



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:30 PM UTC

PDB ID : 4E8N / pdb\_00004e8n  
Title : Structure of Oceanobacillus iheyensis group II intron in a ligand-free state in the presence of NH<sub>4</sub><sup>+</sup> and Mg<sup>2+</sup>  
Authors : Marcia, M.; Pyle, A.M.  
Deposited on : 2012-03-20  
Resolution : 2.96 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

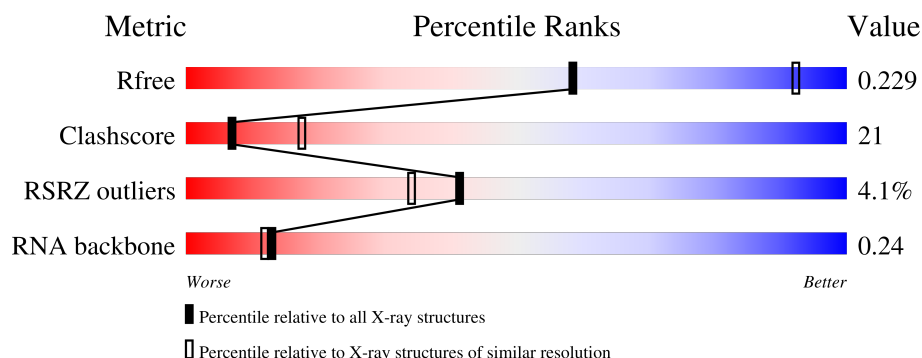
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.96 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<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|---------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$    | 180053                      | 1130 (2.98-2.94)                                      |
| Clashscore    | 190562                      | 1157 (2.98-2.94)                                      |
| RSRZ outliers | 180081                      | 1130 (2.98-2.94)                                      |
| RNA backbone  | 3983                        | 1046 (3.16-2.76)                                      |

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

| Mol | Chain | Length | Quality of chain                                                                       |
|-----|-------|--------|----------------------------------------------------------------------------------------|
| 1   | A     | 393    | <div> <div>4%</div> <div>19%</div> <div>35%</div> <div>33%</div> <div>13%</div> </div> |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 3   | NH4  | A     | 439 | -         | -        | -       | X                |
| 3   | NH4  | A     | 442 | -         | -        | -       | X                |
| 3   | NH4  | A     | 443 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 3   | NH4  | A     | 444 | -         | -        | -       | X                |
| 3   | NH4  | A     | 445 | -         | -        | -       | X                |

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8537 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.

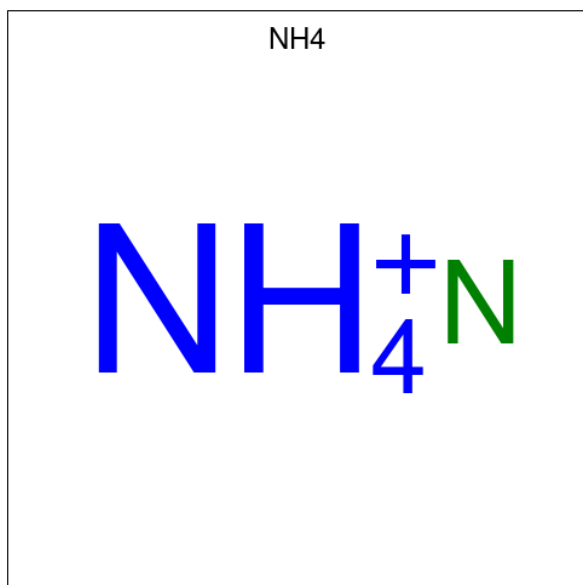
- Molecule 1 is a RNA chain called Group IIC intron.

| Mol | Chain | Residues | Atoms |      |      |      |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|-----|---------|---------|-------|
| 1   | A     | 393      | Total | C    | N    | O    | P   | 0       | 0       | 0     |
|     |       |          | 8412  | 3754 | 1559 | 2707 | 392 |         |         |       |

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | A     | 31       | Total | Mg | 0       | 0       |
|     |       |          | 31    | 31 |         |         |

- Molecule 3 is AMMONIUM ION (CCD ID: NH4) (formula: H<sub>4</sub>N).



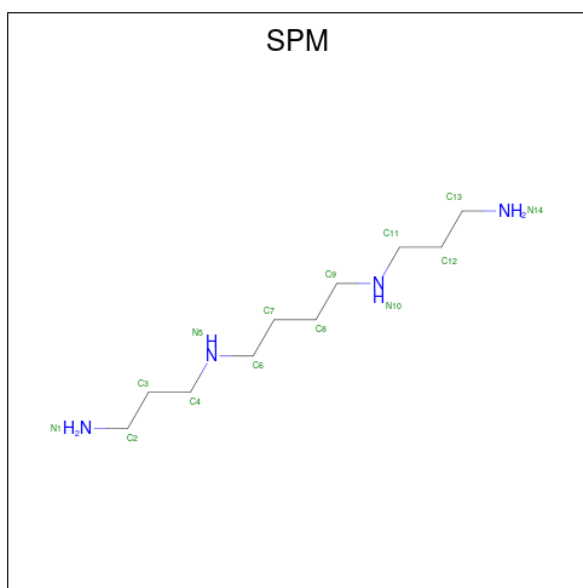
| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 3   | A     | 1        | Total | N | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 3   | A     | 1        | Total | N | 0       | 0       |
|     |       |          | 1     | 1 |         |         |

