



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 3, 2025 – 10:27 PM EST

PDB ID : 4JI5
Title : Crystal Structure of 30S ribosomal subunit from *Thermus thermophilus*
Authors : Demirci, H.; Wang, L.; Murphy IV, F.; Murphy, E.; Carr, J.; Blanchard, S.;
Jogl, G.; Dahlberg, A.E.; Gregory, S.T.
Deposited on : 2013-03-05
Resolution : 3.85 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 types of validation reports are described at

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

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

| | | |
|--------------------------------|---|--|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| Xtriage (Phenix) | : | 1.21 |
| EDS | : | 3.0 |
| Percentile statistics | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| CCP4 | : | 9.0.004 (Gargrove) |
| Density-Fitness | : | 1.0.11 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.40 |

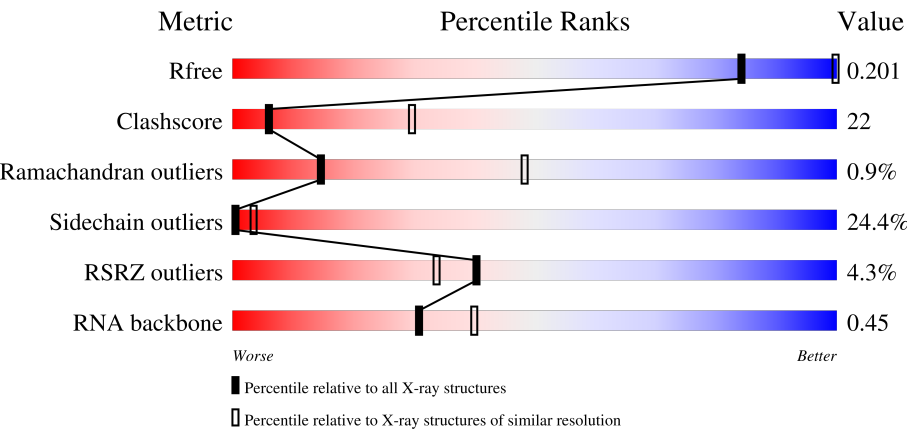
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.85 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} | 164625 | 1056 (4.02-3.70) |
| Clashscore | 180529 | 1117 (4.02-3.70) |
| Ramachandran outliers | 177936 | 1077 (4.02-3.70) |
| Sidechain outliers | 177891 | 1070 (4.02-3.70) |
| RSRZ outliers | 164620 | 1056 (4.02-3.70) |
| RNA backbone | 3690 | 1134 (4.70-3.00) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | A | 1522 | <div><div>3%</div><div>19%</div><div>39%</div><div>33%</div><div>9%</div><div></div></div> |
| 2 | B | 256 | <div><div>2%</div><div>42%</div><div>33%</div><div>14%</div><div>9%</div><div></div></div> |
| 3 | C | 239 | <div><div>2%</div><div>33%</div><div>40%</div><div>12%</div><div>14%</div><div></div></div> |
| 4 | D | 209 | <div><div>10%</div><div>41%</div><div>44%</div><div>15%</div><div></div><div></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 | |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 22 | MG | A | 1630 | - | - | - | X |
| 22 | MG | A | 1632 | - | - | - | X |
| 22 | MG | A | 1745 | - | - | - | X |
| 22 | MG | A | 1749 | - | - | - | X |
| 22 | MG | A | 1757 | - | - | - | X |
| 22 | MG | K | 201 | - | - | - | X |

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 52228 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called RIBOSOMAL PROTEIN S2.

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

- Molecule 3 is a protein called RIBOSOMAL PROTEIN S3.

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

- Molecule 4 is a protein called RIBOSOMAL PROTEIN S4.

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

- Molecule 5 is a protein called RIBOSOMAL PROTEIN S5.

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

- Molecule 6 is a protein called RIBOSOMAL PROTEIN S6.

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

- Molecule 7 is a protein called RIBOSOMAL PROTEIN S7.

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

- Molecule 8 is a protein called RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called RIBOSOMAL PROTEIN S9.

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

- Molecule 10 is a protein called RIBOSOMAL PROTEIN S10.

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

- Molecule 11 is a protein called RIBOSOMAL PROTEIN S11.

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

- Molecule 12 is a protein called RIBOSOMAL PROTEIN S12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | L | 124 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 972 | 612 | 195 | 163 | 2 | | | |

- Molecule 13 is a protein called RIBOSOMAL PROTEIN S13.

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

- Molecule 14 is a protein called RIBOSOMAL PROTEIN S14.

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

- Molecule 15 is a protein called RIBOSOMAL PROTEIN S15.

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

- Molecule 16 is a protein called RIBOSOMAL PROTEIN S16.

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

- Molecule 17 is a protein called RIBOSOMAL PROTEIN S17.

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

- Molecule 18 is a protein called RIBOSOMAL PROTEIN S18.

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

- Molecule 19 is a protein called RIBOSOMAL PROTEIN S19.

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

- Molecule 20 is a protein called RIBOSOMAL PROTEIN S20.

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

- Molecule 21 is a protein called RIBOSOMAL PROTEIN THX.

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

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

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 22 | A | 164 | Total | Mg | 0 | 0 |
| | | | 164 | 164 | | |
| 22 | D | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 22 | E | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 22 | F | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 22 | G | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 22 | H | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 22 | K | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 22 | S | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

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

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

- Molecule 24 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 24 | A | 271 | Total | O | 0 | 0 |
| | | | 271 | 271 | | |

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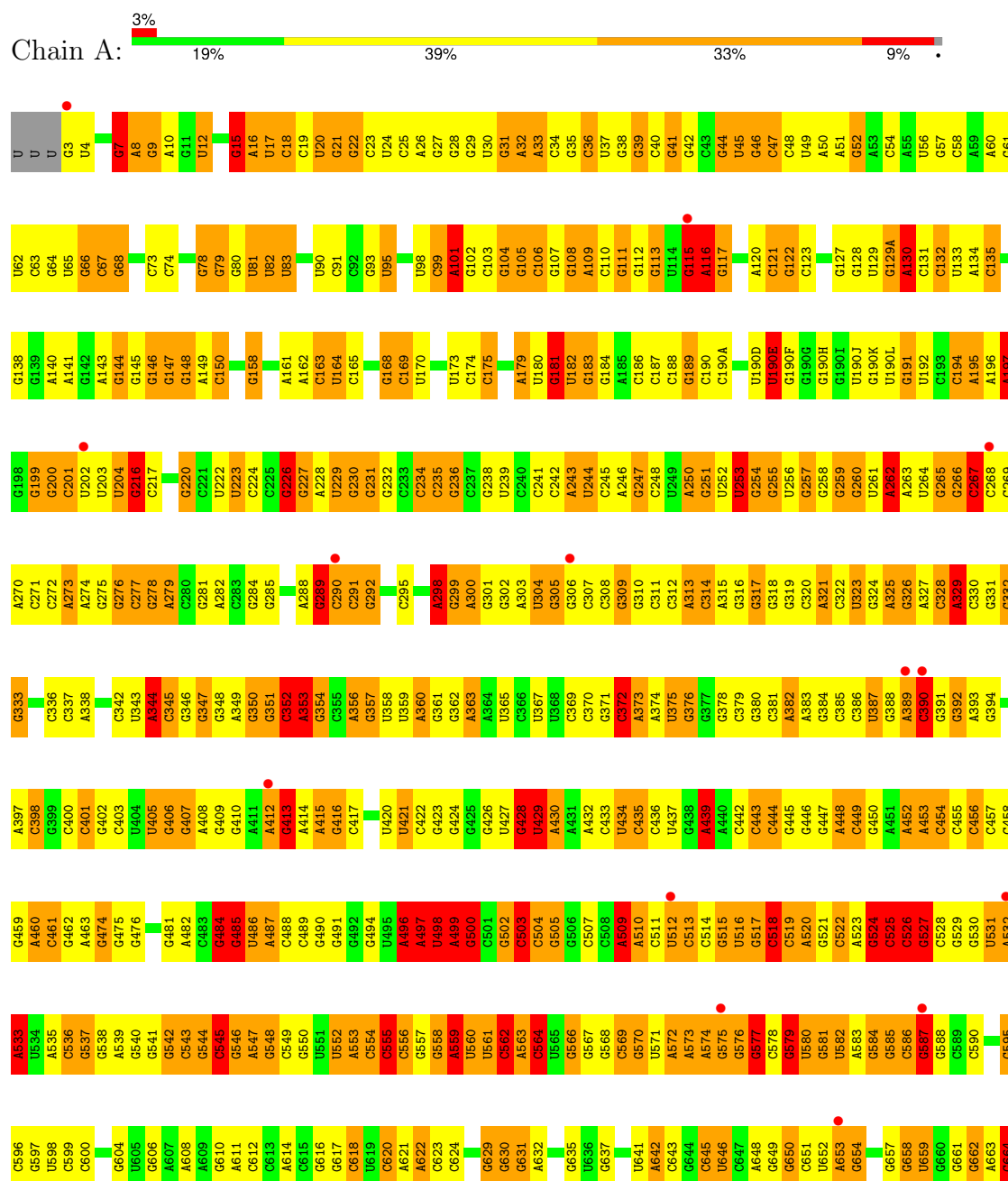
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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 24 | C | 1 | Total 1 | O 1 | 0 | 0 |
| 24 | E | 3 | Total 3 | O 3 | 0 | 0 |
| 24 | L | 1 | Total 1 | O 1 | 0 | 0 |
| 24 | N | 1 | Total 1 | O 1 | 0 | 0 |
| 24 | P | 1 | Total 1 | O 1 | 0 | 0 |
| 24 | T | 1 | Total 1 | O 1 | 0 | 0 |

3 Residue-property plots

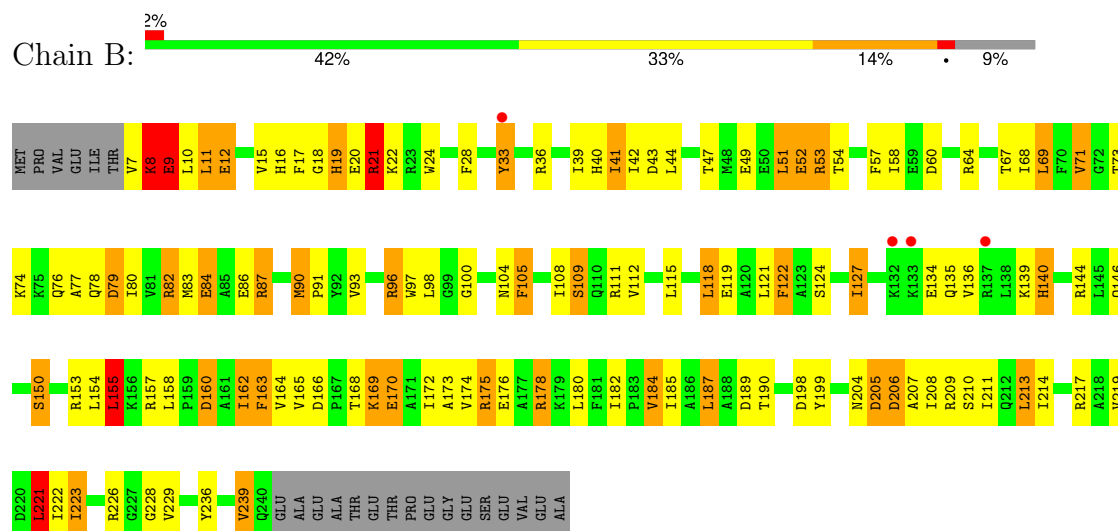
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

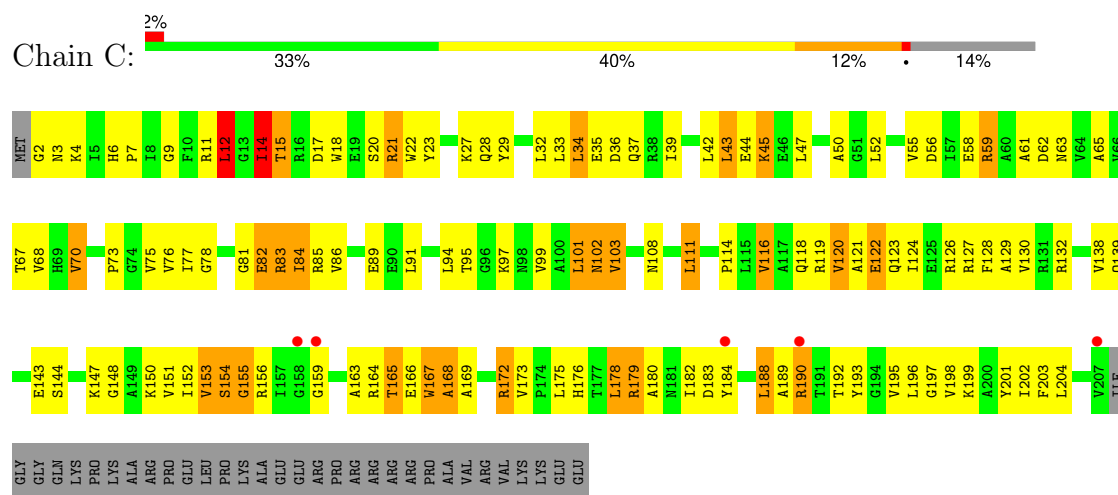




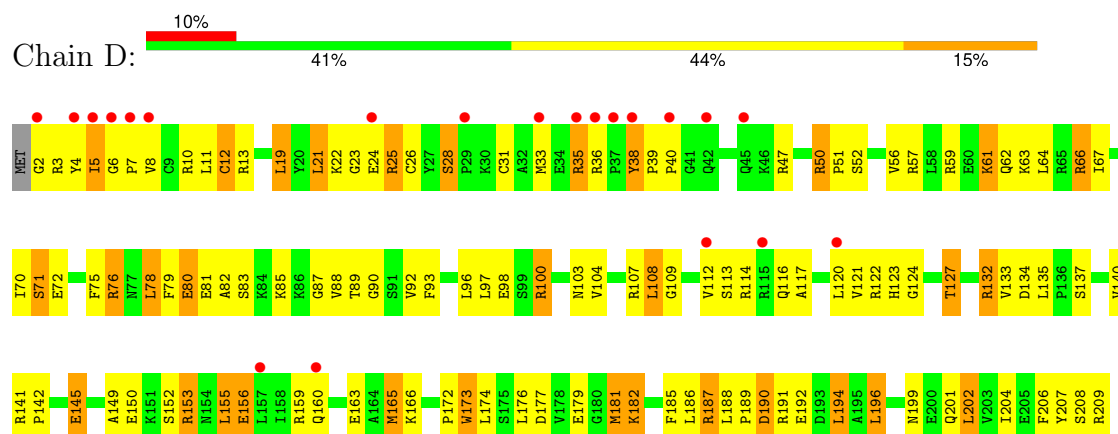
- Molecule 2: RIBOSOMAL PROTEIN S2



- Molecule 3: RIBOSOMAL PROTEIN S3

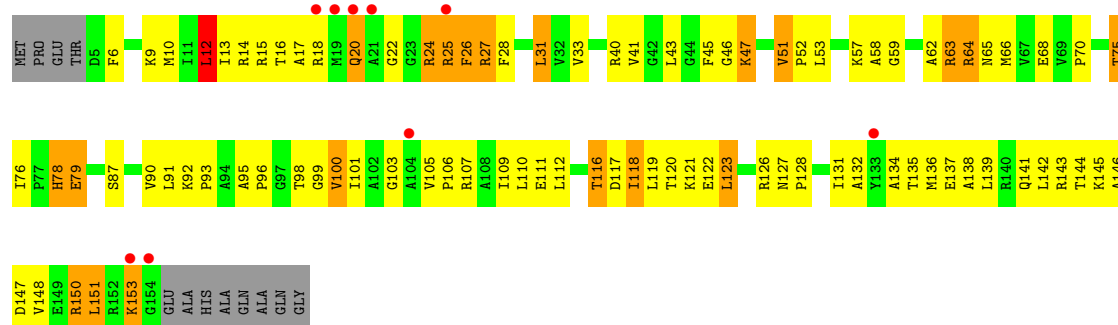


- Molecule 4: RIBOSOMAL PROTEIN S4

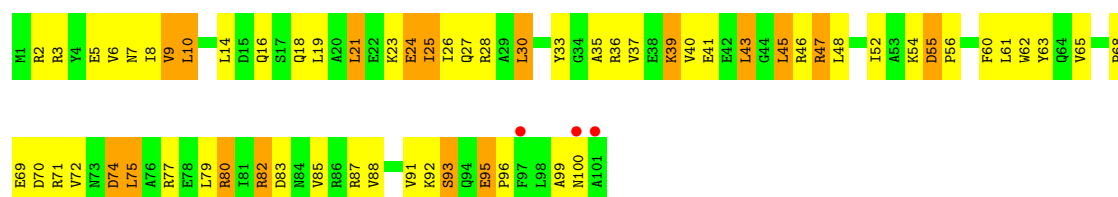


- Molecule 5: RIBOSOMAL PROTEIN S5

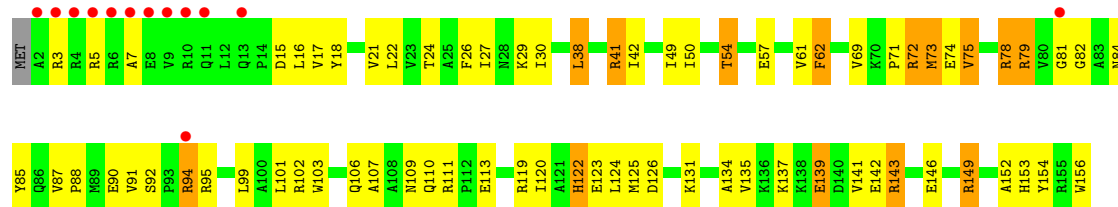




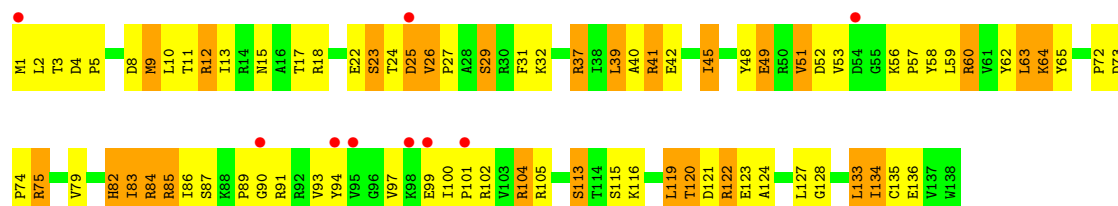
• Molecule 6: RIBOSOMAL PROTEIN S6



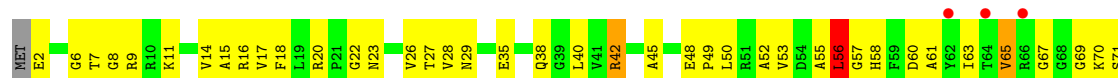
• Molecule 7: RIBOSOMAL PROTEIN S7



• Molecule 8: RIBOSOMAL PROTEIN S8

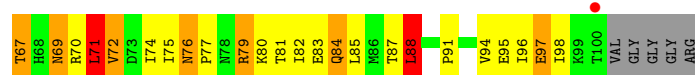


• Molecule 9: RIBOSOMAL PROTEIN S9

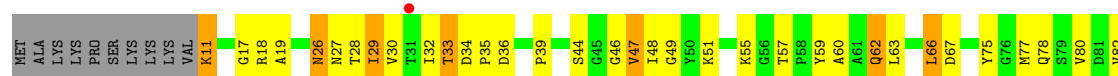




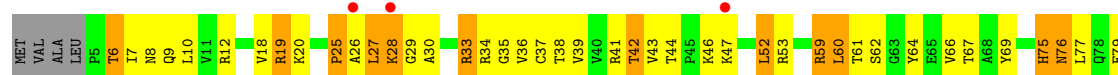
• Molecule 10: RIBOSOMAL PROTEIN S10



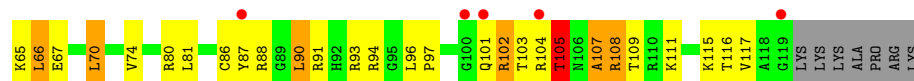
• Molecule 11: RIBOSOMAL PROTEIN S11



• Molecule 12: RIBOSOMAL PROTEIN S12



• Molecule 13: RIBOSOMAL PROTEIN S13

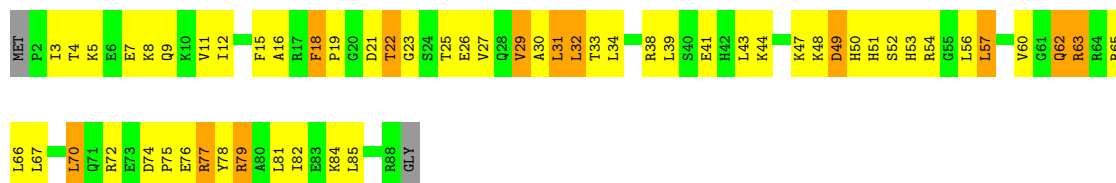


• Molecule 14: RIBOSOMAL PROTEIN S14

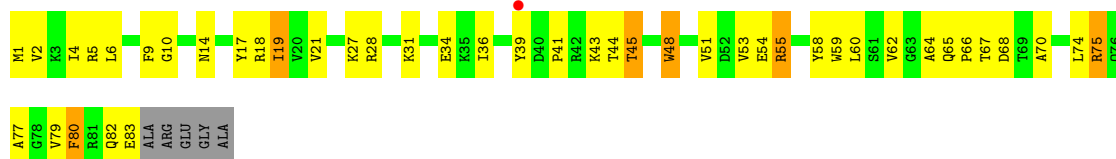
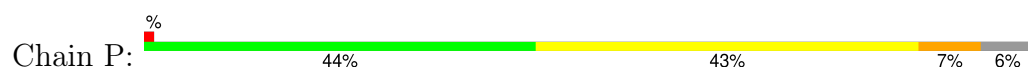




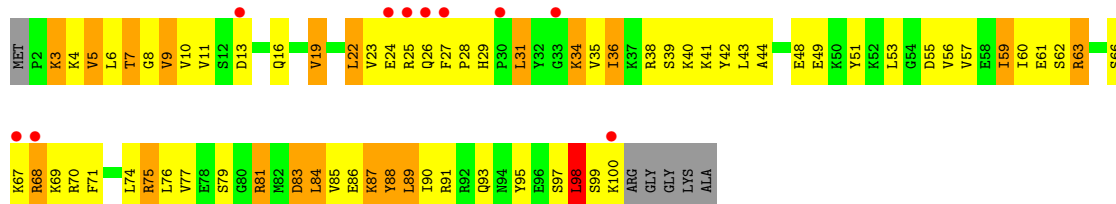
• Molecule 15: RIBOSOMAL PROTEIN S15



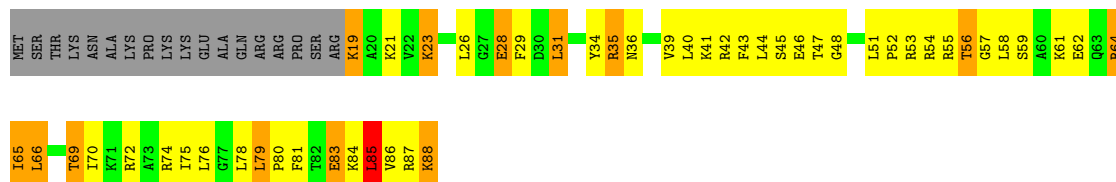
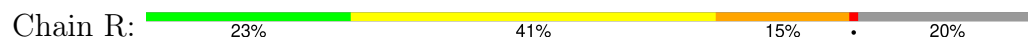
• Molecule 16: RIBOSOMAL PROTEIN S16



• Molecule 17: RIBOSOMAL PROTEIN S17

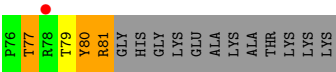


• Molecule 18: RIBOSOMAL PROTEIN S18

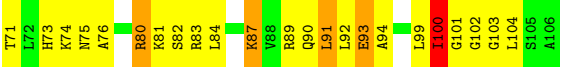
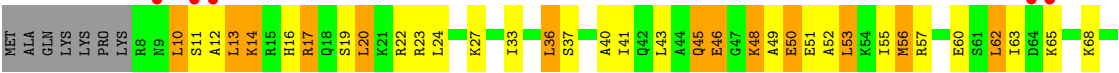


• Molecule 19: RIBOSOMAL PROTEIN S19





• Molecule 20: RIBOSOMAL PROTEIN S20



• Molecule 21: RIBOSOMAL PROTEIN THX



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 41 21 2 | Depositor |
| Cell constants a, b, c, α , β , γ | 399.62Å 399.62Å 216.07Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 47.29 – 3.85 47.29 – 3.85 | Depositor EDS |
| % Data completeness (in resolution range) | 99.3 (47.29-3.85) 99.2 (47.29-3.85) | Depositor EDS |
| R_{merge} | 0.12 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.47 (at 3.88Å) | Xtriage |
| Refinement program | PHENIX dev_1119 | Depositor |
| R, R_{free} | 0.153 , 0.202 0.154 , 0.201 | Depositor DCC |
| R_{free} test set | 8213 reflections (5.04%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 157.0 | Xtriage |
| Anisotropy | 0.232 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.29 , 161.3 | 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 | 52228 | wwPDB-VP |
| Average B, all atoms (Å ²) | 162.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% 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: MA6, MG, 4OC, UR3, 2MG, 7MG, 0TD, ZN, PSU, M2G, 5MC

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 | 1.18 | 129/36187 (0.4%) | 2.02 | 1881/56471 (3.3%) |
| 2 | B | 0.76 | 0/1935 | 1.00 | 6/2609 (0.2%) |
| 3 | C | 0.79 | 0/1636 | 0.98 | 6/2205 (0.3%) |
| 4 | D | 0.77 | 1/1733 (0.1%) | 0.97 | 1/2318 (0.0%) |
| 5 | E | 0.82 | 0/1162 | 1.05 | 4/1564 (0.3%) |
| 6 | F | 0.83 | 0/856 | 1.02 | 3/1154 (0.3%) |
| 7 | G | 0.73 | 0/1276 | 0.87 | 1/1709 (0.1%) |
| 8 | H | 0.83 | 0/1136 | 0.98 | 0/1527 |
| 9 | I | 0.63 | 0/1029 | 0.88 | 1/1379 (0.1%) |
| 10 | J | 0.77 | 0/805 | 1.03 | 4/1082 (0.4%) |
| 11 | K | 0.71 | 0/879 | 0.91 | 0/1187 |
| 12 | L | 0.97 | 2/977 (0.2%) | 1.15 | 2/1306 (0.2%) |
| 13 | M | 0.59 | 0/947 | 0.84 | 0/1270 |
| 14 | N | 0.77 | 0/501 | 1.04 | 3/664 (0.5%) |
| 15 | O | 0.69 | 0/740 | 0.94 | 0/987 |
| 16 | P | 0.74 | 0/716 | 0.92 | 0/963 |
| 17 | Q | 0.87 | 0/836 | 1.05 | 3/1117 (0.3%) |
| 18 | R | 0.71 | 0/579 | 0.99 | 2/768 (0.3%) |
| 19 | S | 0.60 | 0/661 | 1.01 | 4/890 (0.4%) |
| 20 | T | 0.74 | 0/765 | 1.03 | 2/1007 (0.2%) |
| 21 | U | 0.71 | 0/212 | 0.83 | 0/277 |
| All | All | 1.06 | 132/55568 (0.2%) | 1.76 | 1923/82454 (2.3%) |

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 | 2 |
| 3 | C | 0 | 3 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 8 | H | 0 | 1 |
| 9 | I | 0 | 2 |
| 10 | J | 0 | 2 |
| 13 | M | 0 | 3 |
| 14 | N | 0 | 1 |
| 16 | P | 0 | 1 |
| 20 | T | 0 | 3 |
| All | All | 0 | 18 |

All (132) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | A | 672 | U | C4-O4 | 8.76 | 1.30 | 1.23 |
| 1 | A | 563 | A | N9-C4 | -7.63 | 1.33 | 1.37 |
| 1 | A | 729 | A | N3-C4 | -7.49 | 1.30 | 1.34 |
| 1 | A | 1512 | U | C4-O4 | 7.36 | 1.29 | 1.23 |
| 1 | A | 372 | C | C2-O2 | 7.33 | 1.31 | 1.24 |
| 1 | A | 810 | C | N3-C4 | -7.31 | 1.28 | 1.33 |
| 1 | A | 1501 | C | N1-C6 | -6.93 | 1.32 | 1.37 |
| 1 | A | 1513 | A | N9-C4 | -6.92 | 1.33 | 1.37 |
| 1 | A | 802 | A | N7-C5 | -6.88 | 1.35 | 1.39 |
| 12 | L | 26 | ALA | CA-CB | 6.84 | 1.66 | 1.52 |
| 1 | A | 791 | G | C6-O6 | 6.79 | 1.30 | 1.24 |
| 1 | A | 481 | G | N7-C5 | -6.78 | 1.35 | 1.39 |
| 1 | A | 922 | G | C6-O6 | 6.78 | 1.30 | 1.24 |
| 1 | A | 792 | A | N9-C4 | -6.76 | 1.33 | 1.37 |
| 1 | A | 304 | U | C4-O4 | 6.73 | 1.29 | 1.23 |
| 1 | A | 558 | G | C6-O6 | 6.69 | 1.30 | 1.24 |
| 1 | A | 558 | G | N3-C4 | -6.62 | 1.30 | 1.35 |
| 1 | A | 642 | A | N3-C4 | -6.55 | 1.30 | 1.34 |
| 1 | A | 1392 | G | C6-N1 | -6.55 | 1.34 | 1.39 |
| 1 | A | 631 | G | C6-N1 | 6.53 | 1.44 | 1.39 |
| 1 | A | 723 | U | C2-N3 | 6.50 | 1.42 | 1.37 |
| 1 | A | 288 | A | N9-C4 | -6.49 | 1.33 | 1.37 |
| 1 | A | 523 | A | N9-C4 | -6.47 | 1.33 | 1.37 |
| 1 | A | 239 | U | C4-O4 | 6.41 | 1.28 | 1.23 |
| 1 | A | 305 | G | C6-O6 | 6.40 | 1.29 | 1.24 |
| 1 | A | 965 | A | N9-C4 | -6.40 | 1.34 | 1.37 |
| 1 | A | 790 | A | N3-C4 | -6.36 | 1.31 | 1.34 |
| 1 | A | 1335 | C | N1-C2 | 6.35 | 1.46 | 1.40 |
| 1 | A | 1394 | A | C6-N1 | -6.33 | 1.31 | 1.35 |
| 1 | A | 1394 | A | N3-C4 | -6.32 | 1.31 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1 | A | 715 | A | N9-C4 | -6.28 | 1.34 | 1.37 |
| 1 | A | 781 | A | N9-C4 | -6.27 | 1.34 | 1.37 |
| 1 | A | 484 | G | C6-N1 | -6.20 | 1.35 | 1.39 |
| 1 | A | 562 | C | N1-C6 | -6.19 | 1.33 | 1.37 |
| 1 | A | 509 | A | N7-C5 | -6.17 | 1.35 | 1.39 |
| 1 | A | 642 | A | N9-C4 | -6.16 | 1.34 | 1.37 |
| 1 | A | 1529 | G | N7-C5 | -6.15 | 1.35 | 1.39 |
| 1 | A | 32 | A | N3-C4 | -6.14 | 1.31 | 1.34 |
| 1 | A | 47 | C | N3-C4 | -6.08 | 1.29 | 1.33 |
| 1 | A | 439 | A | N3-C4 | -6.07 | 1.31 | 1.34 |
| 1 | A | 563 | A | N3-C4 | -6.05 | 1.31 | 1.34 |
| 1 | A | 238 | G | N3-C4 | -6.01 | 1.31 | 1.35 |
| 1 | A | 871 | U | N1-C2 | 5.99 | 1.44 | 1.38 |
| 1 | A | 266 | G | N9-C4 | -5.99 | 1.33 | 1.38 |
| 1 | A | 550 | G | C6-N1 | -5.97 | 1.35 | 1.39 |
| 1 | A | 1230 | C | C2-O2 | 5.97 | 1.29 | 1.24 |
| 1 | A | 26 | A | N9-C4 | -5.92 | 1.34 | 1.37 |
| 1 | A | 1005 | A | N9-C4 | 5.91 | 1.41 | 1.37 |
| 1 | A | 1377 | A | N9-C4 | -5.86 | 1.34 | 1.37 |
| 1 | A | 309 | G | C6-N1 | 5.86 | 1.43 | 1.39 |
| 1 | A | 50 | A | N9-C4 | -5.84 | 1.34 | 1.37 |
| 1 | A | 204 | U | C2-N3 | 5.77 | 1.41 | 1.37 |
| 1 | A | 748 | C | N1-C2 | 5.76 | 1.46 | 1.40 |
| 1 | A | 893 | C | C2-O2 | 5.73 | 1.29 | 1.24 |
| 1 | A | 622 | A | N9-C4 | -5.73 | 1.34 | 1.37 |
| 1 | A | 1527 | C | N3-C4 | -5.73 | 1.29 | 1.33 |
| 1 | A | 1392 | G | N1-C2 | -5.72 | 1.33 | 1.37 |
| 1 | A | 262 | A | N9-C4 | -5.69 | 1.34 | 1.37 |
| 1 | A | 768 | A | N9-C4 | -5.68 | 1.34 | 1.37 |
| 12 | L | 98 | TYR | CD2-CE2 | 5.68 | 1.47 | 1.39 |
| 1 | A | 267 | C | N3-C4 | -5.67 | 1.29 | 1.33 |
| 1 | A | 279 | A | N9-C4 | -5.65 | 1.34 | 1.37 |
| 1 | A | 382 | A | C6-N1 | -5.63 | 1.31 | 1.35 |
| 1 | A | 18 | C | N1-C6 | -5.63 | 1.33 | 1.37 |
| 1 | A | 250 | A | C5-C4 | 5.62 | 1.42 | 1.38 |
| 1 | A | 859 | A | N9-C4 | -5.62 | 1.34 | 1.37 |
| 1 | A | 523 | A | N3-C4 | -5.60 | 1.31 | 1.34 |
| 1 | A | 108 | G | N9-C4 | -5.57 | 1.33 | 1.38 |
| 1 | A | 828 | A | N9-C4 | -5.55 | 1.34 | 1.37 |
| 1 | A | 878 | G | C6-N1 | -5.55 | 1.35 | 1.39 |
| 1 | A | 45 | U | C4-O4 | 5.53 | 1.28 | 1.23 |
| 1 | A | 817 | C | N1-C6 | -5.53 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | A | 728 | A | N3-C4 | -5.52 | 1.31 | 1.34 |
| 1 | A | 809 | G | C5-C4 | -5.52 | 1.34 | 1.38 |
| 1 | A | 357 | G | C6-O6 | 5.52 | 1.29 | 1.24 |
| 1 | A | 32 | A | C6-N1 | -5.51 | 1.31 | 1.35 |
| 1 | A | 830 | G | C6-O6 | 5.50 | 1.29 | 1.24 |
| 1 | A | 839 | U | N1-C2 | 5.50 | 1.43 | 1.38 |
| 1 | A | 382 | A | N3-C4 | -5.49 | 1.31 | 1.34 |
| 1 | A | 108 | G | N7-C5 | -5.48 | 1.35 | 1.39 |
| 1 | A | 120 | A | N7-C5 | -5.47 | 1.35 | 1.39 |
| 1 | A | 505 | G | C6-N1 | -5.44 | 1.35 | 1.39 |
| 1 | A | 724 | G | N7-C5 | -5.44 | 1.35 | 1.39 |
| 1 | A | 969 | A | N9-C4 | -5.42 | 1.34 | 1.37 |
| 1 | A | 298 | A | N3-C4 | -5.41 | 1.31 | 1.34 |
| 1 | A | 553 | A | N9-C4 | -5.41 | 1.34 | 1.37 |
| 1 | A | 1531 | A | N9-C8 | 5.40 | 1.42 | 1.37 |
| 4 | D | 173 | TRP | CB-CG | -5.40 | 1.40 | 1.50 |
| 1 | A | 631 | G | N1-C2 | 5.40 | 1.42 | 1.37 |
| 1 | A | 1124 | G | C6-N1 | 5.40 | 1.43 | 1.39 |
| 1 | A | 1157 | A | N9-C4 | 5.38 | 1.41 | 1.37 |
| 1 | A | 27 | G | N7-C5 | -5.38 | 1.36 | 1.39 |
| 1 | A | 1225 | A | N3-C4 | -5.37 | 1.31 | 1.34 |
| 1 | A | 375 | U | C4-O4 | 5.36 | 1.27 | 1.23 |
| 1 | A | 703 | G | C5-C6 | 5.36 | 1.47 | 1.42 |
| 1 | A | 919 | A | C5-C4 | -5.36 | 1.35 | 1.38 |
| 1 | A | 532 | A | N3-C4 | 5.35 | 1.38 | 1.34 |
| 1 | A | 1493 | A | N9-C4 | 5.33 | 1.41 | 1.37 |
| 1 | A | 964 | A | N3-C4 | -5.33 | 1.31 | 1.34 |
| 1 | A | 510 | A | N3-C4 | -5.31 | 1.31 | 1.34 |
| 1 | A | 47 | C | N1-C6 | -5.30 | 1.33 | 1.37 |
| 1 | A | 729 | A | N7-C5 | -5.30 | 1.36 | 1.39 |
| 1 | A | 1531 | A | C5-C4 | 5.30 | 1.42 | 1.38 |
| 1 | A | 390 | C | N1-C6 | -5.29 | 1.33 | 1.37 |
| 1 | A | 9 | G | N9-C8 | -5.28 | 1.34 | 1.37 |
| 1 | A | 919 | A | N7-C5 | -5.25 | 1.36 | 1.39 |
| 1 | A | 122 | G | C5-C4 | -5.25 | 1.34 | 1.38 |
| 1 | A | 864 | A | N3-C4 | -5.23 | 1.31 | 1.34 |
| 1 | A | 325 | A | N3-C4 | -5.23 | 1.31 | 1.34 |
| 1 | A | 1530 | G | C6-N1 | 5.23 | 1.43 | 1.39 |
| 1 | A | 1393 | U | C4-O4 | 5.20 | 1.27 | 1.23 |
| 1 | A | 802 | A | C5-C6 | -5.20 | 1.36 | 1.41 |
| 1 | A | 67 | C | N3-C4 | -5.19 | 1.30 | 1.33 |
| 1 | A | 543 | C | N1-C6 | -5.19 | 1.34 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | A | 704 | A | N9-C4 | -5.19 | 1.34 | 1.37 |
| 1 | A | 889 | A | N3-C4 | -5.18 | 1.31 | 1.34 |
| 1 | A | 1403 | C | N1-C6 | -5.18 | 1.34 | 1.37 |
| 1 | A | 1004 | A | N9-C4 | 5.14 | 1.41 | 1.37 |
| 1 | A | 379 | C | N1-C6 | -5.14 | 1.34 | 1.37 |
| 1 | A | 357 | G | C2-N3 | -5.12 | 1.28 | 1.32 |
| 1 | A | 919 | A | N9-C4 | -5.09 | 1.34 | 1.37 |
| 1 | A | 791 | G | N3-C4 | -5.09 | 1.31 | 1.35 |
| 1 | A | 10 | A | C6-N1 | -5.09 | 1.31 | 1.35 |
| 1 | A | 728 | A | C5-C6 | -5.09 | 1.36 | 1.41 |
| 1 | A | 1506 | U | N1-C2 | 5.08 | 1.43 | 1.38 |
| 1 | A | 1084 | G | C6-O6 | 5.07 | 1.28 | 1.24 |
| 1 | A | 230 | G | C6-O6 | 5.07 | 1.28 | 1.24 |
| 1 | A | 859 | A | N3-C4 | -5.06 | 1.31 | 1.34 |
| 1 | A | 964 | A | N9-C4 | -5.05 | 1.34 | 1.37 |
| 1 | A | 1084 | G | C5-C6 | 5.05 | 1.47 | 1.42 |
| 1 | A | 66 | G | N9-C4 | -5.01 | 1.33 | 1.38 |
| 1 | A | 487 | A | N9-C4 | -5.00 | 1.34 | 1.37 |

