



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:24 PM GMT

PDB ID : 1FFZ
Title : LARGE RIBOSOMAL SUBUNIT COMPLEXED WITH R(CC)-DA-PUROMYCIN
Authors : Nissen, P.; Hansen, J.; Ban, N.; Moore, P.B.; Steitz, T.A.
Deposited on : 2000-07-26
Resolution : 3.20 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

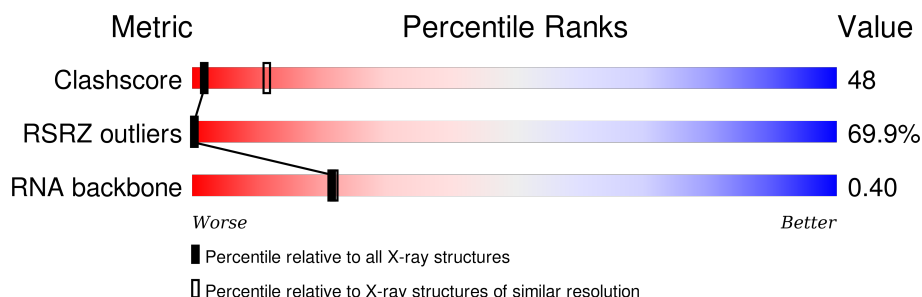
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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)) |
|---------------|-----------------------------|---|
| Clashscore | 102246 | 1024 (3.22-3.18) |
| RSRZ outliers | 91569 | 1129 (3.24-3.16) |
| RNA backbone | 2183 | 1079 (3.70-2.70) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 602 | <div> <div>58%</div> <div> <div>22%</div> <div>42%</div> <div>14%</div> <div>18%</div> </div> </div> |
| 2 | B | 4 | <div> <div>25%</div> <div>75%</div> <div>25%</div> </div> |

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10725 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 23S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|-----|---------|---------|-------|
| 1 | A | 496 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 10627 | 4738 | 1937 | 3456 | 496 | | | |

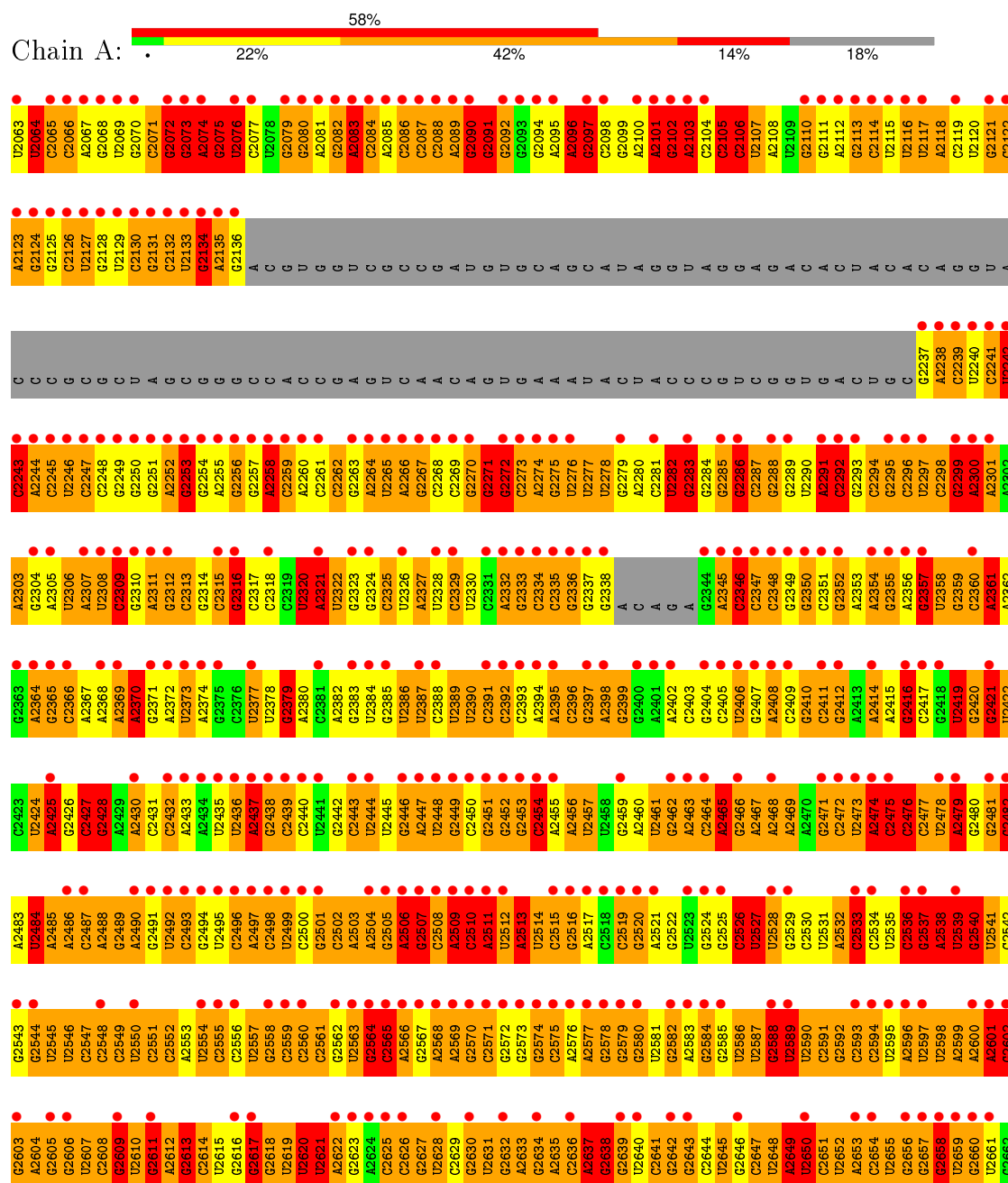
- Molecule 2 is DNA/RNA hybrid called R(P*CP*C*)-D(P*A)-R(P*(PU)).

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 2 | B | 4 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 98 | 50 | 18 | 26 | 4 | | | |

3 Residue-property plots

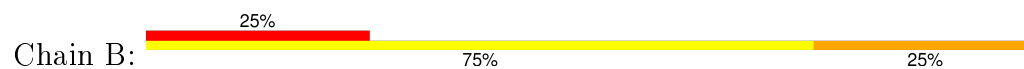
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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: 23S RIBOSOMAL RNA





- Molecule 2: R(P*CP*C*)-D(P*A)-R(P*(PU))



4 Data and refinement statistics

| Property | Value | Source |
|---|--|------------------|
| Space group | C 2 2 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 212.00Å 300.00Å 574.00Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 70.00 – 3.20 59.88 – 3.00 | Depositor EDS |
| % Data completeness (in resolution range) | (Not available) (70.00-3.20) 100.0 (59.88-3.00) | Depositor EDS |
| R_{merge} | 0.19 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.16 (at 3.01Å) | Xtriage |
| Refinement program | O | Depositor |
| R, R_{free} | (Not available) , (Not available) 0.520 , (Not available) | Depositor DCC |
| R_{free} test set | No test flags present. | DCC |
| Wilson B-factor (Å ²) | 41.6 | Xtriage |
| Anisotropy | 0.162 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.09 , -10.0 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$ | Xtriage |
| Outliers | 0 of 361686 reflections | Xtriage |
| F_o, F_c correlation | 0.30 | EDS |
| Total number of atoms | 10725 | wwPDB-VP |
| Average B, all atoms (Å ²) | 40.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: PU

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|------------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | A | 0.96 | 21/11890 (0.2%) | 2.05 | 627/18540 (3.4%) |
| 2 | B | 0.91 | 0/67 | 2.07 | 4/101 (4.0%) |
| All | All | 0.96 | 21/11957 (0.2%) | 2.05 | 631/18641 (3.4%) |

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 |
|-----|-------|---------------------|---------------------|
| 1 | A | 36 | 5 |

All (21) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 1 | A | 2299 | G | C5-C6 | -16.37 | 1.25 | 1.42 |
| 1 | A | 2299 | G | C6-O6 | -14.87 | 1.10 | 1.24 |
| 1 | A | 2299 | G | N1-C2 | 14.47 | 1.49 | 1.37 |
| 1 | A | 2437 | A | C6-N6 | -11.07 | 1.25 | 1.33 |
| 1 | A | 2299 | G | C6-N1 | 11.06 | 1.47 | 1.39 |
| 1 | A | 2437 | A | C5-C4 | 10.81 | 1.46 | 1.38 |
| 1 | A | 2437 | A | C8-N7 | 10.42 | 1.38 | 1.31 |
| 1 | A | 2299 | G | C2-N3 | 8.52 | 1.39 | 1.32 |
| 1 | A | 2564 | G | C2-N3 | -8.08 | 1.26 | 1.32 |
| 1 | A | 2634 | G | P-OP2 | 7.51 | 1.61 | 1.49 |
| 1 | A | 2437 | A | C6-N1 | 6.97 | 1.40 | 1.35 |
| 1 | A | 2437 | A | C5-C6 | -6.79 | 1.34 | 1.41 |
| 1 | A | 2437 | A | C2'-C1' | 6.71 | 1.60 | 1.53 |
| 1 | A | 2564 | G | N9-C8 | 6.25 | 1.42 | 1.37 |
| 1 | A | 2438 | G | C5-C6 | -5.53 | 1.36 | 1.42 |
| 1 | A | 2492 | U | N1-C2 | 5.52 | 1.43 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1 | A | 2320 | U | O3'-P | 5.41 | 1.67 | 1.61 |
| 1 | A | 2564 | G | C2-N2 | 5.31 | 1.39 | 1.34 |
| 1 | A | 2588 | G | C3'-O3' | 5.28 | 1.49 | 1.42 |
| 1 | A | 2437 | A | C4'-C3' | -5.21 | 1.47 | 1.52 |
| 1 | A | 2509 | A | C6-N6 | 5.20 | 1.38 | 1.33 |