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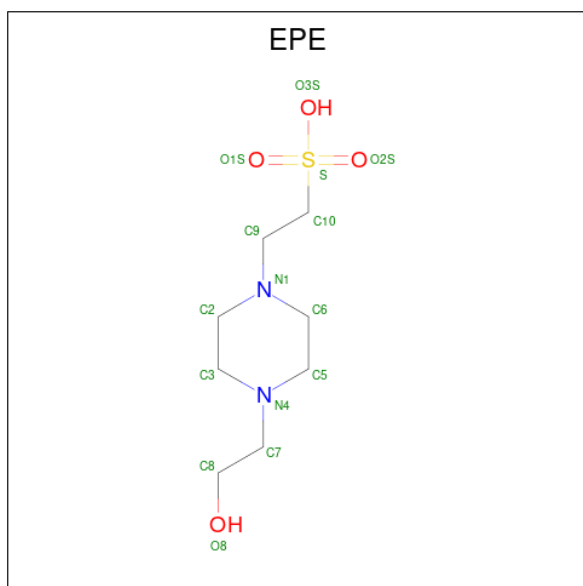
| Mol | Chain | Residues | Atoms          | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 3   | A     | 1        | Total N<br>1 1 | 0       | 0       |
| 3   | A     | 1        | Total N<br>1 1 | 0       | 0       |
| 3   | A     | 1        | Total N<br>1 1 | 0       | 0       |
| 3   | A     | 1        | Total N<br>1 1 | 0       | 0       |
| 3   | A     | 1        | Total N<br>1 1 | 0       | 0       |
| 3   | A     | 1        | Total N<br>1 1 | 0       | 0       |
| 3   | A     | 1        | Total N<br>1 1 | 0       | 0       |
| 3   | A     | 1        | Total N<br>1 1 | 0       | 0       |
| 3   | A     | 1        | Total N<br>1 1 | 0       | 0       |
| 3   | A     | 1        | Total N<br>1 1 | 0       | 0       |
| 3   | A     | 1        | Total N<br>1 1 | 0       | 0       |
| 3   | A     | 1        | Total N<br>1 1 | 0       | 0       |

- Molecule 4 is SPERMINE (CCD ID: SPM) (formula:  $C_{10}H_{26}N_4$ ).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 4   | A     | 1        | Total | C  | N | 0       | 0       |
|     |       |          | 14    | 10 | 4 |         |         |

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 5   | A     | 1        | Total | O | S |   |   | 0       | 0       |
|     |       |          | 4     | 3 | 1 |   |   |         |         |
| 5   | A     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 12    | 6 | 2 | 3 | 1 |         |         |
| 5   | A     | 1        | Total | O | S |   |   | 0       | 0       |
|     |       |          | 4     | 3 | 1 |   |   |         |         |
| 5   | A     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 15    | 8 | 2 | 4 | 1 |         |         |