All (1923) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 1 | A | 1528 | U | O5'-P-OP2 | -17.17 | 90.09 | 110.70 |
| 1 | A | 309 | G | N1-C6-O6 | 16.92 | 130.05 | 119.90 |
| 1 | A | 922 | G | N1-C6-O6 | 15.33 | 129.10 | 119.90 |
| 1 | A | 558 | G | C5-C6-N1 | -15.09 | 103.95 | 111.50 |
| 1 | A | 1335 | C | N1-C2-O2 | 14.44 | 127.56 | 118.90 |
| 1 | A | 117 | G | N1-C6-O6 | 14.31 | 128.49 | 119.90 |
| 1 | A | 791 | G | C5-C6-N1 | -13.57 | 104.72 | 111.50 |
| 1 | A | 325 | A | N1-C6-N6 | -13.50 | 110.50 | 118.60 |
| 1 | A | 922 | G | C5-C6-N1 | -13.29 | 104.86 | 111.50 |
| 1 | A | 970 | C | N1-C2-O2 | 13.22 | 126.83 | 118.90 |
| 1 | A | 672 | U | N3-C4-C5 | -13.21 | 106.67 | 114.60 |
| 1 | A | 305 | G | C5-C6-N1 | -13.20 | 104.90 | 111.50 |
| 1 | A | 239 | U | N3-C4-C5 | -13.17 | 106.70 | 114.60 |
| 1 | A | 1512 | U | N3-C4-C5 | -13.00 | 106.80 | 114.60 |
| 1 | A | 1435 | G | N1-C6-O6 | 12.82 | 127.59 | 119.90 |
| 1 | A | 541 | G | N1-C6-O6 | 12.58 | 127.45 | 119.90 |
| 1 | A | 147 | G | N1-C6-O6 | 12.50 | 127.40 | 119.90 |
| 1 | A | 1531 | A | N7-C8-N9 | 12.41 | 120.01 | 113.80 |
| 1 | A | 58 | C | C6-N1-C2 | -12.22 | 115.41 | 120.30 |
| 1 | A | 1531 | A | N1-C6-N6 | 12.19 | 125.91 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 1 | A | 1531 | A | C5-N7-C8 | -12.04 | 97.88 | 103.90 |
| 1 | A | 304 | U | N3-C4-C5 | -11.95 | 107.43 | 114.60 |
| 1 | A | 730 | G | C4-C5-N7 | -11.91 | 106.04 | 110.80 |
| 1 | A | 518 | C | N1-C2-O2 | 11.81 | 125.99 | 118.90 |
| 1 | A | 481 | G | O5'-P-OP2 | -11.75 | 95.13 | 105.70 |
| 1 | A | 871 | U | N1-C2-O2 | 11.72 | 131.00 | 122.80 |
| 1 | A | 830 | G | C5-C6-N1 | -11.51 | 105.75 | 111.50 |
| 1 | A | 1064 | G | C5-C6-O6 | -11.50 | 121.70 | 128.60 |
| 1 | A | 1050 | G | N1-C6-O6 | 11.43 | 126.76 | 119.90 |
| 1 | A | 1335 | C | N3-C2-O2 | -11.43 | 113.90 | 121.90 |
| 1 | A | 1530 | G | N3-C4-C5 | 11.43 | 134.31 | 128.60 |
| 1 | A | 34 | C | C6-N1-C2 | 11.40 | 124.86 | 120.30 |
| 1 | A | 309 | G | C5-C6-O6 | -11.38 | 121.78 | 128.60 |
| 1 | A | 1532 | U | C5-C6-N1 | 11.23 | 128.32 | 122.70 |
| 1 | A | 285 | G | C8-N9-C4 | 11.23 | 110.89 | 106.40 |
| 1 | A | 624 | C | C6-N1-C2 | 11.23 | 124.79 | 120.30 |
| 1 | A | 27 | G | N1-C6-O6 | 11.18 | 126.61 | 119.90 |
| 1 | A | 710 | G | N1-C6-O6 | 11.13 | 126.58 | 119.90 |
| 1 | A | 1397 | C | O5'-P-OP1 | -11.08 | 95.73 | 105.70 |
| 1 | A | 1233 | G | N1-C6-O6 | 11.06 | 126.53 | 119.90 |
| 1 | A | 254 | G | O5'-P-OP1 | -11.01 | 95.79 | 105.70 |
| 1 | A | 1124 | G | C2-N3-C4 | 10.97 | 117.38 | 111.90 |
| 1 | A | 117 | G | C6-C5-N7 | -10.92 | 123.85 | 130.40 |
| 1 | A | 897 | C | N3-C4-C5 | 10.91 | 126.27 | 121.90 |
| 1 | A | 769 | G | O5'-P-OP2 | -10.88 | 95.91 | 105.70 |
| 1 | A | 1514 | C | C6-N1-C2 | 10.87 | 124.65 | 120.30 |
| 1 | A | 902 | G | N1-C6-O6 | 10.78 | 126.36 | 119.90 |
| 1 | A | 718 | G | C8-N9-C4 | 10.73 | 110.69 | 106.40 |
| 1 | A | 555 | C | O5'-P-OP2 | -10.66 | 96.11 | 105.70 |
| 1 | A | 1277 | C | C6-N1-C2 | -10.62 | 116.05 | 120.30 |
| 1 | A | 1125 | U | N3-C2-O2 | 10.61 | 129.63 | 122.20 |
| 1 | A | 922 | G | C4-C5-C6 | 10.61 | 125.17 | 118.80 |
| 1 | A | 1222 | G | C5-C6-N1 | -10.61 | 106.20 | 111.50 |
| 1 | A | 122 | G | C8-N9-C4 | 10.58 | 110.63 | 106.40 |
| 1 | A | 54 | C | C6-N1-C2 | 10.55 | 124.52 | 120.30 |
| 1 | A | 1064 | G | N1-C6-O6 | 10.55 | 126.23 | 119.90 |
| 1 | A | 333 | G | N1-C6-O6 | 10.50 | 126.20 | 119.90 |
| 1 | A | 1256 | A | C8-N9-C4 | 10.43 | 109.97 | 105.80 |
| 1 | A | 1522 | U | O5'-P-OP2 | -10.40 | 96.34 | 105.70 |
| 1 | A | 893 | C | N1-C2-N3 | -10.37 | 111.94 | 119.20 |
| 1 | A | 357 | G | C5-C6-N1 | -10.32 | 106.34 | 111.50 |
| 1 | A | 710 | G | C5-C6-N1 | -10.31 | 106.35 | 111.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | A | 1227 | A | N1-C6-N6 | 10.30 | 124.78 | 118.60 |
| 1 | A | 251 | G | N1-C6-O6 | 10.17 | 126.00 | 119.90 |
| 1 | A | 314 | C | C6-N1-C2 | 10.16 | 124.36 | 120.30 |
| 1 | A | 108 | G | N1-C6-O6 | 10.15 | 125.99 | 119.90 |
| 1 | A | 975 | A | C2-N3-C4 | -10.11 | 105.54 | 110.60 |
| 1 | A | 300 | A | N1-C6-N6 | -10.11 | 112.54 | 118.60 |
| 1 | A | 522 | C | C6-N1-C2 | 10.07 | 124.33 | 120.30 |
| 1 | A | 234 | C | C6-N1-C2 | 10.06 | 124.32 | 120.30 |
| 1 | A | 1531 | A | C4-C5-N7 | 10.04 | 115.72 | 110.70 |
| 1 | A | 204 | U | C5-C6-N1 | 9.88 | 127.64 | 122.70 |
| 1 | A | 277 | C | C6-N1-C2 | 9.84 | 124.24 | 120.30 |
| 1 | A | 325 | A | N9-C4-C5 | 9.80 | 109.72 | 105.80 |
| 1 | A | 147 | G | C5-C6-N1 | -9.79 | 106.61 | 111.50 |
| 1 | A | 266 | G | N3-C4-C5 | 9.78 | 133.49 | 128.60 |
| 1 | A | 724 | G | N3-C4-C5 | -9.77 | 123.72 | 128.60 |
| 1 | A | 1377 | A | C2-N3-C4 | -9.75 | 105.72 | 110.60 |
| 1 | A | 372 | C | C6-N1-C2 | 9.72 | 124.19 | 120.30 |
| 1 | A | 372 | C | N1-C2-N3 | -9.72 | 112.39 | 119.20 |
| 1 | A | 814 | A | C2-N3-C4 | -9.72 | 105.74 | 110.60 |
| 1 | A | 830 | G | N1-C6-O6 | 9.72 | 125.73 | 119.90 |
| 1 | A | 920 | U | N3-C4-O4 | -9.70 | 112.61 | 119.40 |
| 1 | A | 1233 | G | C5-C6-N1 | -9.66 | 106.67 | 111.50 |
| 1 | A | 922 | G | N3-C2-N2 | -9.66 | 113.14 | 119.90 |
| 1 | A | 309 | G | C6-C5-N7 | -9.64 | 124.61 | 130.40 |
| 1 | A | 332 | G | N1-C6-O6 | 9.61 | 125.67 | 119.90 |
| 1 | A | 255 | G | N1-C6-O6 | 9.61 | 125.66 | 119.90 |
| 1 | A | 1084 | G | C4-C5-N7 | -9.61 | 106.96 | 110.80 |
| 1 | A | 32 | A | C6-N1-C2 | -9.59 | 112.85 | 118.60 |
| 1 | A | 1531 | A | C8-N9-C4 | -9.51 | 101.99 | 105.80 |
| 1 | A | 557 | G | N1-C6-O6 | 9.51 | 125.61 | 119.90 |
| 1 | A | 829 | G | C8-N9-C4 | 9.50 | 110.20 | 106.40 |
| 1 | A | 855 | G | C5-C6-N1 | -9.50 | 106.75 | 111.50 |
| 1 | A | 27 | G | C6-C5-N7 | -9.49 | 124.71 | 130.40 |
| 1 | A | 113 | G | N1-C6-O6 | 9.44 | 125.57 | 119.90 |
| 1 | A | 333 | G | C5-C6-N1 | -9.41 | 106.80 | 111.50 |
| 1 | A | 541 | G | C5-C6-O6 | -9.41 | 122.96 | 128.60 |
| 1 | A | 871 | U | N3-C2-O2 | -9.40 | 115.62 | 122.20 |
| 1 | A | 604 | G | N1-C6-O6 | 9.39 | 125.53 | 119.90 |
| 1 | A | 325 | A | C5-C6-N6 | 9.37 | 131.20 | 123.70 |
| 1 | A | 886 | G | N1-C6-O6 | 9.36 | 125.52 | 119.90 |
| 1 | A | 298 | A | C2-N3-C4 | -9.34 | 105.93 | 110.60 |
| 1 | A | 855 | G | C2-N3-C4 | -9.29 | 107.25 | 111.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 1054 | C | N1-C2-O2 | 9.29 | 124.48 | 118.90 |
| 1 | A | 267 | C | N3-C4-N4 | -9.29 | 111.50 | 118.00 |
| 1 | A | 558 | G | C5-C6-O6 | 9.26 | 134.16 | 128.60 |
| 1 | A | 518 | C | N3-C2-O2 | -9.23 | 115.44 | 121.90 |
| 1 | A | 635 | G | N1-C6-O6 | 9.23 | 125.44 | 119.90 |
| 1 | A | 761 | G | N1-C6-O6 | 9.23 | 125.44 | 119.90 |
| 1 | A | 562 | C | N1-C2-O2 | 9.22 | 124.43 | 118.90 |
| 1 | A | 500 | G | O5'-P-OP1 | -9.21 | 97.41 | 105.70 |
| 1 | A | 893 | C | N1-C2-O2 | 9.21 | 124.42 | 118.90 |
| 1 | A | 830 | G | N3-C2-N2 | -9.16 | 113.49 | 119.90 |
| 1 | A | 31 | G | N3-C4-N9 | 9.15 | 131.49 | 126.00 |
| 1 | A | 313 | A | N1-C6-N6 | 9.15 | 124.09 | 118.60 |
| 1 | A | 28 | G | N1-C6-O6 | 9.14 | 125.39 | 119.90 |
| 1 | A | 398 | C | C6-N1-C2 | 9.11 | 123.94 | 120.30 |
| 1 | A | 887 | G | N1-C6-O6 | 9.11 | 125.36 | 119.90 |
| 1 | A | 610 | G | C8-N9-C4 | -9.09 | 102.76 | 106.40 |
| 1 | A | 1166 | G | N3-C4-C5 | -9.09 | 124.06 | 128.60 |
| 1 | A | 661 | G | N1-C6-O6 | 9.08 | 125.35 | 119.90 |
| 1 | A | 810 | C | N3-C4-N4 | -9.08 | 111.65 | 118.00 |
| 1 | A | 1512 | U | C5-C4-O4 | 9.07 | 131.34 | 125.90 |
| 1 | A | 27 | G | O5'-P-OP1 | -9.06 | 97.55 | 105.70 |
| 3 | C | 179 | ARG | N-CA-C | -9.04 | 86.59 | 111.00 |
| 1 | A | 811 | C | C5-C6-N1 | -9.03 | 116.49 | 121.00 |
| 1 | A | 1426 | C | C6-N1-C2 | 9.02 | 123.91 | 120.30 |
| 1 | A | 228 | A | N1-C6-N6 | -8.98 | 113.21 | 118.60 |
| 1 | A | 901 | A | O5'-P-OP1 | -8.98 | 97.62 | 105.70 |
| 1 | A | 1026 | G | N7-C8-N9 | 8.98 | 117.59 | 113.10 |
| 1 | A | 1087 | G | N1-C6-O6 | 8.98 | 125.29 | 119.90 |
| 1 | A | 381 | C | C6-N1-C2 | -8.98 | 116.71 | 120.30 |
| 1 | A | 1057 | G | N3-C2-N2 | -8.92 | 113.66 | 119.90 |
| 1 | A | 535 | A | N1-C6-N6 | -8.91 | 113.25 | 118.60 |
| 1 | A | 1070 | U | O5'-P-OP2 | -8.90 | 97.69 | 105.70 |
| 1 | A | 749 | C | C6-N1-C2 | -8.90 | 116.74 | 120.30 |
| 1 | A | 204 | U | C2-N1-C1' | 8.88 | 128.36 | 117.70 |
| 1 | A | 828 | A | C8-N9-C4 | 8.88 | 109.35 | 105.80 |
| 1 | A | 1530 | G | N3-C4-N9 | -8.86 | 120.69 | 126.00 |
| 1 | A | 372 | C | N3-C4-C5 | 8.83 | 125.43 | 121.90 |
| 1 | A | 19 | C | O5'-P-OP2 | -8.82 | 97.76 | 105.70 |
| 1 | A | 1004 | A | O4'-C1'-N9 | 8.80 | 115.24 | 108.20 |
| 1 | A | 1277 | C | C5-C6-N1 | 8.78 | 125.39 | 121.00 |
| 1 | A | 661 | G | C5-C6-N1 | -8.77 | 107.11 | 111.50 |
| 1 | A | 1479 | C | C6-N1-C2 | -8.76 | 116.80 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 1 | A | 113 | G | C6-C5-N7 | -8.76 | 125.14 | 130.40 |
| 1 | A | 400 | C | C6-N1-C2 | 8.75 | 123.80 | 120.30 |
| 1 | A | 251 | G | C5-C6-O6 | -8.74 | 123.36 | 128.60 |
| 1 | A | 817 | C | C2-N1-C1' | 8.72 | 128.39 | 118.80 |
| 1 | A | 811 | C | C6-N1-C2 | 8.72 | 123.79 | 120.30 |
| 1 | A | 544 | G | C4-C5-N7 | 8.71 | 114.28 | 110.80 |
| 1 | A | 387 | U | O5'-P-OP2 | -8.71 | 97.86 | 105.70 |
| 1 | A | 590 | C | C6-N1-C2 | 8.71 | 123.78 | 120.30 |
| 1 | A | 239 | U | N3-C4-O4 | 8.70 | 125.49 | 119.40 |
| 1 | A | 664 | G | C5-N7-C8 | 8.70 | 108.65 | 104.30 |
| 1 | A | 241 | C | C6-N1-C2 | 8.70 | 123.78 | 120.30 |
| 1 | A | 265 | G | N3-C4-N9 | -8.70 | 120.78 | 126.00 |
| 1 | A | 557 | G | C6-C5-N7 | -8.70 | 125.18 | 130.40 |
| 1 | A | 1393 | U | C4-C5-C6 | 8.69 | 124.92 | 119.70 |
| 1 | A | 1075 | C | O5'-P-OP2 | -8.69 | 97.88 | 105.70 |
| 1 | A | 1531 | A | C6-C5-N7 | -8.68 | 126.23 | 132.30 |
| 1 | A | 247 | G | N1-C6-O6 | 8.66 | 125.10 | 119.90 |
| 1 | A | 484 | G | N1-C2-N2 | -8.65 | 108.41 | 116.20 |
| 1 | A | 113 | G | N3-C4-N9 | 8.65 | 131.19 | 126.00 |
| 1 | A | 503 | C | O5'-P-OP2 | -8.65 | 97.92 | 105.70 |
| 1 | A | 1290 | G | N1-C6-O6 | 8.63 | 125.08 | 119.90 |
| 1 | A | 31 | G | C8-N9-C1' | -8.61 | 115.81 | 127.00 |
| 1 | A | 1516[A] | G | N3-C4-N9 | -8.60 | 120.84 | 126.00 |
| 1 | A | 1516[B] | G | N3-C4-N9 | -8.60 | 120.84 | 126.00 |
| 1 | A | 403 | C | O5'-P-OP2 | -8.60 | 97.96 | 105.70 |
| 1 | A | 927 | G | O5'-P-OP1 | -8.60 | 97.96 | 105.70 |
| 1 | A | 922 | G | C6-C5-N7 | -8.60 | 125.24 | 130.40 |
| 1 | A | 728 | A | C8-N9-C4 | -8.60 | 102.36 | 105.80 |
| 1 | A | 783 | C | C6-N1-C2 | 8.59 | 123.73 | 120.30 |
| 1 | A | 731 | G | C4-C5-N7 | 8.59 | 114.23 | 110.80 |
| 1 | A | 10 | A | O5'-P-OP2 | -8.58 | 97.98 | 105.70 |
| 1 | A | 113 | G | C5-C6-O6 | -8.57 | 123.45 | 128.60 |
| 1 | A | 1512 | U | C6-N1-C2 | -8.57 | 115.86 | 121.00 |
| 1 | A | 266 | G | C5-N7-C8 | -8.56 | 100.02 | 104.30 |
| 1 | A | 99 | C | C6-N1-C2 | -8.54 | 116.89 | 120.30 |
| 1 | A | 1256 | A | N7-C8-N9 | -8.52 | 109.54 | 113.80 |
| 1 | A | 1528 | U | OP1-P-OP2 | 8.52 | 132.38 | 119.60 |
| 1 | A | 46 | G | C8-N9-C4 | -8.51 | 103.00 | 106.40 |
| 1 | A | 794 | A | O5'-P-OP2 | -8.51 | 98.04 | 105.70 |
| 1 | A | 108 | G | C6-C5-N7 | -8.49 | 125.30 | 130.40 |
| 1 | A | 1432 | G | C8-N9-C4 | -8.49 | 103.00 | 106.40 |
| 1 | A | 1026 | G | C8-N9-C4 | -8.48 | 103.01 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 1432 | G | C5-C6-N1 | -8.45 | 107.27 | 111.50 |
| 1 | A | 1305 | G | C8-N9-C4 | -8.45 | 103.02 | 106.40 |
| 1 | A | 47 | C | N3-C2-O2 | -8.45 | 115.99 | 121.90 |
| 1 | A | 277 | C | O5'-P-OP1 | -8.44 | 98.10 | 105.70 |
| 1 | A | 664 | G | C4-C5-N7 | -8.44 | 107.43 | 110.80 |
| 1 | A | 121 | C | C6-N1-C2 | 8.43 | 123.67 | 120.30 |
| 1 | A | 15 | G | N1-C6-O6 | 8.42 | 124.95 | 119.90 |
| 1 | A | 284 | G | N1-C6-O6 | 8.42 | 124.95 | 119.90 |
| 1 | A | 818 | G | OP1-P-OP2 | 8.41 | 132.22 | 119.60 |
| 1 | A | 21 | G | C6-C5-N7 | -8.41 | 125.36 | 130.40 |
| 1 | A | 541 | G | C6-C5-N7 | -8.39 | 125.36 | 130.40 |
| 1 | A | 1087 | G | C6-C5-N7 | -8.38 | 125.37 | 130.40 |
| 1 | A | 372 | C | N1-C2-O2 | 8.38 | 123.92 | 118.90 |
| 1 | A | 699 | C | C6-N1-C2 | 8.37 | 123.65 | 120.30 |
| 1 | A | 729 | A | OP1-P-O3' | 8.37 | 123.62 | 105.20 |
| 1 | A | 500 | G | N1-C6-O6 | 8.36 | 124.91 | 119.90 |
| 1 | A | 25 | C | C6-N1-C2 | 8.34 | 123.64 | 120.30 |
| 1 | A | 485 | G | C8-N9-C4 | 8.34 | 109.74 | 106.40 |
| 1 | A | 1205 | U | N3-C4-C5 | -8.33 | 109.60 | 114.60 |
| 1 | A | 526 | C | O5'-P-OP1 | 8.32 | 120.69 | 110.70 |
| 1 | A | 122 | G | N7-C8-N9 | -8.30 | 108.95 | 113.10 |
| 1 | A | 987 | G | N1-C6-O6 | 8.30 | 124.88 | 119.90 |
| 1 | A | 304 | U | C4-C5-C6 | 8.29 | 124.67 | 119.70 |
| 1 | A | 774 | G | C6-C5-N7 | -8.28 | 125.43 | 130.40 |
| 1 | A | 1050 | G | C5-C6-O6 | -8.28 | 123.63 | 128.60 |
| 1 | A | 20 | U | C5-C4-O4 | -8.26 | 120.94 | 125.90 |
| 1 | A | 117 | G | C5-C6-O6 | -8.26 | 123.65 | 128.60 |
| 1 | A | 1211 | U | C5-C6-N1 | 8.26 | 126.83 | 122.70 |
| 1 | A | 58 | C | C5-C6-N1 | 8.24 | 125.12 | 121.00 |
| 1 | A | 724 | G | C8-N9-C4 | -8.24 | 103.11 | 106.40 |
| 1 | A | 45 | U | N3-C4-C5 | -8.23 | 109.66 | 114.60 |
| 1 | A | 122 | G | N9-C4-C5 | -8.22 | 102.11 | 105.40 |
| 1 | A | 113 | G | C8-N9-C1' | -8.21 | 116.32 | 127.00 |
| 1 | A | 1393 | U | N3-C4-C5 | -8.21 | 109.67 | 114.60 |
| 1 | A | 408 | A | C8-N9-C4 | -8.20 | 102.52 | 105.80 |
| 1 | A | 906 | G | N1-C6-O6 | 8.20 | 124.82 | 119.90 |
| 1 | A | 133 | U | C5-C4-O4 | 8.19 | 130.81 | 125.90 |
| 1 | A | 239 | U | C6-N1-C2 | -8.19 | 116.09 | 121.00 |
| 1 | A | 766 | A | O5'-P-OP2 | -8.18 | 98.33 | 105.70 |
| 1 | A | 284 | G | C2-N3-C4 | -8.18 | 107.81 | 111.90 |
| 1 | A | 1230 | C | C2-N3-C4 | 8.18 | 123.99 | 119.90 |
| 1 | A | 724 | G | C6-C5-N7 | -8.15 | 125.51 | 130.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 111 | G | N3-C4-N9 | -8.14 | 121.11 | 126.00 |
| 1 | A | 703 | G | C8-N9-C1' | -8.14 | 116.41 | 127.00 |
| 1 | A | 730 | G | C5-N7-C8 | 8.14 | 108.37 | 104.30 |
| 1 | A | 886 | G | C2-N3-C4 | -8.13 | 107.83 | 111.90 |
| 1 | A | 877 | C | C6-N1-C2 | -8.13 | 117.05 | 120.30 |
| 1 | A | 266 | G | N3-C4-N9 | -8.12 | 121.13 | 126.00 |
| 1 | A | 674 | G | N1-C6-O6 | 8.12 | 124.77 | 119.90 |
| 1 | A | 819 | A | N1-C6-N6 | 8.12 | 123.47 | 118.60 |
| 1 | A | 117 | G | N9-C4-C5 | -8.10 | 102.16 | 105.40 |
| 1 | A | 500 | G | C8-N9-C4 | 8.09 | 109.64 | 106.40 |
| 1 | A | 7 | G | C5-C6-O6 | -8.09 | 123.75 | 128.60 |
| 1 | A | 306 | G | N1-C6-O6 | 8.08 | 124.75 | 119.90 |
| 1 | A | 799 | G | C6-C5-N7 | -8.07 | 125.56 | 130.40 |
| 1 | A | 731 | G | C5-N7-C8 | -8.05 | 100.27 | 104.30 |
| 1 | A | 147 | G | C6-C5-N7 | -8.05 | 125.57 | 130.40 |
| 1 | A | 509 | A | C8-N9-C4 | -8.05 | 102.58 | 105.80 |
| 1 | A | 484 | G | P-O3'-C3' | 8.05 | 129.36 | 119.70 |
| 1 | A | 1435 | G | C2-N3-C4 | -8.05 | 107.88 | 111.90 |
| 1 | A | 1050 | G | C6-C5-N7 | -8.04 | 125.57 | 130.40 |
| 1 | A | 1064 | G | C4-C5-N7 | 8.04 | 114.01 | 110.80 |
| 1 | A | 893 | C | C2-N3-C4 | 8.03 | 123.92 | 119.90 |
| 1 | A | 1523 | G | N1-C6-O6 | 8.03 | 124.72 | 119.90 |
| 1 | A | 1491 | G | C8-N9-C4 | -8.02 | 103.19 | 106.40 |
| 1 | A | 507 | C | C6-N1-C2 | 8.02 | 123.51 | 120.30 |
| 1 | A | 785 | G | N1-C6-O6 | 8.01 | 124.71 | 119.90 |
| 1 | A | 646 | U | N3-C4-C5 | -8.01 | 109.80 | 114.60 |
| 1 | A | 976 | G | C5-C6-N1 | -8.01 | 107.50 | 111.50 |
| 1 | A | 1173 | G | C8-N9-C4 | 8.01 | 109.60 | 106.40 |
| 1 | A | 32 | A | N1-C2-N3 | 8.00 | 133.30 | 129.30 |
| 1 | A | 1539 | C | C6-N1-C2 | -8.00 | 117.10 | 120.30 |
| 1 | A | 484 | G | N1-C6-O6 | -8.00 | 115.10 | 119.90 |
| 1 | A | 1202 | G | N9-C4-C5 | 7.99 | 108.60 | 105.40 |
| 1 | A | 260 | G | C8-N9-C4 | -7.99 | 103.20 | 106.40 |
| 1 | A | 314 | C | N3-C4-C5 | 7.99 | 125.09 | 121.90 |
| 1 | A | 906 | G | C6-C5-N7 | -7.99 | 125.61 | 130.40 |
| 1 | A | 133 | U | N3-C2-O2 | -7.98 | 116.61 | 122.20 |
| 1 | A | 791 | G | C4-C5-C6 | 7.98 | 123.59 | 118.80 |
| 1 | A | 1131 | G | N1-C6-O6 | 7.98 | 124.69 | 119.90 |
| 1 | A | 1202 | G | N3-C4-N9 | -7.97 | 121.22 | 126.00 |
| 1 | A | 27 | G | C5-C6-O6 | -7.97 | 123.82 | 128.60 |
| 1 | A | 333 | G | N3-C2-N2 | -7.95 | 114.33 | 119.90 |
| 17 | Q | 98 | LEU | CA-CB-CG | 7.95 | 133.59 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 1 | A | 190(H) | G | N1-C6-O6 | 7.95 | 124.67 | 119.90 |
| 1 | A | 290 | C | O5'-P-OP2 | -7.93 | 98.56 | 105.70 |
| 1 | A | 830 | G | N3-C4-C5 | 7.93 | 132.57 | 128.60 |
| 1 | A | 104 | G | C5-C6-N1 | -7.93 | 107.53 | 111.50 |
| 1 | A | 1084 | G | C5-C6-O6 | 7.93 | 133.36 | 128.60 |
| 1 | A | 799 | G | N1-C6-O6 | 7.92 | 124.65 | 119.90 |
| 1 | A | 1304 | G | C5-C6-N1 | -7.92 | 107.54 | 111.50 |
| 1 | A | 1211 | U | N1-C2-O2 | 7.92 | 128.34 | 122.80 |
| 1 | A | 257 | G | N1-C6-O6 | 7.91 | 124.65 | 119.90 |
| 1 | A | 936 | C | O5'-P-OP2 | 7.91 | 120.19 | 110.70 |
| 1 | A | 401 | C | N3-C4-N4 | 7.91 | 123.53 | 118.00 |
| 1 | A | 1393 | U | N3-C4-O4 | 7.89 | 124.93 | 119.40 |
| 1 | A | 102 | G | C6-C5-N7 | -7.89 | 125.66 | 130.40 |
| 1 | A | 1104 | G | N1-C2-N3 | 7.89 | 128.63 | 123.90 |
| 1 | A | 1257 | U | C2-N1-C1' | 7.89 | 127.17 | 117.70 |
| 1 | A | 852 | G | N1-C6-O6 | 7.89 | 124.63 | 119.90 |
| 1 | A | 481 | G | C6-C5-N7 | -7.89 | 125.67 | 130.40 |
| 1 | A | 1166 | G | N3-C4-N9 | 7.89 | 130.73 | 126.00 |
| 1 | A | 276 | G | N1-C2-N3 | 7.88 | 128.63 | 123.90 |
| 1 | A | 1189 | C | C6-N1-C2 | -7.88 | 117.15 | 120.30 |
| 1 | A | 288 | A | C2-N3-C4 | -7.88 | 106.66 | 110.60 |
| 1 | A | 1230 | C | N1-C2-N3 | -7.88 | 113.69 | 119.20 |
| 1 | A | 113 | G | C4-N9-C1' | 7.87 | 136.74 | 126.50 |
| 1 | A | 965 | A | C8-N9-C4 | 7.87 | 108.95 | 105.80 |
| 1 | A | 204 | U | C6-N1-C2 | -7.86 | 116.28 | 121.00 |
| 1 | A | 579 | G | N1-C6-O6 | 7.85 | 124.61 | 119.90 |
| 1 | A | 252 | U | N1-C2-O2 | -7.85 | 117.30 | 122.80 |
| 1 | A | 1079 | G | N3-C4-C5 | -7.84 | 124.68 | 128.60 |
| 1 | A | 674 | G | C6-C5-N7 | -7.83 | 125.70 | 130.40 |
| 1 | A | 329 | A | O5'-P-OP1 | -7.81 | 98.67 | 105.70 |
| 1 | A | 232 | G | C6-C5-N7 | -7.81 | 125.71 | 130.40 |
| 1 | A | 928 | G | C5-C6-N1 | -7.81 | 107.59 | 111.50 |
| 1 | A | 672 | U | C4-C5-C6 | 7.80 | 124.38 | 119.70 |
| 1 | A | 49 | U | N3-C2-O2 | 7.80 | 127.66 | 122.20 |
| 1 | A | 1532 | U | C4-C5-C6 | -7.80 | 115.02 | 119.70 |
| 1 | A | 254 | G | OP2-P-O3' | 7.79 | 122.35 | 105.20 |
| 1 | A | 558 | G | N3-C4-N9 | -7.79 | 121.33 | 126.00 |
| 1 | A | 562 | C | C6-N1-C2 | 7.78 | 123.41 | 120.30 |
| 1 | A | 902 | G | N9-C4-C5 | -7.78 | 102.29 | 105.40 |
| 1 | A | 1516[A] | G | C2-N3-C4 | -7.78 | 108.01 | 111.90 |
| 1 | A | 1516[B] | G | C2-N3-C4 | -7.78 | 108.01 | 111.90 |
| 1 | A | 928 | G | N1-C6-O6 | 7.77 | 124.56 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 401 | C | N1-C2-O2 | -7.77 | 114.24 | 118.90 |
| 1 | A | 830 | G | N3-C4-N9 | -7.77 | 121.34 | 126.00 |
| 1 | A | 646 | U | C6-N1-C2 | -7.77 | 116.34 | 121.00 |
| 1 | A | 1532 | U | N3-C2-O2 | 7.77 | 127.64 | 122.20 |
| 1 | A | 1524 | C | O5'-P-OP1 | -7.76 | 98.72 | 105.70 |
| 1 | A | 761 | G | C5-C6-N1 | -7.75 | 107.62 | 111.50 |
| 1 | A | 789 | U | N3-C4-C5 | -7.75 | 109.95 | 114.60 |
| 1 | A | 902 | G | C5-C6-O6 | -7.75 | 123.95 | 128.60 |
| 1 | A | 976 | G | N1-C6-O6 | 7.75 | 124.55 | 119.90 |
| 1 | A | 703 | G | C5-C6-O6 | 7.74 | 133.25 | 128.60 |
| 1 | A | 1189 | C | N3-C2-O2 | -7.74 | 116.48 | 121.90 |
| 1 | A | 920 | U | C5-C4-O4 | 7.73 | 130.54 | 125.90 |
| 1 | A | 864 | A | N9-C4-C5 | 7.73 | 108.89 | 105.80 |
| 1 | A | 500 | G | C5-C6-O6 | -7.72 | 123.97 | 128.60 |
| 1 | A | 1502 | A | C2-N3-C4 | -7.71 | 106.74 | 110.60 |
| 1 | A | 761 | G | C2-N3-C4 | -7.71 | 108.05 | 111.90 |
| 1 | A | 746 | A | C6-N1-C2 | -7.71 | 113.97 | 118.60 |
| 1 | A | 1433 | A | O5'-P-OP1 | -7.71 | 98.76 | 105.70 |
| 1 | A | 372 | C | C5-C4-N4 | -7.70 | 114.81 | 120.20 |
| 1 | A | 1530 | G | C4-N9-C1' | -7.70 | 116.49 | 126.50 |
| 1 | A | 830 | G | C2-N3-C4 | -7.70 | 108.05 | 111.90 |
| 1 | A | 659 | U | N1-C2-N3 | 7.69 | 119.51 | 114.90 |
| 1 | A | 786 | G | N1-C6-O6 | 7.68 | 124.51 | 119.90 |
| 1 | A | 251 | G | C4-C5-N7 | 7.66 | 113.86 | 110.80 |
| 1 | A | 1124 | G | N1-C2-N3 | -7.66 | 119.31 | 123.90 |
| 1 | A | 239 | U | C4-C5-C6 | 7.66 | 124.29 | 119.70 |
| 1 | A | 654 | G | N3-C4-N9 | -7.66 | 121.41 | 126.00 |
| 1 | A | 558 | G | C4-C5-N7 | -7.64 | 107.75 | 110.80 |
| 1 | A | 637 | G | N1-C6-O6 | 7.64 | 124.48 | 119.90 |
| 1 | A | 120 | A | C4-C5-C6 | 7.63 | 120.82 | 117.00 |
| 1 | A | 1100 | C | C5-C6-N1 | 7.62 | 124.81 | 121.00 |
| 1 | A | 786 | G | C5-C6-N1 | -7.62 | 107.69 | 111.50 |
| 1 | A | 829 | G | O5'-P-OP2 | -7.60 | 98.86 | 105.70 |
| 1 | A | 1047 | G | C5-C6-N1 | -7.59 | 107.71 | 111.50 |
| 1 | A | 659 | U | N3-C2-O2 | -7.57 | 116.90 | 122.20 |
| 1 | A | 485 | G | C5-C6-N1 | -7.56 | 107.72 | 111.50 |
| 1 | A | 1182 | G | N3-C4-C5 | -7.55 | 124.82 | 128.60 |
| 1 | A | 392 | G | C8-N9-C4 | 7.54 | 109.42 | 106.40 |
| 1 | A | 902 | G | C6-C5-N7 | -7.54 | 125.88 | 130.40 |
| 1 | A | 108 | G | C2-N3-C4 | -7.53 | 108.13 | 111.90 |
| 1 | A | 387 | U | N3-C4-C5 | -7.53 | 110.08 | 114.60 |
| 1 | A | 491 | G | C5-C6-N1 | -7.53 | 107.73 | 111.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 1 | A | 1104 | G | C2-N3-C4 | -7.53 | 108.14 | 111.90 |
| 1 | A | 446 | G | O5'-P-OP1 | -7.53 | 98.93 | 105.70 |
| 1 | A | 1084 | G | C5-N7-C8 | 7.53 | 108.06 | 104.30 |
| 1 | A | 117 | G | C4-C5-N7 | 7.52 | 113.81 | 110.80 |
| 1 | A | 740 | U | N1-C2-O2 | -7.52 | 117.54 | 122.80 |
| 1 | A | 1129 | C | C6-N1-C2 | -7.52 | 117.29 | 120.30 |
| 1 | A | 1465 | C | N1-C2-O2 | 7.51 | 123.41 | 118.90 |
| 1 | A | 1030(C) | G | C4-N9-C1' | 7.51 | 136.26 | 126.50 |
| 2 | B | 71 | VAL | CB-CA-C | -7.51 | 97.13 | 111.40 |
| 1 | A | 481 | G | OP1-P-OP2 | 7.49 | 130.84 | 119.60 |
| 1 | A | 724 | G | N3-C4-N9 | 7.49 | 130.50 | 126.00 |
| 1 | A | 1395 | C | C6-N1-C2 | 7.49 | 123.30 | 120.30 |
| 1 | A | 1516[A] | G | N3-C4-C5 | 7.49 | 132.35 | 128.60 |
| 1 | A | 1516[B] | G | N3-C4-C5 | 7.49 | 132.35 | 128.60 |
| 1 | A | 494 | G | C8-N9-C4 | -7.49 | 103.40 | 106.40 |
| 1 | A | 120 | A | N1-C2-N3 | 7.49 | 133.04 | 129.30 |
| 17 | Q | 84 | LEU | CA-CB-CG | -7.49 | 98.08 | 115.30 |
| 1 | A | 833 | U | N3-C4-C5 | -7.48 | 110.11 | 114.60 |
| 1 | A | 1222 | G | N1-C6-O6 | 7.48 | 124.39 | 119.90 |
| 1 | A | 494 | G | O5'-P-OP1 | -7.47 | 98.98 | 105.70 |
| 1 | A | 829 | G | N7-C8-N9 | -7.47 | 109.36 | 113.10 |
| 1 | A | 314 | C | C2-N1-C1' | -7.47 | 110.59 | 118.80 |
| 1 | A | 774 | G | N3-C4-N9 | 7.46 | 130.48 | 126.00 |
| 1 | A | 1539 | C | C5-C6-N1 | 7.46 | 124.73 | 121.00 |
| 1 | A | 1075 | C | C5-C6-N1 | -7.45 | 117.27 | 121.00 |
| 1 | A | 1411 | C | N1-C2-O2 | 7.45 | 123.37 | 118.90 |
| 1 | A | 309 | G | N3-C2-N2 | -7.44 | 114.69 | 119.90 |
| 1 | A | 689 | C | N3-C2-O2 | 7.44 | 127.11 | 121.90 |
| 1 | A | 276 | G | C2-N3-C4 | -7.43 | 108.18 | 111.90 |
| 1 | A | 729 | A | N9-C4-C5 | 7.43 | 108.77 | 105.80 |
| 1 | A | 26 | A | C2-N3-C4 | -7.43 | 106.89 | 110.60 |
| 1 | A | 535 | A | N9-C4-C5 | 7.42 | 108.77 | 105.80 |
| 1 | A | 275 | G | N1-C6-O6 | 7.42 | 124.35 | 119.90 |
| 1 | A | 746 | A | N1-C2-N3 | 7.42 | 133.01 | 129.30 |
| 1 | A | 730 | G | N9-C4-C5 | 7.42 | 108.37 | 105.40 |
| 1 | A | 1197 | G | C4-N9-C1' | 7.41 | 136.14 | 126.50 |
| 1 | A | 1420 | C | C6-N1-C2 | -7.41 | 117.34 | 120.30 |
| 1 | A | 244 | U | N1-C2-N3 | -7.41 | 110.45 | 114.90 |
| 1 | A | 108 | G | C4-C5-N7 | 7.40 | 113.76 | 110.80 |
| 1 | A | 975 | A | N7-C8-N9 | 7.40 | 117.50 | 113.80 |
| 2 | B | 11 | LEU | CA-CB-CG | 7.40 | 132.31 | 115.30 |
| 1 | A | 394 | G | C5-C6-N1 | -7.39 | 107.80 | 111.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 29 | G | N1-C6-O6 | 7.39 | 124.34 | 119.90 |
| 1 | A | 715 | A | C8-N9-C4 | 7.39 | 108.76 | 105.80 |
| 1 | A | 83 | U | N1-C2-N3 | -7.38 | 110.47 | 114.90 |
| 1 | A | 1121 | U | C5-C6-N1 | -7.38 | 119.01 | 122.70 |
| 1 | A | 1286 | A | N1-C6-N6 | 7.38 | 123.03 | 118.60 |
| 1 | A | 1495 | U | N3-C4-C5 | -7.36 | 110.18 | 114.60 |
| 1 | A | 662 | G | N9-C4-C5 | -7.36 | 102.46 | 105.40 |
| 1 | A | 61 | G | N1-C6-O6 | 7.36 | 124.31 | 119.90 |
| 1 | A | 499 | A | N1-C6-N6 | -7.36 | 114.19 | 118.60 |
| 1 | A | 549 | C | C5-C6-N1 | -7.36 | 117.32 | 121.00 |
| 1 | A | 1092 | A | O5'-P-OP2 | -7.35 | 99.09 | 105.70 |
| 1 | A | 1222 | G | C2-N3-C4 | -7.34 | 108.23 | 111.90 |
| 1 | A | 864 | A | N1-C6-N6 | -7.34 | 114.20 | 118.60 |
| 1 | A | 881 | G | C8-N9-C4 | 7.34 | 109.33 | 106.40 |
| 1 | A | 672 | U | C5-C4-O4 | 7.34 | 130.30 | 125.90 |
| 1 | A | 378 | G | N1-C6-O6 | 7.33 | 124.30 | 119.90 |
| 1 | A | 66 | G | N3-C4-C5 | 7.33 | 132.26 | 128.60 |
| 1 | A | 558 | G | C6-N1-C2 | 7.32 | 129.49 | 125.10 |
| 1 | A | 1075 | C | C4-C5-C6 | 7.32 | 121.06 | 117.40 |
| 1 | A | 197 | A | N1-C6-N6 | -7.30 | 114.22 | 118.60 |
| 1 | A | 730 | G | C5-C6-O6 | 7.30 | 132.98 | 128.60 |
| 1 | A | 9 | G | C8-N9-C4 | 7.30 | 109.32 | 106.40 |
| 1 | A | 1530 | G | N1-C6-O6 | 7.30 | 124.28 | 119.90 |
| 1 | A | 818 | G | C4-C5-N7 | -7.29 | 107.88 | 110.80 |
| 1 | A | 741 | G | C4-C5-N7 | -7.29 | 107.89 | 110.80 |
| 1 | A | 446 | G | C5-C6-O6 | -7.28 | 124.23 | 128.60 |
| 1 | A | 122 | G | N3-C4-N9 | 7.28 | 130.37 | 126.00 |
| 1 | A | 556 | C | C5-C4-N4 | -7.27 | 115.11 | 120.20 |
| 1 | A | 1183 | A | N1-C6-N6 | 7.27 | 122.96 | 118.60 |
| 1 | A | 117 | G | C5-C6-N1 | -7.27 | 107.87 | 111.50 |
| 1 | A | 1125 | U | C6-N1-C2 | 7.27 | 125.36 | 121.00 |
| 1 | A | 61 | G | N3-C4-C5 | 7.26 | 132.23 | 128.60 |
| 1 | A | 27 | G | C4-C5-N7 | 7.25 | 113.70 | 110.80 |
| 2 | B | 155 | LEU | CA-CB-CG | 7.25 | 131.97 | 115.30 |
| 1 | A | 300 | A | N9-C4-C5 | 7.24 | 108.70 | 105.80 |
| 1 | A | 524 | G | O5'-P-OP1 | -7.24 | 99.18 | 105.70 |
| 1 | A | 1528 | U | O5'-P-OP1 | 7.23 | 119.38 | 110.70 |
| 1 | A | 522 | C | N3-C2-O2 | 7.23 | 126.96 | 121.90 |
| 1 | A | 902 | G | C8-N9-C4 | 7.23 | 109.29 | 106.40 |
| 1 | A | 928 | G | C2-N3-C4 | -7.23 | 108.28 | 111.90 |
| 1 | A | 1212 | U | O4'-C1'-N1 | 7.22 | 113.98 | 108.20 |
| 1 | A | 289 | G | N1-C6-O6 | 7.22 | 124.23 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 1490 | C | C5-C6-N1 | 7.21 | 124.61 | 121.00 |
| 1 | A | 31 | G | N9-C4-C5 | -7.20 | 102.52 | 105.40 |
| 1 | A | 1328 | C | C6-N1-C2 | 7.20 | 123.18 | 120.30 |
| 1 | A | 306 | G | N3-C2-N2 | -7.20 | 114.86 | 119.90 |
| 1 | A | 549 | C | C6-N1-C2 | 7.20 | 123.18 | 120.30 |
| 1 | A | 885 | G | C5-C6-N1 | -7.20 | 107.90 | 111.50 |
| 1 | A | 47 | C | C5-C6-N1 | -7.19 | 117.40 | 121.00 |
| 1 | A | 894 | G | C2-N3-C4 | -7.19 | 108.30 | 111.90 |
| 1 | A | 181 | G | C4-N9-C1' | 7.18 | 135.83 | 126.50 |
| 1 | A | 66 | G | N3-C4-N9 | -7.17 | 121.70 | 126.00 |
| 1 | A | 611 | A | N1-C6-N6 | -7.17 | 114.30 | 118.60 |
| 1 | A | 889 | A | N9-C4-C5 | 7.17 | 108.67 | 105.80 |
| 1 | A | 651 | C | C6-N1-C2 | 7.17 | 123.17 | 120.30 |
| 1 | A | 235 | C | C6-N1-C2 | 7.16 | 123.17 | 120.30 |
| 1 | A | 1258 | G | C8-N9-C4 | -7.16 | 103.54 | 106.40 |
| 1 | A | 674 | G | C2-N3-C4 | -7.16 | 108.32 | 111.90 |
| 1 | A | 833 | U | C5-C4-O4 | 7.16 | 130.19 | 125.90 |
| 1 | A | 504 | C | C6-N1-C2 | -7.15 | 117.44 | 120.30 |
| 1 | A | 1435 | G | C5-C6-O6 | -7.14 | 124.32 | 128.60 |
| 1 | A | 1166 | G | C4-N9-C1' | 7.14 | 135.78 | 126.50 |
| 4 | D | 12 | CYS | CA-CB-SG | 7.14 | 126.85 | 114.00 |
| 1 | A | 584 | G | N7-C8-N9 | -7.14 | 109.53 | 113.10 |
| 1 | A | 729 | A | C8-N9-C4 | -7.14 | 102.94 | 105.80 |
| 1 | A | 1526 | G | N3-C2-N2 | -7.14 | 114.90 | 119.90 |
| 1 | A | 672 | U | C2-N3-C4 | 7.13 | 131.28 | 127.00 |
| 1 | A | 522 | C | C2-N1-C1' | -7.12 | 110.96 | 118.80 |
| 1 | A | 1513 | A | C8-N9-C4 | 7.12 | 108.65 | 105.80 |
| 1 | A | 1432 | G | N3-C4-N9 | -7.11 | 121.73 | 126.00 |
| 1 | A | 299 | G | C4-C5-C6 | 7.11 | 123.07 | 118.80 |
| 1 | A | 803 | G | OP2-P-O3' | 7.11 | 120.83 | 105.20 |
| 1 | A | 285 | G | N9-C4-C5 | -7.11 | 102.56 | 105.40 |
| 1 | A | 1104 | G | N1-C2-N2 | -7.11 | 109.81 | 116.20 |
| 1 | A | 735 | C | C6-N1-C2 | 7.10 | 123.14 | 120.30 |
| 1 | A | 765 | G | C8-N9-C4 | 7.10 | 109.24 | 106.40 |
| 1 | A | 20 | U | C6-N1-C2 | 7.09 | 125.26 | 121.00 |
| 1 | A | 1392 | G | N1-C6-O6 | -7.09 | 115.64 | 119.90 |
| 1 | A | 789 | U | N1-C2-N3 | 7.09 | 119.15 | 114.90 |
| 1 | A | 817 | C | C6-N1-C1' | -7.08 | 112.30 | 120.80 |
| 1 | A | 230 | G | C5-C6-N1 | -7.08 | 107.96 | 111.50 |
| 1 | A | 630 | G | C8-N9-C4 | 7.08 | 109.23 | 106.40 |
| 1 | A | 1155 | G | C8-N9-C1' | -7.07 | 117.81 | 127.00 |
| 1 | A | 586 | C | C5-C4-N4 | -7.07 | 115.25 | 120.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 21 | G | N3-C2-N2 | 7.07 | 124.85 | 119.90 |
| 1 | A | 1126 | U | C5-C6-N1 | 7.07 | 126.23 | 122.70 |
| 1 | A | 1155 | G | C5-C6-N1 | -7.07 | 107.97 | 111.50 |
| 1 | A | 566 | G | C8-N9-C4 | 7.07 | 109.23 | 106.40 |
| 1 | A | 494 | G | O5'-P-OP2 | 7.06 | 119.17 | 110.70 |
| 1 | A | 497 | A | N1-C6-N6 | -7.06 | 114.37 | 118.60 |
| 1 | A | 748 | C | C2-N1-C1' | 7.05 | 126.56 | 118.80 |
| 1 | A | 1397 | C | OP1-P-OP2 | 7.05 | 130.18 | 119.60 |
| 1 | A | 1155 | G | C4-C5-C6 | 7.05 | 123.03 | 118.80 |
| 1 | A | 1257 | U | C5-C6-N1 | 7.04 | 126.22 | 122.70 |
| 1 | A | 578 | C | N3-C2-O2 | -7.04 | 116.97 | 121.90 |
| 1 | A | 44 | G | C6-C5-N7 | -7.03 | 126.18 | 130.40 |
| 1 | A | 703 | G | C4-N9-C1' | 7.03 | 135.64 | 126.50 |
| 1 | A | 484 | G | C5-C6-O6 | 7.03 | 132.82 | 128.60 |
| 1 | A | 299 | G | C6-C5-N7 | -7.03 | 126.18 | 130.40 |
| 1 | A | 22 | G | N1-C6-O6 | 7.02 | 124.11 | 119.90 |
| 1 | A | 353 | A | O5'-P-OP2 | -7.01 | 99.39 | 105.70 |
| 1 | A | 1529 | G | O5'-P-OP1 | -7.01 | 99.39 | 105.70 |
| 1 | A | 674 | G | N9-C4-C5 | -7.01 | 102.60 | 105.40 |
| 1 | A | 1478 | C | C5-C6-N1 | 7.00 | 124.50 | 121.00 |
| 1 | A | 95 | U | N3-C4-C5 | -7.00 | 110.40 | 114.60 |
| 1 | A | 734 | G | C5-C6-O6 | -7.00 | 124.40 | 128.60 |
| 1 | A | 746 | A | N1-C6-N6 | -7.00 | 114.40 | 118.60 |
| 1 | A | 232 | G | N1-C6-O6 | 6.99 | 124.09 | 119.90 |
| 1 | A | 862 | C | O5'-P-OP1 | -6.99 | 99.41 | 105.70 |
| 1 | A | 949 | A | N1-C6-N6 | 6.97 | 122.78 | 118.60 |
| 1 | A | 67 | C | N3-C4-C5 | 6.97 | 124.69 | 121.90 |
| 1 | A | 523 | A | C2-N3-C4 | -6.96 | 107.12 | 110.60 |
| 1 | A | 854 | G | C6-C5-N7 | -6.96 | 126.22 | 130.40 |
| 1 | A | 308 | C | N3-C4-N4 | 6.96 | 122.87 | 118.00 |
| 1 | A | 168 | G | C5-C6-N1 | -6.96 | 108.02 | 111.50 |
| 1 | A | 382 | A | N1-C2-N3 | 6.96 | 132.78 | 129.30 |
| 1 | A | 940 | C | C6-N1-C2 | 6.96 | 123.08 | 120.30 |
| 1 | A | 277 | C | C2-N1-C1' | -6.95 | 111.15 | 118.80 |
| 1 | A | 784 | C | O5'-P-OP2 | -6.95 | 99.44 | 105.70 |
| 1 | A | 577 | G | N3-C4-C5 | 6.95 | 132.07 | 128.60 |
| 1 | A | 859 | A | C8-N9-C4 | 6.94 | 108.58 | 105.80 |
| 1 | A | 279 | A | N7-C8-N9 | 6.94 | 117.27 | 113.80 |
| 1 | A | 1394 | A | N1-C6-N6 | -6.93 | 114.44 | 118.60 |
| 1 | A | 550 | G | C2-N3-C4 | -6.93 | 108.43 | 111.90 |
| 1 | A | 703 | G | C4-C5-N7 | -6.92 | 108.03 | 110.80 |
| 1 | A | 645 | C | N3-C4-C5 | 6.92 | 124.67 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 1 | A | 955 | U | N3-C4-C5 | -6.92 | 110.45 | 114.60 |
| 1 | A | 587 | G | C5-C6-N1 | 6.92 | 114.96 | 111.50 |
| 1 | A | 724 | G | C4-C5-C6 | 6.91 | 122.94 | 118.80 |
| 1 | A | 880 | C | C6-N1-C2 | 6.91 | 123.06 | 120.30 |
| 1 | A | 216 | G | N3-C4-C5 | 6.90 | 132.05 | 128.60 |
| 1 | A | 667 | G | N1-C6-O6 | 6.90 | 124.04 | 119.90 |
| 20 | T | 94 | ALA | N-CA-C | -6.90 | 92.37 | 111.00 |
| 1 | A | 20 | U | C5-C6-N1 | -6.90 | 119.25 | 122.70 |
| 1 | A | 253 | U | O5'-P-OP2 | -6.89 | 99.50 | 105.70 |
| 1 | A | 584 | G | C5-N7-C8 | 6.89 | 107.74 | 104.30 |
| 1 | A | 774 | G | N9-C4-C5 | -6.89 | 102.64 | 105.40 |
| 1 | A | 859 | A | N1-C6-N6 | 6.89 | 122.73 | 118.60 |
| 1 | A | 734 | G | C4-C5-N7 | 6.88 | 113.55 | 110.80 |
| 1 | A | 190(H) | G | C6-C5-N7 | -6.88 | 126.27 | 130.40 |
| 1 | A | 1237 | C | N3-C2-O2 | -6.88 | 117.08 | 121.90 |
| 1 | A | 1373 | G | N3-C4-C5 | -6.88 | 125.16 | 128.60 |
| 1 | A | 817 | C | C4-C5-C6 | 6.87 | 120.83 | 117.40 |
| 1 | A | 200 | G | N1-C6-O6 | 6.86 | 124.02 | 119.90 |
| 1 | A | 873 | A | O5'-P-OP2 | -6.86 | 99.52 | 105.70 |
| 1 | A | 306 | G | N3-C4-C5 | 6.86 | 132.03 | 128.60 |
| 9 | I | 56 | LEU | CA-CB-CG | 6.86 | 131.07 | 115.30 |
| 1 | A | 326 | G | C5-C6-N1 | -6.85 | 108.07 | 111.50 |
| 1 | A | 763 | G | C5-C6-O6 | -6.85 | 124.49 | 128.60 |
| 1 | A | 1432 | G | N9-C4-C5 | 6.85 | 108.14 | 105.40 |
| 1 | A | 893 | C | C4-C5-C6 | -6.85 | 113.97 | 117.40 |
| 1 | A | 1094 | G | N3-C4-C5 | -6.85 | 125.18 | 128.60 |
| 1 | A | 555 | C | O5'-P-OP1 | 6.85 | 118.92 | 110.70 |
| 1 | A | 1390 | U | N3-C4-C5 | -6.84 | 110.49 | 114.60 |
| 1 | A | 518 | C | O5'-P-OP2 | 6.84 | 118.91 | 110.70 |
| 1 | A | 884 | U | C4-C5-C6 | 6.84 | 123.80 | 119.70 |
| 1 | A | 1100 | C | C2-N1-C1' | 6.84 | 126.32 | 118.80 |
| 1 | A | 1197 | G | O5'-P-OP2 | 6.83 | 118.90 | 110.70 |
| 1 | A | 481 | G | C5-C6-O6 | -6.83 | 124.50 | 128.60 |
| 1 | A | 799 | G | C2-N3-C4 | -6.83 | 108.48 | 111.90 |
| 1 | A | 1411 | C | N3-C2-O2 | -6.83 | 117.12 | 121.90 |
| 1 | A | 1155 | G | C4-N9-C1' | 6.83 | 135.38 | 126.50 |
| 1 | A | 1189 | C | C2-N1-C1' | 6.83 | 126.31 | 118.80 |
| 1 | A | 370 | C | N1-C2-O2 | 6.83 | 123.00 | 118.90 |
| 1 | A | 429 | U | O4'-C1'-N1 | 6.82 | 113.66 | 108.20 |
| 1 | A | 759 | A | N1-C6-N6 | -6.82 | 114.51 | 118.60 |
| 1 | A | 975 | A | C5-C6-N1 | -6.82 | 114.29 | 117.70 |
| 1 | A | 1435 | G | C5-C6-N1 | -6.82 | 108.09 | 111.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 1 | A | 544 | G | C5-C6-O6 | -6.82 | 124.51 | 128.60 |
| 1 | A | 1287 | A | C8-N9-C4 | -6.82 | 103.07 | 105.80 |
| 1 | A | 216 | G | C4-N9-C1' | -6.81 | 117.65 | 126.50 |
| 1 | A | 230 | G | C8-N9-C4 | 6.81 | 109.12 | 106.40 |
| 1 | A | 147 | G | C4-C5-C6 | 6.81 | 122.89 | 118.80 |
| 1 | A | 758 | G | N9-C4-C5 | -6.80 | 102.68 | 105.40 |
| 1 | A | 548 | G | N1-C6-O6 | 6.80 | 123.98 | 119.90 |
| 1 | A | 376 | G | N7-C8-N9 | -6.78 | 109.71 | 113.10 |
| 1 | A | 944 | G | N3-C4-C5 | -6.78 | 125.21 | 128.60 |
| 1 | A | 579 | G | C6-C5-N7 | -6.78 | 126.33 | 130.40 |
| 1 | A | 1088 | G | C5-C6-O6 | -6.78 | 124.53 | 128.60 |
| 1 | A | 688 | G | C5-C6-N1 | -6.77 | 108.11 | 111.50 |
| 1 | A | 308 | C | C5-C4-N4 | -6.77 | 115.46 | 120.20 |
| 1 | A | 190(L) | U | O5'-P-OP2 | 6.76 | 118.81 | 110.70 |
| 1 | A | 45 | U | C4-C5-C6 | 6.76 | 123.75 | 119.70 |
| 1 | A | 579 | G | C2-N3-C4 | -6.76 | 108.52 | 111.90 |
| 1 | A | 1227 | A | C6-C5-N7 | -6.76 | 127.57 | 132.30 |
| 1 | A | 276 | G | N1-C6-O6 | 6.75 | 123.95 | 119.90 |
| 1 | A | 357 | G | C8-N9-C4 | 6.75 | 109.10 | 106.40 |
| 1 | A | 661 | G | C2-N3-C4 | -6.75 | 108.52 | 111.90 |
| 1 | A | 32 | A | C5-C6-N1 | 6.75 | 121.08 | 117.70 |
| 1 | A | 174 | C | OP2-P-O3' | 6.75 | 120.05 | 105.20 |
| 1 | A | 729 | A | C4-C5-C6 | 6.75 | 120.37 | 117.00 |
| 1 | A | 47 | C | C2-N3-C4 | -6.74 | 116.53 | 119.90 |
| 1 | A | 31 | G | C4-N9-C1' | 6.74 | 135.26 | 126.50 |
| 1 | A | 266 | G | C4-C5-N7 | 6.74 | 113.50 | 110.80 |
| 1 | A | 289 | G | C6-C5-N7 | -6.74 | 126.36 | 130.40 |
| 1 | A | 783 | C | N3-C2-O2 | 6.74 | 126.61 | 121.90 |
| 1 | A | 833 | U | C4-C5-C6 | 6.74 | 123.74 | 119.70 |
| 1 | A | 899 | C | C6-N1-C2 | 6.74 | 122.99 | 120.30 |
| 1 | A | 1435 | G | C6-C5-N7 | -6.73 | 126.36 | 130.40 |
| 1 | A | 1053 | G | N3-C4-N9 | -6.73 | 121.96 | 126.00 |
| 1 | A | 557 | G | C4-C5-C6 | 6.72 | 122.83 | 118.80 |
| 1 | A | 718 | G | N7-C8-N9 | -6.72 | 109.74 | 113.10 |
| 1 | A | 1168 | A | C2-N3-C4 | 6.72 | 113.96 | 110.60 |
| 1 | A | 1516[A] | G | N3-C2-N2 | -6.72 | 115.19 | 119.90 |
| 1 | A | 1516[B] | G | N3-C2-N2 | -6.72 | 115.19 | 119.90 |
| 1 | A | 1053 | G | C4-N9-C1' | -6.72 | 117.77 | 126.50 |
| 1 | A | 260 | G | N9-C4-C5 | 6.72 | 108.09 | 105.40 |
| 1 | A | 662 | G | N1-C6-O6 | 6.71 | 123.93 | 119.90 |
| 19 | S | 81 | ARG | NE-CZ-NH1 | 6.71 | 123.66 | 120.30 |
| 1 | A | 1527 | C | C5-C6-N1 | -6.71 | 117.64 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 46 | G | C5-C6-N1 | -6.71 | 108.14 | 111.50 |
| 1 | A | 791 | G | C2-N3-C4 | -6.71 | 108.55 | 111.90 |
| 1 | A | 789 | U | C6-N1-C2 | -6.71 | 116.98 | 121.00 |
| 1 | A | 144 | G | N1-C6-O6 | 6.70 | 123.92 | 119.90 |
| 1 | A | 361 | G | C8-N9-C4 | 6.70 | 109.08 | 106.40 |
| 1 | A | 631 | G | N3-C4-C5 | 6.70 | 131.95 | 128.60 |
| 1 | A | 774 | G | C4-C5-N7 | 6.70 | 113.48 | 110.80 |
| 1 | A | 1236 | A | C8-N9-C4 | 6.70 | 108.48 | 105.80 |
| 1 | A | 906 | G | C4-C5-N7 | 6.69 | 113.48 | 110.80 |
| 1 | A | 587 | G | N1-C6-O6 | -6.69 | 115.89 | 119.90 |
| 1 | A | 1498 | UR3 | P-O3'-C3' | 6.69 | 127.73 | 119.70 |
| 1 | A | 50 | A | C8-N9-C4 | 6.69 | 108.47 | 105.80 |
| 1 | A | 1286 | A | C5-N7-C8 | -6.68 | 100.56 | 103.90 |
| 1 | A | 922 | G | C4-N9-C1' | 6.67 | 135.18 | 126.50 |
| 1 | A | 1195 | C | C6-N1-C2 | -6.67 | 117.63 | 120.30 |
| 1 | A | 1370 | G | C5-C6-N1 | -6.67 | 108.16 | 111.50 |
| 1 | A | 169 | C | C6-N1-C2 | -6.67 | 117.63 | 120.30 |
| 1 | A | 304 | U | N3-C4-O4 | 6.67 | 124.07 | 119.40 |
| 1 | A | 1442 | G | C8-N9-C1' | -6.67 | 118.33 | 127.00 |
| 1 | A | 285 | G | N3-C4-C5 | 6.67 | 131.93 | 128.60 |
| 1 | A | 736 | C | N3-C2-O2 | -6.66 | 117.24 | 121.90 |
| 1 | A | 309 | G | C5-C6-N1 | -6.66 | 108.17 | 111.50 |
| 1 | A | 257 | G | C2-N3-C4 | -6.65 | 108.57 | 111.90 |
| 1 | A | 1442 | G | C4-N9-C1' | 6.65 | 135.14 | 126.50 |
| 1 | A | 1487 | G | N3-C4-N9 | 6.65 | 129.99 | 126.00 |
| 1 | A | 810 | C | C5-C4-N4 | 6.64 | 124.85 | 120.20 |
| 1 | A | 317 | G | C5-C6-O6 | -6.64 | 124.62 | 128.60 |
| 1 | A | 376 | G | C8-N9-C4 | 6.64 | 109.06 | 106.40 |
| 1 | A | 111 | G | C5-C6-O6 | 6.64 | 132.58 | 128.60 |
| 1 | A | 407 | G | O5'-P-OP1 | -6.63 | 99.73 | 105.70 |
| 1 | A | 799 | G | C4-C5-N7 | 6.63 | 113.45 | 110.80 |
| 1 | A | 1530 | G | C8-N9-C1' | 6.63 | 135.62 | 127.00 |
| 1 | A | 200 | G | C2-N3-C4 | -6.63 | 108.58 | 111.90 |
| 1 | A | 595 | G | N3-C4-N9 | 6.63 | 129.98 | 126.00 |
| 1 | A | 731 | G | N7-C8-N9 | 6.62 | 116.41 | 113.10 |
| 1 | A | 1394 | A | N9-C4-C5 | 6.62 | 108.45 | 105.80 |
| 1 | A | 24 | U | C5-C6-N1 | -6.62 | 119.39 | 122.70 |
| 1 | A | 279 | A | C5-N7-C8 | -6.62 | 100.59 | 103.90 |
| 1 | A | 766 | A | C5-N7-C8 | -6.62 | 100.59 | 103.90 |
| 1 | A | 855 | G | N1-C6-O6 | 6.62 | 123.87 | 119.90 |
| 1 | A | 120 | A | C2-N3-C4 | -6.61 | 107.29 | 110.60 |
| 1 | A | 721 | G | C5-C6-N1 | -6.61 | 108.19 | 111.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | A | 1228 | C | N1-C2-O2 | 6.61 | 122.87 | 118.90 |
| 1 | A | 28 | G | C6-C5-N7 | -6.61 | 126.44 | 130.40 |
| 1 | A | 732 | C | N3-C2-O2 | -6.61 | 117.28 | 121.90 |
| 1 | A | 712 | A | C6-N1-C2 | -6.61 | 114.64 | 118.60 |
| 1 | A | 445 | G | C8-N9-C4 | -6.60 | 103.76 | 106.40 |
| 1 | A | 693 | G | N3-C2-N2 | -6.60 | 115.28 | 119.90 |
| 1 | A | 1512 | U | N1-C2-N3 | 6.60 | 118.86 | 114.90 |
| 1 | A | 21 | G | N9-C4-C5 | -6.60 | 102.76 | 105.40 |
| 1 | A | 922 | G | C8-N9-C1' | -6.60 | 118.42 | 127.00 |
| 1 | A | 1124 | G | C5-C6-O6 | -6.60 | 124.64 | 128.60 |
| 1 | A | 584 | G | C8-N9-C4 | 6.59 | 109.04 | 106.40 |
| 1 | A | 570 | G | C4-N9-C1' | 6.59 | 135.07 | 126.50 |
| 1 | A | 1125 | U | O5'-P-OP1 | -6.59 | 99.77 | 105.70 |
| 1 | A | 1415 | G | OP1-P-O3' | 6.59 | 119.69 | 105.20 |
| 1 | A | 190(E) | U | N3-C2-O2 | -6.59 | 117.59 | 122.20 |
| 1 | A | 288 | A | N3-C4-C5 | 6.59 | 131.41 | 126.80 |
| 1 | A | 1527 | C | O5'-P-OP2 | -6.59 | 99.77 | 105.70 |
| 1 | A | 285 | G | C2-N3-C4 | -6.58 | 108.61 | 111.90 |
| 1 | A | 298 | A | N1-C2-N3 | 6.58 | 132.59 | 129.30 |
| 1 | A | 428 | G | P-O3'-C3' | 6.58 | 127.59 | 119.70 |
| 1 | A | 1392 | G | N1-C2-N2 | -6.58 | 110.28 | 116.20 |
| 1 | A | 353 | A | O5'-P-OP1 | 6.58 | 118.59 | 110.70 |
| 1 | A | 608 | A | N1-C6-N6 | -6.58 | 114.66 | 118.60 |
| 1 | A | 610 | G | N7-C8-N9 | 6.57 | 116.38 | 113.10 |
| 1 | A | 616 | G | C5-C6-N1 | -6.57 | 108.22 | 111.50 |
| 1 | A | 1166 | G | C6-C5-N7 | -6.57 | 126.46 | 130.40 |
| 1 | A | 147 | G | C2-N3-C4 | -6.56 | 108.62 | 111.90 |
| 1 | A | 735 | C | N3-C4-C5 | 6.56 | 124.53 | 121.90 |
| 1 | A | 761 | G | C6-C5-N7 | -6.56 | 126.46 | 130.40 |
| 1 | A | 46 | G | O5'-P-OP1 | -6.56 | 99.80 | 105.70 |
| 1 | A | 401 | C | N3-C4-C5 | -6.56 | 119.28 | 121.90 |
| 1 | A | 387 | U | C5-C4-O4 | 6.56 | 129.83 | 125.90 |
| 1 | A | 757 | U | C5-C4-O4 | 6.56 | 129.83 | 125.90 |
| 1 | A | 95 | U | C5-C4-O4 | 6.55 | 129.83 | 125.90 |
| 1 | A | 200 | G | C5-C6-N1 | -6.55 | 108.22 | 111.50 |
| 1 | A | 955 | U | C4-C5-C6 | 6.55 | 123.63 | 119.70 |
| 1 | A | 1452 | C | C6-N1-C2 | 6.55 | 122.92 | 120.30 |
| 1 | A | 247 | G | N3-C2-N2 | -6.55 | 115.32 | 119.90 |
| 1 | A | 1092 | A | C8-N9-C4 | -6.55 | 103.18 | 105.80 |
| 1 | A | 158 | G | C8-N9-C4 | -6.55 | 103.78 | 106.40 |
| 1 | A | 403 | C | C5-C6-N1 | -6.55 | 117.73 | 121.00 |
| 1 | A | 618 | C | C6-N1-C2 | 6.54 | 122.92 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 720 | C | C5-C4-N4 | -6.54 | 115.62 | 120.20 |
| 1 | A | 102 | G | N1-C6-O6 | 6.53 | 123.82 | 119.90 |
| 1 | A | 741 | G | C5-N7-C8 | 6.53 | 107.56 | 104.30 |
| 1 | A | 1075 | C | C5-C4-N4 | 6.53 | 124.77 | 120.20 |
| 1 | A | 108 | G | N3-C4-C5 | 6.52 | 131.86 | 128.60 |
| 1 | A | 26 | A | N3-C4-C5 | 6.52 | 131.37 | 126.80 |
| 1 | A | 812 | C | N1-C2-O2 | 6.52 | 122.81 | 118.90 |
| 1 | A | 1512 | U | C4-C5-C6 | 6.52 | 123.61 | 119.70 |
| 1 | A | 849 | C | C6-N1-C2 | -6.52 | 117.69 | 120.30 |
| 1 | A | 631 | G | C4-N9-C1' | -6.52 | 118.03 | 126.50 |
| 1 | A | 1231 | G | N1-C6-O6 | 6.52 | 123.81 | 119.90 |
| 1 | A | 949 | A | C4-C5-N7 | 6.51 | 113.96 | 110.70 |
| 1 | A | 1108 | G | C5-C6-O6 | 6.51 | 132.51 | 128.60 |
| 3 | C | 14 | ILE | CB-CA-C | -6.51 | 98.57 | 111.60 |
| 1 | A | 975 | A | N1-C2-N3 | 6.51 | 132.56 | 129.30 |
| 1 | A | 529 | G | O5'-P-OP2 | -6.51 | 99.84 | 105.70 |
| 1 | A | 707 | C | N1-C2-O2 | 6.51 | 122.81 | 118.90 |
| 1 | A | 1338 | G | C4-N9-C1' | 6.51 | 134.96 | 126.50 |
| 1 | A | 150 | C | C6-N1-C2 | 6.51 | 122.90 | 120.30 |
| 1 | A | 248 | C | C5-C6-N1 | -6.51 | 117.75 | 121.00 |
| 1 | A | 1506 | U | N1-C2-O2 | 6.51 | 127.36 | 122.80 |
| 1 | A | 1104 | G | C6-C5-N7 | -6.50 | 126.50 | 130.40 |
| 1 | A | 614 | A | N1-C6-N6 | 6.50 | 122.50 | 118.60 |
| 1 | A | 413 | G | O4'-C1'-N9 | 6.49 | 113.39 | 108.20 |
| 1 | A | 703 | G | N3-C4-C5 | -6.49 | 125.36 | 128.60 |
| 1 | A | 106 | C | OP2-P-O3' | 6.49 | 119.47 | 105.20 |
| 1 | A | 917 | G | N1-C6-O6 | -6.48 | 116.01 | 119.90 |
| 1 | A | 1531 | A | C5-C6-N6 | -6.48 | 118.52 | 123.70 |
| 1 | A | 724 | G | C4-N9-C1' | 6.48 | 134.93 | 126.50 |
| 1 | A | 677 | U | O5'-P-OP2 | -6.48 | 99.87 | 105.70 |
| 1 | A | 289 | G | O5'-P-OP2 | -6.47 | 99.87 | 105.70 |
| 1 | A | 579 | G | N9-C4-C5 | -6.47 | 102.81 | 105.40 |
| 1 | A | 577 | G | C2-N3-C4 | -6.47 | 108.67 | 111.90 |
| 1 | A | 1093 | A | C5-C6-N1 | 6.47 | 120.94 | 117.70 |
| 1 | A | 21 | G | N3-C4-N9 | 6.46 | 129.88 | 126.00 |
| 1 | A | 703 | G | C5-N7-C8 | 6.46 | 107.53 | 104.30 |
| 1 | A | 710 | G | C4-C5-C6 | 6.46 | 122.68 | 118.80 |
| 1 | A | 902 | G | N1-C2-N3 | 6.46 | 127.78 | 123.90 |
| 1 | A | 1526 | G | N1-C6-O6 | 6.46 | 123.78 | 119.90 |
| 1 | A | 809 | G | C5-C6-N1 | 6.46 | 114.73 | 111.50 |
| 1 | A | 481 | G | C4-C5-N7 | 6.45 | 113.38 | 110.80 |
| 1 | A | 975 | A | C5-N7-C8 | -6.45 | 100.67 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | A | 1166 | G | C4-C5-C6 | 6.45 | 122.67 | 118.80 |
| 1 | A | 520 | A | O5'-P-OP2 | -6.45 | 99.89 | 105.70 |
| 1 | A | 535 | A | O5'-P-OP2 | -6.45 | 99.89 | 105.70 |
| 1 | A | 1432 | G | O5'-P-OP2 | -6.45 | 99.90 | 105.70 |
| 1 | A | 111 | G | C5-C6-N1 | -6.44 | 108.28 | 111.50 |
| 1 | A | 833 | U | N1-C2-N3 | 6.44 | 118.77 | 114.90 |
| 1 | A | 893 | C | C6-N1-C2 | 6.44 | 122.88 | 120.30 |
| 1 | A | 190(E) | U | O5'-P-OP2 | -6.44 | 99.91 | 105.70 |
| 1 | A | 135 | C | O5'-P-OP2 | -6.43 | 99.91 | 105.70 |
| 1 | A | 314 | C | N1-C2-O2 | -6.43 | 115.04 | 118.90 |
| 1 | A | 517 | G | C4-C5-N7 | -6.43 | 108.23 | 110.80 |
| 1 | A | 723 | U | N3-C4-C5 | -6.43 | 110.74 | 114.60 |
| 1 | A | 726 | C | O5'-P-OP1 | -6.43 | 99.92 | 105.70 |
| 1 | A | 1050 | G | C4-C5-N7 | 6.43 | 113.37 | 110.80 |
| 1 | A | 122 | G | N3-C2-N2 | 6.42 | 124.40 | 119.90 |
| 1 | A | 484 | G | N1-C2-N3 | 6.42 | 127.75 | 123.90 |
| 1 | A | 885 | G | C4-C5-N7 | -6.42 | 108.23 | 110.80 |
| 1 | A | 579 | G | C8-N9-C4 | 6.42 | 108.97 | 106.40 |
| 1 | A | 1465 | C | N3-C4-C5 | 6.41 | 124.46 | 121.90 |
| 1 | A | 1502 | A | C5-N7-C8 | -6.41 | 100.69 | 103.90 |
| 1 | A | 1525 | G | C2-N3-C4 | -6.41 | 108.69 | 111.90 |
| 1 | A | 631 | G | N1-C2-N2 | 6.41 | 121.97 | 116.20 |
| 1 | A | 307 | C | O5'-P-OP2 | -6.41 | 99.93 | 105.70 |
| 1 | A | 1485 | U | N1-C2-N3 | 6.41 | 118.74 | 114.90 |
| 1 | A | 449 | C | N3-C4-C5 | -6.40 | 119.34 | 121.90 |
| 1 | A | 617 | G | N1-C2-N3 | 6.40 | 127.74 | 123.90 |
| 1 | A | 1512 | U | C6-N1-C1' | 6.40 | 130.15 | 121.20 |
| 1 | A | 255 | G | C6-C5-N7 | -6.39 | 126.56 | 130.40 |
| 1 | A | 981 | U | N3-C4-O4 | 6.39 | 123.88 | 119.40 |
| 1 | A | 900 | A | N1-C6-N6 | 6.39 | 122.44 | 118.60 |
| 1 | A | 857 | C | N3-C2-O2 | -6.39 | 117.43 | 121.90 |
| 1 | A | 285 | G | N7-C8-N9 | -6.39 | 109.91 | 113.10 |
| 1 | A | 871 | U | C5-C6-N1 | -6.39 | 119.51 | 122.70 |
| 1 | A | 910 | C | N1-C2-O2 | -6.39 | 115.07 | 118.90 |
| 1 | A | 313 | A | N9-C4-C5 | -6.39 | 103.25 | 105.80 |
| 1 | A | 1502 | A | C4-C5-N7 | 6.38 | 113.89 | 110.70 |
| 1 | A | 232 | G | C4-N9-C1' | 6.38 | 134.79 | 126.50 |
| 1 | A | 265 | G | N9-C4-C5 | 6.38 | 107.95 | 105.40 |
| 1 | A | 49 | U | C6-N1-C2 | 6.38 | 124.83 | 121.00 |
| 19 | S | 81 | ARG | NE-CZ-NH2 | -6.38 | 117.11 | 120.30 |
| 1 | A | 535 | A | C4-C5-N7 | -6.37 | 107.52 | 110.70 |
| 1 | A | 657 | G | N1-C6-O6 | 6.37 | 123.72 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 1 | A | 1240 | U | C5-C6-N1 | -6.36 | 119.52 | 122.70 |
| 1 | A | 1341 | U | C5-C4-O4 | 6.36 | 129.72 | 125.90 |
| 1 | A | 36 | C | O5'-P-OP2 | -6.36 | 99.98 | 105.70 |
| 1 | A | 1057 | G | N1-C2-N2 | 6.36 | 121.92 | 116.20 |
| 1 | A | 1030(C) | G | C8-N9-C1' | -6.36 | 118.74 | 127.00 |
| 1 | A | 654 | G | N3-C4-C5 | 6.35 | 131.78 | 128.60 |
| 1 | A | 190(L) | U | O5'-P-OP1 | -6.35 | 99.98 | 105.70 |
| 1 | A | 779 | C | C5-C6-N1 | -6.35 | 117.83 | 121.00 |
| 1 | A | 927 | G | N1-C6-O6 | 6.35 | 123.71 | 119.90 |
| 1 | A | 1087 | G | C4-C5-C6 | 6.35 | 122.61 | 118.80 |
| 1 | A | 1442 | G | N3-C4-N9 | 6.35 | 129.81 | 126.00 |
| 1 | A | 799 | G | O5'-P-OP2 | -6.34 | 99.99 | 105.70 |
| 1 | A | 700 | G | C5-C6-N1 | -6.34 | 108.33 | 111.50 |
| 1 | A | 965 | A | N3-C4-C5 | 6.34 | 131.24 | 126.80 |
| 1 | A | 1058 | G | C8-N9-C4 | 6.34 | 108.94 | 106.40 |
| 1 | A | 104 | G | N1-C6-O6 | 6.34 | 123.70 | 119.90 |
| 1 | A | 1542 | U | N1-C2-N3 | -6.34 | 111.10 | 114.90 |
| 1 | A | 635 | G | C6-C5-N7 | -6.33 | 126.60 | 130.40 |
| 1 | A | 1197 | G | C8-N9-C1' | -6.33 | 118.77 | 127.00 |
| 1 | A | 1374 | A | N1-C2-N3 | 6.33 | 132.47 | 129.30 |
| 1 | A | 630 | G | C6-C5-N7 | 6.33 | 134.20 | 130.40 |
| 1 | A | 725 | G | C5-C6-O6 | -6.33 | 124.80 | 128.60 |
| 1 | A | 1030(B) | C | C6-N1-C2 | -6.33 | 117.77 | 120.30 |
| 1 | A | 507 | C | N3-C4-C5 | 6.32 | 124.43 | 121.90 |
| 1 | A | 834 | C | C6-N1-C2 | 6.32 | 122.83 | 120.30 |
| 1 | A | 1514 | C | N3-C4-C5 | 6.32 | 124.43 | 121.90 |
| 1 | A | 1227 | A | C5-N7-C8 | -6.32 | 100.74 | 103.90 |
| 1 | A | 1506 | U | O5'-P-OP2 | -6.32 | 100.01 | 105.70 |
| 1 | A | 1512 | U | C2-N3-C4 | 6.32 | 130.79 | 127.00 |
| 1 | A | 488 | C | N3-C4-C5 | 6.31 | 124.43 | 121.90 |
| 1 | A | 517 | G | C4-C5-C6 | 6.31 | 122.59 | 118.80 |
| 1 | A | 834 | C | O5'-P-OP2 | -6.31 | 100.02 | 105.70 |
| 1 | A | 950 | U | C5-C4-O4 | 6.31 | 129.69 | 125.90 |
| 1 | A | 1197 | G | O5'-P-OP1 | -6.31 | 100.02 | 105.70 |
| 1 | A | 1338 | G | N3-C4-C5 | -6.31 | 125.44 | 128.60 |
| 1 | A | 1528 | U | C6-N1-C2 | 6.31 | 124.79 | 121.00 |
| 1 | A | 703 | G | N3-C4-N9 | 6.31 | 129.78 | 126.00 |
| 1 | A | 1390 | U | C4-C5-C6 | 6.31 | 123.48 | 119.70 |
| 1 | A | 758 | G | OP2-P-O3' | 6.30 | 119.07 | 105.20 |
| 1 | A | 1544 | U | C6-N1-C2 | -6.30 | 117.22 | 121.00 |
| 1 | A | 816 | A | N1-C6-N6 | -6.30 | 114.82 | 118.60 |
| 1 | A | 309 | G | C4-C5-C6 | 6.30 | 122.58 | 118.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 1323 | G | N1-C6-O6 | 6.30 | 123.68 | 119.90 |
| 1 | A | 654 | G | C2-N3-C4 | -6.29 | 108.75 | 111.90 |
| 1 | A | 1432 | G | N3-C2-N2 | -6.29 | 115.50 | 119.90 |
| 1 | A | 133 | U | N1-C2-O2 | 6.29 | 127.20 | 122.80 |
| 1 | A | 314 | C | C5-C6-N1 | -6.29 | 117.86 | 121.00 |
| 1 | A | 314 | C | N3-C4-N4 | -6.29 | 113.60 | 118.00 |
| 1 | A | 266 | G | C2-N3-C4 | -6.29 | 108.76 | 111.90 |
| 1 | A | 1126 | U | C6-N1-C2 | -6.29 | 117.23 | 121.00 |
| 1 | A | 599 | C | C6-N1-C2 | 6.28 | 122.81 | 120.30 |
| 1 | A | 535 | A | C2-N3-C4 | 6.28 | 113.74 | 110.60 |
| 1 | A | 817 | C | N3-C4-C5 | -6.28 | 119.39 | 121.90 |
| 1 | A | 723 | U | C6-N1-C2 | -6.27 | 117.24 | 121.00 |
| 1 | A | 765 | G | O5'-P-OP1 | -6.27 | 100.06 | 105.70 |
| 1 | A | 835 | U | N3-C2-O2 | -6.27 | 117.81 | 122.20 |
| 1 | A | 890 | G | C5-C6-O6 | 6.27 | 132.36 | 128.60 |
| 1 | A | 1397 | C | N1-C2-O2 | 6.27 | 122.66 | 118.90 |
| 1 | A | 1525 | G | N1-C2-N3 | 6.27 | 127.66 | 123.90 |
| 1 | A | 662 | G | C8-N9-C1' | -6.26 | 118.86 | 127.00 |
| 1 | A | 1124 | G | N1-C2-N2 | 6.26 | 121.84 | 116.20 |
| 1 | A | 710 | G | C6-C5-N7 | -6.25 | 126.65 | 130.40 |
| 1 | A | 916 | G | N1-C6-O6 | -6.25 | 116.15 | 119.90 |
| 1 | A | 1394 | A | C5-C6-N6 | 6.24 | 128.69 | 123.70 |
| 1 | A | 113 | G | N9-C4-C5 | -6.24 | 102.90 | 105.40 |
| 1 | A | 818 | G | O5'-P-OP1 | -6.24 | 100.08 | 105.70 |
| 1 | A | 790 | A | N1-C2-N3 | 6.24 | 132.42 | 129.30 |
| 3 | C | 155 | GLY | N-CA-C | 6.24 | 128.70 | 113.10 |
| 1 | A | 498 | U | O5'-P-OP2 | -6.24 | 100.09 | 105.70 |
| 1 | A | 889 | A | N1-C6-N6 | -6.24 | 114.86 | 118.60 |
| 1 | A | 401 | C | N3-C2-O2 | 6.23 | 126.26 | 121.90 |
| 1 | A | 544 | G | N9-C4-C5 | -6.23 | 102.91 | 105.40 |
| 1 | A | 542 | G | N3-C4-C5 | -6.23 | 125.49 | 128.60 |
| 1 | A | 1334 | G | C8-N9-C4 | -6.22 | 103.91 | 106.40 |
| 1 | A | 117 | G | C2-N3-C4 | -6.22 | 108.79 | 111.90 |
| 1 | A | 192 | U | N3-C2-O2 | -6.22 | 117.84 | 122.20 |
| 1 | A | 975 | A | C6-C5-N7 | -6.22 | 127.94 | 132.30 |
| 1 | A | 504 | C | C2-N1-C1' | 6.22 | 125.64 | 118.80 |
| 1 | A | 815 | A | OP1-P-OP2 | -6.22 | 110.27 | 119.60 |
| 1 | A | 392 | G | N7-C8-N9 | -6.22 | 109.99 | 113.10 |
| 1 | A | 29 | G | C5-C6-N1 | -6.22 | 108.39 | 111.50 |
| 1 | A | 631 | G | C8-N9-C1' | 6.21 | 135.08 | 127.00 |
| 1 | A | 731 | G | C8-N9-C4 | -6.21 | 103.92 | 106.40 |
| 1 | A | 38 | G | C5-C6-N1 | -6.21 | 108.39 | 111.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 1286 | A | C4-C5-N7 | 6.21 | 113.81 | 110.70 |
| 1 | A | 497 | A | C5-C6-N6 | 6.21 | 128.66 | 123.70 |
| 1 | A | 1401 | G | C8-N9-C4 | 6.21 | 108.88 | 106.40 |
| 1 | A | 1513 | A | N7-C8-N9 | -6.21 | 110.70 | 113.80 |
| 1 | A | 641 | U | C2-N1-C1' | 6.20 | 125.14 | 117.70 |
| 1 | A | 1305 | G | N7-C8-N9 | 6.20 | 116.20 | 113.10 |
| 1 | A | 385 | C | O5'-P-OP1 | -6.19 | 100.13 | 105.70 |
| 1 | A | 115 | G | P-O3'-C3' | 6.19 | 127.13 | 119.70 |
| 1 | A | 101 | A | C2-N3-C4 | -6.19 | 107.51 | 110.60 |
| 1 | A | 610 | G | N9-C4-C5 | 6.19 | 107.88 | 105.40 |
| 1 | A | 832 | C | OP2-P-O3' | 6.19 | 118.81 | 105.20 |
| 1 | A | 1239 | A | C8-N9-C4 | 6.18 | 108.27 | 105.80 |
| 1 | A | 148 | G | N3-C4-N9 | 6.18 | 129.71 | 126.00 |
| 1 | A | 305 | G | C4-C5-C6 | 6.18 | 122.51 | 118.80 |
| 1 | A | 733 | A | N1-C2-N3 | 6.18 | 132.39 | 129.30 |
| 1 | A | 435 | C | O5'-P-OP1 | -6.18 | 100.14 | 105.70 |
| 1 | A | 836 | G | N1-C6-O6 | 6.18 | 123.61 | 119.90 |
| 1 | A | 331 | G | C6-C5-N7 | -6.17 | 126.69 | 130.40 |
| 1 | A | 536 | C | C6-N1-C2 | -6.17 | 117.83 | 120.30 |
| 1 | A | 1094 | G | N3-C4-N9 | 6.17 | 129.71 | 126.00 |
| 1 | A | 267 | C | C5-C4-N4 | 6.17 | 124.52 | 120.20 |
| 1 | A | 652 | U | N3-C4-C5 | 6.16 | 118.30 | 114.60 |
| 1 | A | 161 | A | C5-C6-N6 | 6.16 | 128.63 | 123.70 |
| 1 | A | 104 | G | C4-C5-C6 | 6.16 | 122.49 | 118.80 |
| 1 | A | 284 | G | N3-C2-N2 | -6.16 | 115.59 | 119.90 |
| 1 | A | 925 | G | C2-N3-C4 | -6.16 | 108.82 | 111.90 |
| 1 | A | 1079 | G | N3-C4-N9 | 6.16 | 129.69 | 126.00 |
| 1 | A | 1341 | U | N3-C4-O4 | -6.16 | 115.09 | 119.40 |
| 1 | A | 232 | G | C8-N9-C1' | -6.15 | 119.00 | 127.00 |
| 1 | A | 1259 | C | N1-C2-O2 | 6.15 | 122.59 | 118.90 |
| 1 | A | 587 | G | C2-N3-C4 | 6.15 | 114.97 | 111.90 |
| 1 | A | 774 | G | C8-N9-C1' | -6.15 | 119.01 | 127.00 |
| 1 | A | 187 | C | N3-C4-C5 | -6.14 | 119.44 | 121.90 |
| 1 | A | 1206 | G | C2-N3-C4 | -6.14 | 108.83 | 111.90 |
| 1 | A | 1478 | C | C6-N1-C2 | -6.14 | 117.84 | 120.30 |
| 1 | A | 105 | G | N1-C6-O6 | 6.14 | 123.59 | 119.90 |
| 1 | A | 255 | G | C2-N3-C4 | -6.14 | 108.83 | 111.90 |
| 1 | A | 1058 | G | N1-C6-O6 | 6.14 | 123.59 | 119.90 |
| 1 | A | 1227 | A | N9-C4-C5 | -6.14 | 103.34 | 105.80 |
| 1 | A | 944 | G | C4-N9-C1' | 6.14 | 134.48 | 126.50 |
| 1 | A | 26 | A | N3-C4-N9 | -6.14 | 122.49 | 127.40 |
| 1 | A | 357 | G | N1-C6-O6 | 6.14 | 123.58 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 406 | G | C8-N9-C4 | -6.14 | 103.94 | 106.40 |
| 1 | A | 564 | C | C6-N1-C2 | 6.13 | 122.75 | 120.30 |
| 1 | A | 570 | G | C8-N9-C4 | -6.13 | 103.95 | 106.40 |
| 1 | A | 705 | U | O5'-P-OP2 | -6.13 | 100.18 | 105.70 |
| 1 | A | 375 | U | N3-C4-C5 | -6.13 | 110.92 | 114.60 |
| 1 | A | 352 | C | N3-C4-C5 | -6.12 | 119.45 | 121.90 |
| 1 | A | 1069 | C | N3-C2-O2 | 6.12 | 126.19 | 121.90 |
| 1 | A | 1131 | G | C5-C6-N1 | -6.12 | 108.44 | 111.50 |
| 1 | A | 1125 | U | N1-C2-N3 | -6.12 | 111.23 | 114.90 |
| 1 | A | 61 | G | O5'-P-OP1 | -6.11 | 100.20 | 105.70 |
| 1 | A | 976 | G | C8-N9-C4 | 6.11 | 108.84 | 106.40 |
| 1 | A | 631 | G | N1-C2-N3 | -6.11 | 120.23 | 123.90 |
| 1 | A | 776 | G | OP1-P-O3' | 6.10 | 118.63 | 105.20 |
| 1 | A | 1435 | G | N3-C2-N2 | -6.10 | 115.63 | 119.90 |
| 1 | A | 1490 | C | C4-C5-C6 | -6.10 | 114.35 | 117.40 |
| 1 | A | 562 | C | C5-C6-N1 | -6.10 | 117.95 | 121.00 |
| 1 | A | 1341 | U | C5-C6-N1 | -6.10 | 119.65 | 122.70 |
| 1 | A | 1530 | G | O5'-P-OP2 | -6.09 | 100.22 | 105.70 |
| 1 | A | 47 | C | C4-C5-C6 | 6.09 | 120.44 | 117.40 |
| 1 | A | 773 | G | N1-C2-N3 | 6.09 | 127.55 | 123.90 |
| 1 | A | 941 | G | C8-N9-C4 | 6.08 | 108.83 | 106.40 |
| 1 | A | 1202 | G | C8-N9-C4 | -6.08 | 103.97 | 106.40 |
| 1 | A | 1342 | C | N3-C4-C5 | 6.08 | 124.33 | 121.90 |
| 1 | A | 67 | C | C2-N3-C4 | -6.08 | 116.86 | 119.90 |
| 1 | A | 1528 | U | OP1-P-O3' | 6.08 | 118.57 | 105.20 |
| 1 | A | 517 | G | N3-C4-C5 | -6.08 | 125.56 | 128.60 |
| 1 | A | 819 | A | N9-C4-C5 | -6.07 | 103.37 | 105.80 |
| 1 | A | 1342 | C | C6-N1-C2 | 6.07 | 122.73 | 120.30 |
| 1 | A | 1188 | A | N1-C2-N3 | 6.07 | 132.34 | 129.30 |
| 1 | A | 945 | G | C5-C6-N1 | 6.07 | 114.53 | 111.50 |
| 1 | A | 1454 | G | C2-N3-C4 | -6.07 | 108.87 | 111.90 |
| 1 | A | 778 | G | C4-C5-C6 | 6.06 | 122.44 | 118.80 |
| 1 | A | 641 | U | C6-N1-C1' | -6.06 | 112.72 | 121.20 |
| 1 | A | 707 | C | N3-C2-O2 | -6.06 | 117.66 | 121.90 |
| 1 | A | 774 | G | C4-N9-C1' | 6.05 | 134.37 | 126.50 |
| 1 | A | 652 | U | C6-N1-C2 | 6.05 | 124.63 | 121.00 |
| 1 | A | 1054 | C | C2-N1-C1' | 6.05 | 125.45 | 118.80 |
| 1 | A | 710 | G | C2-N3-C4 | -6.05 | 108.88 | 111.90 |
| 1 | A | 513 | C | C6-N1-C2 | 6.04 | 122.72 | 120.30 |
| 1 | A | 66 | G | N3-C2-N2 | -6.04 | 115.67 | 119.90 |
| 1 | A | 642 | A | N1-C2-N3 | 6.04 | 132.32 | 129.30 |
| 1 | A | 105 | G | C6-C5-N7 | -6.04 | 126.78 | 130.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 1227 | A | O4'-C1'-N9 | -6.04 | 103.37 | 108.20 |
| 1 | A | 10 | A | C6-N1-C2 | -6.03 | 114.98 | 118.60 |
| 1 | A | 698 | G | N1-C6-O6 | 6.03 | 123.52 | 119.90 |
| 1 | A | 1491 | G | N7-C8-N9 | 6.03 | 116.12 | 113.10 |
| 1 | A | 28 | G | C4-C5-C6 | 6.03 | 122.42 | 118.80 |
| 1 | A | 325 | A | C4-C5-N7 | -6.03 | 107.69 | 110.70 |
| 1 | A | 1100 | C | N1-C2-O2 | 6.03 | 122.52 | 118.90 |
| 1 | A | 1479 | C | N3-C4-C5 | -6.03 | 119.49 | 121.90 |
| 1 | A | 1530 | G | N1-C2-N2 | 6.03 | 121.62 | 116.20 |
| 1 | A | 16 | A | O5'-P-OP1 | -6.02 | 100.28 | 105.70 |
| 1 | A | 1227 | A | C5-C6-N6 | -6.02 | 118.88 | 123.70 |
| 1 | A | 809 | G | C2-N3-C4 | 6.02 | 114.91 | 111.90 |
| 1 | A | 234 | C | C5-C6-N1 | -6.02 | 117.99 | 121.00 |
| 1 | A | 584 | G | C4-C5-N7 | -6.02 | 108.39 | 110.80 |
| 1 | A | 811 | C | C2-N3-C4 | -6.02 | 116.89 | 119.90 |
| 1 | A | 1227 | A | C4-C5-N7 | 6.02 | 113.71 | 110.70 |
| 1 | A | 1424 | C | C6-N1-C2 | 6.02 | 122.71 | 120.30 |
| 1 | A | 1054 | C | N3-C2-O2 | -6.02 | 117.69 | 121.90 |
| 1 | A | 24 | U | C2-N3-C4 | -6.01 | 123.39 | 127.00 |
| 1 | A | 635 | G | C5-C6-N1 | -6.01 | 108.49 | 111.50 |
| 1 | A | 658 | G | N1-C2-N3 | 6.01 | 127.50 | 123.90 |
| 1 | A | 1253 | G | C8-N9-C4 | -6.01 | 104.00 | 106.40 |
| 1 | A | 1437 | C | C6-N1-C2 | 6.01 | 122.70 | 120.30 |
| 1 | A | 563 | A | C2-N3-C4 | -6.01 | 107.60 | 110.60 |
| 1 | A | 1053 | G | C8-N9-C1' | 6.00 | 134.81 | 127.00 |
| 1 | A | 1392 | G | N3-C4-C5 | -6.00 | 125.60 | 128.60 |
| 1 | A | 111 | G | N9-C4-C5 | 6.00 | 107.80 | 105.40 |
| 1 | A | 234 | C | N3-C4-C5 | 6.00 | 124.30 | 121.90 |
| 3 | C | 12 | LEU | CA-CB-CG | -6.00 | 101.51 | 115.30 |
| 1 | A | 1453 | G | N9-C4-C5 | -6.00 | 103.00 | 105.40 |
| 1 | A | 1064 | G | N9-C4-C5 | -5.99 | 103.00 | 105.40 |
| 1 | A | 1167 | A | C2-N3-C4 | -5.99 | 107.61 | 110.60 |
| 1 | A | 22 | G | C6-C5-N7 | -5.99 | 126.81 | 130.40 |
| 1 | A | 864 | A | C5-C6-N6 | 5.99 | 128.49 | 123.70 |
| 1 | A | 791 | G | C8-N9-C1' | -5.99 | 119.22 | 127.00 |
| 1 | A | 1302 | U | N3-C4-O4 | -5.99 | 115.21 | 119.40 |
| 1 | A | 1054 | C | O4'-C1'-N1 | 5.98 | 112.98 | 108.20 |
| 1 | A | 1522 | U | O5'-P-OP1 | 5.98 | 117.88 | 110.70 |
| 1 | A | 549 | C | C2-N3-C4 | -5.98 | 116.91 | 119.90 |
| 1 | A | 557 | G | C5-C6-N1 | -5.98 | 108.51 | 111.50 |
| 1 | A | 228 | A | C6-N1-C2 | -5.97 | 115.02 | 118.60 |
| 1 | A | 553 | A | C8-N9-C4 | 5.97 | 108.19 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 1 | A | 1387 | G | OP1-P-O3' | 5.97 | 118.34 | 105.20 |
| 1 | A | 761 | G | N1-C2-N3 | 5.97 | 127.48 | 123.90 |
| 1 | A | 385 | C | O5'-P-OP2 | 5.97 | 117.86 | 110.70 |
| 1 | A | 970 | C | C6-N1-C2 | 5.97 | 122.69 | 120.30 |
| 1 | A | 748 | C | C6-N1-C2 | -5.96 | 117.91 | 120.30 |
| 1 | A | 251 | G | N9-C4-C5 | -5.96 | 103.02 | 105.40 |
| 1 | A | 9 | G | N7-C8-N9 | -5.96 | 110.12 | 113.10 |
| 1 | A | 181 | G | C8-N9-C1' | -5.96 | 119.25 | 127.00 |
| 1 | A | 724 | G | N7-C8-N9 | 5.96 | 116.08 | 113.10 |
| 1 | A | 1149 | C | N1-C2-O2 | -5.96 | 115.33 | 118.90 |
| 1 | A | 474 | G | N1-C6-O6 | 5.96 | 123.47 | 119.90 |
| 1 | A | 1211 | U | C5-C4-O4 | -5.96 | 122.33 | 125.90 |
| 1 | A | 1333 | A | N1-C2-N3 | 5.95 | 132.28 | 129.30 |
| 1 | A | 1502 | A | OP2-P-O3' | 5.95 | 118.30 | 105.20 |
| 1 | A | 498 | U | N1-C2-O2 | -5.95 | 118.63 | 122.80 |
| 1 | A | 132 | C | C5-C6-N1 | -5.95 | 118.03 | 121.00 |
| 1 | A | 575 | G | OP1-P-O3' | 5.95 | 118.28 | 105.20 |
| 1 | A | 243 | A | O5'-P-OP2 | -5.95 | 100.35 | 105.70 |
| 1 | A | 481 | G | N1-C6-O6 | 5.95 | 123.47 | 119.90 |
| 1 | A | 31 | G | C6-C5-N7 | -5.94 | 126.83 | 130.40 |
| 1 | A | 365 | U | N3-C2-O2 | -5.94 | 118.04 | 122.20 |
| 1 | A | 242 | C | C5-C6-N1 | -5.94 | 118.03 | 121.00 |
| 1 | A | 805 | C | C5-C4-N4 | -5.94 | 116.04 | 120.20 |
| 1 | A | 1396 | A | OP1-P-OP2 | 5.94 | 128.51 | 119.60 |
| 12 | L | 27 | LEU | CA-CB-CG | 5.93 | 128.95 | 115.30 |
| 18 | R | 85 | LEU | CA-CB-CG | 5.93 | 128.94 | 115.30 |
| 1 | A | 1309 | G | N1-C6-O6 | -5.93 | 116.34 | 119.90 |
| 1 | A | 1061 | G | N1-C6-O6 | 5.93 | 123.46 | 119.90 |
| 1 | A | 196 | A | C4-C5-C6 | -5.92 | 114.04 | 117.00 |
| 1 | A | 1026 | G | C5-N7-C8 | -5.92 | 101.34 | 104.30 |
| 1 | A | 168 | G | N1-C6-O6 | 5.92 | 123.45 | 119.90 |
| 1 | A | 388 | G | C8-N9-C4 | 5.92 | 108.77 | 106.40 |
| 1 | A | 957 | U | N1-C2-N3 | 5.92 | 118.45 | 114.90 |
| 1 | A | 300 | A | C5-C6-N6 | 5.92 | 128.43 | 123.70 |
| 1 | A | 1200 | C | N1-C2-O2 | -5.91 | 115.35 | 118.90 |
| 1 | A | 1516[A] | G | C8-N9-C1' | 5.91 | 134.69 | 127.00 |
| 1 | A | 1516[B] | G | C8-N9-C1' | 5.91 | 134.69 | 127.00 |
| 1 | A | 719 | C | N3-C4-C5 | -5.91 | 119.53 | 121.90 |
| 1 | A | 970 | C | N3-C2-O2 | -5.91 | 117.76 | 121.90 |
| 1 | A | 113 | G | C4-C5-C6 | 5.91 | 122.35 | 118.80 |
| 1 | A | 381 | C | C5-C6-N1 | 5.91 | 123.95 | 121.00 |
| 1 | A | 553 | A | C2-N3-C4 | -5.91 | 107.65 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 554 | C | C4-C5-C6 | 5.91 | 120.35 | 117.40 |
| 1 | A | 174 | C | C6-N1-C2 | -5.90 | 117.94 | 120.30 |
| 1 | A | 886 | G | C6-C5-N7 | -5.90 | 126.86 | 130.40 |
| 1 | A | 1502 | A | C6-C5-N7 | -5.90 | 128.17 | 132.30 |
| 1 | A | 117 | G | C4-C5-C6 | 5.90 | 122.34 | 118.80 |
| 1 | A | 641 | U | N1-C2-O2 | 5.90 | 126.93 | 122.80 |
| 1 | A | 766 | A | C4-C5-N7 | 5.90 | 113.65 | 110.70 |
| 1 | A | 650 | G | C5-C6-O6 | -5.89 | 125.06 | 128.60 |
| 1 | A | 133 | U | N3-C4-C5 | -5.89 | 111.06 | 114.60 |
| 1 | A | 357 | G | N7-C8-N9 | -5.89 | 110.15 | 113.10 |
| 1 | A | 791 | G | C4-C5-N7 | -5.89 | 108.44 | 110.80 |
| 1 | A | 858 | G | N3-C4-N9 | 5.89 | 129.54 | 126.00 |
| 1 | A | 61 | G | C5-N7-C8 | -5.89 | 101.36 | 104.30 |
| 1 | A | 861 | G | C4-C5-N7 | 5.89 | 113.16 | 110.80 |
| 1 | A | 313 | A | C5-C6-N6 | -5.89 | 118.99 | 123.70 |
| 1 | A | 712 | A | N1-C2-N3 | 5.89 | 132.24 | 129.30 |
| 1 | A | 116 | A | C2-N3-C4 | -5.89 | 107.66 | 110.60 |
| 1 | A | 807 | A | N1-C6-N6 | 5.89 | 122.13 | 118.60 |
| 1 | A | 216 | G | N3-C4-N9 | -5.88 | 122.47 | 126.00 |
| 1 | A | 630 | G | N7-C8-N9 | -5.88 | 110.16 | 113.10 |
| 1 | A | 1453 | G | N3-C4-N9 | 5.88 | 129.53 | 126.00 |
| 1 | A | 485 | G | O4'-C1'-N9 | 5.88 | 112.90 | 108.20 |
| 1 | A | 491 | G | C4-C5-C6 | 5.87 | 122.32 | 118.80 |
| 1 | A | 993 | G | C4-C5-N7 | 5.87 | 113.15 | 110.80 |
| 1 | A | 1054 | C | C6-N1-C1' | -5.87 | 113.75 | 120.80 |
| 1 | A | 25 | C | O5'-P-OP1 | 5.87 | 117.75 | 110.70 |
| 1 | A | 216 | G | C8-N9-C4 | 5.87 | 108.75 | 106.40 |
| 1 | A | 1005 | A | C4-C5-C6 | 5.87 | 119.94 | 117.00 |
| 1 | A | 45 | U | N1-C2-N3 | 5.87 | 118.42 | 114.90 |
| 1 | A | 102 | G | C5-C6-O6 | -5.87 | 125.08 | 128.60 |
| 1 | A | 173 | U | N3-C4-O4 | -5.87 | 115.29 | 119.40 |
| 1 | A | 41 | G | N1-C6-O6 | 5.87 | 123.42 | 119.90 |
| 1 | A | 400 | C | N3-C2-O2 | 5.87 | 126.01 | 121.90 |
| 1 | A | 1287 | A | N7-C8-N9 | 5.87 | 116.73 | 113.80 |
| 1 | A | 1463 | C | C6-N1-C2 | 5.86 | 122.65 | 120.30 |
| 1 | A | 578 | C | C2-N3-C4 | -5.86 | 116.97 | 119.90 |
| 1 | A | 505 | G | N1-C6-O6 | -5.86 | 116.38 | 119.90 |
| 1 | A | 362 | G | C5-C6-N1 | -5.86 | 108.57 | 111.50 |
| 1 | A | 388 | G | C5-C6-N1 | -5.86 | 108.57 | 111.50 |
| 1 | A | 405 | U | C5-C4-O4 | 5.86 | 129.41 | 125.90 |
| 1 | A | 657 | G | N3-C2-N2 | -5.86 | 115.80 | 119.90 |
| 1 | A | 778 | G | C5-C6-N1 | -5.86 | 108.57 | 111.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 1 | A | 1524 | C | N1-C2-O2 | -5.86 | 115.39 | 118.90 |
| 1 | A | 887 | G | N3-C2-N2 | -5.85 | 115.80 | 119.90 |
| 1 | A | 1129 | C | O4'-C1'-N1 | 5.85 | 112.88 | 108.20 |
| 1 | A | 15 | G | C6-C5-N7 | -5.85 | 126.89 | 130.40 |
| 1 | A | 251 | G | C6-C5-N7 | -5.85 | 126.89 | 130.40 |
| 1 | A | 1030(A) | G | C2-N3-C4 | 5.85 | 114.82 | 111.90 |
| 1 | A | 780 | A | C5-C6-N1 | 5.84 | 120.62 | 117.70 |
| 1 | A | 317 | G | N1-C6-O6 | 5.84 | 123.40 | 119.90 |
| 1 | A | 553 | A | N1-C6-N6 | 5.84 | 122.10 | 118.60 |
| 1 | A | 1333 | A | C6-N1-C2 | -5.84 | 115.10 | 118.60 |
| 1 | A | 595 | G | C8-N9-C1' | -5.83 | 119.42 | 127.00 |
| 1 | A | 719 | C | N3-C4-N4 | 5.83 | 122.08 | 118.00 |
| 1 | A | 1198 | G | C2-N3-C4 | -5.83 | 108.98 | 111.90 |
| 1 | A | 188 | C | N3-C4-C5 | -5.83 | 119.57 | 121.90 |
| 1 | A | 284 | G | N3-C4-C5 | 5.83 | 131.51 | 128.60 |
| 1 | A | 190(D) | U | C5-C6-N1 | -5.83 | 119.79 | 122.70 |
| 1 | A | 1528 | U | C5-C6-N1 | -5.82 | 119.79 | 122.70 |
| 1 | A | 23 | C | OP2-P-O3' | 5.82 | 118.00 | 105.20 |
| 1 | A | 1205 | U | N3-C4-O4 | 5.82 | 123.47 | 119.40 |
| 1 | A | 305 | G | N1-C6-O6 | 5.82 | 123.39 | 119.90 |
| 6 | F | 21 | LEU | CA-CB-CG | -5.82 | 101.92 | 115.30 |
| 1 | A | 572 | A | N1-C6-N6 | -5.81 | 115.11 | 118.60 |
| 1 | A | 1157 | A | C8-N9-C4 | -5.81 | 103.48 | 105.80 |
| 1 | A | 378 | G | C5-C6-O6 | -5.81 | 125.11 | 128.60 |
| 1 | A | 859 | A | C5-C6-N1 | -5.81 | 114.80 | 117.70 |
| 1 | A | 189 | G | C8-N9-C4 | 5.80 | 108.72 | 106.40 |
| 1 | A | 810 | C | N3-C2-O2 | -5.80 | 117.84 | 121.90 |
| 1 | A | 260 | G | C5-C6-N1 | -5.80 | 108.60 | 111.50 |
| 1 | A | 1100 | C | C5-C4-N4 | -5.80 | 116.14 | 120.20 |
| 1 | A | 631 | G | N3-C4-N9 | -5.80 | 122.52 | 126.00 |
| 1 | A | 728 | A | N7-C8-N9 | 5.80 | 116.70 | 113.80 |
| 1 | A | 877 | C | N3-C4-N4 | 5.80 | 122.06 | 118.00 |
| 1 | A | 1205 | U | C4-C5-C6 | 5.79 | 123.18 | 119.70 |
| 1 | A | 25 | C | O5'-P-OP2 | -5.79 | 100.49 | 105.70 |
| 1 | A | 1079 | G | C8-N9-C4 | -5.79 | 104.08 | 106.40 |
| 1 | A | 305 | G | C2-N3-C4 | -5.79 | 109.00 | 111.90 |
| 1 | A | 571 | U | C6-N1-C2 | -5.79 | 117.53 | 121.00 |
| 1 | A | 885 | G | N3-C2-N2 | -5.79 | 115.85 | 119.90 |
| 1 | A | 1220 | G | N1-C6-O6 | 5.79 | 123.37 | 119.90 |
| 1 | A | 769 | G | OP2-P-O3' | 5.78 | 117.92 | 105.20 |
| 1 | A | 907 | A | N1-C6-N6 | -5.78 | 115.13 | 118.60 |
| 19 | S | 4 | SER | N-CA-C | 5.78 | 126.61 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 1 | A | 670 | G | O5'-P-OP2 | -5.78 | 100.50 | 105.70 |
| 1 | A | 720 | C | N3-C4-C5 | 5.78 | 124.21 | 121.90 |
| 1 | A | 1470 | G | C8-N9-C1' | -5.78 | 119.49 | 127.00 |
| 1 | A | 108 | G | C5-C6-O6 | -5.78 | 125.14 | 128.60 |
| 1 | A | 194 | C | C6-N1-C2 | 5.78 | 122.61 | 120.30 |
| 1 | A | 548 | G | C5-C6-O6 | -5.78 | 125.14 | 128.60 |
| 1 | A | 562 | C | C6-N1-C1' | -5.78 | 113.87 | 120.80 |
| 1 | A | 1182 | G | N3-C4-N9 | 5.77 | 129.46 | 126.00 |
| 1 | A | 448 | A | O5'-P-OP2 | -5.77 | 100.51 | 105.70 |
| 1 | A | 703 | G | N3-C2-N2 | 5.77 | 123.94 | 119.90 |
| 1 | A | 943 | U | N3-C2-O2 | 5.77 | 126.24 | 122.20 |
| 1 | A | 1377 | A | N1-C2-N3 | 5.77 | 132.18 | 129.30 |
| 1 | A | 79 | G | C6-C5-N7 | -5.76 | 126.94 | 130.40 |
| 1 | A | 485 | G | N7-C8-N9 | -5.76 | 110.22 | 113.10 |
| 1 | A | 1426 | C | C5-C6-N1 | -5.76 | 118.12 | 121.00 |
| 1 | A | 533 | A | O5'-P-OP2 | -5.76 | 100.52 | 105.70 |
| 1 | A | 122 | G | O5'-P-OP1 | -5.75 | 100.52 | 105.70 |
| 1 | A | 314 | C | N3-C2-O2 | 5.75 | 125.93 | 121.90 |
| 1 | A | 1432 | G | N7-C8-N9 | 5.75 | 115.98 | 113.10 |
| 1 | A | 821 | G | C2-N3-C4 | -5.75 | 109.03 | 111.90 |
| 1 | A | 1030(B) | C | C5-C6-N1 | 5.75 | 123.87 | 121.00 |
| 1 | A | 1053 | G | C6-C5-N7 | 5.75 | 133.85 | 130.40 |
| 1 | A | 255 | G | C5-C6-O6 | -5.75 | 125.15 | 128.60 |
| 1 | A | 712 | A | O5'-P-OP1 | -5.74 | 100.53 | 105.70 |
| 1 | A | 637 | G | C8-N9-C4 | 5.74 | 108.70 | 106.40 |
| 1 | A | 21 | G | C4-C5-N7 | 5.74 | 113.10 | 110.80 |
| 1 | A | 1542 | U | N1-C2-O2 | 5.74 | 126.82 | 122.80 |
| 1 | A | 664 | G | N7-C8-N9 | -5.74 | 110.23 | 113.10 |
| 1 | A | 562 | C | N3-C2-O2 | -5.74 | 117.89 | 121.90 |
| 1 | A | 61 | G | C4-C5-N7 | 5.73 | 113.09 | 110.80 |
| 1 | A | 295 | C | N3-C4-C5 | 5.73 | 124.19 | 121.90 |
| 1 | A | 1257 | U | N1-C2-O2 | 5.73 | 126.81 | 122.80 |
| 1 | A | 104 | G | C6-C5-N7 | -5.72 | 126.97 | 130.40 |
| 1 | A | 566 | G | N7-C8-N9 | -5.72 | 110.24 | 113.10 |
| 1 | A | 817 | C | N3-C2-O2 | -5.72 | 117.89 | 121.90 |
| 1 | A | 31 | G | N3-C2-N2 | 5.72 | 123.91 | 119.90 |
| 1 | A | 1487 | G | N3-C4-C5 | -5.72 | 125.74 | 128.60 |
| 1 | A | 791 | G | N1-C6-O6 | 5.72 | 123.33 | 119.90 |
| 1 | A | 502 | G | O5'-P-OP2 | -5.72 | 100.55 | 105.70 |
| 1 | A | 164 | U | O5'-P-OP1 | -5.72 | 100.56 | 105.70 |
| 1 | A | 304 | U | C6-N1-C2 | -5.72 | 117.57 | 121.00 |
| 1 | A | 50 | A | C2-N3-C4 | -5.71 | 107.74 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 181 | G | C6-C5-N7 | -5.71 | 126.97 | 130.40 |
| 1 | A | 816 | A | C4-C5-N7 | -5.71 | 107.84 | 110.70 |
| 1 | A | 1100 | C | C6-N1-C1' | -5.71 | 113.95 | 120.80 |
| 1 | A | 1230 | C | C5-C6-N1 | 5.71 | 123.86 | 121.00 |
| 1 | A | 1083 | U | C4-C5-C6 | 5.71 | 123.13 | 119.70 |
| 1 | A | 1193 | G | C4-C5-C6 | 5.71 | 122.23 | 118.80 |
| 1 | A | 502 | G | N3-C4-N9 | -5.71 | 122.58 | 126.00 |
| 1 | A | 1514 | C | C5-C6-N1 | -5.71 | 118.15 | 121.00 |
| 1 | A | 381 | C | N3-C4-C5 | -5.70 | 119.62 | 121.90 |
| 1 | A | 541 | G | N3-C2-N2 | -5.70 | 115.91 | 119.90 |
| 1 | A | 1523 | G | N3-C2-N2 | -5.70 | 115.91 | 119.90 |
| 1 | A | 1125 | U | N3-C4-O4 | 5.70 | 123.39 | 119.40 |
| 1 | A | 169 | C | C5-C6-N1 | 5.70 | 123.85 | 121.00 |
| 1 | A | 1055 | A | C4-C5-C6 | 5.70 | 119.85 | 117.00 |
| 1 | A | 1240 | U | C2-N1-C1' | -5.70 | 110.87 | 117.70 |
| 1 | A | 381 | C | C2-N1-C1' | 5.69 | 125.06 | 118.80 |
| 1 | A | 146 | G | O5'-P-OP1 | -5.69 | 100.58 | 105.70 |
| 1 | A | 859 | A | C2-N3-C4 | -5.69 | 107.75 | 110.60 |
| 1 | A | 897 | C | C2-N3-C4 | -5.69 | 117.05 | 119.90 |
| 1 | A | 1470 | G | C4-C5-C6 | 5.69 | 122.22 | 118.80 |
| 1 | A | 299 | G | C8-N9-C1' | -5.69 | 119.60 | 127.00 |
| 1 | A | 729 | A | N3-C4-C5 | -5.69 | 122.82 | 126.80 |
| 1 | A | 558 | G | N3-C4-C5 | 5.69 | 131.44 | 128.60 |
| 1 | A | 380 | G | O5'-P-OP2 | -5.69 | 100.58 | 105.70 |
| 1 | A | 555 | C | N3-C4-C5 | 5.68 | 124.17 | 121.90 |
| 1 | A | 917 | G | C8-N9-C4 | -5.68 | 104.13 | 106.40 |
| 1 | A | 1139 | G | N3-C4-C5 | -5.68 | 125.76 | 128.60 |
| 1 | A | 229 | U | C4-C5-C6 | 5.68 | 123.11 | 119.70 |
| 1 | A | 604 | G | N3-C2-N2 | -5.68 | 115.92 | 119.90 |
| 1 | A | 227 | G | C6-C5-N7 | -5.68 | 126.99 | 130.40 |
| 1 | A | 854 | G | N1-C6-O6 | 5.68 | 123.31 | 119.90 |
| 1 | A | 1157 | A | C2-N3-C4 | 5.68 | 113.44 | 110.60 |
| 1 | A | 1394 | A | O5'-P-OP1 | -5.67 | 100.59 | 105.70 |
| 1 | A | 1109 | C | N3-C2-O2 | -5.67 | 117.93 | 121.90 |
| 1 | A | 1232 | U | N3-C4-O4 | 5.67 | 123.37 | 119.40 |
| 10 | J | 65 | LEU | CA-CB-CG | 5.67 | 128.34 | 115.30 |
| 1 | A | 7 | G | N9-C4-C5 | -5.67 | 103.13 | 105.40 |
| 1 | A | 830 | G | N1-C2-N2 | 5.67 | 121.30 | 116.20 |
| 1 | A | 1432 | G | C5-C6-O6 | 5.67 | 132.00 | 128.60 |
| 1 | A | 12 | U | C2-N1-C1' | 5.67 | 124.50 | 117.70 |
| 1 | A | 789 | U | C5-C4-O4 | 5.67 | 129.30 | 125.90 |
| 1 | A | 1023 | G | N9-C4-C5 | -5.67 | 103.13 | 105.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 1 | A | 993 | G | C6-C5-N7 | -5.66 | 127.00 | 130.40 |
| 1 | A | 1286 | A | N7-C8-N9 | 5.66 | 116.63 | 113.80 |
| 1 | A | 45 | U | C5-C4-O4 | 5.66 | 129.30 | 125.90 |
| 1 | A | 485 | G | OP2-P-O3' | 5.66 | 117.65 | 105.20 |
| 1 | A | 1090 | U | N3-C2-O2 | -5.66 | 118.24 | 122.20 |
| 1 | A | 292 | G | N1-C6-O6 | 5.66 | 123.30 | 119.90 |
| 1 | A | 289 | G | C4-N9-C1' | 5.66 | 133.85 | 126.50 |
| 1 | A | 902 | G | C4-C5-N7 | 5.66 | 113.06 | 110.80 |
| 1 | A | 23 | C | C2-N1-C1' | -5.66 | 112.58 | 118.80 |
| 1 | A | 242 | C | C2-N3-C4 | -5.66 | 117.07 | 119.90 |
| 1 | A | 709 | G | N1-C6-O6 | 5.65 | 123.29 | 119.90 |
| 1 | A | 862 | C | C6-N1-C2 | 5.65 | 122.56 | 120.30 |
| 1 | A | 790 | A | C2-N3-C4 | -5.65 | 107.78 | 110.60 |
| 1 | A | 499 | A | OP1-P-O3' | 5.65 | 117.63 | 105.20 |
| 1 | A | 566 | G | C2-N3-C4 | -5.65 | 109.08 | 111.90 |
| 1 | A | 635 | G | C2-N3-C4 | -5.65 | 109.08 | 111.90 |
| 1 | A | 752 | G | C8-N9-C4 | 5.65 | 108.66 | 106.40 |
| 18 | R | 66 | LEU | CA-CB-CG | -5.65 | 102.31 | 115.30 |
| 1 | A | 372 | C | C6-N1-C1' | -5.65 | 114.03 | 120.80 |
| 1 | A | 1098 | C | C6-N1-C2 | 5.64 | 122.56 | 120.30 |
| 1 | A | 265 | G | C8-N9-C1' | 5.64 | 134.33 | 127.00 |
| 1 | A | 394 | G | N1-C6-O6 | 5.64 | 123.28 | 119.90 |
| 1 | A | 456 | C | O5'-P-OP1 | 5.64 | 117.47 | 110.70 |
| 1 | A | 120 | A | C8-N9-C4 | -5.64 | 103.55 | 105.80 |
| 1 | A | 828 | A | N9-C4-C5 | -5.64 | 103.55 | 105.80 |
| 1 | A | 239 | U | C2-N3-C4 | 5.63 | 130.38 | 127.00 |
| 1 | A | 911 | U | C5-C4-O4 | 5.63 | 129.28 | 125.90 |
| 1 | A | 1204 | A | N1-C6-N6 | 5.63 | 121.98 | 118.60 |
| 1 | A | 884 | U | C5-C6-N1 | -5.63 | 119.89 | 122.70 |
| 1 | A | 28 | G | C5-C6-N1 | -5.63 | 108.69 | 111.50 |
| 1 | A | 279 | A | C8-N9-C4 | -5.63 | 103.55 | 105.80 |
| 1 | A | 44 | G | C4-C5-N7 | 5.63 | 113.05 | 110.80 |
| 1 | A | 1139 | G | C4-C5-N7 | -5.63 | 108.55 | 110.80 |
| 1 | A | 292 | G | C4-C5-C6 | 5.62 | 122.17 | 118.80 |
| 1 | A | 484 | G | N3-C2-N2 | 5.62 | 123.84 | 119.90 |
| 1 | A | 676 | A | C8-N9-C4 | 5.62 | 108.05 | 105.80 |
| 1 | A | 1516[A] | G | C5-C6-N1 | -5.62 | 108.69 | 111.50 |
| 1 | A | 1516[B] | G | C5-C6-N1 | -5.62 | 108.69 | 111.50 |
| 1 | A | 1396 | A | C2-N3-C4 | -5.62 | 107.79 | 110.60 |
| 1 | A | 1462 | G | N1-C6-O6 | 5.62 | 123.27 | 119.90 |
| 1 | A | 1461 | G | N3-C4-C5 | 5.62 | 131.41 | 128.60 |
| 1 | A | 484 | G | C4-N9-C1' | 5.62 | 133.80 | 126.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 1 | A | 1322 | C | N3-C2-O2 | 5.62 | 125.83 | 121.90 |
| 14 | N | 39 | LEU | CA-CB-CG | -5.62 | 102.38 | 115.30 |
| 1 | A | 34 | C | N3-C2-O2 | 5.61 | 125.83 | 121.90 |
| 1 | A | 509 | A | N7-C8-N9 | 5.61 | 116.61 | 113.80 |
| 1 | A | 662 | G | C6-C5-N7 | -5.61 | 127.03 | 130.40 |
| 1 | A | 752 | G | N7-C8-N9 | -5.61 | 110.29 | 113.10 |
| 1 | A | 774 | G | N1-C6-O6 | 5.61 | 123.27 | 119.90 |
| 1 | A | 859 | A | OP1-P-O3' | -5.61 | 92.85 | 105.20 |
| 1 | A | 347 | G | N1-C6-O6 | 5.61 | 123.27 | 119.90 |
| 1 | A | 575 | G | N1-C6-O6 | -5.61 | 116.53 | 119.90 |
| 1 | A | 864 | A | C8-N9-C4 | -5.61 | 103.56 | 105.80 |
| 1 | A | 1451 | A | N1-C6-N6 | -5.61 | 115.23 | 118.60 |
| 1 | A | 22 | G | OP2-P-O3' | 5.61 | 117.53 | 105.20 |
| 1 | A | 672 | U | C6-N1-C2 | -5.61 | 117.64 | 121.00 |
| 1 | A | 945 | G | O5'-P-OP2 | -5.61 | 100.66 | 105.70 |
| 1 | A | 577 | G | N3-C2-N2 | -5.60 | 115.98 | 119.90 |
| 1 | A | 1530 | G | C6-N1-C2 | 5.60 | 128.46 | 125.10 |
| 1 | A | 281 | G | N1-C6-O6 | 5.60 | 123.26 | 119.90 |
| 1 | A | 361 | G | N7-C8-N9 | -5.60 | 110.30 | 113.10 |
| 1 | A | 579 | G | C5-C6-N1 | -5.60 | 108.70 | 111.50 |
| 1 | A | 815 | A | C6-N1-C2 | -5.60 | 115.24 | 118.60 |
| 1 | A | 888 | G | C4-C5-N7 | -5.60 | 108.56 | 110.80 |
| 1 | A | 1014 | A | C2-N3-C4 | 5.60 | 113.40 | 110.60 |
| 1 | A | 1180 | A | C8-N9-C4 | -5.60 | 103.56 | 105.80 |
| 1 | A | 17 | U | N3-C4-O4 | 5.60 | 123.32 | 119.40 |
| 1 | A | 574 | A | C2-N3-C4 | -5.60 | 107.80 | 110.60 |
| 1 | A | 802 | A | N1-C6-N6 | 5.60 | 121.96 | 118.60 |
| 1 | A | 190(H) | G | C5-C6-O6 | -5.60 | 125.24 | 128.60 |
| 1 | A | 1493 | A | O4'-C1'-N9 | 5.60 | 112.68 | 108.20 |
| 1 | A | 552 | U | C2-N3-C4 | -5.59 | 123.64 | 127.00 |
| 1 | A | 901 | A | C2-N3-C4 | -5.59 | 107.80 | 110.60 |
| 1 | A | 928 | G | N3-C2-N2 | -5.59 | 115.98 | 119.90 |
| 1 | A | 949 | A | C5-C6-N6 | -5.59 | 119.23 | 123.70 |
| 1 | A | 1211 | U | C2-N1-C1' | 5.59 | 124.41 | 117.70 |
| 1 | A | 890 | G | O4'-C1'-N9 | 5.59 | 112.67 | 108.20 |
| 1 | A | 266 | G | N7-C8-N9 | 5.58 | 115.89 | 113.10 |
| 1 | A | 344 | A | N7-C8-N9 | 5.58 | 116.59 | 113.80 |
| 1 | A | 791 | G | C5-C6-O6 | 5.58 | 131.95 | 128.60 |
| 1 | A | 1485 | U | C6-N1-C1' | 5.58 | 129.02 | 121.20 |
| 1 | A | 488 | C | C5-C4-N4 | -5.58 | 116.29 | 120.20 |
| 1 | A | 550 | G | C8-N9-C4 | 5.58 | 108.63 | 106.40 |
| 1 | A | 600 | C | OP2-P-O3' | 5.58 | 117.47 | 105.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 830 | G | C6-N1-C2 | 5.58 | 128.44 | 125.10 |
| 1 | A | 360 | A | C6-N1-C2 | -5.57 | 115.26 | 118.60 |
| 1 | A | 1121 | U | C2-N3-C4 | -5.57 | 123.66 | 127.00 |
| 1 | A | 1373 | G | C4-C5-C6 | 5.57 | 122.14 | 118.80 |
| 1 | A | 559 | A | P-O3'-C3' | 5.57 | 126.39 | 119.70 |
| 1 | A | 715 | A | OP1-P-O3' | 5.57 | 117.46 | 105.20 |
| 1 | A | 31 | G | C8-N9-C4 | 5.57 | 108.63 | 106.40 |
| 1 | A | 362 | G | C4-C5-N7 | -5.57 | 108.57 | 110.80 |
| 1 | A | 805 | C | C5-C6-N1 | 5.57 | 123.78 | 121.00 |
| 1 | A | 299 | G | N1-C2-N2 | -5.57 | 111.19 | 116.20 |
| 1 | A | 21 | G | C4-N9-C1' | 5.57 | 133.73 | 126.50 |
| 1 | A | 1117 | G | N3-C4-N9 | 5.56 | 129.34 | 126.00 |
| 1 | A | 1166 | G | C8-N9-C4 | -5.56 | 104.17 | 106.40 |
| 1 | A | 575 | G | C5-C6-N1 | 5.56 | 114.28 | 111.50 |
| 1 | A | 785 | G | N9-C4-C5 | -5.56 | 103.18 | 105.40 |
| 1 | A | 839 | U | N1-C2-O2 | 5.56 | 126.69 | 122.80 |
| 1 | A | 872 | A | N1-C2-N3 | 5.56 | 132.08 | 129.30 |
| 1 | A | 1134 | G | C4-C5-N7 | -5.56 | 108.58 | 110.80 |
| 1 | A | 27 | G | C5-N7-C8 | -5.56 | 101.52 | 104.30 |
| 1 | A | 279 | A | O5'-P-OP2 | -5.56 | 100.70 | 105.70 |
| 1 | A | 741 | G | N3-C4-C5 | -5.56 | 125.82 | 128.60 |
| 1 | A | 899 | C | C2-N1-C1' | -5.56 | 112.69 | 118.80 |
| 1 | A | 733 | A | C2-N3-C4 | -5.56 | 107.82 | 110.60 |
| 1 | A | 604 | G | C5-C6-N1 | -5.55 | 108.72 | 111.50 |
| 1 | A | 761 | G | N3-C2-N2 | -5.55 | 116.01 | 119.90 |
| 1 | A | 783 | C | N3-C4-C5 | 5.55 | 124.12 | 121.90 |
| 1 | A | 893 | C | C5-C6-N1 | 5.55 | 123.78 | 121.00 |
| 1 | A | 1076 | C | N3-C4-C5 | 5.55 | 124.12 | 121.90 |
| 17 | Q | 31 | LEU | CA-CB-CG | -5.55 | 102.53 | 115.30 |
| 1 | A | 658 | G | O5'-P-OP2 | -5.55 | 100.70 | 105.70 |
| 1 | A | 1405 | G | N1-C6-O6 | 5.55 | 123.23 | 119.90 |
| 1 | A | 299 | G | C4-N9-C1' | 5.55 | 133.71 | 126.50 |
| 1 | A | 1399 | C | N3-C4-C5 | -5.54 | 119.68 | 121.90 |
| 1 | A | 788 | U | N3-C4-O4 | 5.54 | 123.28 | 119.40 |
| 1 | A | 1479 | C | C5-C6-N1 | 5.54 | 123.77 | 121.00 |
| 19 | S | 5 | LEU | N-CA-C | 5.54 | 125.96 | 111.00 |
| 1 | A | 711 | G | N1-C6-O6 | 5.54 | 123.22 | 119.90 |
| 1 | A | 332 | G | N3-C2-N2 | -5.53 | 116.03 | 119.90 |
| 1 | A | 1093 | A | C6-N1-C2 | -5.53 | 115.28 | 118.60 |
| 1 | A | 1124 | G | C5-C6-N1 | 5.53 | 114.27 | 111.50 |
| 1 | A | 1147 | C | C4-C5-C6 | 5.53 | 120.17 | 117.40 |
| 1 | A | 944 | G | N3-C4-N9 | 5.53 | 129.32 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 66 | G | O5'-P-OP1 | -5.53 | 100.72 | 105.70 |
| 1 | A | 421 | U | N1-C2-O2 | 5.53 | 126.67 | 122.80 |
| 1 | A | 905 | U | C6-N1-C2 | 5.53 | 124.32 | 121.00 |
| 1 | A | 1380 | U | P-O3'-C3' | 5.53 | 126.33 | 119.70 |
| 1 | A | 1435 | G | N3-C4-C5 | 5.53 | 131.36 | 128.60 |
| 1 | A | 1501 | C | N3-C4-C5 | 5.53 | 124.11 | 121.90 |
| 7 | G | 120 | ILE | CB-CA-C | -5.53 | 100.55 | 111.60 |
| 1 | A | 1323 | G | C6-C5-N7 | -5.52 | 127.09 | 130.40 |
| 1 | A | 121 | C | O5'-P-OP2 | -5.52 | 100.73 | 105.70 |
| 1 | A | 814 | A | N1-C2-N3 | 5.52 | 132.06 | 129.30 |
| 1 | A | 1352 | C | O5'-P-OP2 | -5.52 | 100.73 | 105.70 |
| 1 | A | 21 | G | C8-N9-C1' | -5.52 | 119.83 | 127.00 |
| 1 | A | 1188 | A | C2-N3-C4 | -5.52 | 107.84 | 110.60 |
| 1 | A | 1259 | C | N3-C2-O2 | -5.52 | 118.04 | 121.90 |
| 1 | A | 1053 | G | N3-C4-C5 | 5.51 | 131.36 | 128.60 |
| 1 | A | 1529 | G | C4-C5-C6 | 5.51 | 122.11 | 118.80 |
| 1 | A | 443 | C | C6-N1-C2 | 5.51 | 122.50 | 120.30 |
| 1 | A | 23 | C | N1-C2-O2 | -5.51 | 115.59 | 118.90 |
| 1 | A | 1193 | G | C4-N9-C1' | 5.51 | 133.66 | 126.50 |
| 1 | A | 1160 | G | N1-C6-O6 | 5.51 | 123.20 | 119.90 |
| 1 | A | 235 | C | C5-C6-N1 | -5.50 | 118.25 | 121.00 |
| 1 | A | 314 | C | C2-N3-C4 | -5.50 | 117.15 | 119.90 |
| 1 | A | 1197 | G | C6-C5-N7 | -5.50 | 127.10 | 130.40 |
| 1 | A | 1376 | U | N3-C2-O2 | -5.50 | 118.35 | 122.20 |
| 1 | A | 617 | G | C2-N3-C4 | -5.50 | 109.15 | 111.90 |
| 1 | A | 922 | G | N1-C2-N3 | 5.50 | 127.20 | 123.90 |
| 1 | A | 829 | G | OP1-P-OP2 | 5.50 | 127.84 | 119.60 |
| 1 | A | 1087 | G | C4-N9-C1' | 5.50 | 133.65 | 126.50 |
| 1 | A | 1121 | U | C6-N1-C2 | 5.49 | 124.30 | 121.00 |
| 1 | A | 1139 | G | C5-C6-O6 | 5.49 | 131.90 | 128.60 |
| 1 | A | 504 | C | C5-C6-N1 | 5.49 | 123.75 | 121.00 |
| 1 | A | 445 | G | C4-C5-N7 | 5.49 | 113.00 | 110.80 |
| 1 | A | 692 | U | C6-N1-C2 | 5.49 | 124.30 | 121.00 |
| 1 | A | 902 | G | C8-N9-C1' | -5.49 | 119.86 | 127.00 |
| 10 | J | 71 | LEU | CA-CB-CG | -5.49 | 102.67 | 115.30 |
| 1 | A | 148 | G | C6-C5-N7 | -5.49 | 127.11 | 130.40 |
| 1 | A | 290 | C | C5-C4-N4 | -5.49 | 116.36 | 120.20 |
| 1 | A | 855 | G | N1-C2-N3 | 5.49 | 127.19 | 123.90 |
| 1 | A | 1146 | A | N1-C6-N6 | 5.49 | 121.89 | 118.60 |
| 1 | A | 1501 | C | C6-N1-C1' | -5.49 | 114.21 | 120.80 |
| 1 | A | 780 | A | C4-C5-C6 | -5.49 | 114.26 | 117.00 |
| 1 | A | 928 | G | N1-C2-N3 | 5.49 | 127.19 | 123.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 1 | A | 1118 | C | C6-N1-C2 | -5.49 | 118.11 | 120.30 |
| 1 | A | 1388 | C | N3-C4-C5 | 5.49 | 124.09 | 121.90 |
| 1 | A | 1485 | U | C6-N1-C2 | -5.49 | 117.71 | 121.00 |
| 1 | A | 732 | C | C6-N1-C2 | -5.48 | 118.11 | 120.30 |
| 1 | A | 284 | G | C5-C6-N1 | -5.48 | 108.76 | 111.50 |
| 1 | A | 323 | U | O5'-P-OP2 | -5.48 | 100.77 | 105.70 |
| 1 | A | 860 | A | C8-N9-C4 | 5.48 | 107.99 | 105.80 |
| 1 | A | 748 | C | P-O3'-C3' | 5.47 | 126.27 | 119.70 |
| 1 | A | 975 | A | C4-C5-C6 | 5.47 | 119.74 | 117.00 |
| 1 | A | 741 | G | C8-N9-C1' | -5.47 | 119.89 | 127.00 |
| 1 | A | 325 | A | N3-C4-N9 | -5.47 | 123.03 | 127.40 |
| 1 | A | 1030(C) | G | N3-C4-C5 | -5.47 | 125.86 | 128.60 |
| 1 | A | 1507 | A | O5'-P-OP1 | -5.47 | 100.78 | 105.70 |
| 5 | E | 12 | LEU | CB-CG-CD1 | -5.47 | 101.70 | 111.00 |
| 1 | A | 856 | C | N1-C2-O2 | -5.47 | 115.62 | 118.90 |
| 1 | A | 325 | A | C6-C5-N7 | 5.47 | 136.13 | 132.30 |
| 1 | A | 975 | A | C8-N9-C4 | -5.47 | 103.61 | 105.80 |
| 1 | A | 33 | A | O5'-P-OP2 | -5.46 | 100.78 | 105.70 |
| 1 | A | 102 | G | N3-C4-N9 | 5.46 | 129.28 | 126.00 |
| 1 | A | 1068 | G | OP2-P-O3' | 5.46 | 117.22 | 105.20 |
| 1 | A | 1256 | A | C5-N7-C8 | 5.46 | 106.63 | 103.90 |
| 1 | A | 29 | G | OP1-P-OP2 | 5.46 | 127.80 | 119.60 |
| 1 | A | 376 | G | C5-N7-C8 | 5.46 | 107.03 | 104.30 |
| 1 | A | 668 | G | C2-N3-C4 | -5.46 | 109.17 | 111.90 |
| 1 | A | 251 | G | C5-N7-C8 | -5.46 | 101.57 | 104.30 |
| 1 | A | 434 | U | C6-N1-C2 | -5.46 | 117.72 | 121.00 |
| 1 | A | 538 | G | N1-C6-O6 | -5.46 | 116.62 | 119.90 |
| 1 | A | 1416 | G | C8-N9-C4 | -5.46 | 104.22 | 106.40 |
| 1 | A | 317 | G | C4-C5-N7 | 5.46 | 112.98 | 110.80 |
| 1 | A | 542 | G | N1-C6-O6 | -5.46 | 116.62 | 119.90 |
| 1 | A | 814 | A | OP1-P-O3' | 5.46 | 117.21 | 105.20 |
| 1 | A | 728 | A | C5-N7-C8 | -5.46 | 101.17 | 103.90 |
| 1 | A | 867 | G | O5'-P-OP2 | -5.46 | 100.79 | 105.70 |
| 1 | A | 904 | C | O5'-P-OP2 | 5.46 | 117.25 | 110.70 |
| 1 | A | 1193 | G | N1-C2-N3 | 5.46 | 127.17 | 123.90 |
| 1 | A | 35 | G | C8-N9-C4 | 5.45 | 108.58 | 106.40 |
| 1 | A | 1399 | C | C4-C5-C6 | 5.45 | 120.13 | 117.40 |
| 1 | A | 957 | U | C5-C4-O4 | 5.45 | 129.17 | 125.90 |
| 1 | A | 332 | G | C5-C6-O6 | -5.45 | 125.33 | 128.60 |
| 1 | A | 1131 | G | C6-C5-N7 | -5.45 | 127.13 | 130.40 |
| 1 | A | 1063 | C | C4-C5-C6 | 5.45 | 120.12 | 117.40 |
| 1 | A | 570 | G | N7-C8-N9 | 5.45 | 115.82 | 113.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 1 | A | 47 | C | N1-C2-N3 | 5.45 | 123.01 | 119.20 |
| 1 | A | 108 | G | C5-N7-C8 | -5.45 | 101.58 | 104.30 |
| 1 | A | 199 | G | C8-N9-C4 | 5.45 | 108.58 | 106.40 |
| 1 | A | 1350 | A | O5'-P-OP2 | -5.45 | 100.80 | 105.70 |
| 1 | A | 1511 | G | C8-N9-C1' | -5.44 | 119.92 | 127.00 |
| 1 | A | 239 | U | N1-C2-O2 | -5.44 | 118.99 | 122.80 |
| 1 | A | 976 | G | C2-N3-C4 | -5.44 | 109.18 | 111.90 |
| 1 | A | 1230 | C | N1-C2-O2 | 5.44 | 122.17 | 118.90 |
| 6 | F | 75 | LEU | CA-CB-CG | 5.44 | 127.81 | 115.30 |
| 1 | A | 871 | U | C6-N1-C2 | 5.44 | 124.26 | 121.00 |
| 1 | A | 1467 | G | C2-N3-C4 | 5.44 | 114.62 | 111.90 |
| 1 | A | 278 | G | N3-C4-N9 | -5.44 | 122.74 | 126.00 |
| 1 | A | 852 | G | C2-N3-C4 | -5.44 | 109.18 | 111.90 |
| 1 | A | 961 | U | N3-C4-O4 | 5.44 | 123.20 | 119.40 |
| 1 | A | 935 | A | OP1-P-OP2 | 5.43 | 127.75 | 119.60 |
| 1 | A | 234 | C | C2-N1-C1' | -5.43 | 112.82 | 118.80 |
| 1 | A | 374 | A | C8-N9-C4 | 5.43 | 107.97 | 105.80 |
| 1 | A | 976 | G | O5'-P-OP1 | -5.43 | 100.81 | 105.70 |
| 1 | A | 117 | G | C8-N9-C1' | -5.43 | 119.94 | 127.00 |
| 1 | A | 1396 | A | C8-N9-C4 | 5.43 | 107.97 | 105.80 |
| 1 | A | 564 | C | C6-N1-C1' | -5.43 | 114.28 | 120.80 |
| 1 | A | 190(E) | U | N1-C2-O2 | 5.43 | 126.60 | 122.80 |
| 1 | A | 336 | C | C6-N1-C2 | 5.43 | 122.47 | 120.30 |
| 1 | A | 224 | C | N1-C2-O2 | 5.43 | 122.16 | 118.90 |
| 1 | A | 672 | U | O4'-C1'-N1 | 5.43 | 112.54 | 108.20 |
| 1 | A | 839 | U | N3-C2-O2 | -5.43 | 118.40 | 122.20 |
| 1 | A | 1064 | G | C6-C5-N7 | -5.42 | 127.15 | 130.40 |
| 1 | A | 1249 | C | C6-N1-C2 | 5.42 | 122.47 | 120.30 |
| 1 | A | 970 | C | N1-C2-N3 | -5.42 | 115.40 | 119.20 |
| 1 | A | 886 | G | N3-C4-C5 | 5.42 | 131.31 | 128.60 |
| 1 | A | 947 | G | N1-C6-O6 | 5.42 | 123.15 | 119.90 |
| 1 | A | 955 | U | N1-C2-N3 | 5.42 | 118.15 | 114.90 |
| 14 | N | 7 | ILE | CB-CA-C | 5.42 | 122.44 | 111.60 |
| 1 | A | 877 | C | C5-C6-N1 | 5.42 | 123.71 | 121.00 |
| 1 | A | 1377 | A | N3-C4-C5 | 5.42 | 130.59 | 126.80 |
| 1 | A | 36 | C | O5'-P-OP1 | 5.42 | 117.20 | 110.70 |
| 1 | A | 504 | C | N3-C4-N4 | 5.42 | 121.79 | 118.00 |
| 1 | A | 820 | U | C6-N1-C2 | 5.42 | 124.25 | 121.00 |
| 1 | A | 936 | C | O5'-P-OP1 | -5.42 | 100.82 | 105.70 |
| 1 | A | 170 | U | N3-C4-O4 | 5.42 | 123.19 | 119.40 |
| 1 | A | 509 | A | C4-C5-C6 | 5.42 | 119.71 | 117.00 |
| 1 | A | 785 | G | C5-C6-O6 | -5.42 | 125.35 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 1 | A | 902 | G | C2-N3-C4 | -5.41 | 109.19 | 111.90 |
| 1 | A | 41 | G | C8-N9-C4 | -5.41 | 104.23 | 106.40 |
| 1 | A | 1494 | G | C4-N9-C1' | 5.41 | 133.53 | 126.50 |
| 1 | A | 820 | U | N3-C2-O2 | 5.41 | 125.98 | 122.20 |
| 1 | A | 113 | G | N3-C4-C5 | -5.40 | 125.90 | 128.60 |
| 1 | A | 316 | G | C5-C6-O6 | -5.40 | 125.36 | 128.60 |
| 1 | A | 1490 | C | C2-N3-C4 | 5.40 | 122.60 | 119.90 |
| 1 | A | 161 | A | N1-C6-N6 | -5.40 | 115.36 | 118.60 |
| 1 | A | 661 | G | N3-C2-N2 | -5.40 | 116.12 | 119.90 |
| 1 | A | 819 | A | C6-C5-N7 | -5.40 | 128.52 | 132.30 |
| 1 | A | 1166 | G | C8-N9-C1' | -5.40 | 119.98 | 127.00 |
| 1 | A | 590 | C | C5-C6-N1 | -5.40 | 118.30 | 121.00 |
| 1 | A | 234 | C | N3-C4-N4 | -5.40 | 114.22 | 118.00 |
| 1 | A | 102 | G | C4-C5-C6 | 5.39 | 122.04 | 118.80 |
| 1 | A | 281 | G | C6-C5-N7 | -5.39 | 127.16 | 130.40 |
| 1 | A | 729 | A | C6-N1-C2 | -5.39 | 115.37 | 118.60 |
| 1 | A | 651 | C | N3-C2-O2 | 5.39 | 125.67 | 121.90 |
| 1 | A | 817 | C | O4'-C1'-N1 | -5.39 | 103.89 | 108.20 |
| 1 | A | 890 | G | OP2-P-O3' | 5.39 | 117.05 | 105.20 |
| 1 | A | 54 | C | OP1-P-O3' | 5.38 | 117.05 | 105.20 |
| 1 | A | 792 | A | C2-N3-C4 | -5.38 | 107.91 | 110.60 |
| 1 | A | 1234 | C | C6-N1-C2 | 5.38 | 122.45 | 120.30 |
| 1 | A | 276 | G | C6-C5-N7 | -5.38 | 127.17 | 130.40 |
| 1 | A | 445 | G | C5-C6-O6 | -5.38 | 125.37 | 128.60 |
| 1 | A | 1240 | U | C5-C4-O4 | 5.38 | 129.13 | 125.90 |
| 1 | A | 444 | C | N3-C2-O2 | -5.38 | 118.13 | 121.90 |
| 1 | A | 934 | C | C6-N1-C2 | -5.38 | 118.15 | 120.30 |
| 1 | A | 525 | C | C5-C6-N1 | 5.38 | 123.69 | 121.00 |
| 1 | A | 250 | A | N1-C2-N3 | 5.37 | 131.99 | 129.30 |
| 1 | A | 659 | U | C6-N1-C2 | -5.37 | 117.78 | 121.00 |
| 1 | A | 1516[A] | G | C4-N9-C1' | -5.37 | 119.52 | 126.50 |
| 1 | A | 1516[B] | G | C4-N9-C1' | -5.37 | 119.52 | 126.50 |
| 1 | A | 175 | C | O5'-P-OP1 | 5.37 | 117.14 | 110.70 |
| 1 | A | 1201 | A | P-O3'-C3' | 5.37 | 126.14 | 119.70 |
| 1 | A | 313 | A | C6-C5-N7 | -5.37 | 128.54 | 132.30 |
| 1 | A | 1239 | A | N1-C6-N6 | 5.37 | 121.82 | 118.60 |
| 1 | A | 1304 | G | C4-C5-C6 | 5.37 | 122.02 | 118.80 |
| 1 | A | 970 | C | C6-N1-C1' | -5.37 | 114.36 | 120.80 |
| 1 | A | 1117 | G | N3-C2-N2 | 5.37 | 123.66 | 119.90 |
| 20 | T | 13 | LEU | CB-CG-CD1 | 5.37 | 120.12 | 111.00 |
| 1 | A | 161 | A | N1-C2-N3 | 5.36 | 131.98 | 129.30 |
| 1 | A | 861 | G | C5-N7-C8 | -5.36 | 101.62 | 104.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 133 | U | C4-C5-C6 | 5.36 | 122.92 | 119.70 |
| 1 | A | 517 | G | C8-N9-C4 | -5.36 | 104.25 | 106.40 |
| 1 | A | 496 | A | O5'-P-OP2 | 5.36 | 117.13 | 110.70 |
| 1 | A | 1373 | G | N3-C4-N9 | 5.36 | 129.22 | 126.00 |
| 1 | A | 769 | G | O5'-P-OP1 | 5.36 | 117.13 | 110.70 |
| 1 | A | 1418 | A | C8-N9-C4 | -5.36 | 103.66 | 105.80 |
| 1 | A | 228 | A | N9-C4-C5 | 5.36 | 107.94 | 105.80 |
| 1 | A | 284 | G | OP2-P-O3' | 5.36 | 116.98 | 105.20 |
| 1 | A | 446 | G | N1-C6-O6 | 5.36 | 123.11 | 119.90 |
| 1 | A | 1118 | C | C5-C6-N1 | 5.36 | 123.68 | 121.00 |
| 1 | A | 1440 | C | N3-C4-N4 | 5.36 | 121.75 | 118.00 |
| 1 | A | 275 | G | C6-C5-N7 | -5.35 | 127.19 | 130.40 |
| 1 | A | 899 | C | N3-C2-O2 | 5.35 | 125.65 | 121.90 |
| 1 | A | 216 | G | N7-C8-N9 | -5.35 | 110.42 | 113.10 |
| 1 | A | 497 | A | N9-C4-C5 | 5.35 | 107.94 | 105.80 |
| 1 | A | 1139 | G | C8-N9-C4 | -5.35 | 104.26 | 106.40 |
| 1 | A | 1464 | G | N1-C6-O6 | 5.35 | 123.11 | 119.90 |
| 1 | A | 148 | G | C8-N9-C1' | -5.35 | 120.05 | 127.00 |
| 1 | A | 292 | G | C5-C6-N1 | -5.34 | 108.83 | 111.50 |
| 1 | A | 900 | A | OP1-P-OP2 | -5.34 | 111.58 | 119.60 |
| 1 | A | 446 | G | N3-C2-N2 | -5.34 | 116.16 | 119.90 |
| 1 | A | 818 | G | C5-C6-O6 | 5.34 | 131.81 | 128.60 |
| 14 | N | 39 | LEU | CB-CG-CD2 | -5.34 | 101.92 | 111.00 |
| 1 | A | 238 | G | O5'-P-OP2 | -5.34 | 100.89 | 105.70 |
| 1 | A | 541 | G | C4-C5-N7 | 5.34 | 112.94 | 110.80 |
| 1 | A | 886 | G | C5-C6-N1 | -5.34 | 108.83 | 111.50 |
| 2 | B | 122 | PHE | N-CA-C | 5.34 | 125.41 | 111.00 |
| 1 | A | 299 | G | N1-C2-N3 | 5.34 | 127.10 | 123.90 |
| 1 | A | 1142 | G | O5'-P-OP1 | -5.34 | 100.90 | 105.70 |
| 1 | A | 1230 | C | N3-C4-N4 | 5.34 | 121.74 | 118.00 |
| 1 | A | 853 | G | C4-C5-C6 | 5.33 | 122.00 | 118.80 |
| 1 | A | 1233 | G | C6-C5-N7 | -5.33 | 127.20 | 130.40 |
| 1 | A | 265 | G | C4-N9-C1' | -5.33 | 119.56 | 126.50 |
| 1 | A | 321 | A | C8-N9-C4 | 5.33 | 107.93 | 105.80 |
| 1 | A | 1522 | U | OP2-P-O3' | 5.33 | 116.94 | 105.20 |
| 1 | A | 61 | G | C2-N3-C4 | -5.33 | 109.23 | 111.90 |
| 1 | A | 306 | G | N1-C2-N2 | 5.33 | 121.00 | 116.20 |
| 1 | A | 363 | A | C5-N7-C8 | -5.33 | 101.23 | 103.90 |
| 1 | A | 148 | G | C4-N9-C1' | 5.33 | 133.43 | 126.50 |
| 1 | A | 573 | A | OP2-P-O3' | 5.33 | 116.92 | 105.20 |
| 1 | A | 893 | C | C5-C4-N4 | -5.33 | 116.47 | 120.20 |
| 1 | A | 197 | A | C5-C6-N6 | 5.33 | 127.96 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 759 | A | C2-N3-C4 | 5.33 | 113.26 | 110.60 |
| 1 | A | 1083 | U | N3-C4-C5 | -5.33 | 111.41 | 114.60 |
| 1 | A | 624 | C | N1-C2-N3 | -5.32 | 115.47 | 119.20 |
| 1 | A | 1353 | G | C4-C5-N7 | 5.32 | 112.93 | 110.80 |
| 1 | A | 1507 | A | OP1-P-O3' | 5.32 | 116.91 | 105.20 |
| 10 | J | 54 | PHE | N-CA-C | 5.32 | 125.37 | 111.00 |
| 1 | A | 748 | C | N3-C2-O2 | -5.32 | 118.18 | 121.90 |
| 1 | A | 987 | G | C5-C6-N1 | -5.32 | 108.84 | 111.50 |
| 1 | A | 1478 | C | C2-N3-C4 | 5.32 | 122.56 | 119.90 |
| 2 | B | 221 | LEU | CA-CB-CG | 5.32 | 127.54 | 115.30 |
| 1 | A | 436 | C | O5'-P-OP1 | -5.32 | 100.91 | 105.70 |
| 1 | A | 487 | A | C2-N3-C4 | -5.32 | 107.94 | 110.60 |
| 1 | A | 204 | U | C2-N3-C4 | 5.32 | 130.19 | 127.00 |
| 1 | A | 265 | G | N3-C4-C5 | 5.32 | 131.26 | 128.60 |
| 1 | A | 913 | A | N1-C6-N6 | -5.32 | 115.41 | 118.60 |
| 1 | A | 1440 | C | C5-C4-N4 | -5.32 | 116.48 | 120.20 |
| 1 | A | 52 | G | N3-C4-N9 | -5.31 | 122.81 | 126.00 |
| 1 | A | 120 | A | N9-C4-C5 | 5.31 | 107.92 | 105.80 |
| 1 | A | 242 | C | C6-N1-C2 | 5.31 | 122.42 | 120.30 |
| 1 | A | 299 | G | C5-C6-N1 | -5.31 | 108.85 | 111.50 |
| 1 | A | 583 | A | C4-C5-C6 | 5.31 | 119.65 | 117.00 |
| 1 | A | 1005 | A | C4-N9-C1' | 5.31 | 135.85 | 126.30 |
| 1 | A | 1034 | G | O4'-C1'-N9 | 5.31 | 112.44 | 108.20 |
| 1 | A | 1533 | C | C5-C6-N1 | 5.31 | 123.65 | 121.00 |
| 1 | A | 313 | A | O4'-C1'-N9 | -5.31 | 103.95 | 108.20 |
| 1 | A | 1302 | U | N3-C2-O2 | -5.30 | 118.49 | 122.20 |
| 1 | A | 1369 | C | N3-C4-C5 | -5.30 | 119.78 | 121.90 |
| 1 | A | 66 | G | N1-C2-N2 | 5.30 | 120.97 | 116.20 |
| 1 | A | 265 | G | C4-C5-N7 | -5.30 | 108.68 | 110.80 |
| 1 | A | 1077 | G | N3-C4-C5 | 5.30 | 131.25 | 128.60 |
| 1 | A | 531 | U | N3-C2-O2 | -5.30 | 118.49 | 122.20 |
| 1 | A | 241 | C | N3-C4-C5 | 5.30 | 124.02 | 121.90 |
| 1 | A | 515 | G | C6-C5-N7 | -5.30 | 127.22 | 130.40 |
| 1 | A | 1206 | G | N1-C6-O6 | 5.30 | 123.08 | 119.90 |
| 1 | A | 1443 | G | O4'-C1'-N9 | -5.29 | 103.97 | 108.20 |
| 1 | A | 1497 | G | N1-C2-N3 | 5.29 | 127.08 | 123.90 |
| 1 | A | 546 | G | C8-N9-C4 | -5.29 | 104.28 | 106.40 |
| 1 | A | 1393 | U | O5'-P-OP1 | 5.29 | 117.05 | 110.70 |
| 1 | A | 243 | A | O4'-C1'-N9 | -5.29 | 103.97 | 108.20 |
| 1 | A | 676 | A | N7-C8-N9 | -5.29 | 111.16 | 113.80 |
| 6 | F | 9 | VAL | CB-CA-C | -5.29 | 101.36 | 111.40 |
| 1 | A | 41 | G | C5-C6-O6 | -5.28 | 125.43 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | A | 95 | U | C4-C5-C6 | 5.28 | 122.87 | 119.70 |
| 1 | A | 1100 | C | C4-C5-C6 | -5.28 | 114.76 | 117.40 |
| 1 | A | 1215 | G | N1-C6-O6 | 5.28 | 123.07 | 119.90 |
| 1 | A | 1530 | G | C5-C6-N1 | -5.28 | 108.86 | 111.50 |
| 1 | A | 190(A) | C | C5-C4-N4 | -5.28 | 116.50 | 120.20 |
| 1 | A | 320 | C | C6-N1-C2 | 5.28 | 122.41 | 120.30 |
| 1 | A | 1328 | C | N3-C4-C5 | 5.28 | 124.01 | 121.90 |
| 1 | A | 763 | G | C4-C5-N7 | 5.28 | 112.91 | 110.80 |
| 1 | A | 1125 | U | N1-C2-O2 | -5.28 | 119.11 | 122.80 |
| 1 | A | 1073 | U | C6-N1-C2 | -5.28 | 117.83 | 121.00 |
| 1 | A | 330 | C | OP2-P-O3' | 5.27 | 116.80 | 105.20 |
| 1 | A | 1099 | G | N3-C4-N9 | -5.27 | 122.84 | 126.00 |
| 1 | A | 1389 | C | C6-N1-C2 | -5.27 | 118.19 | 120.30 |
| 1 | A | 415 | A | C8-N9-C4 | -5.27 | 103.69 | 105.80 |
| 1 | A | 1084 | G | C4-C5-C6 | 5.27 | 121.96 | 118.80 |
| 1 | A | 1172 | C | C6-N1-C2 | 5.27 | 122.41 | 120.30 |
| 1 | A | 31 | G | N3-C4-C5 | -5.26 | 125.97 | 128.60 |
| 1 | A | 321 | A | O5'-P-OP2 | -5.26 | 100.96 | 105.70 |
| 1 | A | 687 | A | OP1-P-O3' | 5.26 | 116.78 | 105.20 |
| 1 | A | 36 | C | C5-C6-N1 | -5.26 | 118.37 | 121.00 |
| 1 | A | 282 | A | C4-C5-N7 | 5.26 | 113.33 | 110.70 |
| 1 | A | 900 | A | C5-C6-N6 | -5.26 | 119.49 | 123.70 |
| 1 | A | 1508 | G | N1-C2-N2 | 5.26 | 120.94 | 116.20 |
| 1 | A | 1396 | A | C5-C6-N1 | -5.26 | 115.07 | 117.70 |
| 1 | A | 200 | G | C6-C5-N7 | -5.26 | 127.25 | 130.40 |
| 1 | A | 1338 | G | C4-C5-C6 | 5.26 | 121.95 | 118.80 |
| 1 | A | 108 | G | C5-C6-N1 | -5.25 | 108.87 | 111.50 |
| 1 | A | 344 | A | C8-N9-C4 | -5.25 | 103.70 | 105.80 |
| 1 | A | 348 | G | C5-C6-O6 | -5.25 | 125.45 | 128.60 |
| 1 | A | 387 | U | C4-C5-C6 | 5.25 | 122.85 | 119.70 |
| 1 | A | 885 | G | OP1-P-OP2 | 5.25 | 127.48 | 119.60 |
| 1 | A | 1358 | U | C5-C6-N1 | -5.25 | 120.07 | 122.70 |
| 1 | A | 127 | G | N1-C6-O6 | 5.25 | 123.05 | 119.90 |
| 1 | A | 799 | G | OP1-P-OP2 | 5.25 | 127.48 | 119.60 |
| 1 | A | 405 | U | N3-C2-O2 | -5.25 | 118.53 | 122.20 |
| 1 | A | 791 | G | C4-N9-C1' | 5.25 | 133.32 | 126.50 |
| 1 | A | 1304 | G | N1-C6-O6 | 5.25 | 123.05 | 119.90 |
| 1 | A | 10 | A | N1-C2-N3 | 5.25 | 131.92 | 129.30 |
| 1 | A | 587 | G | C8-N9-C4 | -5.25 | 104.30 | 106.40 |
| 1 | A | 1222 | G | C4-C5-C6 | 5.24 | 121.95 | 118.80 |
| 1 | A | 689 | C | N1-C2-O2 | -5.24 | 115.76 | 118.90 |
| 1 | A | 993 | G | C5-C6-O6 | -5.24 | 125.46 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 908 | A | N1-C6-N6 | -5.24 | 115.46 | 118.60 |
| 1 | A | 977 | A | C2-N3-C4 | 5.24 | 113.22 | 110.60 |
| 1 | A | 1391 | U | C6-N1-C2 | 5.24 | 124.14 | 121.00 |
| 1 | A | 10 | A | C5-C6-N1 | 5.24 | 120.32 | 117.70 |
| 1 | A | 348 | G | N1-C6-O6 | 5.23 | 123.04 | 119.90 |
| 1 | A | 537 | G | C8-N9-C4 | 5.23 | 108.49 | 106.40 |
| 1 | A | 1193 | G | C5-C6-N1 | -5.23 | 108.88 | 111.50 |
| 1 | A | 1261 | A | N9-C4-C5 | -5.23 | 103.71 | 105.80 |
| 2 | B | 41 | ILE | CB-CA-C | -5.23 | 101.13 | 111.60 |
| 5 | E | 12 | LEU | CA-CB-CG | 5.23 | 127.33 | 115.30 |
| 1 | A | 254 | G | C2-N3-C4 | -5.23 | 109.28 | 111.90 |
| 1 | A | 853 | G | C4-N9-C1' | 5.23 | 133.30 | 126.50 |
| 1 | A | 1069 | C | C5-C4-N4 | -5.23 | 116.54 | 120.20 |
| 1 | A | 140 | A | N1-C6-N6 | 5.23 | 121.74 | 118.60 |
| 1 | A | 1532 | U | N1-C2-N3 | -5.23 | 111.76 | 114.90 |
| 1 | A | 509 | A | C6-C5-N7 | -5.23 | 128.64 | 132.30 |
| 1 | A | 748 | C | N1-C2-O2 | 5.23 | 122.04 | 118.90 |
| 1 | A | 1084 | G | N3-C4-C5 | -5.23 | 125.99 | 128.60 |
| 1 | A | 78 | G | C5-C6-N1 | -5.22 | 108.89 | 111.50 |
| 1 | A | 1359 | C | N1-C2-O2 | 5.22 | 122.03 | 118.90 |
| 1 | A | 8 | A | C2-N3-C4 | -5.22 | 107.99 | 110.60 |
| 1 | A | 578 | C | C5-C6-N1 | -5.22 | 118.39 | 121.00 |
| 1 | A | 183 | G | C6-C5-N7 | -5.22 | 127.27 | 130.40 |
| 1 | A | 944 | G | OP2-P-O3' | 5.22 | 116.68 | 105.20 |
| 1 | A | 50 | A | C5-C6-N6 | 5.22 | 127.88 | 123.70 |
| 1 | A | 597 | G | C2-N3-C4 | -5.22 | 109.29 | 111.90 |
| 1 | A | 712 | A | N1-C6-N6 | -5.22 | 115.47 | 118.60 |
| 1 | A | 673 | G | C6-C5-N7 | 5.22 | 133.53 | 130.40 |
| 1 | A | 715 | A | N7-C8-N9 | -5.22 | 111.19 | 113.80 |
| 1 | A | 949 | A | C6-C5-N7 | -5.22 | 128.65 | 132.30 |
| 1 | A | 1124 | G | O4'-C1'-N9 | 5.22 | 112.37 | 108.20 |
| 1 | A | 1125 | U | OP2-P-O3' | 5.22 | 116.68 | 105.20 |
| 1 | A | 1511 | G | C8-N9-C4 | 5.22 | 108.49 | 106.40 |
| 1 | A | 61 | G | C5-C6-O6 | -5.21 | 125.47 | 128.60 |
| 1 | A | 267 | C | N3-C4-C5 | 5.21 | 123.99 | 121.90 |
| 1 | A | 352 | C | C2-N3-C4 | 5.21 | 122.51 | 119.90 |
| 1 | A | 284 | G | N1-C2-N3 | 5.21 | 127.03 | 123.90 |
| 1 | A | 1195 | C | N3-C4-C5 | -5.21 | 119.81 | 121.90 |
| 1 | A | 1452 | C | N1-C2-N3 | -5.21 | 115.55 | 119.20 |
| 1 | A | 764 | C | C2-N1-C1' | 5.21 | 124.53 | 118.80 |
| 1 | A | 403 | C | C4-C5-C6 | 5.21 | 120.00 | 117.40 |
| 1 | A | 1290 | G | C6-C5-N7 | -5.21 | 127.27 | 130.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 289 | G | C8-N9-C1' | -5.21 | 120.23 | 127.00 |
| 1 | A | 852 | G | C5-C6-N1 | -5.21 | 108.90 | 111.50 |
| 1 | A | 791 | G | N1-C2-N3 | 5.20 | 127.02 | 123.90 |
| 1 | A | 1055 | A | C6-C5-N7 | -5.20 | 128.66 | 132.30 |
| 1 | A | 1058 | G | C2-N3-C4 | -5.20 | 109.30 | 111.90 |
| 1 | A | 1079 | G | C6-C5-N7 | -5.20 | 127.28 | 130.40 |
| 1 | A | 1098 | C | C5-C6-N1 | -5.20 | 118.40 | 121.00 |
| 1 | A | 229 | U | N3-C4-O4 | 5.20 | 123.04 | 119.40 |
| 1 | A | 144 | G | C5-C6-N1 | -5.20 | 108.90 | 111.50 |
| 1 | A | 255 | G | N1-C2-N3 | 5.20 | 127.02 | 123.90 |
| 1 | A | 610 | G | N3-C2-N2 | -5.20 | 116.26 | 119.90 |
| 1 | A | 1087 | G | N7-C8-N9 | 5.20 | 115.70 | 113.10 |
| 1 | A | 1119 | C | N1-C2-O2 | 5.20 | 122.02 | 118.90 |
| 1 | A | 1143 | G | C8-N9-C4 | 5.20 | 108.48 | 106.40 |
| 1 | A | 949 | A | C5-N7-C8 | -5.20 | 101.30 | 103.90 |
| 1 | A | 1129 | C | C6-N1-C1' | 5.20 | 127.04 | 120.80 |
| 1 | A | 1410 | G | C8-N9-C4 | 5.20 | 108.48 | 106.40 |
| 1 | A | 513 | C | N3-C4-C5 | 5.20 | 123.98 | 121.90 |
| 1 | A | 650 | G | N1-C6-O6 | 5.20 | 123.02 | 119.90 |
| 1 | A | 1102 | A | C8-N9-C4 | -5.20 | 103.72 | 105.80 |
| 1 | A | 1190 | G | C4-C5-N7 | -5.20 | 108.72 | 110.80 |
| 1 | A | 1239 | A | N9-C4-C5 | -5.20 | 103.72 | 105.80 |
| 1 | A | 252 | U | N3-C2-O2 | 5.19 | 125.84 | 122.20 |
| 1 | A | 1353 | G | C6-C5-N7 | -5.19 | 127.28 | 130.40 |
| 1 | A | 809 | G | N1-C2-N3 | -5.19 | 120.78 | 123.90 |
| 1 | A | 818 | G | N9-C4-C5 | 5.19 | 107.48 | 105.40 |
| 1 | A | 1450 | U | O5'-P-OP2 | -5.19 | 101.03 | 105.70 |
| 1 | A | 439 | A | N9-C4-C5 | 5.19 | 107.88 | 105.80 |
| 1 | A | 869 | G | N1-C6-O6 | -5.19 | 116.78 | 119.90 |
| 5 | E | 12 | LEU | CB-CG-CD2 | 5.19 | 119.82 | 111.00 |
| 1 | A | 262 | A | N3-C4-C5 | 5.19 | 130.43 | 126.80 |
| 1 | A | 556 | C | N3-C4-N4 | 5.19 | 121.63 | 118.00 |
| 1 | A | 1229 | A | C2-N3-C4 | -5.19 | 108.01 | 110.60 |
| 1 | A | 1467 | G | N3-C4-C5 | -5.19 | 126.01 | 128.60 |
| 1 | A | 658 | G | N1-C2-N2 | -5.18 | 111.53 | 116.20 |
| 1 | A | 1087 | G | C5-C6-N1 | -5.18 | 108.91 | 111.50 |
| 1 | A | 305 | G | C5-C6-O6 | 5.18 | 131.71 | 128.60 |
| 1 | A | 620 | C | C6-N1-C2 | 5.18 | 122.37 | 120.30 |
| 1 | A | 672 | U | N3-C4-O4 | 5.18 | 123.03 | 119.40 |
| 1 | A | 369 | C | O5'-P-OP1 | 5.18 | 116.92 | 110.70 |
| 1 | A | 416 | G | C8-N9-C4 | -5.18 | 104.33 | 106.40 |
| 1 | A | 855 | G | C4-C5-C6 | 5.18 | 121.91 | 118.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 1158 | C | N3-C2-O2 | -5.18 | 118.28 | 121.90 |
| 1 | A | 1495 | U | C6-N1-C2 | -5.18 | 117.89 | 121.00 |
| 1 | A | 629 | G | OP2-P-O3' | 5.17 | 116.58 | 105.20 |
| 1 | A | 1128 | C | N3-C4-C5 | -5.17 | 119.83 | 121.90 |
| 1 | A | 247 | G | C5-C6-O6 | -5.17 | 125.50 | 128.60 |
| 1 | A | 20 | U | C6-N1-C1' | -5.17 | 113.96 | 121.20 |
| 1 | A | 228 | A | N1-C2-N3 | 5.17 | 131.89 | 129.30 |
| 1 | A | 244 | U | N1-C2-O2 | 5.17 | 126.42 | 122.80 |
| 1 | A | 1261 | A | C8-N9-C4 | 5.17 | 107.87 | 105.80 |
| 1 | A | 1155 | G | N1-C2-N3 | 5.17 | 127.00 | 123.90 |
| 1 | A | 50 | A | C5-C6-N1 | -5.17 | 115.12 | 117.70 |
| 1 | A | 762 | C | C2-N3-C4 | -5.17 | 117.32 | 119.90 |
| 1 | A | 259 | G | N1-C6-O6 | 5.17 | 123.00 | 119.90 |
| 1 | A | 668 | G | N1-C6-O6 | 5.17 | 123.00 | 119.90 |
| 1 | A | 798 | G | N1-C2-N3 | -5.17 | 120.80 | 123.90 |
| 1 | A | 841 | U | C5-C6-N1 | 5.16 | 125.28 | 122.70 |
| 1 | A | 910 | C | N3-C2-O2 | 5.16 | 125.52 | 121.90 |
| 1 | A | 360 | A | N1-C2-N3 | 5.16 | 131.88 | 129.30 |
| 1 | A | 444 | C | N1-C2-O2 | 5.16 | 122.00 | 118.90 |
| 1 | A | 895 | G | N1-C2-N3 | 5.16 | 127.00 | 123.90 |
| 1 | A | 147 | G | N3-C2-N2 | -5.16 | 116.29 | 119.90 |
| 1 | A | 254 | G | C8-N9-C4 | 5.16 | 108.46 | 106.40 |
| 1 | A | 281 | G | C2-N3-C4 | -5.16 | 109.32 | 111.90 |
| 1 | A | 965 | A | C4-C5-C6 | -5.16 | 114.42 | 117.00 |
| 1 | A | 528 | C | O5'-P-OP1 | -5.16 | 101.06 | 105.70 |
| 1 | A | 818 | G | C5-N7-C8 | 5.16 | 106.88 | 104.30 |
| 1 | A | 614 | A | C4-C5-N7 | 5.15 | 113.28 | 110.70 |
| 1 | A | 226 | G | N1-C6-O6 | 5.15 | 122.99 | 119.90 |
| 1 | A | 1099 | G | C4-N9-C1' | -5.15 | 119.80 | 126.50 |
| 1 | A | 1522 | U | C4-C5-C6 | 5.15 | 122.79 | 119.70 |
| 1 | A | 303 | A | C8-N9-C4 | -5.15 | 103.74 | 105.80 |
| 1 | A | 499 | A | N9-C4-C5 | 5.14 | 107.86 | 105.80 |
| 1 | A | 553 | A | OP2-P-O3' | 5.14 | 116.52 | 105.20 |
| 1 | A | 590 | C | N3-C4-C5 | 5.14 | 123.96 | 121.90 |
| 1 | A | 731 | G | C5-C6-O6 | -5.14 | 125.51 | 128.60 |
| 1 | A | 866 | C | C5-C4-N4 | 5.14 | 123.80 | 120.20 |
| 1 | A | 1136 | U | C5-C6-N1 | 5.14 | 125.27 | 122.70 |
| 1 | A | 257 | G | C6-C5-N7 | -5.14 | 127.31 | 130.40 |
| 1 | A | 1075 | C | C2-N1-C1' | -5.14 | 113.14 | 118.80 |
| 1 | A | 1532 | U | C2-N3-C4 | 5.14 | 130.09 | 127.00 |
| 1 | A | 273 | A | C2-N3-C4 | -5.14 | 108.03 | 110.60 |
| 1 | A | 570 | G | C6-C5-N7 | -5.14 | 127.32 | 130.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 502 | G | C4-N9-C1' | -5.14 | 119.82 | 126.50 |
| 1 | A | 894 | G | C5-C6-N1 | -5.14 | 108.93 | 111.50 |
| 1 | A | 1084 | G | C5-C6-N1 | -5.14 | 108.93 | 111.50 |
| 1 | A | 382 | A | N9-C4-C5 | 5.14 | 107.86 | 105.80 |
| 1 | A | 1510 | U | O5'-P-OP1 | -5.14 | 101.08 | 105.70 |
| 1 | A | 34 | C | N1-C2-N3 | -5.13 | 115.61 | 119.20 |
| 1 | A | 1394 | A | C2-N3-C4 | -5.13 | 108.03 | 110.60 |
| 1 | A | 577 | G | N3-C4-N9 | -5.13 | 122.92 | 126.00 |
| 1 | A | 799 | G | C5-N7-C8 | -5.13 | 101.73 | 104.30 |
| 1 | A | 612 | C | C5-C4-N4 | 5.13 | 123.79 | 120.20 |
| 1 | A | 779 | C | O5'-P-OP2 | -5.13 | 101.08 | 105.70 |
| 1 | A | 908 | A | N9-C4-C5 | 5.13 | 107.85 | 105.80 |
| 1 | A | 641 | U | C5-C4-O4 | -5.13 | 122.82 | 125.90 |
| 1 | A | 1278 | U | O5'-P-OP2 | -5.13 | 101.08 | 105.70 |
| 1 | A | 658 | G | C6-N1-C2 | -5.13 | 122.03 | 125.10 |
| 1 | A | 912 | C | N1-C2-O2 | -5.13 | 115.82 | 118.90 |
| 1 | A | 532 | A | C8-N9-C4 | 5.12 | 107.85 | 105.80 |
| 1 | A | 734 | G | C6-C5-N7 | -5.12 | 127.33 | 130.40 |
| 1 | A | 821 | G | N1-C2-N3 | 5.12 | 126.97 | 123.90 |
| 1 | A | 1453 | G | C6-C5-N7 | -5.12 | 127.33 | 130.40 |
| 1 | A | 792 | A | C5-C6-N1 | -5.12 | 115.14 | 117.70 |
| 1 | A | 1290 | G | C5-C6-O6 | -5.12 | 125.53 | 128.60 |
| 12 | L | 27 | LEU | CB-CG-CD2 | 5.12 | 119.70 | 111.00 |
| 1 | A | 7 | G | C8-N9-C4 | 5.12 | 108.45 | 106.40 |
| 1 | A | 740 | U | C2-N1-C1' | -5.12 | 111.56 | 117.70 |
| 1 | A | 111 | G | OP1-P-OP2 | 5.12 | 127.27 | 119.60 |
| 1 | A | 382 | A | N1-C6-N6 | -5.12 | 115.53 | 118.60 |
| 1 | A | 794 | A | N1-C6-N6 | -5.12 | 115.53 | 118.60 |
| 1 | A | 897 | C | C6-N1-C2 | 5.12 | 122.35 | 120.30 |
| 1 | A | 453 | A | C8-N9-C4 | -5.11 | 103.75 | 105.80 |
| 1 | A | 851 | G | N1-C6-O6 | 5.11 | 122.97 | 119.90 |
| 1 | A | 665 | A | C2-N3-C4 | 5.11 | 113.16 | 110.60 |
| 1 | A | 1232 | U | C2-N1-C1' | 5.11 | 123.83 | 117.70 |
| 1 | A | 329 | A | C5-C6-N6 | 5.11 | 127.79 | 123.70 |
| 1 | A | 1085 | U | N1-C2-N3 | -5.11 | 111.84 | 114.90 |
| 1 | A | 46 | G | N9-C4-C5 | 5.11 | 107.44 | 105.40 |
| 1 | A | 631 | G | C6-N1-C2 | 5.11 | 128.16 | 125.10 |
| 1 | A | 665 | A | C5-C6-N1 | 5.11 | 120.25 | 117.70 |
| 1 | A | 512 | U | C5-C4-O4 | -5.10 | 122.84 | 125.90 |
| 1 | A | 130 | A | N1-C6-N6 | 5.10 | 121.66 | 118.60 |
| 1 | A | 292 | G | C6-C5-N7 | -5.10 | 127.34 | 130.40 |
| 1 | A | 509 | A | C2'-C3'-O3' | 5.10 | 121.86 | 113.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 870 | U | C5-C6-N1 | -5.10 | 120.15 | 122.70 |
| 1 | A | 1257 | U | C6-N1-C2 | -5.10 | 117.94 | 121.00 |
| 1 | A | 68 | G | N3-C4-N9 | -5.10 | 122.94 | 126.00 |
| 1 | A | 674 | G | C4-C5-N7 | 5.10 | 112.84 | 110.80 |
| 1 | A | 816 | A | OP1-P-O3' | 5.10 | 116.42 | 105.20 |
| 1 | A | 1128 | C | C6-N1-C2 | -5.10 | 118.26 | 120.30 |
| 1 | A | 1198 | G | C5-C6-N1 | -5.10 | 108.95 | 111.50 |
| 1 | A | 191 | G | N3-C4-C5 | -5.09 | 126.05 | 128.60 |
| 1 | A | 500 | G | N9-C4-C5 | -5.09 | 103.36 | 105.40 |
| 1 | A | 1399 | C | N1-C2-N3 | 5.09 | 122.77 | 119.20 |
| 1 | A | 1525 | G | N9-C1'-C2' | -5.09 | 106.40 | 112.00 |
| 1 | A | 1531 | A | C2-N3-C4 | -5.09 | 108.05 | 110.60 |
| 1 | A | 362 | G | C5-N7-C8 | 5.09 | 106.85 | 104.30 |
| 1 | A | 585 | G | N3-C4-C5 | 5.09 | 131.15 | 128.60 |
| 1 | A | 1299 | A | N7-C8-N9 | 5.09 | 116.35 | 113.80 |
| 1 | A | 397 | A | C8-N9-C4 | -5.09 | 103.76 | 105.80 |
| 1 | A | 407 | G | C2-N3-C4 | -5.09 | 109.35 | 111.90 |
| 1 | A | 507 | C | N3-C2-O2 | 5.09 | 125.46 | 121.90 |
| 1 | A | 1023 | G | N3-C4-N9 | 5.09 | 129.06 | 126.00 |
| 1 | A | 148 | G | N3-C4-C5 | -5.09 | 126.06 | 128.60 |
| 1 | A | 184 | G | C5-N7-C8 | 5.09 | 106.84 | 104.30 |
| 1 | A | 389 | A | C8-N9-C4 | -5.09 | 103.76 | 105.80 |
| 1 | A | 499 | A | C5-C6-N6 | 5.09 | 127.77 | 123.70 |
| 1 | A | 900 | A | C4-C5-N7 | 5.09 | 113.25 | 110.70 |
| 1 | A | 1529 | G | C8-N9-C4 | -5.09 | 104.36 | 106.40 |
| 1 | A | 872 | A | C4-C5-C6 | 5.09 | 119.54 | 117.00 |
| 1 | A | 46 | G | N7-C8-N9 | 5.09 | 115.64 | 113.10 |
| 1 | A | 889 | A | C8-N9-C4 | -5.09 | 103.77 | 105.80 |
| 1 | A | 331 | G | N7-C8-N9 | 5.08 | 115.64 | 113.10 |
| 1 | A | 728 | A | C6-C5-N7 | -5.08 | 128.74 | 132.30 |
| 1 | A | 833 | U | C6-N1-C1' | 5.08 | 128.32 | 121.20 |
| 1 | A | 9 | G | O5'-P-OP2 | -5.08 | 101.12 | 105.70 |
| 1 | A | 747 | C | C4-C5-C6 | 5.08 | 119.94 | 117.40 |
| 1 | A | 667 | G | C5-C6-N1 | -5.08 | 108.96 | 111.50 |
| 1 | A | 1379 | G | C6-C5-N7 | -5.08 | 127.35 | 130.40 |
| 1 | A | 502 | G | N3-C4-C5 | 5.08 | 131.14 | 128.60 |
| 1 | A | 1079 | G | C4-N9-C1' | 5.08 | 133.10 | 126.50 |
| 1 | A | 1138 | G | N3-C2-N2 | -5.08 | 116.35 | 119.90 |
| 1 | A | 497 | A | C4-C5-N7 | -5.08 | 108.16 | 110.70 |
| 1 | A | 1416 | G | N7-C8-N9 | 5.08 | 115.64 | 113.10 |
| 1 | A | 880 | C | N1-C2-N3 | -5.07 | 115.65 | 119.20 |
| 1 | A | 1322 | C | OP1-P-OP2 | -5.07 | 111.99 | 119.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 904 | C | C6-N1-C2 | 5.07 | 122.33 | 120.30 |
| 1 | A | 223 | U | C5-C6-N1 | -5.07 | 120.17 | 122.70 |
| 1 | A | 917 | G | C2-N3-C4 | 5.07 | 114.43 | 111.90 |
| 1 | A | 363 | A | C5-C6-N6 | -5.07 | 119.65 | 123.70 |
| 1 | A | 1502 | A | N7-C8-N9 | 5.07 | 116.33 | 113.80 |
| 1 | A | 58 | C | N3-C4-N4 | 5.07 | 121.55 | 118.00 |
| 1 | A | 60 | A | C8-N9-C4 | -5.07 | 103.77 | 105.80 |
| 1 | A | 435 | C | O5'-P-OP2 | 5.07 | 116.78 | 110.70 |
| 1 | A | 887 | G | C5-C6-N1 | -5.07 | 108.97 | 111.50 |
| 3 | C | 14 | ILE | CG1-CB-CG2 | 5.07 | 122.54 | 111.40 |
| 3 | C | 21 | ARG | NE-CZ-NH1 | 5.07 | 122.83 | 120.30 |
| 1 | A | 116 | A | OP1-P-OP2 | 5.06 | 127.20 | 119.60 |
| 1 | A | 857 | C | OP2-P-O3' | 5.06 | 116.34 | 105.20 |
| 1 | A | 881 | G | N9-C4-C5 | -5.06 | 103.37 | 105.40 |
| 1 | A | 612 | C | N3-C4-N4 | -5.06 | 114.46 | 118.00 |
| 1 | A | 820 | U | C5-C6-N1 | -5.06 | 120.17 | 122.70 |
| 1 | A | 148 | G | C4-C5-C6 | 5.06 | 121.84 | 118.80 |
| 1 | A | 231 | G | O5'-P-OP2 | 5.06 | 116.77 | 110.70 |
| 1 | A | 1240 | U | N3-C4-O4 | -5.06 | 115.86 | 119.40 |
| 1 | A | 248 | C | C2-N3-C4 | -5.06 | 117.37 | 119.90 |
| 1 | A | 504 | C | N3-C4-C5 | -5.06 | 119.88 | 121.90 |
| 1 | A | 934 | C | O5'-P-OP2 | -5.06 | 101.15 | 105.70 |
| 1 | A | 277 | C | N3-C4-C5 | 5.06 | 123.92 | 121.90 |
| 1 | A | 406 | G | N7-C8-N9 | 5.06 | 115.63 | 113.10 |
| 1 | A | 599 | C | N3-C2-O2 | 5.06 | 125.44 | 121.90 |
| 1 | A | 300 | A | C4-C5-N7 | -5.06 | 108.17 | 110.70 |
| 1 | A | 595 | G | N3-C2-N2 | 5.05 | 123.44 | 119.90 |
| 10 | J | 5 | ARG | CG-CD-NE | 5.05 | 122.41 | 111.80 |
| 1 | A | 564 | C | N1-C2-O2 | 5.05 | 121.93 | 118.90 |
| 1 | A | 788 | U | N3-C4-C5 | -5.05 | 111.57 | 114.60 |
| 1 | A | 1193 | G | OP1-P-OP2 | 5.05 | 127.18 | 119.60 |
| 1 | A | 1373 | G | C4-N9-C1' | 5.05 | 133.06 | 126.50 |
| 1 | A | 688 | G | N1-C6-O6 | 5.05 | 122.93 | 119.90 |
| 1 | A | 993 | G | N3-C4-N9 | 5.05 | 129.03 | 126.00 |
| 1 | A | 382 | A | C5-C6-N6 | 5.05 | 127.74 | 123.70 |
| 1 | A | 500 | G | C2-N3-C4 | -5.05 | 109.38 | 111.90 |
| 1 | A | 546 | G | N7-C8-N9 | 5.05 | 115.62 | 113.10 |
| 1 | A | 1125 | U | C2-N1-C1' | -5.05 | 111.64 | 117.70 |
| 1 | A | 1494 | G | C8-N9-C1' | -5.04 | 120.44 | 127.00 |
| 1 | A | 316 | G | N3-C4-N9 | 5.04 | 129.03 | 126.00 |
| 1 | A | 224 | C | N3-C2-O2 | -5.04 | 118.37 | 121.90 |
| 1 | A | 535 | A | C5-N7-C8 | 5.04 | 106.42 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 1166 | G | N7-C8-N9 | 5.04 | 115.62 | 113.10 |
| 1 | A | 1338 | G | C8-N9-C1' | -5.04 | 120.45 | 127.00 |
| 1 | A | 1397 | C | N3-C4-C5 | 5.04 | 123.92 | 121.90 |
| 1 | A | 1304 | G | C4-N9-C1' | 5.04 | 133.05 | 126.50 |
| 1 | A | 1391 | U | C2-N1-C1' | -5.04 | 111.65 | 117.70 |
| 1 | A | 585 | G | N3-C4-N9 | -5.04 | 122.98 | 126.00 |
| 1 | A | 879 | C | C2-N1-C1' | -5.04 | 113.26 | 118.80 |
| 1 | A | 918 | A | C5-C6-N6 | -5.04 | 119.67 | 123.70 |
| 1 | A | 232 | G | N3-C4-N9 | 5.04 | 129.02 | 126.00 |
| 1 | A | 787 | A | C6-N1-C2 | -5.04 | 115.58 | 118.60 |
| 1 | A | 1370 | G | C2-N3-C4 | -5.04 | 109.38 | 111.90 |
| 1 | A | 1524 | C | OP2-P-O3' | 5.04 | 116.28 | 105.20 |
| 1 | A | 517 | G | C5-C6-N1 | -5.03 | 108.98 | 111.50 |
| 1 | A | 580 | U | N3-C4-C5 | -5.03 | 111.58 | 114.60 |
| 1 | A | 834 | C | N3-C4-C5 | 5.03 | 123.91 | 121.90 |
| 1 | A | 1227 | A | O5'-P-OP1 | -5.03 | 101.17 | 105.70 |
| 1 | A | 375 | U | N3-C4-O4 | 5.03 | 122.92 | 119.40 |
| 1 | A | 918 | A | C5-C6-N1 | 5.03 | 120.22 | 117.70 |
| 1 | A | 79 | G | N1-C6-O6 | 5.03 | 122.92 | 119.90 |
| 1 | A | 545 | C | OP1-P-OP2 | 5.03 | 127.14 | 119.60 |
| 5 | E | 123 | LEU | CB-CG-CD2 | -5.03 | 102.45 | 111.00 |
| 1 | A | 951 | G | N1-C6-O6 | 5.03 | 122.92 | 119.90 |
| 1 | A | 1386 | G | O5'-P-OP2 | -5.03 | 101.18 | 105.70 |
| 1 | A | 575 | G | N3-C2-N2 | 5.02 | 123.42 | 119.90 |
| 1 | A | 542 | G | C5-C6-N1 | 5.02 | 114.01 | 111.50 |
| 1 | A | 28 | G | O5'-P-OP1 | -5.02 | 101.18 | 105.70 |
| 1 | A | 42 | G | N3-C2-N2 | -5.02 | 116.39 | 119.90 |
| 1 | A | 1397 | C | N3-C2-O2 | -5.02 | 118.39 | 121.90 |
| 1 | A | 1526 | G | C2-N3-C4 | -5.02 | 109.39 | 111.90 |
| 1 | A | 352 | C | C5-C6-N1 | 5.02 | 123.51 | 121.00 |
| 1 | A | 1148 | U | N3-C2-O2 | -5.02 | 118.69 | 122.20 |
| 1 | A | 1395 | C | N3-C2-O2 | 5.02 | 125.41 | 121.90 |
| 1 | A | 582 | U | C4-C5-C6 | 5.02 | 122.71 | 119.70 |
| 1 | A | 406 | G | C6-C5-N7 | -5.01 | 127.39 | 130.40 |
| 1 | A | 517 | G | N9-C4-C5 | 5.01 | 107.41 | 105.40 |
| 1 | A | 786 | G | C4-C5-C6 | 5.01 | 121.81 | 118.80 |
| 1 | A | 1202 | G | C8-N9-C1' | 5.01 | 133.52 | 127.00 |
| 1 | A | 886 | G | C4-C5-N7 | 5.01 | 112.80 | 110.80 |
| 1 | A | 906 | G | C5-C6-O6 | -5.01 | 125.59 | 128.60 |
| 1 | A | 646 | U | C2-N3-C4 | 5.01 | 130.00 | 127.00 |
| 1 | A | 1417 | G | O4'-C1'-N9 | 5.01 | 112.21 | 108.20 |
| 1 | A | 1435 | G | C4-C5-N7 | 5.01 | 112.80 | 110.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | A | 710 | G | N3-C2-N2 | -5.01 | 116.39 | 119.90 |
| 1 | A | 1494 | G | N3-C4-N9 | 5.01 | 129.00 | 126.00 |
| 1 | A | 1495 | U | C2-N3-C4 | 5.01 | 130.00 | 127.00 |
| 1 | A | 357 | G | C6-N1-C2 | 5.00 | 128.10 | 125.10 |
| 1 | A | 654 | G | OP2-P-O3' | 5.00 | 116.21 | 105.20 |
| 1 | A | 190(H) | G | C8-N9-C1' | -5.00 | 120.49 | 127.00 |
| 1 | A | 869 | G | N3-C4-N9 | 5.00 | 129.00 | 126.00 |
| 1 | A | 332 | G | C5-C6-N1 | -5.00 | 109.00 | 111.50 |
| 1 | A | 518 | C | C2-N1-C1' | 5.00 | 124.30 | 118.80 |
| 1 | A | 662 | G | C5-C6-N1 | -5.00 | 109.00 | 111.50 |
| 1 | A | 770 | C | N1-C2-O2 | 5.00 | 121.90 | 118.90 |
| 1 | A | 786 | G | C8-N9-C1' | -5.00 | 120.50 | 127.00 |
| 1 | A | 1079 | G | C6-N1-C2 | -5.00 | 122.10 | 125.10 |

