,90,90,90 | 0 |
| 24 | MG | A | 1745 | 1/1 | 0.91 | 0.69 | 82,82,82,82 | 0 |
| 24 | MG | A | 1653 | 1/1 | 0.91 | 0.65 | 89,89,89,89 | 0 |
| 24 | MG | A | 1764 | 1/1 | 0.91 | 0.27 | 104,104,104,104 | 0 |
| 24 | MG | A | 1751 | 1/1 | 0.91 | 0.25 | 83,83,83,83 | 0 |
| 24 | MG | A | 1717 | 1/1 | 0.91 | 0.53 | 125,125,125,125 | 0 |
| 24 | MG | A | 1661 | 1/1 | 0.91 | 0.22 | 121,121,121,121 | 0 |
| 24 | MG | A | 1688 | 1/1 | 0.92 | 0.15 | 120,120,120,120 | 0 |
| 24 | MG | A | 1817 | 1/1 | 0.92 | 0.28 | 180,180,180,180 | 0 |
| 24 | MG | A | 1756 | 1/1 | 0.92 | 0.18 | 101,101,101,101 | 0 |
| 24 | MG | A | 1780 | 1/1 | 0.92 | 0.70 | 80,80,80,80 | 0 |
| 24 | MG | A | 1685 | 1/1 | 0.92 | 0.26 | 134,134,134,134 | 0 |
| 24 | MG | A | 1849 | 1/1 | 0.92 | 0.25 | 74,74,74,74 | 0 |
| 24 | MG | A | 1742 | 1/1 | 0.92 | 0.35 | 89,89,89,89 | 0 |
| 24 | MG | A | 1824 | 1/1 | 0.92 | 0.17 | 202,202,202,202 | 0 |
| 24 | MG | Q | 201 | 1/1 | 0.92 | 0.26 | 84,84,84,84 | 0 |
| 24 | MG | A | 1680 | 1/1 | 0.92 | 0.22 | 250,250,250,250 | 0 |
| 24 | MG | A | 1737 | 1/1 | 0.92 | 0.35 | 81,81,81,81 | 0 |
| 24 | MG | A | 1793 | 1/1 | 0.92 | 0.46 | 80,80,80,80 | 0 |
| 24 | MG | A | 1670 | 1/1 | 0.92 | 0.21 | 109,109,109,109 | 0 |
| 24 | MG | A | 1681 | 1/1 | 0.92 | 0.10 | 160,160,160,160 | 0 |
| 24 | MG | A | 1785 | 1/1 | 0.92 | 0.41 | 92,92,92,92 | 0 |
| 24 | MG | A | 1854 | 1/1 | 0.92 | 0.64 | 89,89,89,89 | 0 |
| 24 | MG | A | 1845 | 1/1 | 0.92 | 0.20 | 293,293,293,293 | 0 |
| 24 | MG | A | 1802 | 1/1 | 0.93 | 0.42 | 206,206,206,206 | 0 |
| 24 | MG | E | 201 | 1/1 | 0.93 | 0.57 | 87,87,87,87 | 0 |
| 24 | MG | A | 1705 | 1/1 | 0.93 | 0.43 | 69,69,69,69 | 0 |
| 24 | MG | A | 1728 | 1/1 | 0.93 | 0.17 | 95,95,95,95 | 0 |
| 24 | MG | A | 1844 | 1/1 | 0.93 | 0.44 | 310,310,310,310 | 0 |
| 24 | MG | A | 1714 | 1/1 | 0.93 | 0.53 | 99,99,99,99 | 0 |
| 24 | MG | A | 1830 | 1/1 | 0.93 | 0.25 | 273,273,273,273 | 0 |
| 24 | MG | A | 1786 | 1/1 | 0.93 | 0.31 | 96,96,96,96 | 0 |
| 24 | MG | A | 1796 | 1/1 | 0.93 | 0.28 | 98,98,98,98 | 0 |
| 24 | MG | A | 1639 | 1/1 | 0.93 | 0.32 | 73,73,73,73 | 0 |
| 24 | MG | A | 1684 | 1/1 | 0.93 | 0.28 | 90,90,90,90 | 0 |