All (631) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1 | A | 2474 | A | O4'-C1'-N9 | -30.35 | 83.92 | 108.20 |
| 1 | A | 2275 | G | O5'-P-OP2 | -28.22 | 76.83 | 110.70 |
| 1 | A | 2589 | U | O5'-P-OP2 | 26.79 | 142.85 | 110.70 |
| 1 | A | 2579 | G | O4'-C1'-N9 | -24.89 | 88.29 | 108.20 |
| 1 | A | 2489 | G | OP2-P-O3' | -23.09 | 54.39 | 105.20 |
| 1 | A | 2437 | A | N9-C1'-C2' | 22.55 | 143.31 | 114.00 |
| 1 | A | 2274 | A | OP2-P-O3' | 22.33 | 154.34 | 105.20 |
| 1 | A | 2463 | A | N9-C1'-C2' | 22.21 | 142.87 | 114.00 |
| 1 | A | 2490 | A | O5'-P-OP2 | 21.85 | 136.92 | 110.70 |
| 1 | A | 2490 | A | O5'-P-OP1 | -20.65 | 85.92 | 110.70 |
| 1 | A | 2608 | C | OP2-P-O3' | -20.55 | 59.99 | 105.20 |
| 1 | A | 2577 | A | O4'-C1'-N9 | -19.36 | 92.72 | 108.20 |
| 1 | A | 2313 | C | O4'-C1'-N1 | 18.86 | 123.28 | 108.20 |
| 1 | A | 2588 | G | OP2-P-O3' | -18.16 | 65.24 | 105.20 |
| 1 | A | 2597 | U | N1-C1'-C2' | -18.09 | 90.48 | 114.00 |
| 1 | A | 2536 | C | O4'-C1'-N1 | -17.99 | 93.81 | 108.20 |
| 1 | A | 2397 | G | O5'-P-OP2 | -17.85 | 89.28 | 110.70 |
| 1 | A | 2637 | A | O4'-C1'-N9 | -17.83 | 93.94 | 108.20 |
| 1 | A | 2299 | G | C5-C6-N1 | 17.81 | 120.41 | 111.50 |
| 1 | A | 2616 | G | N9-C1'-C2' | 17.63 | 136.92 | 114.00 |
| 1 | A | 2632 | G | O4'-C1'-N9 | -17.51 | 94.19 | 108.20 |
| 1 | A | 2299 | G | C6-N1-C2 | -17.46 | 114.62 | 125.10 |
| 1 | A | 2386 | U | O4'-C1'-N1 | -17.19 | 94.45 | 108.20 |
| 1 | A | 2437 | A | O4'-C1'-N9 | -16.74 | 94.81 | 108.20 |
| 1 | A | 2539 | U | O4'-C1'-N1 | -16.46 | 95.03 | 108.20 |
| 1 | A | 2538 | A | N9-C1'-C2' | 16.16 | 135.01 | 114.00 |
| 1 | A | 2564 | G | N9-C1'-C2' | -16.04 | 93.15 | 114.00 |
| 1 | A | 2596 | A | N9-C1'-C2' | -16.03 | 93.16 | 114.00 |
| 1 | A | 2632 | G | OP2-P-O3' | -16.02 | 69.95 | 105.20 |
| 1 | A | 2468 | A | O4'-C1'-N9 | 15.84 | 120.87 | 108.20 |
| 1 | A | 2511 | A | O4'-C1'-N9 | -15.74 | 95.61 | 108.20 |
| 1 | A | 2474 | A | N9-C1'-C2' | 15.46 | 134.10 | 114.00 |
| 1 | A | 2608 | C | OP1-P-O3' | -15.34 | 71.45 | 105.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 1 | A | 2528 | U | N1-C1'-C2' | 15.30 | 133.89 | 114.00 |
| 1 | A | 2102 | G | O4'-C1'-N9 | -15.29 | 95.97 | 108.20 |
| 1 | A | 2274 | A | N9-C1'-C2' | -15.26 | 94.16 | 114.00 |
| 1 | A | 2586 | U | O4'-C1'-N1 | 14.95 | 120.16 | 108.20 |
| 1 | A | 2484 | U | C2'-C3'-O3' | 14.86 | 142.18 | 109.50 |
| 1 | A | 2072 | G | O4'-C1'-N9 | -14.68 | 96.46 | 108.20 |
| 1 | A | 2333 | G | N9-C1'-C2' | -14.65 | 94.95 | 114.00 |
| 1 | A | 2333 | G | O4'-C1'-N9 | -14.40 | 96.68 | 108.20 |
| 1 | A | 2329 | C | O4'-C1'-N1 | 14.38 | 119.70 | 108.20 |
| 1 | A | 2466 | G | O4'-C1'-N9 | -14.10 | 96.92 | 108.20 |
| 1 | A | 2579 | G | N9-C1'-C2' | -14.02 | 95.77 | 114.00 |
| 1 | A | 2589 | U | O5'-P-OP1 | -13.80 | 93.28 | 105.70 |
| 1 | A | 2521 | A | C1'-C2'-O2' | -13.77 | 69.30 | 110.60 |
| 1 | A | 2448 | U | O4'-C1'-N1 | 13.62 | 119.10 | 108.20 |
| 1 | A | 2107 | U | O4'-C1'-N1 | 13.60 | 119.08 | 108.20 |
| 1 | A | 2316 | G | N9-C1'-C2' | 13.54 | 131.60 | 114.00 |
| 1 | A | 2366 | C | O4'-C1'-N1 | -13.53 | 97.37 | 108.20 |
| 1 | A | 2572 | G | O4'-C1'-N9 | 13.52 | 119.01 | 108.20 |
| 1 | A | 2604 | A | O4'-C1'-N9 | 13.51 | 119.01 | 108.20 |
| 1 | A | 2090 | G | N9-C1'-C2' | -13.44 | 96.53 | 114.00 |
| 1 | A | 2437 | A | C4-N9-C1' | -13.42 | 102.14 | 126.30 |
| 1 | A | 2658 | G | N9-C1'-C2' | -13.40 | 96.58 | 114.00 |
| 1 | A | 2602 | G | O5'-P-OP2 | -13.27 | 93.76 | 105.70 |
| 1 | A | 2498 | C | N1-C1'-C2' | -13.26 | 96.76 | 114.00 |
| 1 | A | 2611 | G | O4'-C1'-N9 | -13.02 | 97.78 | 108.20 |
| 1 | A | 2594 | C | N1-C1'-C2' | -12.92 | 97.21 | 114.00 |
| 1 | A | 2092 | G | O4'-C1'-N9 | 12.77 | 118.41 | 108.20 |
| 1 | A | 2293 | G | N9-C1'-C2' | -12.71 | 97.48 | 114.00 |
| 2 | B | 76 | DA | O5'-P-OP2 | -12.56 | 94.39 | 105.70 |
| 1 | A | 2630 | G | O4'-C1'-N9 | 12.36 | 118.09 | 108.20 |
| 1 | A | 2572 | G | O5'-P-OP1 | -12.29 | 94.64 | 105.70 |
| 1 | A | 2279 | G | N9-C1'-C2' | -12.27 | 98.04 | 114.00 |
| 1 | A | 2308 | U | N1-C1'-C2' | -12.17 | 98.17 | 114.00 |
| 1 | A | 2103 | A | O5'-P-OP2 | -12.16 | 94.75 | 105.70 |
| 1 | A | 2332 | A | O4'-C1'-N9 | -12.14 | 98.49 | 108.20 |
| 1 | A | 2389 | U | O4'-C1'-N1 | 12.10 | 117.88 | 108.20 |
| 1 | A | 2569 | A | N9-C1'-C2' | -12.00 | 98.40 | 114.00 |
| 1 | A | 2547 | C | N1-C1'-C2' | -11.78 | 98.68 | 114.00 |
| 1 | A | 2272 | G | O4'-C1'-N9 | -11.68 | 98.86 | 108.20 |
| 1 | A | 2273 | C | N1-C1'-C2' | -11.58 | 98.95 | 114.00 |
| 1 | A | 2274 | A | O3'-P-O5' | -11.53 | 82.10 | 104.00 |
| 1 | A | 2550 | U | O4'-C1'-N1 | 11.51 | 117.41 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 1 | A | 2456 | A | O4'-C1'-N9 | 11.50 | 117.40 | 108.20 |
| 1 | A | 2466 | G | N9-C1'-C2' | 11.48 | 128.92 | 114.00 |
| 1 | A | 2514 | U | O4'-C1'-N1 | -11.47 | 99.02 | 108.20 |
| 1 | A | 2420 | G | O4'-C1'-N9 | 11.40 | 117.32 | 108.20 |
| 1 | A | 2626 | C | C3'-C2'-O2' | 11.38 | 146.29 | 113.30 |
| 1 | A | 2364 | A | N9-C1'-C2' | -11.35 | 99.25 | 114.00 |
| 1 | A | 2095 | A | O5'-P-OP1 | -11.33 | 95.50 | 105.70 |
| 1 | A | 2296 | C | O4'-C1'-N1 | 11.33 | 117.27 | 108.20 |
| 1 | A | 2538 | A | C2'-C3'-O3' | 11.31 | 134.39 | 109.50 |
| 1 | A | 2370 | A | O4'-C1'-N9 | -11.30 | 99.16 | 108.20 |
| 1 | A | 2312 | G | O4'-C1'-N9 | 11.23 | 117.19 | 108.20 |
| 1 | A | 2513 | A | O4'-C1'-N9 | -11.16 | 99.27 | 108.20 |
| 1 | A | 2307 | A | O4'-C1'-N9 | -11.15 | 99.28 | 108.20 |
| 1 | A | 2451 | G | N9-C1'-C2' | -11.13 | 99.53 | 114.00 |
| 1 | A | 2489 | G | O3'-P-O5' | -11.12 | 82.87 | 104.00 |
| 1 | A | 2613 | G | N9-C1'-C2' | -11.12 | 99.54 | 114.00 |
| 1 | A | 2578 | G | O4'-C1'-N9 | -11.12 | 99.31 | 108.20 |
| 1 | A | 2482 | G | C4'-C3'-O3' | 11.09 | 135.17 | 113.00 |
| 1 | A | 2499 | U | O4'-C1'-N1 | 11.08 | 117.06 | 108.20 |
| 1 | A | 2256 | G | O4'-C1'-N9 | 11.05 | 117.04 | 108.20 |
| 1 | A | 2444 | U | N1-C1'-C2' | -11.04 | 99.65 | 114.00 |
| 1 | A | 2100 | A | O4'-C1'-N9 | 11.02 | 117.02 | 108.20 |
| 1 | A | 2088 | C | O4'-C1'-N1 | -10.99 | 99.41 | 108.20 |
| 1 | A | 2386 | U | N1-C1'-C2' | -10.98 | 99.73 | 114.00 |
| 1 | A | 2497 | A | N9-C1'-C2' | -10.91 | 99.82 | 114.00 |
| 1 | A | 2623 | G | O4'-C1'-N9 | -10.89 | 99.49 | 108.20 |
| 1 | A | 2588 | G | O3'-P-O5' | -10.83 | 83.43 | 104.00 |
| 1 | A | 2071 | C | O4'-C1'-N1 | 10.81 | 116.85 | 108.20 |
| 1 | A | 2489 | G | OP1-P-O3' | 10.78 | 128.91 | 105.20 |
| 1 | A | 2274 | A | OP1-P-O3' | -10.74 | 81.58 | 105.20 |
| 1 | A | 2506 | A | N9-C1'-C2' | -10.69 | 100.11 | 114.00 |
| 1 | A | 2612 | A | O4'-C1'-N9 | -10.60 | 99.72 | 108.20 |
| 1 | A | 2063 | U | OP2-P-O3' | -10.58 | 81.92 | 105.20 |
| 1 | A | 2584 | G | O4'-C1'-N9 | -10.55 | 99.76 | 108.20 |
| 1 | A | 2437 | A | C8-N9-C1' | 10.54 | 146.67 | 127.70 |
| 1 | A | 2452 | G | N9-C1'-C2' | -10.52 | 100.32 | 114.00 |
| 1 | A | 2419 | U | N1-C1'-C2' | 10.48 | 127.63 | 114.00 |
| 1 | A | 2245 | C | O5'-P-OP1 | -10.46 | 96.28 | 105.70 |
| 1 | A | 2657 | G | N9-C1'-C2' | -10.45 | 100.41 | 114.00 |
| 1 | A | 2555 | C | O4'-C1'-N1 | -10.39 | 99.89 | 108.20 |
| 1 | A | 2476 | C | N1-C1'-C2' | -10.35 | 100.54 | 114.00 |
| 1 | A | 2621 | U | O5'-P-OP1 | 10.34 | 123.11 | 110.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1 | A | 2123 | A | O4'-C1'-N9 | -10.27 | 99.99 | 108.20 |
| 1 | A | 2321 | A | O4'-C1'-N9 | 10.27 | 116.42 | 108.20 |
| 1 | A | 2294 | C | O4'-C1'-N1 | 10.18 | 116.34 | 108.20 |
| 1 | A | 2453 | G | N9-C1'-C2' | -10.14 | 100.81 | 114.00 |
| 1 | A | 2094 | G | O4'-C1'-N9 | 10.12 | 116.30 | 108.20 |
| 1 | A | 2607 | U | N1-C1'-C2' | 10.11 | 127.14 | 114.00 |
| 1 | A | 2660 | G | O4'-C1'-N9 | -10.09 | 100.13 | 108.20 |
| 1 | A | 2435 | U | O4'-C1'-N1 | 10.07 | 116.26 | 108.20 |
| 1 | A | 2482 | G | O4'-C1'-N9 | 10.03 | 116.22 | 108.20 |
| 1 | A | 2628 | U | O4'-C1'-N1 | 10.03 | 116.22 | 108.20 |
| 1 | A | 2620 | U | OP2-P-O3' | -10.01 | 83.18 | 105.20 |
| 1 | A | 2432 | C | O5'-P-OP1 | 9.95 | 122.64 | 110.70 |
| 1 | A | 2490 | A | N9-C1'-C2' | -9.94 | 101.07 | 112.00 |
| 1 | A | 2593 | C | N1-C1'-C2' | -9.82 | 101.19 | 112.00 |
| 1 | A | 2508 | C | O4'-C1'-N1 | 9.82 | 116.06 | 108.20 |
| 1 | A | 2503 | A | O4'-C1'-N9 | 9.77 | 116.02 | 108.20 |
| 1 | A | 2622 | A | N9-C1'-C2' | 9.69 | 126.59 | 114.00 |
| 1 | A | 2089 | A | N9-C1'-C2' | -9.64 | 101.40 | 112.00 |
| 1 | A | 2076 | U | O4'-C1'-N1 | 9.63 | 115.91 | 108.20 |
| 1 | A | 2608 | C | N1-C1'-C2' | 9.61 | 126.50 | 114.00 |
| 1 | A | 2065 | C | N1-C1'-C2' | -9.61 | 101.43 | 112.00 |
| 1 | A | 2531 | U | O4'-C1'-N1 | 9.60 | 115.88 | 108.20 |
| 1 | A | 2574 | G | N9-C1'-C2' | 9.59 | 126.46 | 114.00 |
| 1 | A | 2544 | G | N9-C1'-C2' | -9.56 | 101.48 | 112.00 |
| 1 | A | 2663 | U | N1-C1'-C2' | 9.55 | 126.42 | 114.00 |
| 1 | A | 2526 | C | O4'-C1'-N1 | -9.53 | 100.57 | 108.20 |
| 1 | A | 2391 | C | O4'-C1'-N1 | 9.51 | 115.81 | 108.20 |
| 1 | A | 2425 | A | N9-C1'-C2' | -9.50 | 101.55 | 112.00 |
| 1 | A | 2465 | A | N9-C1'-C2' | 9.50 | 126.35 | 114.00 |
| 1 | A | 2564 | G | O4'-C1'-N9 | -9.49 | 100.61 | 108.20 |
| 1 | A | 2571 | C | O4'-C1'-N1 | 9.47 | 115.77 | 108.20 |
| 1 | A | 2365 | G | N9-C1'-C2' | -9.46 | 101.60 | 112.00 |
| 1 | A | 2265 | U | O5'-P-OP1 | -9.41 | 97.23 | 105.70 |
| 1 | A | 2073 | G | N9-C1'-C2' | 9.40 | 126.22 | 114.00 |
| 1 | A | 2299 | G | N1-C6-O6 | -9.39 | 114.27 | 119.90 |
| 1 | A | 2602 | G | O4'-C1'-N9 | -9.38 | 100.69 | 108.20 |
| 1 | A | 2451 | G | O4'-C1'-N9 | -9.38 | 100.70 | 108.20 |
| 1 | A | 2271 | G | O4'-C1'-N9 | -9.36 | 100.71 | 108.20 |
| 1 | A | 2614 | C | N1-C1'-C2' | -9.36 | 101.70 | 112.00 |
| 1 | A | 2565 | C | O4'-C1'-N1 | -9.35 | 100.72 | 108.20 |
| 1 | A | 2620 | U | O4'-C1'-N1 | -9.34 | 100.73 | 108.20 |
| 1 | A | 2298 | C | N1-C1'-C2' | 9.29 | 126.08 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 2309 | C | O4'-C1'-N1 | 9.25 | 115.60 | 108.20 |
| 1 | A | 2472 | C | O4'-C1'-N1 | -9.22 | 100.82 | 108.20 |
| 1 | A | 2079 | G | N9-C1'-C2' | 9.21 | 125.98 | 114.00 |
| 1 | A | 2277 | U | O4'-C1'-N1 | 9.21 | 115.56 | 108.20 |
| 1 | A | 2642 | G | N9-C1'-C2' | -9.18 | 101.91 | 112.00 |
| 1 | A | 2610 | U | O4'-C1'-N1 | -9.17 | 100.86 | 108.20 |
| 1 | A | 2603 | G | O4'-C1'-N9 | 9.17 | 115.53 | 108.20 |
| 1 | A | 2438 | G | C4'-C3'-O3' | 9.16 | 131.31 | 113.00 |
| 1 | A | 2095 | A | N9-C1'-C2' | 9.14 | 125.88 | 114.00 |
| 1 | A | 2097 | G | O4'-C1'-N9 | -9.14 | 100.89 | 108.20 |
| 1 | A | 2481 | G | C1'-C2'-O2' | -9.13 | 83.20 | 110.60 |
| 1 | A | 2463 | A | C4'-C3'-O3' | -9.13 | 90.22 | 109.40 |
| 1 | A | 2484 | U | O4'-C1'-N1 | -9.13 | 100.89 | 108.20 |
| 1 | A | 2589 | U | O4'-C1'-N1 | -9.13 | 100.90 | 108.20 |
| 1 | A | 2493 | C | N1-C1'-C2' | -9.05 | 102.04 | 112.00 |
| 1 | A | 2533 | C | O5'-P-OP1 | -9.06 | 97.55 | 105.70 |
| 1 | A | 2605 | G | O4'-C1'-N9 | 9.03 | 115.42 | 108.20 |
| 1 | A | 2431 | C | N1-C1'-C2' | -9.03 | 102.07 | 112.00 |
| 1 | A | 2117 | U | N1-C1'-C2' | -8.99 | 102.11 | 112.00 |
| 1 | A | 2637 | A | C5'-C4'-O4' | 8.90 | 119.78 | 109.10 |
| 1 | A | 2477 | C | N1-C1'-C2' | -8.84 | 102.27 | 112.00 |
| 1 | A | 2123 | A | N9-C1'-C2' | -8.84 | 102.28 | 112.00 |
| 1 | A | 2105 | C | C1'-C2'-O2' | -8.83 | 84.10 | 110.60 |
| 1 | A | 2493 | C | O4'-C1'-N1 | 8.83 | 115.27 | 108.20 |
| 1 | A | 2080 | G | OP1-P-O3' | -8.82 | 85.78 | 105.20 |
| 1 | A | 2600 | A | C1'-C2'-O2' | -8.82 | 84.14 | 110.60 |
| 1 | A | 2559 | C | N1-C1'-C2' | -8.81 | 102.30 | 112.00 |
| 1 | A | 2281 | C | O4'-C1'-N1 | 8.79 | 115.23 | 108.20 |
| 1 | A | 2638 | G | O5'-P-OP2 | -8.76 | 97.82 | 105.70 |
| 1 | A | 2566 | A | O4'-C1'-N9 | -8.75 | 101.20 | 108.20 |
| 1 | A | 2637 | A | C2'-C3'-O3' | 8.74 | 128.74 | 109.50 |
| 1 | A | 2105 | C | O4'-C1'-N1 | 8.74 | 115.19 | 108.20 |
| 1 | A | 2481 | G | O4'-C1'-N9 | 8.73 | 115.19 | 108.20 |
| 1 | A | 2126 | C | O4'-C1'-N1 | 8.72 | 115.18 | 108.20 |
| 1 | A | 2588 | G | N9-C1'-C2' | -8.69 | 102.44 | 112.00 |
| 1 | A | 2633 | A | O5'-P-OP1 | 8.68 | 121.12 | 110.70 |
| 1 | A | 2481 | G | N9-C1'-C2' | 8.68 | 125.28 | 114.00 |
| 1 | A | 2482 | G | O5'-P-OP1 | -8.68 | 97.89 | 105.70 |
| 1 | A | 2510 | C | N1-C1'-C2' | 8.67 | 125.27 | 114.00 |
| 1 | A | 2626 | C | O4'-C1'-N1 | 8.67 | 115.13 | 108.20 |
| 1 | A | 2558 | G | N9-C1'-C2' | -8.66 | 102.47 | 112.00 |
| 1 | A | 2560 | C | O5'-P-OP2 | -8.66 | 97.91 | 105.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 2412 | G | N9-C1'-C2' | 8.64 | 125.23 | 114.00 |
| 1 | A | 2322 | U | N1-C1'-C2' | 8.63 | 125.22 | 114.00 |
| 1 | A | 2655 | U | N1-C1'-C2' | 8.62 | 125.21 | 114.00 |
| 1 | A | 2321 | A | C2'-C3'-O3' | 8.61 | 128.45 | 109.50 |
| 1 | A | 2291 | A | N9-C1'-C2' | 8.60 | 125.18 | 114.00 |
| 1 | A | 2521 | A | N9-C1'-C2' | 8.58 | 125.16 | 114.00 |
| 1 | A | 2519 | C | O4'-C1'-N1 | 8.56 | 115.05 | 108.20 |
| 1 | A | 2323 | G | O5'-P-OP1 | -8.55 | 98.01 | 105.70 |
| 1 | A | 2600 | A | O5'-P-OP1 | -8.55 | 98.01 | 105.70 |
| 1 | A | 2348 | C | O4'-C1'-N1 | 8.53 | 115.03 | 108.20 |
| 1 | A | 2134 | G | N9-C1'-C2' | -8.53 | 102.62 | 112.00 |
| 1 | A | 2591 | C | N1-C1'-C2' | -8.52 | 102.63 | 112.00 |
| 1 | A | 2613 | G | O5'-P-OP1 | -8.50 | 98.05 | 105.70 |
| 1 | A | 2623 | G | O5'-P-OP1 | -8.49 | 98.06 | 105.70 |
| 1 | A | 2301 | A | N9-C1'-C2' | 8.47 | 125.02 | 114.00 |
| 1 | A | 2419 | U | O4'-C1'-N1 | -8.47 | 101.42 | 108.20 |
| 1 | A | 2359 | G | O4'-C1'-N9 | 8.47 | 114.98 | 108.20 |
| 1 | A | 2449 | G | N9-C1'-C2' | -8.47 | 102.68 | 112.00 |
| 1 | A | 2548 | C | C3'-C2'-O2' | 8.47 | 137.86 | 113.30 |
| 1 | A | 2502 | C | O4'-C1'-N1 | 8.46 | 114.97 | 108.20 |
| 1 | A | 2350 | G | O4'-C1'-N9 | 8.45 | 114.96 | 108.20 |
| 1 | A | 2443 | C | O4'-C1'-N1 | -8.45 | 101.44 | 108.20 |
| 1 | A | 2370 | A | C4'-C3'-O3' | 8.42 | 129.85 | 113.00 |
| 1 | A | 2611 | G | C3'-C2'-O2' | 8.39 | 137.63 | 113.30 |
| 1 | A | 2625 | C | N1-C1'-C2' | -8.38 | 102.78 | 112.00 |
| 1 | A | 2291 | A | C4'-C3'-O3' | -8.37 | 91.81 | 109.40 |
| 1 | A | 2656 | G | N9-C1'-C2' | -8.38 | 102.79 | 112.00 |
| 1 | A | 2243 | C | O4'-C1'-N1 | 8.37 | 114.89 | 108.20 |
| 1 | A | 2598 | U | O5'-P-OP1 | -8.33 | 98.20 | 105.70 |
| 1 | A | 2404 | G | O4'-C1'-N9 | -8.29 | 101.57 | 108.20 |
| 1 | A | 2091 | G | N9-C1'-C2' | -8.27 | 102.90 | 112.00 |
| 1 | A | 2531 | U | N1-C1'-C2' | 8.22 | 124.68 | 114.00 |
| 1 | A | 2416 | G | O4'-C1'-N9 | 8.20 | 114.76 | 108.20 |
| 1 | A | 2516 | G | O4'-C1'-N9 | 8.20 | 114.76 | 108.20 |
| 1 | A | 2652 | U | O5'-P-OP1 | -8.19 | 98.33 | 105.70 |
| 1 | A | 2530 | C | O4'-C1'-N1 | 8.11 | 114.69 | 108.20 |
| 1 | A | 2108 | A | N9-C1'-C2' | 8.09 | 124.51 | 114.00 |
| 1 | A | 2588 | G | O4'-C1'-N9 | 8.06 | 114.65 | 108.20 |
| 1 | A | 2515 | C | C3'-C2'-O2' | 8.04 | 136.60 | 113.30 |
| 1 | A | 2533 | C | O4'-C1'-N1 | -8.02 | 101.78 | 108.20 |
| 1 | A | 2247 | C | O4'-C1'-N1 | 7.96 | 114.57 | 108.20 |
| 1 | A | 2101 | A | OP2-P-O3' | -7.96 | 87.69 | 105.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 2637 | A | C5'-C4'-C3' | 7.96 | 128.73 | 116.00 |
| 1 | A | 2649 | A | O4'-C1'-N9 | -7.91 | 101.87 | 108.20 |
| 1 | A | 2364 | A | O4'-C1'-N9 | 7.91 | 114.52 | 108.20 |
| 1 | A | 2097 | G | N9-C1'-C2' | -7.90 | 103.31 | 112.00 |
| 1 | A | 2457 | U | O5'-P-OP1 | -7.88 | 98.61 | 105.70 |
| 1 | A | 2607 | U | O4'-C1'-N1 | -7.83 | 101.94 | 108.20 |
| 1 | A | 2582 | G | O4'-C1'-N9 | 7.82 | 114.46 | 108.20 |
| 1 | A | 2504 | A | O4'-C1'-N9 | 7.80 | 114.44 | 108.20 |
| 1 | A | 2492 | U | N1-C1'-C2' | 7.78 | 124.11 | 114.00 |
| 1 | A | 2361 | A | O4'-C1'-N9 | -7.76 | 101.99 | 108.20 |
| 1 | A | 2637 | A | C4'-C3'-O3' | 7.73 | 128.46 | 113.00 |
| 1 | A | 2081 | A | O5'-P-OP1 | 7.72 | 119.97 | 110.70 |
| 1 | A | 2521 | A | C3'-C2'-O2' | -7.70 | 90.98 | 113.30 |
| 1 | A | 2551 | C | N1-C1'-C2' | 7.70 | 124.00 | 114.00 |
| 1 | A | 2427 | C | O4'-C1'-N1 | 7.68 | 114.35 | 108.20 |
| 1 | A | 2473 | U | O4'-C1'-N1 | -7.68 | 102.05 | 108.20 |
| 1 | A | 2334 | C | O4'-C1'-N1 | 7.67 | 114.34 | 108.20 |
| 1 | A | 2446 | G | O4'-C1'-N9 | 7.67 | 114.34 | 108.20 |
| 1 | A | 2484 | U | C4'-C3'-O3' | -7.67 | 93.29 | 109.40 |
| 1 | A | 2135 | A | O5'-P-OP2 | -7.64 | 98.82 | 105.70 |
| 1 | A | 2421 | G | O4'-C1'-N9 | 7.63 | 114.30 | 108.20 |
| 1 | A | 2590 | U | O4'-C1'-N1 | 7.63 | 114.30 | 108.20 |
| 1 | A | 2635 | A | N9-C1'-C2' | -7.57 | 103.67 | 112.00 |
| 1 | A | 2563 | U | O4'-C1'-N1 | 7.57 | 114.25 | 108.20 |
| 1 | A | 2253 | G | N9-C1'-C2' | -7.55 | 103.69 | 112.00 |
| 1 | A | 2597 | U | O5'-P-OP1 | -7.55 | 98.91 | 105.70 |
| 1 | A | 2320 | U | N1-C1'-C2' | 7.53 | 123.79 | 114.00 |
| 1 | A | 2439 | C | O5'-P-OP1 | 7.53 | 119.74 | 110.70 |
| 1 | A | 2281 | C | O5'-P-OP1 | -7.53 | 98.92 | 105.70 |
| 1 | A | 2242 | U | C3'-C2'-O2' | 7.53 | 135.12 | 113.30 |
| 1 | A | 2561 | C | O4'-C1'-N1 | 7.51 | 114.21 | 108.20 |
| 1 | A | 2463 | A | C2'-C3'-O3' | 7.50 | 126.01 | 109.50 |
| 1 | A | 2298 | C | O4'-C1'-N1 | 7.50 | 114.20 | 108.20 |
| 1 | A | 2084 | C | O4'-C1'-N1 | 7.49 | 114.19 | 108.20 |
| 1 | A | 2564 | G | N3-C4-N9 | -7.49 | 121.50 | 126.00 |
| 1 | A | 2110 | G | N9-C1'-C2' | -7.49 | 103.76 | 112.00 |
| 1 | A | 2103 | A | O5'-P-OP1 | 7.48 | 119.67 | 110.70 |
| 1 | A | 2427 | C | C2'-C3'-O3' | 7.47 | 125.93 | 109.50 |
| 1 | A | 2404 | G | P-O5'-C5' | 7.46 | 132.84 | 120.90 |
| 1 | A | 2101 | A | C4'-C3'-O3' | -7.45 | 93.75 | 109.40 |
| 1 | A | 2114 | C | O4'-C1'-N1 | -7.44 | 102.25 | 108.20 |
| 1 | A | 2411 | C | O5'-P-OP1 | -7.42 | 99.03 | 105.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 2557 | U | N1-C1'-C2' | -7.41 | 103.85 | 112.00 |
| 1 | A | 2424 | U | O4'-C1'-N1 | 7.41 | 114.12 | 108.20 |
| 1 | A | 2292 | C | O4'-C1'-N1 | 7.38 | 114.11 | 108.20 |
| 1 | A | 2648 | U | OP1-P-O3' | 7.35 | 121.36 | 105.20 |
| 1 | A | 2361 | A | N9-C1'-C2' | 7.33 | 123.53 | 114.00 |
| 1 | A | 2370 | A | C2'-C3'-O3' | 7.31 | 125.59 | 109.50 |
| 1 | A | 2531 | U | C3'-C2'-O2' | -7.31 | 92.09 | 113.30 |
| 1 | A | 2521 | A | C4'-C3'-O3' | 7.31 | 127.62 | 113.00 |
| 1 | A | 2316 | G | C4'-C3'-O3' | -7.29 | 94.08 | 109.40 |
| 1 | A | 2360 | C | N1-C1'-C2' | 7.29 | 123.48 | 114.00 |
| 1 | A | 2658 | G | OP1-P-O3' | 7.29 | 121.23 | 105.20 |
| 1 | A | 2306 | U | N1-C1'-C2' | -7.28 | 104.00 | 112.00 |
| 1 | A | 2620 | U | C3'-C2'-O2' | 7.28 | 134.41 | 113.30 |
| 2 | B | 75 | C | O5'-P-OP1 | -7.27 | 99.16 | 105.70 |
| 1 | A | 2463 | A | OP1-P-O3' | 7.27 | 121.20 | 105.20 |
| 1 | A | 2607 | U | O5'-P-OP2 | -7.25 | 99.17 | 105.70 |
| 1 | A | 2083 | A | C4'-C3'-O3' | 7.25 | 127.49 | 113.00 |
| 1 | A | 2439 | C | C4'-C3'-O3' | 7.24 | 127.48 | 113.00 |
| 1 | A | 2473 | U | OP1-P-O3' | 7.23 | 121.11 | 105.20 |
| 1 | A | 2083 | A | O4'-C1'-N9 | -7.23 | 102.42 | 108.20 |
| 1 | A | 2348 | C | O5'-P-OP1 | -7.22 | 99.20 | 105.70 |
| 1 | A | 2099 | G | OP2-P-O3' | -7.20 | 89.36 | 105.20 |
| 1 | A | 2588 | G | OP1-P-O3' | 7.14 | 120.91 | 105.20 |
| 1 | A | 2278 | U | O5'-P-OP1 | -7.12 | 99.29 | 105.70 |
| 1 | A | 2437 | A | C1'-C2'-O2' | 7.12 | 131.97 | 110.60 |
| 1 | A | 2478 | U | N1-C1'-C2' | -7.11 | 104.18 | 112.00 |
| 1 | A | 2437 | A | C5-N7-C8 | -7.09 | 100.36 | 103.90 |
| 1 | A | 2299 | G | C5-C6-O6 | -7.08 | 124.35 | 128.60 |
| 1 | A | 2507 | G | N9-C1'-C2' | -7.07 | 104.22 | 112.00 |