There are no chirality outliers.

All (18) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 2 | B | 8 | LYS | Peptide |
| 2 | B | 9 | GLU | Peptide |
| 3 | C | 154 | SER | Peptide |
| 3 | C | 166 | GLU | Peptide |
| 3 | C | 168 | ALA | Peptide |
| 8 | H | 90 | GLY | Peptide |
| 9 | I | 56 | LEU | Peptide |
| 9 | I | 57 | GLY | Peptide |
| 10 | J | 34 | VAL | Peptide |
| 10 | J | 88 | LEU | Peptide |
| 13 | M | 105 | THR | Peptide |
| 13 | M | 107 | ALA | Peptide |
| 13 | M | 62 | ASN | Peptide |
| 14 | N | 7 | ILE | Peptide |
| 16 | P | 19 | ILE | Peptide |
| 20 | T | 12 | ALA | Peptide |
| 20 | T | 92 | LEU | Peptide |
| 20 | T | 93 | GLU | 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 | 32687 | 0 | 16528 | 920 | 0 |
| 2 | B | 1900 | 0 | 1951 | 96 | 0 |
| 3 | C | 1612 | 0 | 1677 | 97 | 0 |
| 4 | D | 1703 | 0 | 1763 | 104 | 0 |
| 5 | E | 1146 | 0 | 1207 | 78 | 0 |
| 6 | F | 843 | 0 | 857 | 62 | 0 |
| 7 | G | 1257 | 0 | 1296 | 69 | 0 |
| 8 | H | 1116 | 0 | 1177 | 74 | 0 |
| 9 | I | 1010 | 0 | 1037 | 65 | 0 |
| 10 | J | 792 | 0 | 835 | 73 | 0 |
| 11 | K | 864 | 0 | 881 | 44 | 0 |
| 12 | L | 972 | 0 | 1058 | 59 | 0 |
| 13 | M | 937 | 0 | 995 | 59 | 0 |
| 14 | N | 492 | 0 | 529 | 47 | 0 |
| 15 | O | 729 | 0 | 768 | 49 | 0 |
| 16 | P | 700 | 0 | 720 | 34 | 0 |
| 17 | Q | 823 | 0 | 891 | 55 | 0 |
| 18 | R | 574 | 0 | 644 | 49 | 0 |
| 19 | S | 647 | 0 | 673 | 48 | 0 |
| 20 | T | 763 | 0 | 861 | 51 | 0 |
| 21 | U | 208 | 0 | 221 | 9 | 0 |
| 22 | A | 164 | 0 | 0 | 0 | 0 |
| 22 | D | 1 | 0 | 0 | 0 | 0 |
| 22 | E | 1 | 0 | 0 | 0 | 0 |
| 22 | F | 1 | 0 | 0 | 0 | 0 |
| 22 | G | 1 | 0 | 0 | 0 | 0 |
| 22 | H | 1 | 0 | 0 | 0 | 0 |
| 22 | K | 2 | 0 | 0 | 0 | 0 |
| 22 | S | 1 | 0 | 0 | 0 | 0 |
| 23 | D | 1 | 0 | 0 | 0 | 0 |
| 23 | N | 1 | 0 | 0 | 0 | 0 |
| 24 | A | 271 | 0 | 0 | 14 | 0 |
| 24 | C | 1 | 0 | 0 | 0 | 0 |
| 24 | E | 3 | 0 | 0 | 0 | 0 |
| 24 | L | 1 | 0 | 0 | 0 | 0 |
| 24 | N | 1 | 0 | 0 | 0 | 0 |
| 24 | P | 1 | 0 | 0 | 0 | 0 |
| 24 | T | 1 | 0 | 0 | 0 | 0 |
| All | All | 52228 | 0 | 36569 | 1946 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 22.