| 24 | MG | A | 1846 | 1/1 | 0.93 | 0.13 | 225,225,225,225 | 0 |
| 24 | MG | A | 1826 | 1/1 | 0.93 | 0.28 | 354,354,354,354 | 0 |
| 24 | MG | A | 1782 | 1/1 | 0.93 | 0.17 | 65,65,65,65 | 0 |
| 24 | MG | A | 1813 | 1/1 | 0.94 | 0.27 | 181,181,181,181 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 24 | MG | A | 1797 | 1/1 | 0.94 | 0.19 | 94,94,94,94 | 0 |
| 24 | MG | A | 1810 | 1/1 | 0.94 | 0.34 | 295,295,295,295 | 0 |
| 24 | MG | A | 1805 | 1/1 | 0.94 | 0.39 | 280,280,280,280 | 0 |
| 24 | MG | A | 1837 | 1/1 | 0.94 | 0.14 | 244,244,244,244 | 0 |
| 24 | MG | A | 1748 | 1/1 | 0.94 | 0.26 | 77,77,77,77 | 0 |
| 24 | MG | A | 1637 | 1/1 | 0.94 | 0.20 | 86,86,86,86 | 0 |
| 24 | MG | A | 1638 | 1/1 | 0.94 | 0.32 | 87,87,87,87 | 0 |
| 24 | MG | A | 1832 | 1/1 | 0.94 | 0.18 | 112,112,112,112 | 0 |
| 24 | MG | A | 1618 | 1/1 | 0.94 | 0.60 | 85,85,85,85 | 0 |
| 24 | MG | A | 1833 | 1/1 | 0.94 | 0.15 | 335,335,335,335 | 0 |
| 24 | MG | A | 1806 | 1/1 | 0.94 | 0.51 | 211,211,211,211 | 0 |
| 24 | MG | A | 1723 | 1/1 | 0.94 | 0.22 | 117,117,117,117 | 0 |
| 24 | MG | A | 1702 | 1/1 | 0.94 | 0.11 | 163,163,163,163 | 0 |
| 24 | MG | A | 1620 | 1/1 | 0.94 | 0.19 | 141,141,141,141 | 0 |
| 24 | MG | A | 1834 | 1/1 | 0.94 | 0.41 | 231,231,231,231 | 0 |
| 24 | MG | A | 1776 | 1/1 | 0.94 | 0.23 | 96,96,96,96 | 0 |
| 24 | MG | A | 1692 | 1/1 | 0.94 | 0.17 | 119,119,119,119 | 0 |
| 24 | MG | A | 1678 | 1/1 | 0.94 | 0.19 | 133,133,133,133 | 0 |
| 24 | MG | A | 1700 | 1/1 | 0.94 | 0.19 | 272,272,272,272 | 0 |
| 24 | MG | A | 1698 | 1/1 | 0.94 | 0.16 | 218,218,218,218 | 0 |
| 24 | MG | A | 1754 | 1/1 | 0.95 | 0.24 | 105,105,105,105 | 0 |
| 24 | MG | A | 1699 | 1/1 | 0.95 | 0.49 | 100,100,100,100 | 0 |
| 24 | MG | A | 1701 | 1/1 | 0.95 | 0.54 | 73,73,73,73 | 0 |
| 24 | MG | A | 1613 | 1/1 | 0.95 | 0.14 | 88,88,88,88 | 0 |
| 24 | MG | A | 1647 | 1/1 | 0.95 | 0.17 | 127,127,127,127 | 0 |
| 24 | MG | A | 1843 | 1/1 | 0.95 | 0.12 | 115,115,115,115 | 0 |
| 24 | MG | A | 1822 | 1/1 | 0.95 | 0.25 | 209,209,209,209 | 0 |
| 24 | MG | A | 1829 | 1/1 | 0.95 | 0.19 | 267,267,267,267 | 0 |
| 24 | MG | A | 1821 | 1/1 | 0.95 | 0.18 | 178,178,178,178 | 0 |