| 1 | A | 2439 | C | O4'-C1'-N1 | 7.05 | 113.84 | 108.20 |
| 1 | A | 2239 | C | O4'-C1'-N1 | 7.05 | 113.84 | 108.20 |
| 1 | A | 2505 | G | O4'-C1'-N9 | 7.03 | 113.82 | 108.20 |
| 1 | A | 2600 | A | O4'-C1'-N9 | 7.02 | 113.82 | 108.20 |
| 1 | A | 2118 | A | OP2-P-O3' | 7.02 | 120.64 | 105.20 |
| 1 | A | 2574 | G | O4'-C1'-N9 | 7.01 | 113.81 | 108.20 |
| 1 | A | 2617 | G | O4'-C1'-N9 | 7.01 | 113.81 | 108.20 |
| 1 | A | 2345 | A | O4'-C1'-N9 | -7.00 | 102.60 | 108.20 |
| 1 | A | 2506 | A | O4'-C1'-N9 | 6.97 | 113.78 | 108.20 |
| 1 | A | 2641 | C | N1-C1'-C2' | -6.97 | 104.33 | 112.00 |
| 1 | A | 2552 | C | O5'-P-OP1 | -6.96 | 99.43 | 105.70 |
| 1 | A | 2427 | C | O5'-P-OP1 | 6.96 | 119.05 | 110.70 |
| 1 | A | 2507 | G | O5'-P-OP1 | 6.94 | 119.03 | 110.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 2074 | A | C3'-C2'-O2' | 6.93 | 133.39 | 113.30 |
| 1 | A | 2653 | A | O4'-C1'-N9 | 6.92 | 113.74 | 108.20 |
| 1 | A | 2087 | C | O4'-C1'-N1 | -6.92 | 102.66 | 108.20 |
| 1 | A | 2527 | U | OP2-P-O3' | -6.91 | 89.99 | 105.20 |
| 1 | A | 2635 | A | C4'-C3'-O3' | -6.91 | 94.90 | 109.40 |
| 1 | A | 2457 | U | O4'-C1'-N1 | 6.90 | 113.72 | 108.20 |
| 1 | A | 2444 | U | O4'-C1'-N1 | 6.87 | 113.70 | 108.20 |
| 1 | A | 2649 | A | N9-C1'-C2' | -6.84 | 104.47 | 112.00 |
| 1 | A | 2267 | G | O4'-C1'-N9 | 6.84 | 113.67 | 108.20 |
| 1 | A | 2099 | G | O4'-C1'-N9 | -6.84 | 102.73 | 108.20 |
| 1 | A | 2083 | A | N9-C1'-C2' | -6.83 | 104.48 | 112.00 |
| 1 | A | 2252 | A | N9-C1'-C2' | -6.83 | 104.49 | 112.00 |
| 1 | A | 2559 | C | OP2-P-O3' | 6.83 | 120.22 | 105.20 |
| 1 | A | 2134 | G | O4'-C1'-N9 | 6.81 | 113.65 | 108.20 |
| 1 | A | 2572 | G | P-O5'-C5' | -6.81 | 110.01 | 120.90 |
| 1 | A | 2548 | C | O4'-C1'-N1 | 6.78 | 113.62 | 108.20 |
| 1 | A | 2377 | U | O4'-C1'-N1 | 6.78 | 113.62 | 108.20 |
| 1 | A | 2321 | A | C4'-C3'-O3' | 6.78 | 126.56 | 113.00 |
| 1 | A | 2398 | A | N9-C1'-C2' | -6.78 | 104.54 | 112.00 |
| 1 | A | 2473 | U | C2'-C3'-O3' | -6.78 | 94.59 | 109.50 |
| 1 | A | 2282 | U | N1-C1'-C2' | 6.77 | 122.80 | 114.00 |
| 1 | A | 2305 | A | N9-C1'-C2' | -6.77 | 104.56 | 112.00 |
| 1 | A | 2096 | A | O4'-C1'-N9 | -6.76 | 102.79 | 108.20 |
| 1 | A | 2560 | C | O4'-C1'-N1 | 6.76 | 113.61 | 108.20 |
| 1 | A | 2092 | G | C1'-C2'-O2' | -6.74 | 90.37 | 110.60 |
| 1 | A | 2358 | U | O4'-C1'-N1 | -6.72 | 102.82 | 108.20 |
| 1 | A | 2488 | A | O4'-C1'-N9 | 6.72 | 113.58 | 108.20 |
| 1 | A | 2244 | A | O5'-P-OP1 | -6.72 | 99.65 | 105.70 |
| 1 | A | 2081 | A | O4'-C1'-N9 | -6.70 | 102.84 | 108.20 |
| 1 | A | 2459 | G | O5'-P-OP1 | -6.69 | 99.68 | 105.70 |
| 1 | A | 2599 | A | N9-C1'-C2' | 6.68 | 122.68 | 114.00 |
| 1 | A | 2480 | G | O4'-C1'-N9 | 6.68 | 113.54 | 108.20 |
| 1 | A | 2563 | U | N1-C1'-C2' | 6.67 | 122.66 | 114.00 |
| 1 | A | 2090 | G | O4'-C1'-N9 | 6.66 | 113.53 | 108.20 |
| 1 | A | 2426 | G | O4'-C1'-N9 | -6.66 | 102.87 | 108.20 |
| 1 | A | 2113 | G | C4'-C3'-O3' | 6.66 | 126.31 | 113.00 |
| 1 | A | 2127 | U | C1'-C2'-O2' | 6.65 | 130.55 | 110.60 |
| 1 | A | 2431 | C | OP2-P-O3' | -6.64 | 90.60 | 105.20 |
| 1 | A | 2411 | C | O4'-C1'-N1 | 6.63 | 113.51 | 108.20 |
| 1 | A | 2617 | G | O5'-P-OP1 | -6.63 | 99.73 | 105.70 |
| 1 | A | 2526 | C | C3'-C2'-O2' | 6.60 | 132.45 | 113.30 |
| 1 | A | 2634 | G | O4'-C1'-N9 | -6.60 | 102.92 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 2501 | G | O4'-C1'-N9 | 6.58 | 113.46 | 108.20 |
| 1 | A | 2102 | G | C2'-C3'-O3' | -6.58 | 95.03 | 109.50 |
| 1 | A | 2580 | G | N9-C1'-C2' | -6.57 | 104.77 | 112.00 |
| 1 | A | 2355 | G | C1'-C2'-O2' | 6.55 | 130.24 | 110.60 |
| 1 | A | 2266 | A | O5'-P-OP2 | -6.54 | 99.81 | 105.70 |
| 1 | A | 2601 | A | OP1-P-O3' | 6.54 | 119.59 | 105.20 |
| 1 | A | 2545 | U | N1-C1'-C2' | -6.53 | 104.81 | 112.00 |
| 1 | A | 2437 | A | N3-C4-C5 | 6.53 | 131.37 | 126.80 |
| 1 | A | 2379 | G | O4'-C1'-N9 | 6.52 | 113.41 | 108.20 |
| 1 | A | 2438 | G | OP1-P-O3' | -6.51 | 90.87 | 105.20 |
| 1 | A | 2345 | A | C1'-C2'-O2' | 6.51 | 130.13 | 110.60 |
| 1 | A | 2113 | G | N9-C1'-C2' | -6.51 | 104.84 | 112.00 |
| 1 | A | 2100 | A | N9-C1'-C2' | -6.48 | 104.87 | 112.00 |
| 1 | A | 2438 | G | O5'-P-OP2 | 6.48 | 118.48 | 110.70 |
| 1 | A | 2570 | G | N9-C1'-C2' | -6.48 | 104.88 | 112.00 |
| 1 | A | 2285 | G | N9-C1'-C2' | -6.46 | 104.90 | 112.00 |
| 1 | A | 2266 | A | N9-C1'-C2' | 6.45 | 122.39 | 114.00 |
| 1 | A | 2075 | G | OP2-P-O3' | 6.45 | 119.39 | 105.20 |
| 1 | A | 2287 | C | O5'-P-OP1 | -6.45 | 99.90 | 105.70 |
| 1 | A | 2135 | A | N9-C1'-C2' | -6.44 | 104.92 | 112.00 |
| 1 | A | 2280 | A | N9-C1'-C2' | -6.44 | 104.92 | 112.00 |
| 1 | A | 2633 | A | N9-C1'-C2' | -6.43 | 104.92 | 112.00 |
| 1 | A | 2600 | A | C3'-C2'-O2' | -6.40 | 94.73 | 113.30 |
| 1 | A | 2427 | C | C4'-C3'-O3' | 6.39 | 125.77 | 113.00 |
| 1 | A | 2558 | G | OP2-P-O3' | 6.39 | 119.25 | 105.20 |
| 1 | A | 2327 | A | C1'-C2'-O2' | 6.36 | 129.69 | 110.60 |
| 1 | A | 2582 | G | N9-C1'-C2' | -6.35 | 105.01 | 112.00 |
| 1 | A | 2130 | C | O4'-C1'-N1 | -6.35 | 103.12 | 108.20 |
| 1 | A | 2570 | G | O4'-C1'-N9 | 6.35 | 113.28 | 108.20 |
| 1 | A | 2482 | G | OP2-P-O3' | 6.34 | 119.15 | 105.20 |
| 1 | A | 2406 | U | O4'-C1'-N1 | -6.34 | 103.13 | 108.20 |
| 1 | A | 2646 | G | O4'-C1'-N9 | -6.33 | 103.14 | 108.20 |
| 1 | A | 2374 | A | O5'-P-OP1 | 6.30 | 118.26 | 110.70 |
| 1 | A | 2643 | G | N9-C1'-C2' | -6.29 | 105.08 | 112.00 |
| 1 | A | 2547 | C | C1'-C2'-O2' | 6.29 | 129.47 | 110.60 |
| 1 | A | 2621 | U | O5'-P-OP2 | -6.29 | 100.04 | 105.70 |
| 1 | A | 2126 | C | OP1-P-O3' | -6.27 | 91.41 | 105.20 |
| 1 | A | 2649 | A | C4'-C3'-O3' | -6.27 | 96.24 | 109.40 |
| 1 | A | 2623 | G | N9-C1'-C2' | -6.26 | 105.11 | 112.00 |
| 1 | A | 2122 | C | O5'-P-OP1 | 6.25 | 118.20 | 110.70 |
| 1 | A | 2659 | U | C1'-C2'-O2' | 6.25 | 129.35 | 110.60 |
| 1 | A | 2647 | C | N1-C1'-C2' | -6.25 | 105.13 | 112.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 2262 | C | O4'-C1'-N1 | -6.24 | 103.21 | 108.20 |
| 1 | A | 2313 | C | C5'-C4'-C3' | 6.24 | 125.98 | 116.00 |
| 1 | A | 2437 | A | N3-C4-N9 | -6.23 | 122.41 | 127.40 |
| 1 | A | 2244 | A | OP1-P-O3' | 6.23 | 118.90 | 105.20 |
| 1 | A | 2461 | U | N1-C1'-C2' | -6.23 | 105.15 | 112.00 |
| 1 | A | 2264 | A | OP2-P-O3' | 6.22 | 118.89 | 105.20 |
| 1 | A | 2651 | C | OP2-P-O3' | 6.22 | 118.89 | 105.20 |
| 1 | A | 2102 | G | OP2-P-O3' | -6.22 | 91.52 | 105.20 |
| 1 | A | 2356 | A | C4'-C3'-O3' | -6.22 | 96.34 | 109.40 |
| 1 | A | 2465 | A | OP2-P-O3' | 6.21 | 118.87 | 105.20 |
| 1 | A | 2610 | U | N1-C1'-C2' | 6.21 | 122.07 | 114.00 |
| 1 | A | 2069 | U | C4'-C3'-O3' | -6.21 | 96.36 | 109.40 |
| 1 | A | 2352 | G | O5'-P-OP1 | -6.19 | 100.13 | 105.70 |
| 1 | A | 2652 | U | O4'-C1'-N1 | 6.18 | 113.14 | 108.20 |
| 1 | A | 2271 | G | N9-C1'-C2' | -6.17 | 105.21 | 112.00 |
| 1 | A | 2064 | U | O5'-P-OP1 | 6.17 | 118.10 | 110.70 |
| 1 | A | 2073 | G | O5'-P-OP1 | 6.17 | 118.10 | 110.70 |
| 1 | A | 2485 | A | O4'-C1'-N9 | 6.16 | 113.12 | 108.20 |
| 1 | A | 2609 | G | O4'-C1'-N9 | 6.13 | 113.10 | 108.20 |
| 1 | A | 2283 | G | O4'-C1'-N9 | -6.12 | 103.30 | 108.20 |
| 1 | A | 2512 | U | O4'-C1'-N1 | -6.12 | 103.30 | 108.20 |
| 1 | A | 2620 | U | C2'-C3'-O3' | -6.12 | 96.03 | 109.50 |
| 1 | A | 2395 | A | O4'-C1'-N9 | -6.11 | 103.31 | 108.20 |
| 1 | A | 2368 | A | O5'-P-OP2 | -6.11 | 100.20 | 105.70 |
| 1 | A | 2594 | C | O5'-P-OP2 | 6.11 | 118.03 | 110.70 |
| 1 | A | 2537 | G | O5'-P-OP2 | 6.10 | 118.02 | 110.70 |
| 1 | A | 2522 | G | C1'-C2'-O2' | 6.08 | 128.85 | 110.60 |
| 1 | A | 2432 | C | N1-C1'-C2' | -6.07 | 105.32 | 112.00 |
| 1 | A | 2241 | C | C3'-C2'-O2' | 6.06 | 130.88 | 113.30 |
| 1 | A | 2612 | A | OP2-P-O3' | 6.06 | 118.52 | 105.20 |
| 1 | A | 2116 | U | O4'-C1'-N1 | 6.05 | 113.04 | 108.20 |
| 1 | A | 2360 | C | O4'-C1'-N1 | -6.05 | 103.36 | 108.20 |
| 1 | A | 2367 | A | O4'-C1'-N9 | -6.04 | 103.36 | 108.20 |
| 1 | A | 2369 | A | O4'-C1'-N9 | -6.04 | 103.36 | 108.20 |
| 1 | A | 2616 | G | O4'-C1'-N9 | 6.03 | 113.03 | 108.20 |
| 1 | A | 2082 | G | N9-C1'-C2' | -6.03 | 105.37 | 112.00 |
| 1 | A | 2300 | A | C2-N3-C4 | -6.02 | 107.59 | 110.60 |
| 1 | A | 2086 | C | N1-C1'-C2' | -6.02 | 105.38 | 112.00 |
| 1 | A | 2447 | A | C3'-C2'-O2' | 6.02 | 130.76 | 113.30 |
| 1 | A | 2335 | C | O5'-P-OP1 | -6.01 | 100.29 | 105.70 |
| 1 | A | 2637 | A | N9-C1'-C2' | 6.01 | 121.82 | 114.00 |
| 1 | A | 2311 | A | N9-C1'-C2' | -6.01 | 105.39 | 112.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 2535 | U | C1'-C2'-O2' | 6.01 | 128.63 | 110.60 |
| 1 | A | 2634 | G | O5'-P-OP2 | -6.00 | 100.30 | 105.70 |
| 1 | A | 2410 | G | O4'-C1'-N9 | 5.99 | 112.99 | 108.20 |
| 1 | A | 2637 | A | OP2-P-O3' | 5.98 | 118.36 | 105.20 |
| 1 | A | 2247 | C | N1-C1'-C2' | 5.98 | 121.77 | 114.00 |
| 1 | A | 2473 | U | OP2-P-O3' | -5.98 | 92.05 | 105.20 |
| 1 | A | 2606 | G | O4'-C1'-N9 | 5.97 | 112.98 | 108.20 |
| 1 | A | 2294 | C | OP2-P-O3' | 5.97 | 118.33 | 105.20 |
| 1 | A | 2373 | U | OP1-P-O3' | -5.95 | 92.11 | 105.20 |
| 1 | A | 2466 | G | C3'-C2'-O2' | -5.95 | 96.05 | 113.30 |
| 1 | A | 2647 | C | C3'-C2'-O2' | 5.95 | 130.54 | 113.30 |
| 1 | A | 2452 | G | O4'-C1'-N9 | -5.94 | 103.44 | 108.20 |
| 1 | A | 2478 | U | O4'-C1'-N1 | 5.94 | 112.95 | 108.20 |
| 1 | A | 2101 | A | OP1-P-O3' | 5.93 | 118.25 | 105.20 |
| 1 | A | 2540 | G | O5'-P-OP2 | -5.93 | 100.37 | 105.70 |
| 1 | A | 2574 | G | C3'-C2'-O2' | -5.92 | 96.13 | 113.30 |
| 1 | A | 2299 | G | C6-C5-N7 | -5.92 | 126.85 | 130.40 |
| 1 | A | 2550 | U | N1-C1'-C2' | 5.91 | 121.69 | 114.00 |
| 1 | A | 2454 | C | C1'-C2'-O2' | 5.91 | 128.32 | 110.60 |
| 1 | A | 2067 | A | O4'-C1'-N9 | 5.90 | 112.92 | 108.20 |
| 1 | A | 2430 | A | O4'-C1'-N9 | -5.89 | 103.49 | 108.20 |
| 1 | A | 2365 | G | O4'-C1'-N9 | -5.88 | 103.49 | 108.20 |
| 1 | A | 2568 | A | O4'-C1'-N9 | -5.88 | 103.50 | 108.20 |
| 1 | A | 2437 | A | C4-C5-C6 | -5.88 | 114.06 | 117.00 |
| 1 | A | 2551 | C | O4'-C1'-N1 | 5.87 | 112.90 | 108.20 |
| 1 | A | 2652 | U | P-O5'-C5' | -5.87 | 111.51 | 120.90 |
| 1 | A | 2575 | C | N1-C1'-C2' | 5.86 | 121.62 | 114.00 |
| 1 | A | 2608 | C | C2'-C3'-O3' | 5.86 | 123.08 | 113.70 |
| 1 | A | 2357 | G | N9-C1'-C2' | -5.86 | 105.56 | 112.00 |
| 1 | A | 2571 | C | O5'-P-OP1 | -5.85 | 100.43 | 105.70 |
| 1 | A | 2605 | G | N9-C1'-C2' | 5.85 | 121.61 | 114.00 |
| 1 | A | 2390 | U | N1-C1'-C2' | 5.85 | 121.61 | 114.00 |
| 1 | A | 2068 | G | O4'-C1'-N9 | 5.83 | 112.87 | 108.20 |
| 1 | A | 2631 | U | O4'-C1'-N1 | -5.83 | 103.53 | 108.20 |
| 1 | A | 2271 | G | C2'-C3'-O3' | -5.83 | 96.68 | 109.50 |
| 1 | A | 2598 | U | C5'-C4'-C3' | -5.83 | 106.68 | 116.00 |
| 1 | A | 2536 | C | C1'-O4'-C4' | -5.82 | 105.24 | 109.90 |
| 1 | A | 2406 | U | N1-C1'-C2' | -5.82 | 105.60 | 112.00 |
| 1 | A | 2490 | A | O4'-C1'-N9 | 5.82 | 112.86 | 108.20 |
| 1 | A | 2245 | C | OP2-P-O3' | 5.82 | 118.00 | 105.20 |
| 1 | A | 2382 | A | O4'-C1'-N9 | -5.81 | 103.55 | 108.20 |
| 1 | A | 2118 | A | N9-C1'-C2' | 5.81 | 121.55 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 2463 | A | P-O3'-C3' | 5.81 | 126.67 | 119.70 |
| 1 | A | 2332 | A | OP2-P-O3' | 5.80 | 117.97 | 105.20 |
| 1 | A | 2478 | U | OP2-P-O3' | 5.79 | 117.94 | 105.20 |
| 1 | A | 2066 | C | O4'-C1'-N1 | 5.77 | 112.81 | 108.20 |
| 1 | A | 2305 | A | C4'-C3'-O3' | -5.75 | 97.32 | 109.40 |
| 1 | A | 2637 | A | O5'-P-OP1 | -5.74 | 100.53 | 105.70 |
| 1 | A | 2620 | U | OP1-P-O3' | 5.74 | 117.82 | 105.20 |
| 1 | A | 2246 | U | C4'-C3'-O3' | -5.74 | 97.35 | 109.40 |
| 1 | A | 2473 | U | C4'-C3'-O3' | 5.73 | 124.46 | 113.00 |
| 1 | A | 2571 | C | OP2-P-O3' | 5.73 | 117.81 | 105.20 |
| 1 | A | 2092 | G | N9-C1'-C2' | 5.73 | 121.45 | 114.00 |
| 1 | A | 2436 | U | OP2-P-O3' | 5.72 | 117.78 | 105.20 |
| 1 | A | 2336 | G | O4'-C1'-N9 | 5.71 | 112.77 | 108.20 |
| 1 | A | 2410 | G | OP2-P-O3' | 5.71 | 117.75 | 105.20 |
| 1 | A | 2303 | A | OP2-P-O3' | 5.69 | 117.72 | 105.20 |
| 1 | A | 2496 | C | C4'-C3'-O3' | 5.69 | 124.38 | 113.00 |
| 1 | A | 2527 | U | P-O3'-C3' | -5.68 | 112.88 | 119.70 |
| 1 | A | 2661 | U | O4'-C1'-N1 | 5.68 | 112.75 | 108.20 |
| 2 | B | 74 | C | N1-C1'-C2' | 5.68 | 121.38 | 114.00 |
| 1 | A | 2473 | U | N1-C1'-C2' | -5.67 | 105.77 | 112.00 |
| 1 | A | 2437 | A | C2-N3-C4 | -5.65 | 107.78 | 110.60 |
| 1 | A | 2507 | G | C4'-C3'-O3' | 5.62 | 124.24 | 113.00 |
| 1 | A | 2598 | U | O5'-C5'-C4' | -5.62 | 101.02 | 111.70 |
| 1 | A | 2106 | C | N1-C1'-C2' | 5.61 | 121.30 | 114.00 |
| 1 | A | 2561 | C | O5'-P-OP1 | -5.61 | 100.65 | 105.70 |
| 1 | A | 2479 | A | O4'-C1'-N9 | -5.59 | 103.73 | 108.20 |
| 1 | A | 2402 | A | O4'-C1'-N9 | 5.59 | 112.67 | 108.20 |
| 1 | A | 2130 | C | OP2-P-O3' | -5.59 | 92.91 | 105.20 |
| 1 | A | 2132 | C | N1-C1'-C2' | -5.58 | 105.86 | 112.00 |
| 1 | A | 2356 | A | C3'-C2'-O2' | 5.58 | 129.48 | 113.30 |
| 1 | A | 2396 | C | OP2-P-O3' | 5.58 | 117.47 | 105.20 |
| 1 | A | 2590 | U | OP2-P-O3' | 5.58 | 117.47 | 105.20 |
| 1 | A | 2463 | A | O4'-C1'-N9 | -5.57 | 103.74 | 108.20 |
| 1 | A | 2124 | G | O5'-C5'-C4' | -5.57 | 101.13 | 111.70 |
| 1 | A | 2454 | C | C3'-C2'-O2' | 5.54 | 129.35 | 113.30 |
| 1 | A | 2095 | A | C5'-C4'-O4' | 5.53 | 115.73 | 109.10 |
| 1 | A | 2347 | C | O4'-C1'-N1 | 5.52 | 112.62 | 108.20 |
| 1 | A | 2488 | A | OP2-P-O3' | 5.52 | 117.35 | 105.20 |
| 1 | A | 2619 | U | C2'-C3'-O3' | 5.52 | 122.53 | 113.70 |
| 1 | A | 2638 | G | N9-C1'-C2' | -5.52 | 105.93 | 112.00 |
| 1 | A | 2286 | G | N9-C1'-C2' | -5.51 | 105.94 | 112.00 |
| 1 | A | 2635 | A | O4'-C1'-N9 | 5.51 | 112.61 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 2069 | U | OP2-P-O3' | 5.51 | 117.31 | 105.20 |
| 1 | A | 2467 | A | N9-C1'-C2' | 5.50 | 121.15 | 114.00 |
| 1 | A | 2616 | G | C4'-C3'-O3' | -5.50 | 97.85 | 109.40 |
| 1 | A | 2074 | A | N9-C1'-C2' | 5.50 | 121.14 | 114.00 |
| 1 | A | 2313 | C | P-O5'-C5' | -5.50 | 112.11 | 120.90 |
| 1 | A | 2122 | C | C4'-C3'-O3' | 5.49 | 123.97 | 113.00 |
| 1 | A | 2486 | A | O4'-C1'-N9 | 5.46 | 112.57 | 108.20 |
| 1 | A | 2633 | A | O4'-C1'-N9 | -5.46 | 103.83 | 108.20 |
| 1 | A | 2607 | U | C4'-C3'-O3' | -5.45 | 97.96 | 109.40 |
| 2 | B | 75 | C | OP1-P-O3' | 5.45 | 117.19 | 105.20 |
| 1 | A | 2106 | C | O4'-C1'-N1 | 5.45 | 112.56 | 108.20 |
| 1 | A | 2362 | A | O5'-P-OP1 | -5.45 | 100.80 | 105.70 |
| 1 | A | 2584 | G | N9-C1'-C2' | -5.44 | 106.02 | 112.00 |
| 1 | A | 2300 | A | N9-C1'-C2' | 5.43 | 121.06 | 114.00 |
| 1 | A | 2295 | G | O5'-P-OP1 | -5.43 | 100.81 | 105.70 |
| 1 | A | 2439 | C | OP1-P-O3' | 5.42 | 117.13 | 105.20 |
| 1 | A | 2274 | A | O4'-C1'-N9 | 5.42 | 112.53 | 108.20 |
| 1 | A | 2632 | G | P-O3'-C3' | -5.42 | 113.20 | 119.70 |
| 1 | A | 2325 | C | O5'-P-OP1 | -5.42 | 100.82 | 105.70 |
| 1 | A | 2607 | U | O5'-P-OP1 | 5.41 | 117.19 | 110.70 |
| 1 | A | 2654 | C | OP1-P-O3' | 5.41 | 117.09 | 105.20 |
| 1 | A | 2299 | G | C3'-C2'-C1' | 5.40 | 105.82 | 101.50 |
| 1 | A | 2336 | G | OP2-P-O3' | 5.39 | 117.07 | 105.20 |
| 1 | A | 2611 | G | N9-C1'-C2' | 5.39 | 121.01 | 114.00 |
| 1 | A | 2124 | G | C3'-C2'-O2' | 5.39 | 128.92 | 113.30 |
| 1 | A | 2121 | G | OP1-P-O3' | -5.38 | 93.37 | 105.20 |
| 1 | A | 2469 | A | O4'-C1'-N9 | 5.38 | 112.50 | 108.20 |
| 1 | A | 2290 | U | C4'-C3'-O3' | -5.37 | 98.13 | 109.40 |
| 1 | A | 2074 | A | C1'-C2'-O2' | -5.37 | 94.50 | 110.60 |
| 1 | A | 2520 | G | C3'-C2'-O2' | -5.37 | 97.74 | 113.30 |
| 1 | A | 2546 | U | O4'-C1'-N1 | -5.36 | 103.91 | 108.20 |
| 1 | A | 2559 | C | O5'-P-OP2 | -5.36 | 100.88 | 105.70 |
| 1 | A | 2487 | C | OP1-P-O3' | 5.35 | 116.97 | 105.20 |
| 1 | A | 2647 | C | C1'-C2'-O2' | 5.32 | 126.57 | 110.60 |
| 1 | A | 2619 | U | O4'-C1'-N1 | 5.32 | 112.46 | 108.20 |
| 1 | A | 2487 | C | N1-C1'-C2' | -5.31 | 106.16 | 112.00 |
| 1 | A | 2270 | G | O4'-C1'-N9 | -5.31 | 103.95 | 108.20 |
| 1 | A | 2652 | U | O5'-P-OP2 | 5.31 | 117.07 | 110.70 |
| 1 | A | 2439 | C | N1-C1'-C2' | -5.30 | 106.17 | 112.00 |
| 1 | A | 2438 | G | OP2-P-O3' | -5.30 | 93.54 | 105.20 |
| 1 | A | 2619 | U | OP1-P-O3' | 5.28 | 116.81 | 105.20 |
| 1 | A | 2408 | A | C3'-C2'-O2' | -5.27 | 98.02 | 113.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 2063 | U | O3'-P-O5' | 5.26 | 114.00 | 104.00 |
| 1 | A | 2266 | A | OP2-P-O3' | 5.26 | 116.76 | 105.20 |
| 1 | A | 2632 | G | N9-C1'-C2' | 5.25 | 120.83 | 114.00 |
| 1 | A | 2096 | A | C4'-C3'-O3' | -5.25 | 98.38 | 109.40 |
| 1 | A | 2600 | A | O5'-P-OP2 | 5.25 | 117.00 | 110.70 |
| 1 | A | 2573 | G | O4'-C1'-N9 | 5.24 | 112.39 | 108.20 |
| 1 | A | 2475 | C | O4'-C1'-N1 | -5.22 | 104.02 | 108.20 |
| 1 | A | 2101 | A | O4'-C1'-N9 | 5.22 | 112.38 | 108.20 |
| 1 | A | 2241 | C | C1'-C2'-O2' | 5.22 | 126.25 | 110.60 |
| 1 | A | 2424 | U | O5'-C5'-C4' | -5.21 | 101.79 | 111.70 |
| 1 | A | 2428 | G | C2'-C3'-O3' | -5.21 | 98.03 | 109.50 |
| 1 | A | 2414 | A | O5'-C5'-C4' | -5.21 | 101.80 | 111.70 |
| 1 | A | 2346 | C | O5'-C5'-C4' | -5.21 | 101.80 | 111.70 |
| 1 | A | 2471 | G | C1'-C2'-O2' | 5.20 | 126.19 | 110.60 |
| 1 | A | 2403 | C | O4'-C1'-N1 | 5.20 | 112.36 | 108.20 |
| 1 | A | 2602 | G | C3'-C2'-O2' | 5.20 | 128.37 | 113.30 |
| 1 | A | 2474 | A | C4'-C3'-O3' | 5.19 | 123.38 | 113.00 |
| 1 | A | 2591 | C | C4'-C3'-O3' | -5.19 | 98.51 | 109.40 |
| 1 | A | 2439 | C | P-O3'-C3' | -5.18 | 113.48 | 119.70 |
| 1 | A | 2618 | G | OP2-P-O3' | 5.18 | 116.60 | 105.20 |
| 1 | A | 2320 | U | OP1-P-O3' | 5.18 | 116.59 | 105.20 |
| 1 | A | 2288 | G | O4'-C1'-N9 | 5.13 | 112.31 | 108.20 |
| 1 | A | 2636 | C | O5'-P-OP1 | -5.13 | 101.08 | 105.70 |
| 1 | A | 2438 | G | N9-C1'-C2' | -5.13 | 106.36 | 112.00 |
| 1 | A | 2391 | C | N1-C1'-C2' | -5.12 | 106.37 | 112.00 |
| 1 | A | 2560 | C | OP2-P-O3' | 5.12 | 116.45 | 105.20 |
| 1 | A | 2282 | U | O4'-C1'-N1 | 5.11 | 112.28 | 108.20 |
| 1 | A | 2095 | A | O4'-C1'-N9 | 5.10 | 112.28 | 108.20 |
| 1 | A | 2650 | U | O4'-C1'-N1 | -5.08 | 104.13 | 108.20 |
| 1 | A | 2498 | C | O4'-C1'-N1 | 5.08 | 112.26 | 108.20 |
| 1 | A | 2619 | U | O5'-P-OP1 | -5.08 | 101.13 | 105.70 |
| 1 | A | 2639 | G | O4'-C1'-N9 | 5.08 | 112.26 | 108.20 |
| 1 | A | 2663 | U | O4'-C1'-N1 | 5.07 | 112.26 | 108.20 |
| 1 | A | 2258 | A | C2'-C3'-O3' | 5.07 | 121.81 | 113.70 |
| 1 | A | 2392 | C | O4'-C1'-N1 | 5.07 | 112.26 | 108.20 |
| 1 | A | 2558 | G | C1'-C2'-O2' | 5.07 | 125.81 | 110.60 |
| 1 | A | 2620 | U | N1-C1'-C2' | 5.07 | 120.59 | 114.00 |
| 1 | A | 2431 | C | P-O3'-C3' | -5.07 | 113.62 | 119.70 |
| 1 | A | 2550 | U | OP2-P-O3' | 5.06 | 116.34 | 105.20 |
| 1 | A | 2627 | G | O4'-C1'-N9 | 5.06 | 112.25 | 108.20 |
| 1 | A | 2387 | U | C4'-C3'-O3' | -5.06 | 98.78 | 109.40 |
| 1 | A | 2303 | A | O5'-P-OP1 | 5.05 | 116.76 | 110.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | A | 2516 | G | N9-C1'-C2' | -5.05 | 106.44 | 112.00 |
| 1 | A | 2131 | G | O5'-P-OP1 | 5.05 | 116.76 | 110.70 |
| 1 | A | 2554 | U | C2'-C3'-O3' | -5.04 | 98.41 | 109.50 |
| 1 | A | 2566 | A | N9-C1'-C2' | 5.04 | 120.55 | 114.00 |
| 1 | A | 2617 | G | C2'-C3'-O3' | 5.03 | 121.74 | 113.70 |
| 1 | A | 2383 | G | N9-C1'-C2' | -5.02 | 106.48 | 112.00 |
| 1 | A | 2395 | A | C2'-C3'-O3' | 5.01 | 121.72 | 113.70 |
| 1 | A | 2122 | C | P-O3'-C3' | -5.01 | 113.69 | 119.70 |
| 1 | A | 2265 | U | OP1-P-O3' | 5.01 | 116.22 | 105.20 |
| 1 | A | 2481 | G | OP2-P-O3' | 5.00 | 116.20 | 105.20 |