All (1946) 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) |
|------------------|------------------|--------------------------|-------------------|
| 9:I:8:GLY:HA2 | 9:I:79:LEU:HD13 | 1.48 | 0.95 |
| 8:H:10:LEU:HD22 | 8:H:83:ILE:HD11 | 1.49 | 0.94 |
| 1:A:664:G:H22 | 1:A:741:G:H1 | 1.17 | 0.92 |
| 1:A:1002:G:N1 | 1:A:1003(A):G:O6 | 2.04 | 0.91 |
| 4:D:187:ARG:HH22 | 4:D:188:LEU:HD12 | 1.36 | 0.91 |
| 1:A:1026:G:H8 | 1:A:1027:C:H5'' | 1.34 | 0.90 |
| 1:A:1003:G:O2' | 1:A:1003(A):G:N7 | 2.04 | 0.90 |
| 1:A:1366:C:O2' | 10:J:60:ARG:NH2 | 2.05 | 0.89 |
| 15:O:5:LYS:H | 15:O:5:LYS:HZ3 | 1.18 | 0.88 |
| 13:M:48:LEU:HD12 | 13:M:53:VAL:HG22 | 1.55 | 0.88 |
| 19:S:18:LYS:HG2 | 19:S:31:ILE:HD11 | 1.55 | 0.87 |
| 7:G:85:TYR:HD1 | 7:G:154:TYR:HE1 | 1.23 | 0.87 |
| 8:H:113:SER:HB3 | 8:H:134:ILE:HD11 | 1.56 | 0.87 |
| 11:K:57:THR:HG22 | 11:K:59:TYR:H | 1.40 | 0.85 |
| 2:B:17:PHE:HD1 | 2:B:18:GLY:H | 1.22 | 0.85 |
| 1:A:1443:G:H4' | 1:A:1446:A:H5' | 1.59 | 0.85 |
| 1:A:677:U:H3 | 1:A:713:G:H22 | 1.23 | 0.85 |
| 7:G:122:HIS:HA | 7:G:125:MET:HB2 | 1.57 | 0.84 |
| 1:A:1028:C:H6 | 1:A:1033:G:H22 | 1.25 | 0.84 |
| 10:J:55:LYS:HG2 | 10:J:56:HIS:H | 1.44 | 0.83 |
| 1:A:598:U:H4' | 8:H:94:TYR:CD1 | 2.13 | 0.82 |
| 8:H:9:MET:HG3 | 8:H:26:VAL:HG21 | 1.60 | 0.82 |
| 4:D:187:ARG:CZ | 4:D:188:LEU:H | 1.93 | 0.82 |
| 1:A:1026:G:C8 | 1:A:1027:C:H5'' | 2.15 | 0.81 |
| 15:O:70:LEU:HD11 | 15:O:77:ARG:HB2 | 1.61 | 0.81 |
| 15:O:32:LEU:HD12 | 15:O:63:ARG:HB3 | 1.63 | 0.81 |
| 1:A:1543:C:H2' | 1:A:1544:U:H5'' | 1.63 | 0.80 |
| 19:S:39:THR:HG22 | 19:S:70:LYS:HD2 | 1.61 | 0.80 |
| 1:A:1238:A:H5' | 1:A:1336:C:H41 | 1.47 | 0.79 |
| 1:A:1425:U:H3 | 1:A:1475:G:H1 | 1.26 | 0.79 |
| 6:F:2:ARG:HH11 | 6:F:69:GLU:HG2 | 1.47 | 0.79 |
| 1:A:1527:C:H2' | 1:A:1528:U:C6 | 2.17 | 0.79 |
| 1:A:103:C:OP1 | 20:T:17:ARG:NH1 | 2.15 | 0.79 |
| 12:L:27:LEU:O | 12:L:29:GLY:N | 2.16 | 0.79 |
| 1:A:1178:G:OP1 | 9:I:93:ARG:NH1 | 2.16 | 0.78 |
| 4:D:98:GLU:OE1 | 4:D:103:ASN:ND2 | 2.16 | 0.78 |
| 3:C:155:GLY:HA3 | 3:C:163:ALA:HB1 | 1.65 | 0.78 |
| 2:B:16:HIS:HB3 | 2:B:210:SER:HB2 | 1.65 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:123:GLN:HB2 | 3:C:128:PHE:HD1 | 1.47 | 0.78 |
| 11:K:85:ARG:HD3 | 11:K:113:PRO:HD3 | 1.65 | 0.78 |
| 1:A:298:A:N6 | 24:A:1868:HOH:O | 2.18 | 0.77 |
| 1:A:254:G:H2' | 1:A:255:G:H8 | 1.48 | 0.77 |
| 1:A:758:G:N7 | 24:A:2070:HOH:O | 2.17 | 0.77 |
| 3:C:95:THR:HB | 3:C:97:LYS:HG2 | 1.67 | 0.77 |
| 4:D:153:ARG:HD3 | 4:D:181:MET:HG3 | 1.67 | 0.76 |
| 1:A:677:U:O4 | 1:A:713:G:N1 | 2.15 | 0.76 |
| 19:S:80:TYR:CE1 | 19:S:81:ARG:HD3 | 2.20 | 0.76 |
| 1:A:1262:C:H42 | 1:A:1273:G:H1 | 1.31 | 0.76 |
| 2:B:91:PRO:HG3 | 2:B:155:LEU:HB3 | 1.67 | 0.76 |
| 18:R:79:LEU:HD23 | 18:R:80:PRO:HD2 | 1.66 | 0.76 |
| 1:A:1001:A:H61 | 1:A:1039:C:H42 | 1.34 | 0.76 |
| 3:C:35:GLU:OE1 | 3:C:59:ARG:NH1 | 2.18 | 0.76 |
| 7:G:27:ILE:HA | 7:G:30:ILE:HD12 | 1.66 | 0.76 |
| 1:A:1073:U:OP2 | 5:E:57:LYS:NZ | 2.18 | 0.75 |
| 1:A:1249:C:O2' | 9:I:73:GLN:NE2 | 2.20 | 0.75 |
| 15:O:62:GLN:HG2 | 15:O:65:ARG:HH21 | 1.52 | 0.75 |
| 1:A:673:G:H2' | 1:A:674:G:C8 | 2.21 | 0.75 |
| 1:A:902:G:H2' | 1:A:903:G:H8 | 1.50 | 0.75 |
| 5:E:64:ARG:HE | 5:E:65:ASN:HB2 | 1.51 | 0.75 |
| 20:T:40:ALA:HB2 | 20:T:55:ILE:HG22 | 1.68 | 0.75 |
| 18:R:34:TYR:HB3 | 18:R:69:THR:HG22 | 1.69 | 0.75 |
| 1:A:695:A:H2' | 1:A:696:A:C8 | 2.21 | 0.74 |
| 4:D:57:ARG:HG3 | 4:D:202:LEU:HD12 | 1.68 | 0.74 |
| 8:H:40:ALA:HB2 | 8:H:45:ILE:HD13 | 1.68 | 0.74 |
| 1:A:967:5MC:O2' | 9:I:128:ARG:NH1 | 2.20 | 0.74 |
| 16:P:9:PHE:CD1 | 16:P:18:ARG:HD2 | 2.23 | 0.74 |
| 7:G:85:TYR:HD1 | 7:G:154:TYR:CE1 | 2.05 | 0.74 |
| 1:A:299:G:N1 | 24:A:1868:HOH:O | 2.19 | 0.74 |
| 4:D:149:ALA:HB3 | 4:D:152:SER:HB3 | 1.69 | 0.74 |
| 11:K:92:GLU:HB3 | 11:K:96:ARG:HH21 | 1.52 | 0.74 |
| 1:A:1236:A:H4' | 1:A:1304:G:H4' | 1.70 | 0.73 |
| 1:A:669:U:H2' | 1:A:670:G:C8 | 2.24 | 0.73 |
| 1:A:1367:C:H5' | 10:J:60:ARG:HH21 | 1.53 | 0.73 |
| 1:A:1423:G:N2 | 1:A:1477:C:O2 | 2.19 | 0.73 |
| 1:A:562:C:H4' | 1:A:563:A:H5'' | 1.71 | 0.73 |
| 1:A:1026:G:OP1 | 1:A:1030(D):A:O2' | 2.07 | 0.73 |
| 1:A:1316:G:H4' | 14:N:18:VAL:HG11 | 1.71 | 0.73 |
| 9:I:29:ASN:HD21 | 9:I:65:VAL:HB | 1.52 | 0.73 |
| 1:A:925:G:O2' | 1:A:927:G:OP1 | 2.07 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:F:5:GLU:HB3 | 6:F:62:TRP:HE1 | 1.53 | 0.73 |
| 12:L:25:PRO:C | 12:L:27:LEU:H | 1.91 | 0.73 |
| 1:A:920:U:H2' | 1:A:921:U:C6 | 2.23 | 0.72 |
| 6:F:14:LEU:HD13 | 6:F:19:LEU:HA | 1.71 | 0.72 |
| 8:H:11:THR:O | 8:H:15:ASN:ND2 | 2.21 | 0.72 |
| 20:T:53:LEU:HD13 | 20:T:103:GLY:H | 1.55 | 0.72 |
| 1:A:1033:G:H3' | 1:A:1034:G:H5' | 1.70 | 0.72 |
| 3:C:50:ALA:HB2 | 3:C:75:VAL:HB | 1.71 | 0.72 |
| 1:A:669:U:OP1 | 15:O:48:LYS:NZ | 2.15 | 0.72 |
| 2:B:15:VAL:HG13 | 2:B:209:ARG:HG3 | 1.72 | 0.72 |
| 1:A:62:U:H2' | 1:A:63:C:H6 | 1.55 | 0.72 |
| 1:A:413:G:H8 | 1:A:428:G:H21 | 1.35 | 0.72 |
| 2:B:178:ARG:HB2 | 2:B:178:ARG:HH11 | 1.55 | 0.71 |
| 5:E:79:GLU:HG3 | 8:H:105:ARG:HG2 | 1.72 | 0.71 |
| 15:O:56:LEU:O | 15:O:60:VAL:HG23 | 1.90 | 0.71 |
| 1:A:1258:G:H2' | 1:A:1259:C:H5' | 1.72 | 0.71 |
| 1:A:1316:G:N1 | 1:A:1319:A:OP2 | 2.22 | 0.71 |
| 20:T:50:GLU:HB2 | 20:T:99:LEU:HD23 | 1.70 | 0.71 |
| 1:A:45:U:H2' | 1:A:46:G:C8 | 2.25 | 0.71 |
| 1:A:108:G:H5' | 1:A:109:A:H5' | 1.72 | 0.71 |
| 1:A:1348:U:H4' | 9:I:120:ARG:HG3 | 1.71 | 0.71 |
| 20:T:57:ARG:HH22 | 20:T:100:ILE:HD12 | 1.55 | 0.71 |
| 1:A:1288:A:N3 | 1:A:1352:C:O2' | 2.24 | 0.71 |
| 7:G:113:GLU:HG2 | 7:G:119:ARG:HG2 | 1.73 | 0.71 |
| 7:G:111:ARG:HH21 | 7:G:123:GLU:HA | 1.56 | 0.70 |
| 3:C:77:ILE:HG22 | 3:C:81:GLY:HA2 | 1.73 | 0.70 |
| 4:D:155:LEU:HD23 | 4:D:156:GLU:H | 1.56 | 0.70 |
| 11:K:85:ARG:HE | 11:K:111:ASP:HB3 | 1.55 | 0.70 |
| 1:A:390:C:H2' | 1:A:391:G:C8 | 2.26 | 0.70 |
| 1:A:975:A:H4' | 1:A:976:G:H5'' | 1.71 | 0.70 |
| 8:H:41:ARG:HH12 | 8:H:42:GLU:HG2 | 1.56 | 0.70 |
| 4:D:186:LEU:HD23 | 4:D:186:LEU:H | 1.56 | 0.70 |
| 6:F:77:ARG:HA | 6:F:80:ARG:HG2 | 1.74 | 0.70 |
| 1:A:337:C:H2' | 1:A:338:A:H8 | 1.57 | 0.70 |
| 1:A:981:U:H5' | 14:N:21:TYR:CE1 | 2.27 | 0.70 |
| 8:H:124:ALA:O | 8:H:128:GLY:N | 2.25 | 0.70 |
| 10:J:57:LYS:HG3 | 10:J:60:ARG:HH12 | 1.57 | 0.69 |
| 1:A:1005:A:N7 | 1:A:1025:U:H1' | 2.07 | 0.69 |
| 17:Q:3:LYS:NZ | 17:Q:61:GLU:O | 2.24 | 0.69 |
| 1:A:337:C:H2' | 1:A:338:A:C8 | 2.27 | 0.69 |
| 4:D:23:GLY:HA3 | 4:D:112:VAL:HG12 | 1.73 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 11:K:44:SER:H | 11:K:47:VAL:HB | 1.55 | 0.69 |
| 1:A:343:U:O2' | 1:A:346:G:O6 | 2.09 | 0.69 |
| 1:A:878:G:H5' | 8:H:89:PRO:HG2 | 1.74 | 0.69 |
| 14:N:32:SER:O | 14:N:40:CYS:HA | 1.91 | 0.69 |
| 1:A:1320:C:O2 | 19:S:36:ARG:NH1 | 2.26 | 0.69 |
| 11:K:86:GLY:N | 11:K:112:THR:OG1 | 2.20 | 0.69 |
| 16:P:60:LEU:HD23 | 16:P:64:ALA:HB3 | 1.75 | 0.69 |
| 1:A:948:C:H42 | 1:A:1233:G:H1 | 1.41 | 0.69 |
| 6:F:33:TYR:HB2 | 6:F:75:LEU:HD23 | 1.75 | 0.69 |
| 1:A:253:U:H2' | 1:A:254:G:H8 | 1.59 | 0.68 |
| 1:A:1391:U:H2' | 1:A:1392:G:C8 | 2.28 | 0.68 |
| 2:B:136:VAL:HA | 2:B:139:LYS:HZ2 | 1.58 | 0.68 |
| 10:J:34:VAL:HG13 | 10:J:74:ILE:HA | 1.75 | 0.68 |
| 13:M:12:ASN:H | 13:M:45:VAL:CG1 | 2.05 | 0.68 |
| 15:O:16:ALA:HB1 | 15:O:21:ASP:HB3 | 1.73 | 0.68 |
| 17:Q:9:VAL:HG23 | 17:Q:56:VAL:HG22 | 1.74 | 0.68 |
| 9:I:50:LEU:HA | 9:I:53:VAL:HG22 | 1.75 | 0.68 |
| 1:A:1128:C:O2' | 1:A:1130:A:OP1 | 2.09 | 0.68 |
| 1:A:1147:C:O2 | 9:I:16:ARG:NH1 | 2.26 | 0.68 |
| 2:B:79:ASP:HA | 2:B:82:ARG:HG2 | 1.75 | 0.68 |
| 1:A:259:G:H1 | 1:A:267:C:H42 | 1.42 | 0.68 |
| 17:Q:61:GLU:HA | 17:Q:71:PHE:CE2 | 2.29 | 0.68 |
| 1:A:770:C:H1' | 1:A:899:C:H42 | 1.57 | 0.68 |
| 1:A:1366:C:H2' | 1:A:1367:C:C6 | 2.28 | 0.68 |
| 19:S:49:ILE:HG21 | 19:S:71:LEU:HD11 | 1.74 | 0.68 |
| 2:B:77:ALA:HB2 | 2:B:211:ILE:HD13 | 1.74 | 0.68 |
| 4:D:76:ARG:HB2 | 4:D:207:TYR:HE2 | 1.59 | 0.68 |
| 6:F:14:LEU:HD22 | 6:F:18:GLN:HB3 | 1.76 | 0.67 |
| 1:A:1030(D):A:H5'' | 1:A:1031:G:H5'' | 1.77 | 0.67 |
| 2:B:90:MET:N | 2:B:90:MET:SD | 2.67 | 0.67 |
| 1:A:310:G:H2' | 1:A:311:C:H6 | 1.59 | 0.67 |
| 2:B:96:ARG:HG3 | 2:B:97:TRP:N | 2.09 | 0.67 |
| 1:A:17:U:H2' | 1:A:18:C:C6 | 2.30 | 0.67 |
| 1:A:527:7MG:H5'' | 1:A:527:7MG:H81 | 1.76 | 0.67 |
| 1:A:669:U:H2' | 1:A:670:G:H8 | 1.56 | 0.67 |
| 2:B:76:GLN:HE22 | 2:B:206:ASP:HB3 | 1.58 | 0.67 |
| 1:A:664:G:N2 | 1:A:741:G:H1 | 1.92 | 0.67 |
| 11:K:80:VAL:HG13 | 11:K:103:LEU:HD21 | 1.76 | 0.67 |
| 1:A:967:5MC:H4' | 9:I:128:ARG:HG3 | 1.76 | 0.66 |
| 1:A:1367:C:H5' | 10:J:60:ARG:NH2 | 2.10 | 0.66 |
| 3:C:14:ILE:HB | 3:C:15:THR:HG23 | 1.76 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1427:U:H2' | 1:A:1428:A:C8 | 2.29 | 0.66 |
| 15:O:29:VAL:HG11 | 15:O:81:LEU:HD11 | 1.77 | 0.66 |
| 1:A:1343:G:H4' | 9:I:122:ALA:HB3 | 1.75 | 0.66 |
| 2:B:119:GLU:OE2 | 2:B:153:ARG:NH2 | 2.29 | 0.66 |
| 1:A:720:C:H5'' | 1:A:721:G:H5'' | 1.77 | 0.66 |
| 1:A:1326:C:H5'' | 21:U:12:LYS:HE3 | 1.78 | 0.66 |
| 8:H:29:SER:HG | 8:H:32:LYS:H | 1.43 | 0.66 |
| 5:E:31:LEU:HG | 5:E:45:PHE:HD1 | 1.61 | 0.66 |
| 13:M:4:ILE:HD12 | 13:M:22:ILE:HD11 | 1.78 | 0.66 |
| 20:T:53:LEU:HD22 | 20:T:56:MET:HG2 | 1.77 | 0.66 |
| 1:A:1127:G:H1 | 1:A:1145:C:H42 | 1.40 | 0.66 |
| 6:F:30:LEU:HA | 6:F:75:LEU:HD21 | 1.77 | 0.66 |
| 1:A:514:C:H2' | 1:A:515:G:H8 | 1.60 | 0.66 |
| 8:H:11:THR:HG23 | 8:H:15:ASN:HD21 | 1.60 | 0.66 |
| 13:M:96:LEU:HB3 | 13:M:97:PRO:HD2 | 1.78 | 0.66 |
| 17:Q:6:LEU:H | 17:Q:59:ILE:HG22 | 1.59 | 0.66 |
| 1:A:1035:A:H2' | 1:A:1036:G:H8 | 1.59 | 0.66 |
| 13:M:8:GLU:N | 13:M:8:GLU:OE2 | 2.29 | 0.66 |
| 6:F:91:VAL:HG13 | 18:R:72:ARG:HH22 | 1.61 | 0.65 |
| 6:F:8:ILE:HD11 | 6:F:79:LEU:HD13 | 1.78 | 0.65 |
| 8:H:4:ASP:OD2 | 8:H:85:ARG:NH1 | 2.29 | 0.65 |
| 6:F:91:VAL:HG12 | 6:F:92:LYS:O | 1.95 | 0.65 |
| 7:G:95:ARG:HG3 | 7:G:99:LEU:HD12 | 1.77 | 0.65 |
| 16:P:74:LEU:HD22 | 16:P:79:VAL:HG21 | 1.79 | 0.65 |
| 1:A:1527:C:H2' | 1:A:1528:U:H6 | 1.58 | 0.65 |
| 4:D:206:PHE:HD2 | 4:D:207:TYR:CE1 | 2.15 | 0.65 |
| 3:C:164:ARG:HG2 | 3:C:165:THR:H | 1.61 | 0.65 |
| 5:E:99:GLY:N | 5:E:117:ASP:OD1 | 2.29 | 0.65 |
| 1:A:259:G:OP2 | 20:T:83:ARG:NH1 | 2.29 | 0.65 |
| 1:A:1332:A:H2' | 1:A:1333:A:H8 | 1.61 | 0.65 |
| 1:A:1226:C:OP2 | 13:M:91:ARG:NH2 | 2.30 | 0.65 |
| 9:I:118:LYS:O | 9:I:120:ARG:N | 2.30 | 0.65 |
| 8:H:25:ASP:OD1 | 8:H:25:ASP:N | 2.30 | 0.64 |
| 10:J:29:ARG:NH2 | 10:J:84:GLN:OE1 | 2.30 | 0.64 |
| 1:A:1130:A:OP1 | 1:A:1130:A:H8 | 1.79 | 0.64 |
| 11:K:17:GLY:HA2 | 11:K:35:PRO:HD3 | 1.80 | 0.64 |
| 15:O:26:GLU:O | 15:O:29:VAL:HG12 | 1.97 | 0.64 |
| 1:A:1320:C:H4' | 19:S:73:GLU:HG3 | 1.80 | 0.64 |
| 1:A:1541:PSU:H5' | 1:A:1542:U:OP1 | 1.97 | 0.64 |
| 9:I:6:GLY:HA3 | 9:I:83:ARG:HG3 | 1.79 | 0.64 |
| 10:J:4:ILE:HB | 10:J:74:ILE:CG1 | 2.27 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 17:Q:7:THR:O | 17:Q:23:VAL:HG13 | 1.97 | 0.64 |
| 17:Q:88:TYR:HA | 17:Q:91:ARG:HD3 | 1.79 | 0.64 |
| 1:A:312:C:H2' | 1:A:313:A:C8 | 2.32 | 0.64 |
| 1:A:537:G:OP1 | 12:L:113:ARG:NH2 | 2.30 | 0.64 |
| 13:M:22:ILE:HG21 | 13:M:66:LEU:HD13 | 1.79 | 0.64 |
| 14:N:25:VAL:HG12 | 14:N:38:GLY:O | 1.97 | 0.64 |
| 1:A:579:G:H4' | 15:O:54:ARG:HH21 | 1.63 | 0.64 |
| 5:E:116:THR:OG1 | 5:E:117:ASP:OD2 | 2.16 | 0.64 |
| 6:F:45:LEU:O | 6:F:46:ARG:NH1 | 2.31 | 0.64 |
| 14:N:47:LEU:O | 14:N:50:LYS:N | 2.31 | 0.64 |
| 1:A:793:U:O2 | 1:A:1516[A]:G:H4' | 1.96 | 0.64 |
| 4:D:199:ASN:HB3 | 4:D:202:LEU:HD23 | 1.78 | 0.64 |
| 12:L:27:LEU:HG | 12:L:28:LYS:H | 1.62 | 0.64 |
| 1:A:352:C:H5' | 24:A:2004:HOH:O | 1.97 | 0.64 |
| 1:A:62:U:H2' | 1:A:63:C:C6 | 2.33 | 0.64 |
| 1:A:426:G:OP1 | 4:D:36:ARG:NH1 | 2.31 | 0.64 |
| 1:A:1125:U:O2' | 1:A:1126:U:OP2 | 2.12 | 0.64 |
| 1:A:1258:G:OP2 | 1:A:1258:G:H8 | 1.80 | 0.64 |
| 2:B:68:ILE:H | 2:B:90:MET:HG3 | 1.63 | 0.64 |
| 7:G:78:ARG:HH12 | 7:G:156:TRP:HB2 | 1.63 | 0.64 |
| 15:O:15:PHE:CE2 | 15:O:84:LYS:HG2 | 2.33 | 0.64 |
| 1:A:937:A:H5'' | 1:A:938:A:OP2 | 1.98 | 0.63 |
| 1:A:1121:U:H2' | 1:A:1122:U:C6 | 2.33 | 0.63 |
| 3:C:76:VAL:O | 3:C:83:ARG:HG2 | 1.98 | 0.63 |
| 7:G:15:ASP:OD2 | 7:G:18:TYR:N | 2.29 | 0.63 |
| 9:I:77:ILE:O | 9:I:81:ILE:HG12 | 1.98 | 0.63 |
| 1:A:1146:A:H2' | 1:A:1147:C:O4' | 1.98 | 0.63 |
| 1:A:1418:A:H2' | 1:A:1419:G:O4' | 1.99 | 0.63 |
| 14:N:42:ILE:O | 14:N:46:GLU:HG3 | 1.99 | 0.63 |
| 15:O:18:PHE:CE2 | 15:O:21:ASP:HB2 | 2.32 | 0.63 |
| 18:R:26:LEU:HD11 | 18:R:42:ARG:HD3 | 1.81 | 0.63 |
| 18:R:56:THR:OG1 | 18:R:57:GLY:N | 2.28 | 0.63 |
| 1:A:1171:G:O2' | 1:A:1172:C:H5' | 1.98 | 0.63 |
| 1:A:1366:C:H2' | 1:A:1367:C:H6 | 1.62 | 0.63 |
| 1:A:1510:U:H2' | 1:A:1511:G:C8 | 2.32 | 0.63 |
| 4:D:31:CYS:C | 4:D:33:MET:H | 2.02 | 0.63 |
| 12:L:66:VAL:HG21 | 12:L:98:TYR:CE1 | 2.33 | 0.63 |
| 19:S:13:ASP:OD2 | 19:S:13:ASP:N | 2.28 | 0.63 |
| 1:A:444:C:O2 | 1:A:490:G:N2 | 2.27 | 0.63 |
| 1:A:940:C:OP1 | 7:G:29:LYS:NZ | 2.31 | 0.63 |
| 1:A:115:G:O2' | 1:A:116:A:OP2 | 2.13 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1342:C:H2' | 1:A:1343:G:C8 | 2.33 | 0.63 |
| 10:J:88:LEU:HD22 | 10:J:88:LEU:N | 2.12 | 0.63 |
| 1:A:711:G:H2' | 1:A:712:A:H8 | 1.64 | 0.63 |
| 4:D:71:SER:OG | 4:D:72:GLU:N | 2.32 | 0.63 |
| 5:E:151:LEU:HD11 | 8:H:79:VAL:HA | 1.80 | 0.63 |
| 10:J:4:ILE:HG13 | 10:J:77:PRO:HG2 | 1.81 | 0.63 |
| 20:T:49:ALA:O | 20:T:53:LEU:HB2 | 1.99 | 0.63 |
| 1:A:782:A:OP1 | 1:A:1521:G:N2 | 2.31 | 0.63 |
| 7:G:72:ARG:NE | 7:G:142:GLU:OE1 | 2.20 | 0.63 |
| 20:T:63:ILE:HD13 | 20:T:80:ARG:HB3 | 1.81 | 0.63 |
| 1:A:664:G:OP1 | 18:R:64:ARG:HD2 | 1.99 | 0.63 |
| 10:J:53:PRO:HA | 14:N:41:ARG:HH21 | 1.64 | 0.63 |
| 1:A:1057:G:H4' | 3:C:197:GLY:H | 1.64 | 0.62 |
| 2:B:16:HIS:CB | 2:B:210:SER:HB2 | 2.28 | 0.62 |
| 7:G:85:TYR:CD1 | 7:G:154:TYR:HE1 | 2.10 | 0.62 |
| 1:A:881:G:OP2 | 12:L:12:ARG:NH2 | 2.30 | 0.62 |
| 1:A:1523:G:OP1 | 11:K:123:LYS:NZ | 2.18 | 0.62 |
| 6:F:9:VAL:HG22 | 6:F:60:PHE:CD2 | 2.34 | 0.62 |
| 13:M:5:ALA:HA | 13:M:61:GLU:HG3 | 1.80 | 0.62 |
| 3:C:91:LEU:HB3 | 3:C:99:VAL:HG21 | 1.81 | 0.62 |
| 7:G:41:ARG:NH1 | 7:G:41:ARG:HB2 | 2.15 | 0.62 |
| 2:B:236:TYR:O | 2:B:239:VAL:HG23 | 2.00 | 0.62 |
| 1:A:750:G:H1' | 15:O:23:GLY:H | 1.65 | 0.62 |
| 1:A:1388:C:H2' | 1:A:1389:C:H6 | 1.64 | 0.62 |
| 1:A:1481:U:H2' | 1:A:1482:G:C8 | 2.35 | 0.62 |
| 4:D:36:ARG:HD2 | 4:D:38:TYR:CE2 | 2.33 | 0.62 |
| 1:A:489:C:H2' | 1:A:490:G:H8 | 1.63 | 0.62 |
| 1:A:880:C:OP1 | 12:L:8:ASN:ND2 | 2.33 | 0.62 |
| 21:U:10:ARG:HA | 21:U:13:ILE:HB | 1.82 | 0.62 |
| 3:C:153:VAL:HG23 | 3:C:198:VAL:HG22 | 1.81 | 0.62 |
| 5:E:33:VAL:HG11 | 5:E:109:ILE:HA | 1.81 | 0.62 |
| 10:J:88:LEU:HD22 | 10:J:88:LEU:H | 1.65 | 0.62 |
| 11:K:26:ASN:O | 11:K:26:ASN:ND2 | 2.30 | 0.62 |
| 1:A:390:C:O3' | 16:P:28:ARG:NH2 | 2.32 | 0.62 |
| 2:B:19:HIS:CE1 | 2:B:206:ASP:HB2 | 2.35 | 0.62 |
| 2:B:80:ILE:HG21 | 2:B:211:ILE:HG22 | 1.80 | 0.62 |
| 3:C:121:ALA:HA | 3:C:124:ILE:HD12 | 1.81 | 0.62 |
| 5:E:18:ARG:HG2 | 5:E:25:ARG:O | 1.99 | 0.61 |
| 10:J:8:LEU:HD22 | 10:J:96:ILE:HG22 | 1.81 | 0.61 |
| 1:A:1196:U:H3' | 24:A:1871:HOH:O | 1.99 | 0.61 |
| 2:B:9:GLU:OE2 | 2:B:12:GLU:N | 2.33 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:H:116:LYS:HG3 | 8:H:127:LEU:HD11 | 1.82 | 0.61 |
| 1:A:861:G:HO2' | 1:A:874:G:HO2' | 1.47 | 0.61 |
| 4:D:21:LEU:HD12 | 4:D:22:LYS:H | 1.65 | 0.61 |
| 9:I:50:LEU:HD11 | 9:I:81:ILE:HG21 | 1.81 | 0.61 |
| 1:A:1228:C:OP1 | 13:M:108:ARG:NH2 | 2.33 | 0.61 |
| 1:A:1258:G:C2' | 1:A:1259:C:H5' | 2.30 | 0.61 |
| 1:A:1060:C:C5 | 3:C:2:GLY:HA2 | 2.35 | 0.61 |
| 1:A:1368:G:OP2 | 9:I:112:LYS:NZ | 2.27 | 0.61 |
| 1:A:1504:G:OP1 | 1:A:1507:A:H4' | 2.00 | 0.61 |
| 7:G:146:GLU:HA | 7:G:149:ARG:HB2 | 1.80 | 0.61 |
| 13:M:4:ILE:HD11 | 13:M:10:PRO:HG3 | 1.81 | 0.61 |
| 15:O:5:LYS:H | 15:O:5:LYS:NZ | 1.97 | 0.61 |
| 15:O:18:PHE:CD2 | 15:O:21:ASP:HB2 | 2.35 | 0.61 |
| 18:R:87:ARG:O | 18:R:88:LYS:HB2 | 2.00 | 0.61 |
| 1:A:322:C:H4' | 20:T:23:ARG:HD2 | 1.82 | 0.61 |
| 1:A:955:U:H1' | 1:A:1227:A:H61 | 1.66 | 0.61 |
| 1:A:1060:C:OP1 | 14:N:45:ARG:NH2 | 2.33 | 0.61 |
| 13:M:5:ALA:N | 13:M:8:GLU:OE1 | 2.34 | 0.61 |
| 1:A:643:C:H5' | 8:H:31:PHE:CD1 | 2.36 | 0.61 |
| 8:H:85:ARG:NE | 8:H:87:SER:O | 2.34 | 0.61 |
| 14:N:29:ARG:HH22 | 14:N:41:ARG:HH12 | 1.49 | 0.61 |
| 1:A:264:U:H2' | 1:A:265:G:O4' | 2.00 | 0.61 |
| 1:A:737:A:H2' | 1:A:738:C:C6 | 2.36 | 0.61 |
| 1:A:1127:G:O6 | 1:A:1144:G:N1 | 2.30 | 0.61 |
| 1:A:1505:G:H4' | 1:A:1506:U:H5'' | 1.82 | 0.61 |
| 1:A:1511:G:H2' | 1:A:1512:U:O4' | 2.01 | 0.61 |
| 3:C:6:HIS:CD2 | 3:C:9:GLY:H | 2.19 | 0.61 |
| 19:S:47:HIS:HB3 | 19:S:49:ILE:HD11 | 1.82 | 0.61 |
| 1:A:1243:C:H2' | 1:A:1244:C:C6 | 2.36 | 0.61 |
| 1:A:1321:C:H5'' | 1:A:1322:C:H5'' | 1.82 | 0.61 |
| 12:L:83:VAL:HG21 | 12:L:100:ILE:HD13 | 1.83 | 0.61 |
| 15:O:22:THR:O | 15:O:27:VAL:HG11 | 2.00 | 0.61 |
| 1:A:1491:G:C6 | 1:A:1493:A:H2 | 2.19 | 0.60 |
| 3:C:150:LYS:HB3 | 3:C:201:TYR:HB2 | 1.82 | 0.60 |
| 6:F:91:VAL:HG13 | 18:R:72:ARG:NH2 | 2.17 | 0.60 |
| 12:L:77:LEU:HD21 | 12:L:107:ALA:HA | 1.82 | 0.60 |
| 1:A:1425:U:H2' | 1:A:1426:C:C6 | 2.36 | 0.60 |
| 8:H:23:SER:HB2 | 8:H:62:TYR:HA | 1.82 | 0.60 |
| 1:A:310:G:OP2 | 16:P:27:LYS:NZ | 2.35 | 0.60 |
| 1:A:1103:C:H5'' | 2:B:98:LEU:HD22 | 1.84 | 0.60 |
| 1:A:1435:G:H2' | 1:A:1436:U:C6 | 2.36 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 4:D:155:LEU:HD23 | 4:D:156:GLU:N | 2.16 | 0.60 |
| 3:C:18:TRP:CD1 | 14:N:54:PRO:HA | 2.36 | 0.60 |
| 18:R:39:VAL:HG13 | 18:R:40:LEU:HD23 | 1.84 | 0.60 |
| 1:A:253:U:H2' | 1:A:254:G:C8 | 2.35 | 0.60 |
| 1:A:976:G:H5' | 1:A:1358:U:O2' | 2.02 | 0.60 |
| 1:A:1307:U:H2' | 1:A:1308:U:C6 | 2.37 | 0.60 |
| 11:K:48:ILE:HG22 | 11:K:49:GLY:H | 1.66 | 0.60 |
| 1:A:1124:G:H5' | 10:J:35:SER:HB2 | 1.83 | 0.60 |
| 2:B:178:ARG:HD3 | 8:H:72:PRO:HA | 1.82 | 0.60 |
| 3:C:188:LEU:HD11 | 3:C:195:VAL:HG13 | 1.84 | 0.60 |
| 1:A:448:A:OP2 | 1:A:485:G:N2 | 2.31 | 0.60 |
| 1:A:499:A:H4' | 1:A:500:G:OP1 | 2.01 | 0.60 |
| 1:A:1134:G:H2' | 1:A:1135:U:O4' | 2.01 | 0.60 |
| 5:E:64:ARG:NE | 5:E:65:ASN:HB2 | 2.16 | 0.60 |
| 6:F:2:ARG:HD2 | 6:F:69:GLU:HG2 | 1.83 | 0.60 |
| 1:A:197:A:H5'' | 24:A:1993:HOH:O | 2.01 | 0.60 |
| 1:A:1255:G:H2' | 1:A:1258:G:H21 | 1.67 | 0.60 |
| 2:B:213:LEU:HD23 | 2:B:214:ILE:HD13 | 1.84 | 0.60 |
| 7:G:38:LEU:O | 7:G:42:ILE:HG13 | 2.02 | 0.60 |
| 10:J:61:GLU:OE2 | 14:N:49:HIS:NE2 | 2.34 | 0.60 |
| 20:T:87:LYS:O | 20:T:91:LEU:HB2 | 2.02 | 0.60 |
| 1:A:1144:G:H2' | 1:A:1145:C:C5 | 2.36 | 0.60 |
| 10:J:24:VAL:HG21 | 10:J:37:PRO:HG3 | 1.84 | 0.60 |
| 11:K:92:GLU:HB3 | 11:K:96:ARG:NH2 | 2.16 | 0.60 |
| 17:Q:87:LYS:HE3 | 17:Q:88:TYR:N | 2.16 | 0.60 |
| 1:A:434:U:H2' | 1:A:435:C:H6 | 1.66 | 0.59 |
| 1:A:1518[B]:MA6:H8 | 1:A:1518[B]:MA6:O5' | 2.01 | 0.59 |
| 2:B:9:GLU:HG2 | 2:B:10:LEU:N | 2.16 | 0.59 |
| 7:G:102:ARG:O | 7:G:106:GLN:HG3 | 2.01 | 0.59 |
| 1:A:447:G:H2' | 1:A:485:G:N2 | 2.17 | 0.59 |
| 20:T:10:LEU:HD22 | 20:T:11:SER:N | 2.16 | 0.59 |
| 20:T:33:ILE:HG13 | 20:T:62:LEU:HD13 | 1.83 | 0.59 |
| 3:C:12:LEU:HD21 | 14:N:51:GLY:HA2 | 1.83 | 0.59 |
| 1:A:1096:C:H2' | 1:A:1097:C:H6 | 1.66 | 0.59 |
| 10:J:50:ILE:HD12 | 10:J:50:ILE:N | 2.17 | 0.59 |
| 4:D:104:VAL:HG21 | 4:D:140:VAL:HG21 | 1.85 | 0.59 |
| 1:A:447:G:H1 | 1:A:485:G:HO2' | 1.50 | 0.59 |
| 1:A:1338:G:H2' | 1:A:1339:A:C8 | 2.38 | 0.59 |
| 3:C:6:HIS:CD2 | 14:N:49:HIS:HB3 | 2.38 | 0.59 |
| 4:D:187:ARG:NH2 | 4:D:188:LEU:HB2 | 2.16 | 0.59 |
| 13:M:50:GLU:HA | 13:M:53:VAL:HB | 1.85 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:8:A:N7 | 4:D:208:SER:OG | 2.36 | 0.59 |
| 4:D:206:PHE:HD2 | 4:D:207:TYR:CD1 | 2.20 | 0.59 |
| 1:A:514:C:O2' | 1:A:515:G:H5' | 2.03 | 0.59 |
| 2:B:180:LEU:HB2 | 2:B:182:ILE:HG13 | 1.84 | 0.59 |
| 9:I:26:VAL:HG13 | 9:I:61:ALA:HB3 | 1.83 | 0.59 |
| 9:I:65:VAL:HG11 | 9:I:73:GLN:OE1 | 2.03 | 0.59 |
| 1:A:948:C:H5' | 1:A:1306:A:O2' | 2.02 | 0.59 |
| 1:A:1399:C:H4' | 1:A:1400:5MC:H5'' | 1.84 | 0.59 |
| 2:B:189:ASP:OD1 | 2:B:190:THR:N | 2.30 | 0.59 |
| 4:D:196:LEU:HD23 | 4:D:196:LEU:H | 1.67 | 0.59 |
| 16:P:19:ILE:HG22 | 16:P:36:ILE:HG13 | 1.85 | 0.59 |
| 1:A:579:G:H5' | 1:A:728:A:H1' | 1.84 | 0.58 |
| 1:A:1190:G:H5' | 3:C:176:HIS:CE1 | 2.38 | 0.58 |
| 6:F:5:GLU:HB3 | 6:F:62:TRP:NE1 | 2.18 | 0.58 |
| 8:H:64:LYS:HG2 | 8:H:79:VAL:HG21 | 1.84 | 0.58 |
| 1:A:1099:G:H2' | 1:A:1100:C:C6 | 2.38 | 0.58 |
| 8:H:51:VAL:HG12 | 8:H:58:TYR:O | 2.03 | 0.58 |
| 2:B:74:LYS:NZ | 2:B:74:LYS:HB3 | 2.18 | 0.58 |
| 6:F:39:LYS:HD3 | 6:F:40:VAL:N | 2.18 | 0.58 |
| 6:F:41:GLU:OE1 | 18:R:35:ARG:NH2 | 2.36 | 0.58 |
| 6:F:77:ARG:O | 6:F:77:ARG:HG2 | 2.04 | 0.58 |
| 1:A:234:C:H2' | 1:A:235:C:C6 | 2.39 | 0.58 |
| 1:A:243:A:C2 | 1:A:246:A:C8 | 2.91 | 0.58 |
| 1:A:457:C:H2' | 1:A:458:C:H6 | 1.68 | 0.58 |
| 1:A:1027:C:O2 | 1:A:1028:C:N4 | 2.36 | 0.58 |
| 1:A:1332:A:H2' | 1:A:1333:A:C8 | 2.38 | 0.58 |
| 18:R:87:ARG:HG2 | 18:R:88:LYS:H | 1.67 | 0.58 |
| 1:A:437:U:HO2' | 4:D:123:HIS:HD1 | 1.50 | 0.58 |
| 2:B:121:LEU:O | 2:B:124:SER:OG | 2.21 | 0.58 |
| 2:B:170:GLU:O | 2:B:173:ALA:N | 2.37 | 0.58 |
| 6:F:33:TYR:HD2 | 6:F:71:ARG:HD2 | 1.68 | 0.58 |
| 17:Q:22:LEU:HD11 | 17:Q:39:SER:HB2 | 1.85 | 0.58 |
| 20:T:14:LYS:HA | 20:T:17:ARG:HG3 | 1.86 | 0.58 |
| 1:A:1003(A):G:N2 | 1:A:1038:C:O2 | 2.36 | 0.58 |
| 1:A:1234:C:H1' | 1:A:1364:U:O2 | 2.03 | 0.58 |
| 21:U:5:ASP:O | 21:U:11:GLY:HA3 | 2.02 | 0.58 |
| 2:B:158:LEU:H | 2:B:158:LEU:HD12 | 1.69 | 0.58 |
| 3:C:21:ARG:HH11 | 3:C:21:ARG:HG3 | 1.69 | 0.58 |
| 4:D:21:LEU:O | 4:D:113:SER:HB2 | 2.04 | 0.58 |
| 1:A:426:G:OP1 | 4:D:38:TYR:OH | 2.14 | 0.58 |
| 3:C:28:GLN:HB3 | 3:C:32:LEU:HD13 | 1.86 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:I:35:GLU:HA | 9:I:38:GLN:HB2 | 1.85 | 0.58 |
| 10:J:53:PRO:HA | 14:N:41:ARG:NH2 | 2.18 | 0.58 |
| 18:R:51:LEU:HD13 | 18:R:55:ARG:HE | 1.69 | 0.58 |
| 1:A:132:C:O3' | 20:T:74:LYS:NZ | 2.37 | 0.58 |
| 1:A:190(J):U:H2' | 1:A:190(K):G:C8 | 2.39 | 0.58 |
| 3:C:9:GLY:HA2 | 3:C:12:LEU:HD13 | 1.84 | 0.58 |
| 13:M:23:TYR:HB3 | 13:M:67:GLU:HA | 1.85 | 0.58 |
| 13:M:40:ASN:HB3 | 13:M:43:THR:HG23 | 1.86 | 0.58 |
| 1:A:390:C:H2' | 1:A:391:G:H8 | 1.65 | 0.57 |
| 1:A:811:C:H4' | 1:A:900:A:N6 | 2.19 | 0.57 |
| 1:A:1005:A:H3' | 1:A:1006:C:C6 | 2.39 | 0.57 |
| 6:F:100:ASN:ND2 | 18:R:23:LYS:O | 2.36 | 0.57 |
| 8:H:65:TYR:HA | 8:H:79:VAL:HG23 | 1.86 | 0.57 |
| 2:B:122:PHE:CD2 | 2:B:127:ILE:HG21 | 2.38 | 0.57 |
| 11:K:62:GLN:HG2 | 11:K:63:LEU:HD23 | 1.86 | 0.57 |
| 12:L:19:ARG:H | 12:L:19:ARG:CZ | 2.16 | 0.57 |
| 15:O:25:THR:HG21 | 15:O:70:LEU:HD23 | 1.87 | 0.57 |
| 19:S:12:ASP:O | 19:S:15:LEU:HD23 | 2.04 | 0.57 |
| 1:A:353:A:H5' | 1:A:353:A:H8 | 1.70 | 0.57 |
| 1:A:1310:G:OP2 | 13:M:88:ARG:NH2 | 2.24 | 0.57 |
| 1:A:1531:A:O5' | 1:A:1531:A:H8 | 1.87 | 0.57 |
| 4:D:78:LEU:HD21 | 4:D:96:LEU:HB3 | 1.86 | 0.57 |
| 9:I:102:LEU:H | 9:I:102:LEU:HD12 | 1.69 | 0.57 |
| 12:L:66:VAL:HG22 | 12:L:67:THR:N | 2.20 | 0.57 |
| 1:A:606:G:H1' | 1:A:632:A:H61 | 1.69 | 0.57 |
| 1:A:665:A:H3' | 1:A:725:G:N2 | 2.18 | 0.57 |
| 1:A:1412:C:H2' | 1:A:1413:A:C8 | 2.40 | 0.57 |
| 5:E:107:ARG:HG3 | 5:E:111:GLU:HG3 | 1.85 | 0.57 |
| 15:O:18:PHE:HB2 | 15:O:19:PRO:HD2 | 1.87 | 0.57 |
| 17:Q:83:ASP:OD2 | 17:Q:83:ASP:N | 2.36 | 0.57 |
| 1:A:509:A:C8 | 1:A:509:A:H3' | 2.40 | 0.57 |
| 1:A:1392:G:H21 | 1:A:1502:A:H8 | 1.50 | 0.57 |
| 8:H:82:HIS:NE2 | 8:H:84:ARG:HD2 | 2.19 | 0.57 |
| 9:I:106:ALA:O | 9:I:108:VAL:HG22 | 2.04 | 0.57 |
| 12:L:7:ILE:O | 12:L:10:LEU:N | 2.37 | 0.57 |
| 17:Q:74:LEU:HG | 17:Q:75:ARG:HG2 | 1.85 | 0.57 |
| 1:A:1314:C:H5 | 19:S:6:LYS:HZ2 | 1.52 | 0.57 |
| 2:B:33:TYR:CD2 | 2:B:43:ASP:HA | 2.40 | 0.57 |
| 2:B:97:TRP:HH2 | 2:B:176:GLU:CD | 2.07 | 0.57 |
| 3:C:17:ASP:OD1 | 3:C:18:TRP:N | 2.37 | 0.57 |
| 6:F:46:ARG:HB2 | 6:F:60:PHE:CE1 | 2.40 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:922:G:H4' | 5:E:20:GLN:HA | 1.87 | 0.57 |
| 2:B:7:VAL:N | 2:B:8:LYS:HD2 | 2.19 | 0.57 |
| 18:R:45:SER:OG | 18:R:46:GLU:N | 2.38 | 0.57 |
| 16:P:34:GLU:OE1 | 16:P:55:ARG:NH1 | 2.38 | 0.57 |
| 17:Q:10:VAL:HG23 | 17:Q:55:ASP:O | 2.05 | 0.57 |
| 1:A:517:G:N2 | 1:A:533:A:OP2 | 2.33 | 0.57 |
| 1:A:807:A:H2' | 1:A:808:C:C6 | 2.39 | 0.57 |
| 1:A:1118:C:H1' | 1:A:1179:A:C4 | 2.40 | 0.57 |
| 1:A:1226:C:H4' | 1:A:1227:A:OP1 | 2.05 | 0.57 |
| 1:A:201:C:H42 | 1:A:216:G:H1 | 1.53 | 0.56 |
| 1:A:527:7MG:H5'' | 1:A:527:7MG:C8 | 2.40 | 0.56 |
| 16:P:10:GLY:HA3 | 16:P:14:ASN:O | 2.05 | 0.56 |
| 1:A:1032:G:H2' | 1:A:1033:G:H5' | 1.86 | 0.56 |
| 1:A:1280:A:O2' | 1:A:1281:U:H5' | 2.05 | 0.56 |
| 4:D:52:SER:O | 4:D:56:VAL:HG23 | 2.04 | 0.56 |
| 10:J:5:ARG:O | 10:J:98:ILE:HA | 2.04 | 0.56 |
| 18:R:29:PHE:HZ | 18:R:43:PHE:HE1 | 1.52 | 0.56 |
| 1:A:922:G:H2' | 1:A:923:A:C8 | 2.39 | 0.56 |
| 1:A:1033:G:H2' | 1:A:1033:G:N3 | 2.20 | 0.56 |
| 1:A:1041:A:H2' | 1:A:1042:G:O4' | 2.05 | 0.56 |
| 2:B:21:ARG:HA | 2:B:39:ILE:HA | 1.86 | 0.56 |
| 2:B:80:ILE:O | 2:B:84:GLU:HB2 | 2.06 | 0.56 |
| 4:D:8:VAL:HG12 | 4:D:21:LEU:HD22 | 1.87 | 0.56 |
| 6:F:41:GLU:HB3 | 6:F:43:LEU:HD11 | 1.87 | 0.56 |
| 20:T:37:SER:HB3 | 20:T:84:LEU:HD13 | 1.87 | 0.56 |
| 2:B:84:GLU:OE1 | 2:B:87:ARG:NH2 | 2.37 | 0.56 |
| 4:D:176:LEU:HD12 | 4:D:177:ASP:N | 2.20 | 0.56 |
| 6:F:47:ARG:NH1 | 6:F:48:LEU:O | 2.37 | 0.56 |
| 7:G:73:MET:HG3 | 7:G:90:GLU:HA | 1.86 | 0.56 |
| 1:A:269:C:H2' | 1:A:270:A:C8 | 2.40 | 0.56 |
| 1:A:485:G:O2' | 1:A:486:U:P | 2.63 | 0.56 |
| 1:A:693:G:H2' | 1:A:694:A:C8 | 2.41 | 0.56 |
| 1:A:838:G:H1 | 1:A:848:C:H42 | 1.54 | 0.56 |
| 9:I:50:LEU:HD23 | 9:I:55:ALA:HB3 | 1.87 | 0.56 |
| 9:I:79:LEU:O | 9:I:83:ARG:HG2 | 2.06 | 0.56 |
| 6:F:80:ARG:NE | 6:F:88:VAL:HB | 2.20 | 0.56 |
| 1:A:129:U:O3' | 1:A:129(A):G:H3' | 2.05 | 0.56 |
| 1:A:676:A:H1' | 11:K:115:PRO:HB3 | 1.88 | 0.56 |
| 2:B:208:ILE:H | 2:B:208:ILE:HD12 | 1.71 | 0.56 |
| 1:A:277:C:H5' | 17:Q:68:ARG:NH1 | 2.21 | 0.56 |
| 5:E:138:ALA:O | 5:E:141:GLN:HB2 | 2.06 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:F:75:LEU:HD13 | 6:F:79:LEU:HD11 | 1.86 | 0.56 |
| 15:O:33:THR:OG1 | 15:O:63:ARG:NH1 | 2.39 | 0.56 |
| 16:P:74:LEU:O | 16:P:77:ALA:HB3 | 2.06 | 0.56 |
| 17:Q:19:VAL:HG22 | 17:Q:44:ALA:HB3 | 1.85 | 0.56 |
| 1:A:40:C:H2' | 1:A:41:G:O4' | 2.06 | 0.56 |
| 1:A:254:G:H2' | 1:A:255:G:C8 | 2.36 | 0.56 |
| 1:A:691:G:H2' | 1:A:692:U:H6 | 1.71 | 0.56 |
| 1:A:841:U:C6 | 1:A:848:C:H5' | 2.41 | 0.56 |
| 12:L:27:LEU:C | 12:L:29:GLY:H | 2.04 | 0.56 |
| 2:B:118:LEU:O | 2:B:121:LEU:HB3 | 2.06 | 0.56 |
| 16:P:58:TYR:O | 16:P:62:VAL:HG13 | 2.06 | 0.56 |
| 20:T:74:LYS:HB2 | 20:T:76:ALA:H | 1.69 | 0.56 |
| 1:A:496:A:H4' | 1:A:497:A:H5' | 1.87 | 0.55 |
| 1:A:680:C:H42 | 1:A:710:G:H1 | 1.55 | 0.55 |
| 2:B:22:LYS:HE2 | 2:B:40:HIS:HE1 | 1.71 | 0.55 |
| 4:D:82:ALA:HB1 | 4:D:92:VAL:HG13 | 1.87 | 0.55 |
| 15:O:50:HIS:O | 15:O:53:HIS:HB3 | 2.06 | 0.55 |
| 1:A:141:A:H1' | 1:A:182:U:O2 | 2.06 | 0.55 |
| 1:A:975:A:H5' | 1:A:975:A:H8 | 1.71 | 0.55 |
| 1:A:1030(A):G:H2' | 1:A:1030(B):C:H5'' | 1.89 | 0.55 |
| 1:A:1414:U:H2' | 1:A:1415:G:C8 | 2.41 | 0.55 |
| 1:A:1501:C:N4 | 1:A:1504:G:C2 | 2.73 | 0.55 |
| 2:B:9:GLU:HG2 | 2:B:10:LEU:H | 1.70 | 0.55 |
| 2:B:82:ARG:NH2 | 2:B:86:GLU:OE2 | 2.39 | 0.55 |
| 4:D:159:ARG:O | 4:D:163:GLU:HB2 | 2.06 | 0.55 |
| 18:R:36:ASN:OD1 | 18:R:39:VAL:HG12 | 2.06 | 0.55 |
| 18:R:52:PRO:HG3 | 18:R:54:ARG:NH2 | 2.20 | 0.55 |
| 1:A:553:A:O2' | 12:L:29:GLY:O | 2.23 | 0.55 |
| 1:A:1060:C:H5'' | 10:J:51:ARG:HG2 | 1.88 | 0.55 |
| 7:G:79:ARG:HA | 7:G:84:ASN:HB3 | 1.88 | 0.55 |
| 1:A:922:G:H1 | 1:A:1395:C:H42 | 1.53 | 0.55 |
| 3:C:77:ILE:HD11 | 3:C:103:VAL:HG21 | 1.88 | 0.55 |
| 10:J:49:VAL:HG13 | 14:N:41:ARG:HG3 | 1.88 | 0.55 |
| 16:P:59:TRP:HB3 | 16:P:64:ALA:HB2 | 1.89 | 0.55 |
| 1:A:1211:U:O2' | 1:A:1213:A:N3 | 2.34 | 0.55 |
| 3:C:36:ASP:HA | 3:C:39:ILE:HD12 | 1.88 | 0.55 |
| 9:I:79:LEU:HD22 | 9:I:83:ARG:NE | 2.22 | 0.55 |
| 1:A:1118:C:OP1 | 9:I:9:ARG:HD2 | 2.06 | 0.55 |
| 12:L:75:HIS:HA | 12:L:102:ARG:HH22 | 1.72 | 0.55 |
| 18:R:51:LEU:HD22 | 18:R:52:PRO:HD2 | 1.88 | 0.55 |
| 18:R:85:LEU:HD11 | 18:R:88:LYS:HG2 | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 19:S:7:LYS:HE2 | 19:S:7:LYS:O | 2.06 | 0.55 |
| 19:S:31:ILE:HA | 19:S:32:LYS:HZ3 | 1.70 | 0.55 |
| 1:A:1040:U:O4 | 1:A:1041:A:N6 | 2.40 | 0.55 |
| 1:A:1194:U:H4' | 5:E:22:GLY:HA2 | 1.89 | 0.55 |
| 6:F:75:LEU:O | 6:F:79:LEU:HG | 2.06 | 0.55 |
| 1:A:106:C:O2' | 1:A:107:G:H5' | 2.07 | 0.55 |
| 1:A:1275:A:H2' | 1:A:1276:G:O4' | 2.07 | 0.55 |
| 1:A:1287:A:H2' | 1:A:1288:A:C8 | 2.42 | 0.55 |
| 4:D:12:CYS:HA | 4:D:19:LEU:HG | 1.89 | 0.55 |
| 4:D:174:LEU:HD23 | 4:D:185:PHE:HA | 1.89 | 0.55 |
| 5:E:20:GLN:OE1 | 5:E:25:ARG:NH2 | 2.28 | 0.55 |
| 5:E:27:ARG:NH1 | 5:E:27:ARG:HB2 | 2.22 | 0.55 |
| 1:A:20:U:H1' | 1:A:916:G:N2 | 2.22 | 0.55 |
| 1:A:706:A:H1' | 11:K:29:ILE:HD11 | 1.89 | 0.55 |
| 1:A:1089:G:C5 | 1:A:1090:U:C5 | 2.95 | 0.55 |
| 1:A:1322:C:H4' | 1:A:1323:G:OP1 | 2.06 | 0.55 |
| 3:C:95:THR:C | 3:C:97:LYS:H | 2.10 | 0.55 |
| 4:D:4:TYR:OH | 4:D:7:PRO:O | 2.21 | 0.55 |
| 7:G:26:PHE:HA | 7:G:101:LEU:HD23 | 1.89 | 0.55 |
| 9:I:28:VAL:HG12 | 9:I:29:ASN:HD22 | 1.72 | 0.55 |
| 1:A:881:G:P | 12:L:12:ARG:HH22 | 2.30 | 0.54 |
| 1:A:976:G:OP2 | 1:A:1358:U:O2' | 2.24 | 0.54 |
| 15:O:15:PHE:HE2 | 15:O:84:LYS:HG2 | 1.72 | 0.54 |
| 15:O:15:PHE:HD1 | 15:O:30:ALA:HB2 | 1.72 | 0.54 |
| 1:A:325:A:H2' | 1:A:326:G:O4' | 2.07 | 0.54 |
| 1:A:563:A:H2' | 1:A:567:G:C8 | 2.42 | 0.54 |
| 4:D:70:ILE:HG22 | 4:D:71:SER:N | 2.21 | 0.54 |
| 12:L:28:LYS:HD2 | 12:L:33:ARG:CZ | 2.37 | 0.54 |
| 12:L:93:LEU:HB3 | 12:L:96:VAL:HG21 | 1.88 | 0.54 |
| 21:U:5:ASP:HB3 | 21:U:8:THR:HG23 | 1.90 | 0.54 |
| 1:A:1443:G:C4' | 1:A:1446:A:H5' | 2.34 | 0.54 |
| 4:D:100:ARG:HD2 | 4:D:137:SER:HA | 1.90 | 0.54 |
| 1:A:299:G:C6 | 1:A:300:A:C6 | 2.96 | 0.54 |
| 4:D:70:ILE:HG22 | 4:D:71:SER:H | 1.72 | 0.54 |
| 2:B:79:ASP:OD2 | 2:B:79:ASP:N | 2.31 | 0.54 |
| 4:D:187:ARG:NH2 | 4:D:188:LEU:HD12 | 2.15 | 0.54 |
| 4:D:196:LEU:HD23 | 4:D:196:LEU:N | 2.22 | 0.54 |
| 7:G:139:GLU:HG3 | 7:G:143:ARG:HH22 | 1.71 | 0.54 |
| 9:I:96:LEU:HG | 9:I:101:PHE:HD1 | 1.72 | 0.54 |
| 19:S:40:ILE:HB | 19:S:67:VAL:O | 2.08 | 0.54 |
| 1:A:375:U:C2 | 1:A:376:G:C8 | 2.96 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:668:G:O4' | 15:O:49:ASP:HB2 | 2.08 | 0.54 |
| 1:A:1499:A:H1' | 1:A:1520[B]:G:OP1 | 2.07 | 0.54 |
| 2:B:71:VAL:O | 2:B:164:VAL:HA | 2.06 | 0.54 |
| 5:E:93:PRO:HG2 | 8:H:105:ARG:NH1 | 2.22 | 0.54 |
| 10:J:4:ILE:HB | 10:J:74:ILE:HD11 | 1.90 | 0.54 |
| 1:A:560:U:H4' | 1:A:561:U:H5'' | 1.88 | 0.54 |
| 1:A:1286:A:H2' | 1:A:1287:A:H4' | 1.88 | 0.54 |
| 12:L:76:ASN:OD1 | 12:L:108:ALA:N | 2.38 | 0.54 |
| 13:M:11:ARG:HA | 13:M:45:VAL:HG11 | 1.90 | 0.54 |
| 1:A:216:G:O2' | 1:A:217:C:O5' | 2.26 | 0.54 |
| 1:A:292:G:N2 | 1:A:309:G:C4 | 2.76 | 0.54 |
| 1:A:620:C:H2' | 1:A:621:A:O4' | 2.08 | 0.54 |
| 1:A:986:A:C2 | 1:A:1220:G:C2 | 2.96 | 0.54 |
| 2:B:19:HIS:NE2 | 2:B:206:ASP:HB2 | 2.22 | 0.54 |
| 16:P:6:LEU:HD23 | 16:P:17:TYR:CG | 2.42 | 0.54 |
| 1:A:81:U:H2' | 1:A:82:U:H5'' | 1.89 | 0.54 |
| 1:A:691:G:O2' | 1:A:797:C:H4' | 2.08 | 0.54 |
| 1:A:1016:A:H2' | 1:A:1017:G:O4' | 2.07 | 0.54 |
| 1:A:1496:C:O2 | 1:A:1517[A]:G:N2 | 2.41 | 0.54 |
| 3:C:156:ARG:H | 3:C:163:ALA:HA | 1.73 | 0.54 |
| 7:G:109:ASN:OD1 | 7:G:119:ARG:NH2 | 2.40 | 0.54 |
| 13:M:91:ARG:NH2 | 13:M:103:THR:HG21 | 2.23 | 0.54 |
| 21:U:6:ARG:HG2 | 21:U:15:ARG:HH21 | 1.73 | 0.54 |
| 1:A:182:U:H6 | 1:A:182:U:H5' | 1.72 | 0.53 |
| 1:A:950:U:H2' | 1:A:951:G:C8 | 2.43 | 0.53 |
| 7:G:50:ILE:HD11 | 7:G:124:LEU:HD11 | 1.89 | 0.53 |
| 10:J:84:GLN:HA | 10:J:84:GLN:HE21 | 1.73 | 0.53 |
| 1:A:356:A:H2' | 1:A:357:G:O4' | 2.09 | 0.53 |
| 3:C:73:PRO:O | 3:C:77:ILE:HG12 | 2.08 | 0.53 |
| 5:E:137:GLU:O | 5:E:141:GLN:HG2 | 2.08 | 0.53 |
| 1:A:1465:C:H2' | 1:A:1466:C:O4' | 2.08 | 0.53 |
| 3:C:68:VAL:HG12 | 3:C:70:VAL:HG22 | 1.91 | 0.53 |
| 5:E:15:ARG:HH11 | 5:E:15:ARG:HG3 | 1.72 | 0.53 |
| 10:J:76:ASN:N | 10:J:77:PRO:HD3 | 2.22 | 0.53 |
| 11:K:85:ARG:NE | 11:K:111:ASP:HB3 | 2.21 | 0.53 |
| 12:L:90:VAL:HG23 | 12:L:93:LEU:HB2 | 1.90 | 0.53 |
| 13:M:2:ALA:O | 13:M:10:PRO:HD2 | 2.09 | 0.53 |
| 13:M:2:ALA:N | 13:M:9:ILE:HG23 | 2.23 | 0.53 |
| 1:A:1095:U:N3 | 1:A:1096:C:C4 | 2.77 | 0.53 |
| 1:A:1361:G:H2' | 1:A:1361(A):C:C6 | 2.43 | 0.53 |
| 12:L:28:LYS:HB2 | 12:L:33:ARG:HE | 1.74 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:547:A:OP2 | 4:D:2:GLY:N | 2.42 | 0.53 |
| 1:A:1190:G:H5' | 3:C:176:HIS:NE2 | 2.24 | 0.53 |
| 1:A:1202:G:N2 | 14:N:43:CYS:SG | 2.81 | 0.53 |
| 1:A:1425:U:H2' | 1:A:1426:C:H6 | 1.74 | 0.53 |
| 4:D:36:ARG:HD2 | 4:D:38:TYR:HE2 | 1.71 | 0.53 |
| 4:D:152:SER:O | 4:D:152:SER:OG | 2.25 | 0.53 |
| 7:G:113:GLU:CG | 7:G:119:ARG:HG2 | 2.38 | 0.53 |
| 12:L:84:LEU:HD23 | 12:L:101:VAL:HG21 | 1.90 | 0.53 |
| 1:A:44:G:H5'' | 1:A:44:G:H8 | 1.73 | 0.53 |
| 1:A:147:G:C2 | 1:A:148:G:C8 | 2.96 | 0.53 |
| 1:A:1502:A:H2 | 1:A:1505:G:H1 | 1.57 | 0.53 |
| 8:H:23:SER:HA | 8:H:63:LEU:HD13 | 1.89 | 0.53 |
| 9:I:71:SER:O | 9:I:74:ILE:HB | 2.08 | 0.53 |
| 10:J:79:ARG:O | 10:J:82:ILE:N | 2.42 | 0.53 |
| 18:R:51:LEU:HD11 | 18:R:55:ARG:HH21 | 1.74 | 0.53 |
| 20:T:33:ILE:HD11 | 20:T:63:ILE:HA | 1.91 | 0.53 |
| 1:A:258:G:H2' | 1:A:259:G:H8 | 1.73 | 0.53 |
| 1:A:514:C:H2' | 1:A:515:G:C8 | 2.42 | 0.53 |
| 1:A:1119:C:H42 | 1:A:1154:G:H1 | 1.55 | 0.53 |
| 1:A:1163:C:H2' | 1:A:1164:G:O4' | 2.09 | 0.53 |
| 4:D:127:THR:HG21 | 4:D:150:GLU:OE1 | 2.08 | 0.53 |
| 5:E:27:ARG:HB2 | 5:E:27:ARG:HH11 | 1.74 | 0.53 |
| 5:E:43:LEU:HB2 | 5:E:136:MET:HG3 | 1.91 | 0.53 |
| 16:P:6:LEU:HB3 | 16:P:17:TYR:CD2 | 2.44 | 0.53 |
| 1:A:658:G:H2' | 1:A:659:U:O4' | 2.08 | 0.53 |
| 1:A:734:G:N2 | 18:R:75:ILE:HD11 | 2.23 | 0.53 |
| 1:A:770:C:O2' | 1:A:899:C:N3 | 2.39 | 0.53 |
| 1:A:965:A:C2 | 1:A:969:A:C2 | 2.96 | 0.53 |
| 2:B:84:GLU:O | 2:B:219:VAL:HG21 | 2.09 | 0.53 |
| 13:M:62:ASN:OD1 | 13:M:62:ASN:N | 2.41 | 0.53 |
| 1:A:130:A:H1' | 1:A:263:A:O2' | 2.09 | 0.53 |
| 1:A:375:U:H2' | 1:A:376:G:H8 | 1.74 | 0.53 |
| 1:A:671:G:C2 | 1:A:672:U:H1' | 2.44 | 0.53 |
| 1:A:778:G:H8 | 1:A:778:G:O5' | 1.91 | 0.53 |
| 5:E:40:ARG:HH21 | 5:E:66:MET:HG3 | 1.73 | 0.53 |
| 5:E:144:THR:HB | 5:E:147:ASP:H | 1.74 | 0.53 |
| 9:I:17:VAL:HG21 | 9:I:80:GLY:HA3 | 1.91 | 0.53 |
| 12:L:25:PRO:C | 12:L:27:LEU:N | 2.61 | 0.53 |
| 20:T:20:LEU:HD22 | 20:T:20:LEU:H | 1.73 | 0.53 |
| 1:A:276:G:O2' | 17:Q:68:ARG:NH1 | 2.42 | 0.53 |
| 1:A:1241:G:H2' | 1:A:1242:C:H6 | 1.73 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:103:GLY:O | 5:E:106:PRO:HD2 | 2.09 | 0.53 |
| 1:A:123:C:OP1 | 1:A:311:C:O2' | 2.25 | 0.52 |
| 1:A:569:C:H42 | 1:A:881:G:H1 | 1.55 | 0.52 |
| 4:D:187:ARG:HH22 | 4:D:188:LEU:CD1 | 2.17 | 0.52 |
| 5:E:150:ARG:NH1 | 5:E:150:ARG:HB2 | 2.25 | 0.52 |
| 6:F:30:LEU:HD23 | 6:F:35:ALA:HB3 | 1.90 | 0.52 |
| 12:L:84:LEU:HB3 | 12:L:101:VAL:CG2 | 2.39 | 0.52 |
| 13:M:108:ARG:O | 13:M:111:LYS:N | 2.42 | 0.52 |
| 1:A:414:A:H3' | 24:A:1969:HOH:O | 2.10 | 0.52 |
| 1:A:881:G:H2' | 1:A:882:C:O4' | 2.09 | 0.52 |
| 1:A:975:A:H5' | 1:A:975:A:C8 | 2.43 | 0.52 |
| 1:A:1144:G:H2' | 1:A:1145:C:C6 | 2.44 | 0.52 |
| 5:E:144:THR:HG22 | 5:E:146:ALA:H | 1.74 | 0.52 |
| 9:I:48:GLU:N | 9:I:49:PRO:HD2 | 2.24 | 0.52 |
| 10:J:34:VAL:HG13 | 10:J:74:ILE:HG22 | 1.90 | 0.52 |
| 20:T:53:LEU:HD12 | 20:T:101:GLY:H | 1.74 | 0.52 |
| 1:A:1491:G:C6 | 1:A:1493:A:C2 | 2.98 | 0.52 |
| 7:G:99:LEU:O | 7:G:103:TRP:HB2 | 2.10 | 0.52 |
| 10:J:65:LEU:HD12 | 14:N:56:VAL:HG22 | 1.91 | 0.52 |
| 17:Q:97:SER:O | 17:Q:98:LEU:HD12 | 2.09 | 0.52 |
| 1:A:254:G:OP1 | 17:Q:67:LYS:O | 2.27 | 0.52 |
| 2:B:60:ASP:O | 2:B:64:ARG:HG3 | 2.10 | 0.52 |
| 21:U:10:ARG:HA | 21:U:13:ILE:HD12 | 1.92 | 0.52 |
| 1:A:279:A:OP2 | 17:Q:95:TYR:OH | 2.17 | 0.52 |
| 1:A:946:A:H2' | 1:A:947:G:C8 | 2.45 | 0.52 |
| 1:A:1031:G:O2' | 1:A:1032:G:N2 | 2.43 | 0.52 |
| 1:A:1476:G:C2' | 1:A:1477:C:H5' | 2.39 | 0.52 |
| 2:B:93:VAL:HG21 | 2:B:97:TRP:CD1 | 2.44 | 0.52 |
| 4:D:142:PRO:HA | 4:D:185:PHE:HD2 | 1.74 | 0.52 |
| 9:I:18:PHE:HB3 | 9:I:20:ARG:HH12 | 1.74 | 0.52 |
| 1:A:926:G:C6 | 1:A:1505:G:C6 | 2.97 | 0.52 |
| 1:A:1148:U:H2' | 1:A:1149:C:O4' | 2.10 | 0.52 |
| 1:A:1313:U:H5 | 19:S:4:SER:HB2 | 1.74 | 0.52 |
| 2:B:47:THR:O | 2:B:51:LEU:HB2 | 2.10 | 0.52 |
| 6:F:47:ARG:CZ | 6:F:47:ARG:HB2 | 2.33 | 0.52 |
| 16:P:58:TYR:CZ | 16:P:62:VAL:HG11 | 2.45 | 0.52 |
| 1:A:78:G:C2 | 1:A:79:G:C8 | 2.97 | 0.52 |
| 1:A:474:G:O2' | 1:A:475:G:H5' | 2.09 | 0.52 |
| 1:A:562:C:H4' | 1:A:563:A:C5' | 2.40 | 0.52 |
| 1:A:877:C:O2 | 8:H:3:THR:HG21 | 2.09 | 0.52 |
| 17:Q:34:LYS:HG2 | 17:Q:35:VAL:H | 1.74 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 18:R:58:LEU:HB3 | 18:R:62:GLU:HB3 | 1.91 | 0.52 |
| 1:A:164:U:H2' | 1:A:165:C:C6 | 2.44 | 0.52 |
| 1:A:563:A:H5' | 1:A:564:C:OP1 | 2.09 | 0.52 |
| 1:A:1313:U:OP2 | 19:S:6:LYS:HA | 2.09 | 0.52 |
| 1:A:1451:A:H5'' | 1:A:1452:C:C5 | 2.45 | 0.52 |
| 1:A:1483:A:H2' | 1:A:1483:A:N3 | 2.23 | 0.52 |
| 1:A:1518[B]:MA6:O2' | 1:A:1519[B]:MA6:OP1 | 2.27 | 0.52 |
| 5:E:40:ARG:HE | 5:E:66:MET:HE2 | 1.75 | 0.52 |
| 7:G:41:ARG:HB2 | 7:G:41:ARG:HH11 | 1.74 | 0.52 |
| 12:L:6:THR:HG23 | 12:L:9:GLN:OE1 | 2.09 | 0.52 |
| 15:O:72:ARG:NH1 | 15:O:72:ARG:HB3 | 2.25 | 0.52 |
| 1:A:143:A:O3' | 1:A:144:G:H8 | 1.93 | 0.52 |
| 1:A:924:C:O2' | 1:A:1502:A:N6 | 2.43 | 0.52 |
| 1:A:1124:G:OP1 | 10:J:33:GLN:NE2 | 2.43 | 0.52 |
| 1:A:1192:C:OP2 | 3:C:4:LYS:NZ | 2.42 | 0.52 |
| 1:A:1234:C:H2' | 1:A:1235:U:H6 | 1.74 | 0.52 |
| 1:A:1324:A:H2' | 1:A:1325:C:O4' | 2.09 | 0.52 |
| 2:B:189:ASP:HB2 | 2:B:205:ASP:H | 1.75 | 0.52 |
| 14:N:33:VAL:HA | 14:N:39:LEU:O | 2.10 | 0.52 |
| 1:A:474:G:OP2 | 16:P:75:ARG:HD2 | 2.10 | 0.52 |
| 1:A:1277:C:H3' | 1:A:1277:C:C6 | 2.44 | 0.52 |
| 1:A:1342:C:H2' | 1:A:1343:G:H8 | 1.75 | 0.52 |
| 5:E:43:LEU:O | 5:E:62:ALA:HA | 2.10 | 0.52 |
| 7:G:99:LEU:HD22 | 7:G:103:TRP:CH2 | 2.45 | 0.52 |
| 14:N:26:ARG:HH22 | 14:N:47:LEU:HD13 | 1.74 | 0.52 |
| 18:R:36:ASN:O | 18:R:40:LEU:HG | 2.10 | 0.52 |
| 19:S:18:LYS:O | 19:S:22:LEU:HG | 2.10 | 0.52 |
| 1:A:17:U:H2' | 1:A:18:C:H6 | 1.73 | 0.51 |
| 1:A:924:C:O2' | 1:A:925:G:H5' | 2.09 | 0.51 |
| 5:E:78:HIS:HB2 | 8:H:104:ARG:HG2 | 1.91 | 0.51 |
| 6:F:69:GLU:O | 6:F:72:VAL:HG23 | 2.10 | 0.51 |
| 12:L:25:PRO:HB2 | 12:L:64:TYR:CE2 | 2.45 | 0.51 |
| 1:A:279:A:C6 | 17:Q:98:LEU:HD13 | 2.45 | 0.51 |
| 1:A:671:G:N2 | 1:A:672:U:H1' | 2.25 | 0.51 |
| 1:A:814:A:N7 | 1:A:816:A:C4 | 2.79 | 0.51 |
| 1:A:830:G:C6 | 1:A:831:U:C4 | 2.98 | 0.51 |
| 1:A:1023:G:H3' | 1:A:1024:G:H5'' | 1.91 | 0.51 |
| 1:A:1134:G:H1 | 1:A:1140:C:H42 | 1.57 | 0.51 |
| 1:A:1321:C:C5' | 1:A:1322:C:H5'' | 2.39 | 0.51 |
| 2:B:97:TRP:CH2 | 2:B:173:ALA:HA | 2.46 | 0.51 |
| 10:J:85:LEU:HA | 10:J:88:LEU:HD11 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 11:K:57:THR:HB | 11:K:60:ALA:H | 1.76 | 0.51 |
| 14:N:14:PRO:O | 14:N:15:LYS:HB3 | 2.09 | 0.51 |
| 19:S:31:ILE:HG22 | 19:S:49:ILE:HA | 1.92 | 0.51 |
| 1:A:39:G:O2' | 1:A:40:C:H5' | 2.10 | 0.51 |
| 1:A:168:G:C2 | 1:A:169:C:C5 | 2.98 | 0.51 |
| 1:A:547:A:H4' | 1:A:548:G:O5' | 2.09 | 0.51 |
| 1:A:667:G:C2 | 1:A:740:U:O2 | 2.63 | 0.51 |
| 1:A:839:U:O2 | 1:A:839:U:H3' | 2.11 | 0.51 |
| 1:A:1005:A:H1' | 1:A:1026:G:H1 | 1.75 | 0.51 |
| 2:B:105:PHE:CE1 | 2:B:109:SER:HB3 | 2.45 | 0.51 |
| 1:A:181:G:H4' | 1:A:182:U:C5' | 2.41 | 0.51 |
| 1:A:1323:G:H2' | 1:A:1324:A:C8 | 2.45 | 0.51 |
| 1:A:1366:C:O3' | 10:J:60:ARG:NH2 | 2.42 | 0.51 |
| 1:A:1403:C:C2 | 1:A:1404:5MC:HM52 | 2.45 | 0.51 |
| 12:L:110:VAL:O | 12:L:122:THR:HG21 | 2.11 | 0.51 |
| 19:S:11:VAL:HG12 | 19:S:15:LEU:HD21 | 1.92 | 0.51 |
| 20:T:43:LEU:HA | 20:T:46:GLU:HB2 | 1.93 | 0.51 |
| 1:A:734:G:H21 | 18:R:75:ILE:HD11 | 1.76 | 0.51 |
| 1:A:951:G:OP2 | 13:M:102:ARG:NH2 | 2.44 | 0.51 |
| 1:A:956:U:H2' | 1:A:957:U:O4' | 2.11 | 0.51 |
| 1:A:1169:A:C5 | 1:A:1171:G:H1' | 2.45 | 0.51 |
| 1:A:1216:G:H5'' | 14:N:5:ALA:CB | 2.40 | 0.51 |
| 1:A:1493:A:HO2' | 1:A:1494:G:H8 | 1.58 | 0.51 |
| 8:H:86:ILE:HG22 | 8:H:93:VAL:HG21 | 1.92 | 0.51 |
| 13:M:10:PRO:O | 13:M:45:VAL:HG21 | 2.11 | 0.51 |
| 18:R:47:THR:HB | 18:R:83:GLU:O | 2.10 | 0.51 |
| 1:A:708:C:H2' | 1:A:709:G:H8 | 1.76 | 0.51 |
| 1:A:781:A:H2' | 1:A:782:A:H5' | 1.92 | 0.51 |
| 10:J:50:ILE:HD12 | 10:J:50:ILE:H | 1.76 | 0.51 |
| 10:J:55:LYS:HG2 | 10:J:56:HIS:N | 2.22 | 0.51 |
| 18:R:61:LYS:O | 18:R:65:ILE:HG12 | 2.09 | 0.51 |
| 19:S:50:ALA:HB1 | 19:S:57:HIS:HB3 | 1.92 | 0.51 |
| 20:T:43:LEU:HB2 | 20:T:52:ALA:HB2 | 1.93 | 0.51 |
| 1:A:8:A:N6 | 4:D:209:ARG:HB2 | 2.26 | 0.51 |
| 1:A:143:A:H2 | 1:A:220:G:H22 | 1.58 | 0.51 |
| 1:A:825:G:H21 | 8:H:11:THR:HG21 | 1.76 | 0.51 |
| 2:B:22:LYS:HE2 | 2:B:40:HIS:CE1 | 2.46 | 0.51 |
| 2:B:160:ASP:OD2 | 2:B:160:ASP:N | 2.37 | 0.51 |
| 4:D:145:GLU:OE2 | 4:D:182:LYS:NZ | 2.43 | 0.51 |
| 1:A:546:G:P | 4:D:72:GLU:HB3 | 2.51 | 0.51 |
| 1:A:710:G:H2' | 1:A:711:G:H8 | 1.75 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:860:A:H2' | 1:A:861:G:O4' | 2.10 | 0.51 |
| 1:A:1057:G:H5'' | 3:C:154:SER:HB2 | 1.93 | 0.51 |
| 1:A:1403:C:O2 | 1:A:1403:C:H2' | 2.11 | 0.51 |
| 2:B:53:ARG:HG3 | 2:B:54:THR:N | 2.25 | 0.51 |
| 4:D:57:ARG:HB3 | 4:D:206:PHE:HB2 | 1.91 | 0.51 |
| 5:E:131:ILE:O | 5:E:134:ALA:HB3 | 2.11 | 0.51 |
| 8:H:73:ASP:OD2 | 8:H:75:ARG:HG3 | 2.11 | 0.51 |
| 1:A:439:A:C4 | 1:A:497:A:C2 | 2.99 | 0.51 |
| 2:B:17:PHE:CD1 | 2:B:18:GLY:N | 2.77 | 0.51 |
| 3:C:159:GLY:HA2 | 3:C:193:TYR:CD1 | 2.46 | 0.51 |
| 17:Q:89:LEU:O | 17:Q:93:GLN:HG3 | 2.11 | 0.51 |
| 1:A:748:C:H6 | 1:A:748:C:O5' | 1.93 | 0.51 |
| 1:A:858:G:O6 | 1:A:869:G:H3' | 2.10 | 0.51 |
| 1:A:1064:G:H1' | 1:A:1190:G:N2 | 2.25 | 0.51 |
| 1:A:1070:U:H2' | 1:A:1071:C:C6 | 2.46 | 0.51 |
| 1:A:1313:U:C5 | 19:S:4:SER:HB2 | 2.46 | 0.51 |
| 4:D:156:GLU:O | 4:D:160:GLN:HG3 | 2.10 | 0.51 |
| 5:E:101:ILE:O | 5:E:120:THR:HB | 2.11 | 0.51 |
| 10:J:19:SER:HB2 | 10:J:91:PRO:HG2 | 1.93 | 0.51 |
| 16:P:48:TRP:N | 16:P:48:TRP:CD1 | 2.79 | 0.51 |
| 20:T:93:GLU:N | 20:T:93:GLU:OE2 | 2.44 | 0.51 |
| 1:A:1238:A:OP2 | 1:A:1335:C:O2 | 2.29 | 0.50 |
| 1:A:1299:A:C8 | 1:A:1301:U:H1' | 2.46 | 0.50 |
| 1:A:1372:U:OP2 | 9:I:11:LYS:NZ | 2.35 | 0.50 |
| 2:B:105:PHE:O | 2:B:108:ILE:N | 2.44 | 0.50 |
| 8:H:27:PRO:HG3 | 8:H:58:TYR:CE2 | 2.46 | 0.50 |
| 1:A:1133:G:H1 | 1:A:1141:C:H42 | 1.59 | 0.50 |
| 1:A:1189:C:H5' | 14:N:58:LYS:HZ1 | 1.77 | 0.50 |
| 3:C:130:VAL:HG11 | 3:C:153:VAL:HG11 | 1.93 | 0.50 |
| 12:L:113:ARG:HH11 | 12:L:116:SER:H | 1.58 | 0.50 |
| 19:S:41:VAL:HG23 | 19:S:43:GLU:HG2 | 1.92 | 0.50 |
| 1:A:116:A:O5' | 1:A:116:A:H8 | 1.94 | 0.50 |
| 1:A:235:C:O2' | 1:A:236:G:H5' | 2.11 | 0.50 |
| 1:A:1029:C:N3 | 1:A:1030:C:N4 | 2.55 | 0.50 |
| 1:A:1122:U:O2' | 1:A:1123:A:H5' | 2.11 | 0.50 |
| 1:A:1223:C:H3' | 1:A:1224:G:H5'' | 1.92 | 0.50 |
| 3:C:150:LYS:HA | 3:C:169:ALA:HA | 1.94 | 0.50 |
| 10:J:16:LEU:HD22 | 10:J:94:VAL:HG23 | 1.93 | 0.50 |
| 13:M:14:ARG:HB2 | 13:M:17:VAL:HG22 | 1.92 | 0.50 |
| 1:A:836:G:C6 | 1:A:851:G:C6 | 3.00 | 0.50 |
| 1:A:1001:A:H61 | 1:A:1039:C:N4 | 2.06 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1238:A:N7 | 1:A:1303:C:H1' | 2.26 | 0.50 |
| 1:A:1426:C:H2' | 1:A:1427:U:C6 | 2.46 | 0.50 |
| 4:D:12:CYS:SG | 4:D:21:LEU:HD11 | 2.51 | 0.50 |
| 8:H:51:VAL:HG22 | 8:H:52:ASP:H | 1.76 | 0.50 |
| 19:S:31:ILE:HG21 | 19:S:49:ILE:HD12 | 1.93 | 0.50 |
| 1:A:512:U:H2' | 1:A:513:C:H6 | 1.76 | 0.50 |
| 1:A:665:A:H1' | 1:A:733:A:O4' | 2.12 | 0.50 |
| 1:A:811:C:H4' | 1:A:900:A:H61 | 1.76 | 0.50 |
| 1:A:1194:U:H2' | 1:A:1195:C:C6 | 2.46 | 0.50 |
| 1:A:1504:G:H4' | 1:A:1505:G:O5' | 2.11 | 0.50 |
| 3:C:7:PRO:O | 3:C:11:ARG:HD2 | 2.11 | 0.50 |
| 3:C:85:ARG:HH11 | 3:C:86:VAL:HG23 | 1.77 | 0.50 |
| 3:C:139:GLN:HG3 | 3:C:143:GLU:OE1 | 2.10 | 0.50 |
| 11:K:11:LYS:HB2 | 11:K:11:LYS:NZ | 2.27 | 0.50 |
| 16:P:9:PHE:HD1 | 16:P:18:ARG:HD2 | 1.72 | 0.50 |
| 18:R:19:LYS:O | 18:R:21:LYS:NZ | 2.45 | 0.50 |
| 1:A:774:G:C4 | 1:A:775:G:C8 | 2.99 | 0.50 |
| 1:A:804:U:H5'' | 1:A:805:C:OP2 | 2.11 | 0.50 |
| 1:A:1221:G:H4' | 19:S:77:THR:HG21 | 1.93 | 0.50 |
| 3:C:184:TYR:OH | 3:C:199:LYS:HD3 | 2.11 | 0.50 |
| 16:P:51:VAL:HG11 | 16:P:77:ALA:HB1 | 1.93 | 0.50 |
| 1:A:134:A:H2' | 1:A:135:C:O4' | 2.12 | 0.50 |
| 1:A:227:G:O2' | 24:A:1959:HOH:O | 2.20 | 0.50 |
| 1:A:310:G:H2' | 1:A:311:C:C6 | 2.43 | 0.50 |
| 1:A:1073:U:P | 5:E:57:LYS:HZ1 | 2.34 | 0.50 |
| 1:A:1451:A:H5'' | 1:A:1452:C:H5 | 1.77 | 0.50 |
| 4:D:163:GLU:OE1 | 4:D:166:LYS:HE2 | 2.11 | 0.50 |
| 6:F:33:TYR:CD2 | 6:F:71:ARG:HD2 | 2.46 | 0.50 |
| 9:I:22:GLY:HA3 | 9:I:60:ASP:N | 2.26 | 0.50 |
| 9:I:79:LEU:HD22 | 9:I:83:ARG:HE | 1.77 | 0.50 |
| 12:L:6:THR:O | 12:L:9:GLN:HB2 | 2.12 | 0.50 |
| 12:L:19:ARG:H | 12:L:19:ARG:NE | 2.09 | 0.50 |
| 16:P:58:TYR:CE2 | 16:P:62:VAL:HG11 | 2.46 | 0.50 |
| 17:Q:83:ASP:OD2 | 17:Q:84:LEU:HG | 2.12 | 0.50 |
| 1:A:179:A:H2' | 1:A:180:U:C6 | 2.47 | 0.50 |
| 1:A:350:G:H5'' | 1:A:350:G:H8 | 1.77 | 0.50 |
| 1:A:410:G:C2 | 1:A:429:U:C2 | 3.00 | 0.50 |
| 1:A:681:C:N4 | 1:A:682:G:O6 | 2.45 | 0.50 |
| 2:B:204:ASN:HB3 | 2:B:206:ASP:O | 2.12 | 0.50 |
| 4:D:172:PRO:HD2 | 4:D:173:TRP:CE3 | 2.47 | 0.50 |
| 6:F:39:LYS:HD3 | 6:F:40:VAL:H | 1.77 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:138:G:C2 | 1:A:226:G:N3 | 2.80 | 0.50 |
| 1:A:736:C:H2' | 1:A:737:A:C8 | 2.46 | 0.50 |
| 1:A:1349:A:H1' | 1:A:1374:A:N6 | 2.27 | 0.50 |
| 1:A:1410:G:H2' | 1:A:1411:C:C6 | 2.46 | 0.50 |
| 5:E:99:GLY:O | 5:E:101:ILE:HG13 | 2.11 | 0.50 |
| 9:I:50:LEU:HD12 | 9:I:50:LEU:H | 1.77 | 0.50 |
| 9:I:124:GLN:HG3 | 9:I:125:TYR:N | 2.26 | 0.50 |
| 18:R:74:ARG:HB3 | 18:R:81:PHE:CE2 | 2.46 | 0.50 |
| 1:A:259:G:H2' | 1:A:260:G:O4' | 2.12 | 0.49 |
| 1:A:1502:A:H2 | 1:A:1505:G:H22 | 1.54 | 0.49 |
| 6:F:82:ARG:HB2 | 6:F:85:VAL:HG23 | 1.93 | 0.49 |
| 9:I:81:ILE:HG22 | 9:I:85:LEU:HD22 | 1.94 | 0.49 |
| 1:A:763:G:H2' | 1:A:764:C:H6 | 1.77 | 0.49 |
| 1:A:966:M2G:HM22 | 1:A:967:5MC:O2 | 2.12 | 0.49 |
| 1:A:975:A:N6 | 1:A:1366:C:O2' | 2.41 | 0.49 |
| 1:A:1133:G:H1 | 1:A:1141:C:N4 | 2.10 | 0.49 |
| 1:A:1352:C:H2' | 1:A:1353:G:C8 | 2.47 | 0.49 |
| 12:L:35:GLY:HA3 | 12:L:59:ARG:O | 2.12 | 0.49 |
| 17:Q:26:GLN:HA | 17:Q:36:ILE:O | 2.13 | 0.49 |
| 1:A:278:G:C6 | 17:Q:95:TYR:CD2 | 3.00 | 0.49 |
| 1:A:346:G:H2' | 1:A:347:G:O4' | 2.13 | 0.49 |
| 1:A:727:G:N2 | 1:A:730:G:OP2 | 2.45 | 0.49 |
| 2:B:146:GLN:O | 2:B:150:SER:HB2 | 2.11 | 0.49 |
| 13:M:11:ARG:HD2 | 13:M:45:VAL:HG11 | 1.94 | 0.49 |
| 1:A:260:G:H2' | 1:A:261:U:C6 | 2.47 | 0.49 |
| 1:A:1095:U:C4 | 1:A:1096:C:N4 | 2.80 | 0.49 |
| 1:A:1400:5MC:H3' | 1:A:1401:G:H5' | 1.93 | 0.49 |
| 12:L:66:VAL:HG21 | 12:L:98:TYR:HE1 | 1.75 | 0.49 |
| 13:M:34:LEU:HD13 | 13:M:41:PRO:HA | 1.94 | 0.49 |
| 15:O:18:PHE:CD2 | 15:O:18:PHE:N | 2.80 | 0.49 |
| 20:T:57:ARG:HH22 | 20:T:100:ILE:CD1 | 2.25 | 0.49 |
| 1:A:191:G:O2' | 20:T:101:GLY:O | 2.30 | 0.49 |
| 1:A:270:A:H2' | 1:A:271:C:O4' | 2.13 | 0.49 |
| 1:A:767:A:H2' | 1:A:768:A:O4' | 2.13 | 0.49 |
| 1:A:1112:C:O2 | 3:C:179:ARG:HB2 | 2.13 | 0.49 |
| 1:A:1112:C:N3 | 3:C:178:LEU:HD12 | 2.27 | 0.49 |
| 3:C:116:VAL:HG21 | 3:C:202:ILE:HD11 | 1.94 | 0.49 |
| 4:D:31:CYS:O | 4:D:31:CYS:SG | 2.71 | 0.49 |
| 5:E:15:ARG:HG3 | 5:E:15:ARG:NH1 | 2.27 | 0.49 |
| 10:J:3:LYS:NZ | 10:J:3:LYS:HB3 | 2.27 | 0.49 |
| 15:O:18:PHE:N | 15:O:18:PHE:HD2 | 2.11 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:62:U:C2 | 1:A:63:C:C5 | 3.01 | 0.49 |
| 1:A:460:A:O2' | 1:A:461:C:H5' | 2.13 | 0.49 |
| 1:A:522:C:OP2 | 12:L:69:TYR:OH | 2.24 | 0.49 |
| 1:A:927:G:O2' | 1:A:1503:A:N7 | 2.44 | 0.49 |
| 3:C:150:LYS:HG3 | 3:C:169:ALA:HB2 | 1.93 | 0.49 |
| 4:D:173:TRP:O | 4:D:186:LEU:HD23 | 2.13 | 0.49 |
| 5:E:76:ILE:HD13 | 5:E:76:ILE:N | 2.27 | 0.49 |
| 3:C:67:THR:HA | 3:C:102:ASN:OD1 | 2.13 | 0.49 |
| 5:E:14:ARG:O | 5:E:28:PHE:HD2 | 1.95 | 0.49 |
| 9:I:118:LYS:C | 9:I:120:ARG:H | 2.16 | 0.49 |
| 10:J:15:THR:O | 10:J:19:SER:HB3 | 2.13 | 0.49 |
| 10:J:61:GLU:OE1 | 14:N:58:LYS:HD2 | 2.13 | 0.49 |
| 11:K:48:ILE:HD13 | 11:K:63:LEU:HB2 | 1.93 | 0.49 |
| 13:M:10:PRO:HB2 | 13:M:18:ALA:HB1 | 1.95 | 0.49 |
| 13:M:50:GLU:HG3 | 13:M:53:VAL:HB | 1.93 | 0.49 |
| 19:S:11:VAL:HG13 | 19:S:38:SER:HB3 | 1.95 | 0.49 |
| 1:A:680:C:N3 | 1:A:710:G:N2 | 2.46 | 0.49 |
| 1:A:718:G:O6 | 18:R:74:ARG:NH1 | 2.46 | 0.49 |
| 1:A:770:C:N4 | 24:A:1934:HOH:O | 2.18 | 0.49 |
| 1:A:933:G:N2 | 1:A:1384:C:O2 | 2.40 | 0.49 |
| 1:A:1442:G:N1 | 1:A:1446:A:N6 | 2.60 | 0.49 |
| 11:K:80:VAL:HG22 | 11:K:103:LEU:HD22 | 1.93 | 0.49 |
| 20:T:16:HIS:O | 20:T:20:LEU:HD22 | 2.13 | 0.49 |
| 1:A:106:C:C2' | 1:A:107:G:H5' | 2.43 | 0.49 |
| 1:A:116:A:H61 | 1:A:313:A:H1' | 1.77 | 0.49 |
| 1:A:432:A:H2' | 1:A:433:C:O4' | 2.13 | 0.49 |
| 1:A:1505:G:H5' | 24:A:1809:HOH:O | 2.12 | 0.49 |
| 13:M:19:LEU:HD11 | 13:M:56:LEU:HD11 | 1.94 | 0.49 |
| 1:A:642:A:H2' | 1:A:643:C:C6 | 2.48 | 0.49 |
| 1:A:725:G:C5 | 1:A:726:C:C5 | 3.01 | 0.49 |
| 1:A:939:G:C6 | 1:A:940:C:N4 | 2.81 | 0.49 |
| 1:A:1345:U:C4 | 1:A:1377:A:C2 | 3.01 | 0.49 |
| 5:E:92:LYS:HB3 | 5:E:119:LEU:HB2 | 1.94 | 0.49 |
| 8:H:116:LYS:CG | 8:H:127:LEU:HD11 | 2.43 | 0.49 |
| 14:N:35:ARG:HG2 | 14:N:35:ARG:HH11 | 1.77 | 0.49 |
| 16:P:53:VAL:HG23 | 16:P:54:GLU:H | 1.77 | 0.49 |
| 17:Q:5:VAL:HB | 17:Q:60:ILE:CD1 | 2.43 | 0.49 |
| 18:R:29:PHE:HZ | 18:R:43:PHE:CE1 | 2.30 | 0.49 |
| 18:R:46:GLU:N | 18:R:46:GLU:OE2 | 2.37 | 0.49 |
| 1:A:350:G:O2' | 1:A:351:G:H5' | 2.13 | 0.48 |
| 1:A:358:U:H2' | 1:A:359:U:H6 | 1.78 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:642:A:N7 | 8:H:115:SER:HA | 2.28 | 0.48 |
| 3:C:164:ARG:HG2 | 3:C:165:THR:N | 2.27 | 0.48 |
| 13:M:91:ARG:HH21 | 13:M:103:THR:HG21 | 1.77 | 0.48 |
| 1:A:7:G:C5 | 1:A:298:A:C2 | 3.01 | 0.48 |
| 3:C:121:ALA:O | 3:C:124:ILE:HB | 2.13 | 0.48 |
| 6:F:30:LEU:HD21 | 6:F:65:VAL:HG11 | 1.95 | 0.48 |
| 7:G:69:VAL:HG11 | 7:G:134:ALA:HB1 | 1.95 | 0.48 |
| 7:G:78:ARG:NH1 | 7:G:154:TYR:O | 2.46 | 0.48 |
| 10:J:13:HIS:CD2 | 10:J:14:LYS:N | 2.80 | 0.48 |
| 17:Q:40:LYS:HD3 | 17:Q:42:TYR:CZ | 2.48 | 0.48 |
| 1:A:291:C:O2 | 1:A:291:C:H2' | 2.12 | 0.48 |
| 1:A:730:G:N2 | 1:A:765:G:H5'' | 2.27 | 0.48 |
| 1:A:826:C:H2' | 1:A:827:U:H6 | 1.78 | 0.48 |
| 1:A:1461:G:H2' | 1:A:1462:G:H8 | 1.77 | 0.48 |
| 2:B:76:GLN:NE2 | 2:B:206:ASP:HB3 | 2.27 | 0.48 |
| 5:E:51:VAL:N | 5:E:52:PRO:HD2 | 2.28 | 0.48 |
| 6:F:99:ALA:HB2 | 18:R:31:LEU:HG | 1.94 | 0.48 |
| 13:M:87:TYR:HA | 13:M:90:LEU:HD22 | 1.95 | 0.48 |
| 1:A:1118:C:OP1 | 9:I:104:ARG:NE | 2.45 | 0.48 |
| 1:A:1378:C:N4 | 1:A:1379:G:N3 | 2.62 | 0.48 |
| 1:A:1378:C:C5 | 1:A:1379:G:C8 | 3.02 | 0.48 |
| 1:A:1481:U:H2' | 1:A:1482:G:H8 | 1.76 | 0.48 |
| 2:B:69:LEU:HB3 | 2:B:162:ILE:HD11 | 1.95 | 0.48 |
| 2:B:178:ARG:CD | 8:H:72:PRO:HA | 2.44 | 0.48 |
| 3:C:147:LYS:NZ | 3:C:172:ARG:HE | 2.10 | 0.48 |
| 5:E:121:LYS:HG3 | 5:E:122:GLU:O | 2.13 | 0.48 |
| 6:F:25:ILE:HA | 6:F:28:ARG:HG2 | 1.94 | 0.48 |
| 7:G:88:PRO:HG2 | 7:G:152:ALA:HA | 1.95 | 0.48 |
| 13:M:12:ASN:H | 13:M:45:VAL:HG12 | 1.76 | 0.48 |
| 15:O:3:ILE:HA | 15:O:7:GLU:OE1 | 2.13 | 0.48 |
| 16:P:19:ILE:HD11 | 16:P:39:TYR:HB2 | 1.95 | 0.48 |
| 1:A:15:G:H5' | 1:A:1396:A:O2' | 2.14 | 0.48 |
| 1:A:44:G:H2' | 1:A:45:U:O4' | 2.13 | 0.48 |
| 1:A:414:A:H2' | 1:A:415:A:C8 | 2.48 | 0.48 |
| 1:A:1025:U:H5 | 1:A:1034:G:H1 | 1.62 | 0.48 |
| 1:A:1168:A:H2' | 1:A:1169:A:C8 | 2.48 | 0.48 |
| 1:A:1371:G:O3' | 9:I:69:GLY:HA3 | 2.13 | 0.48 |
| 2:B:28:PHE:CE2 | 2:B:190:THR:HG22 | 2.49 | 0.48 |
| 1:A:389:A:C6 | 1:A:390:C:H1' | 2.49 | 0.48 |
| 1:A:648:A:H2' | 1:A:649:G:O4' | 2.14 | 0.48 |
| 1:A:1026:G:C8 | 1:A:1026:G:H3' | 2.49 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1508:G:C5 | 1:A:1509:C:C5 | 3.02 | 0.48 |
| 5:E:78:HIS:CE1 | 5:E:143:ARG:H | 2.31 | 0.48 |