| 24 | MG | A | 1706 | 1/1 | 0.95 | 0.28 | 174,174,174,174 | 0 |
| 24 | MG | A | 1788 | 1/1 | 0.95 | 0.19 | 84,84,84,84 | 0 |
| 24 | MG | A | 1842 | 1/1 | 0.95 | 0.65 | 334,334,334,334 | 0 |
| 24 | MG | A | 1663 | 1/1 | 0.95 | 0.33 | 94,94,94,94 | 0 |
| 24 | MG | A | 1840 | 1/1 | 0.95 | 0.21 | 289,289,289,289 | 0 |
| 24 | MG | A | 1804 | 1/1 | 0.95 | 0.26 | 304,304,304,304 | 0 |
| 24 | MG | A | 1733 | 1/1 | 0.95 | 0.34 | 68,68,68,68 | 0 |
| 24 | MG | A | 1734 | 1/1 | 0.95 | 0.19 | 99,99,99,99 | 0 |
| 24 | MG | A | 1799 | 1/1 | 0.95 | 0.29 | 277,277,277,277 | 0 |
| 24 | MG | A | 1696 | 1/1 | 0.95 | 0.39 | 99,99,99,99 | 0 |
| 24 | MG | A | 1839 | 1/1 | 0.96 | 0.23 | 205,205,205,205 | 1 |
| 24 | MG | A | 1759 | 1/1 | 0.96 | 0.30 | 75,75,75,75 | 0 |
| 24 | MG | A | 1831 | 1/1 | 0.96 | 0.33 | 160,160,160,160 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 24 | MG | A | 1629 | 1/1 | 0.96 | 0.06 | 151,151,151,151 | 0 |
| 24 | MG | A | 1708 | 1/1 | 0.96 | 0.12 | 211,211,211,211 | 0 |
| 24 | MG | A | 1654 | 1/1 | 0.96 | 0.15 | 97,97,97,97 | 0 |
| 24 | MG | A | 1729 | 1/1 | 0.96 | 0.72 | 111,111,111,111 | 0 |
| 24 | MG | A | 1607 | 1/1 | 0.96 | 0.10 | 102,102,102,102 | 0 |
| 24 | MG | P | 101 | 1/1 | 0.96 | 0.41 | 67,67,67,67 | 0 |
| 24 | MG | A | 1710 | 1/1 | 0.96 | 0.30 | 177,177,177,177 | 0 |
| 24 | MG | A | 1838 | 1/1 | 0.96 | 0.25 | 181,181,181,181 | 0 |
| 24 | MG | A | 1627 | 1/1 | 0.96 | 0.23 | 102,102,102,102 | 0 |
| 24 | MG | A | 1617 | 1/1 | 0.96 | 0.14 | 81,81,81,81 | 0 |
| 24 | MG | A | 1674 | 1/1 | 0.96 | 0.10 | 125,125,125,125 | 0 |
| 24 | MG | A | 1716 | 1/1 | 0.96 | 0.09 | 70,70,70,70 | 0 |
| 25 | SRY | A | 1860 | 40/40 | 0.96 | 0.17 | 60,79,97,101 | 0 |
| 24 | MG | A | 1811 | 1/1 | 0.96 | 0.06 | 121,121,121,121 | 0 |
| 24 | MG | A | 1783 | 1/1 | 0.96 | 0.29 | 89,89,89,89 | 0 |
| 24 | MG | A | 1635 | 1/1 | 0.97 | 0.15 | 75,75,75,75 | 0 |
| 24 | MG | A | 1636 | 1/1 | 0.97 | 0.19 | 94,94,94,94 | 0 |
| 26 | ZN | D | 301 | 1/1 | 0.97 | 0.34 | 114,114,114,114 | 0 |
| 24 | MG | A | 1713 | 1/1 | 0.97 | 0.08 | 112,112,112,112 | 0 |
| 24 | MG | A | 1841 | 1/1 | 0.97 | 0.14 | 266,266,266,266 | 0 |
| 24 | MG | A | 1675 | 1/1 | 0.97 | 0.12 | 223,223,223,223 | 0 |