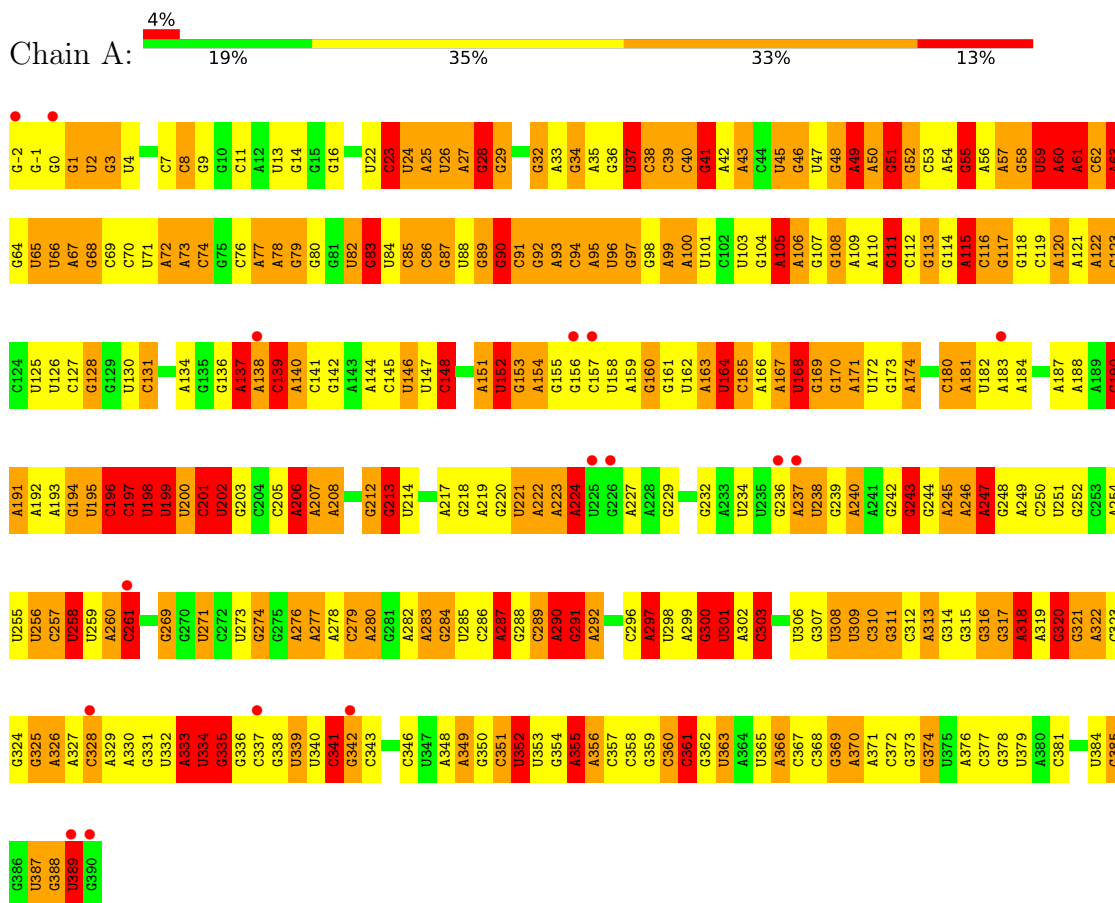
- Molecule 6 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 6   | A     | 31       | Total | O  | 0       | 0       |
|     |       |          | 31    | 31 |         |         |

### 3 Residue-property plots

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

• Molecule 1: Group IIC intron



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 88.89Å 95.43Å 224.55Å<br>90.00° 90.00° 90.00°               | Depositor        |
| Resolution (Å)                                                          | 49.10 – 2.96<br>49.10 – 2.96                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.8 (49.10-2.96)<br>98.8 (49.10-2.96)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.04                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.64 (at 2.96Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.6.0117                                             | Depositor        |
| R, $R_{free}$                                                           | 0.196 , 0.235<br>0.193 , 0.229                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2015 reflections (5.01%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 91.4                                                        | Xtriage          |
| Anisotropy                                                              | 0.282                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 109.9                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.95                                                        | EDS              |
| Total number of atoms                                                   | 8537                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 109.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, EPE, SPM, NH4

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     | 0.61         | 3/9427 (0.0%) | 1.58        | 306/14705 (2.1%) |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 49  | A    | O3'-P   | -5.61 | 1.52        | 1.61     |
| 1   | A     | 168 | U    | O3'-P   | -5.33 | 1.53        | 1.61     |
| 1   | A     | 60  | A    | C3'-O3' | -5.02 | 1.34        | 1.42     |