All (36) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 1 | A | 2083 | A | C3' |
| 1 | A | 2124 | G | C2' |
| 1 | A | 2127 | U | C2' |
| 1 | A | 2130 | C | C2' |
| 1 | A | 2241 | C | C2' |
| 1 | A | 2263 | G | C2' |
| 1 | A | 2321 | A | C3' |
| 1 | A | 2327 | A | C2' |
| 1 | A | 2345 | A | C2' |
| 1 | A | 2355 | G | C2' |
| 1 | A | 2370 | A | C3' |
| 1 | A | 2408 | A | C2' |
| 1 | A | 2427 | C | C3' |
| 1 | A | 2437 | A | C2' |
| 1 | A | 2447 | A | C2' |
| 1 | A | 2454 | C | C2' |
| 1 | A | 2482 | G | C3' |
| 1 | A | 2515 | C | C2' |
| 1 | A | 2532 | A | C2' |
| 1 | A | 2535 | U | C2' |
| 1 | A | 2547 | C | C2' |
| 1 | A | 2548 | C | C2' |
| 1 | A | 2602 | G | C2' |
| 1 | A | 2610 | U | C2' |
| 1 | A | 2611 | G | C2' |
| 1 | A | 2615 | U | C2' |
| 1 | A | 2616 | G | C1' |
| 1 | A | 2624 | A | C2' |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|---------|
| 1 | A | 2626 | C | C2' |
| 1 | A | 2637 | A | C4',C3' |
| 1 | A | 2647 | C | C2' |
| 1 | A | 2650 | U | C2' |
| 1 | A | 2656 | G | C2' |
| 1 | A | 2657 | G | C2' |
| 1 | A | 2659 | U | C2' |