| 24 | MG | A | 1601 | 1/1 | 0.97 | 0.12 | 86,86,86,86 | 0 |
| 24 | MG | A | 1621 | 1/1 | 0.97 | 0.46 | 131,131,131,131 | 0 |
| 24 | MG | D | 302 | 1/1 | 0.97 | 0.13 | 86,86,86,86 | 0 |
| 24 | MG | S | 101 | 1/1 | 0.97 | 0.22 | 80,80,80,80 | 0 |
| 24 | MG | A | 1645 | 1/1 | 0.97 | 0.09 | 108,108,108,108 | 0 |
| 24 | MG | A | 1758 | 1/1 | 0.97 | 0.15 | 70,70,70,70 | 0 |
| 24 | MG | A | 1778 | 1/1 | 0.97 | 0.33 | 78,78,78,78 | 0 |
| 24 | MG | A | 1721 | 1/1 | 0.97 | 0.21 | 95,95,95,95 | 0 |
| 24 | MG | A | 1665 | 1/1 | 0.97 | 0.15 | 99,99,99,99 | 0 |
| 24 | MG | A | 1823 | 1/1 | 0.97 | 0.22 | 281,281,281,281 | 0 |
| 24 | MG | A | 1691 | 1/1 | 0.97 | 0.19 | 139,139,139,139 | 0 |
| 24 | MG | A | 1835 | 1/1 | 0.97 | 0.16 | 299,299,299,299 | 0 |
| 24 | MG | A | 1763 | 1/1 | 0.97 | 0.16 | 72,72,72,72 | 0 |
| 24 | MG | A | 1820 | 1/1 | 0.97 | 0.30 | 152,152,152,152 | 0 |
| 24 | MG | A | 1690 | 1/1 | 0.97 | 0.35 | 193,193,193,193 | 0 |
| 24 | MG | A | 1604 | 1/1 | 0.97 | 0.10 | 153,153,153,153 | 0 |
| 24 | MG | A | 1671 | 1/1 | 0.98 | 0.33 | 99,99,99,99 | 0 |
| 24 | MG | A | 1787 | 1/1 | 0.98 | 0.15 | 78,78,78,78 | 0 |
| 24 | MG | A | 1602 | 1/1 | 0.98 | 0.11 | 108,108,108,108 | 0 |
| 24 | MG | A | 1611 | 1/1 | 0.98 | 0.14 | 120,120,120,120 | 0 |
| 24 | MG | A | 1606 | 1/1 | 0.98 | 0.29 | 87,87,87,87 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 24 | MG | A | 1648 | 1/1 | 0.98 | 0.10 | 96,96,96,96 | 0 |
| 24 | MG | A | 1738 | 1/1 | 0.98 | 0.24 | 58,58,58,58 | 0 |
| 24 | MG | A | 1712 | 1/1 | 0.98 | 0.16 | 107,107,107,107 | 0 |
| 24 | MG | A | 1741 | 1/1 | 0.98 | 0.20 | 101,101,101,101 | 0 |
| 24 | MG | A | 1736 | 1/1 | 0.98 | 0.14 | 119,119,119,119 | 0 |
| 24 | MG | A | 1669 | 1/1 | 0.98 | 0.43 | 134,134,134,134 | 0 |
| 24 | MG | A | 1608 | 1/1 | 0.98 | 0.48 | 84,84,84,84 | 0 |
| 24 | MG | A | 1628 | 1/1 | 0.98 | 0.43 | 104,104,104,104 | 0 |
| 24 | MG | A | 1760 | 1/1 | 0.98 | 0.15 | 101,101,101,101 | 0 |
| 24 | MG | A | 1612 | 1/1 | 0.98 | 0.19 | 97,97,97,97 | 0 |
| 24 | MG | A | 1614 | 1/1 | 0.98 | 0.19 | 79,79,79,79 | 0 |
| 24 | MG | A | 1814 | 1/1 | 0.98 | 0.07 | 113,113,113,113 | 0 |