All (306) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 1   | A     | 58  | G    | O3'-P-O5'   | -17.08 | 78.38       | 104.00   |
| 1   | A     | 197 | C    | O3'-P-O5'   | 16.57  | 128.85      | 104.00   |
| 1   | A     | 168 | U    | C2'-C3'-O3' | 13.47  | 129.70      | 109.50   |
| 1   | A     | 63  | A    | O3'-P-O5'   | 12.91  | 123.37      | 104.00   |
| 1   | A     | 59  | U    | O3'-P-O5'   | -12.56 | 85.16       | 104.00   |
| 1   | A     | 120 | A    | C1'-C2'-O2' | -12.40 | 89.80       | 108.40   |
| 1   | A     | 91  | C    | O3'-P-O5'   | -12.32 | 85.53       | 104.00   |
| 1   | A     | 86  | C    | O3'-P-O5'   | -11.84 | 86.23       | 104.00   |
| 1   | A     | 239 | G    | O3'-P-O5'   | -11.45 | 86.83       | 104.00   |
| 1   | A     | 55  | G    | O3'-P-O5'   | -11.27 | 87.10       | 104.00   |
| 1   | A     | 41  | G    | O3'-P-O5'   | -11.13 | 87.31       | 104.00   |
| 1   | A     | 243 | G    | O3'-P-O5'   | -10.95 | 87.57       | 104.00   |
| 1   | A     | 91  | C    | C1'-C2'-O2' | -10.92 | 92.02       | 108.40   |
| 1   | A     | 115 | A    | O3'-P-O5'   | -10.75 | 87.87       | 104.00   |
| 1   | A     | 199 | U    | C4'-C3'-O3' | -10.38 | 97.43       | 113.00   |
| 1   | A     | 3   | G    | O3'-P-O5'   | -10.12 | 88.83       | 104.00   |
| 1   | A     | 59  | U    | C2'-C3'-O3' | -10.03 | 98.66       | 113.70   |
| 1   | A     | 51  | G    | O3'-P-O5'   | -9.64  | 89.54       | 104.00   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 196 | C    | O3'-P-O5'   | 9.33  | 118.00      | 104.00   |
| 1   | A     | 389 | U    | C1'-C2'-O2' | 9.27  | 125.71      | 111.80   |
| 1   | A     | 280 | A    | C1'-C2'-O2' | -9.09 | 94.77       | 108.40   |
| 1   | A     | 359 | G    | O3'-P-O5'   | -9.08 | 90.38       | 104.00   |
| 1   | A     | 346 | C    | O3'-P-O5'   | -9.07 | 90.40       | 104.00   |
| 1   | A     | 201 | C    | P-O3'-C3'   | -9.06 | 106.62      | 120.20   |
| 1   | A     | 49  | A    | C2'-C3'-O3' | -9.01 | 100.18      | 113.70   |
| 1   | A     | 100 | A    | O3'-P-O5'   | -8.91 | 90.63       | 104.00   |
| 1   | A     | 37  | U    | P-O3'-C3'   | -8.88 | 106.88      | 120.20   |
| 1   | A     | 120 | A    | O3'-P-O5'   | -8.87 | 90.70       | 104.00   |
| 1   | A     | 171 | A    | P-O3'-C3'   | -8.80 | 107.00      | 120.20   |
| 1   | A     | 85  | C    | O3'-P-O5'   | -8.79 | 90.81       | 104.00   |
| 1   | A     | 117 | G    | C3'-C2'-O2' | 8.78  | 123.87      | 110.70   |
| 1   | A     | 73  | A    | O3'-P-O5'   | -8.78 | 90.83       | 104.00   |
| 1   | A     | 62  | C    | O3'-P-O5'   | 8.78  | 117.17      | 104.00   |
| 1   | A     | 348 | A    | O3'-P-O5'   | -8.70 | 90.94       | 104.00   |
| 1   | A     | 60  | A    | C4'-C3'-O3' | -8.58 | 100.13      | 113.00   |
| 1   | A     | 245 | A    | P-O3'-C3'   | -8.48 | 107.49      | 120.20   |
| 1   | A     | 274 | G    | C1'-C2'-O2' | -8.47 | 95.69       | 108.40   |
| 1   | A     | 154 | A    | P-O3'-C3'   | -8.32 | 107.72      | 120.20   |
| 1   | A     | 256 | U    | C3'-C2'-O2' | 8.32  | 123.17      | 110.70   |
| 1   | A     | 79  | G    | C2'-C3'-O3' | -8.18 | 101.44      | 113.70   |
| 1   | A     | 355 | A    | O3'-P-O5'   | -8.13 | 91.81       | 104.00   |
| 1   | A     | 271 | U    | O3'-P-O5'   | -8.05 | 91.93       | 104.00   |
| 1   | A     | 43  | A    | C1'-C2'-O2' | 8.00  | 120.41      | 108.40   |
| 1   | A     | 125 | U    | O3'-P-O5'   | -8.00 | 92.00       | 104.00   |
| 1   | A     | 242 | G    | P-O3'-C3'   | -8.00 | 108.20      | 120.20   |
| 1   | A     | 99  | A    | O3'-P-O5'   | -7.95 | 92.07       | 104.00   |