All (5) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 1 | A | 2299 | G | Sidechain |
| 1 | A | 2300 | A | Sidechain |
| 1 | A | 2437 | A | Sidechain |
| 1 | A | 2549 | C | Sidechain |
| 1 | A | 2564 | G | Sidechain |

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 | 10627 | 0 | 5357 | 744 | 0 |
| 2 | B | 98 | 0 | 61 | 12 | 0 |
| All | All | 10725 | 0 | 5418 | 747 | 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 48.

All (747) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:A:2299:G:H1 | 1:A:2300:A:N6 | 1.42 | 1.16 |
| 1:A:2473:U:H4' | 1:A:2474:A:H5' | 1.35 | 1.08 |
| 1:A:2478:U:H2' | 1:A:2479:A:H8 | 1.27 | 1.00 |
| 1:A:2299:G:N1 | 1:A:2300:A:N6 | 2.15 | 0.95 |
| 1:A:2316:G:H2' | 1:A:2427:C:N4 | 1.85 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:A:2546:U:H2' | 1:A:2547:C:C6 | 2.08 | 0.89 |
| 1:A:2252:A:C5 | 1:A:2253:G:H1' | 2.09 | 0.87 |
| 1:A:2264:A:H2' | 1:A:2265:U:C6 | 2.11 | 0.86 |
| 1:A:2312:G:H2' | 1:A:2313:C:H5' | 1.56 | 0.85 |
| 1:A:2619:U:H2' | 1:A:2620:U:C5 | 2.11 | 0.85 |
| 1:A:2253:G:H2' | 1:A:2254:G:H8 | 1.41 | 0.85 |
| 1:A:2256:G:H2' | 1:A:2257:G:H5' | 1.56 | 0.85 |
| 1:A:2541:U:H3 | 1:A:2618:G:H1 | 1.25 | 0.84 |
| 1:A:2509:A:N6 | 1:A:2564:G:N2 | 2.26 | 0.84 |
| 1:A:2635:A:H2' | 1:A:2636:C:C6 | 2.14 | 0.83 |
| 1:A:2488:A:H61 | 1:A:2534:C:H42 | 1.27 | 0.82 |
| 1:A:2542:C:C2' | 1:A:2543:G:H5' | 2.10 | 0.81 |
| 1:A:2502:C:C2' | 1:A:2503:A:H5' | 2.10 | 0.81 |
| 1:A:2266:A:H2' | 1:A:2267:G:H8 | 1.45 | 0.81 |
| 1:A:2478:U:H2' | 1:A:2479:A:C8 | 2.12 | 0.81 |
| 1:A:2264:A:H2' | 1:A:2265:U:H6 | 1.47 | 0.80 |
| 1:A:2262:C:H2' | 1:A:2263:G:H8 | 1.46 | 0.80 |
| 1:A:2266:A:H2' | 1:A:2267:G:C8 | 2.16 | 0.79 |
| 1:A:2087:C:O2' | 1:A:2088:C:H5' | 1.82 | 0.79 |
| 1:A:2494:G:H2' | 1:A:2495:U:H5' | 1.65 | 0.79 |
| 1:A:2326:U:H2' | 1:A:2327:A:H8 | 1.46 | 0.79 |
| 1:A:2619:U:H2' | 1:A:2620:U:C6 | 2.18 | 0.79 |
| 1:A:2345:A:H3' | 1:A:2346:C:C5 | 2.19 | 0.78 |
| 1:A:2509:A:H62 | 1:A:2564:G:N2 | 1.80 | 0.78 |
| 1:A:2487:C:C2' | 1:A:2488:A:H5' | 2.14 | 0.77 |
| 1:A:2515:C:H2' | 1:A:2516:G:H5' | 1.66 | 0.77 |
| 1:A:2505:G:C2' | 1:A:2506:A:H5' | 2.14 | 0.77 |
| 1:A:2496:C:H1' | 1:A:2527:U:N3 | 1.99 | 0.77 |
| 1:A:2445:U:H2' | 1:A:2446:G:C8 | 2.20 | 0.77 |
| 1:A:2507:G:H2' | 1:A:2510:C:H42 | 1.50 | 0.77 |
| 1:A:2542:C:H2' | 1:A:2543:G:H5' | 1.66 | 0.76 |
| 1:A:2473:U:C4' | 1:A:2474:A:H5' | 2.13 | 0.76 |
| 1:A:2237:G:H1' | 1:A:2238:A:C8 | 2.20 | 0.76 |
| 1:A:2326:U:H2' | 1:A:2327:A:C8 | 2.20 | 0.75 |
| 1:A:2590:U:H2' | 1:A:2591:C:H5' | 1.67 | 0.75 |
| 1:A:2605:G:C2' | 1:A:2606:G:H5' | 2.16 | 0.75 |
| 1:A:2299:G:H1' | 1:A:2310:G:N2 | 2.02 | 0.74 |
| 1:A:2299:G:N1 | 1:A:2300:A:C6 | 2.54 | 0.74 |
| 1:A:2546:U:H2' | 1:A:2547:C:H6 | 1.52 | 0.74 |
| 1:A:2114:C:O2' | 1:A:2115:U:H5' | 1.87 | 0.74 |
| 1:A:2256:G:C2' | 1:A:2257:G:H5' | 2.16 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:2269:C:C2' | 1:A:2270:G:H5' | 2.18 | 0.73 |
| 1:A:2271:G:N3 | 1:A:2271:G:H2' | 2.02 | 0.73 |
| 1:A:2104:C:H2' | 1:A:2105:C:H5' | 1.71 | 0.72 |
| 1:A:2121:G:O2' | 1:A:2122:C:H5' | 1.88 | 0.72 |
| 1:A:2265:U:H2' | 1:A:2266:A:C8 | 2.24 | 0.71 |
| 1:A:2488:A:H61 | 1:A:2534:C:N4 | 1.86 | 0.71 |
| 1:A:2085:A:O2' | 1:A:2086:C:H5' | 1.90 | 0.71 |
| 1:A:2486:A:C2 | 2:B:77:PU:HE2 | 2.25 | 0.71 |
| 1:A:2332:A:H3' | 1:A:2333:G:C8 | 2.25 | 0.71 |
| 1:A:2105:C:N4 | 1:A:2481:G:N1 | 2.37 | 0.71 |
| 1:A:2419:U:H5'' | 1:A:2420:G:H5'' | 1.73 | 0.71 |
| 1:A:2439:C:N4 | 1:A:2440:C:H41 | 1.89 | 0.71 |
| 1:A:2488:A:N6 | 1:A:2534:C:H42 | 1.87 | 0.71 |
| 1:A:2325:C:H2' | 1:A:2326:U:C6 | 2.26 | 0.71 |
| 1:A:2568:A:C2' | 1:A:2569:A:H5' | 2.21 | 0.71 |
| 1:A:2591:C:H2' | 1:A:2592:G:O4' | 1.91 | 0.71 |
| 1:A:2082:G:O2' | 1:A:2083:A:H5' | 1.92 | 0.70 |
| 1:A:2654:C:O2' | 1:A:2655:U:H5' | 1.90 | 0.70 |
| 1:A:2508:C:OP1 | 1:A:2510:C:N4 | 2.24 | 0.70 |
| 1:A:2253:G:H2' | 1:A:2254:G:C8 | 2.25 | 0.70 |
| 1:A:2291:A:H5'' | 1:A:2292:C:C5' | 2.22 | 0.70 |
| 1:A:2414:A:H2' | 1:A:2415:A:C8 | 2.26 | 0.70 |
| 1:A:2453:G:O2' | 1:A:2454:C:H5' | 1.92 | 0.69 |
| 1:A:2478:U:O2' | 1:A:2479:A:H5' | 1.92 | 0.69 |
| 1:A:2312:G:C2' | 1:A:2313:C:H5' | 2.20 | 0.69 |
| 1:A:2460:A:H2' | 1:A:2461:U:C6 | 2.27 | 0.69 |
| 1:A:2238:A:O2' | 1:A:2239:C:H5' | 1.92 | 0.69 |
| 1:A:2509:A:H62 | 1:A:2564:G:H22 | 1.38 | 0.69 |
| 1:A:2446:G:H2' | 1:A:2447:A:H8 | 1.57 | 0.69 |
| 1:A:2568:A:H2' | 1:A:2569:A:H5' | 1.75 | 0.69 |
| 1:A:2507:G:H2' | 1:A:2510:C:N4 | 2.07 | 0.69 |
| 1:A:2505:G:O2' | 1:A:2506:A:H5' | 1.92 | 0.69 |
| 1:A:2492:U:C2' | 1:A:2493:C:H5' | 2.23 | 0.69 |
| 1:A:2614:C:O2' | 1:A:2615:U:H5' | 1.93 | 0.69 |
| 1:A:2112:A:O2' | 1:A:2113:G:H5' | 1.92 | 0.68 |
| 1:A:2621:U:N3 | 1:A:2622:A:N7 | 2.40 | 0.68 |
| 1:A:2391:C:N4 | 1:A:2397:G:OP2 | 2.26 | 0.68 |
| 1:A:2502:C:H2' | 1:A:2503:A:H5' | 1.74 | 0.68 |
| 1:A:2345:A:H3' | 1:A:2346:C:C6 | 2.28 | 0.68 |
| 1:A:2630:G:N2 | 1:A:2633:A:OP2 | 2.26 | 0.68 |
| 1:A:2262:C:H2' | 1:A:2263:G:C8 | 2.29 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|----------------|--------------------------|-------------------|
| 1:A:2605:G:H2' | 1:A:2606:G:H5' | 1.75 | 0.68 |
| 1:A:2495:U:C2' | 1:A:2496:C:H5' | 2.23 | 0.68 |
| 1:A:2509:A:N6 | 1:A:2564:G:H22 | 1.89 | 0.68 |
| 1:A:2487:C:H2' | 1:A:2488:A:H5' | 1.76 | 0.68 |
| 1:A:2252:A:C6 | 1:A:2253:G:H1' | 2.28 | 0.68 |
| 1:A:2412:G:N2 | 1:A:2415:A:OP2 | 2.27 | 0.67 |
| 1:A:2065:C:H2' | 1:A:2066:C:C6 | 2.30 | 0.67 |
| 1:A:2090:G:H2' | 1:A:2091:G:C8 | 2.30 | 0.67 |
| 1:A:2314:G:H2' | 1:A:2315:C:H5' | 1.75 | 0.67 |
| 1:A:2594:C:O2' | 1:A:2595:U:H5' | 1.94 | 0.67 |
| 1:A:2325:C:H2' | 1:A:2326:U:H6 | 1.59 | 0.67 |
| 1:A:2612:A:H5'' | 1:A:2613:G:O5' | 1.94 | 0.67 |
| 1:A:2106:C:H2' | 1:A:2107:U:C6 | 2.30 | 0.67 |
| 1:A:2398:A:H2' | 1:A:2399:G:O4' | 1.94 | 0.67 |
| 1:A:2628:U:H3 | 1:A:2635:A:H61 | 1.43 | 0.67 |
| 1:A:2065:C:H2' | 1:A:2066:C:H6 | 1.61 | 0.66 |
| 1:A:2582:G:O2' | 1:A:2583:A:H5' | 1.95 | 0.66 |
| 1:A:2102:G:OP2 | 1:A:2537:G:H5' | 1.96 | 0.66 |
| 1:A:2105:C:N4 | 1:A:2536:C:N3 | 2.44 | 0.65 |
| 1:A:2265:U:H2' | 1:A:2266:A:H8 | 1.61 | 0.65 |
| 1:A:2456:A:H2' | 1:A:2457:U:C6 | 2.31 | 0.65 |
| 1:A:2485:A:O2' | 2:B:76:DA:N1 | 2.20 | 0.65 |
| 1:A:2255:A:H2' | 1:A:2256:G:O4' | 1.96 | 0.65 |
| 1:A:2385:G:H2' | 1:A:2386:U:C6 | 2.31 | 0.65 |
| 1:A:2242:U:O2' | 1:A:2243:C:H2' | 1.96 | 0.65 |
| 1:A:2246:U:H2' | 1:A:2247:C:C6 | 2.31 | 0.65 |
| 1:A:2449:G:H2' | 1:A:2450:C:C6 | 2.31 | 0.65 |
| 1:A:2387:U:H2' | 1:A:2388:C:C6 | 2.32 | 0.64 |
| 1:A:2611:G:H3' | 1:A:2611:G:N3 | 2.11 | 0.64 |
| 1:A:2300:A:C2 | 1:A:2306:U:C5 | 2.85 | 0.64 |
| 1:A:2332:A:H3' | 1:A:2333:G:H8 | 1.60 | 0.64 |
| 1:A:2124:G:HO2' | 1:A:2125:G:H8 | 1.43 | 0.64 |
| 1:A:2316:G:H4' | 1:A:2316:G:OP1 | 1.97 | 0.64 |
| 1:A:2299:G:H1 | 1:A:2300:A:H62 | 1.32 | 0.64 |
| 1:A:2452:G:N2 | 1:A:2453:G:H1' | 2.13 | 0.64 |
| 1:A:2105:C:N4 | 1:A:2481:G:H1 | 1.96 | 0.64 |
| 1:A:2428:G:N1 | 1:A:2462:G:OP1 | 2.28 | 0.63 |
| 1:A:2115:U:O4' | 1:A:2633:A:H1' | 1.98 | 0.63 |
| 1:A:2364:A:O2' | 1:A:2365:G:H5' | 1.99 | 0.62 |
| 1:A:2419:U:H5'' | 1:A:2420:G:C5' | 2.28 | 0.62 |
| 1:A:2569:A:C2 | 1:A:2570:G:H1' | 2.34 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|----------------|--------------------------|-------------------|
| 1:A:2618:G:H2' | 1:A:2619:U:O4' | 1.99 | 0.62 |
| 1:A:2291:A:C8 | 1:A:2309:C:H5' | 2.35 | 0.62 |
| 1:A:2439:C:N4 | 1:A:2440:C:N4 | 2.47 | 0.62 |
| 1:A:2637:A:H61 | 2:B:77:PU:H3' | 1.64 | 0.61 |
| 1:A:2590:U:C2' | 1:A:2591:C:H5' | 2.29 | 0.61 |
| 1:A:2570:G:H2' | 1:A:2571:C:C6 | 2.35 | 0.61 |
| 1:A:2133:U:H4' | 1:A:2134:G:H5' | 1.82 | 0.61 |
| 1:A:2613:G:O2' | 1:A:2614:C:H5' | 1.99 | 0.61 |
| 1:A:2291:A:H5'' | 1:A:2292:C:H5' | 1.82 | 0.61 |
| 1:A:2239:C:O2' | 1:A:2240:U:H5' | 2.00 | 0.61 |
| 1:A:2073:G:OP2 | 1:A:2490:A:H5' | 2.00 | 0.61 |
| 1:A:2515:C:O2' | 1:A:2516:G:H5' | 1.99 | 0.61 |
| 1:A:2102:G:OP2 | 1:A:2537:G:OP2 | 2.19 | 0.61 |
| 1:A:2634:G:N2 | 1:A:2635:A:C5 | 2.69 | 0.61 |
| 1:A:2489:G:H2' | 1:A:2490:A:O4' | 2.00 | 0.61 |
| 1:A:2505:G:H2' | 1:A:2506:A:H5' | 1.81 | 0.61 |
| 1:A:2430:A:H62 | 1:A:2460:A:H2 | 1.49 | 0.60 |
| 1:A:2353:A:H4' | 1:A:2354:A:O5' | 2.01 | 0.60 |
| 1:A:2554:U:N1 | 1:A:2577:A:N6 | 2.48 | 0.60 |
| 1:A:2296:C:H2' | 1:A:2297:U:C6 | 2.36 | 0.60 |
| 1:A:2244:A:C6 | 1:A:2245:C:C2 | 2.90 | 0.60 |
| 1:A:2320:U:H4' | 1:A:2321:A:O4' | 2.00 | 0.60 |
| 1:A:2261:C:H2' | 1:A:2262:C:C6 | 2.36 | 0.60 |
| 1:A:2082:G:C2' | 1:A:2083:A:H5' | 2.31 | 0.60 |
| 1:A:2074:A:H4' | 1:A:2075:G:OP1 | 2.00 | 0.60 |
| 2:B:76:DA:H2'' | 2:B:77:PU:OP1 | 2.01 | 0.60 |
| 1:A:2250:G:O2' | 1:A:2251:G:H5' | 2.01 | 0.60 |
| 1:A:2299:G:N1 | 1:A:2300:A:C5 | 2.70 | 0.60 |
| 1:A:2625:C:O5' | 1:A:2625:C:H6 | 1.84 | 0.59 |
| 1:A:2269:C:H2' | 1:A:2270:G:O4' | 2.02 | 0.59 |
| 1:A:2447:A:HO2' | 1:A:2448:U:H6 | 1.51 | 0.59 |
| 1:A:2104:C:N4 | 1:A:2105:C:H5 | 2.01 | 0.59 |
| 1:A:2471:G:O2' | 1:A:2472:C:H5' | 2.03 | 0.59 |
| 1:A:2430:A:N6 | 1:A:2460:A:H2 | 1.99 | 0.59 |
| 1:A:2490:A:N6 | 1:A:2491:G:O6 | 2.36 | 0.59 |
| 1:A:2492:U:O2' | 1:A:2493:C:H5' | 2.03 | 0.59 |
| 1:A:2495:U:O2' | 1:A:2496:C:H5' | 2.03 | 0.59 |
| 1:A:2448:U:O2' | 1:A:2449:G:H5' | 2.03 | 0.59 |
| 1:A:2451:G:H2' | 1:A:2451:G:N3 | 2.18 | 0.59 |
| 1:A:2637:A:N6 | 2:B:77:PU:H3' | 2.18 | 0.58 |
| 1:A:2495:U:H2' | 1:A:2496:C:H5' | 1.83 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:A:2504:A:H2' | 1:A:2505:G:O4' | 2.03 | 0.58 |
| 1:A:2405:C:O2' | 1:A:2406:U:H5' | 2.03 | 0.58 |
| 1:A:2486:A:N1 | 2:B:77:PU:HE2 | 2.17 | 0.58 |
| 1:A:2437:A:C2' | 1:A:2437:A:N3 | 2.67 | 0.58 |
| 1:A:2346:C:H6 | 1:A:2346:C:O5' | 1.87 | 0.58 |
| 1:A:2345:A:OP1 | 1:A:2346:C:H5 | 1.87 | 0.57 |
| 1:A:2271:G:H4' | 1:A:2272:G:OP1 | 2.02 | 0.57 |
| 1:A:2333:G:O2' | 1:A:2334:C:H5' | 2.04 | 0.57 |
| 1:A:2268:C:H2' | 1:A:2269:C:C6 | 2.39 | 0.57 |
| 1:A:2114:C:H2' | 1:A:2115:U:H6 | 1.69 | 0.57 |
| 1:A:2491:G:C5 | 1:A:2492:U:C5 | 2.92 | 0.57 |
| 1:A:2064:U:H2' | 1:A:2065:C:C6 | 2.39 | 0.57 |
| 1:A:2086:C:O2' | 1:A:2087:C:H5' | 2.04 | 0.57 |
| 1:A:2090:G:H4' | 1:A:2091:G:OP1 | 2.05 | 0.57 |
| 1:A:2245:C:C2 | 1:A:2246:U:C5 | 2.91 | 0.57 |
| 1:A:2252:A:H2' | 1:A:2253:G:O4' | 2.04 | 0.57 |
| 1:A:2659:U:O5' | 1:A:2659:U:H6 | 1.88 | 0.57 |
| 1:A:2566:A:H2' | 1:A:2567:G:H5' | 1.87 | 0.57 |
| 1:A:2107:U:H1' | 1:A:2484:U:O4 | 2.05 | 0.57 |
| 1:A:2416:G:H2' | 1:A:2417:C:H6 | 1.69 | 0.57 |
| 1:A:2641:C:O2' | 1:A:2642:G:H5' | 2.04 | 0.57 |
| 1:A:2106:C:H1' | 1:A:2484:U:O2 | 2.05 | 0.57 |
| 1:A:2549:C:C2 | 1:A:2606:G:N2 | 2.73 | 0.56 |
| 1:A:2630:G:H2' | 1:A:2632:G:OP2 | 2.04 | 0.56 |
| 1:A:2366:C:H4' | 1:A:2370:A:N6 | 2.21 | 0.56 |
| 1:A:2372:A:H2' | 1:A:2373:U:H6 | 1.70 | 0.56 |
| 1:A:2324:G:H2' | 1:A:2325:C:C6 | 2.39 | 0.56 |
| 1:A:2273:C:O2' | 1:A:2274:A:H5' | 2.04 | 0.56 |
| 1:A:2618:G:C2 | 1:A:2619:U:H1' | 2.40 | 0.56 |
| 1:A:2088:C:H2' | 1:A:2089:A:H8 | 1.70 | 0.56 |
| 1:A:2311:A:N6 | 1:A:2312:G:C6 | 2.74 | 0.56 |
| 1:A:2473:U:H5' | 1:A:2474:A:C5' | 2.35 | 0.56 |
| 1:A:2245:C:O2 | 1:A:2259:C:N4 | 2.39 | 0.56 |
| 1:A:2549:C:N4 | 1:A:2606:G:N1 | 2.53 | 0.56 |
| 1:A:2251:G:C6 | 1:A:2252:A:C6 | 2.94 | 0.56 |
| 1:A:2584:G:H2' | 1:A:2585:G:H8 | 1.69 | 0.55 |
| 1:A:2064:U:H4' | 1:A:2652:U:O3' | 2.07 | 0.55 |
| 1:A:2366:C:O5' | 1:A:2366:C:H6 | 1.89 | 0.55 |
| 1:A:2508:C:H2' | 1:A:2509:A:H8 | 1.71 | 0.55 |
| 1:A:2273:C:H2' | 1:A:2274:A:C8 | 2.41 | 0.55 |
| 1:A:2111:G:H1 | 1:A:2476:C:H42 | 1.53 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:A:2526:C:C6 | 1:A:2526:C:C3' | 2.90 | 0.55 |
| 1:A:2438:G:C6 | 1:A:2439:C:N3 | 2.75 | 0.55 |
| 1:A:2613:G:H2' | 1:A:2614:C:C6 | 2.41 | 0.55 |
| 1:A:2269:C:H2' | 1:A:2270:G:H5' | 1.88 | 0.55 |
| 1:A:2326:U:H4' | 1:A:2412:G:H4' | 1.88 | 0.55 |
| 1:A:2246:U:O2' | 1:A:2247:C:O4' | 2.25 | 0.55 |
| 1:A:2114:C:H2' | 1:A:2115:U:C6 | 2.42 | 0.55 |
| 1:A:2104:C:C4 | 1:A:2105:C:H5 | 2.24 | 0.55 |
| 1:A:2337:G:N1 | 1:A:2348:C:C4 | 2.75 | 0.55 |
| 1:A:2399:G:H4' | 1:A:2428:G:OP1 | 2.07 | 0.55 |
| 1:A:2453:G:N2 | 1:A:2454:C:C2 | 2.74 | 0.55 |
| 1:A:2525:G:H4' | 1:A:2526:C:OP1 | 2.07 | 0.55 |
| 1:A:2588:G:H1' | 1:A:2617:G:N3 | 2.21 | 0.55 |
| 1:A:2617:G:C2' | 1:A:2618:G:H5' | 2.37 | 0.55 |
| 1:A:2111:G:O2' | 1:A:2112:A:H5' | 2.07 | 0.55 |
| 1:A:2133:U:H4' | 1:A:2134:G:C5' | 2.36 | 0.55 |
| 1:A:2075:G:H2' | 1:A:2075:G:N3 | 2.20 | 0.55 |
| 1:A:2447:A:O2' | 1:A:2448:U:H6 | 1.90 | 0.54 |
| 1:A:2085:A:C6 | 1:A:2660:G:C2 | 2.95 | 0.54 |
| 1:A:2554:U:C6 | 1:A:2577:A:N6 | 2.76 | 0.54 |
| 1:A:2090:G:O5' | 1:A:2090:G:H8 | 1.91 | 0.54 |
| 1:A:2365:G:O2' | 1:A:2370:A:N1 | 2.35 | 0.54 |
| 1:A:2251:G:H2' | 1:A:2252:A:H8 | 1.71 | 0.54 |
| 1:A:2635:A:C5 | 1:A:2636:C:C4 | 2.96 | 0.54 |
| 1:A:2379:G:H4' | 1:A:2380:A:O5' | 2.08 | 0.54 |
| 1:A:2090:G:C8 | 1:A:2090:G:H3' | 2.43 | 0.54 |
| 1:A:2583:A:C2 | 1:A:2584:G:C4 | 2.95 | 0.54 |
| 1:A:2578:G:H8 | 1:A:2578:G:H5' | 1.72 | 0.54 |
| 1:A:2586:U:H3 | 1:A:2592:G:H22 | 1.55 | 0.54 |
| 1:A:2119:C:O2' | 1:A:2120:U:H5' | 2.08 | 0.54 |
| 1:A:2621:U:C5 | 1:A:2643:G:N2 | 2.76 | 0.54 |
| 1:A:2445:U:H2' | 1:A:2446:G:H8 | 1.70 | 0.54 |
| 1:A:2509:A:N6 | 1:A:2564:G:C2 | 2.76 | 0.54 |
| 1:A:2494:G:C2' | 1:A:2495:U:H5' | 2.35 | 0.54 |
| 1:A:2299:G:C6 | 1:A:2300:A:C5 | 2.97 | 0.53 |
| 1:A:2070:G:H2' | 1:A:2072:G:OP1 | 2.08 | 0.53 |
| 1:A:2650:U:O2' | 1:A:2651:C:O4' | 2.26 | 0.53 |
| 1:A:2251:G:C2 | 1:A:2252:A:C4 | 2.96 | 0.53 |
| 1:A:2346:C:C2 | 1:A:2347:C:C5 | 2.97 | 0.53 |
| 1:A:2106:C:H1' | 1:A:2484:U:H3 | 1.73 | 0.53 |
| 1:A:2526:C:H6 | 1:A:2526:C:C5' | 2.20 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:A:2456:A:H2' | 1:A:2457:U:H6 | 1.72 | 0.53 |
| 1:A:2492:U:H2' | 1:A:2493:C:H5' | 1.89 | 0.53 |
| 1:A:2554:U:O4' | 1:A:2577:A:N6 | 2.33 | 0.53 |
| 1:A:2548:C:C2 | 1:A:2549:C:C5 | 2.96 | 0.53 |
| 1:A:2249:G:N1 | 1:A:2253:G:C6 | 2.77 | 0.53 |
| 1:A:2439:C:N3 | 1:A:2440:C:C5 | 2.76 | 0.53 |
| 1:A:2551:C:C2 | 1:A:2552:C:C5 | 2.97 | 0.53 |
| 1:A:2619:U:C2' | 1:A:2620:U:C5 | 2.90 | 0.53 |
| 1:A:2621:U:C4 | 1:A:2622:A:N7 | 2.77 | 0.53 |
| 1:A:2449:G:C5 | 1:A:2450:C:C4 | 2.96 | 0.53 |
| 1:A:2307:A:C2 | 1:A:2308:U:N3 | 2.77 | 0.53 |
| 1:A:2514:U:O5' | 1:A:2514:U:H6 | 1.91 | 0.53 |
| 1:A:2432:C:O5' | 1:A:2432:C:H6 | 1.91 | 0.53 |
| 1:A:2246:U:C4 | 1:A:2256:G:N2 | 2.77 | 0.53 |
| 1:A:2064:U:H4' | 1:A:2653:A:P | 2.49 | 0.53 |
| 1:A:2285:G:H2' | 1:A:2286:G:H8 | 1.73 | 0.52 |
| 1:A:2104:C:N3 | 1:A:2485:A:N6 | 2.47 | 0.52 |
| 1:A:2102:G:N7 | 1:A:2538:A:O4' | 2.42 | 0.52 |
| 1:A:2316:G:C6 | 1:A:2462:G:C2 | 2.97 | 0.52 |
| 1:A:2492:U:N3 | 1:A:2493:C:C4 | 2.78 | 0.52 |
| 1:A:2065:C:H6 | 1:A:2065:C:O5' | 1.92 | 0.52 |
| 1:A:2447:A:C4 | 1:A:2448:U:C5 | 2.97 | 0.52 |
| 1:A:2449:G:C5 | 1:A:2450:C:C5 | 2.97 | 0.52 |
| 1:A:2438:G:C6 | 1:A:2439:C:C4 | 2.98 | 0.52 |
| 1:A:2298:C:H2' | 1:A:2299:G:O4' | 2.10 | 0.52 |
| 1:A:2104:C:O2 | 1:A:2485:A:N1 | 2.43 | 0.52 |
| 1:A:2071:C:O2' | 1:A:2534:C:H4' | 2.09 | 0.52 |
| 1:A:2575:C:C4 | 1:A:2576:A:C5 | 2.98 | 0.52 |
| 1:A:2645:U:O5' | 1:A:2645:U:H6 | 1.93 | 0.52 |
| 1:A:2410:G:H2' | 1:A:2411:C:C6 | 2.44 | 0.52 |
| 1:A:2554:U:C5 | 1:A:2576:A:C5 | 2.97 | 0.52 |
| 1:A:2555:C:N3 | 1:A:2602:G:C8 | 2.78 | 0.52 |
| 1:A:2338:G:N1 | 1:A:2347:C:C4 | 2.77 | 0.52 |
| 1:A:2406:U:C4 | 1:A:2407:G:N7 | 2.77 | 0.52 |
| 1:A:2273:C:H2' | 1:A:2274:A:H8 | 1.75 | 0.52 |
| 1:A:2357:G:C6 | 1:A:2358:U:C4 | 2.98 | 0.52 |
| 1:A:2397:G:C5 | 1:A:2465:A:C6 | 2.98 | 0.52 |
| 1:A:2245:C:C2 | 1:A:2246:U:H5 | 2.27 | 0.52 |
| 1:A:2250:G:C6 | 1:A:2251:G:C4 | 2.98 | 0.52 |
| 1:A:2490:A:H2' | 1:A:2491:G:C8 | 2.45 | 0.52 |
| 1:A:2414:A:O5' | 1:A:2414:A:H8 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:A:2242:U:C2 | 1:A:2257:G:C2 | 2.98 | 0.52 |
| 1:A:2527:U:C4 | 1:A:2528:U:C4 | 2.97 | 0.52 |
| 1:A:2551:C:C4 | 1:A:2604:A:N1 | 2.78 | 0.52 |
| 1:A:2136:G:N2 | 1:A:2239:C:O2 | 2.42 | 0.52 |
| 1:A:2261:C:H2' | 1:A:2262:C:H6 | 1.74 | 0.52 |
| 1:A:2365:G:C2 | 1:A:2422:U:N3 | 2.78 | 0.52 |
| 1:A:2574:G:C4 | 1:A:2575:C:C5 | 2.98 | 0.52 |
| 1:A:2558:G:C6 | 1:A:2559:C:C4 | 2.97 | 0.52 |
| 1:A:2512:U:O5' | 1:A:2512:U:H6 | 1.92 | 0.52 |
| 1:A:2492:U:N3 | 1:A:2493:C:N3 | 2.57 | 0.52 |
| 1:A:2073:G:C6 | 1:A:2607:U:C2 | 2.98 | 0.52 |
| 1:A:2650:U:O2 | 1:A:2650:U:O2' | 2.28 | 0.52 |
| 1:A:2287:C:C2' | 1:A:2288:G:H5' | 2.39 | 0.52 |
| 1:A:2507:G:H2' | 1:A:2508:C:OP1 | 2.10 | 0.52 |
| 1:A:2619:U:O2' | 2:B:77:PU:H2' | 2.09 | 0.51 |
| 1:A:2113:G:C6 | 1:A:2472:C:N3 | 2.78 | 0.51 |
| 1:A:2297:U:C2 | 1:A:2312:G:N2 | 2.79 | 0.51 |
| 1:A:2455:A:C6 | 1:A:2456:A:C5 | 2.97 | 0.51 |
| 1:A:2129:U:H2' | 1:A:2130:C:C6 | 2.45 | 0.51 |
| 1:A:2251:G:C4 | 1:A:2252:A:C8 | 2.99 | 0.51 |
| 1:A:2630:G:N1 | 1:A:2634:G:C6 | 2.78 | 0.51 |
| 1:A:2657:G:O2' | 1:A:2658:G:O4' | 2.28 | 0.51 |
| 1:A:2064:U:H5' | 1:A:2652:U:O3' | 2.10 | 0.51 |
| 1:A:2365:G:N3 | 1:A:2370:A:C2 | 2.79 | 0.51 |
| 1:A:2559:C:C4 | 1:A:2560:C:C5 | 2.99 | 0.51 |
| 1:A:2472:C:O2' | 1:A:2634:G:H4' | 2.10 | 0.51 |
| 1:A:2630:G:H22 | 1:A:2633:A:P | 2.33 | 0.51 |
| 1:A:2085:A:C6 | 1:A:2660:G:N1 | 2.79 | 0.51 |
| 1:A:2585:G:N2 | 1:A:2594:C:H1' | 2.25 | 0.51 |
| 1:A:2314:G:C2' | 1:A:2315:C:H5' | 2.39 | 0.51 |
| 1:A:2385:G:N2 | 1:A:2386:U:C2 | 2.79 | 0.51 |
| 1:A:2097:G:N2 | 1:A:2098:C:H1' | 2.26 | 0.51 |
| 1:A:2542:C:C2 | 1:A:2618:G:C2 | 2.98 | 0.51 |
| 1:A:2251:G:C6 | 1:A:2252:A:C5 | 2.99 | 0.51 |
| 1:A:2497:A:C6 | 1:A:2498:C:C4 | 2.98 | 0.51 |
| 1:A:2128:G:C6 | 1:A:2129:U:C4 | 2.98 | 0.51 |
| 1:A:2134:G:C6 | 1:A:2258:A:C8 | 2.98 | 0.51 |
| 1:A:2408:A:O2' | 1:A:2409:C:O5' | 2.28 | 0.51 |
| 1:A:2551:C:N3 | 1:A:2552:C:C4 | 2.79 | 0.51 |
| 1:A:2311:A:C6 | 1:A:2312:G:C5 | 2.98 | 0.51 |
| 1:A:2473:U:H4' | 1:A:2475:C:OP1 | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|----------------|--------------------------|-------------------|
| 1:A:2316:G:C5 | 1:A:2462:G:C2 | 2.98 | 0.51 |
| 1:A:2548:C:O2' | 1:A:2549:C:O4' | 2.28 | 0.51 |
| 1:A:2593:C:C2' | 1:A:2594:C:H5' | 2.40 | 0.51 |
| 1:A:2594:C:N3 | 1:A:2595:U:C5 | 2.78 | 0.51 |
| 1:A:2357:G:C6 | 1:A:2358:U:N3 | 2.79 | 0.51 |
| 1:A:2582:G:C2 | 1:A:2583:A:C8 | 2.99 | 0.51 |
| 1:A:2407:G:O2' | 1:A:2408:A:H5' | 2.11 | 0.51 |
| 1:A:2105:C:C4 | 1:A:2481:G:N2 | 2.77 | 0.51 |
| 1:A:2316:G:H2' | 1:A:2427:C:C4 | 2.43 | 0.51 |
| 1:A:2135:A:C2 | 1:A:2136:G:C5 | 2.98 | 0.51 |
| 1:A:2253:G:N3 | 1:A:2254:G:C8 | 2.79 | 0.51 |
| 1:A:2554:U:C2 | 1:A:2577:A:C6 | 2.99 | 0.51 |
| 1:A:2096:A:N7 | 1:A:2539:U:C4 | 2.78 | 0.51 |
| 1:A:2562:G:C6 | 1:A:2563:U:N3 | 2.79 | 0.51 |
| 1:A:2307:A:C2 | 1:A:2308:U:C4 | 2.99 | 0.51 |
| 1:A:2501:G:C5 | 1:A:2502:C:C5 | 2.99 | 0.51 |
| 1:A:2416:G:N2 | 1:A:2417:C:C2 | 2.79 | 0.51 |
| 1:A:2582:G:C6 | 1:A:2601:A:N7 | 2.79 | 0.51 |
| 1:A:2123:A:H3' | 1:A:2124:G:H8 | 1.75 | 0.51 |
| 1:A:2296:C:H2' | 1:A:2297:U:H6 | 1.75 | 0.50 |
| 1:A:2105:C:N4 | 1:A:2536:C:C4 | 2.75 | 0.50 |
| 1:A:2260:A:C5 | 1:A:2261:C:C5 | 2.99 | 0.50 |
| 1:A:2113:G:C6 | 1:A:2114:C:C4 | 2.99 | 0.50 |
| 1:A:2632:G:H8 | 1:A:2632:G:O5' | 1.94 | 0.50 |
| 1:A:2494:G:C6 | 1:A:2529:G:C2 | 3.00 | 0.50 |
| 1:A:2451:G:C2 | 1:A:2452:G:C8 | 2.99 | 0.50 |
| 1:A:2350:G:O2' | 1:A:2351:C:H5' | 2.11 | 0.50 |
| 1:A:2105:C:C5 | 1:A:2485:A:N6 | 2.79 | 0.50 |
| 1:A:2106:C:H2' | 1:A:2107:U:C1' | 2.41 | 0.50 |
| 1:A:2618:G:C6 | 1:A:2619:U:C2 | 2.99 | 0.50 |
| 1:A:2416:G:H2' | 1:A:2417:C:C6 | 2.47 | 0.50 |
| 1:A:2439:C:H42 | 1:A:2440:C:N4 | 2.08 | 0.50 |
| 1:A:2574:G:C5 | 1:A:2575:C:C5 | 2.99 | 0.50 |
| 1:A:2393:C:H6 | 1:A:2393:C:O5' | 1.94 | 0.50 |
| 1:A:2285:G:H2' | 1:A:2286:G:C8 | 2.46 | 0.50 |
| 1:A:2620:U:H5'' | 1:A:2621:U:OP1 | 2.11 | 0.50 |
| 1:A:2406:U:C2 | 1:A:2407:G:C8 | 2.99 | 0.50 |
| 1:A:2253:G:H8 | 1:A:2253:G:OP2 | 1.95 | 0.50 |
| 1:A:2255:A:C6 | 1:A:2256:G:C5 | 2.99 | 0.50 |