| 20:T:55:ILE:HA | 20:T:55:ILE:HD13 | 1.72 | 0.48 |
| 1:A:323:U:H2' | 1:A:324:G:O4' | 2.12 | 0.48 |
| 1:A:539:A:H2' | 1:A:540:G:C8 | 2.49 | 0.48 |
| 1:A:745:C:H5'' | 1:A:851:G:O2' | 2.13 | 0.48 |
| 1:A:806:C:O2' | 1:A:807:A:H5' | 2.13 | 0.48 |
| 1:A:1029:C:OP1 | 1:A:1033:G:N2 | 2.47 | 0.48 |
| 1:A:1138:G:H3' | 1:A:1138:G:N3 | 2.29 | 0.48 |
| 2:B:93:VAL:HG21 | 2:B:97:TRP:HD1 | 1.79 | 0.48 |
| 3:C:108:ASN:ND2 | 3:C:111:LEU:HD22 | 2.29 | 0.48 |
| 1:A:109:A:C6 | 1:A:326:G:C6 | 3.02 | 0.48 |
| 1:A:463:A:O2' | 16:P:82:GLN:HG2 | 2.14 | 0.48 |
| 1:A:780:A:OP2 | 11:K:122:LYS:HE3 | 2.13 | 0.48 |
| 1:A:1096:C:H2' | 1:A:1097:C:C6 | 2.48 | 0.48 |
| 1:A:1152:A:H5'' | 10:J:13:HIS:HB2 | 1.94 | 0.48 |
| 1:A:1374:A:C4 | 1:A:1375:A:C8 | 3.01 | 0.48 |
| 2:B:10:LEU:O | 2:B:12:GLU:N | 2.47 | 0.48 |
| 4:D:72:GLU:O | 4:D:75:PHE:N | 2.47 | 0.48 |
| 12:L:113:ARG:NH1 | 12:L:116:SER:H | 2.11 | 0.48 |
| 13:M:101:GLN:OE1 | 13:M:101:GLN:N | 2.46 | 0.48 |
| 1:A:485:G:O2' | 1:A:486:U:OP2 | 2.29 | 0.48 |
| 1:A:586:C:C2' | 1:A:587:G:H5' | 2.44 | 0.48 |
| 1:A:662:G:H2' | 1:A:663:A:C8 | 2.49 | 0.48 |
| 1:A:683:G:H3' | 1:A:684:A:H8 | 1.78 | 0.48 |
| 1:A:691:G:H2' | 1:A:692:U:C6 | 2.48 | 0.48 |
| 1:A:1070:U:H2' | 1:A:1071:C:H6 | 1.77 | 0.48 |
| 1:A:1150:U:C2' | 1:A:1151:A:H5' | 2.43 | 0.48 |
| 1:A:1195:C:O3' | 1:A:1196:U:H4' | 2.14 | 0.48 |
| 1:A:1224:G:O2' | 1:A:1322:C:OP1 | 2.20 | 0.48 |
| 1:A:1238:A:H5' | 1:A:1336:C:N4 | 2.23 | 0.48 |
| 4:D:201:GLN:HG2 | 4:D:204:ILE:HD12 | 1.96 | 0.48 |
| 5:E:9:LYS:HG2 | 5:E:112:LEU:HD11 | 1.95 | 0.48 |
| 7:G:17:VAL:HG12 | 7:G:18:TYR:CD1 | 2.49 | 0.48 |
| 9:I:90:PRO:O | 9:I:93:ARG:HG3 | 2.14 | 0.48 |
| 16:P:6:LEU:HD23 | 16:P:17:TYR:CD2 | 2.49 | 0.48 |
| 17:Q:75:ARG:NH1 | 17:Q:75:ARG:HB2 | 2.29 | 0.48 |
| 19:S:11:VAL:HG12 | 19:S:12:ASP:H | 1.79 | 0.48 |
| 20:T:57:ARG:NH1 | 20:T:100:ILE:HG21 | 2.29 | 0.48 |
| 1:A:558:G:H3' | 1:A:559:A:H3' | 1.96 | 0.48 |
| 1:A:682:G:C2 | 1:A:683:G:C8 | 3.02 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:716:A:N3 | 11:K:118:GLY:HA2 | 2.29 | 0.48 |
| 1:A:949:A:C2 | 1:A:1233:G:N3 | 2.82 | 0.48 |
| 1:A:1044:A:C6 | 1:A:1045:C:H1' | 2.49 | 0.48 |
| 3:C:20:SER:HB3 | 3:C:22:TRP:HE1 | 1.79 | 0.48 |
| 3:C:120:VAL:HG12 | 3:C:198:VAL:HG11 | 1.95 | 0.48 |
| 7:G:50:ILE:O | 7:G:54:THR:OG1 | 2.23 | 0.48 |
| 16:P:44:THR:OG1 | 16:P:45:THR:HG22 | 2.13 | 0.48 |
| 18:R:45:SER:HB2 | 18:R:51:LEU:HD21 | 1.96 | 0.48 |
| 1:A:98:U:O2' | 1:A:99:C:H5' | 2.14 | 0.47 |
| 1:A:429:U:H1' | 1:A:430:A:H5'' | 1.96 | 0.47 |
| 1:A:512:U:H2' | 1:A:513:C:C6 | 2.49 | 0.47 |
| 1:A:622:A:C8 | 1:A:623:C:C5 | 3.02 | 0.47 |
| 1:A:910:C:C4 | 1:A:911:U:C5 | 3.03 | 0.47 |
| 1:A:918:A:H2' | 1:A:919:A:C8 | 2.48 | 0.47 |
| 1:A:1137:C:O2 | 1:A:1138:G:N1 | 2.45 | 0.47 |
| 3:C:43:LEU:HD13 | 3:C:47:LEU:HD22 | 1.95 | 0.47 |
| 4:D:38:TYR:H | 4:D:38:TYR:HD2 | 1.62 | 0.47 |
| 17:Q:66:SER:OG | 17:Q:69:LYS:HB2 | 2.14 | 0.47 |
| 19:S:5:LEU:HD22 | 19:S:6:LYS:NZ | 2.29 | 0.47 |
| 1:A:416:G:C6 | 1:A:417:C:N3 | 2.82 | 0.47 |
| 1:A:705:U:H5'' | 1:A:706:A:OP2 | 2.14 | 0.47 |
| 1:A:1086:U:O5' | 1:A:1086:U:H6 | 1.96 | 0.47 |
| 1:A:1381:U:O2' | 1:A:1382:C:H5' | 2.14 | 0.47 |
| 2:B:178:ARG:HH21 | 8:H:74:PRO:HG3 | 1.78 | 0.47 |
| 5:E:40:ARG:HB3 | 5:E:66:MET:CE | 2.43 | 0.47 |
| 7:G:16:LEU:HD22 | 9:I:42:ARG:HA | 1.96 | 0.47 |
| 11:K:126:ARG:HH11 | 11:K:126:ARG:HG3 | 1.79 | 0.47 |
| 18:R:46:GLU:OE2 | 18:R:55:ARG:NH2 | 2.47 | 0.47 |
| 1:A:149:A:H2' | 1:A:150:C:C6 | 2.49 | 0.47 |
| 1:A:344:A:C5' | 1:A:345:C:H5 | 2.28 | 0.47 |
| 1:A:454:C:H5'' | 1:A:455:C:C5 | 2.49 | 0.47 |
| 1:A:709:G:H2' | 1:A:710:G:H8 | 1.79 | 0.47 |
| 1:A:725:G:H2' | 1:A:726:C:H6 | 1.79 | 0.47 |
| 1:A:1075:C:O3' | 2:B:175:ARG:NH2 | 2.47 | 0.47 |
| 1:A:1304:G:C6 | 1:A:1305:G:N1 | 2.82 | 0.47 |
| 3:C:34:LEU:HD23 | 14:N:25:VAL:HG21 | 1.96 | 0.47 |
| 10:J:6:ILE:HB | 10:J:72:VAL:CG2 | 2.44 | 0.47 |
| 13:M:48:LEU:H | 13:M:48:LEU:HG | 1.42 | 0.47 |
| 15:O:11:VAL:HG21 | 15:O:34:LEU:HD22 | 1.95 | 0.47 |
| 19:S:39:THR:HA | 19:S:70:LYS:HA | 1.95 | 0.47 |
| 1:A:434:U:H2' | 1:A:435:C:C6 | 2.48 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:A:737:A:H2' | 1:A:738:C:H6 | 1.79 | 0.47 |
| 1:A:1233:G:N2 | 1:A:1234:C:N3 | 2.62 | 0.47 |
| 1:A:1519[B]:MA6:C5 | 1:A:1520[B]:G:H1' | 2.44 | 0.47 |
| 2:B:54:THR:OG1 | 2:B:199:TYR:HB3 | 2.13 | 0.47 |
| 14:N:9:LYS:HD3 | 14:N:10:ALA:N | 2.29 | 0.47 |
| 18:R:69:THR:O | 18:R:72:ARG:HB2 | 2.14 | 0.47 |
| 1:A:107:G:C2 | 1:A:108:G:H1' | 2.50 | 0.47 |
| 1:A:109:A:C4 | 1:A:327:A:C2 | 3.02 | 0.47 |
| 1:A:448:A:C4 | 1:A:487:A:C2 | 3.03 | 0.47 |
| 1:A:452:A:C2 | 1:A:453:A:C4 | 3.03 | 0.47 |
| 1:A:1191:A:H2' | 1:A:1192:C:C6 | 2.49 | 0.47 |
| 2:B:109:SER:O | 2:B:112:VAL:HB | 2.14 | 0.47 |
| 3:C:148:GLY:HA3 | 3:C:172:ARG:O | 2.14 | 0.47 |
| 4:D:190:ASP:OD2 | 4:D:192:GLU:N | 2.39 | 0.47 |
| 9:I:52:ALA:O | 9:I:95:LYS:HD3 | 2.15 | 0.47 |
| 10:J:6:ILE:HB | 10:J:72:VAL:HG23 | 1.96 | 0.47 |
| 11:K:62:GLN:O | 11:K:66:LEU:HB2 | 2.14 | 0.47 |
| 13:M:49:THR:OG1 | 13:M:52:GLU:HG3 | 2.14 | 0.47 |
| 1:A:37:U:O2' | 1:A:500:G:H4' | 2.14 | 0.47 |
| 1:A:1309:G:C6 | 1:A:1329:A:C2 | 3.02 | 0.47 |
| 2:B:112:VAL:O | 2:B:115:LEU:HB3 | 2.15 | 0.47 |
| 3:C:151:VAL:O | 3:C:152:ILE:HD13 | 2.14 | 0.47 |
| 12:L:117:ARG:NH2 | 12:L:124:LYS:HB2 | 2.29 | 0.47 |
| 13:M:23:TYR:CE2 | 13:M:70:LEU:HD13 | 2.50 | 0.47 |
| 13:M:108:ARG:NH2 | 13:M:111:LYS:HG2 | 2.30 | 0.47 |
| 21:U:8:THR:HG1 | 21:U:11:GLY:H | 1.61 | 0.47 |
| 1:A:375:U:H2' | 1:A:376:G:C8 | 2.50 | 0.47 |
| 1:A:729:A:C2' | 1:A:730:G:H5' | 2.44 | 0.47 |
| 1:A:975:A:H4' | 1:A:976:G:C5' | 2.40 | 0.47 |
| 1:A:1057:G:O6 | 1:A:1203:C:N4 | 2.44 | 0.47 |
| 1:A:1127:G:N2 | 1:A:1145:C:N3 | 2.62 | 0.47 |
| 1:A:1315:U:H2' | 1:A:1316:G:O4' | 2.15 | 0.47 |
| 1:A:1327:C:H2' | 1:A:1328:C:C6 | 2.50 | 0.47 |
| 3:C:20:SER:O | 14:N:54:PRO:HB3 | 2.15 | 0.47 |
| 3:C:126:ARG:O | 3:C:127:ARG:HG2 | 2.15 | 0.47 |
| 3:C:182:ILE:HD12 | 3:C:203:PHE:HB2 | 1.96 | 0.47 |
| 8:H:10:LEU:O | 8:H:13:ILE:HB | 2.15 | 0.47 |
| 8:H:39:LEU:HA | 8:H:39:LEU:HD22 | 1.54 | 0.47 |
| 10:J:87:THR:C | 10:J:88:LEU:HD13 | 2.34 | 0.47 |
| 11:K:120:ARG:HH22 | 11:K:126:ARG:HH12 | 1.62 | 0.47 |
| 15:O:15:PHE:HD1 | 15:O:30:ALA:CB | 2.27 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:292:G:C2 | 1:A:309:G:C2 | 3.03 | 0.47 |
| 1:A:376:G:H5'' | 16:P:5:ARG:HD2 | 1.96 | 0.47 |
| 1:A:564:C:C5 | 17:Q:31:LEU:HD21 | 2.50 | 0.47 |
| 1:A:710:G:H5'' | 6:F:54:LYS:HE3 | 1.97 | 0.47 |
| 1:A:1508:G:H2' | 1:A:1509:C:O4' | 2.15 | 0.47 |
| 2:B:18:GLY:H | 2:B:41:ILE:HG23 | 1.80 | 0.47 |
| 3:C:167:TRP:HE3 | 3:C:168:ALA:H | 1.59 | 0.47 |
| 12:L:36:VAL:HG12 | 12:L:37:CYS:O | 2.15 | 0.47 |
| 1:A:475:G:H2' | 1:A:476:G:H8 | 1.80 | 0.47 |
| 1:A:674:G:H2' | 1:A:675:A:C8 | 2.49 | 0.47 |
| 1:A:902:G:O2' | 1:A:903:G:H5' | 2.15 | 0.47 |
| 3:C:23:TYR:HD1 | 10:J:11:PHE:CE2 | 2.33 | 0.47 |
| 5:E:59:GLY:C | 5:E:63:ARG:HH21 | 2.18 | 0.47 |
| 6:F:14:LEU:HA | 6:F:18:GLN:OE1 | 2.14 | 0.47 |
| 8:H:51:VAL:HG11 | 8:H:60:ARG:NH1 | 2.30 | 0.47 |
| 11:K:27:ASN:OD1 | 11:K:28:THR:N | 2.47 | 0.47 |
| 13:M:53:VAL:O | 13:M:57:ARG:HB2 | 2.14 | 0.47 |
| 14:N:6:LEU:HD13 | 14:N:23:ARG:HH22 | 1.80 | 0.47 |
| 1:A:263:A:O2' | 1:A:264:U:H5' | 2.15 | 0.47 |
| 1:A:500:G:C5 | 1:A:546:G:N2 | 2.83 | 0.47 |
| 4:D:206:PHE:CD2 | 4:D:207:TYR:CE1 | 2.99 | 0.47 |
| 5:E:100:VAL:HA | 5:E:118:ILE:HG22 | 1.97 | 0.47 |
| 5:E:106:PRO:O | 5:E:110:LEU:HG | 2.14 | 0.47 |
| 7:G:62:PHE:HD1 | 7:G:124:LEU:HD22 | 1.80 | 0.47 |
| 11:K:19:ALA:HB2 | 11:K:32:ILE:HG23 | 1.96 | 0.47 |
| 13:M:4:ILE:CD1 | 13:M:22:ILE:HD11 | 2.44 | 0.47 |
| 16:P:67:THR:O | 16:P:70:ALA:HB3 | 2.15 | 0.47 |
| 1:A:405:U:C2 | 1:A:498:U:C5 | 3.03 | 0.46 |
| 1:A:530:G:H2' | 1:A:530:G:N3 | 2.30 | 0.46 |
| 1:A:1377:A:N6 | 7:G:5:ARG:HH22 | 2.14 | 0.46 |
| 2:B:163:PHE:CE2 | 2:B:185:ILE:HG22 | 2.50 | 0.46 |
| 6:F:52:ILE:O | 6:F:55:ASP:HB2 | 2.15 | 0.46 |
| 11:K:17:GLY:O | 11:K:80:VAL:HA | 2.15 | 0.46 |
| 19:S:51:VAL:O | 19:S:57:HIS:HA | 2.16 | 0.46 |
| 1:A:595:G:H1' | 1:A:596:C:H5 | 1.80 | 0.46 |
| 1:A:750:G:N3 | 15:O:23:GLY:HA3 | 2.30 | 0.46 |
| 1:A:1057:G:N2 | 1:A:1204:A:H1' | 2.30 | 0.46 |
| 1:A:1172:C:H2' | 1:A:1173:G:H8 | 1.80 | 0.46 |
| 1:A:1226:C:C5 | 13:M:104:ARG:HA | 2.50 | 0.46 |
| 3:C:18:TRP:O | 3:C:21:ARG:NH1 | 2.49 | 0.46 |
| 3:C:102:ASN:OD1 | 3:C:102:ASN:N | 2.48 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:26:ILE:O | 6:F:30:LEU:HB2 | 2.15 | 0.46 |
| 8:H:49:GLU:HB2 | 8:H:62:TYR:CE2 | 2.50 | 0.46 |
| 12:L:123:LYS:H | 12:L:123:LYS:HG2 | 1.27 | 0.46 |
| 19:S:53:ASN:O | 19:S:77:THR:HG22 | 2.15 | 0.46 |
| 20:T:50:GLU:CB | 20:T:99:LEU:HD23 | 2.42 | 0.46 |
| 1:A:3:G:H1 | 4:D:87:GLY:H | 1.64 | 0.46 |
| 1:A:17:U:C2 | 1:A:18:C:C5 | 3.04 | 0.46 |
| 1:A:66:G:N3 | 1:A:66:G:H2' | 2.29 | 0.46 |
| 1:A:128:G:H4' | 17:Q:3:LYS:HG2 | 1.97 | 0.46 |
| 1:A:710:G:C2 | 1:A:711:G:C5 | 3.03 | 0.46 |
| 1:A:949:A:H1' | 1:A:1364:U:N3 | 2.30 | 0.46 |
| 1:A:1310:G:C2 | 1:A:1328:C:N3 | 2.84 | 0.46 |
| 1:A:1310:G:N7 | 19:S:2:PRO:HD3 | 2.30 | 0.46 |
| 1:A:1487:G:C5 | 1:A:1488:G:C8 | 3.03 | 0.46 |
| 1:A:1539:C:H5'' | 7:G:82:GLY:CA | 2.46 | 0.46 |
| 2:B:223:ILE:CD1 | 2:B:228:GLY:HA3 | 2.45 | 0.46 |
| 5:E:33:VAL:HG22 | 5:E:43:LEU:HD13 | 1.98 | 0.46 |
| 8:H:1:MET:HG2 | 8:H:2:LEU:H | 1.79 | 0.46 |
| 9:I:63:ILE:HG21 | 9:I:77:ILE:HD11 | 1.96 | 0.46 |
| 16:P:21:VAL:HG21 | 16:P:59:TRP:CD1 | 2.50 | 0.46 |
| 1:A:138:G:C2 | 1:A:226:G:C2 | 3.03 | 0.46 |
| 1:A:442:C:H2' | 1:A:443:C:C6 | 2.50 | 0.46 |
| 1:A:452:A:O2' | 1:A:453:A:H8 | 1.97 | 0.46 |
| 1:A:948:C:OP2 | 13:M:108:ARG:HB2 | 2.16 | 0.46 |
| 2:B:223:ILE:HD12 | 2:B:228:GLY:HA3 | 1.97 | 0.46 |
| 3:C:11:ARG:HH12 | 3:C:180:ALA:HB3 | 1.81 | 0.46 |
| 6:F:43:LEU:HD22 | 6:F:43:LEU:H | 1.80 | 0.46 |
| 8:H:87:SER:HB2 | 8:H:93:VAL:HG22 | 1.95 | 0.46 |
| 11:K:66:LEU:HD23 | 11:K:97:ALA:HB1 | 1.97 | 0.46 |
| 20:T:43:LEU:HD13 | 20:T:51:GLU:HB3 | 1.97 | 0.46 |
| 1:A:448:A:P | 1:A:485:G:H22 | 2.38 | 0.46 |
| 1:A:1048:G:H1 | 1:A:1209:C:H42 | 1.63 | 0.46 |
| 1:A:1248:A:O2' | 9:I:70:LYS:NZ | 2.28 | 0.46 |
| 1:A:1438:G:H2' | 1:A:1439:C:H6 | 1.80 | 0.46 |
| 1:A:1491:G:C2' | 1:A:1492:A:H5' | 2.45 | 0.46 |
| 2:B:69:LEU:HD23 | 2:B:91:PRO:O | 2.15 | 0.46 |
| 7:G:95:ARG:CZ | 7:G:99:LEU:HD11 | 2.46 | 0.46 |
| 13:M:90:LEU:HA | 13:M:93:ARG:HB3 | 1.98 | 0.46 |
| 1:A:463:A:H2' | 1:A:474:G:O4' | 2.15 | 0.46 |
| 1:A:500:G:C6 | 1:A:546:G:C2 | 3.04 | 0.46 |
| 1:A:502:G:OP1 | 12:L:117:ARG:N | 2.47 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:544:G:OP1 | 4:D:59:ARG:NH2 | 2.33 | 0.46 |
| 1:A:833:U:H2' | 1:A:834:C:C6 | 2.50 | 0.46 |
| 1:A:935:A:N6 | 7:G:3:ARG:HG3 | 2.31 | 0.46 |
| 1:A:992:U:H3 | 1:A:1044:A:H62 | 1.63 | 0.46 |
| 1:A:1499:A:H1' | 1:A:1520[A]:G:H5' | 1.98 | 0.46 |
| 2:B:36:ARG:HB3 | 2:B:41:ILE:HD11 | 1.96 | 0.46 |
| 3:C:129:ALA:HB3 | 3:C:132:ARG:HD2 | 1.97 | 0.46 |
| 3:C:195:VAL:C | 3:C:196:LEU:HD12 | 2.35 | 0.46 |
| 10:J:4:ILE:HB | 10:J:74:ILE:CD1 | 2.46 | 0.46 |
| 14:N:23:ARG:HD3 | 14:N:29:ARG:O | 2.16 | 0.46 |
| 14:N:41:ARG:HG2 | 14:N:42:ILE:HG23 | 1.97 | 0.46 |
| 15:O:50:HIS:O | 15:O:53:HIS:N | 2.48 | 0.46 |
| 20:T:53:LEU:CD2 | 20:T:56:MET:HG2 | 2.46 | 0.46 |
| 21:U:6:ARG:HG2 | 21:U:15:ARG:NH2 | 2.31 | 0.46 |
| 1:A:229:U:H2' | 1:A:230:G:H8 | 1.81 | 0.46 |
| 1:A:542:G:H2' | 1:A:543:C:H6 | 1.80 | 0.46 |
| 1:A:693:G:O2' | 7:G:81:GLY:O | 2.25 | 0.46 |
| 1:A:867:G:O2' | 1:A:868:C:H5' | 2.15 | 0.46 |
| 1:A:869:G:C8 | 24:A:2036:HOH:O | 2.68 | 0.46 |
| 1:A:1079:G:C6 | 1:A:1080:A:N6 | 2.84 | 0.46 |
| 1:A:1333:A:H2' | 1:A:1334:G:O4' | 2.15 | 0.46 |
| 3:C:81:GLY:O | 3:C:84:ILE:HG22 | 2.16 | 0.46 |
| 4:D:202:LEU:HD13 | 4:D:202:LEU:HA | 1.80 | 0.46 |
| 7:G:101:LEU:N | 7:G:101:LEU:HD12 | 2.31 | 0.46 |
| 10:J:32:ALA:HB3 | 10:J:75:ILE:HB | 1.97 | 0.46 |
| 13:M:12:ASN:H | 13:M:45:VAL:HG11 | 1.79 | 0.46 |
| 15:O:85:LEU:HD23 | 15:O:85:LEU:HA | 1.54 | 0.46 |
| 1:A:310:G:C5 | 1:A:311:C:C5 | 3.04 | 0.46 |
| 1:A:448:A:C2 | 1:A:449:C:C2 | 3.03 | 0.46 |
| 1:A:872:A:C5 | 1:A:874:G:C8 | 3.04 | 0.46 |
| 1:A:1443:G:H5'' | 1:A:1443:G:H8 | 1.81 | 0.46 |
| 1:A:1502:A:H5'' | 1:A:1504:G:N7 | 2.31 | 0.46 |
| 4:D:19:LEU:HB2 | 4:D:21:LEU:HD23 | 1.98 | 0.46 |
| 7:G:50:ILE:HD13 | 7:G:61:VAL:HG11 | 1.98 | 0.46 |
| 7:G:87:VAL:HA | 7:G:88:PRO:HD2 | 1.75 | 0.46 |
| 9:I:86:VAL:HA | 9:I:89:ASN:O | 2.16 | 0.46 |
| 18:R:66:LEU:O | 18:R:70:ILE:HG13 | 2.15 | 0.46 |
| 19:S:53:ASN:HB2 | 19:S:56:GLN:O | 2.15 | 0.46 |
| 1:A:93:G:H2' | 1:A:95:U:O4' | 2.16 | 0.46 |
| 1:A:690:G:N7 | 11:K:55:LYS:NZ | 2.63 | 0.46 |
| 1:A:839:U:H5'' | 1:A:840:C:OP2 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:920:U:O4' | 1:A:1080:A:C2 | 2.68 | 0.46 |
| 1:A:1035:A:C4 | 1:A:1036:G:N7 | 2.84 | 0.46 |
| 1:A:1367:C:N3 | 1:A:1368:G:C8 | 2.84 | 0.46 |
| 1:A:1486:G:H2' | 1:A:1487:G:O4' | 2.16 | 0.46 |
| 3:C:150:LYS:HD2 | 3:C:173:VAL:HG21 | 1.98 | 0.46 |
| 5:E:12:LEU:HD23 | 5:E:13:ILE:CA | 2.46 | 0.46 |
| 5:E:135:THR:O | 5:E:138:ALA:HB3 | 2.16 | 0.46 |
| 7:G:75:VAL:HA | 7:G:87:VAL:O | 2.16 | 0.46 |
| 12:L:10:LEU:HD23 | 12:L:10:LEU:HA | 1.57 | 0.46 |
| 12:L:117:ARG:HB3 | 12:L:122:THR:OG1 | 2.16 | 0.46 |
| 17:Q:31:LEU:HD12 | 17:Q:31:LEU:HA | 1.65 | 0.46 |
| 18:R:53:ARG:HA | 18:R:56:THR:HG23 | 1.98 | 0.46 |
| 20:T:89:ARG:HH21 | 20:T:104:LEU:HD22 | 1.81 | 0.46 |
| 1:A:401:C:H2' | 1:A:402:G:H8 | 1.81 | 0.46 |
| 1:A:499:A:N6 | 1:A:547:A:C8 | 2.84 | 0.46 |
| 1:A:520:A:OP1 | 12:L:52:LEU:HD12 | 2.16 | 0.46 |
| 1:A:800:G:O2' | 1:A:801:U:H5' | 2.16 | 0.46 |
| 1:A:1151:A:H1' | 1:A:1152:A:C8 | 2.51 | 0.46 |
| 1:A:1487:G:H2' | 1:A:1488:G:H5' | 1.97 | 0.46 |
| 17:Q:8:GLY:HA3 | 17:Q:22:LEU:O | 2.16 | 0.46 |
| 17:Q:60:ILE:HA | 17:Q:60:ILE:HD12 | 1.68 | 0.46 |
| 1:A:7:G:H5' | 1:A:298:A:O4' | 2.16 | 0.45 |
| 1:A:56:U:O2' | 1:A:57:G:H5' | 2.16 | 0.45 |
| 1:A:130:A:H4' | 1:A:190(F):G:C2 | 2.51 | 0.45 |
| 1:A:515:G:H2' | 1:A:516:PSU:O4' | 2.16 | 0.45 |
| 1:A:645:C:H2' | 1:A:646:U:O4' | 2.15 | 0.45 |
| 1:A:1491:G:N1 | 1:A:1493:A:H2 | 2.14 | 0.45 |
| 5:E:12:LEU:HD21 | 5:E:14:ARG:HB3 | 1.98 | 0.45 |
| 8:H:120:THR:HG23 | 8:H:123:GLU:HG3 | 1.99 | 0.45 |
| 10:J:3:LYS:N | 10:J:74:ILE:O | 2.50 | 0.45 |
| 19:S:25:LYS:HE3 | 19:S:25:LYS:HB3 | 1.75 | 0.45 |
| 1:A:352:C:H6 | 1:A:352:C:H5'' | 1.81 | 0.45 |
| 1:A:401:C:H2' | 1:A:402:G:C8 | 2.51 | 0.45 |
| 1:A:452:A:HO2' | 1:A:453:A:H8 | 1.64 | 0.45 |
| 1:A:689:C:P | 11:K:46:GLY:HA3 | 2.56 | 0.45 |
| 1:A:728:A:H2' | 1:A:729:A:O4' | 2.16 | 0.45 |
| 1:A:938:A:C6 | 1:A:939:G:C5 | 3.04 | 0.45 |
| 1:A:942:G:C2 | 1:A:1342:C:C2 | 3.05 | 0.45 |
| 1:A:1171:G:H2' | 1:A:1172:C:C6 | 2.51 | 0.45 |
| 1:A:1309:G:N2 | 1:A:1329:A:H1' | 2.31 | 0.45 |
| 1:A:1378:C:N4 | 1:A:1379:G:C4 | 2.85 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 13:M:80:ARG:HB3 | 13:M:80:ARG:CZ | 2.45 | 0.45 |
| 17:Q:70:ARG:O | 17:Q:71:PHE:HD2 | 1.99 | 0.45 |
| 1:A:496:A:C2 | 1:A:497:A:C5 | 3.04 | 0.45 |
| 1:A:581:G:C2 | 1:A:582:U:C5 | 3.04 | 0.45 |
| 1:A:581:G:N2 | 1:A:760:G:N7 | 2.63 | 0.45 |
| 1:A:665:A:C5 | 1:A:733:A:C5 | 3.04 | 0.45 |
| 1:A:682:G:H1 | 1:A:708:C:H42 | 1.65 | 0.45 |
| 1:A:993:G:H2' | 1:A:995:C:H41 | 1.81 | 0.45 |
| 1:A:1126:U:C4 | 1:A:1127:G:C2 | 3.04 | 0.45 |
| 1:A:1402:4OC:O2 | 1:A:1500:A:N1 | 2.49 | 0.45 |
| 3:C:122:GLU:OE1 | 3:C:126:ARG:HD2 | 2.16 | 0.45 |
| 6:F:23:LYS:O | 6:F:26:ILE:HB | 2.17 | 0.45 |
| 17:Q:81:ARG:HE | 17:Q:81:ARG:HB3 | 1.45 | 0.45 |
| 17:Q:85:VAL:O | 17:Q:89:LEU:HB2 | 2.17 | 0.45 |
| 18:R:83:GLU:OE1 | 18:R:84:LYS:HG3 | 2.16 | 0.45 |
| 1:A:665:A:H3' | 1:A:725:G:H21 | 1.82 | 0.45 |
| 1:A:1234:C:H2' | 1:A:1235:U:C6 | 2.49 | 0.45 |
| 1:A:1461:G:H2' | 1:A:1462:G:C8 | 2.51 | 0.45 |
| 7:G:5:ARG:HE | 7:G:7:ALA:HA | 1.81 | 0.45 |
| 8:H:9:MET:O | 8:H:13:ILE:HD12 | 2.17 | 0.45 |
| 8:H:29:SER:OG | 8:H:32:LYS:N | 2.31 | 0.45 |
| 8:H:100:ILE:HA | 8:H:101:PRO:HD2 | 1.77 | 0.45 |
| 10:J:8:LEU:CD2 | 10:J:96:ILE:HG22 | 2.44 | 0.45 |
| 17:Q:4:LYS:HE2 | 17:Q:6:LEU:HD21 | 1.98 | 0.45 |
| 1:A:222:U:H2' | 1:A:223:U:C6 | 2.51 | 0.45 |
| 1:A:342:C:H42 | 1:A:347:G:H1 | 1.62 | 0.45 |
| 1:A:561:U:HO2' | 1:A:562:C:P | 2.40 | 0.45 |
| 1:A:584:G:H2' | 1:A:585:G:C8 | 2.51 | 0.45 |
| 1:A:709:G:H2' | 1:A:710:G:C8 | 2.52 | 0.45 |
| 1:A:1119:C:N4 | 1:A:1154:G:H1 | 2.13 | 0.45 |
| 1:A:1256:A:H4' | 1:A:1257:U:O5' | 2.16 | 0.45 |
| 6:F:40:VAL:HG22 | 6:F:63:TYR:HD2 | 1.80 | 0.45 |
| 8:H:121:ASP:OD2 | 8:H:122:ARG:N | 2.49 | 0.45 |
| 10:J:6:ILE:HA | 10:J:97:GLU:O | 2.17 | 0.45 |
| 11:K:18:ARG:HG3 | 11:K:33:THR:HG23 | 1.99 | 0.45 |
| 15:O:70:LEU:HD22 | 15:O:70:LEU:HA | 1.68 | 0.45 |
| 17:Q:95:TYR:O | 17:Q:98:LEU:HD12 | 2.17 | 0.45 |
| 20:T:53:LEU:HD23 | 20:T:53:LEU:HA | 1.82 | 0.45 |
| 20:T:100:ILE:HG22 | 20:T:102:GLY:H | 1.81 | 0.45 |
| 21:U:6:ARG:H | 21:U:6:ARG:HG3 | 1.57 | 0.45 |
| 1:A:629:G:H2' | 1:A:630:G:O4' | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 1:A:710:G:H2' | 1:A:711:G:C8 | 2.50 | 0.45 |
| 1:A:899:C:H2' | 1:A:900:A:O4' | 2.16 | 0.45 |
| 1:A:1510:U:H2' | 1:A:1511:G:N7 | 2.32 | 0.45 |
| 1:A:1518[B]:MA6:HO2' | 1:A:1519[B]:MA6:P | 2.40 | 0.45 |
| 2:B:184:VAL:O | 2:B:198:ASP:HB2 | 2.16 | 0.45 |
| 7:G:71:PRO:HG3 | 7:G:103:TRP:HZ3 | 1.81 | 0.45 |
| 7:G:107:ALA:HA | 7:G:110:GLN:HG2 | 1.99 | 0.45 |
| 7:G:139:GLU:CG | 7:G:143:ARG:HH22 | 2.28 | 0.45 |
| 8:H:86:ILE:HG21 | 8:H:133:LEU:HD13 | 1.99 | 0.45 |
| 9:I:111:ARG:O | 9:I:111:ARG:HG3 | 2.16 | 0.45 |
| 16:P:41:PRO:O | 16:P:43:LYS:HD2 | 2.17 | 0.45 |
| 19:S:16:LEU:HD11 | 19:S:20:LEU:HD23 | 1.98 | 0.45 |
| 1:A:509:A:C8 | 1:A:509:A:C3' | 3.00 | 0.45 |
| 1:A:542:G:O2' | 1:A:543:C:H5' | 2.16 | 0.45 |
| 1:A:725:G:C4 | 1:A:726:C:C5 | 3.05 | 0.45 |
| 1:A:782:A:H2' | 1:A:783:C:O4' | 2.17 | 0.45 |
| 1:A:1403:C:N4 | 1:A:1544:U:OP1 | 2.50 | 0.45 |
| 1:A:1414:U:H2' | 1:A:1415:G:H8 | 1.82 | 0.45 |
| 1:A:1503:A:N6 | 1:A:1532:U:O2' | 2.49 | 0.45 |
| 3:C:182:ILE:HG22 | 3:C:183:ASP:O | 2.16 | 0.45 |
| 4:D:35:ARG:O | 4:D:36:ARG:HG2 | 2.15 | 0.45 |
| 4:D:63:LYS:O | 4:D:67:ILE:HG13 | 2.17 | 0.45 |
| 5:E:17:ALA:HB2 | 5:E:26:PHE:CD2 | 2.52 | 0.45 |
| 5:E:79:GLU:HG3 | 8:H:105:ARG:CG | 2.45 | 0.45 |
| 10:J:6:ILE:O | 10:J:72:VAL:HG23 | 2.17 | 0.45 |
| 15:O:41:GLU:OE2 | 15:O:44:LYS:HD3 | 2.16 | 0.45 |
| 1:A:112:G:H21 | 1:A:354:G:C4' | 2.30 | 0.45 |
| 1:A:502:G:H2' | 1:A:503:C:O4' | 2.16 | 0.45 |
| 1:A:933:G:N1 | 1:A:935:A:H1' | 2.32 | 0.45 |
| 1:A:966:M2G:C8 | 1:A:967:5MC:HM52 | 2.52 | 0.45 |
| 1:A:1233:G:C2 | 1:A:1234:C:C4 | 3.05 | 0.45 |
| 1:A:1514:C:H2' | 1:A:1515[A]:C:O4' | 2.16 | 0.45 |
| 4:D:10:ARG:HG3 | 4:D:40:PRO:HG3 | 1.98 | 0.45 |
| 8:H:51:VAL:HG11 | 8:H:60:ARG:HH12 | 1.82 | 0.45 |
| 1:A:950:U:H2' | 1:A:951:G:H8 | 1.82 | 0.45 |
| 1:A:1015:A:H2' | 1:A:1016:A:C8 | 2.52 | 0.45 |
| 1:A:1349:A:OP1 | 9:I:120:ARG:HB2 | 2.16 | 0.45 |
| 1:A:1518[A]:MA6:N6 | 1:A:1519[A]:MA6:H103 | 2.32 | 0.45 |
| 1:A:1539:C:H5'' | 7:G:82:GLY:HA2 | 1.99 | 0.45 |
| 3:C:150:LYS:CG | 3:C:169:ALA:HB2 | 2.46 | 0.45 |
| 5:E:75:THR:C | 5:E:76:ILE:HD13 | 2.37 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:7:ASN:HD22 | 6:F:7:ASN:N | 2.14 | 0.45 |
| 20:T:10:LEU:HD22 | 20:T:11:SER:H | 1.82 | 0.45 |
| 1:A:499:A:C6 | 1:A:547:A:C8 | 3.05 | 0.45 |
| 1:A:711:G:N3 | 1:A:712:A:C8 | 2.85 | 0.45 |
| 1:A:1377:A:OP2 | 7:G:94:ARG:NE | 2.50 | 0.45 |
| 7:G:99:LEU:HD22 | 7:G:103:TRP:CZ3 | 2.52 | 0.45 |
| 14:N:6:LEU:HA | 14:N:6:LEU:HD23 | 1.63 | 0.45 |
| 14:N:31:ARG:O | 14:N:33:VAL:HG22 | 2.17 | 0.45 |
| 1:A:73:C:O2' | 1:A:74:C:H5' | 2.17 | 0.44 |
| 1:A:874:G:C6 | 1:A:875:C:C4 | 3.04 | 0.44 |
| 1:A:936:C:H2' | 1:A:937:A:O4' | 2.17 | 0.44 |
| 1:A:1392:G:H8 | 1:A:1392:G:O5' | 2.01 | 0.44 |
| 1:A:1481:U:O2' | 1:A:1482:G:H5' | 2.17 | 0.44 |
| 4:D:107:ARG:NH1 | 4:D:114:ARG:HH22 | 2.15 | 0.44 |
| 5:E:46:GLY:N | 5:E:58:ALA:HB2 | 2.31 | 0.44 |
| 11:K:33:THR:OG1 | 11:K:34:ASP:N | 2.49 | 0.44 |
| 12:L:38:THR:HB | 12:L:39:VAL:H | 1.66 | 0.44 |
| 12:L:111:LYS:O | 12:L:112:ASP:HB2 | 2.17 | 0.44 |
| 14:N:32:SER:HB2 | 14:N:41:ARG:HB3 | 1.98 | 0.44 |
| 15:O:49:ASP:OD1 | 15:O:52:SER:OG | 2.22 | 0.44 |
| 17:Q:29:HIS:HB2 | 17:Q:36:ILE:HD12 | 2.00 | 0.44 |
| 19:S:5:LEU:C | 19:S:6:LYS:HZ3 | 2.20 | 0.44 |
| 1:A:226:G:C2 | 1:A:227:G:C8 | 3.05 | 0.44 |
| 1:A:489:C:H2' | 1:A:490:G:C8 | 2.48 | 0.44 |
| 1:A:711:G:H2' | 1:A:712:A:C8 | 2.49 | 0.44 |
| 1:A:792:A:H4' | 1:A:793:U:H5'' | 1.99 | 0.44 |
| 1:A:1250:A:H4' | 9:I:67:GLY:HA2 | 2.00 | 0.44 |
| 1:A:1307:U:H2' | 1:A:1308:U:H6 | 1.82 | 0.44 |
| 1:A:1416:G:H2' | 1:A:1417:G:H5' | 1.99 | 0.44 |
| 1:A:1506:U:N3 | 1:A:1522:U:OP1 | 2.29 | 0.44 |
| 2:B:221:LEU:HD13 | 2:B:222:ILE:N | 2.32 | 0.44 |
| 5:E:28:PHE:O | 5:E:47:LYS:HA | 2.16 | 0.44 |
| 5:E:91:LEU:HA | 5:E:91:LEU:HD23 | 1.59 | 0.44 |
| 5:E:127:ASN:HA | 5:E:128:PRO:HD2 | 1.81 | 0.44 |
| 6:F:3:ARG:HG2 | 6:F:93:SER:HB2 | 1.99 | 0.44 |
| 8:H:119:LEU:N | 8:H:119:LEU:HD12 | 2.33 | 0.44 |
| 9:I:48:GLU:HB3 | 9:I:101:PHE:CZ | 2.52 | 0.44 |
| 12:L:28:LYS:HD2 | 12:L:33:ARG:NE | 2.32 | 0.44 |
| 15:O:51:HIS:O | 15:O:54:ARG:HB3 | 2.18 | 0.44 |
| 15:O:74:ASP:HA | 15:O:75:PRO:HD2 | 1.85 | 0.44 |
| 17:Q:27:PHE:HA | 17:Q:28:PRO:HD3 | 1.66 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 19:S:7:LYS:H | 19:S:7:LYS:HZ3 | 1.65 | 0.44 |
| 20:T:36:LEU:HD22 | 20:T:36:LEU:HA | 1.83 | 0.44 |
| 20:T:65:LYS:O | 20:T:68:LYS:HB2 | 2.18 | 0.44 |
| 1:A:106:C:H2' | 1:A:107:G:H8 | 1.81 | 0.44 |
| 1:A:414:A:OP2 | 1:A:428:G:N2 | 2.43 | 0.44 |
| 1:A:785:G:C2 | 1:A:786:G:C8 | 3.06 | 0.44 |
| 1:A:929:G:C5 | 1:A:930:C:C5 | 3.05 | 0.44 |
| 1:A:1086:U:O2' | 1:A:1087:G:H5' | 2.18 | 0.44 |
| 1:A:1143:G:H2' | 1:A:1144:G:C8 | 2.53 | 0.44 |
| 1:A:1254:C:O4' | 1:A:1356:G:H5'' | 2.17 | 0.44 |
| 1:A:1356:G:H2' | 1:A:1357:A:C8 | 2.52 | 0.44 |
| 1:A:1539:C:H2' | 1:A:1540:PSU:H5'' | 1.98 | 0.44 |
| 3:C:123:GLN:HB2 | 3:C:128:PHE:CD1 | 2.37 | 0.44 |
| 4:D:61:LYS:HG3 | 4:D:62:GLN:N | 2.27 | 0.44 |
| 4:D:177:ASP:OD2 | 4:D:179:GLU:HG2 | 2.17 | 0.44 |
| 9:I:28:VAL:HG22 | 9:I:63:ILE:HB | 1.98 | 0.44 |
| 10:J:38:ILE:HG13 | 10:J:71:LEU:HB2 | 1.99 | 0.44 |
| 17:Q:57:VAL:HG12 | 17:Q:76:LEU:HA | 1.98 | 0.44 |
| 1:A:147:G:H1 | 1:A:175:C:H42 | 1.65 | 0.44 |
| 1:A:412:A:N6 | 4:D:35:ARG:HB3 | 2.33 | 0.44 |
| 1:A:484:G:H5' | 1:A:486:U:O4' | 2.17 | 0.44 |
| 1:A:486:U:H2' | 1:A:487:A:H8 | 1.82 | 0.44 |
| 1:A:762:C:H2' | 1:A:763:G:H8 | 1.83 | 0.44 |
| 1:A:1053:G:C3' | 1:A:1054:C:H5' | 2.47 | 0.44 |
| 1:A:1438:G:H2' | 1:A:1439:C:C6 | 2.52 | 0.44 |
| 1:A:1476:G:O2' | 1:A:1477:C:H5' | 2.17 | 0.44 |
| 1:A:1496:C:H2' | 1:A:1497:G:O4' | 2.18 | 0.44 |
| 2:B:71:VAL:HG13 | 2:B:93:VAL:HB | 2.00 | 0.44 |
| 4:D:172:PRO:HD2 | 4:D:173:TRP:CZ3 | 2.53 | 0.44 |
| 6:F:40:VAL:HG22 | 6:F:63:TYR:CD2 | 2.52 | 0.44 |
| 6:F:68:PRO:HG2 | 6:F:71:ARG:NH2 | 2.33 | 0.44 |
| 14:N:23:ARG:HA | 14:N:29:ARG:O | 2.16 | 0.44 |
| 1:A:138:G:N2 | 1:A:226:G:N3 | 2.66 | 0.44 |
| 1:A:255:G:C2 | 1:A:256:U:C4 | 3.05 | 0.44 |
| 1:A:372:C:H4' | 1:A:373:A:OP1 | 2.17 | 0.44 |
| 1:A:1387:G:C6 | 1:A:1388:C:N4 | 2.85 | 0.44 |
| 2:B:136:VAL:O | 2:B:140:HIS:HB2 | 2.17 | 0.44 |
| 4:D:190:ASP:OD2 | 4:D:190:ASP:C | 2.56 | 0.44 |
| 6:F:10:LEU:H | 6:F:10:LEU:HD12 | 1.82 | 0.44 |
| 7:G:74:GLU:HG2 | 7:G:91:VAL:HG11 | 2.00 | 0.44 |
| 8:H:52:ASP:OD1 | 8:H:56:LYS:N | 2.51 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 10:J:7:LYS:O | 10:J:8:LEU:HD23 | 2.18 | 0.44 |
| 13:M:91:ARG:HA | 13:M:91:ARG:HD2 | 1.81 | 0.44 |
| 1:A:79:G:C2 | 1:A:80:G:C8 | 3.06 | 0.44 |
| 1:A:194:C:H2' | 1:A:195:A:H5'' | 1.99 | 0.44 |
| 1:A:386:C:H2' | 1:A:387:U:H5' | 1.99 | 0.44 |
| 1:A:693:G:H2' | 1:A:694:A:H8 | 1.82 | 0.44 |
| 1:A:764:C:H5'' | 1:A:765:G:OP2 | 2.18 | 0.44 |
| 1:A:1072:G:C5 | 1:A:1073:U:C4 | 3.06 | 0.44 |
| 1:A:1241:G:H2' | 1:A:1242:C:C6 | 2.52 | 0.44 |
| 1:A:1484:C:H2' | 1:A:1485:U:O4' | 2.17 | 0.44 |
| 2:B:166:ASP:HB3 | 2:B:169:LYS:HB3 | 2.00 | 0.44 |
| 9:I:7:THR:HG22 | 9:I:8:GLY:N | 2.32 | 0.44 |
| 10:J:25:GLU:HA | 10:J:28:ARG:HB2 | 2.00 | 0.44 |
| 17:Q:59:ILE:HD13 | 17:Q:59:ILE:HA | 1.77 | 0.44 |
| 1:A:622:A:C8 | 1:A:623:C:C6 | 3.05 | 0.44 |
| 1:A:826:C:H5' | 8:H:12:ARG:CZ | 2.47 | 0.44 |
| 1:A:1221:G:H4' | 19:S:77:THR:CG2 | 2.48 | 0.44 |
| 1:A:1417:G:H2' | 1:A:1482:G:N2 | 2.33 | 0.44 |
| 1:A:1484:C:C4 | 1:A:1485:U:O2 | 2.71 | 0.44 |
| 3:C:11:ARG:O | 3:C:14:ILE:O | 2.34 | 0.44 |
| 5:E:116:THR:OG1 | 5:E:117:ASP:N | 2.51 | 0.44 |
| 8:H:86:ILE:HG21 | 8:H:133:LEU:HD22 | 1.99 | 0.44 |
| 9:I:48:GLU:HB3 | 9:I:101:PHE:HZ | 1.83 | 0.44 |
| 17:Q:29:HIS:HB2 | 17:Q:36:ILE:CD1 | 2.48 | 0.44 |
| 1:A:544:G:P | 4:D:59:ARG:HH22 | 2.39 | 0.44 |
| 1:A:932:C:H2' | 1:A:933:G:C8 | 2.52 | 0.44 |
| 3:C:35:GLU:HG3 | 3:C:95:THR:HG21 | 1.99 | 0.44 |
| 7:G:17:VAL:HG12 | 7:G:18:TYR:HD1 | 1.83 | 0.44 |
| 8:H:56:LYS:HA | 8:H:57:PRO:HD3 | 1.80 | 0.44 |
| 13:M:14:ARG:HB3 | 13:M:41:PRO:O | 2.17 | 0.44 |
| 13:M:86:CYS:O | 13:M:90:LEU:HD22 | 2.18 | 0.44 |
| 15:O:57:LEU:HA | 15:O:57:LEU:HD13 | 1.45 | 0.44 |
| 1:A:254:G:N3 | 1:A:255:G:C8 | 2.86 | 0.44 |
| 1:A:427:U:C4 | 1:A:428:G:C6 | 3.06 | 0.44 |
| 1:A:803:G:H2' | 1:A:804:U:O4' | 2.18 | 0.44 |
| 1:A:1459:C:H2' | 1:A:1460:A:O4' | 2.18 | 0.44 |
| 1:A:1478:C:H2' | 1:A:1479:C:O4' | 2.18 | 0.44 |
| 4:D:104:VAL:O | 4:D:108:LEU:HB2 | 2.18 | 0.44 |
| 8:H:13:ILE:O | 8:H:17:THR:HG23 | 2.18 | 0.44 |
| 8:H:40:ALA:O | 8:H:42:GLU:N | 2.51 | 0.44 |
| 11:K:59:TYR:CE2 | 11:K:63:LEU:HD11 | 2.52 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 14:N:15:LYS:HB3 | 14:N:15:LYS:HE2 | 1.74 | 0.44 |
| 17:Q:26:GLN:O | 17:Q:27:PHE:HB3 | 2.18 | 0.44 |
| 20:T:87:LYS:HE2 | 20:T:87:LYS:HB2 | 1.91 | 0.44 |
| 1:A:67:C:H2' | 1:A:68:G:C8 | 2.53 | 0.43 |
| 1:A:113:G:H1 | 1:A:314:C:H42 | 1.66 | 0.43 |
| 1:A:670:G:H1 | 1:A:736:C:H42 | 1.66 | 0.43 |
| 1:A:967:5MC:H2' | 1:A:968:A:C8 | 2.53 | 0.43 |
| 4:D:194:LEU:HB3 | 4:D:196:LEU:CD2 | 2.48 | 0.43 |
| 8:H:86:ILE:HG21 | 8:H:133:LEU:HB3 | 1.99 | 0.43 |
| 10:J:57:LYS:HG3 | 10:J:57:LYS:O | 2.18 | 0.43 |
| 13:M:29:ARG:HB3 | 13:M:64:TRP:CZ3 | 2.53 | 0.43 |
| 19:S:39:THR:HG22 | 19:S:70:LYS:CD | 2.42 | 0.43 |
| 1:A:235:C:N4 | 24:A:1842:HOH:O | 2.51 | 0.43 |
| 1:A:518:C:H2' | 1:A:530:G:C8 | 2.53 | 0.43 |
| 1:A:707:C:OP1 | 11:K:85:ARG:NH1 | 2.51 | 0.43 |
| 1:A:954:G:H2' | 1:A:955:U:C6 | 2.54 | 0.43 |
| 1:A:1104:G:H5'' | 1:A:1104:G:H8 | 1.82 | 0.43 |
| 1:A:1399:C:O2 | 1:A:1401:G:C5 | 2.71 | 0.43 |
| 2:B:57:PHE:CG | 2:B:199:TYR:CE1 | 3.06 | 0.43 |
| 8:H:63:LEU:HD13 | 8:H:63:LEU:H | 1.83 | 0.43 |
| 10:J:57:LYS:HG3 | 10:J:60:ARG:NH1 | 2.29 | 0.43 |
| 12:L:33:ARG:HG2 | 12:L:62:SER:HB3 | 2.00 | 0.43 |
| 13:M:94:ARG:HB3 | 13:M:96:LEU:HD12 | 2.00 | 0.43 |
| 14:N:11:LYS:HE2 | 14:N:11:LYS:HB3 | 1.78 | 0.43 |
| 17:Q:43:LEU:HD23 | 17:Q:68:ARG:NH2 | 2.32 | 0.43 |
| 1:A:64:G:H4' | 1:A:65:U:H3' | 2.00 | 0.43 |
| 1:A:104:G:C2 | 1:A:105:G:C8 | 3.06 | 0.43 |
| 1:A:277:C:OP2 | 17:Q:41:LYS:HE3 | 2.19 | 0.43 |
| 1:A:382:A:C2 | 1:A:383:A:C4 | 3.06 | 0.43 |
| 1:A:673:G:H5'' | 6:F:87:ARG:NH1 | 2.33 | 0.43 |
| 1:A:841:U:H6 | 1:A:848:C:H5' | 1.82 | 0.43 |
| 1:A:1297:C:H4' | 1:A:1298:C:H5' | 2.00 | 0.43 |
| 4:D:117:ALA:O | 4:D:121:VAL:HG23 | 2.18 | 0.43 |
| 5:E:142:LEU:O | 5:E:143:ARG:HD3 | 2.17 | 0.43 |
| 9:I:65:VAL:HG11 | 9:I:73:GLN:CD | 2.38 | 0.43 |
| 9:I:117:HIS:HB2 | 9:I:121:ARG:HG2 | 2.00 | 0.43 |
| 12:L:33:ARG:HB3 | 12:L:60:LEU:CD1 | 2.49 | 0.43 |
| 1:A:186:C:O3' | 20:T:82:SER:HB2 | 2.19 | 0.43 |
| 1:A:392:G:H2' | 1:A:393:A:C8 | 2.54 | 0.43 |
| 1:A:949:A:N1 | 1:A:1233:G:N3 | 2.67 | 0.43 |
| 1:A:1005:A:C2 | 1:A:1006:C:C2 | 3.07 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:A:1022:G:H2' | 1:A:1023:G:O4' | 2.17 | 0.43 |
| 1:A:1052:U:O4 | 1:A:1200:C:C2 | 2.71 | 0.43 |
| 1:A:1198:G:C6 | 1:A:1199:U:C4 | 3.07 | 0.43 |
| 1:A:1468:A:O5' | 1:A:1468:A:H8 | 2.02 | 0.43 |
| 1:A:1519[B]:MA6:N7 | 1:A:1520[B]:G:H1' | 2.33 | 0.43 |
| 4:D:5:ILE:O | 4:D:5:ILE:HG12 | 2.19 | 0.43 |
| 8:H:23:SER:HA | 8:H:63:LEU:CD1 | 2.48 | 0.43 |
| 13:M:87:TYR:HA | 13:M:90:LEU:CD2 | 2.48 | 0.43 |
| 15:O:79:ARG:HE | 15:O:79:ARG:HB2 | 1.56 | 0.43 |
| 16:P:34:GLU:OE2 | 16:P:55:ARG:HD2 | 2.18 | 0.43 |
| 17:Q:24:GLU:HA | 17:Q:38:ARG:O | 2.18 | 0.43 |
| 17:Q:68:ARG:N | 17:Q:70:ARG:HH12 | 2.16 | 0.43 |
| 18:R:23:LYS:HE3 | 18:R:57:GLY:O | 2.17 | 0.43 |
| 1:A:261:U:O2 | 1:A:263:A:C8 | 2.71 | 0.43 |
| 1:A:358:U:H2' | 1:A:359:U:C6 | 2.53 | 0.43 |
| 1:A:778:G:H1 | 1:A:804:U:H3 | 1.67 | 0.43 |
| 1:A:947:G:H1 | 1:A:1234:C:H42 | 1.65 | 0.43 |
| 1:A:1124:G:H22 | 1:A:1280:A:N6 | 2.17 | 0.43 |
| 3:C:114:PRO:O | 3:C:118:GLN:HG3 | 2.19 | 0.43 |
| 4:D:31:CYS:C | 4:D:33:MET:N | 2.71 | 0.43 |
| 4:D:79:PHE:HA | 4:D:93:PHE:CE2 | 2.53 | 0.43 |
| 9:I:49:PRO:HG2 | 9:I:50:LEU:HD12 | 1.99 | 0.43 |
| 11:K:77:MET:O | 11:K:78:GLN:NE2 | 2.43 | 0.43 |
| 1:A:200:G:H2' | 1:A:201:C:O4' | 2.19 | 0.43 |
| 1:A:352:C:O2' | 1:A:354:G:OP1 | 2.33 | 0.43 |
| 1:A:585:G:O5' | 1:A:585:G:H8 | 2.00 | 0.43 |
| 1:A:674:G:H2' | 1:A:675:A:H8 | 1.83 | 0.43 |
| 1:A:1213:A:C4 | 1:A:1215:G:C8 | 3.07 | 0.43 |
| 1:A:1256:A:N3 | 1:A:1256:A:O4' | 2.51 | 0.43 |
| 3:C:101:LEU:HD23 | 3:C:101:LEU:HA | 1.77 | 0.43 |
| 6:F:99:ALA:O | 18:R:28:GLU:HG3 | 2.19 | 0.43 |
| 7:G:111:ARG:HB3 | 7:G:113:GLU:OE2 | 2.19 | 0.43 |
| 10:J:50:ILE:H | 10:J:50:ILE:CD1 | 2.31 | 0.43 |
| 20:T:48:LYS:H | 20:T:48:LYS:HG2 | 1.39 | 0.43 |
| 1:A:110:C:H2' | 1:A:111:G:O4' | 2.19 | 0.43 |
| 1:A:229:U:H2' | 1:A:230:G:C8 | 2.54 | 0.43 |
| 1:A:332:G:H2' | 1:A:333:G:H8 | 1.83 | 0.43 |
| 1:A:429:U:O3' | 4:D:22:LYS:HE3 | 2.18 | 0.43 |
| 1:A:443:C:H2' | 1:A:444:C:H6 | 1.82 | 0.43 |
| 1:A:925:G:O2' | 1:A:926:G:H5'' | 2.18 | 0.43 |
| 1:A:1172:C:H2' | 1:A:1173:G:C8 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1192:C:P | 3:C:4:LYS:HZ1 | 2.41 | 0.43 |
| 1:A:1220:G:H2' | 1:A:1221:G:H8 | 1.84 | 0.43 |
| 1:A:1427:U:H2' | 1:A:1428:A:H8 | 1.80 | 0.43 |
| 3:C:188:LEU:CD1 | 3:C:195:VAL:HG13 | 2.49 | 0.43 |
| 4:D:25:ARG:HA | 4:D:28:SER:HB3 | 2.00 | 0.43 |
| 11:K:91:ARG:HB3 | 11:K:92:GLU:OE1 | 2.19 | 0.43 |
| 12:L:28:LYS:HB3 | 12:L:30:ALA:CB | 2.49 | 0.43 |
| 15:O:32:LEU:HD22 | 15:O:32:LEU:HA | 1.64 | 0.43 |
| 20:T:10:LEU:HD13 | 20:T:13:LEU:H | 1.84 | 0.43 |
| 1:A:162:A:C5 | 1:A:163:C:H1' | 2.54 | 0.43 |
| 1:A:1095:U:C4 | 1:A:1096:C:C4 | 3.06 | 0.43 |
| 1:A:1179:A:O3' | 9:I:103:THR:HG23 | 2.19 | 0.43 |
| 1:A:1196:U:O2' | 1:A:1197:G:OP1 | 2.33 | 0.43 |
| 1:A:1233:G:N2 | 1:A:1234:C:C2 | 2.87 | 0.43 |
| 1:A:1480:G:C6 | 1:A:1481:U:C4 | 3.06 | 0.43 |
| 1:A:1485:U:C6 | 1:A:1486:G:N7 | 2.87 | 0.43 |
| 3:C:23:TYR:CD1 | 10:J:11:PHE:CE2 | 3.07 | 0.43 |
| 4:D:90:GLY:N | 4:D:204:ILE:HD11 | 2.34 | 0.43 |
| 5:E:79:GLU:HG3 | 5:E:79:GLU:H | 1.48 | 0.43 |
| 6:F:21:LEU:HD12 | 6:F:21:LEU:HA | 1.78 | 0.43 |
| 10:J:69:ASN:O | 10:J:70:ARG:HG3 | 2.18 | 0.43 |
| 17:Q:29:HIS:O | 17:Q:31:LEU:N | 2.51 | 0.43 |
| 1:A:262:A:C6 | 1:A:263:A:C6 | 3.06 | 0.43 |
| 1:A:349:A:H2' | 1:A:350:G:H5'' | 2.00 | 0.43 |
| 1:A:429:U:H4' | 1:A:430:A:O5' | 2.18 | 0.43 |
| 1:A:869:G:N7 | 24:A:2036:HOH:O | 2.36 | 0.43 |
| 1:A:1525:G:C8 | 1:A:1525:G:H3' | 2.54 | 0.43 |
| 3:C:91:LEU:HD23 | 3:C:99:VAL:HG21 | 2.00 | 0.43 |
| 10:J:50:ILE:N | 10:J:50:ILE:CD1 | 2.81 | 0.43 |
| 12:L:84:LEU:HD13 | 12:L:105:TYR:HE1 | 1.84 | 0.43 |
| 16:P:80:PHE:N | 16:P:80:PHE:CD1 | 2.87 | 0.43 |
| 1:A:449:C:C5 | 1:A:450:G:C5 | 3.06 | 0.43 |
| 1:A:695:A:H2' | 1:A:696:A:H8 | 1.78 | 0.43 |
| 1:A:780:A:P | 11:K:122:LYS:HG3 | 2.58 | 0.43 |
| 1:A:947:G:H2' | 1:A:948:C:O4' | 2.19 | 0.43 |
| 1:A:973:G:OP1 | 10:J:57:LYS:HD3 | 2.19 | 0.43 |
| 1:A:1124:G:H4' | 1:A:1125:U:OP1 | 2.19 | 0.43 |
| 1:A:1152:A:H2' | 1:A:1153:C:C6 | 2.54 | 0.43 |
| 1:A:1233:G:OP2 | 9:I:124:GLN:HB3 | 2.18 | 0.43 |
| 3:C:33:LEU:HD21 | 14:N:53:LEU:HD22 | 1.99 | 0.43 |
| 3:C:78:GLY:HA3 | 3:C:83:ARG:HB3 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:80:GLU:O | 4:D:83:SER:N | 2.50 | 0.43 |
| 6:F:8:ILE:HG21 | 6:F:26:ILE:HD11 | 2.01 | 0.43 |
| 12:L:28:LYS:HB3 | 12:L:30:ALA:H | 1.84 | 0.43 |
| 14:N:26:ARG:HH12 | 14:N:47:LEU:HD22 | 1.82 | 0.43 |
| 15:O:8:LYS:O | 15:O:12:ILE:HG13 | 2.19 | 0.43 |
| 18:R:64:ARG:HE | 18:R:64:ARG:HB2 | 1.50 | 0.43 |
| 1:A:554:C:C2' | 1:A:555:C:H5' | 2.49 | 0.42 |
| 1:A:788:U:H2' | 1:A:789:U:C6 | 2.54 | 0.42 |
| 1:A:1023:G:H2' | 1:A:1023:G:N3 | 2.33 | 0.42 |
| 1:A:1361:G:H2' | 1:A:1361(A):C:H6 | 1.84 | 0.42 |
| 2:B:49:GLU:O | 2:B:52:GLU:HB3 | 2.19 | 0.42 |
| 4:D:67:ILE:O | 4:D:114:ARG:HD2 | 2.18 | 0.42 |
| 10:J:47:PHE:HB2 | 10:J:63:PHE:HB2 | 2.01 | 0.42 |
| 13:M:22:ILE:HB | 13:M:25:ILE:HB | 2.01 | 0.42 |
| 14:N:22:THR:OG1 | 14:N:33:VAL:HG21 | 2.19 | 0.42 |
| 14:N:24:CYS:HB3 | 14:N:29:ARG:HB2 | 2.01 | 0.42 |
| 18:R:58:LEU:HD22 | 18:R:62:GLU:HB3 | 2.00 | 0.42 |
| 19:S:41:VAL:HB | 19:S:42:PRO:HD2 | 2.01 | 0.42 |
| 1:A:267:C:H2' | 1:A:268:C:H6 | 1.85 | 0.42 |
| 1:A:576:G:H3' | 1:A:577:G:H5'' | 2.01 | 0.42 |
| 1:A:1029:C:H1' | 1:A:1033:G:H1' | 2.01 | 0.42 |
| 1:A:1039:C:H2' | 1:A:1040:U:C6 | 2.54 | 0.42 |
| 1:A:1063:C:N4 | 1:A:1064:G:C2 | 2.87 | 0.42 |
| 1:A:1188:A:N7 | 1:A:1189:C:C5 | 2.87 | 0.42 |
| 3:C:152:ILE:HB | 3:C:199:LYS:HB2 | 2.01 | 0.42 |
| 4:D:13:ARG:NH1 | 4:D:38:TYR:O | 2.52 | 0.42 |
| 8:H:119:LEU:HD12 | 8:H:119:LEU:H | 1.83 | 0.42 |
| 9:I:17:VAL:HG22 | 9:I:63:ILE:HD12 | 2.01 | 0.42 |
| 11:K:29:ILE:HD12 | 11:K:30:VAL:N | 2.34 | 0.42 |
| 12:L:102:ARG:HE | 12:L:102:ARG:HB3 | 1.52 | 0.42 |
| 17:Q:89:LEU:HA | 17:Q:89:LEU:HD22 | 1.78 | 0.42 |
| 18:R:44:LEU:HD12 | 18:R:48:GLY:O | 2.18 | 0.42 |
| 18:R:53:ARG:NH1 | 18:R:59:SER:HA | 2.33 | 0.42 |
| 19:S:30:LEU:O | 19:S:31:ILE:HB | 2.18 | 0.42 |
| 1:A:148:G:H2' | 1:A:149:A:H8 | 1.85 | 0.42 |
| 1:A:304:U:O2' | 1:A:305:G:H5' | 2.18 | 0.42 |
| 1:A:575:G:O2' | 1:A:821:G:OP2 | 2.24 | 0.42 |
| 1:A:1178:G:N2 | 1:A:1180:A:H3' | 2.34 | 0.42 |
| 6:F:95:GLU:HA | 6:F:96:PRO:HD3 | 1.79 | 0.42 |
| 7:G:57:GLU:O | 7:G:61:VAL:HG23 | 2.19 | 0.42 |
| 7:G:95:ARG:HG3 | 7:G:99:LEU:CD1 | 2.46 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 12:L:28:LYS:HB3 | 12:L:30:ALA:HB2 | 2.01 | 0.42 |
| 19:S:10:PHE:O | 19:S:39:THR:HG23 | 2.18 | 0.42 |
| 20:T:20:LEU:HD13 | 20:T:20:LEU:N | 2.34 | 0.42 |
| 20:T:60:GLU:HG3 | 20:T:81:LYS:HD2 | 2.01 | 0.42 |
| 1:A:52:G:C5 | 1:A:360:A:C2 | 3.07 | 0.42 |
| 1:A:134:A:C6 | 1:A:135:C:C2 | 3.08 | 0.42 |
| 1:A:328:C:H4' | 1:A:329:A:H5' | 2.00 | 0.42 |
| 1:A:526:C:H3' | 1:A:527:7MG:O4' | 2.19 | 0.42 |
| 1:A:561:U:O2' | 1:A:562:C:P | 2.78 | 0.42 |
| 1:A:1502:A:C2 | 1:A:1504:G:C2 | 3.07 | 0.42 |
| 2:B:17:PHE:HA | 2:B:44:LEU:HD21 | 2.01 | 0.42 |
| 4:D:187:ARG:HD2 | 4:D:187:ARG:HA | 1.35 | 0.42 |
| 5:E:63:ARG:HE | 5:E:63:ARG:HB2 | 1.53 | 0.42 |
| 8:H:83:ILE:HA | 8:H:136:GLU:O | 2.18 | 0.42 |
| 9:I:40:LEU:CD1 | 9:I:70:LYS:HD2 | 2.50 | 0.42 |
| 12:L:66:VAL:HG22 | 12:L:67:THR:H | 1.82 | 0.42 |
| 14:N:40:CYS:O | 14:N:44:LEU:HB3 | 2.20 | 0.42 |
| 1:A:122:G:O2' | 1:A:123:C:H5' | 2.19 | 0.42 |
| 2:B:21:ARG:H | 2:B:21:ARG:HG2 | 1.51 | 0.42 |
| 3:C:61:ALA:O | 3:C:63:ASN:N | 2.53 | 0.42 |
| 4:D:24:GLU:O | 4:D:25:ARG:HB3 | 2.19 | 0.42 |
| 4:D:109:GLY:HA3 | 4:D:165:MET:SD | 2.59 | 0.42 |
| 5:E:24:ARG:O | 5:E:25:ARG:HG2 | 2.20 | 0.42 |
| 5:E:139:LEU:HA | 5:E:142:LEU:HG | 2.02 | 0.42 |
| 6:F:9:VAL:HG22 | 6:F:60:PHE:CE2 | 2.55 | 0.42 |
| 8:H:120:THR:OG1 | 8:H:122:ARG:HG3 | 2.20 | 0.42 |
| 9:I:124:GLN:HE21 | 9:I:124:GLN:HB2 | 1.57 | 0.42 |
| 20:T:13:LEU:HD12 | 20:T:14:LYS:N | 2.34 | 0.42 |
| 1:A:115:G:H1' | 1:A:116:A:N7 | 2.34 | 0.42 |
| 1:A:719:C:C5 | 1:A:720:C:C4 | 3.07 | 0.42 |
| 1:A:749:C:O2' | 1:A:750:G:H5' | 2.20 | 0.42 |
| 1:A:986:A:H2' | 1:A:987:G:O4' | 2.19 | 0.42 |
| 1:A:1130:A:OP1 | 1:A:1130:A:C8 | 2.67 | 0.42 |
| 1:A:1532:U:H3' | 1:A:1532:U:H6 | 1.83 | 0.42 |
| 5:E:78:HIS:NE2 | 5:E:142:LEU:HA | 2.35 | 0.42 |
| 6:F:16:GLN:OE1 | 6:F:16:GLN:HA | 2.18 | 0.42 |
| 14:N:57:ARG:HG2 | 14:N:58:LYS:N | 2.34 | 0.42 |
| 15:O:70:LEU:HD12 | 15:O:78:TYR:N | 2.34 | 0.42 |
| 17:Q:87:LYS:O | 17:Q:90:ILE:N | 2.52 | 0.42 |
| 20:T:100:ILE:HG22 | 20:T:102:GLY:N | 2.34 | 0.42 |
| 1:A:99:C:H2' | 1:A:101:A:C8 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|----------------------|--------------------------|-------------------|
| 1:A:289:G:P | 24:A:1801:HOH:O | 2.77 | 0.42 |
| 1:A:437:U:H5'' | 4:D:155:LEU:HD11 | 2.01 | 0.42 |
| 1:A:620:C:C2 | 4:D:135:LEU:HD22 | 2.54 | 0.42 |
| 1:A:687:A:H2' | 1:A:701:C:H41 | 1.84 | 0.42 |
| 4:D:186:LEU:HD23 | 4:D:186:LEU:N | 2.30 | 0.42 |
| 5:E:43:LEU:HD21 | 5:E:132:ALA:HB1 | 2.01 | 0.42 |
| 5:E:153:LYS:O | 5:E:153:LYS:HG2 | 2.20 | 0.42 |
| 7:G:38:LEU:O | 7:G:41:ARG:HB3 | 2.18 | 0.42 |
| 8:H:40:ALA:HB2 | 8:H:45:ILE:CD1 | 2.44 | 0.42 |
| 11:K:126:ARG:HG3 | 11:K:126:ARG:NH1 | 2.35 | 0.42 |
| 13:M:3:ARG:O | 13:M:57:ARG:NE | 2.50 | 0.42 |
| 14:N:43:CYS:O | 14:N:46:GLU:N | 2.53 | 0.42 |
| 16:P:36:ILE:HD13 | 16:P:36:ILE:HG21 | 1.76 | 0.42 |
| 20:T:74:LYS:HE2 | 20:T:74:LYS:HA | 2.02 | 0.42 |
| 1:A:642:A:H2' | 1:A:643:C:H6 | 1.84 | 0.42 |
| 1:A:653:A:O4' | 8:H:56:LYS:HD3 | 2.19 | 0.42 |
| 1:A:807:A:C6 | 1:A:808:C:N4 | 2.87 | 0.42 |
| 1:A:1239:A:C4 | 1:A:1298:C:N4 | 2.88 | 0.42 |
| 1:A:1251:A:H2' | 1:A:1252:A:C8 | 2.55 | 0.42 |
| 4:D:89:THR:O | 4:D:92:VAL:HG12 | 2.20 | 0.42 |
| 4:D:108:LEU:HD23 | 4:D:108:LEU:HA | 1.89 | 0.42 |
| 5:E:64:ARG:O | 5:E:65:ASN:HB3 | 2.19 | 0.42 |
| 6:F:47:ARG:HH22 | 6:F:56:PRO:HB3 | 1.85 | 0.42 |
| 7:G:5:ARG:HH21 | 7:G:7:ALA:HA | 1.84 | 0.42 |
| 9:I:69:GLY:O | 9:I:73:GLN:HG3 | 2.19 | 0.42 |
| 10:J:23:ILE:HD12 | 10:J:72:VAL:HG21 | 2.01 | 0.42 |
| 10:J:88:LEU:N | 10:J:88:LEU:CD2 | 2.80 | 0.42 |
| 19:S:70:LYS:HE3 | 19:S:70:LYS:HB3 | 1.76 | 0.42 |
| 1:A:363:A:OP2 | 12:L:34:ARG:NH1 | 2.52 | 0.42 |
| 1:A:390:C:H4' | 16:P:28:ARG:HH21 | 1.85 | 0.42 |
| 1:A:514:C:C2' | 1:A:515:G:H5' | 2.49 | 0.42 |
| 1:A:849:C:H2' | 1:A:850:U:H6 | 1.84 | 0.42 |
| 1:A:1309:G:N1 | 1:A:1329:A:C4 | 2.88 | 0.42 |
| 1:A:1518[A]:MA6:C6 | 1:A:1519[A]:MA6:H103 | 2.50 | 0.42 |
| 5:E:15:ARG:HA | 5:E:28:PHE:CE2 | 2.55 | 0.42 |
| 5:E:26:PHE:CD1 | 5:E:26:PHE:N | 2.88 | 0.42 |
| 7:G:38:LEU:HD23 | 7:G:38:LEU:HA | 1.85 | 0.42 |
| 14:N:14:PRO:C | 14:N:16:PHE:H | 2.23 | 0.42 |
| 1:A:36:C:O2' | 12:L:117:ARG:NH2 | 2.53 | 0.42 |
| 1:A:519:C:H2' | 1:A:520:A:C8 | 2.55 | 0.42 |
| 1:A:1097:C:H2' | 1:A:1098:C:C6 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1127:G:H8 | 1:A:1127:G:H3' | 1.83 | 0.42 |
| 1:A:1316:G:O6 | 19:S:5:LEU:HD21 | 2.20 | 0.42 |
| 2:B:69:LEU:HB3 | 2:B:162:ILE:CD1 | 2.50 | 0.42 |
| 5:E:98:THR:N | 5:E:117:ASP:OD1 | 2.53 | 0.42 |
| 6:F:37:VAL:HG12 | 6:F:39:LYS:O | 2.20 | 0.42 |
| 15:O:4:THR:OG1 | 15:O:7:GLU:HG3 | 2.20 | 0.42 |
| 18:R:78:LEU:H | 18:R:78:LEU:HG | 1.60 | 0.42 |
| 1:A:579:G:H2' | 1:A:580:U:C6 | 2.55 | 0.41 |
| 1:A:1108:G:H2' | 1:A:1109:C:H5' | 2.02 | 0.41 |
| 1:A:1112:C:C4 | 3:C:178:LEU:HD12 | 2.55 | 0.41 |
| 1:A:1226:C:H5'' | 19:S:80:TYR:CE2 | 2.54 | 0.41 |
| 1:A:1326:C:H2' | 1:A:1327:C:C6 | 2.55 | 0.41 |
| 1:A:1350:A:H2' | 1:A:1351:U:C6 | 2.55 | 0.41 |
| 2:B:209:ARG:HD3 | 2:B:239:VAL:HG11 | 2.02 | 0.41 |
| 5:E:95:ALA:HB1 | 5:E:96:PRO:HD2 | 2.01 | 0.41 |
| 9:I:7:THR:O | 9:I:15:ALA:O | 2.38 | 0.41 |
| 20:T:89:ARG:HG2 | 20:T:90:GLN:N | 2.35 | 0.41 |
| 1:A:257:G:C2 | 1:A:270:A:C2 | 3.08 | 0.41 |
| 1:A:373:A:C2 | 1:A:482:A:C6 | 3.08 | 0.41 |
| 1:A:671:G:N3 | 1:A:671:G:H2' | 2.34 | 0.41 |
| 1:A:801:U:H2' | 1:A:802:A:C8 | 2.55 | 0.41 |
| 1:A:829:G:N2 | 1:A:830:G:H1' | 2.35 | 0.41 |
| 1:A:1107:C:OP1 | 3:C:172:ARG:HB2 | 2.20 | 0.41 |
| 1:A:1136:U:H6 | 1:A:1136:U:H2' | 1.61 | 0.41 |
| 1:A:1453:G:H2' | 1:A:1454:G:O4' | 2.20 | 0.41 |
| 1:A:1497:G:C2' | 1:A:1498:UR3:H5' | 2.50 | 0.41 |
| 2:B:74:LYS:NZ | 2:B:76:GLN:HG3 | 2.35 | 0.41 |
| 2:B:100:GLY:O | 2:B:104:ASN:N | 2.50 | 0.41 |
| 2:B:213:LEU:O | 2:B:217:ARG:HG2 | 2.20 | 0.41 |
| 5:E:90:VAL:O | 5:E:120:THR:HA | 2.20 | 0.41 |
| 8:H:5:PRO:O | 8:H:8:ASP:HB3 | 2.19 | 0.41 |
| 15:O:29:VAL:HG21 | 15:O:67:LEU:HG | 2.03 | 0.41 |
| 1:A:33:A:O2' | 1:A:363:A:H1' | 2.20 | 0.41 |
| 1:A:146:G:C2 | 1:A:147:G:C8 | 3.09 | 0.41 |
| 1:A:273:A:N6 | 1:A:274:A:C6 | 2.89 | 0.41 |
| 1:A:289:G:N2 | 1:A:290:C:C2 | 2.88 | 0.41 |
| 1:A:552:U:O2' | 12:L:86:ARG:O | 2.34 | 0.41 |
| 1:A:672:U:H2' | 1:A:673:G:H8 | 1.86 | 0.41 |
| 1:A:1026:G:C8 | 1:A:1026:G:C3' | 3.02 | 0.41 |
| 6:F:74:ASP:HA | 6:F:77:ARG:HH11 | 1.85 | 0.41 |
| 8:H:99:GLU:O | 8:H:101:PRO:HD3 | 2.19 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 10:J:80:LYS:HG2 | 10:J:83:GLU:OE2 | 2.21 | 0.41 |
| 13:M:37:THR:HG21 | 13:M:56:LEU:HA | 2.01 | 0.41 |
| 13:M:90:LEU:O | 13:M:93:ARG:HB3 | 2.21 | 0.41 |
| 1:A:563:A:N7 | 1:A:567:G:H1' | 2.36 | 0.41 |
| 1:A:670:G:C4 | 1:A:671:G:C8 | 3.08 | 0.41 |
| 1:A:688:G:H5' | 11:K:46:GLY:O | 2.19 | 0.41 |
| 1:A:1071:C:H2' | 1:A:1072:G:C8 | 2.55 | 0.41 |
| 1:A:1516[A]:G:H2' | 1:A:1518[A]:MA6:OP2 | 2.20 | 0.41 |
| 3:C:75:VAL:O | 3:C:83:ARG:HD3 | 2.21 | 0.41 |
| 4:D:13:ARG:HD2 | 4:D:36:ARG:O | 2.21 | 0.41 |
| 4:D:124:GLY:HA3 | 4:D:132:ARG:NH1 | 2.35 | 0.41 |
| 5:E:43:LEU:HD12 | 5:E:43:LEU:HA | 1.72 | 0.41 |
| 5:E:110:LEU:HD13 | 5:E:118:ILE:HD13 | 2.01 | 0.41 |
| 7:G:101:LEU:HD12 | 7:G:101:LEU:H | 1.84 | 0.41 |
| 8:H:101:PRO:HG3 | 8:H:133:LEU:HD11 | 2.00 | 0.41 |
| 12:L:98:TYR:CD1 | 12:L:98:TYR:N | 2.89 | 0.41 |
| 1:A:486:U:C2 | 1:A:487:A:C8 | 3.08 | 0.41 |
| 1:A:524:G:C6 | 1:A:525:C:N4 | 2.89 | 0.41 |
| 1:A:667:G:H4' | 15:O:51:HIS:CE1 | 2.55 | 0.41 |
| 1:A:996:A:N1 | 1:A:1045:C:O2' | 2.47 | 0.41 |
| 1:A:1104:G:H4' | 2:B:111:ARG:HD3 | 2.03 | 0.41 |
| 2:B:187:LEU:HA | 2:B:187:LEU:HD23 | 1.81 | 0.41 |
| 3:C:77:ILE:CG2 | 3:C:81:GLY:HA2 | 2.47 | 0.41 |
| 3:C:95:THR:O | 3:C:97:LYS:N | 2.53 | 0.41 |
| 4:D:4:TYR:CE2 | 4:D:11:LEU:HD11 | 2.54 | 0.41 |
| 6:F:24:GLU:O | 6:F:27:GLN:N | 2.53 | 0.41 |
| 10:J:34:VAL:CG1 | 10:J:74:ILE:HG22 | 2.49 | 0.41 |
| 10:J:75:ILE:HG22 | 10:J:76:ASN:OD1 | 2.21 | 0.41 |
| 13:M:105:THR:O | 13:M:107:ALA:N | 2.53 | 0.41 |
| 19:S:36:ARG:HG2 | 19:S:51:VAL:HG12 | 2.02 | 0.41 |
| 1:A:103:C:P | 20:T:17:ARG:HH12 | 2.41 | 0.41 |
| 1:A:179:A:H2' | 1:A:180:U:H6 | 1.86 | 0.41 |
| 1:A:1417:G:N2 | 1:A:1484:C:N4 | 2.69 | 0.41 |
| 4:D:6:GLY:O | 4:D:8:VAL:HG23 | 2.20 | 0.41 |
| 7:G:26:PHE:CA | 7:G:101:LEU:HD23 | 2.50 | 0.41 |
| 1:A:21:G:H2' | 1:A:22:G:C8 | 2.55 | 0.41 |
| 1:A:344:A:H5' | 1:A:345:C:H5 | 1.85 | 0.41 |
| 1:A:666:G:C2 | 1:A:741:G:C4 | 3.08 | 0.41 |
| 1:A:682:G:N1 | 1:A:709:G:C6 | 2.89 | 0.41 |
| 1:A:833:U:O2 | 1:A:854:G:C2 | 2.73 | 0.41 |
| 1:A:1220:G:H2' | 1:A:1221:G:C8 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1367:C:C2 | 1:A:1368:G:C8 | 3.08 | 0.41 |
| 1:A:1469:G:H8 | 1:A:1469:G:O5' | 2.03 | 0.41 |
| 2:B:52:GLU:HG3 | 2:B:53:ARG:N | 2.35 | 0.41 |
| 3:C:45:LYS:NZ | 3:C:45:LYS:HA | 2.36 | 0.41 |
| 4:D:206:PHE:CD2 | 4:D:207:TYR:CD1 | 3.07 | 0.41 |
| 7:G:18:TYR:N | 7:G:18:TYR:CD1 | 2.88 | 0.41 |
| 12:L:42:THR:HA | 12:L:53:ARG:O | 2.21 | 0.41 |
| 18:R:87:ARG:CG | 18:R:88:LYS:H | 2.30 | 0.41 |
| 19:S:18:LYS:HE3 | 19:S:31:ILE:HG12 | 2.01 | 0.41 |
| 1:A:254:G:C4 | 1:A:255:G:C8 | 3.09 | 0.41 |
| 1:A:264:U:O2' | 17:Q:63:ARG:HG2 | 2.20 | 0.41 |
| 1:A:353:A:H5' | 1:A:353:A:C8 | 2.52 | 0.41 |
| 1:A:682:G:N3 | 1:A:683:G:C8 | 2.88 | 0.41 |
| 1:A:806:C:H2' | 1:A:807:A:C8 | 2.56 | 0.41 |
| 1:A:1023:G:H3' | 1:A:1024:G:C5' | 2.49 | 0.41 |
| 1:A:1134:G:N2 | 1:A:1140:C:N3 | 2.54 | 0.41 |
| 1:A:1189:C:H5' | 14:N:58:LYS:NZ | 2.35 | 0.41 |
| 1:A:1277:C:H3' | 1:A:1277:C:H6 | 1.84 | 0.41 |
| 1:A:1403:C:H3' | 1:A:1404:5MC:HM51 | 2.02 | 0.41 |
| 1:A:1464:G:O2' | 1:A:1465:C:H5' | 2.21 | 0.41 |
| 10:J:23:ILE:HD13 | 10:J:23:ILE:HG21 | 1.86 | 0.41 |
| 10:J:55:LYS:CG | 10:J:56:HIS:H | 2.19 | 0.41 |
| 18:R:36:ASN:CG | 18:R:39:VAL:HG12 | 2.41 | 0.41 |
| 20:T:45:GLN:HB2 | 20:T:91:LEU:HG | 2.01 | 0.41 |
| 1:A:190(J):U:H2' | 1:A:190(K):G:H8 | 1.84 | 0.41 |
| 1:A:199:G:O2' | 1:A:200:G:H5' | 2.21 | 0.41 |
| 1:A:420:U:O2' | 1:A:423:G:O6 | 2.30 | 0.41 |
| 1:A:475:G:H2' | 1:A:476:G:C8 | 2.56 | 0.41 |
| 1:A:519:C:H41 | 1:A:533:A:N6 | 2.18 | 0.41 |
| 1:A:587:G:O2' | 1:A:588:G:OP2 | 2.32 | 0.41 |
| 1:A:665:A:C2 | 1:A:732:C:C2 | 3.09 | 0.41 |
| 1:A:794:A:H2' | 1:A:795:C:C6 | 2.55 | 0.41 |
| 1:A:875:C:H1' | 8:H:15:ASN:OD1 | 2.21 | 0.41 |
| 1:A:939:G:H5' | 7:G:102:ARG:NH1 | 2.36 | 0.41 |
| 1:A:1068:G:N3 | 1:A:1191:A:C2 | 2.89 | 0.41 |
| 1:A:1326:C:H2' | 1:A:1327:C:H6 | 1.86 | 0.41 |
| 1:A:1428:A:H2' | 1:A:1429:C:C6 | 2.55 | 0.41 |
| 1:A:1442:G:N1 | 1:A:1446:A:C6 | 2.89 | 0.41 |
| 2:B:74:LYS:HB3 | 2:B:74:LYS:HZ2 | 1.84 | 0.41 |
| 2:B:76:GLN:OE1 | 2:B:207:ALA:N | 2.54 | 0.41 |
| 3:C:85:ARG:NH1 | 3:C:86:VAL:HG23 | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|---------------------|--------------------------|-------------------|
| 5:E:68:GLU:OE1 | 5:E:68:GLU:N | 2.54 | 0.41 |
| 5:E:123:LEU:HA | 5:E:123:LEU:HD23 | 1.73 | 0.41 |
| 7:G:15:ASP:HB3 | 7:G:24:THR:HG23 | 2.02 | 0.41 |
| 7:G:22:LEU:HD23 | 7:G:62:PHE:HE2 | 1.85 | 0.41 |
| 7:G:149:ARG:HD2 | 11:K:59:TYR:CD1 | 2.55 | 0.41 |
| 8:H:4:ASP:HA | 8:H:5:PRO:HD2 | 1.91 | 0.41 |
| 8:H:24:THR:O | 8:H:24:THR:HG23 | 2.21 | 0.41 |
| 10:J:8:LEU:O | 10:J:69:ASN:HA | 2.20 | 0.41 |
| 10:J:57:LYS:O | 10:J:60:ARG:NH1 | 2.53 | 0.41 |
| 13:M:15:VAL:CG1 | 13:M:34:LEU:HD21 | 2.51 | 0.41 |
| 13:M:59:TYR:O | 13:M:60:VAL:C | 2.59 | 0.41 |
| 13:M:64:TRP:CD1 | 13:M:64:TRP:N | 2.84 | 0.41 |
| 17:Q:51:TYR:CD1 | 17:Q:51:TYR:N | 2.89 | 0.41 |
| 1:A:189:G:H2' | 1:A:190:C:O4' | 2.21 | 0.41 |
| 1:A:696:A:H8 | 1:A:696:A:O5' | 2.04 | 0.41 |
| 1:A:1039:C:O2' | 1:A:1040:U:O4' | 2.36 | 0.41 |
| 1:A:1350:A:OP2 | 9:I:118:LYS:NZ | 2.35 | 0.41 |
| 1:A:1406:U:H4' | 1:A:1518[B]:MA6:H1' | 2.03 | 0.41 |
| 1:A:1415:G:O6 | 1:A:1485:U:C4 | 2.74 | 0.41 |
| 1:A:1424:C:C4 | 1:A:1425:U:C5 | 3.08 | 0.41 |
| 2:B:60:ASP:OD2 | 2:B:64:ARG:HD2 | 2.21 | 0.41 |
| 3:C:190:ARG:H | 3:C:190:ARG:HG2 | 1.65 | 0.41 |
| 4:D:11:LEU:HD13 | 4:D:66:ARG:HG2 | 2.03 | 0.41 |
| 6:F:6:VAL:HB | 6:F:63:TYR:HB2 | 2.03 | 0.41 |
| 10:J:11:PHE:HE2 | 10:J:67:THR:HG23 | 1.86 | 0.41 |
| 10:J:27:ALA:O | 10:J:30:SER:N | 2.54 | 0.41 |
| 12:L:111:LYS:HE2 | 12:L:111:LYS:HB2 | 1.83 | 0.41 |
| 19:S:36:ARG:NH2 | 19:S:75:ALA:O | 2.54 | 0.41 |
| 20:T:52:ALA:O | 20:T:56:MET:HB3 | 2.20 | 0.41 |
| 1:A:90:U:H2' | 1:A:91:C:C6 | 2.56 | 0.40 |
| 1:A:459:G:H8 | 1:A:459:G:O5' | 2.04 | 0.40 |
| 1:A:569:C:H1' | 1:A:574:A:C4 | 2.56 | 0.40 |
| 1:A:755:G:OP2 | 15:O:65:ARG:HD2 | 2.21 | 0.40 |
| 1:A:855:G:C6 | 1:A:856:C:C4 | 3.09 | 0.40 |
| 1:A:901:A:C5 | 1:A:902:G:H1' | 2.57 | 0.40 |
| 1:A:939:G:OP1 | 7:G:102:ARG:NH1 | 2.50 | 0.40 |
| 1:A:1014:A:H2' | 1:A:1015:A:C8 | 2.56 | 0.40 |
| 1:A:1084:G:H5' | 1:A:1102:A:OP2 | 2.22 | 0.40 |
| 1:A:1116:C:C2' | 1:A:1117:G:H5' | 2.51 | 0.40 |
| 3:C:121:ALA:HB1 | 3:C:189:ALA:HB2 | 2.02 | 0.40 |
| 5:E:12:LEU:HD23 | 5:E:13:ILE:C | 2.41 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 13:M:70:LEU:O | 13:M:74:VAL:HG23 | 2.21 | 0.40 |
| 17:Q:56:VAL:O | 17:Q:77:VAL:HB | 2.21 | 0.40 |
| 1:A:544:G:C6 | 1:A:545:C:C4 | 3.09 | 0.40 |
| 1:A:993:G:H4' | 1:A:994:A:OP2 | 2.20 | 0.40 |
| 1:A:1096:C:C2 | 1:A:1097:C:C5 | 3.10 | 0.40 |
| 1:A:1116:C:C2 | 1:A:1185:G:C2 | 3.09 | 0.40 |
| 1:A:1253:G:H1' | 1:A:1355:G:O2' | 2.21 | 0.40 |
| 1:A:1434:A:H61 | 1:A:1467:G:H1' | 1.86 | 0.40 |
| 2:B:41:ILE:HG22 | 2:B:42:ILE:N | 2.36 | 0.40 |
| 3:C:58:GLU:HB2 | 3:C:65:ALA:HB2 | 2.03 | 0.40 |
| 4:D:189:PRO:HB2 | 4:D:194:LEU:HD22 | 2.03 | 0.40 |
| 6:F:77:ARG:O | 6:F:80:ARG:HB2 | 2.21 | 0.40 |
| 7:G:26:PHE:CD2 | 7:G:62:PHE:HE1 | 2.39 | 0.40 |
| 11:K:33:THR:HB | 11:K:39:PRO:HA | 2.03 | 0.40 |
| 12:L:120:TYR:O | 12:L:122:THR:HG23 | 2.22 | 0.40 |
| 20:T:73:HIS:HB3 | 20:T:74:LYS:H | 1.66 | 0.40 |
| 1:A:725:G:O2' | 1:A:726:C:H5' | 2.20 | 0.40 |
| 1:A:763:G:H2' | 1:A:764:C:C6 | 2.57 | 0.40 |
| 1:A:1375:A:H4' | 7:G:29:LYS:HE2 | 2.02 | 0.40 |
| 1:A:1416:G:N2 | 1:A:1485:U:O2' | 2.55 | 0.40 |
| 1:A:1440:C:H5'' | 1:A:1441:G:OP2 | 2.21 | 0.40 |
| 1:A:1515[B]:C:N4 | 1:A:1520[B]:G:O6 | 2.51 | 0.40 |
| 2:B:54:THR:O | 2:B:58:ILE:HG13 | 2.21 | 0.40 |
| 3:C:152:ILE:HD13 | 3:C:152:ILE:HA | 1.70 | 0.40 |
| 4:D:50:ARG:HA | 4:D:51:PRO:HD3 | 1.59 | 0.40 |
| 6:F:62:TRP:HB2 | 18:R:35:ARG:NH1 | 2.36 | 0.40 |
| 7:G:16:LEU:HD23 | 9:I:45:ALA:HB2 | 2.02 | 0.40 |
| 9:I:8:GLY:N | 9:I:83:ARG:HD2 | 2.36 | 0.40 |
| 15:O:43:LEU:HA | 15:O:43:LEU:HD23 | 1.83 | 0.40 |
| 1:A:190(E):U:C2 | 17:Q:63:ARG:NH1 | 2.89 | 0.40 |
| 1:A:317:G:C2' | 1:A:318:G:H5' | 2.51 | 0.40 |
| 1:A:407:G:H4' | 4:D:116:GLN:HA | 2.04 | 0.40 |
| 1:A:721:G:H8 | 1:A:721:G:O5' | 2.04 | 0.40 |
| 1:A:1133:G:H2' | 1:A:1134:G:O4' | 2.21 | 0.40 |
| 3:C:44:GLU:HA | 3:C:52:LEU:HD21 | 2.03 | 0.40 |
| 3:C:82:GLU:OE2 | 3:C:83:ARG:N | 2.54 | 0.40 |
| 5:E:53:LEU:HA | 5:E:53:LEU:HD13 | 1.63 | 0.40 |
| 5:E:118:ILE:O | 5:E:119:LEU:HD23 | 2.21 | 0.40 |
| 7:G:74:GLU:OE2 | 7:G:95:ARG:NH2 | 2.49 | 0.40 |
| 8:H:37:ARG:HH11 | 8:H:37:ARG:HB3 | 1.86 | 0.40 |
| 8:H:41:ARG:NH1 | 8:H:42:GLU:HG2 | 2.27 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 10:J:54:PHE:O | 10:J:55:LYS:HB3 | 2.21 | 0.40 |
| 14:N:8:GLU:O | 14:N:11:LYS:HB3 | 2.21 | 0.40 |
| 15:O:5:LYS:O | 15:O:9:GLN:HB2 | 2.22 | 0.40 |
| 15:O:27:VAL:HG12 | 15:O:31:LEU:HD22 | 2.04 | 0.40 |
| 17:Q:66:SER:O | 17:Q:70:ARG:NH1 | 2.54 | 0.40 |
| 19:S:31:ILE:HA | 19:S:32:LYS:NZ | 2.36 | 0.40 |
| 19:S:40:ILE:HG23 | 19:S:44:MET:SD | 2.62 | 0.40 |
| 1:A:134:A:C6 | 1:A:135:C:N3 | 2.89 | 0.40 |
| 1:A:148:G:C2 | 1:A:149:A:C5 | 3.10 | 0.40 |
| 1:A:302:G:N3 | 1:A:556:C:H4' | 2.37 | 0.40 |
| 1:A:392:G:H2' | 1:A:393:A:H8 | 1.85 | 0.40 |
| 1:A:463:A:OP2 | 16:P:75:ARG:NH1 | 2.54 | 0.40 |
| 1:A:673:G:H5'' | 6:F:87:ARG:CZ | 2.51 | 0.40 |
| 1:A:745:C:O5' | 1:A:745:C:H6 | 2.04 | 0.40 |
| 1:A:965:A:OP1 | 1:A:1198:G:H5'' | 2.21 | 0.40 |
| 1:A:1072:G:C6 | 1:A:1073:U:N3 | 2.89 | 0.40 |
| 1:A:1127:G:H3' | 1:A:1127:G:C8 | 2.57 | 0.40 |
| 10:J:91:PRO:O | 10:J:94:VAL:HG12 | 2.21 | 0.40 |
| 11:K:120:ARG:HH22 | 11:K:126:ARG:NH1 | 2.19 | 0.40 |
| 14:N:12:ARG:NH1 | 14:N:21:TYR:O | 2.55 | 0.40 |
| 16:P:4:ILE:H | 16:P:66:PRO:HA | 1.86 | 0.40 |
| 18:R:46:GLU:CD | 18:R:55:ARG:HH22 | 2.24 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 2 | B | 232/256 (91%) | 198 (85%) | 29 (12%) | 5 (2%) | 5 | 32 |
| 3 | C | 204/239 (85%) | 175 (86%) | 27 (13%) | 2 (1%) | 13 | 46 |
| 4 | D | 206/209 (99%) | 190 (92%) | 16 (8%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 5 | E | 148/162 (91%) | 139 (94%) | 6 (4%) | 3 (2%) | 6 | 34 |
| 6 | F | 99/101 (98%) | 97 (98%) | 2 (2%) | 0 | 100 | 100 |
| 7 | G | 153/156 (98%) | 137 (90%) | 16 (10%) | 0 | 100 | 100 |
| 8 | H | 136/138 (99%) | 127 (93%) | 9 (7%) | 0 | 100 | 100 |
| 9 | I | 125/128 (98%) | 111 (89%) | 12 (10%) | 2 (2%) | 8 | 37 |
| 10 | J | 96/105 (91%) | 81 (84%) | 13 (14%) | 2 (2%) | 5 | 33 |
| 11 | K | 114/129 (88%) | 99 (87%) | 15 (13%) | 0 | 100 | 100 |
| 12 | L | 121/135 (90%) | 106 (88%) | 12 (10%) | 3 (2%) | 4 | 30 |
| 13 | M | 116/126 (92%) | 94 (81%) | 21 (18%) | 1 (1%) | 14 | 48 |
| 14 | N | 58/61 (95%) | 48 (83%) | 10 (17%) | 0 | 100 | 100 |
| 15 | O | 85/89 (96%) | 78 (92%) | 7 (8%) | 0 | 100 | 100 |
| 16 | P | 81/88 (92%) | 70 (86%) | 11 (14%) | 0 | 100 | 100 |
| 17 | Q | 97/105 (92%) | 89 (92%) | 8 (8%) | 0 | 100 | 100 |
| 18 | R | 68/88 (77%) | 59 (87%) | 9 (13%) | 0 | 100 | 100 |
| 19 | S | 78/93 (84%) | 67 (86%) | 9 (12%) | 2 (3%) | 4 | 29 |
| 20 | T | 97/106 (92%) | 79 (81%) | 16 (16%) | 2 (2%) | 5 | 33 |
| 21 | U | 22/27 (82%) | 21 (96%) | 1 (4%) | 0 | 100 | 100 |
| All | All | 2336/2541 (92%) | 2065 (88%) | 249 (11%) | 22 (1%) | 14 | 48 |