| 1   | A     | 223 | A    | C2'-C3'-O3' | -7.93 | 97.61       | 109.50   |
| 1   | A     | 170 | G    | O3'-P-O5'   | 7.92  | 115.88      | 104.00   |
| 1   | A     | 276 | A    | C1'-C2'-O2' | -7.91 | 96.53       | 108.40   |
| 1   | A     | 87  | G    | O3'-P-O5'   | -7.86 | 92.20       | 104.00   |
| 1   | A     | 334 | U    | C2'-C3'-O3' | -7.84 | 101.94      | 113.70   |
| 1   | A     | 56  | A    | C1'-C2'-O2' | 7.83  | 120.14      | 108.40   |
| 1   | A     | 291 | G    | C2'-C3'-O3' | 7.81  | 121.21      | 109.50   |
| 1   | A     | 354 | G    | O3'-P-O5'   | -7.79 | 92.32       | 104.00   |
| 1   | A     | 352 | U    | O3'-P-O5'   | 7.78  | 115.67      | 104.00   |
| 1   | A     | 98  | G    | O4'-C4'-C3' | -7.73 | 96.27       | 104.00   |
| 1   | A     | 173 | G    | C4'-C3'-O3' | -7.72 | 101.42      | 113.00   |
| 1   | A     | 97  | G    | P-O3'-C3'   | -7.71 | 108.63      | 120.20   |
| 1   | A     | 195 | U    | O3'-P-O5'   | -7.70 | 92.44       | 104.00   |
| 1   | A     | 291 | G    | P-O3'-C3'   | 7.66  | 131.70      | 120.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 33  | A    | P-O3'-C3'   | -7.65 | 108.72      | 120.20   |
| 1   | A     | 110 | A    | C3'-C2'-O2' | -7.62 | 103.16      | 114.60   |
| 1   | A     | 69  | C    | C4'-C3'-O3' | 7.58  | 124.37      | 113.00   |
| 1   | A     | 328 | C    | P-O3'-C3'   | -7.58 | 108.83      | 120.20   |
| 1   | A     | 271 | U    | P-O3'-C3'   | -7.53 | 108.91      | 120.20   |
| 1   | A     | 171 | A    | O3'-P-O5'   | 7.52  | 115.28      | 104.00   |
| 1   | A     | 137 | A    | P-O3'-C3'   | 7.48  | 131.43      | 120.20   |
| 1   | A     | 103 | U    | O3'-P-O5'   | 7.46  | 115.18      | 104.00   |
| 1   | A     | 352 | U    | C1'-C2'-O2' | 7.41  | 119.51      | 108.40   |
| 1   | A     | 286 | C    | C3'-C2'-O2' | -7.40 | 103.49      | 114.60   |
| 1   | A     | 388 | G    | O3'-P-O5'   | -7.38 | 92.92       | 104.00   |
| 1   | A     | 335 | G    | P-O3'-C3'   | -7.34 | 109.19      | 120.20   |
| 1   | A     | 52  | G    | O3'-P-O5'   | -7.33 | 93.00       | 104.00   |
| 1   | A     | 24  | U    | C4'-C3'-O3' | -7.33 | 102.00      | 113.00   |
| 1   | A     | 374 | G    | O3'-P-O5'   | -7.33 | 93.01       | 104.00   |
| 1   | A     | 85  | C    | C2'-C3'-O3' | -7.31 | 102.73      | 113.70   |
| 1   | A     | 29  | G    | C1'-C2'-O2' | 7.31  | 119.36      | 108.40   |
| 1   | A     | 346 | C    | C3'-C2'-O2' | 7.29  | 121.63      | 110.70   |
| 1   | A     | 70  | C    | OP1-P-O3'   | -7.27 | 86.19       | 108.00   |
| 1   | A     | 57  | A    | C2'-C3'-O3' | -7.24 | 102.84      | 113.70   |
| 1   | A     | 297 | A    | P-O3'-C3'   | 7.22  | 131.03      | 120.20   |
| 1   | A     | 351 | C    | P-O3'-C3'   | 7.19  | 130.99      | 120.20   |
| 1   | A     | 46  | G    | O3'-P-O5'   | -7.13 | 93.31       | 104.00   |
| 1   | A     | 49  | A    | O3'-P-O5'   | -7.09 | 93.36       | 104.00   |
| 1   | A     | 83  | G    | P-O3'-C3'   | 7.09  | 130.83      | 120.20   |
| 1   | A     | 336 | G    | P-O3'-C3'   | -7.06 | 109.61      | 120.20   |
| 1   | A     | 303 | C    | O3'-P-O5'   | -7.03 | 93.46       | 104.00   |
| 1   | A     | 317 | G    | C1'-C2'-O2' | -7.01 | 97.88       | 108.40   |
| 1   | A     | 319 | A    | C4'-C3'-O3' | -7.00 | 102.50      | 113.00   |
| 1   | A     | 297 | A    | C2'-C3'-O3' | 6.97  | 124.15      | 113.70   |
| 1   | A     | 376 | A    | O3'-P-O5'   | -6.94 | 93.58       | 104.00   |
| 1   | A     | 194 | G    | O3'-P-O5'   | -6.91 | 93.63       | 104.00   |
| 1   | A     | 257 | C    | P-O3'-C3'   | -6.88 | 109.87      | 120.20   |
| 1   | A     | 69  | C    | P-O3'-C3'   | -6.86 | 109.92      | 120.20   |