| 1:A:2337:G:C6 | 1:A:2348:C:N4 | 2.79 | 0.50 |
| 1:A:2447:A:O2' | 1:A:2448:U:O4' | 2.29 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:A:2377:U:H6 | 1:A:2377:U:O5' | 1.93 | 0.50 |
| 1:A:2384:U:O5' | 1:A:2384:U:H6 | 1.93 | 0.50 |
| 1:A:2442:G:C6 | 1:A:2451:G:C5 | 3.00 | 0.50 |
| 1:A:2105:C:N4 | 1:A:2481:G:C2 | 2.79 | 0.50 |
| 1:A:2629:C:C2 | 1:A:2634:G:N2 | 2.75 | 0.50 |
| 1:A:2527:U:H2' | 1:A:2528:U:O4' | 2.12 | 0.50 |
| 1:A:2416:G:C2 | 1:A:2417:C:C2 | 2.99 | 0.50 |
| 1:A:2297:U:N3 | 1:A:2312:G:C2 | 2.79 | 0.50 |
| 1:A:2473:U:C5' | 1:A:2474:A:H5' | 2.42 | 0.50 |
| 1:A:2478:U:C2 | 1:A:2479:A:C8 | 3.00 | 0.50 |
| 1:A:2526:C:C6 | 1:A:2526:C:H3' | 2.46 | 0.50 |
| 1:A:2526:C:H6 | 1:A:2526:C:H5' | 1.77 | 0.50 |
| 1:A:2126:C:C4 | 1:A:2127:U:C4 | 2.99 | 0.50 |
| 1:A:2372:A:H2' | 1:A:2373:U:C6 | 2.46 | 0.50 |
| 1:A:2489:G:C6 | 1:A:2534:C:N4 | 2.79 | 0.50 |
| 1:A:2088:C:H2' | 1:A:2089:A:C8 | 2.46 | 0.50 |
| 1:A:2447:A:N3 | 1:A:2448:U:C6 | 2.80 | 0.50 |
| 1:A:2332:A:H5' | 1:A:2333:G:OP2 | 2.11 | 0.50 |
| 1:A:2088:C:C2 | 1:A:2657:G:C2 | 3.00 | 0.49 |
| 1:A:2338:G:C6 | 1:A:2347:C:N4 | 2.80 | 0.49 |
| 1:A:2582:G:C5 | 1:A:2601:A:C5 | 3.00 | 0.49 |
| 1:A:2106:C:H2' | 1:A:2107:U:O4' | 2.12 | 0.49 |
| 1:A:2113:G:N1 | 1:A:2114:C:C2 | 2.81 | 0.49 |
| 1:A:2496:C:C2 | 1:A:2497:A:C8 | 2.99 | 0.49 |
| 1:A:2446:G:H2' | 1:A:2447:A:C8 | 2.42 | 0.49 |
| 1:A:2593:C:O2' | 1:A:2594:C:H5' | 2.11 | 0.49 |
| 1:A:2582:G:C6 | 1:A:2601:A:C8 | 3.00 | 0.49 |
| 1:A:2482:G:C4 | 1:A:2536:C:C4 | 2.99 | 0.49 |
| 1:A:2114:C:C2' | 1:A:2115:U:H5' | 2.41 | 0.49 |
| 1:A:2087:C:C2' | 1:A:2088:C:H5' | 2.43 | 0.49 |
| 1:A:2524:G:C6 | 1:A:2525:G:C6 | 3.00 | 0.49 |
| 1:A:2276:U:H2' | 1:A:2277:U:C6 | 2.48 | 0.49 |
| 1:A:2499:U:H2' | 1:A:2500:C:H6 | 1.77 | 0.49 |
| 1:A:2286:G:C6 | 1:A:2287:C:C4 | 3.00 | 0.49 |
| 1:A:2486:A:O2' | 2:B:76:DA:H2' | 2.13 | 0.49 |
| 1:A:2549:C:C2 | 1:A:2550:U:C6 | 3.00 | 0.49 |
| 1:A:2574:G:C6 | 1:A:2575:C:C4 | 3.00 | 0.49 |
| 1:A:2626:C:O2' | 1:A:2627:G:O4' | 2.25 | 0.49 |
| 1:A:2298:C:C2 | 1:A:2311:A:C2 | 3.01 | 0.49 |
| 1:A:2298:C:O2' | 1:A:2299:G:H5' | 2.11 | 0.49 |
| 1:A:2114:C:H2' | 1:A:2115:U:O4' | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|----------------|--------------------------|-------------------|
| 1:A:2587:U:C2' | 1:A:2589:U:H5 | 2.26 | 0.49 |
| 1:A:2628:U:H3 | 1:A:2635:A:N6 | 2.11 | 0.49 |
| 1:A:2599:A:C5 | 1:A:2600:A:C6 | 3.01 | 0.49 |
| 1:A:2609:G:C6 | 1:A:2610:U:N3 | 2.81 | 0.49 |
| 1:A:2578:G:H2' | 1:A:2579:G:H8 | 1.77 | 0.49 |
| 1:A:2104:C:C4 | 1:A:2105:C:C5 | 3.01 | 0.49 |
| 1:A:2241:C:HO2' | 1:A:2242:U:H6 | 1.60 | 0.49 |
| 1:A:2634:G:N2 | 1:A:2635:A:C6 | 2.81 | 0.49 |
| 1:A:2513:A:C8 | 1:A:2564:G:N7 | 2.81 | 0.49 |
| 1:A:2347:C:C2 | 1:A:2348:C:C5 | 3.00 | 0.49 |
| 1:A:2516:G:HO2' | 1:A:2517:A:H8 | 1.61 | 0.49 |
| 1:A:2584:G:C2 | 1:A:2585:G:N7 | 2.80 | 0.49 |
| 1:A:2365:G:C2 | 1:A:2422:U:C2 | 3.01 | 0.49 |
| 1:A:2251:G:C5 | 1:A:2252:A:C5 | 3.01 | 0.48 |
| 1:A:2253:G:O2' | 1:A:2254:G:O5' | 2.31 | 0.48 |
| 1:A:2659:U:O2' | 1:A:2660:G:O5' | 2.30 | 0.48 |
| 1:A:2584:G:H2' | 1:A:2585:G:C8 | 2.48 | 0.48 |
| 1:A:2289:G:N2 | 1:A:2309:C:C5 | 2.82 | 0.48 |
| 1:A:2250:G:C5 | 1:A:2251:G:C5 | 3.01 | 0.48 |
| 1:A:2114:C:C2 | 1:A:2471:G:N2 | 2.76 | 0.48 |
| 1:A:2575:C:N4 | 1:A:2576:A:C6 | 2.81 | 0.48 |
| 1:A:2638:G:H2' | 1:A:2639:G:H8 | 1.78 | 0.48 |
| 1:A:2250:G:H2' | 1:A:2251:G:O5' | 2.13 | 0.48 |
| 1:A:2346:C:H2' | 1:A:2347:C:H6 | 1.77 | 0.48 |
| 1:A:2583:A:C2 | 1:A:2584:G:N9 | 2.81 | 0.48 |
| 1:A:2452:G:N2 | 1:A:2453:G:C1' | 2.76 | 0.48 |
| 1:A:2365:G:N3 | 1:A:2370:A:H2 | 2.11 | 0.48 |
| 1:A:2359:G:C6 | 1:A:2360:C:N4 | 2.81 | 0.48 |
| 1:A:2251:G:H2' | 1:A:2252:A:C8 | 2.49 | 0.48 |
| 1:A:2113:G:O6 | 1:A:2472:C:N3 | 2.46 | 0.48 |
| 1:A:2337:G:C2 | 1:A:2348:C:N3 | 2.81 | 0.48 |
| 1:A:2348:C:H2' | 1:A:2349:G:H8 | 1.78 | 0.48 |
| 1:A:2449:G:C6 | 1:A:2450:C:C4 | 3.01 | 0.48 |
| 1:A:2449:G:C6 | 1:A:2450:C:N3 | 2.81 | 0.48 |
| 1:A:2592:G:O2' | 1:A:2593:C:H5' | 2.13 | 0.48 |
| 1:A:2246:U:C2 | 1:A:2247:C:C5 | 3.02 | 0.48 |
| 1:A:2249:G:C2 | 1:A:2253:G:C6 | 3.01 | 0.48 |
| 1:A:2634:G:H2' | 1:A:2635:A:H8 | 1.77 | 0.48 |
| 1:A:2495:U:H2' | 1:A:2496:C:C5' | 2.44 | 0.48 |
| 1:A:2439:C:C4 | 1:A:2440:C:C5 | 3.01 | 0.48 |
| 1:A:2127:U:O2' | 1:A:2128:G:O4' | 2.32 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:A:2106:C:H1' | 1:A:2484:U:C2 | 2.49 | 0.48 |
| 1:A:2282:U:O2' | 1:A:2283:G:OP1 | 2.30 | 0.48 |
| 1:A:2656:G:O2' | 1:A:2657:G:O4' | 2.32 | 0.48 |
| 1:A:2130:C:O2' | 1:A:2131:G:O4' | 2.31 | 0.48 |
| 1:A:2283:G:N3 | 1:A:2283:G:O4' | 2.47 | 0.48 |
| 1:A:2649:A:H8 | 1:A:2649:A:OP2 | 1.97 | 0.48 |
| 1:A:2490:A:C6 | 1:A:2491:G:C5 | 3.02 | 0.47 |
| 1:A:2610:U:O2' | 1:A:2613:G:N7 | 2.40 | 0.47 |
| 1:A:2103:A:N7 | 1:A:2538:A:C6 | 2.82 | 0.47 |
| 1:A:2244:A:C5 | 1:A:2245:C:C2 | 3.03 | 0.47 |
| 1:A:2250:G:C6 | 1:A:2251:G:C5 | 3.03 | 0.47 |
| 1:A:2254:G:N2 | 1:A:2255:A:C4 | 2.82 | 0.47 |
| 1:A:2406:U:N3 | 1:A:2407:G:N7 | 2.61 | 0.47 |
| 1:A:2556:C:C4 | 1:A:2557:U:C4 | 3.01 | 0.47 |
| 1:A:2486:A:C6 | 2:B:77:PU:HE2 | 2.50 | 0.47 |
| 1:A:2541:U:O4 | 1:A:2618:G:O6 | 2.32 | 0.47 |
| 1:A:2135:A:C2 | 1:A:2136:G:C8 | 3.01 | 0.47 |
| 1:A:2471:G:O2' | 1:A:2633:A:N1 | 2.45 | 0.47 |
| 1:A:2407:G:H2' | 1:A:2408:A:C8 | 2.49 | 0.47 |
| 1:A:2539:U:O2' | 1:A:2540:G:O5' | 2.32 | 0.47 |
| 1:A:2303:A:N1 | 1:A:2304:G:C4 | 2.83 | 0.47 |
| 1:A:2303:A:C2 | 1:A:2304:G:N9 | 2.82 | 0.47 |
| 1:A:2248:C:C2 | 1:A:2254:G:C2 | 3.02 | 0.47 |
| 1:A:2346:C:N3 | 1:A:2347:C:C5 | 2.82 | 0.47 |
| 1:A:2132:C:H6 | 1:A:2132:C:O5' | 1.96 | 0.47 |
| 1:A:2277:U:C4 | 1:A:2278:U:C4 | 3.03 | 0.47 |
| 1:A:2585:G:N1 | 1:A:2594:C:C2 | 2.82 | 0.47 |
| 1:A:2460:A:C5 | 1:A:2461:U:C4 | 3.03 | 0.47 |
| 1:A:2064:U:H4' | 1:A:2653:A:OP1 | 2.13 | 0.47 |
| 1:A:2256:G:H2' | 1:A:2257:G:C5' | 2.38 | 0.47 |
| 1:A:2513:A:C4 | 1:A:2564:G:C8 | 3.02 | 0.47 |
| 1:A:2547:C:O2' | 1:A:2548:C:O4' | 2.33 | 0.47 |
| 1:A:2252:A:C4 | 1:A:2253:G:H1' | 2.48 | 0.47 |
| 1:A:2502:C:O2' | 1:A:2503:A:H5' | 2.14 | 0.47 |
| 1:A:2449:G:H2' | 1:A:2450:C:H6 | 1.77 | 0.47 |
| 1:A:2125:G:O2' | 1:A:2126:C:H5' | 2.14 | 0.47 |
| 1:A:2602:G:O2' | 1:A:2603:G:O4' | 2.32 | 0.47 |
| 1:A:2103:A:N7 | 1:A:2538:A:N1 | 2.62 | 0.47 |
| 1:A:2617:G:N2 | 1:A:2618:G:H1' | 2.30 | 0.47 |
| 1:A:2496:C:H1' | 1:A:2527:U:C4 | 2.50 | 0.47 |
| 1:A:2519:C:C2 | 1:A:2520:G:C8 | 3.03 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|----------------|--------------------------|-------------------|
| 1:A:2647:C:O5' | 1:A:2647:C:H6 | 1.98 | 0.47 |
| 1:A:2287:C:H2' | 1:A:2288:G:H5' | 1.95 | 0.47 |
| 1:A:2288:G:H2' | 1:A:2289:G:O4' | 2.15 | 0.47 |
| 1:A:2238:A:C2 | 1:A:2239:C:C6 | 3.02 | 0.47 |
| 1:A:2260:A:C6 | 1:A:2261:C:C4 | 3.02 | 0.47 |
| 1:A:2335:C:H2' | 1:A:2336:G:C8 | 2.50 | 0.47 |
| 1:A:2300:A:N6 | 1:A:2307:A:OP2 | 2.31 | 0.46 |
| 1:A:2644:C:HO2' | 1:A:2645:U:P | 2.37 | 0.46 |
| 1:A:2269:C:O2' | 1:A:2270:G:H5' | 2.15 | 0.46 |
| 1:A:2597:U:C6 | 1:A:2597:U:C3' | 2.98 | 0.46 |
| 1:A:2621:U:C2 | 1:A:2622:A:C8 | 3.04 | 0.46 |
| 1:A:2265:U:C2 | 1:A:2266:A:N7 | 2.84 | 0.46 |
| 1:A:2476:C:O2' | 1:A:2477:C:H5' | 2.16 | 0.46 |
| 1:A:2436:U:N3 | 1:A:2456:A:C2 | 2.83 | 0.46 |
| 1:A:2075:G:C6 | 1:A:2076:U:C4 | 3.03 | 0.46 |
| 1:A:2602:G:O2' | 1:A:2602:G:N3 | 2.49 | 0.46 |
| 1:A:2562:G:C6 | 1:A:2563:U:C4 | 3.03 | 0.46 |
| 1:A:2073:G:C2 | 1:A:2607:U:C5 | 3.03 | 0.46 |
| 1:A:2405:C:H2' | 1:A:2406:U:C6 | 2.50 | 0.46 |
| 1:A:2405:C:H2' | 1:A:2406:U:H6 | 1.79 | 0.46 |
| 1:A:2490:A:C6 | 1:A:2491:G:C6 | 3.03 | 0.46 |
| 1:A:2590:U:C5 | 1:A:2591:C:C6 | 3.03 | 0.46 |
| 1:A:2574:G:C6 | 1:A:2575:C:N4 | 2.82 | 0.46 |
| 1:A:2566:A:C2' | 1:A:2567:G:H5' | 2.44 | 0.46 |
| 1:A:2246:U:C4 | 1:A:2256:G:N1 | 2.83 | 0.46 |
| 1:A:2570:G:H2' | 1:A:2571:C:H6 | 1.79 | 0.46 |
| 1:A:2096:A:C8 | 1:A:2539:U:N3 | 2.83 | 0.46 |
| 1:A:2294:C:H2' | 1:A:2295:G:C8 | 2.51 | 0.46 |
| 1:A:2101:A:O2' | 1:A:2102:G:OP1 | 2.29 | 0.46 |
| 1:A:2549:C:N3 | 1:A:2606:G:C2 | 2.83 | 0.46 |
| 1:A:2595:U:C2 | 1:A:2596:A:C8 | 3.03 | 0.46 |
| 1:A:2244:A:N7 | 1:A:2245:C:C4 | 2.84 | 0.46 |
| 1:A:2253:G:C2 | 1:A:2254:G:C8 | 3.04 | 0.46 |
| 1:A:2254:G:C2 | 1:A:2255:A:C8 | 3.03 | 0.46 |
| 1:A:2513:A:N9 | 1:A:2564:G:C8 | 2.83 | 0.46 |
| 1:A:2524:G:C6 | 1:A:2525:G:N1 | 2.84 | 0.46 |
| 1:A:2597:U:C6 | 1:A:2597:U:H3' | 2.50 | 0.46 |
| 1:A:2079:G:H2' | 1:A:2080:G:O4' | 2.15 | 0.46 |
| 1:A:2594:C:C2' | 1:A:2595:U:H5' | 2.45 | 0.46 |
| 1:A:2335:C:O2' | 1:A:2336:G:H5' | 2.16 | 0.46 |
| 1:A:2249:G:C2 | 1:A:2253:G:C5 | 3.03 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:A:2090:G:C3' | 1:A:2090:G:C8 | 3.00 | 0.45 |
| 1:A:2554:U:C4 | 1:A:2576:A:C4 | 3.04 | 0.45 |
| 1:A:2096:A:C8 | 1:A:2539:U:C2 | 3.04 | 0.45 |
| 1:A:2135:A:C2 | 1:A:2136:G:N7 | 2.85 | 0.45 |
| 1:A:2248:C:N3 | 1:A:2254:G:C2 | 2.84 | 0.45 |
| 1:A:2476:C:N3 | 1:A:2477:C:C5 | 2.84 | 0.45 |
| 1:A:2455:A:N6 | 1:A:2456:A:C6 | 2.85 | 0.45 |
| 1:A:2294:C:H2' | 1:A:2295:G:H8 | 1.81 | 0.45 |
| 1:A:2605:G:H2' | 1:A:2606:G:C5' | 2.43 | 0.45 |
| 1:A:2635:A:C6 | 1:A:2636:C:C4 | 3.04 | 0.45 |
| 1:A:2072:G:O5' | 1:A:2072:G:H8 | 1.98 | 0.45 |
| 1:A:2596:A:H3' | 1:A:2596:A:C8 | 2.51 | 0.45 |
| 1:A:2357:G:C5 | 1:A:2358:U:C4 | 3.05 | 0.45 |
| 1:A:2513:A:H2' | 1:A:2514:U:O4' | 2.17 | 0.45 |
| 1:A:2544:G:O2' | 1:A:2545:U:H5' | 2.16 | 0.45 |
| 1:A:2351:C:H2' | 1:A:2352:G:O4' | 2.16 | 0.45 |
| 1:A:2237:G:H1' | 1:A:2238:A:H8 | 1.75 | 0.45 |
| 1:A:2596:A:C3' | 1:A:2596:A:C8 | 3.00 | 0.45 |
| 1:A:2554:U:C5 | 1:A:2576:A:C6 | 3.05 | 0.45 |
| 1:A:2555:C:N4 | 1:A:2602:G:C5 | 2.84 | 0.45 |
| 1:A:2507:G:C5 | 1:A:2510:C:C4 | 3.04 | 0.45 |
| 1:A:2072:G:C6 | 1:A:2533:C:H1' | 2.51 | 0.45 |
| 1:A:2345:A:H3' | 1:A:2346:C:H5 | 1.79 | 0.45 |
| 1:A:2237:G:N3 | 1:A:2238:A:N7 | 2.64 | 0.45 |
| 1:A:2113:G:H2' | 1:A:2114:C:O5' | 2.16 | 0.45 |
| 1:A:2116:U:H2' | 1:A:2118:A:OP1 | 2.17 | 0.45 |
| 1:A:2533:C:C2 | 1:A:2534:C:C5 | 3.05 | 0.45 |
| 1:A:2325:C:OP1 | 1:A:2417:C:O2' | 2.34 | 0.45 |
| 1:A:2575:C:H2' | 1:A:2576:A:O4' | 2.16 | 0.45 |
| 1:A:2630:G:C2 | 1:A:2634:G:C5 | 3.04 | 0.45 |
| 1:A:2073:G:O6 | 1:A:2488:A:O2' | 2.30 | 0.45 |
| 1:A:2250:G:C6 | 1:A:2251:G:C2 | 3.05 | 0.45 |
| 1:A:2526:C:C6 | 1:A:2526:C:C4' | 3.00 | 0.45 |
| 1:A:2433:A:O5' | 1:A:2433:A:H8 | 2.00 | 0.45 |
| 1:A:2485:A:C2' | 2:B:76:DA:C2 | 3.00 | 0.45 |
| 2:B:77:PU:HN'3 | 2:B:77:PU:HB1 | 1.62 | 0.45 |
| 1:A:2478:U:C2' | 1:A:2479:A:H5' | 2.46 | 0.45 |
| 1:A:2420:G:H2' | 1:A:2421:G:H8 | 1.82 | 0.45 |
| 1:A:2064:U:H2' | 1:A:2065:C:H6 | 1.80 | 0.45 |
| 1:A:2119:C:C4 | 1:A:2120:U:C5 | 3.05 | 0.45 |
| 1:A:2104:C:N4 | 1:A:2105:C:C5 | 2.83 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:A:2542:C:C1' | 1:A:2618:G:N2 | 2.79 | 0.44 |
| 1:A:2613:G:OP2 | 1:A:2613:G:H4' | 2.17 | 0.44 |
| 1:A:2106:C:C2 | 1:A:2481:G:N2 | 2.85 | 0.44 |
| 1:A:2462:G:H4' | 1:A:2464:C:C6 | 2.52 | 0.44 |
| 1:A:2245:C:O2' | 1:A:2260:A:N1 | 2.49 | 0.44 |
| 1:A:2594:C:C3' | 1:A:2594:C:C6 | 3.00 | 0.44 |
| 1:A:2092:G:H2' | 1:A:2613:G:OP1 | 2.17 | 0.44 |
| 1:A:2314:G:C2 | 1:A:2315:C:C6 | 3.04 | 0.44 |
| 1:A:2286:G:C5 | 1:A:2287:C:C5 | 3.05 | 0.44 |
| 1:A:2590:U:C5 | 1:A:2591:C:N1 | 2.85 | 0.44 |
| 1:A:2452:G:N3 | 1:A:2452:G:H2' | 2.33 | 0.44 |
| 1:A:2303:A:C2 | 1:A:2304:G:C1' | 3.01 | 0.44 |
| 1:A:2614:C:H6 | 1:A:2614:C:O5' | 2.00 | 0.44 |
| 1:A:2128:G:C5 | 1:A:2129:U:C4 | 3.05 | 0.44 |
| 1:A:2114:C:H6 | 1:A:2114:C:O5' | 2.01 | 0.44 |
| 1:A:2388:C:O2' | 1:A:2389:U:H5' | 2.17 | 0.44 |
| 1:A:2312:G:H2' | 1:A:2313:C:C5' | 2.39 | 0.44 |
| 1:A:2116:U:H5' | 1:A:2632:G:H1' | 1.98 | 0.44 |
| 1:A:2639:G:C6 | 1:A:2640:U:C4 | 3.04 | 0.44 |
| 1:A:2580:G:C6 | 1:A:2581:U:N3 | 2.86 | 0.44 |
| 1:A:2617:G:C3' | 1:A:2618:G:H5' | 2.47 | 0.44 |
| 1:A:2474:A:H2' | 1:A:2622:A:OP1 | 2.17 | 0.44 |
| 1:A:2135:A:C6 | 1:A:2241:C:N3 | 2.85 | 0.44 |
| 1:A:2252:A:C5 | 1:A:2253:G:C1' | 2.93 | 0.44 |
| 1:A:2250:G:O6 | 1:A:2251:G:N1 | 2.51 | 0.44 |
| 1:A:2492:U:N3 | 1:A:2493:C:C2 | 2.86 | 0.44 |
| 1:A:2533:C:OP2 | 1:A:2534:C:OP2 | 2.36 | 0.44 |
| 1:A:2406:U:N3 | 1:A:2407:G:C8 | 2.85 | 0.44 |
| 1:A:2245:C:H2' | 1:A:2246:U:H6 | 1.83 | 0.43 |
| 1:A:2542:C:H2' | 1:A:2543:G:C5' | 2.42 | 0.43 |
| 1:A:2242:U:C2 | 1:A:2257:G:N1 | 2.87 | 0.43 |
| 1:A:2635:A:H2' | 1:A:2636:C:H6 | 1.75 | 0.43 |
| 1:A:2581:U:H6 | 1:A:2581:U:O5' | 2.01 | 0.43 |
| 1:A:2486:A:OP2 | 1:A:2532:A:N1 | 2.51 | 0.43 |
| 1:A:2237:G:N3 | 1:A:2238:A:C5 | 2.86 | 0.43 |
| 1:A:2336:G:N2 | 1:A:2349:G:C4 | 2.86 | 0.43 |
| 1:A:2448:U:C2 | 1:A:2449:G:C8 | 3.06 | 0.43 |
| 1:A:2491:G:C4 | 1:A:2492:U:C6 | 3.06 | 0.43 |
| 1:A:2124:G:H8 | 1:A:2124:G:O5' | 2.01 | 0.43 |
| 1:A:2366:C:C4' | 1:A:2370:A:N6 | 2.80 | 0.43 |
| 1:A:2096:A:N3 | 1:A:2096:A:H3' | 2.33 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:A:2394:A:OP1 | 1:A:2394:A:H8 | 2.01 | 0.43 |
| 1:A:2542:C:H1' | 1:A:2618:G:N2 | 2.33 | 0.43 |
| 1:A:2250:G:C6 | 1:A:2251:G:C6 | 3.06 | 0.43 |
| 1:A:2492:U:O2 | 1:A:2492:U:H2' | 2.17 | 0.43 |
| 1:A:2527:U:C5 | 1:A:2528:U:C4 | 3.07 | 0.43 |
| 1:A:2562:G:C2' | 1:A:2563:U:H5' | 2.48 | 0.43 |
| 1:A:2237:G:C2 | 1:A:2238:A:C5 | 3.06 | 0.43 |
| 1:A:2659:U:O2' | 1:A:2660:G:O4' | 2.27 | 0.43 |
| 1:A:2332:A:C2 | 1:A:2355:G:C5 | 3.06 | 0.43 |
| 1:A:2379:G:H4' | 1:A:2380:A:C5' | 2.49 | 0.43 |
| 1:A:2361:A:N7 | 1:A:2425:A:N6 | 2.66 | 0.43 |
| 1:A:2658:G:N3 | 1:A:2658:G:H2' | 2.31 | 0.43 |
| 1:A:2129:U:H2' | 1:A:2130:C:H6 | 1.83 | 0.43 |
| 1:A:2578:G:O2' | 1:A:2579:G:H5' | 2.18 | 0.43 |
| 1:A:2329:C:H2' | 1:A:2330:U:C6 | 2.54 | 0.43 |
| 1:A:2487:C:O2' | 1:A:2488:A:H5' | 2.18 | 0.43 |
| 1:A:2489:G:H2' | 1:A:2490:A:C8 | 2.54 | 0.43 |
| 1:A:2496:C:C1' | 1:A:2527:U:N3 | 2.77 | 0.43 |
| 1:A:2631:U:H2' | 1:A:2632:G:O4' | 2.19 | 0.43 |
| 1:A:2563:U:H2' | 1:A:2565:C:O5' | 2.18 | 0.43 |
| 1:A:2102:G:H2' | 1:A:2536:C:O2' | 2.19 | 0.43 |
| 1:A:2102:G:N7 | 1:A:2538:A:C1' | 2.82 | 0.43 |
| 1:A:2347:C:H2' | 1:A:2348:C:C6 | 2.54 | 0.43 |
| 1:A:2397:G:H2' | 1:A:2398:A:C8 | 2.53 | 0.42 |
| 1:A:2487:C:H2' | 1:A:2488:A:C5' | 2.47 | 0.42 |
| 1:A:2544:G:OP1 | 1:A:2590:U:H5'' | 2.18 | 0.42 |
| 2:B:77:PU:N7 | 2:B:77:PU:C9 | 2.81 | 0.42 |
| 1:A:2248:C:O2' | 1:A:2249:G:H5' | 2.19 | 0.42 |
| 1:A:2594:C:H3' | 1:A:2594:C:C6 | 2.54 | 0.42 |
| 1:A:2613:G:H2' | 1:A:2614:C:H6 | 1.84 | 0.42 |
| 1:A:2123:A:H3' | 1:A:2124:G:C8 | 2.54 | 0.42 |
| 1:A:2246:U:C4 | 1:A:2256:G:C2 | 3.07 | 0.42 |
| 1:A:2269:C:H2' | 1:A:2270:G:C5' | 2.48 | 0.42 |
| 1:A:2083:A:O5' | 1:A:2083:A:H8 | 2.03 | 0.42 |
| 1:A:2611:G:N3 | 1:A:2611:G:C3' | 2.81 | 0.42 |
| 1:A:2125:G:C2 | 1:A:2126:C:C2 | 3.07 | 0.42 |
| 1:A:2554:U:C6 | 1:A:2576:A:C6 | 3.07 | 0.42 |
| 1:A:2308:U:C6 | 1:A:2308:U:H3' | 2.54 | 0.42 |
| 1:A:2241:C:O2' | 1:A:2242:U:H6 | 2.02 | 0.42 |
| 1:A:2633:A:O5' | 1:A:2633:A:H8 | 2.02 | 0.42 |
| 1:A:2560:C:H2' | 1:A:2561:C:C6 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|----------------|--------------------------|-------------------|
| 1:A:2308:U:C6 | 1:A:2308:U:C3' | 3.02 | 0.42 |
| 1:A:2106:C:H1' | 1:A:2484:U:N3 | 2.34 | 0.42 |
| 1:A:2253:G:HO2' | 1:A:2254:G:C5' | 2.32 | 0.42 |
| 1:A:2255:A:N1 | 1:A:2256:G:C4 | 2.87 | 0.42 |
| 1:A:2113:G:O6 | 1:A:2472:C:C4 | 2.72 | 0.42 |
| 1:A:2085:A:C5 | 1:A:2660:G:N2 | 2.87 | 0.42 |
| 1:A:2524:G:C5 | 1:A:2525:G:C6 | 3.07 | 0.42 |
| 1:A:2416:G:N3 | 1:A:2417:C:C6 | 2.87 | 0.42 |
| 1:A:2117:U:H6 | 1:A:2117:U:OP1 | 2.02 | 0.42 |
| 1:A:2089:A:O2' | 1:A:2090:G:H5' | 2.20 | 0.42 |
| 1:A:2090:G:C2' | 1:A:2091:G:C8 | 3.01 | 0.42 |
| 1:A:2345:A:C3' | 1:A:2346:C:C6 | 3.00 | 0.42 |
| 1:A:2526:C:O2' | 1:A:2527:U:H5' | 2.20 | 0.42 |
| 1:A:2460:A:H2' | 1:A:2461:U:H6 | 1.83 | 0.42 |
| 1:A:2303:A:C6 | 1:A:2304:G:C5 | 3.07 | 0.42 |
| 1:A:2085:A:N6 | 1:A:2660:G:C6 | 2.87 | 0.42 |
| 1:A:2088:C:N3 | 1:A:2657:G:C2 | 2.88 | 0.42 |
| 1:A:2411:C:N4 | 1:A:2412:G:O6 | 2.51 | 0.42 |
| 1:A:2638:G:H2' | 1:A:2639:G:C8 | 2.54 | 0.42 |
| 1:A:2479:A:OP2 | 1:A:2479:A:C8 | 2.73 | 0.42 |
| 1:A:2442:G:C6 | 1:A:2451:G:C6 | 3.07 | 0.42 |
| 1:A:2511:A:C8 | 1:A:2511:A:H5' | 2.55 | 0.42 |
| 1:A:2106:C:O2' | 1:A:2484:U:N3 | 2.52 | 0.42 |
| 1:A:2449:G:C8 | 1:A:2450:C:C5 | 3.08 | 0.42 |
| 1:A:2582:G:HO2' | 1:A:2583:A:H5' | 1.85 | 0.42 |
| 1:A:2599:A:C6 | 1:A:2600:A:N1 | 2.88 | 0.42 |
| 1:A:2124:G:O2' | 1:A:2125:G:O4' | 2.38 | 0.42 |
| 1:A:2328:U:H2' | 1:A:2329:C:O4' | 2.19 | 0.42 |
| 1:A:2424:U:H6 | 1:A:2424:U:O5' | 2.03 | 0.42 |
| 1:A:2550:U:H1' | 1:A:2605:G:N2 | 2.34 | 0.41 |
| 1:A:2291:A:C4 | 1:A:2309:C:H5' | 2.55 | 0.41 |
| 1:A:2246:U:O4 | 1:A:2256:G:N1 | 2.53 | 0.41 |
| 1:A:2569:A:H8 | 1:A:2569:A:O5' | 2.03 | 0.41 |
| 1:A:2437:A:N7 | 1:A:2455:A:C2 | 2.88 | 0.41 |
| 1:A:2242:U:N3 | 1:A:2257:G:C2 | 2.89 | 0.41 |
| 1:A:2121:G:C2' | 1:A:2122:C:H5' | 2.50 | 0.41 |
| 1:A:2439:C:O2' | 1:A:2440:C:H5' | 2.21 | 0.41 |
| 1:A:2456:A:C4 | 1:A:2457:U:C5 | 3.08 | 0.41 |
| 1:A:2308:U:H5'' | 1:A:2309:C:OP1 | 2.20 | 0.41 |
| 1:A:2264:A:C4 | 1:A:2265:U:C5 | 3.08 | 0.41 |
| 1:A:2411:C:C4 | 1:A:2412:G:N7 | 2.89 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|----------------|--------------------------|-------------------|
| 1:A:2125:G:H8 | 1:A:2125:G:O5' | 2.03 | 0.41 |
| 1:A:2549:C:C4 | 1:A:2606:G:N1 | 2.89 | 0.41 |
| 1:A:2250:G:N1 | 1:A:2251:G:N3 | 2.67 | 0.41 |
| 1:A:2651:C:H2' | 1:A:2652:U:O4' | 2.20 | 0.41 |
| 1:A:2249:G:N2 | 1:A:2253:G:C5 | 2.89 | 0.41 |
| 1:A:2492:U:O2 | 1:A:2493:C:N1 | 2.53 | 0.41 |
| 1:A:2385:G:H2' | 1:A:2385:G:N3 | 2.35 | 0.41 |
| 1:A:2386:U:O5' | 1:A:2386:U:H6 | 2.03 | 0.41 |
| 1:A:2397:G:C5 | 1:A:2465:A:N6 | 2.88 | 0.41 |
| 1:A:2548:C:HO2' | 1:A:2549:C:H6 | 1.67 | 0.41 |
| 1:A:2241:C:O2' | 1:A:2242:U:O4' | 2.39 | 0.41 |
| 1:A:2630:G:N2 | 1:A:2634:G:C5 | 2.88 | 0.41 |
| 1:A:2630:G:N2 | 1:A:2634:G:N7 | 2.68 | 0.41 |
| 1:A:2438:G:H2' | 1:A:2439:C:O5' | 2.19 | 0.41 |
| 1:A:2128:G:C6 | 1:A:2129:U:N3 | 2.89 | 0.41 |
| 1:A:2621:U:C2 | 1:A:2622:A:N7 | 2.89 | 0.41 |
| 1:A:2548:C:N3 | 1:A:2549:C:C5 | 2.89 | 0.41 |
| 1:A:2085:A:C4 | 1:A:2660:G:N2 | 2.89 | 0.41 |
| 1:A:2332:A:H3' | 1:A:2333:G:O4' | 2.20 | 0.41 |
| 1:A:2639:G:N1 | 1:A:2640:U:C4 | 2.89 | 0.41 |
| 1:A:2245:C:H2' | 1:A:2246:U:C6 | 2.55 | 0.41 |
| 1:A:2513:A:C8 | 1:A:2564:G:C8 | 3.09 | 0.41 |
| 1:A:2582:G:N7 | 1:A:2601:A:C4 | 2.88 | 0.41 |
| 1:A:2438:G:C6 | 1:A:2439:C:C2 | 3.08 | 0.41 |
| 1:A:2385:G:C2 | 1:A:2386:U:C2 | 3.09 | 0.41 |
| 1:A:2554:U:C2 | 1:A:2577:A:N6 | 2.89 | 0.41 |
| 1:A:2357:G:C2 | 1:A:2358:U:C2 | 3.09 | 0.41 |
| 1:A:2562:G:O2' | 1:A:2563:U:H5' | 2.20 | 0.41 |
| 1:A:2257:G:H4' | 1:A:2259:C:C2 | 2.56 | 0.41 |
| 1:A:2600:A:H5'' | 1:A:2601:A:OP2 | 2.20 | 0.41 |
| 1:A:2097:G:C2' | 1:A:2098:C:H5' | 2.51 | 0.41 |
| 1:A:2073:G:N1 | 1:A:2607:U:C6 | 2.89 | 0.40 |
| 1:A:2527:U:C6 | 1:A:2528:U:C5 | 3.08 | 0.40 |
| 1:A:2442:G:C4 | 1:A:2451:G:C2 | 3.10 | 0.40 |
| 1:A:2132:C:H3' | 1:A:2133:U:H2' | 2.03 | 0.40 |
| 1:A:2274:A:H2' | 1:A:2275:G:C8 | 2.55 | 0.40 |
| 1:A:2267:G:H2' | 1:A:2268:C:C6 | 2.56 | 0.40 |
| 1:A:2452:G:N1 | 1:A:2453:G:C8 | 2.89 | 0.40 |
| 1:A:2104:C:O2 | 1:A:2486:A:C2 | 2.74 | 0.40 |
| 1:A:2262:C:C2 | 1:A:2263:G:C8 | 3.09 | 0.40 |
| 1:A:2113:G:C2 | 1:A:2114:C:C2 | 3.10 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|---------------|--------------------------|-------------------|
| 1:A:2271:G:C2' | 1:A:2271:G:N3 | 2.75 | 0.40 |
| 1:A:2389:U:C4 | 1:A:2390:U:C4 | 3.09 | 0.40 |
| 1:A:2265:U:O2 | 1:A:2266:A:C8 | 2.74 | 0.40 |
| 1:A:2598:U:O2 | 1:A:2600:A:C8 | 2.74 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.3.3 RNA [i](#)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|---------------|-------------------|-----------------|
| 1 | A | 493/602 (81%) | 114 (23%) | 29 (5%) |
| 2 | B | 1/4 (25%) | 0 | 0 |
| All | All | 494/606 (81%) | 114 (23%) | 29 (5%) |