All (22) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 21 | ARG |
| 12 | L | 28 | LYS |
| 19 | S | 31 | ILE |
| 2 | B | 9 | GLU |
| 3 | C | 62 | ASP |
| 9 | I | 58 | HIS |
| 2 | B | 11 | LEU |
| 5 | E | 16 | THR |
| 9 | I | 119 | ALA |
| 12 | L | 25 | PRO |
| 2 | B | 78 | GLN |
| 3 | C | 27 | LYS |
| 5 | E | 118 | ILE |
| 10 | J | 35 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20 | T | 71 | THR |
| 12 | L | 79 | GLU |
| 19 | S | 30 | LEU |
| 10 | J | 34 | VAL |
| 13 | M | 7 | VAL |
| 5 | E | 70 | PRO |
| 2 | B | 229 | VAL |
| 20 | T | 100 | ILE |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2 | B | 202/220 (92%) | 150 (74%) | 52 (26%) | 0 | 3 |
| 3 | C | 160/188 (85%) | 121 (76%) | 39 (24%) | 0 | 3 |
| 4 | D | 180/181 (99%) | 135 (75%) | 45 (25%) | 0 | 3 |
| 5 | E | 115/123 (94%) | 88 (76%) | 27 (24%) | 0 | 4 |
| 6 | F | 90/90 (100%) | 72 (80%) | 18 (20%) | 1 | 6 |
| 7 | G | 126/127 (99%) | 103 (82%) | 23 (18%) | 1 | 9 |
| 8 | H | 119/119 (100%) | 83 (70%) | 36 (30%) | 0 | 2 |
| 9 | I | 98/99 (99%) | 77 (79%) | 21 (21%) | 1 | 5 |
| 10 | J | 87/92 (95%) | 63 (72%) | 24 (28%) | 0 | 2 |
| 11 | K | 88/99 (89%) | 69 (78%) | 19 (22%) | 1 | 5 |
| 12 | L | 103/110 (94%) | 78 (76%) | 25 (24%) | 0 | 3 |
| 13 | M | 94/101 (93%) | 71 (76%) | 23 (24%) | 0 | 3 |
| 14 | N | 49/50 (98%) | 34 (69%) | 15 (31%) | 0 | 2 |
| 15 | O | 79/80 (99%) | 61 (77%) | 18 (23%) | 0 | 4 |
| 16 | P | 72/74 (97%) | 61 (85%) | 11 (15%) | 2 | 13 |
| 17 | Q | 94/97 (97%) | 64 (68%) | 30 (32%) | 0 | 1 |
| 18 | R | 61/77 (79%) | 45 (74%) | 16 (26%) | 0 | 3 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 19 | S | 71/80 (89%) | 52 (73%) | 19 (27%) | 0 | 3 |
| 20 | T | 76/82 (93%) | 54 (71%) | 22 (29%) | 0 | 2 |
| 21 | U | 19/22 (86%) | 18 (95%) | 1 (5%) | 19 | 45 |
| All | All | 1983/2111 (94%) | 1499 (76%) | 484 (24%) | 0 | 3 |