| 1   | A     | 154 | A    | C3'-C2'-O2' | 6.84  | 120.97      | 110.70   |
| 1   | A     | 36  | G    | C4'-C3'-O3' | -6.84 | 102.74      | 113.00   |
| 1   | A     | 54  | A    | O3'-P-O5'   | -6.81 | 93.78       | 104.00   |
| 1   | A     | 289 | C    | P-O3'-C3'   | 6.79  | 130.38      | 120.20   |
| 1   | A     | 126 | U    | P-O3'-C3'   | -6.78 | 110.03      | 120.20   |
| 1   | A     | 72  | A    | P-O3'-C3'   | -6.76 | 110.05      | 120.20   |
| 1   | A     | 234 | U    | O3'-P-O5'   | -6.74 | 93.89       | 104.00   |
| 1   | A     | 50  | A    | P-O3'-C3'   | 6.70  | 130.25      | 120.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 284 | G    | C2'-C3'-O3' | -6.70 | 103.65      | 113.70   |
| 1   | A     | 246 | A    | P-O3'-C3'   | -6.68 | 110.17      | 120.20   |
| 1   | A     | 361 | C    | C2'-C3'-O3' | -6.67 | 103.69      | 113.70   |
| 1   | A     | 168 | U    | P-O3'-C3'   | 6.67  | 130.20      | 120.20   |
| 1   | A     | 363 | U    | C3'-C2'-O2' | 6.66  | 120.69      | 110.70   |
| 1   | A     | 37  | U    | C2'-C3'-O3' | 6.64  | 119.47      | 109.50   |
| 1   | A     | 261 | C    | P-O3'-C3'   | 6.63  | 130.15      | 120.20   |
| 1   | A     | 297 | A    | O3'-P-O5'   | 6.62  | 113.94      | 104.00   |
| 1   | A     | 336 | G    | C2'-C3'-O3' | -6.62 | 103.77      | 113.70   |
| 1   | A     | 77  | A    | C1'-C2'-O2' | 6.62  | 118.33      | 108.40   |
| 1   | A     | 47  | U    | O3'-P-O5'   | 6.62  | 113.93      | 104.00   |
| 1   | A     | 69  | C    | O4'-C4'-C3' | -6.62 | 97.38       | 104.00   |
| 1   | A     | 105 | A    | C2'-C3'-O3' | -6.59 | 103.82      | 113.70   |
| 1   | A     | 49  | A    | O5'-P-OP2   | -6.53 | 88.42       | 108.00   |
| 1   | A     | 22  | U    | P-O3'-C3'   | -6.51 | 110.44      | 120.20   |
| 1   | A     | 356 | A    | C1'-C2'-O2' | 6.47  | 118.11      | 108.40   |
| 1   | A     | 300 | G    | P-O3'-C3'   | 6.45  | 129.88      | 120.20   |
| 1   | A     | 122 | A    | C2'-C3'-O3' | -6.45 | 104.02      | 113.70   |
| 1   | A     | 27  | A    | P-O3'-C3'   | -6.38 | 110.62      | 120.20   |
| 1   | A     | 119 | C    | C1'-C2'-O2' | 6.38  | 117.96      | 108.40   |
| 1   | A     | 206 | A    | P-O3'-C3'   | 6.37  | 129.75      | 120.20   |
| 1   | A     | 116 | C    | OP1-P-O3'   | -6.36 | 88.92       | 108.00   |
| 1   | A     | 199 | U    | O3'-P-O5'   | -6.35 | 94.48       | 104.00   |
| 1   | A     | 79  | G    | C1'-C2'-O2' | 6.32  | 117.88      | 108.40   |
| 1   | A     | 373 | G    | O3'-P-O5'   | -6.31 | 94.54       | 104.00   |
| 1   | A     | 288 | G    | C2'-C3'-O3' | -6.31 | 104.24      | 113.70   |
| 1   | A     | 68  | G    | P-O3'-C3'   | -6.30 | 110.75      | 120.20   |
| 1   | A     | 90  | G    | O3'-P-O5'   | -6.30 | 94.55       | 104.00   |
| 1   | A     | 290 | A    | C4'-C3'-O3' | -6.30 | 103.55      | 113.00   |
| 1   | A     | 55  | G    | C3'-C2'-O2' | 6.27  | 120.11      | 110.70   |
| 1   | A     | 245 | A    | O3'-P-O5'   | 6.27  | 113.40      | 104.00   |
| 1   | A     | 229 | G    | O3'-P-O5'   | -6.26 | 94.61       | 104.00   |
| 1   | A     | 22  | U    | C4'-C3'-O3' | 6.22  | 122.33      | 113.00   |
| 1   | A     | 51  | G    | P-O3'-C3'   | -6.21 | 110.88      | 120.20   |
| 1   | A     | 45  | U    | C3'-C2'-O2' | 6.16  | 119.94      | 110.70   |
| 1   | A     | 148 | C    | P-O3'-C3'   | -6.16 | 110.96      | 120.20   |
| 1   | A     | 330 | A    | O3'-P-O5'   | 6.15  | 113.23      | 104.00   |
| 1   | A     | 277 | A    | C3'-C2'-O2' | -6.13 | 101.50      | 110.70   |
| 1   | A     | 330 | A    | C3'-C2'-O2' | 6.13  | 119.90      | 110.70   |