All (114) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 2064 | U |
| 1 | A | 2072 | G |
| 1 | A | 2073 | G |
| 1 | A | 2074 | A |
| 1 | A | 2075 | G |
| 1 | A | 2077 | C |
| 1 | A | 2083 | A |
| 1 | A | 2084 | C |
| 1 | A | 2091 | G |
| 1 | A | 2096 | A |
| 1 | A | 2097 | G |
| 1 | A | 2101 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 2102 | G |
| 1 | A | 2103 | A |
| 1 | A | 2105 | C |
| 1 | A | 2106 | C |
| 1 | A | 2110 | G |
| 1 | A | 2134 | G |
| 1 | A | 2238 | A |
| 1 | A | 2243 | C |
| 1 | A | 2253 | G |
| 1 | A | 2258 | A |
| 1 | A | 2259 | C |
| 1 | A | 2271 | G |
| 1 | A | 2272 | G |
| 1 | A | 2276 | U |
| 1 | A | 2283 | G |
| 1 | A | 2284 | G |
| 1 | A | 2286 | G |
| 1 | A | 2291 | A |
| 1 | A | 2292 | C |
| 1 | A | 2297 | U |
| 1 | A | 2301 | A |
| 1 | A | 2309 | C |
| 1 | A | 2316 | G |
| 1 | A | 2317 | C |
| 1 | A | 2318 | C |
| 1 | A | 2320 | U |
| 1 | A | 2321 | A |
| 1 | A | 2322 | U |
| 1 | A | 2346 | C |
| 1 | A | 2354 | A |
| 1 | A | 2357 | G |
| 1 | A | 2361 | A |
| 1 | A | 2369 | A |
| 1 | A | 2370 | A |
| 1 | A | 2371 | G |
| 1 | A | 2378 | U |
| 1 | A | 2379 | G |
| 1 | A | 2392 | C |
| 1 | A | 2396 | C |
| 1 | A | 2399 | G |
| 1 | A | 2416 | G |
| 1 | A | 2419 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 2422 | U |
| 1 | A | 2425 | A |
| 1 | A | 2427 | C |
| 1 | A | 2428 | G |
| 1 | A | 2437 | A |
| 1 | A | 2443 | C |
| 1 | A | 2444 | U |
| 1 | A | 2454 | C |
| 1 | A | 2462 | G |
| 1 | A | 2463 | A |
| 1 | A | 2464 | C |
| 1 | A | 2465 | A |
| 1 | A | 2466 | G |
| 1 | A | 2467 | A |
| 1 | A | 2469 | A |
| 1 | A | 2474 | A |
| 1 | A | 2475 | C |
| 1 | A | 2476 | C |
| 1 | A | 2479 | A |
| 1 | A | 2482 | G |
| 1 | A | 2483 | A |
| 1 | A | 2484 | U |
| 1 | A | 2507 | G |
| 1 | A | 2509 | A |
| 1 | A | 2510 | C |
| 1 | A | 2511 | A |
| 1 | A | 2513 | A |
| 1 | A | 2526 | C |
| 1 | A | 2527 | U |
| 1 | A | 2532 | A |
| 1 | A | 2533 | C |
| 1 | A | 2536 | C |
| 1 | A | 2537 | G |
| 1 | A | 2538 | A |
| 1 | A | 2539 | U |
| 1 | A | 2540 | G |
| 1 | A | 2541 | U |
| 1 | A | 2553 | A |
| 1 | A | 2564 | G |
| 1 | A | 2565 | C |
| 1 | A | 2587 | U |
| 1 | A | 2589 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 2592 | G |
| 1 | A | 2601 | A |
| 1 | A | 2602 | G |
| 1 | A | 2608 | C |
| 1 | A | 2609 | G |
| 1 | A | 2611 | G |
| 1 | A | 2613 | G |
| 1 | A | 2617 | G |
| 1 | A | 2620 | U |
| 1 | A | 2621 | U |
| 1 | A | 2637 | A |
| 1 | A | 2638 | G |
| 1 | A | 2645 | U |
| 1 | A | 2648 | U |
| 1 | A | 2649 | A |
| 1 | A | 2650 | U |
| 1 | A | 2658 | G |
| 1 | A | 2663 | U |