All (484) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 8 | LYS |
| 2 | B | 12 | GLU |
| 2 | B | 19 | HIS |
| 2 | B | 20 | GLU |
| 2 | B | 21 | ARG |
| 2 | B | 24 | TRP |
| 2 | B | 33 | TYR |
| 2 | B | 51 | LEU |
| 2 | B | 52 | GLU |
| 2 | B | 53 | ARG |
| 2 | B | 67 | THR |
| 2 | B | 69 | LEU |
| 2 | B | 73 | THR |
| 2 | B | 79 | ASP |
| 2 | B | 82 | ARG |
| 2 | B | 83 | MET |
| 2 | B | 84 | GLU |
| 2 | B | 87 | ARG |
| 2 | B | 90 | MET |
| 2 | B | 96 | ARG |
| 2 | B | 105 | PHE |
| 2 | B | 109 | SER |
| 2 | B | 118 | LEU |
| 2 | B | 127 | ILE |
| 2 | B | 134 | GLU |
| 2 | B | 135 | GLN |
| 2 | B | 140 | HIS |
| 2 | B | 144 | ARG |
| 2 | B | 150 | SER |
| 2 | B | 154 | LEU |
| 2 | B | 155 | LEU |
| 2 | B | 157 | ARG |
| 2 | B | 160 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 162 | ILE |
| 2 | B | 163 | PHE |
| 2 | B | 165 | VAL |
| 2 | B | 168 | THR |
| 2 | B | 169 | LYS |
| 2 | B | 170 | GLU |
| 2 | B | 172 | ILE |
| 2 | B | 174 | VAL |
| 2 | B | 175 | ARG |
| 2 | B | 178 | ARG |
| 2 | B | 184 | VAL |
| 2 | B | 187 | LEU |
| 2 | B | 205 | ASP |
| 2 | B | 206 | ASP |
| 2 | B | 213 | LEU |
| 2 | B | 221 | LEU |
| 2 | B | 223 | ILE |
| 2 | B | 226 | ARG |
| 2 | B | 239 | VAL |
| 3 | C | 3 | ASN |
| 3 | C | 12 | LEU |
| 3 | C | 14 | ILE |
| 3 | C | 15 | THR |
| 3 | C | 29 | TYR |
| 3 | C | 34 | LEU |
| 3 | C | 37 | GLN |
| 3 | C | 42 | LEU |
| 3 | C | 43 | LEU |
| 3 | C | 45 | LYS |
| 3 | C | 55 | VAL |
| 3 | C | 56 | ASP |
| 3 | C | 59 | ARG |
| 3 | C | 70 | VAL |
| 3 | C | 82 | GLU |
| 3 | C | 83 | ARG |
| 3 | C | 84 | ILE |
| 3 | C | 89 | GLU |
| 3 | C | 94 | LEU |
| 3 | C | 101 | LEU |
| 3 | C | 102 | ASN |
| 3 | C | 103 | VAL |
| 3 | C | 111 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 116 | VAL |
| 3 | C | 119 | ARG |
| 3 | C | 120 | VAL |
| 3 | C | 122 | GLU |
| 3 | C | 138 | VAL |
| 3 | C | 144 | SER |
| 3 | C | 153 | VAL |
| 3 | C | 165 | THR |
| 3 | C | 167 | TRP |
| 3 | C | 172 | ARG |
| 3 | C | 175 | LEU |
| 3 | C | 178 | LEU |
| 3 | C | 188 | LEU |
| 3 | C | 190 | ARG |
| 3 | C | 192 | THR |
| 3 | C | 204 | LEU |
| 4 | D | 3 | ARG |
| 4 | D | 5 | ILE |
| 4 | D | 19 | LEU |
| 4 | D | 21 | LEU |
| 4 | D | 25 | ARG |
| 4 | D | 26 | CYS |
| 4 | D | 28 | SER |
| 4 | D | 35 | ARG |
| 4 | D | 38 | TYR |
| 4 | D | 39 | PRO |
| 4 | D | 47 | ARG |
| 4 | D | 50 | ARG |
| 4 | D | 61 | LYS |
| 4 | D | 64 | LEU |
| 4 | D | 66 | ARG |
| 4 | D | 71 | SER |
| 4 | D | 76 | ARG |
| 4 | D | 78 | LEU |
| 4 | D | 80 | GLU |
| 4 | D | 81 | GLU |
| 4 | D | 85 | LYS |
| 4 | D | 88 | VAL |
| 4 | D | 97 | LEU |
| 4 | D | 100 | ARG |
| 4 | D | 108 | LEU |
| 4 | D | 120 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | D | 122 | ARG |
| 4 | D | 127 | THR |
| 4 | D | 132 | ARG |
| 4 | D | 133 | VAL |
| 4 | D | 134 | ASP |
| 4 | D | 141 | ARG |
| 4 | D | 145 | GLU |
| 4 | D | 153 | ARG |
| 4 | D | 155 | LEU |
| 4 | D | 156 | GLU |
| 4 | D | 165 | MET |
| 4 | D | 181 | MET |
| 4 | D | 182 | LYS |
| 4 | D | 187 | ARG |
| 4 | D | 190 | ASP |
| 4 | D | 191 | ARG |
| 4 | D | 194 | LEU |
| 4 | D | 196 | LEU |
| 4 | D | 202 | LEU |
| 5 | E | 6 | PHE |
| 5 | E | 10 | MET |
| 5 | E | 12 | LEU |
| 5 | E | 20 | GLN |
| 5 | E | 24 | ARG |
| 5 | E | 25 | ARG |
| 5 | E | 26 | PHE |
| 5 | E | 27 | ARG |
| 5 | E | 31 | LEU |
| 5 | E | 41 | VAL |
| 5 | E | 47 | LYS |
| 5 | E | 51 | VAL |
| 5 | E | 63 | ARG |
| 5 | E | 64 | ARG |
| 5 | E | 75 | THR |
| 5 | E | 78 | HIS |
| 5 | E | 79 | GLU |
| 5 | E | 87 | SER |
| 5 | E | 100 | VAL |
| 5 | E | 105 | VAL |
| 5 | E | 116 | THR |
| 5 | E | 126 | ARG |
| 5 | E | 145 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | E | 148 | VAL |
| 5 | E | 150 | ARG |
| 5 | E | 151 | LEU |
| 5 | E | 153 | LYS |
| 6 | F | 10 | LEU |
| 6 | F | 24 | GLU |
| 6 | F | 25 | ILE |
| 6 | F | 30 | LEU |
| 6 | F | 36 | ARG |
| 6 | F | 39 | LYS |
| 6 | F | 43 | LEU |
| 6 | F | 45 | LEU |
| 6 | F | 47 | ARG |
| 6 | F | 55 | ASP |
| 6 | F | 61 | LEU |
| 6 | F | 70 | ASP |
| 6 | F | 74 | ASP |
| 6 | F | 80 | ARG |
| 6 | F | 82 | ARG |
| 6 | F | 83 | ASP |
| 6 | F | 93 | SER |
| 6 | F | 95 | GLU |
| 7 | G | 21 | VAL |
| 7 | G | 38 | LEU |
| 7 | G | 41 | ARG |
| 7 | G | 49 | ILE |
| 7 | G | 54 | THR |
| 7 | G | 62 | PHE |
| 7 | G | 72 | ARG |
| 7 | G | 73 | MET |
| 7 | G | 75 | VAL |
| 7 | G | 78 | ARG |
| 7 | G | 79 | ARG |
| 7 | G | 92 | SER |
| 7 | G | 94 | ARG |
| 7 | G | 122 | HIS |
| 7 | G | 126 | ASP |
| 7 | G | 131 | LYS |
| 7 | G | 135 | VAL |
| 7 | G | 137 | LYS |
| 7 | G | 139 | GLU |
| 7 | G | 141 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | G | 143 | ARG |
| 7 | G | 149 | ARG |
| 7 | G | 153 | HIS |
| 8 | H | 9 | MET |
| 8 | H | 12 | ARG |
| 8 | H | 18 | ARG |
| 8 | H | 22 | GLU |
| 8 | H | 23 | SER |
| 8 | H | 25 | ASP |
| 8 | H | 26 | VAL |
| 8 | H | 29 | SER |
| 8 | H | 37 | ARG |
| 8 | H | 39 | LEU |
| 8 | H | 41 | ARG |
| 8 | H | 45 | ILE |
| 8 | H | 48 | TYR |
| 8 | H | 49 | GLU |
| 8 | H | 51 | VAL |
| 8 | H | 53 | VAL |
| 8 | H | 59 | LEU |
| 8 | H | 60 | ARG |
| 8 | H | 63 | LEU |
| 8 | H | 64 | LYS |
| 8 | H | 75 | ARG |
| 8 | H | 82 | HIS |
| 8 | H | 83 | ILE |
| 8 | H | 84 | ARG |
| 8 | H | 85 | ARG |
| 8 | H | 91 | ARG |
| 8 | H | 97 | VAL |
| 8 | H | 102 | ARG |
| 8 | H | 104 | ARG |
| 8 | H | 113 | SER |
| 8 | H | 119 | LEU |
| 8 | H | 120 | THR |
| 8 | H | 122 | ARG |
| 8 | H | 133 | LEU |
| 8 | H | 134 | ILE |
| 8 | H | 135 | CYS |
| 9 | I | 2 | GLU |
| 9 | I | 14 | VAL |
| 9 | I | 23 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | I | 27 | THR |
| 9 | I | 42 | ARG |
| 9 | I | 56 | LEU |
| 9 | I | 65 | VAL |
| 9 | I | 79 | LEU |
| 9 | I | 85 | LEU |
| 9 | I | 91 | ASP |
| 9 | I | 96 | LEU |
| 9 | I | 102 | LEU |
| 9 | I | 108 | VAL |
| 9 | I | 111 | ARG |
| 9 | I | 113 | LYS |
| 9 | I | 116 | LYS |
| 9 | I | 118 | LYS |
| 9 | I | 121 | ARG |
| 9 | I | 124 | GLN |
| 9 | I | 126 | SER |
| 9 | I | 127 | LYS |
| 10 | J | 3 | LYS |
| 10 | J | 5 | ARG |
| 10 | J | 16 | LEU |
| 10 | J | 19 | SER |
| 10 | J | 21 | GLN |
| 10 | J | 24 | VAL |
| 10 | J | 29 | ARG |
| 10 | J | 44 | VAL |
| 10 | J | 45 | ARG |
| 10 | J | 60 | ARG |
| 10 | J | 61 | GLU |
| 10 | J | 62 | HIS |
| 10 | J | 66 | ARG |
| 10 | J | 67 | THR |
| 10 | J | 69 | ASN |
| 10 | J | 71 | LEU |
| 10 | J | 72 | VAL |
| 10 | J | 76 | ASN |
| 10 | J | 79 | ARG |
| 10 | J | 81 | THR |
| 10 | J | 84 | GLN |
| 10 | J | 88 | LEU |
| 10 | J | 95 | GLU |
| 10 | J | 97 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | K | 11 | LYS |
| 11 | K | 26 | ASN |
| 11 | K | 29 | ILE |
| 11 | K | 33 | THR |
| 11 | K | 36 | ASP |
| 11 | K | 47 | VAL |
| 11 | K | 51 | LYS |
| 11 | K | 62 | GLN |
| 11 | K | 66 | LEU |
| 11 | K | 67 | ASP |
| 11 | K | 75 | TYR |
| 11 | K | 82 | VAL |
| 11 | K | 83 | ILE |
| 11 | K | 87 | THR |
| 11 | K | 92 | GLU |
| 11 | K | 101 | SER |
| 11 | K | 105 | VAL |
| 11 | K | 112 | THR |
| 11 | K | 119 | CYS |
| 12 | L | 6 | THR |
| 12 | L | 18 | VAL |
| 12 | L | 19 | ARG |
| 12 | L | 20 | LYS |
| 12 | L | 33 | ARG |
| 12 | L | 41 | ARG |
| 12 | L | 42 | THR |
| 12 | L | 43 | VAL |
| 12 | L | 44 | THR |
| 12 | L | 46 | LYS |
| 12 | L | 47 | LYS |
| 12 | L | 52 | LEU |
| 12 | L | 59 | ARG |
| 12 | L | 60 | LEU |
| 12 | L | 61 | THR |
| 12 | L | 75 | HIS |
| 12 | L | 76 | ASN |
| 12 | L | 81 | SER |
| 12 | L | 82 | VAL |
| 12 | L | 89 | ARG |
| 12 | L | 97 | ARG |
| 12 | L | 111 | LYS |
| 12 | L | 114 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | L | 123 | LYS |
| 12 | L | 126 | LYS |
| 13 | M | 3 | ARG |
| 13 | M | 4 | ILE |
| 13 | M | 29 | ARG |
| 13 | M | 35 | GLU |
| 13 | M | 45 | VAL |
| 13 | M | 46 | LYS |
| 13 | M | 48 | LEU |
| 13 | M | 50 | GLU |
| 13 | M | 54 | VAL |
| 13 | M | 63 | THR |
| 13 | M | 64 | TRP |
| 13 | M | 65 | LYS |
| 13 | M | 66 | LEU |
| 13 | M | 70 | LEU |
| 13 | M | 81 | LEU |
| 13 | M | 90 | LEU |
| 13 | M | 102 | ARG |
| 13 | M | 105 | THR |
| 13 | M | 108 | ARG |
| 13 | M | 109 | THR |
| 13 | M | 115 | LYS |
| 13 | M | 116 | THR |
| 13 | M | 117 | VAL |
| 14 | N | 3 | ARG |
| 14 | N | 7 | ILE |
| 14 | N | 8 | GLU |
| 14 | N | 9 | LYS |
| 14 | N | 22 | THR |
| 14 | N | 24 | CYS |
| 14 | N | 25 | VAL |
| 14 | N | 26 | ARG |
| 14 | N | 29 | ARG |
| 14 | N | 33 | VAL |
| 14 | N | 41 | ARG |
| 14 | N | 42 | ILE |
| 14 | N | 44 | LEU |
| 14 | N | 47 | LEU |
| 14 | N | 50 | LYS |
| 15 | O | 18 | PHE |
| 15 | O | 22 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15 | O | 29 | VAL |
| 15 | O | 31 | LEU |
| 15 | O | 32 | LEU |
| 15 | O | 38 | ARG |
| 15 | O | 39 | LEU |
| 15 | O | 47 | LYS |
| 15 | O | 49 | ASP |
| 15 | O | 57 | LEU |
| 15 | O | 62 | GLN |
| 15 | O | 63 | ARG |
| 15 | O | 66 | LEU |
| 15 | O | 70 | LEU |
| 15 | O | 76 | GLU |
| 15 | O | 77 | ARG |
| 15 | O | 79 | ARG |
| 15 | O | 82 | ILE |
| 16 | P | 1 | MET |
| 16 | P | 2 | VAL |
| 16 | P | 31 | LYS |
| 16 | P | 45 | THR |
| 16 | P | 48 | TRP |
| 16 | P | 55 | ARG |
| 16 | P | 65 | GLN |
| 16 | P | 68 | ASP |
| 16 | P | 75 | ARG |
| 16 | P | 80 | PHE |
| 16 | P | 83 | GLU |
| 17 | Q | 3 | LYS |
| 17 | Q | 5 | VAL |
| 17 | Q | 7 | THR |
| 17 | Q | 9 | VAL |
| 17 | Q | 11 | VAL |
| 17 | Q | 13 | ASP |
| 17 | Q | 16 | GLN |
| 17 | Q | 19 | VAL |
| 17 | Q | 22 | LEU |
| 17 | Q | 25 | ARG |
| 17 | Q | 34 | LYS |
| 17 | Q | 36 | ILE |
| 17 | Q | 48 | GLU |
| 17 | Q | 49 | GLU |
| 17 | Q | 53 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17 | Q | 59 | ILE |
| 17 | Q | 62 | SER |
| 17 | Q | 63 | ARG |
| 17 | Q | 68 | ARG |
| 17 | Q | 75 | ARG |
| 17 | Q | 79 | SER |
| 17 | Q | 81 | ARG |
| 17 | Q | 83 | ASP |
| 17 | Q | 86 | GLU |
| 17 | Q | 87 | LYS |
| 17 | Q | 88 | TYR |
| 17 | Q | 89 | LEU |
| 17 | Q | 98 | LEU |
| 17 | Q | 99 | SER |
| 17 | Q | 100 | LYS |
| 18 | R | 19 | LYS |
| 18 | R | 23 | LYS |
| 18 | R | 28 | GLU |
| 18 | R | 31 | LEU |
| 18 | R | 35 | ARG |
| 18 | R | 41 | LYS |
| 18 | R | 56 | THR |
| 18 | R | 64 | ARG |
| 18 | R | 65 | ILE |
| 18 | R | 69 | THR |
| 18 | R | 76 | LEU |
| 18 | R | 79 | LEU |
| 18 | R | 83 | GLU |
| 18 | R | 85 | LEU |
| 18 | R | 86 | VAL |
| 18 | R | 88 | LYS |
| 19 | S | 3 | ARG |
| 19 | S | 5 | LEU |
| 19 | S | 6 | LYS |
| 19 | S | 7 | LYS |
| 19 | S | 9 | VAL |
| 19 | S | 13 | ASP |
| 19 | S | 15 | LEU |
| 19 | S | 17 | GLU |
| 19 | S | 20 | LEU |
| 19 | S | 22 | LEU |
| 19 | S | 28 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19 | S | 29 | ARG |
| 19 | S | 32 | LYS |
| 19 | S | 43 | GLU |
| 19 | S | 48 | THR |
| 19 | S | 70 | LYS |
| 19 | S | 77 | THR |
| 19 | S | 79 | THR |
| 19 | S | 80 | TYR |
| 20 | T | 10 | LEU |
| 20 | T | 14 | LYS |
| 20 | T | 17 | ARG |
| 20 | T | 19 | SER |
| 20 | T | 20 | LEU |
| 20 | T | 22 | ARG |
| 20 | T | 24 | LEU |
| 20 | T | 27 | LYS |
| 20 | T | 36 | LEU |
| 20 | T | 41 | ILE |
| 20 | T | 45 | GLN |
| 20 | T | 46 | GLU |
| 20 | T | 48 | LYS |
| 20 | T | 50 | GLU |
| 20 | T | 53 | LEU |
| 20 | T | 56 | MET |
| 20 | T | 62 | LEU |
| 20 | T | 75 | ASN |
| 20 | T | 80 | ARG |
| 20 | T | 87 | LYS |
| 20 | T | 91 | LEU |
| 20 | T | 100 | ILE |
| 21 | U | 10 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 19 | HIS |
| 2 | B | 40 | HIS |
| 3 | C | 6 | HIS |
| 7 | G | 110 | GLN |
| 9 | I | 29 | ASN |
| 9 | I | 73 | GLN |
| 9 | I | 124 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | J | 13 | HIS |
| 10 | J | 33 | GLN |
| 15 | O | 62 | GLN |
| 20 | T | 16 | HIS |

5.3.3 RNA [i](#)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | A | 1505/1522 (98%) | 357 (23%) | 27 (1%) |

All (357) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | A | 4 | U |
| 1 | A | 7 | G |
| 1 | A | 9 | G |
| 1 | A | 12 | U |
| 1 | A | 15 | G |
| 1 | A | 16 | A |
| 1 | A | 30 | U |
| 1 | A | 31 | G |
| 1 | A | 32 | A |
| 1 | A | 39 | G |
| 1 | A | 47 | C |
| 1 | A | 48 | C |
| 1 | A | 51 | A |
| 1 | A | 81 | U |
| 1 | A | 82 | U |
| 1 | A | 83 | U |
| 1 | A | 101 | A |
| 1 | A | 109 | A |
| 1 | A | 115 | G |
| 1 | A | 116 | A |
| 1 | A | 117 | G |
| 1 | A | 121 | C |
| 1 | A | 129(A) | G |
| 1 | A | 130 | A |
| 1 | A | 131 | C |
| 1 | A | 145 | G |
| 1 | A | 158 | G |
| 1 | A | 163 | C |

Continued on next page...