| 24 | MG | A | 1610 | 1/1 | 0.98 | 0.14 | 71,71,71,71 | 0 |
| 24 | MG | A | 1650 | 1/1 | 0.98 | 0.08 | 107,107,107,107 | 0 |
| 24 | MG | A | 1686 | 1/1 | 0.98 | 0.14 | 194,194,194,194 | 0 |
| 24 | MG | A | 1735 | 1/1 | 0.98 | 0.38 | 96,96,96,96 | 0 |
| 24 | MG | A | 1630 | 1/1 | 0.98 | 0.06 | 82,82,82,82 | 0 |
| 24 | MG | A | 1662 | 1/1 | 0.98 | 0.17 | 145,145,145,145 | 0 |
| 24 | MG | A | 1668 | 1/1 | 0.98 | 0.19 | 138,138,138,138 | 0 |
| 24 | MG | A | 1743 | 1/1 | 0.98 | 0.07 | 76,76,76,76 | 0 |
| 24 | MG | A | 1640 | 1/1 | 0.98 | 0.07 | 98,98,98,98 | 0 |
| 24 | MG | A | 1642 | 1/1 | 0.98 | 0.04 | 112,112,112,112 | 0 |
| 24 | MG | A | 1664 | 1/1 | 0.98 | 0.35 | 131,131,131,131 | 0 |
| 24 | MG | A | 1619 | 1/1 | 0.98 | 0.14 | 72,72,72,72 | 0 |
| 24 | MG | A | 1660 | 1/1 | 0.98 | 0.06 | 104,104,104,104 | 0 |
| 24 | MG | A | 1707 | 1/1 | 0.99 | 0.27 | 163,163,163,163 | 0 |
| 24 | MG | A | 1704 | 1/1 | 0.99 | 0.26 | 116,116,116,116 | 0 |
| 24 | MG | A | 1616 | 1/1 | 0.99 | 0.04 | 93,93,93,93 | 0 |
| 24 | MG | A | 1677 | 1/1 | 0.99 | 0.11 | 113,113,113,113 | 0 |
| 24 | MG | A | 1693 | 1/1 | 0.99 | 0.11 | 192,192,192,192 | 0 |
| 24 | MG | A | 1703 | 1/1 | 0.99 | 0.26 | 106,106,106,106 | 0 |
| 24 | MG | A | 1828 | 1/1 | 0.99 | 0.15 | 284,284,284,284 | 0 |
| 24 | MG | A | 1624 | 1/1 | 0.99 | 0.26 | 97,97,97,97 | 0 |
| 26 | ZN | N | 101 | 1/1 | 0.99 | 0.11 | 129,129,129,129 | 0 |
| 24 | MG | A | 1651 | 1/1 | 0.99 | 0.14 | 143,143,143,143 | 0 |
| 24 | MG | A | 1631 | 1/1 | 0.99 | 0.13 | 101,101,101,101 | 0 |
| 24 | MG | A | 1632 | 1/1 | 0.99 | 0.12 | 76,76,76,76 | 0 |
| 24 | MG | A | 1605 | 1/1 | 0.99 | 0.08 | 72,72,72,72 | 0 |
| 24 | MG | A | 1643 | 1/1 | 0.99 | 0.26 | 99,99,99,99 | 0 |
| 24 | MG | A | 1715 | 1/1 | 0.99 | 0.13 | 89,89,89,89 | 0 |
| 24 | MG | A | 1649 | 1/1 | 0.99 | 0.30 | 51,51,51,51 | 0 |
| 24 | MG | A | 1623 | 1/1 | 0.99 | 0.12 | 84,84,84,84 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 24 | MG | A | 1694 | 1/1 | 0.99 | 0.14 | 116,116,116,116 | 0 |
| 24 | MG | A | 1626 | 1/1 | 0.99 | 0.20 | 103,103,103,103 | 0 |
| 24 | MG | A | 1775 | 1/1 | 0.99 | 0.10 | 114,114,114,114 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.