All (29) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 2074 | A |
| 1 | A | 2076 | U |
| 1 | A | 2083 | A |
| 1 | A | 2090 | G |
| 1 | A | 2102 | G |
| 1 | A | 2133 | U |
| 1 | A | 2242 | U |
| 1 | A | 2258 | A |
| 1 | A | 2282 | U |
| 1 | A | 2315 | C |
| 1 | A | 2321 | A |
| 1 | A | 2370 | A |
| 1 | A | 2395 | A |
| 1 | A | 2421 | G |
| 1 | A | 2427 | C |
| 1 | A | 2463 | A |
| 1 | A | 2465 | A |
| 1 | A | 2467 | A |
| 1 | A | 2468 | A |
| 1 | A | 2474 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 2482 | G |
| 1 | A | 2484 | U |
| 1 | A | 2506 | A |
| 1 | A | 2526 | C |
| 1 | A | 2538 | A |
| 1 | A | 2564 | G |
| 1 | A | 2588 | G |
| 1 | A | 2620 | U |
| 1 | A | 2637 | A |

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

1 non-standard protein/DNA/RNA residue is 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 | $\# Z > 2$ |
| 2 | PU | B | 77 | 1,2 | 31,40,41 | 4.13 | 10 (32%) | 36,57,60 | 2.61 | 9 (25%) |

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 |
|-----|------|-------|-----|------|---------|------------|---------|
| 2 | PU | B | 77 | 1,2 | - | 0/20/44/45 | 0/4/4/4 |

All (10) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2 | B | 77 | PU | CE1-CZ | -6.38 | 1.25 | 1.38 |
| 2 | B | 77 | PU | CA-N | -5.53 | 1.41 | 1.47 |
| 2 | B | 77 | PU | OC-CZ | -2.71 | 1.31 | 1.37 |
| 2 | B | 77 | PU | CA-C | 2.09 | 1.58 | 1.52 |
| 2 | B | 77 | PU | C6-N1 | 2.10 | 1.37 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | B | 77 | PU | CB-CA | 2.49 | 1.60 | 1.54 |
| 2 | B | 77 | PU | OC-CM | 2.83 | 1.51 | 1.42 |
| 2 | B | 77 | PU | CB-CG | 3.84 | 1.60 | 1.51 |
| 2 | B | 77 | PU | CE2-CD2 | 13.15 | 1.62 | 1.38 |
| 2 | B | 77 | PU | CE1-CD1 | 15.05 | 1.65 | 1.38 |

All (9) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 2 | B | 77 | PU | O2'-C2'-C3' | -12.16 | 81.88 | 110.62 |
| 2 | B | 77 | PU | CD2-CG-CD1 | -4.32 | 111.22 | 118.13 |
| 2 | B | 77 | PU | OC-CZ-CE2 | -2.09 | 109.73 | 119.78 |
| 2 | B | 77 | PU | CE1-CD1-CG | 2.08 | 123.89 | 121.04 |
| 2 | B | 77 | PU | CE2-CD2-CG | 2.36 | 124.27 | 121.04 |
| 2 | B | 77 | PU | C2-N1-C6 | 2.65 | 117.06 | 111.43 |
| 2 | B | 77 | PU | C-CA-N | 2.69 | 118.48 | 110.88 |
| 2 | B | 77 | PU | CB-CG-CD1 | 2.89 | 126.96 | 120.90 |
| 2 | B | 77 | PU | C2'-C1'-N9 | 4.01 | 120.42 | 114.29 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 9 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2 | B | 77 | PU | 9 | 0 |

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

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 | 496/602 (82%) | 2.39 | 348 (70%) 0 0 | 40, 40, 40, 40 | 0 |
| 2 | B | 3/4 (75%) | 1.91 | 1 (33%) 0 0 | 40, 40, 40, 40 | 0 |
| All | All | 499/606 (82%) | 2.38 | 349 (69%) 0 0 | 40, 40, 40, 40 | 0 |

All (349) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 2249 | G | 4.7 |
| 1 | A | 2238 | A | 4.4 |
| 1 | A | 2254 | G | 4.3 |
| 1 | A | 2449 | G | 4.2 |
| 1 | A | 2251 | G | 4.2 |
| 1 | A | 2255 | A | 4.1 |
| 1 | A | 2642 | G | 4.0 |
| 1 | A | 2452 | G | 4.0 |
| 1 | A | 2237 | G | 4.0 |
| 1 | A | 2562 | G | 4.0 |
| 1 | A | 2135 | A | 3.9 |
| 1 | A | 2131 | G | 3.9 |
| 1 | A | 2337 | G | 3.8 |
| 1 | A | 2125 | G | 3.8 |
| 1 | A | 2136 | G | 3.7 |
| 1 | A | 2364 | A | 3.7 |
| 1 | A | 2250 | G | 3.7 |
| 1 | A | 2263 | G | 3.6 |
| 1 | A | 2494 | G | 3.6 |
| 1 | A | 2657 | G | 3.6 |
| 1 | A | 2253 | G | 3.5 |
| 1 | A | 2564 | G | 3.5 |
| 1 | A | 2567 | G | 3.5 |
| 1 | A | 2264 | A | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 2111 | G | 3.5 |
| 1 | A | 2336 | G | 3.5 |
| 1 | A | 2504 | A | 3.5 |
| 1 | A | 2375 | G | 3.5 |
| 1 | A | 2446 | G | 3.5 |
| 1 | A | 2077 | C | 3.5 |
| 1 | A | 2444 | U | 3.5 |
| 1 | A | 2505 | G | 3.5 |
| 1 | A | 2259 | C | 3.4 |
| 1 | A | 2335 | C | 3.4 |
| 1 | A | 2451 | G | 3.4 |
| 1 | A | 2515 | C | 3.4 |
| 1 | A | 2247 | C | 3.3 |
| 1 | A | 2560 | C | 3.3 |
| 1 | A | 2636 | C | 3.3 |
| 1 | A | 2270 | G | 3.3 |
| 1 | A | 2348 | C | 3.3 |
| 1 | A | 2412 | G | 3.3 |
| 1 | A | 2258 | A | 3.3 |
| 1 | A | 2566 | A | 3.3 |
| 1 | A | 2544 | G | 3.3 |
| 1 | A | 2240 | U | 3.2 |
| 1 | A | 2252 | A | 3.2 |
| 1 | A | 2416 | G | 3.2 |
| 1 | A | 2501 | G | 3.2 |
| 1 | A | 2537 | G | 3.2 |
| 1 | A | 2570 | G | 3.2 |
| 1 | A | 2351 | C | 3.2 |
| 1 | A | 2269 | C | 3.2 |
| 1 | A | 2606 | G | 3.2 |
| 1 | A | 2267 | G | 3.1 |
| 1 | A | 2085 | A | 3.1 |
| 1 | A | 2434 | A | 3.1 |
| 1 | A | 2601 | A | 3.1 |
| 1 | A | 2391 | C | 3.1 |
| 1 | A | 2404 | G | 3.1 |
| 1 | A | 2510 | C | 3.1 |
| 1 | A | 2344 | G | 3.1 |
| 1 | A | 2124 | G | 3.1 |
| 1 | A | 2568 | A | 3.0 |
| 1 | A | 2507 | G | 3.0 |
| 1 | A | 2559 | C | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 2088 | C | 3.0 |
| 1 | A | 2383 | G | 3.0 |
| 1 | A | 2363 | G | 3.0 |
| 1 | A | 2643 | G | 3.0 |
| 1 | A | 2245 | C | 3.0 |
| 1 | A | 2268 | C | 3.0 |
| 1 | A | 2409 | C | 3.0 |
| 1 | A | 2338 | G | 2.9 |
| 1 | A | 2453 | G | 2.9 |
| 1 | A | 2574 | G | 2.9 |
| 1 | A | 2630 | G | 2.9 |
| 1 | A | 2509 | A | 2.9 |
| 1 | A | 2293 | G | 2.9 |
| 1 | A | 2349 | G | 2.9 |
| 1 | A | 2395 | A | 2.9 |
| 1 | A | 2117 | U | 2.9 |
| 1 | A | 2450 | C | 2.9 |
| 1 | A | 2323 | G | 2.9 |
| 1 | A | 2345 | A | 2.9 |
| 1 | A | 2459 | G | 2.9 |
| 1 | A | 2392 | C | 2.9 |
| 1 | A | 2316 | G | 2.9 |
| 1 | A | 2417 | C | 2.9 |
| 1 | A | 2558 | G | 2.9 |
| 1 | A | 2478 | U | 2.9 |
| 1 | A | 2660 | G | 2.9 |
| 1 | A | 2381 | C | 2.9 |
| 1 | A | 2443 | C | 2.9 |
| 1 | A | 2411 | C | 2.9 |
| 1 | A | 2371 | G | 2.8 |
| 1 | A | 2520 | G | 2.8 |
| 1 | A | 2584 | G | 2.8 |
| 1 | A | 2261 | C | 2.8 |
| 1 | A | 2352 | G | 2.8 |
| 1 | A | 2466 | G | 2.8 |
| 1 | A | 2374 | A | 2.8 |
| 1 | A | 2328 | U | 2.8 |
| 1 | A | 2256 | G | 2.8 |
| 1 | A | 2658 | G | 2.8 |
| 1 | A | 2068 | G | 2.8 |
| 1 | A | 2243 | C | 2.8 |
| 1 | A | 2626 | C | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 2448 | U | 2.8 |
| 1 | A | 2087 | C | 2.8 |
| 1 | A | 2490 | A | 2.8 |
| 1 | A | 2596 | A | 2.8 |
| 1 | A | 2080 | G | 2.8 |
| 1 | A | 2094 | G | 2.8 |
| 1 | A | 2462 | G | 2.8 |
| 1 | A | 2482 | G | 2.8 |
| 1 | A | 2569 | A | 2.8 |
| 1 | A | 2098 | C | 2.8 |
| 1 | A | 2385 | G | 2.8 |
| 1 | A | 2414 | A | 2.8 |
| 1 | A | 2661 | U | 2.7 |
| 1 | A | 2437 | A | 2.7 |
| 1 | A | 2496 | C | 2.7 |
| 1 | A | 2369 | A | 2.7 |
| 1 | A | 2408 | A | 2.7 |
| 1 | A | 2134 | G | 2.7 |
| 1 | A | 2122 | C | 2.7 |
| 1 | A | 2260 | A | 2.7 |
| 1 | A | 2481 | G | 2.7 |
| 1 | A | 2543 | G | 2.7 |
| 1 | A | 2086 | C | 2.7 |
| 1 | A | 2305 | A | 2.7 |
| 1 | A | 2082 | G | 2.7 |
| 1 | A | 2407 | G | 2.7 |
| 1 | A | 2471 | G | 2.7 |
| 1 | A | 2585 | G | 2.7 |
| 1 | A | 2602 | G | 2.7 |
| 1 | A | 2623 | G | 2.7 |
| 1 | A | 2132 | C | 2.7 |
| 1 | A | 2285 | G | 2.7 |
| 1 | A | 2288 | G | 2.7 |
| 1 | A | 2333 | G | 2.7 |
| 1 | A | 2603 | G | 2.7 |
| 1 | A | 2529 | G | 2.7 |
| 1 | A | 2063 | U | 2.7 |
| 1 | A | 2133 | U | 2.7 |
| 1 | A | 2321 | A | 2.7 |
| 1 | A | 2110 | G | 2.7 |
| 1 | A | 2582 | G | 2.7 |
| 1 | A | 2095 | A | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 2447 | A | 2.6 |
| 1 | A | 2299 | G | 2.6 |
| 1 | A | 2393 | C | 2.6 |
| 1 | A | 2565 | C | 2.6 |
| 1 | A | 2123 | A | 2.6 |
| 1 | A | 2577 | A | 2.6 |
| 1 | A | 2435 | U | 2.6 |
| 1 | A | 2659 | U | 2.6 |
| 1 | A | 2084 | C | 2.6 |
| 1 | A | 2334 | C | 2.6 |
| 1 | A | 2092 | G | 2.6 |
| 1 | A | 2611 | G | 2.6 |
| 1 | A | 2632 | G | 2.6 |
| 1 | A | 2455 | A | 2.6 |
| 1 | A | 2265 | U | 2.6 |
| 1 | A | 2366 | C | 2.6 |
| 1 | A | 2609 | G | 2.6 |
| 1 | A | 2274 | A | 2.6 |
| 1 | A | 2090 | G | 2.6 |
| 1 | A | 2311 | A | 2.6 |
| 1 | A | 2116 | U | 2.6 |
| 1 | A | 2127 | U | 2.6 |
| 1 | A | 2296 | C | 2.6 |
| 1 | A | 2242 | U | 2.6 |
| 1 | A | 2384 | U | 2.6 |
| 1 | A | 2244 | A | 2.6 |
| 1 | A | 2464 | C | 2.6 |
| 1 | A | 2579 | G | 2.6 |
| 1 | A | 2500 | C | 2.6 |
| 1 | A | 2508 | C | 2.6 |
| 1 | A | 2491 | G | 2.5 |
| 1 | A | 2493 | C | 2.5 |
| 1 | A | 2425 | A | 2.5 |
| 1 | A | 2432 | C | 2.5 |
| 1 | A | 2578 | G | 2.5 |
| 1 | A | 2593 | C | 2.5 |
| 1 | A | 2377 | U | 2.5 |
| 1 | A | 2563 | U | 2.5 |
| 1 | A | 2583 | A | 2.5 |
| 1 | A | 2318 | C | 2.5 |
| 1 | A | 2439 | C | 2.5 |
| 1 | A | 2454 | C | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 2310 | G | 2.5 |
| 1 | A | 2440 | C | 2.5 |
| 1 | A | 2272 | G | 2.5 |
| 1 | A | 2308 | U | 2.5 |
| 1 | A | 2239 | C | 2.5 |
| 1 | A | 2512 | U | 2.5 |
| 1 | A | 2104 | C | 2.5 |
| 1 | A | 2257 | G | 2.5 |
| 1 | A | 2350 | G | 2.5 |
| 1 | A | 2421 | G | 2.5 |
| 1 | A | 2617 | G | 2.5 |
| 1 | A | 2083 | A | 2.5 |
| 1 | A | 2130 | C | 2.5 |
| 1 | A | 2556 | C | 2.5 |
| 1 | A | 2625 | C | 2.5 |
| 1 | A | 2283 | G | 2.4 |
| 1 | A | 2401 | A | 2.4 |
| 1 | A | 2312 | G | 2.4 |
| 1 | A | 2065 | C | 2.4 |
| 1 | A | 2332 | A | 2.4 |
| 1 | A | 2354 | A | 2.4 |
| 1 | A | 2372 | A | 2.4 |
| 1 | A | 2548 | C | 2.4 |
| 1 | A | 2387 | U | 2.4 |
| 1 | A | 2081 | A | 2.4 |
| 1 | A | 2089 | A | 2.4 |
| 1 | A | 2433 | A | 2.4 |
| 1 | A | 2101 | A | 2.4 |
| 1 | A | 2248 | C | 2.4 |
| 1 | A | 2324 | G | 2.4 |
| 1 | A | 2524 | G | 2.4 |
| 1 | A | 2575 | C | 2.4 |
| 1 | A | 2473 | U | 2.4 |
| 1 | A | 2663 | U | 2.4 |
| 1 | A | 2463 | A | 2.4 |
| 1 | A | 2326 | U | 2.4 |
| 1 | A | 2397 | G | 2.4 |
| 1 | A | 2394 | A | 2.4 |
| 1 | A | 2430 | A | 2.4 |
| 1 | A | 2511 | A | 2.4 |
| 1 | A | 2536 | C | 2.4 |
| 1 | A | 2128 | G | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 2400 | G | 2.4 |
| 1 | A | 2634 | G | 2.4 |
| 1 | A | 2246 | U | 2.4 |
| 1 | A | 2273 | C | 2.4 |
| 1 | A | 2475 | C | 2.4 |
| 1 | A | 2486 | A | 2.4 |
| 1 | A | 2070 | G | 2.4 |
| 1 | A | 2114 | C | 2.4 |
| 1 | A | 2622 | A | 2.4 |
| 1 | A | 2438 | G | 2.3 |
| 1 | A | 2499 | U | 2.3 |
| 1 | A | 2241 | C | 2.3 |
| 1 | A | 2347 | C | 2.3 |
| 1 | A | 2571 | C | 2.3 |
| 1 | A | 2093 | G | 2.3 |
| 1 | A | 2067 | A | 2.3 |
| 1 | A | 2286 | G | 2.3 |
| 1 | A | 2516 | G | 2.3 |
| 1 | A | 2588 | G | 2.3 |
| 1 | A | 2518 | C | 2.3 |
| 1 | A | 2534 | C | 2.3 |
| 1 | A | 2594 | C | 2.3 |
| 1 | A | 2112 | A | 2.3 |
| 1 | A | 2069 | U | 2.3 |
| 1 | A | 2373 | U | 2.3 |
| 1 | A | 2495 | U | 2.3 |
| 1 | A | 2113 | G | 2.3 |
| 1 | A | 2580 | G | 2.3 |
| 1 | A | 2616 | G | 2.3 |
| 1 | A | 2639 | G | 2.3 |
| 1 | A | 2307 | A | 2.3 |
| 1 | A | 2506 | A | 2.3 |
| 1 | A | 2276 | U | 2.3 |
| 1 | A | 2126 | C | 2.3 |
| 1 | A | 2072 | G | 2.3 |
| 1 | A | 2102 | G | 2.3 |
| 1 | A | 2279 | G | 2.3 |
| 1 | A | 2355 | G | 2.3 |
| 1 | A | 2525 | G | 2.3 |
| 1 | A | 2656 | G | 2.3 |
| 1 | A | 2653 | A | 2.3 |
| 1 | A | 2600 | A | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 2295 | G | 2.3 |
| 1 | A | 2595 | U | 2.3 |
| 1 | A | 2119 | C | 2.2 |
| 1 | A | 2346 | C | 2.2 |
| 1 | A | 2079 | G | 2.2 |
| 1 | A | 2605 | G | 2.2 |
| 1 | A | 2309 | C | 2.2 |
| 1 | A | 2360 | C | 2.2 |
| 1 | A | 2368 | A | 2.2 |
| 1 | A | 2521 | A | 2.2 |
| 1 | A | 2576 | A | 2.2 |
| 1 | A | 2074 | A | 2.2 |
| 1 | A | 2497 | A | 2.2 |
| 1 | A | 2275 | G | 2.2 |
| 1 | A | 2315 | C | 2.2 |
| 1 | A | 2121 | G | 2.2 |
| 1 | A | 2289 | G | 2.2 |
| 1 | A | 2076 | U | 2.2 |
| 1 | A | 2441 | U | 2.2 |
| 1 | A | 2331 | C | 2.2 |
| 1 | A | 2115 | U | 2.2 |
| 1 | A | 2097 | G | 2.2 |
| 1 | A | 2572 | G | 2.2 |
| 1 | A | 2266 | A | 2.2 |
| 1 | A | 2388 | C | 2.2 |
| 1 | A | 2405 | C | 2.2 |
| 1 | A | 2487 | C | 2.2 |
| 1 | A | 2519 | C | 2.2 |
| 1 | A | 2100 | A | 2.2 |
| 1 | A | 2436 | U | 2.2 |
| 1 | A | 2597 | U | 2.2 |
| 1 | A | 2304 | G | 2.2 |
| 1 | A | 2357 | G | 2.2 |
| 1 | A | 2365 | G | 2.2 |
| 1 | A | 2418 | G | 2.2 |
| 1 | A | 2291 | A | 2.1 |
| 1 | A | 2517 | A | 2.1 |
| 1 | A | 2628 | U | 2.1 |
| 1 | A | 2654 | C | 2.1 |
| 1 | A | 2650 | U | 2.1 |
| 1 | A | 2300 | A | 2.1 |
| 1 | A | 2066 | C | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 2498 | C | 2.1 |
| 2 | B | 75 | C | 2.1 |
| 1 | A | 2640 | U | 2.1 |
| 1 | A | 2129 | U | 2.1 |
| 1 | A | 2356 | A | 2.1 |
| 1 | A | 2402 | A | 2.1 |
| 1 | A | 2624 | A | 2.1 |
| 1 | A | 2555 | C | 2.1 |
| 1 | A | 2492 | U | 2.1 |
| 1 | A | 2073 | G | 2.1 |
| 1 | A | 2479 | A | 2.1 |
| 1 | A | 2528 | U | 2.1 |
| 1 | A | 2472 | C | 2.1 |
| 1 | A | 2301 | A | 2.1 |
| 1 | A | 2468 | A | 2.1 |
| 1 | A | 2554 | U | 2.1 |
| 1 | A | 2406 | U | 2.0 |
| 1 | A | 2539 | U | 2.0 |
| 1 | A | 2292 | C | 2.0 |
| 1 | A | 2646 | G | 2.0 |
| 1 | A | 2398 | A | 2.0 |
| 1 | A | 2589 | U | 2.0 |
| 1 | A | 2281 | C | 2.0 |
| 1 | A | 2573 | G | 2.0 |
| 1 | A | 2523 | U | 2.0 |
| 1 | A | 2103 | A | 2.0 |
| 1 | A | 2533 | C | 2.0 |
| 1 | A | 2550 | U | 2.0 |
| 1 | A | 2329 | C | 2.0 |
| 1 | A | 2474 | A | 2.0 |
| 1 | A | 2297 | U | 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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 | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|-----------------------------|-------|
| 2 | PU | B | 77 | 37/38 | 0.88 | 0.38 | - | 40,40,40,40 | 0 |

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.