| 1   | A     | 245 | A    | C4'-C3'-O3' | -6.13 | 100.21      | 109.40   |
| 1   | A     | 341 | C    | P-O3'-C3'   | 6.11  | 129.37      | 120.20   |
| 1   | A     | 59  | U    | OP2-P-O3'   | 6.11  | 126.32      | 108.00   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 97  | G    | C1'-C2'-O2' | -6.10 | 99.24       | 108.40   |
| 1   | A     | 367 | C    | O3'-P-O5'   | -6.09 | 94.86       | 104.00   |
| 1   | A     | 349 | A    | P-O3'-C3'   | -6.08 | 111.08      | 120.20   |
| 1   | A     | 74  | C    | C3'-C2'-O2' | 6.08  | 119.82      | 110.70   |
| 1   | A     | 385 | G    | P-O3'-C3'   | -6.07 | 111.09      | 120.20   |
| 1   | A     | 236 | G    | C1'-C2'-O2' | -6.07 | 99.29       | 108.40   |
| 1   | A     | 259 | U    | C4'-C3'-O3' | -6.07 | 103.89      | 113.00   |
| 1   | A     | 61  | A    | O3'-P-O5'   | 6.06  | 113.09      | 104.00   |
| 1   | A     | 381 | C    | O3'-P-O5'   | -6.05 | 94.93       | 104.00   |
| 1   | A     | 172 | U    | C4'-C3'-O3' | -6.03 | 103.95      | 113.00   |
| 1   | A     | 389 | U    | C2'-C3'-O3' | 6.03  | 118.55      | 109.50   |
| 1   | A     | 139 | C    | C3'-C2'-O2' | 6.03  | 119.74      | 110.70   |
| 1   | A     | 376 | A    | C1'-C2'-O2' | -6.03 | 102.76      | 111.80   |
| 1   | A     | 331 | G    | P-O3'-C3'   | -5.99 | 111.21      | 120.20   |
| 1   | A     | 61  | A    | C3'-C2'-O2' | 5.99  | 119.69      | 110.70   |
| 1   | A     | 26  | U    | O3'-P-O5'   | 5.98  | 112.97      | 104.00   |
| 1   | A     | 323 | C    | O3'-P-O5'   | -5.96 | 95.07       | 104.00   |
| 1   | A     | 118 | G    | P-O3'-C3'   | -5.95 | 111.28      | 120.20   |
| 1   | A     | 224 | A    | P-O3'-C3'   | 5.95  | 129.12      | 120.20   |
| 1   | A     | 1   | G    | P-O3'-C3'   | 5.93  | 129.10      | 120.20   |
| 1   | A     | 198 | U    | O5'-P-OP2   | -5.92 | 90.25       | 108.00   |
| 1   | A     | 34  | G    | OP1-P-O3'   | -5.92 | 90.25       | 108.00   |
| 1   | A     | 363 | U    | P-O3'-C3'   | -5.91 | 111.33      | 120.20   |
| 1   | A     | 171 | A    | O5'-P-OP1   | -5.91 | 90.28       | 108.00   |
| 1   | A     | 28  | G    | C1'-C2'-O2' | 5.89  | 117.24      | 108.40   |
| 1   | A     | 59  | U    | C3'-C2'-O2' | -5.86 | 101.91      | 110.70   |
| 1   | A     | 283 | A    | O3'-P-O5'   | -5.85 | 95.22       | 104.00   |
| 1   | A     | 96  | U    | C1'-C2'-O2' | -5.85 | 99.62       | 108.40   |
| 1   | A     | 240 | A    | C4'-C3'-O3' | -5.84 | 104.23      | 113.00   |
| 1   | A     | 365 | U    | C4'-C3'-O3' | -5.84 | 104.24      | 113.00   |
| 1   | A     | 47  | U    | O5'-P-OP1   | -5.82 | 90.54       | 108.00   |
| 1   | A     | 96  | U    | C4'-C3'-O3' | -5.81 | 104.29      | 113.00   |
| 1   | A     | 46  | G    | C1'-C2'-O2' | 5.80  | 117.10      | 108.40   |
| 1   | A     | 123 | C    | P-O3'-C3'   | -5.80 | 111.50      | 120.20   |
| 1   | A     | 46  | G    | C2'-C3'-O3' | -5.79 | 105.01      | 113.70   |
| 1   | A     | 152 | U    | O3'-P-O5'   | -5.79 | 95.32       | 104.00   |
| 1   | A     | 352 | U    | C2'-C3'-O3' | -5.79 | 105.02      | 113.70   |
| 1   | A     | 95  | A    | O3'-P-O5'   | 5.78  | 112.67      | 104.00   |
| 1   | A     | 247 | A    | C1'-C2'-O2' | -5.77 | 99.75       | 108.40   |
| 1   | A     | 136 | G    | O3'-P-O5'   | -5.77 | 95.35       | 104.00   |
| 1   | A     | 127 | C    | C3'-C2'-O2' | 5.76  | 119.35      | 110.70   |
| 1   | A     | 191 | A    | C1'-C2'-O2' | 5.76  | 117.05      | 108.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 282 | A    | O3'-P-O5'   | -5.75 | 95.38       | 104.00   |
| 1   | A     | 201 | C    | C1'-C2'-O2' | 5.75  | 117.02      | 108.40   |