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | A | 179 | A |
| 1 | A | 182 | U |
| 1 | A | 183 | G |
| 1 | A | 190(E) | U |
| 1 | A | 195 | A |
| 1 | A | 197 | A |
| 1 | A | 201 | C |
| 1 | A | 202 | U |
| 1 | A | 203 | U |
| 1 | A | 204 | U |
| 1 | A | 216 | G |
| 1 | A | 220 | G |
| 1 | A | 226 | G |
| 1 | A | 231 | G |
| 1 | A | 236 | G |
| 1 | A | 244 | U |
| 1 | A | 245 | C |
| 1 | A | 247 | G |
| 1 | A | 251 | G |
| 1 | A | 253 | U |
| 1 | A | 262 | A |
| 1 | A | 266 | G |
| 1 | A | 267 | C |
| 1 | A | 272 | C |
| 1 | A | 289 | G |
| 1 | A | 291 | C |
| 1 | A | 298 | A |
| 1 | A | 301 | G |
| 1 | A | 315 | A |
| 1 | A | 319 | G |
| 1 | A | 321 | A |
| 1 | A | 328 | C |
| 1 | A | 329 | A |
| 1 | A | 344 | A |
| 1 | A | 345 | C |
| 1 | A | 350 | G |
| 1 | A | 351 | G |
| 1 | A | 352 | C |
| 1 | A | 353 | A |
| 1 | A | 354 | G |
| 1 | A | 356 | A |
| 1 | A | 367 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 371 | G |
| 1 | A | 372 | C |
| 1 | A | 373 | A |
| 1 | A | 384 | G |
| 1 | A | 390 | C |
| 1 | A | 398 | C |
| 1 | A | 406 | G |
| 1 | A | 409 | G |
| 1 | A | 412 | A |
| 1 | A | 413 | G |
| 1 | A | 421 | U |
| 1 | A | 422 | C |
| 1 | A | 424 | G |
| 1 | A | 429 | U |
| 1 | A | 430 | A |
| 1 | A | 439 | A |
| 1 | A | 452 | A |
| 1 | A | 454 | C |
| 1 | A | 456 | C |
| 1 | A | 460 | A |
| 1 | A | 461 | C |
| 1 | A | 462 | G |
| 1 | A | 484 | G |
| 1 | A | 485 | G |
| 1 | A | 486 | U |
| 1 | A | 496 | A |
| 1 | A | 497 | A |
| 1 | A | 498 | U |
| 1 | A | 500 | G |
| 1 | A | 503 | C |
| 1 | A | 504 | C |
| 1 | A | 505 | G |
| 1 | A | 509 | A |
| 1 | A | 510 | A |
| 1 | A | 511 | C |
| 1 | A | 518 | C |
| 1 | A | 519 | C |
| 1 | A | 521 | G |
| 1 | A | 524 | G |
| 1 | A | 526 | C |
| 1 | A | 527 | 7MG |
| 1 | A | 531 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 532 | A |
| 1 | A | 533 | A |
| 1 | A | 536 | C |
| 1 | A | 545 | C |
| 1 | A | 547 | A |
| 1 | A | 555 | C |
| 1 | A | 559 | A |
| 1 | A | 560 | U |
| 1 | A | 561 | U |
| 1 | A | 562 | C |
| 1 | A | 564 | C |
| 1 | A | 566 | G |
| 1 | A | 568 | G |
| 1 | A | 569 | C |
| 1 | A | 570 | G |
| 1 | A | 572 | A |
| 1 | A | 573 | A |
| 1 | A | 576 | G |
| 1 | A | 577 | G |
| 1 | A | 579 | G |
| 1 | A | 581 | G |
| 1 | A | 587 | G |
| 1 | A | 618 | C |
| 1 | A | 631 | G |
| 1 | A | 650 | G |
| 1 | A | 653 | A |
| 1 | A | 654 | G |
| 1 | A | 664 | G |
| 1 | A | 665 | A |
| 1 | A | 666 | G |
| 1 | A | 667 | G |
| 1 | A | 671 | G |
| 1 | A | 687 | A |
| 1 | A | 695 | A |
| 1 | A | 702 | A |
| 1 | A | 703 | G |
| 1 | A | 705 | U |
| 1 | A | 720 | C |
| 1 | A | 721 | G |
| 1 | A | 722 | A |
| 1 | A | 723 | U |
| 1 | A | 724 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 730 | G |
| 1 | A | 734 | G |
| 1 | A | 741 | G |
| 1 | A | 749 | C |
| 1 | A | 751 | U |
| 1 | A | 753 | A |
| 1 | A | 755 | G |
| 1 | A | 760 | G |
| 1 | A | 766 | A |
| 1 | A | 774 | G |
| 1 | A | 777 | A |
| 1 | A | 781 | A |
| 1 | A | 782 | A |
| 1 | A | 783 | C |
| 1 | A | 784 | C |
| 1 | A | 787 | A |
| 1 | A | 789 | U |
| 1 | A | 793 | U |
| 1 | A | 794 | A |
| 1 | A | 798 | G |
| 1 | A | 801 | U |
| 1 | A | 802 | A |
| 1 | A | 815 | A |
| 1 | A | 817 | C |
| 1 | A | 818 | G |
| 1 | A | 821 | G |
| 1 | A | 827 | U |
| 1 | A | 828 | A |
| 1 | A | 839 | U |
| 1 | A | 840 | C |
| 1 | A | 841 | U |
| 1 | A | 848 | C |
| 1 | A | 852 | G |
| 1 | A | 858 | G |
| 1 | A | 870 | U |
| 1 | A | 872 | A |
| 1 | A | 873 | A |
| 1 | A | 874 | G |
| 1 | A | 885 | G |
| 1 | A | 922 | G |
| 1 | A | 926 | G |
| 1 | A | 927 | G |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | A | 934 | C |
| 1 | A | 935 | A |
| 1 | A | 937 | A |
| 1 | A | 939 | G |
| 1 | A | 960 | U |
| 1 | A | 965 | A |
| 1 | A | 966 | M2G |
| 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 | 982 | U |
| 1 | A | 993 | G |
| 1 | A | 998 | G |
| 1 | A | 999 | C |
| 1 | A | 1003 | G |
| 1 | A | 1003(A) | G |
| 1 | A | 1004 | A |
| 1 | A | 1005 | A |
| 1 | A | 1007 | C |
| 1 | A | 1009 | G |
| 1 | A | 1016 | A |
| 1 | A | 1021 | G |
| 1 | A | 1022 | G |
| 1 | A | 1024 | G |
| 1 | A | 1025 | U |
| 1 | A | 1026 | G |
| 1 | A | 1027 | C |
| 1 | A | 1028 | C |
| 1 | A | 1029 | C |
| 1 | A | 1030 | C |
| 1 | A | 1030(A) | G |
| 1 | A | 1030(B) | C |
| 1 | A | 1030(C) | G |
| 1 | A | 1030(D) | A |
| 1 | A | 1031 | G |
| 1 | A | 1032 | G |
| 1 | A | 1034 | G |
| 1 | A | 1035 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1039 | C |
| 1 | A | 1045 | C |
| 1 | A | 1050 | G |
| 1 | A | 1053 | G |
| 1 | A | 1054 | C |
| 1 | A | 1055 | A |
| 1 | A | 1056 | U |
| 1 | A | 1065 | U |
| 1 | A | 1079 | G |
| 1 | A | 1094 | G |
| 1 | A | 1095 | U |
| 1 | A | 1100 | C |
| 1 | A | 1101 | A |
| 1 | A | 1108 | G |
| 1 | A | 1118 | C |
| 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 | 1134 | G |
| 1 | A | 1135 | U |
| 1 | A | 1136 | U |
| 1 | A | 1137 | C |
| 1 | A | 1139 | G |
| 1 | A | 1140 | C |
| 1 | A | 1141 | C |
| 1 | A | 1145 | C |
| 1 | A | 1146 | A |
| 1 | A | 1151 | A |
| 1 | A | 1159 | U |
| 1 | A | 1160 | G |
| 1 | A | 1171 | G |
| 1 | A | 1172 | C |
| 1 | A | 1174 | G |
| 1 | A | 1182 | G |
| 1 | A | 1190 | G |
| 1 | A | 1196 | U |
| 1 | A | 1197 | G |
| 1 | A | 1198 | G |
| 1 | A | 1201 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1202 | G |
| 1 | A | 1203 | C |
| 1 | A | 1205 | U |
| 1 | A | 1211 | U |
| 1 | A | 1212 | U |
| 1 | A | 1213 | A |
| 1 | A | 1214 | C |
| 1 | A | 1224 | G |
| 1 | A | 1225 | A |
| 1 | A | 1227 | A |
| 1 | A | 1233 | G |
| 1 | A | 1238 | A |
| 1 | A | 1253 | G |
| 1 | A | 1256 | A |
| 1 | A | 1257 | U |
| 1 | A | 1258 | G |
| 1 | A | 1259 | C |
| 1 | A | 1270 | C |
| 1 | A | 1277 | C |
| 1 | A | 1278 | U |
| 1 | A | 1279 | A |
| 1 | A | 1280 | A |
| 1 | A | 1286 | A |
| 1 | A | 1287 | A |
| 1 | A | 1296 | C |
| 1 | A | 1298 | C |
| 1 | A | 1300 | G |
| 1 | A | 1302 | U |
| 1 | A | 1307 | U |
| 1 | A | 1320 | C |
| 1 | A | 1322 | C |
| 1 | A | 1323 | G |
| 1 | A | 1336 | C |
| 1 | A | 1338 | G |
| 1 | A | 1353 | G |
| 1 | A | 1363 | A |
| 1 | A | 1370 | G |
| 1 | A | 1379 | G |
| 1 | A | 1381 | U |
| 1 | A | 1394 | A |
| 1 | A | 1398 | A |
| 1 | A | 1399 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1400 | 5MC |
| 1 | A | 1403 | C |
| 1 | A | 1418 | A |
| 1 | A | 1428 | A |
| 1 | A | 1432 | G |
| 1 | A | 1440 | C |
| 1 | A | 1442 | G |
| 1 | A | 1443 | G |
| 1 | A | 1447 | G |
| 1 | A | 1451 | A |
| 1 | A | 1453 | G |
| 1 | A | 1474 | G |
| 1 | A | 1475 | G |
| 1 | A | 1477 | C |
| 1 | A | 1478 | C |
| 1 | A | 1479 | C |
| 1 | A | 1481 | U |
| 1 | A | 1482 | G |
| 1 | A | 1485 | U |
| 1 | A | 1486 | G |
| 1 | A | 1487 | G |
| 1 | A | 1491 | G |
| 1 | A | 1493 | A |
| 1 | A | 1497 | G |
| 1 | A | 1498 | UR3 |
| 1 | A | 1499 | A |
| 1 | A | 1502 | A |
| 1 | A | 1506 | U |
| 1 | A | 1529 | G |
| 1 | A | 1530 | G |
| 1 | A | 1533 | C |
| 1 | A | 1540 | PSU |
| 1 | A | 1541 | PSU |
| 1 | A | 1542 | U |
| 1 | A | 1544 | U |

All (27) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | A | 115 | G |
| 1 | A | 129(A) | G |
| 1 | A | 181 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 204 | U |
| 1 | A | 250 | A |
| 1 | A | 350 | G |
| 1 | A | 428 | G |
| 1 | A | 429 | U |
| 1 | A | 484 | G |
| 1 | A | 485 | G |
| 1 | A | 499 | A |
| 1 | A | 509 | A |
| 1 | A | 518 | C |
| 1 | A | 525 | C |
| 1 | A | 559 | A |
| 1 | A | 748 | C |
| 1 | A | 793 | U |
| 1 | A | 992 | U |
| 1 | A | 1125 | U |
| 1 | A | 1126 | U |
| 1 | A | 1195 | C |
| 1 | A | 1201 | A |
| 1 | A | 1256 | A |
| 1 | A | 1277 | C |
| 1 | A | 1319 | A |
| 1 | A | 1380 | U |
| 1 | A | 1529 | G |

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 | MA6 | A | 1519[A] | 1 | 19,26,27 | 1.23 | 3 (15%) | 18,38,41 | 0.89 | 0 |
| 1 | PSU | A | 516 | 1,22 | 18,21,22 | 1.28 | 3 (16%) | 21,30,33 | 1.14 | 3 (14%) |
| 1 | M2G | A | 966 | 1 | 20,27,28 | 1.57 | 2 (10%) | 19,40,43 | 1.51 | 2 (10%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|---------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | MA6 | A | 1518[B] | 1 | 19,26,27 | 1.43 | 4 (21%) | 18,38,41 | 0.82 | 0 |
| 12 | 0TD | L | 92 | 12 | 8,9,10 | 1.58 | 1 (12%) | 6,11,13 | 2.34 | 2 (33%) |
| 1 | MA6 | A | 1519[B] | 1 | 19,26,27 | 1.86 | 5 (26%) | 18,38,41 | 0.76 | 0 |
| 1 | 7MG | A | 527 | 1 | 23,26,27 | 3.88 | 6 (26%) | 27,39,42 | 2.37 | 8 (29%) |
| 1 | UR3 | A | 1498 | 1 | 19,22,23 | 1.33 | 3 (15%) | 26,32,35 | 1.42 | 4 (15%) |
| 1 | 4OC | A | 1402 | 1 | 20,23,24 | 1.14 | 2 (10%) | 25,32,35 | 0.98 | 2 (8%) |
| 1 | 5MC | A | 1400 | 1 | 19,22,23 | 1.56 | 5 (26%) | 26,32,35 | 1.15 | 4 (15%) |
| 1 | PSU | A | 1540 | 1 | 18,21,22 | 1.01 | 1 (5%) | 21,30,33 | 1.64 | 3 (14%) |
| 1 | 5MC | A | 1407 | 1 | 19,22,23 | 1.08 | 2 (10%) | 26,32,35 | 1.29 | 2 (7%) |
| 1 | 2MG | A | 1207 | 1,22 | 18,26,27 | 1.39 | 2 (11%) | 16,38,41 | 1.23 | 2 (12%) |
| 1 | PSU | A | 1541 | 1 | 18,21,22 | 1.08 | 3 (16%) | 21,30,33 | 1.94 | 6 (28%) |
| 1 | 5MC | A | 1404 | 1 | 19,22,23 | 1.40 | 3 (15%) | 26,32,35 | 1.15 | 3 (11%) |
| 1 | 5MC | A | 967 | 1 | 19,22,23 | 1.14 | 2 (10%) | 26,32,35 | 1.15 | 3 (11%) |
| 1 | MA6 | A | 1518[A] | 1 | 19,26,27 | 1.24 | 1 (5%) | 18,38,41 | 0.83 | 1 (5%) |

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 | MA6 | A | 1519[A] | 1 | - | 4/7/29/30 | 0/3/3/3 |
| 1 | PSU | A | 516 | 1,22 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | M2G | A | 966 | 1 | - | 2/7/29/30 | 0/3/3/3 |
| 1 | MA6 | A | 1518[B] | 1 | - | 6/7/29/30 | 0/3/3/3 |
| 12 | 0TD | L | 92 | 12 | - | 3/7/12/14 | - |
| 1 | MA6 | A | 1519[B] | 1 | - | 4/7/29/30 | 0/3/3/3 |
| 1 | 7MG | A | 527 | 1 | - | 1/7/37/38 | 0/3/3/3 |
| 1 | UR3 | A | 1498 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 4OC | A | 1402 | 1 | - | 2/9/29/30 | 0/2/2/2 |
| 1 | 5MC | A | 1400 | 1 | - | 2/7/25/26 | 0/2/2/2 |
| 1 | PSU | A | 1540 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MC | A | 1407 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 2MG | A | 1207 | 1,22 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | PSU | A | 1541 | 1 | - | 3/7/25/26 | 0/2/2/2 |
| 1 | 5MC | A | 1404 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MC | A | 967 | 1 | - | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|---------|------|---------|-----------|---------|
| 1 | MA6 | A | 1518[A] | 1 | - | 3/7/29/30 | 0/3/3/3 |

All (48) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|---------|--------|-------------|----------|
| 1 | A | 527 | 7MG | C8-N9 | -16.46 | 1.35 | 1.45 |
| 1 | A | 1519[B] | MA6 | C6-N1 | 5.09 | 1.39 | 1.32 |
| 1 | A | 527 | 7MG | C5-N7 | 4.67 | 1.41 | 1.35 |
| 1 | A | 1518[A] | MA6 | C6-C5 | -4.57 | 1.37 | 1.44 |
| 1 | A | 1207 | 2MG | C5-C6 | -4.27 | 1.39 | 1.47 |
| 1 | A | 966 | M2G | C2-N2 | 4.23 | 1.42 | 1.35 |
| 1 | A | 1518[B] | MA6 | C6-N1 | 4.01 | 1.38 | 1.32 |
| 1 | A | 527 | 7MG | C6-N1 | -3.83 | 1.31 | 1.38 |
| 1 | A | 1400 | 5MC | C2-N1 | 3.81 | 1.48 | 1.40 |
| 1 | A | 966 | M2G | C2-N3 | 3.74 | 1.35 | 1.30 |
| 1 | A | 527 | 7MG | C2-N1 | -3.49 | 1.29 | 1.37 |
| 12 | L | 92 | 0TD | CB-CA | -3.44 | 1.53 | 1.54 |
| 1 | A | 516 | PSU | C6-C5 | 3.40 | 1.39 | 1.35 |
| 1 | A | 1540 | PSU | C6-C5 | 3.26 | 1.38 | 1.35 |
| 1 | A | 1519[B] | MA6 | C2-N1 | 3.26 | 1.39 | 1.33 |
| 1 | A | 1400 | 5MC | C2-N3 | 3.21 | 1.42 | 1.36 |
| 1 | A | 1402 | 4OC | O2-C2 | -3.10 | 1.17 | 1.23 |
| 1 | A | 1519[B] | MA6 | C6-N6 | 3.10 | 1.44 | 1.37 |
| 1 | A | 527 | 7MG | C2-N2 | 3.00 | 1.41 | 1.34 |
| 1 | A | 967 | 5MC | C5-C4 | -2.98 | 1.41 | 1.44 |
| 1 | A | 1498 | UR3 | C3U-N3 | -2.97 | 1.41 | 1.47 |
| 1 | A | 1519[B] | MA6 | C2-N3 | 2.94 | 1.36 | 1.32 |
| 1 | A | 1404 | 5MC | O2-C2 | -2.90 | 1.18 | 1.23 |
| 1 | A | 1404 | 5MC | C2-N3 | 2.82 | 1.41 | 1.36 |
| 1 | A | 1519[A] | MA6 | C6-N1 | 2.74 | 1.36 | 1.32 |
| 1 | A | 1541 | PSU | C6-C5 | 2.74 | 1.38 | 1.35 |
| 1 | A | 1400 | 5MC | C6-N1 | -2.73 | 1.33 | 1.38 |
| 1 | A | 1402 | 4OC | C6-N1 | -2.71 | 1.31 | 1.38 |
| 1 | A | 1519[A] | MA6 | C2-N1 | 2.64 | 1.38 | 1.33 |
| 1 | A | 1519[B] | MA6 | C4-N3 | 2.57 | 1.39 | 1.35 |
| 1 | A | 1400 | 5MC | C5-C4 | -2.47 | 1.42 | 1.44 |
| 1 | A | 967 | 5MC | C2-N1 | 2.43 | 1.45 | 1.40 |
| 1 | A | 1518[B] | MA6 | C6-N6 | 2.40 | 1.43 | 1.37 |
| 1 | A | 1498 | UR3 | O4-C4 | 2.39 | 1.28 | 1.23 |
| 1 | A | 1404 | 5MC | C5-C4 | -2.36 | 1.42 | 1.44 |
| 1 | A | 516 | PSU | O4'-C1' | -2.35 | 1.40 | 1.43 |
| 1 | A | 1519[A] | MA6 | C6-C5 | -2.28 | 1.41 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|---------|-------|-------------|----------|
| 1 | A | 1407 | 5MC | C5-C4 | -2.27 | 1.42 | 1.44 |
| 1 | A | 516 | PSU | C4-C5 | -2.27 | 1.38 | 1.44 |
| 1 | A | 1541 | PSU | O4'-C1' | -2.24 | 1.40 | 1.43 |
| 1 | A | 1518[B] | MA6 | C2-N1 | 2.23 | 1.37 | 1.33 |
| 1 | A | 1518[B] | MA6 | C2-N3 | 2.22 | 1.35 | 1.32 |
| 1 | A | 1207 | 2MG | C2-N2 | 2.20 | 1.38 | 1.33 |
| 1 | A | 1407 | 5MC | C2-N3 | 2.20 | 1.40 | 1.36 |
| 1 | A | 1498 | UR3 | C4-N3 | -2.19 | 1.36 | 1.40 |
| 1 | A | 1400 | 5MC | O2-C2 | 2.10 | 1.27 | 1.23 |
| 1 | A | 1541 | PSU | C4-C5 | -2.04 | 1.38 | 1.44 |
| 1 | A | 527 | 7MG | C8-N7 | -2.01 | 1.32 | 1.42 |

All (45) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 527 | 7MG | C5-C6-N1 | 5.06 | 119.84 | 110.94 |
| 12 | L | 92 | 0TD | CSB-SB-CB | -4.67 | 93.96 | 102.36 |
| 1 | A | 527 | 7MG | N9-C8-N7 | 4.66 | 109.97 | 103.37 |
| 1 | A | 527 | 7MG | C2-N3-C4 | 4.54 | 120.12 | 112.30 |
| 1 | A | 527 | 7MG | C5-C4-N3 | -4.43 | 119.81 | 128.13 |
| 1 | A | 1540 | PSU | C4-N3-C2 | -4.42 | 120.28 | 126.37 |
| 1 | A | 527 | 7MG | N9-C4-N3 | 4.37 | 131.87 | 125.46 |
| 1 | A | 1541 | PSU | C4-N3-C2 | -4.15 | 120.65 | 126.37 |
| 1 | A | 966 | M2G | O6-C6-N1 | -3.96 | 115.92 | 120.62 |
| 1 | A | 1541 | PSU | N1-C2-N3 | 3.96 | 119.34 | 115.17 |
| 1 | A | 1541 | PSU | O2-C2-N1 | -3.88 | 118.78 | 122.79 |
| 1 | A | 966 | M2G | O6-C6-C5 | 3.82 | 131.90 | 124.32 |
| 1 | A | 1540 | PSU | N1-C2-N3 | 3.79 | 119.16 | 115.17 |
| 1 | A | 527 | 7MG | C6-C5-C4 | -3.38 | 116.45 | 122.40 |
| 1 | A | 1541 | PSU | C6-C5-C4 | 3.33 | 120.42 | 118.17 |
| 1 | A | 1407 | 5MC | C1'-N1-C6 | -3.32 | 115.68 | 121.15 |
| 1 | A | 1207 | 2MG | O6-C6-N1 | -3.18 | 116.85 | 120.62 |
| 1 | A | 527 | 7MG | C6-C5-N7 | 3.09 | 136.72 | 131.93 |
| 1 | A | 1498 | UR3 | O3'-C3'-C2' | 3.08 | 121.69 | 111.82 |
| 1 | A | 527 | 7MG | C2-N1-C6 | -2.89 | 119.86 | 125.11 |
| 1 | A | 516 | PSU | C4-N3-C2 | -2.89 | 122.38 | 126.37 |
| 1 | A | 1207 | 2MG | O6-C6-C5 | 2.81 | 129.90 | 124.32 |
| 1 | A | 1498 | UR3 | C6-N1-C2 | -2.67 | 119.62 | 121.80 |
| 1 | A | 967 | 5MC | C5-C4-N3 | 2.59 | 124.41 | 121.75 |
| 1 | A | 1400 | 5MC | C1'-N1-C6 | -2.57 | 116.92 | 121.15 |
| 1 | A | 1407 | 5MC | C5-C4-N3 | 2.49 | 124.31 | 121.75 |
| 1 | A | 1400 | 5MC | O2-C2-N1 | 2.44 | 123.67 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-------------|-------|-------------|----------|
| 1 | A | 1404 | 5MC | C1'-N1-C2 | 2.42 | 123.78 | 118.44 |
| 1 | A | 1541 | PSU | O4'-C1'-C2' | 2.36 | 108.42 | 105.15 |
| 1 | A | 1541 | PSU | C6-N1-C2 | -2.34 | 120.52 | 122.69 |
| 1 | A | 1402 | 4OC | C2'-C1'-N1 | -2.34 | 109.80 | 114.24 |
| 1 | A | 1540 | PSU | C6-N1-C2 | -2.23 | 120.62 | 122.69 |
| 1 | A | 1498 | UR3 | C4-N3-C2 | 2.22 | 126.36 | 124.58 |
| 1 | A | 967 | 5MC | C4-N3-C2 | -2.19 | 117.77 | 120.81 |
| 1 | A | 1404 | 5MC | C4-N3-C2 | -2.18 | 117.78 | 120.81 |
| 1 | A | 1404 | 5MC | C1'-N1-C6 | -2.18 | 117.56 | 121.15 |
| 1 | A | 516 | PSU | O4'-C1'-C2' | 2.17 | 108.16 | 105.15 |
| 1 | A | 1402 | 4OC | C5-C4-N4 | -2.16 | 117.65 | 122.40 |
| 1 | A | 967 | 5MC | N4-C4-N3 | -2.13 | 114.65 | 118.51 |
| 1 | A | 1400 | 5MC | C1'-N1-C2 | 2.08 | 123.04 | 118.44 |
| 1 | A | 1518[A] | MA6 | N1-C6-N6 | -2.06 | 114.45 | 116.83 |
| 1 | A | 1400 | 5MC | N4-C4-N3 | -2.06 | 114.77 | 118.51 |
| 1 | A | 1498 | UR3 | C5-C4-N3 | -2.03 | 112.36 | 115.04 |
| 1 | A | 516 | PSU | O4-C4-C5 | -2.03 | 118.96 | 124.01 |
| 12 | L | 92 | 0TD | CB-CA-N | -2.03 | 104.98 | 109.10 |

There are no chirality outliers.

All (30) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|---------|------|-----------------|
| 1 | A | 966 | M2G | O4'-C4'-C5'-O5' |
| 1 | A | 1402 | 4OC | O4'-C4'-C5'-O5' |
| 1 | A | 1402 | 4OC | C3'-C4'-C5'-O5' |
| 1 | A | 1518[A] | MA6 | O4'-C4'-C5'-O5' |
| 1 | A | 1518[A] | MA6 | C3'-C4'-C5'-O5' |
| 1 | A | 1518[B] | MA6 | O4'-C4'-C5'-O5' |
| 1 | A | 1518[B] | MA6 | C3'-C4'-C5'-O5' |
| 1 | A | 1518[B] | MA6 | C5-C6-N6-C9 |
| 1 | A | 1518[B] | MA6 | C5-C6-N6-C10 |
| 1 | A | 1518[B] | MA6 | N1-C6-N6-C9 |
| 1 | A | 1518[B] | MA6 | N1-C6-N6-C10 |
| 1 | A | 1519[A] | MA6 | O4'-C4'-C5'-O5' |
| 1 | A | 1519[A] | MA6 | C3'-C4'-C5'-O5' |
| 1 | A | 1519[A] | MA6 | C5-C6-N6-C10 |
| 12 | L | 92 | 0TD | O-C-CA-CB |
| 1 | A | 1400 | 5MC | O4'-C4'-C5'-O5' |
| 1 | A | 1519[B] | MA6 | C3'-C4'-C5'-O5' |
| 1 | A | 1541 | PSU | O4'-C4'-C5'-O5' |
| 1 | A | 527 | 7MG | C4'-C5'-O5'-P |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|---------|------|-----------------|
| 1 | A | 1519[A] | MA6 | C4'-C5'-O5'-P |
| 1 | A | 966 | M2G | C3'-C4'-C5'-O5' |
| 1 | A | 1519[B] | MA6 | N1-C6-N6-C9 |
| 1 | A | 1519[B] | MA6 | O4'-C4'-C5'-O5' |
| 1 | A | 1400 | 5MC | C3'-C4'-C5'-O5' |
| 1 | A | 1541 | PSU | C3'-C4'-C5'-O5' |
| 12 | L | 92 | 0TD | CG-CB-SB-CSB |
| 1 | A | 1518[A] | MA6 | C5-C6-N6-C10 |
| 1 | A | 1519[B] | MA6 | C5-C6-N6-C9 |
| 12 | L | 92 | 0TD | SB-CB-CG-OD1 |
| 1 | A | 1541 | PSU | O4'-C1'-C5-C4 |

There are no ring outliers.

14 monomers are involved in 26 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|---------|------|---------|--------------|
| 1 | A | 1519[A] | MA6 | 2 | 0 |
| 1 | A | 516 | PSU | 1 | 0 |
| 1 | A | 966 | M2G | 2 | 0 |
| 1 | A | 1518[B] | MA6 | 4 | 0 |
| 1 | A | 1519[B] | MA6 | 4 | 0 |
| 1 | A | 527 | 7MG | 3 | 0 |
| 1 | A | 1498 | UR3 | 1 | 0 |
| 1 | A | 1402 | 4OC | 1 | 0 |
| 1 | A | 1400 | 5MC | 2 | 0 |
| 1 | A | 1540 | PSU | 1 | 0 |
| 1 | A | 1541 | PSU | 1 | 0 |
| 1 | A | 1404 | 5MC | 2 | 0 |
| 1 | A | 967 | 5MC | 5 | 0 |
| 1 | A | 1518[A] | MA6 | 3 | 0 |

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 174 ligands modelled in this entry, 174 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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 | 1500/1522 (98%) | -0.27 | 47 (3%) 51 40 | 59, 152, 229, 333 | 4 (0%) |
| 2 | B | 234/256 (91%) | -0.48 | 4 (1%) 69 52 | 122, 170, 240, 274 | 0 |
| 3 | C | 206/239 (86%) | -0.12 | 5 (2%) 59 46 | 121, 156, 199, 229 | 0 |
| 4 | D | 208/209 (99%) | 0.16 | 21 (10%) 14 15 | 104, 151, 206, 237 | 0 |
| 5 | E | 150/162 (92%) | -0.12 | 9 (6%) 29 26 | 93, 132, 172, 216 | 0 |
| 6 | F | 101/101 (100%) | -0.15 | 3 (2%) 52 41 | 135, 171, 201, 254 | 0 |
| 7 | G | 155/156 (99%) | 0.05 | 13 (8%) 18 18 | 145, 183, 228, 254 | 0 |
| 8 | H | 138/138 (100%) | -0.11 | 9 (6%) 26 24 | 114, 143, 181, 226 | 0 |
| 9 | I | 127/128 (99%) | 0.12 | 7 (5%) 32 27 | 149, 182, 222, 246 | 0 |
| 10 | J | 98/105 (93%) | 0.23 | 4 (4%) 42 34 | 136, 186, 225, 252 | 0 |
| 11 | K | 116/129 (89%) | -0.01 | 3 (2%) 57 44 | 134, 168, 207, 226 | 0 |
| 12 | L | 123/135 (91%) | -0.10 | 7 (5%) 30 27 | 106, 137, 168, 224 | 0 |
| 13 | M | 118/126 (93%) | 0.10 | 9 (7%) 21 20 | 149, 192, 225, 299 | 0 |
| 14 | N | 60/61 (98%) | 0.01 | 0 100 100 | 133, 161, 214, 240 | 0 |
| 15 | O | 87/89 (97%) | -0.56 | 0 100 100 | 128, 160, 194, 201 | 0 |
| 16 | P | 83/88 (94%) | -0.20 | 1 (1%) 76 60 | 126, 148, 181, 205 | 0 |
| 17 | Q | 99/105 (94%) | 0.41 | 10 (10%) 14 15 | 120, 144, 178, 199 | 0 |
| 18 | R | 70/88 (79%) | -0.56 | 0 100 100 | 131, 165, 237, 266 | 0 |
| 19 | S | 80/93 (86%) | -0.01 | 5 (6%) 27 25 | 157, 197, 240, 268 | 0 |
| 20 | T | 99/106 (93%) | 0.33 | 5 (5%) 34 30 | 123, 154, 196, 214 | 0 |
| 21 | U | 24/27 (88%) | 1.05 | 3 (12%) 9 13 | 172, 194, 241, 254 | 0 |
| All | All | 3876/4063 (95%) | -0.13 | 165 (4%) 40 34 | 59, 159, 221, 333 | 4 (0%) |

All (165) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 7 | G | 8 | GLU | 15.5 |
| 7 | G | 6 | ARG | 10.8 |
| 7 | G | 9 | VAL | 8.7 |
| 1 | A | 1516[A] | G | 8.5 |
| 7 | G | 11 | GLN | 8.0 |
| 8 | H | 99 | GLU | 7.2 |
| 9 | I | 66 | ARG | 6.9 |
| 1 | A | 1129 | C | 6.8 |
| 20 | T | 9 | ASN | 6.6 |
| 10 | J | 43 | ARG | 6.0 |
| 4 | D | 6 | GLY | 5.9 |
| 4 | D | 24 | GLU | 5.8 |
| 5 | E | 20 | GLN | 5.8 |
| 21 | U | 25 | LYS | 5.5 |
| 7 | G | 3 | ARG | 5.5 |
| 7 | G | 10 | ARG | 5.2 |
| 20 | T | 11 | SER | 5.1 |
| 6 | F | 101 | ALA | 4.9 |
| 1 | A | 1283 | G | 4.7 |
| 9 | I | 127 | LYS | 4.7 |
| 21 | U | 24 | ARG | 4.6 |
| 7 | G | 2 | ALA | 4.6 |
| 5 | E | 18 | ARG | 4.5 |
| 8 | H | 25 | ASP | 4.5 |
| 10 | J | 45 | ARG | 4.5 |
| 1 | A | 1533 | C | 4.5 |
| 7 | G | 4 | ARG | 4.4 |
| 1 | A | 977 | A | 4.3 |
| 1 | A | 1334 | G | 4.2 |
| 4 | D | 4 | TYR | 4.1 |
| 17 | Q | 25 | ARG | 4.0 |
| 1 | A | 1282 | C | 4.0 |
| 13 | M | 100 | GLY | 4.0 |
| 17 | Q | 24 | GLU | 3.9 |
| 13 | M | 7 | VAL | 3.9 |
| 9 | I | 64 | THR | 3.8 |
| 19 | S | 2 | PRO | 3.8 |
| 19 | S | 8 | GLY | 3.8 |
| 17 | Q | 100 | LYS | 3.8 |
| 1 | A | 1517[A] | G | 3.7 |
| 7 | G | 5 | ARG | 3.7 |
| 12 | L | 115 | LYS | 3.6 |
| 1 | A | 726 | C | 3.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 8 | H | 98 | LYS | 3.6 |
| 2 | B | 137 | ARG | 3.5 |
| 12 | L | 128 | ALA | 3.5 |
| 20 | T | 65 | LYS | 3.5 |
| 8 | H | 1 | MET | 3.5 |
| 1 | A | 1362 | C | 3.4 |
| 1 | A | 727 | G | 3.4 |
| 21 | U | 3 | LYS | 3.4 |
| 1 | A | 776 | G | 3.3 |
| 10 | J | 100 | THR | 3.3 |
| 12 | L | 28 | LYS | 3.3 |
| 20 | T | 12 | ALA | 3.3 |
| 9 | I | 126 | SER | 3.3 |
| 1 | A | 1003 | G | 3.2 |
| 1 | A | 1426 | C | 3.2 |
| 17 | Q | 33 | GLY | 3.1 |
| 16 | P | 39 | TYR | 3.1 |
| 12 | L | 47 | LYS | 3.1 |
| 1 | A | 978 | A | 3.1 |
| 8 | H | 90 | GLY | 3.0 |
| 13 | M | 21 | TYR | 3.0 |
| 1 | A | 1525 | G | 3.0 |
| 2 | B | 133 | LYS | 3.0 |
| 8 | H | 54 | ASP | 3.0 |
| 4 | D | 5 | ILE | 3.0 |
| 1 | A | 1224 | G | 2.9 |
| 5 | E | 21 | ALA | 2.9 |
| 1 | A | 1128 | C | 2.9 |
| 19 | S | 5 | LEU | 2.9 |
| 11 | K | 124 | LYS | 2.9 |
| 1 | A | 921 | U | 2.9 |
| 4 | D | 115 | ARG | 2.9 |
| 5 | E | 19 | MET | 2.9 |
| 4 | D | 2 | GLY | 2.9 |
| 1 | A | 306 | G | 2.9 |
| 4 | D | 35 | ARG | 2.9 |
| 4 | D | 7 | PRO | 2.8 |
| 4 | D | 8 | VAL | 2.8 |
| 7 | G | 7 | ALA | 2.8 |
| 4 | D | 38 | TYR | 2.8 |
| 2 | B | 33 | TYR | 2.7 |
| 4 | D | 112 | VAL | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 8 | H | 95 | VAL | 2.7 |
| 1 | A | 1280 | A | 2.7 |
| 17 | Q | 30 | PRO | 2.7 |
| 5 | E | 154 | GLY | 2.7 |
| 13 | M | 101 | GLN | 2.7 |
| 1 | A | 1333 | A | 2.7 |
| 4 | D | 42 | GLN | 2.7 |
| 13 | M | 119 | GLY | 2.7 |
| 2 | B | 132 | LYS | 2.6 |
| 4 | D | 157 | LEU | 2.6 |
| 1 | A | 731 | G | 2.6 |
| 19 | S | 78 | ARG | 2.6 |
| 1 | A | 202 | U | 2.6 |
| 11 | K | 126 | ARG | 2.6 |
| 6 | F | 97 | PHE | 2.6 |
| 1 | A | 390 | C | 2.6 |
| 7 | G | 13 | GLN | 2.6 |
| 1 | A | 1477 | C | 2.5 |
| 7 | G | 94 | ARG | 2.5 |
| 1 | A | 1427 | U | 2.5 |
| 4 | D | 29 | PRO | 2.5 |
| 3 | C | 207 | VAL | 2.5 |
| 1 | A | 1030(D) | A | 2.5 |
| 5 | E | 153 | LYS | 2.5 |
| 5 | E | 25 | ARG | 2.5 |
| 8 | H | 94 | TYR | 2.5 |
| 1 | A | 653 | A | 2.5 |
| 3 | C | 190 | ARG | 2.4 |
| 13 | M | 4 | ILE | 2.4 |
| 3 | C | 158 | GLY | 2.4 |
| 1 | A | 922 | G | 2.4 |
| 4 | D | 40 | PRO | 2.4 |
| 13 | M | 27 | LYS | 2.4 |
| 8 | H | 101 | PRO | 2.4 |
| 1 | A | 290 | C | 2.4 |
| 1 | A | 1054 | C | 2.4 |
| 12 | L | 116 | SER | 2.4 |
| 11 | K | 31 | THR | 2.3 |
| 7 | G | 81 | GLY | 2.3 |
| 1 | A | 1290 | G | 2.3 |
| 4 | D | 37 | PRO | 2.3 |
| 1 | A | 732 | C | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 20 | T | 64 | ASP | 2.3 |
| 9 | I | 62 | TYR | 2.3 |
| 17 | Q | 13 | ASP | 2.3 |
| 17 | Q | 68 | ARG | 2.3 |
| 13 | M | 104 | ARG | 2.3 |
| 1 | A | 3 | G | 2.3 |
| 1 | A | 587 | G | 2.3 |
| 4 | D | 160 | GLN | 2.2 |
| 1 | A | 1361(A) | C | 2.2 |
| 5 | E | 104 | ALA | 2.2 |
| 17 | Q | 67 | LYS | 2.2 |
| 13 | M | 87 | TYR | 2.2 |
| 19 | S | 9 | VAL | 2.2 |
| 1 | A | 532 | A | 2.2 |
| 10 | J | 47 | PHE | 2.2 |
| 17 | Q | 27 | PHE | 2.2 |
| 3 | C | 159 | GLY | 2.2 |
| 1 | A | 412 | A | 2.2 |
| 3 | C | 184 | TYR | 2.2 |
| 4 | D | 33 | MET | 2.2 |
| 12 | L | 26 | ALA | 2.2 |
| 1 | A | 512 | U | 2.2 |
| 5 | E | 133 | TYR | 2.1 |
| 4 | D | 36 | ARG | 2.1 |
| 1 | A | 115 | G | 2.1 |
| 17 | Q | 26 | GLN | 2.1 |
| 4 | D | 120 | LEU | 2.1 |
| 1 | A | 742 | G | 2.1 |
| 1 | A | 389 | A | 2.1 |
| 1 | A | 1255 | G | 2.1 |
| 6 | F | 100 | ASN | 2.1 |
| 9 | I | 75 | ASP | 2.1 |
| 9 | I | 117 | HIS | 2.1 |
| 12 | L | 120 | TYR | 2.1 |
| 4 | D | 45 | GLN | 2.0 |
| 1 | A | 268 | C | 2.0 |
| 1 | A | 920 | U | 2.0 |
| 1 | A | 575 | G | 2.0 |

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

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|---------|-------|------|------|----------------------------|-------|
| 1 | PSU | A | 1540 | 20/21 | 0.89 | 0.18 | 234,259,275,280 | 0 |
| 1 | 2MG | A | 1207 | 24/25 | 0.93 | 0.08 | 148,156,161,163 | 0 |
| 1 | MA6 | A | 1518[A] | 24/25 | 0.93 | 0.19 | 109,121,135,142 | 24 |
| 1 | MA6 | A | 1518[B] | 24/25 | 0.93 | 0.19 | 126,134,140,141 | 24 |
| 1 | PSU | A | 516 | 20/21 | 0.93 | 0.07 | 143,152,163,165 | 0 |
| 1 | PSU | A | 1541 | 20/21 | 0.93 | 0.15 | 232,243,250,252 | 0 |
| 1 | 7MG | A | 527 | 24/25 | 0.94 | 0.09 | 127,137,152,160 | 0 |
| 1 | M2G | A | 966 | 25/26 | 0.96 | 0.12 | 120,145,181,186 | 0 |
| 1 | 4OC | A | 1402 | 22/23 | 0.96 | 0.09 | 117,134,153,154 | 0 |
| 1 | 5MC | A | 1407 | 21/22 | 0.96 | 0.06 | 140,145,154,161 | 0 |
| 1 | UR3 | A | 1498 | 21/22 | 0.96 | 0.12 | 115,130,138,144 | 0 |
| 1 | 5MC | A | 1400 | 21/22 | 0.97 | 0.07 | 106,127,151,157 | 0 |
| 1 | MA6 | A | 1519[A] | 24/25 | 0.98 | 0.11 | 104,118,124,129 | 24 |
| 1 | MA6 | A | 1519[B] | 24/25 | 0.98 | 0.11 | 105,117,131,134 | 24 |
| 1 | 5MC | A | 967 | 21/22 | 0.98 | 0.07 | 134,149,157,162 | 0 |
| 1 | 5MC | A | 1404 | 21/22 | 0.98 | 0.17 | 132,137,141,146 | 0 |
| 12 | 0TD | L | 92 | 10/11 | 0.99 | 0.07 | 130,141,148,274 | 0 |

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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 |
|-----|------|-------|------|-------|-------|------|----------------------------|-------|
| 22 | MG | A | 1632 | 1/1 | -0.09 | 0.54 | 161,161,161,161 | 0 |
| 22 | MG | A | 1732 | 1/1 | 0.08 | 0.34 | 161,161,161,161 | 0 |
| 22 | MG | A | 1731 | 1/1 | 0.34 | 0.29 | 185,185,185,185 | 0 |
| 22 | MG | A | 1730 | 1/1 | 0.34 | 0.23 | 181,181,181,181 | 0 |
| 22 | MG | A | 1733 | 1/1 | 0.35 | 0.30 | 143,143,143,143 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 22 | MG | A | 1653 | 1/1 | 0.51 | 0.35 | 100,100,100,100 | 0 |
| 22 | MG | A | 1746 | 1/1 | 0.51 | 0.20 | 185,185,185,185 | 0 |
| 22 | MG | G | 201 | 1/1 | 0.51 | 0.38 | 157,157,157,157 | 0 |
| 22 | MG | A | 1630 | 1/1 | 0.52 | 0.47 | 127,127,127,127 | 0 |
| 22 | MG | A | 1749 | 1/1 | 0.58 | 0.41 | 134,134,134,134 | 0 |
| 22 | MG | A | 1650 | 1/1 | 0.60 | 0.34 | 120,120,120,120 | 0 |
| 22 | MG | A | 1728 | 1/1 | 0.62 | 0.32 | 120,120,120,120 | 0 |
| 22 | MG | A | 1684 | 1/1 | 0.62 | 0.23 | 128,128,128,128 | 0 |
| 22 | MG | A | 1755 | 1/1 | 0.69 | 0.10 | 148,148,148,148 | 0 |
| 22 | MG | A | 1706 | 1/1 | 0.70 | 0.13 | 400,400,400,400 | 0 |
| 22 | MG | A | 1671 | 1/1 | 0.70 | 0.22 | 108,108,108,108 | 0 |
| 22 | MG | A | 1737 | 1/1 | 0.72 | 0.28 | 143,143,143,143 | 0 |
| 22 | MG | A | 1639 | 1/1 | 0.73 | 0.16 | 133,133,133,133 | 0 |
| 22 | MG | A | 1757 | 1/1 | 0.73 | 0.43 | 121,121,121,121 | 0 |
| 22 | MG | A | 1673 | 1/1 | 0.73 | 0.24 | 121,121,121,121 | 0 |
| 22 | MG | A | 1675 | 1/1 | 0.74 | 0.35 | 95,95,95,95 | 0 |
| 22 | MG | A | 1735 | 1/1 | 0.74 | 0.17 | 143,143,143,143 | 0 |
| 22 | MG | A | 1734 | 1/1 | 0.75 | 0.22 | 136,136,136,136 | 0 |
| 22 | MG | A | 1619 | 1/1 | 0.76 | 0.19 | 132,132,132,132 | 0 |
| 22 | MG | A | 1628 | 1/1 | 0.76 | 0.18 | 127,127,127,127 | 0 |
| 22 | MG | F | 201 | 1/1 | 0.76 | 0.28 | 127,127,127,127 | 0 |
| 22 | MG | A | 1750 | 1/1 | 0.76 | 0.35 | 137,137,137,137 | 0 |
| 22 | MG | A | 1752 | 1/1 | 0.77 | 0.19 | 156,156,156,156 | 0 |
| 22 | MG | A | 1679 | 1/1 | 0.79 | 0.23 | 140,140,140,140 | 0 |
| 22 | MG | A | 1647 | 1/1 | 0.79 | 0.13 | 141,141,141,141 | 0 |
| 22 | MG | A | 1736 | 1/1 | 0.79 | 0.26 | 112,112,112,112 | 0 |
| 22 | MG | A | 1745 | 1/1 | 0.80 | 0.44 | 107,107,107,107 | 0 |
| 22 | MG | A | 1762 | 1/1 | 0.80 | 0.18 | 136,136,136,136 | 0 |
| 22 | MG | K | 201 | 1/1 | 0.80 | 0.62 | 93,93,93,93 | 0 |
| 22 | MG | A | 1751 | 1/1 | 0.81 | 0.40 | 170,170,170,170 | 0 |
| 22 | MG | A | 1674 | 1/1 | 0.81 | 0.26 | 114,114,114,114 | 0 |
| 22 | MG | A | 1741 | 1/1 | 0.82 | 0.18 | 111,111,111,111 | 0 |
| 22 | MG | A | 1754 | 1/1 | 0.83 | 0.17 | 121,121,121,121 | 0 |
| 22 | MG | A | 1631 | 1/1 | 0.83 | 0.10 | 277,277,277,277 | 0 |
| 22 | MG | A | 1756 | 1/1 | 0.83 | 0.10 | 132,132,132,132 | 0 |
| 22 | MG | A | 1726 | 1/1 | 0.83 | 0.08 | 127,127,127,127 | 0 |
| 22 | MG | A | 1711 | 1/1 | 0.84 | 0.11 | 398,398,398,398 | 0 |
| 22 | MG | A | 1760 | 1/1 | 0.84 | 0.07 | 121,121,121,121 | 0 |
| 22 | MG | A | 1758 | 1/1 | 0.85 | 0.41 | 139,139,139,139 | 0 |
| 22 | MG | A | 1693 | 1/1 | 0.85 | 0.30 | 94,94,94,94 | 0 |
| 22 | MG | A | 1748 | 1/1 | 0.85 | 0.40 | 97,97,97,97 | 0 |
| 22 | MG | A | 1698 | 1/1 | 0.85 | 0.10 | 424,424,424,424 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 22 | MG | A | 1617 | 1/1 | 0.85 | 0.36 | 109,109,109,109 | 0 |
| 22 | MG | A | 1622 | 1/1 | 0.85 | 0.18 | 88,88,88,88 | 0 |
| 22 | MG | S | 101 | 1/1 | 0.85 | 0.15 | 137,137,137,137 | 0 |
| 22 | MG | A | 1761 | 1/1 | 0.86 | 0.10 | 148,148,148,148 | 0 |
| 22 | MG | A | 1607 | 1/1 | 0.86 | 0.10 | 134,134,134,134 | 0 |
| 22 | MG | A | 1738 | 1/1 | 0.87 | 0.30 | 126,126,126,126 | 0 |
| 22 | MG | A | 1764 | 1/1 | 0.87 | 0.18 | 132,132,132,132 | 0 |
| 22 | MG | D | 302 | 1/1 | 0.87 | 0.20 | 130,130,130,130 | 0 |
| 22 | MG | A | 1614 | 1/1 | 0.87 | 0.17 | 113,113,113,113 | 0 |
| 22 | MG | A | 1753 | 1/1 | 0.87 | 0.25 | 118,118,118,118 | 0 |
| 22 | MG | A | 1743 | 1/1 | 0.87 | 0.22 | 104,104,104,104 | 0 |
| 22 | MG | A | 1720 | 1/1 | 0.87 | 0.07 | 324,324,324,324 | 0 |
| 22 | MG | A | 1640 | 1/1 | 0.88 | 0.25 | 141,141,141,141 | 0 |
| 22 | MG | A | 1729 | 1/1 | 0.88 | 0.21 | 94,94,94,94 | 0 |
| 22 | MG | A | 1667 | 1/1 | 0.88 | 0.17 | 93,93,93,93 | 0 |
| 22 | MG | A | 1747 | 1/1 | 0.88 | 0.24 | 102,102,102,102 | 0 |
| 22 | MG | A | 1740 | 1/1 | 0.88 | 0.13 | 130,130,130,130 | 0 |
| 22 | MG | A | 1689 | 1/1 | 0.88 | 0.36 | 107,107,107,107 | 0 |
| 22 | MG | A | 1744 | 1/1 | 0.89 | 0.10 | 115,115,115,115 | 0 |
| 22 | MG | A | 1646 | 1/1 | 0.89 | 0.11 | 153,153,153,153 | 0 |
| 22 | MG | A | 1701 | 1/1 | 0.89 | 0.10 | 383,383,383,383 | 0 |
| 22 | MG | A | 1643 | 1/1 | 0.89 | 0.07 | 245,245,245,245 | 0 |
| 22 | MG | A | 1692 | 1/1 | 0.89 | 0.20 | 126,126,126,126 | 0 |
| 22 | MG | A | 1660 | 1/1 | 0.89 | 0.20 | 107,107,107,107 | 0 |
| 22 | MG | A | 1697 | 1/1 | 0.90 | 0.09 | 411,411,411,411 | 0 |
| 22 | MG | A | 1719 | 1/1 | 0.90 | 0.22 | 320,320,320,320 | 0 |
| 22 | MG | A | 1634 | 1/1 | 0.90 | 0.17 | 113,113,113,113 | 0 |
| 22 | MG | A | 1601 | 1/1 | 0.90 | 0.33 | 96,96,96,96 | 0 |
| 22 | MG | A | 1686 | 1/1 | 0.90 | 0.17 | 118,118,118,118 | 0 |
| 22 | MG | A | 1710 | 1/1 | 0.90 | 0.09 | 470,470,470,470 | 0 |
| 22 | MG | A | 1685 | 1/1 | 0.91 | 0.12 | 136,136,136,136 | 0 |
| 22 | MG | A | 1681 | 1/1 | 0.91 | 0.19 | 107,107,107,107 | 0 |
| 22 | MG | A | 1683 | 1/1 | 0.92 | 0.09 | 264,264,264,264 | 0 |
| 22 | MG | A | 1623 | 1/1 | 0.92 | 0.24 | 90,90,90,90 | 0 |
| 22 | MG | A | 1705 | 1/1 | 0.92 | 0.07 | 310,310,310,310 | 0 |
| 22 | MG | A | 1636 | 1/1 | 0.92 | 0.12 | 186,186,186,186 | 0 |
| 22 | MG | A | 1742 | 1/1 | 0.92 | 0.15 | 97,97,97,97 | 0 |
| 22 | MG | A | 1642 | 1/1 | 0.92 | 0.09 | 191,191,191,191 | 0 |
| 22 | MG | A | 1661 | 1/1 | 0.92 | 0.10 | 105,105,105,105 | 0 |
| 22 | MG | A | 1676 | 1/1 | 0.92 | 0.07 | 153,153,153,153 | 0 |
| 22 | MG | A | 1649 | 1/1 | 0.92 | 0.29 | 102,102,102,102 | 0 |
| 22 | MG | A | 1668 | 1/1 | 0.92 | 0.34 | 115,115,115,115 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 22 | MG | A | 1677 | 1/1 | 0.93 | 0.22 | 89,89,89,89 | 0 |
| 22 | MG | A | 1702 | 1/1 | 0.93 | 0.10 | 259,259,259,259 | 0 |
| 22 | MG | A | 1721 | 1/1 | 0.93 | 0.19 | 259,259,259,259 | 0 |
| 22 | MG | A | 1615 | 1/1 | 0.93 | 0.21 | 92,92,92,92 | 0 |
| 22 | MG | A | 1616 | 1/1 | 0.93 | 0.13 | 127,127,127,127 | 0 |
| 22 | MG | A | 1611 | 1/1 | 0.93 | 0.14 | 153,153,153,153 | 0 |
| 22 | MG | H | 201 | 1/1 | 0.93 | 0.06 | 83,83,83,83 | 0 |
| 22 | MG | A | 1759 | 1/1 | 0.93 | 0.14 | 132,132,132,132 | 0 |
| 22 | MG | A | 1699 | 1/1 | 0.93 | 0.13 | 426,426,426,426 | 0 |
| 22 | MG | A | 1682 | 1/1 | 0.94 | 0.18 | 126,126,126,126 | 0 |
| 22 | MG | A | 1625 | 1/1 | 0.94 | 0.18 | 123,123,123,123 | 0 |
| 22 | MG | A | 1669 | 1/1 | 0.94 | 0.27 | 89,89,89,89 | 0 |
| 22 | MG | A | 1652 | 1/1 | 0.94 | 0.18 | 127,127,127,127 | 0 |
| 22 | MG | A | 1662 | 1/1 | 0.94 | 0.26 | 110,110,110,110 | 0 |
| 22 | MG | A | 1605 | 1/1 | 0.94 | 0.17 | 293,293,293,293 | 0 |
| 22 | MG | A | 1690 | 1/1 | 0.94 | 0.22 | 96,96,96,96 | 0 |
| 22 | MG | A | 1727 | 1/1 | 0.95 | 0.18 | 92,92,92,92 | 0 |
| 22 | MG | A | 1635 | 1/1 | 0.95 | 0.09 | 129,129,129,129 | 0 |
| 22 | MG | A | 1704 | 1/1 | 0.95 | 0.20 | 436,436,436,436 | 0 |
| 22 | MG | A | 1620 | 1/1 | 0.95 | 0.07 | 114,114,114,114 | 0 |
| 22 | MG | A | 1678 | 1/1 | 0.95 | 0.18 | 79,79,79,79 | 0 |
| 22 | MG | A | 1707 | 1/1 | 0.95 | 0.10 | 411,411,411,411 | 0 |
| 22 | MG | A | 1708 | 1/1 | 0.95 | 0.10 | 262,262,262,262 | 0 |
| 22 | MG | A | 1763 | 1/1 | 0.95 | 0.07 | 148,148,148,148 | 0 |
| 22 | MG | A | 1645 | 1/1 | 0.95 | 0.14 | 141,141,141,141 | 0 |
| 22 | MG | A | 1659 | 1/1 | 0.95 | 0.14 | 100,100,100,100 | 0 |
| 22 | MG | A | 1713 | 1/1 | 0.95 | 0.22 | 192,192,192,192 | 0 |
| 22 | MG | A | 1672 | 1/1 | 0.95 | 0.07 | 129,129,129,129 | 0 |
| 22 | MG | A | 1638 | 1/1 | 0.95 | 0.29 | 95,95,95,95 | 0 |
| 22 | MG | A | 1629 | 1/1 | 0.95 | 0.06 | 192,192,192,192 | 0 |
| 22 | MG | A | 1606 | 1/1 | 0.95 | 0.11 | 154,154,154,154 | 0 |
| 22 | MG | A | 1633 | 1/1 | 0.96 | 0.11 | 171,171,171,171 | 0 |
| 22 | MG | A | 1644 | 1/1 | 0.96 | 0.08 | 279,279,279,279 | 0 |
| 22 | MG | A | 1651 | 1/1 | 0.96 | 0.12 | 95,95,95,95 | 0 |
| 22 | MG | A | 1663 | 1/1 | 0.96 | 0.33 | 122,122,122,122 | 0 |
| 22 | MG | A | 1687 | 1/1 | 0.96 | 0.12 | 157,157,157,157 | 0 |
| 22 | MG | A | 1666 | 1/1 | 0.96 | 0.20 | 97,97,97,97 | 0 |
| 22 | MG | A | 1613 | 1/1 | 0.96 | 0.34 | 88,88,88,88 | 0 |
| 22 | MG | A | 1691 | 1/1 | 0.96 | 0.04 | 109,109,109,109 | 0 |
| 22 | MG | A | 1618 | 1/1 | 0.96 | 0.11 | 147,147,147,147 | 0 |
| 22 | MG | A | 1657 | 1/1 | 0.96 | 0.19 | 95,95,95,95 | 0 |
| 22 | MG | E | 201 | 1/1 | 0.96 | 0.25 | 95,95,95,95 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 22 | MG | A | 1696 | 1/1 | 0.96 | 0.17 | 390,390,390,390 | 0 |
| 22 | MG | A | 1716 | 1/1 | 0.96 | 0.20 | 497,497,497,497 | 0 |
| 22 | MG | A | 1717 | 1/1 | 0.96 | 0.10 | 254,254,254,254 | 0 |
| 22 | MG | A | 1670 | 1/1 | 0.96 | 0.31 | 111,111,111,111 | 0 |
| 22 | MG | A | 1612 | 1/1 | 0.96 | 0.08 | 104,104,104,104 | 0 |
| 22 | MG | A | 1665 | 1/1 | 0.97 | 0.07 | 102,102,102,102 | 0 |
| 22 | MG | A | 1658 | 1/1 | 0.97 | 0.18 | 130,130,130,130 | 0 |
| 22 | MG | A | 1700 | 1/1 | 0.97 | 0.05 | 129,129,129,129 | 0 |
| 22 | MG | A | 1723 | 1/1 | 0.97 | 0.11 | 181,181,181,181 | 0 |
| 22 | MG | A | 1724 | 1/1 | 0.97 | 0.11 | 290,290,290,290 | 0 |
| 22 | MG | A | 1709 | 1/1 | 0.97 | 0.27 | 354,354,354,354 | 0 |
| 22 | MG | A | 1739 | 1/1 | 0.97 | 0.17 | 96,96,96,96 | 0 |
| 22 | MG | A | 1688 | 1/1 | 0.97 | 0.17 | 84,84,84,84 | 0 |
| 22 | MG | A | 1694 | 1/1 | 0.97 | 0.10 | 244,244,244,244 | 0 |
| 22 | MG | A | 1703 | 1/1 | 0.97 | 0.14 | 475,475,475,475 | 0 |
| 22 | MG | A | 1714 | 1/1 | 0.97 | 0.11 | 200,200,200,200 | 0 |
| 22 | MG | A | 1603 | 1/1 | 0.97 | 0.05 | 184,184,184,184 | 0 |
| 22 | MG | A | 1648 | 1/1 | 0.97 | 0.11 | 227,227,227,227 | 0 |
| 22 | MG | A | 1680 | 1/1 | 0.98 | 0.05 | 134,134,134,134 | 0 |
| 22 | MG | A | 1664 | 1/1 | 0.98 | 0.13 | 101,101,101,101 | 0 |
| 22 | MG | A | 1627 | 1/1 | 0.98 | 0.04 | 121,121,121,121 | 0 |
| 22 | MG | A | 1604 | 1/1 | 0.98 | 0.08 | 90,90,90,90 | 0 |
| 22 | MG | A | 1602 | 1/1 | 0.98 | 0.12 | 114,114,114,114 | 0 |
| 22 | MG | A | 1715 | 1/1 | 0.98 | 0.04 | 167,167,167,167 | 0 |
| 22 | MG | A | 1624 | 1/1 | 0.98 | 0.05 | 114,114,114,114 | 0 |
| 22 | MG | A | 1695 | 1/1 | 0.98 | 0.06 | 184,184,184,184 | 0 |
| 22 | MG | A | 1621 | 1/1 | 0.98 | 0.11 | 107,107,107,107 | 0 |
| 22 | MG | A | 1654 | 1/1 | 0.98 | 0.06 | 105,105,105,105 | 0 |
| 22 | MG | A | 1655 | 1/1 | 0.98 | 0.11 | 96,96,96,96 | 0 |
| 22 | MG | A | 1722 | 1/1 | 0.98 | 0.05 | 73,73,73,73 | 0 |
| 22 | MG | A | 1656 | 1/1 | 0.99 | 0.04 | 68,68,68,68 | 0 |
| 22 | MG | A | 1610 | 1/1 | 0.99 | 0.09 | 87,87,87,87 | 0 |
| 22 | MG | A | 1626 | 1/1 | 0.99 | 0.08 | 108,108,108,108 | 0 |
| 22 | MG | A | 1725 | 1/1 | 0.99 | 0.06 | 114,114,114,114 | 0 |
| 22 | MG | A | 1608 | 1/1 | 0.99 | 0.05 | 143,143,143,143 | 0 |
| 22 | MG | A | 1641 | 1/1 | 0.99 | 0.15 | 96,96,96,96 | 0 |
| 22 | MG | A | 1718 | 1/1 | 0.99 | 0.11 | 111,111,111,111 | 0 |
| 22 | MG | A | 1609 | 1/1 | 0.99 | 0.06 | 140,140,140,140 | 0 |
| 22 | MG | A | 1637 | 1/1 | 0.99 | 0.10 | 235,235,235,235 | 0 |
| 22 | MG | K | 202 | 1/1 | 0.99 | 0.04 | 110,110,110,110 | 0 |
| 22 | MG | A | 1712 | 1/1 | 0.99 | 0.08 | 376,376,376,376 | 0 |
| 23 | ZN | D | 301 | 1/1 | 0.99 | 0.14 | 136,136,136,136 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 23 | ZN | N | 101 | 1/1 | 1.00 | 0.01 | 148,148,148,148 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.