| 1   | A     | 333 | A    | C2'-C3'-O3' | 5.75  | 118.12      | 109.50   |
| 1   | A     | 91  | C    | O5'-P-OP2   | 5.74  | 125.21      | 108.00   |
| 1   | A     | 112 | C    | C1'-C2'-O2' | -5.74 | 99.79       | 108.40   |
| 1   | A     | 276 | A    | P-O3'-C3'   | -5.74 | 111.59      | 120.20   |
| 1   | A     | 284 | G    | O3'-P-O5'   | -5.74 | 95.39       | 104.00   |
| 1   | A     | 128 | G    | C3'-C2'-O2' | 5.73  | 119.29      | 110.70   |
| 1   | A     | 49  | A    | C4'-C3'-O3' | -5.72 | 104.42      | 113.00   |
| 1   | A     | 48  | G    | O3'-P-O5'   | 5.71  | 112.57      | 104.00   |
| 1   | A     | 288 | G    | C4'-C3'-O3' | -5.71 | 104.43      | 113.00   |
| 1   | A     | 54  | A    | C3'-C2'-O2' | 5.71  | 119.26      | 110.70   |
| 1   | A     | 82  | U    | P-O3'-C3'   | 5.71  | 128.76      | 120.20   |
| 1   | A     | 170 | G    | C1'-C2'-O2' | 5.70  | 116.95      | 108.40   |
| 1   | A     | 91  | C    | C4'-C3'-O3' | -5.68 | 104.47      | 113.00   |
| 1   | A     | 190 | C    | C4'-C3'-O3' | -5.67 | 104.49      | 113.00   |
| 1   | A     | 213 | G    | C3'-C2'-O2' | 5.67  | 119.20      | 110.70   |
| 1   | A     | 277 | A    | N9-C1'-C2'  | 5.67  | 120.50      | 112.00   |
| 1   | A     | 356 | A    | P-O3'-C3'   | -5.66 | 111.71      | 120.20   |
| 1   | A     | 208 | A    | P-O3'-C3'   | -5.66 | 111.71      | 120.20   |
| 1   | A     | 25  | A    | O3'-P-O5'   | -5.66 | 95.52       | 104.00   |
| 1   | A     | 67  | A    | C4'-C3'-O3' | -5.65 | 104.52      | 113.00   |
| 1   | A     | 335 | G    | C2'-C3'-O3' | -5.65 | 105.23      | 113.70   |
| 1   | A     | 166 | A    | P-O3'-C3'   | -5.64 | 111.73      | 120.20   |
| 1   | A     | 45  | U    | P-O3'-C3'   | -5.64 | 111.74      | 120.20   |
| 1   | A     | 60  | A    | C3'-C2'-O2' | 5.64  | 119.16      | 110.70   |
| 1   | A     | 128 | G    | C4'-C3'-O3' | -5.63 | 104.55      | 113.00   |
| 1   | A     | 269 | G    | C1'-C2'-O2' | 5.63  | 116.85      | 108.40   |
| 1   | A     | 116 | C    | C1'-C2'-O2' | 5.62  | 116.84      | 108.40   |
| 1   | A     | 194 | G    | C2'-C3'-O3' | -5.62 | 105.27      | 113.70   |
| 1   | A     | 87  | G    | OP2-P-O3'   | 5.62  | 124.85      | 108.00   |
| 1   | A     | 4   | U    | C2'-C3'-O3' | -5.61 | 105.28      | 113.70   |
| 1   | A     | 187 | A    | C3'-C2'-O2' | 5.61  | 119.12      | 110.70   |
| 1   | A     | 23  | C    | O3'-P-O5'   | -5.56 | 95.65       | 104.00   |
| 1   | A     | 14  | G    | OP1-P-O3'   | -5.54 | 91.38       | 108.00   |
| 1   | A     | 106 | A    | O3'-P-O5'   | -5.53 | 95.70       | 104.00   |
| 1   | A     | 58  | G    | OP2-P-O3'   | 5.51  | 124.54      | 108.00   |
| 1   | A     | 197 | C    | O5'-P-OP1   | -5.51 | 91.47       | 108.00   |
| 1   | A     | 37  | U    | O3'-P-O5'   | -5.50 | 95.75       | 104.00   |
| 1   | A     | 200 | U    | C2'-C3'-O3' | -5.50 | 105.44      | 113.70   |
| 1   | A     | 71  | U    | P-O3'-C3'   | -5.50 | 111.95      | 120.20   |
| 1   | A     | 359 | G    | C2'-C3'-O3' | -5.50 | 105.45      | 113.70   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 43  | A    | P-O3'-C3'   | -5.45 | 112.03      | 120.20   |
| 1   | A     | 278 | A    | C4'-C3'-O3' | -5.45 | 104.83      | 113.00   |
| 1   | A     | 92  | G    | P-O3'-C3'   | -5.44 | 112.05      | 120.20   |
| 1   | A     | 32  | G    | C2'-C3'-O3' | 5.44  | 121.85      | 113.70   |
| 1   | A     | 53  | C    | O3'-P-O5'   | -5.44 | 95.84       | 104.00   |
| 1   | A     | 388 | G    | C4'-C3'-O3' | 5.44  | 117.56      | 109.40   |
| 1   | A     | 148 | C    | C4'-C3'-O3' | -5.42 | 104.88      | 113.00   |
| 1   | A     | 191 | A    | C4'-C3'-O3' | -5.42 | 104.88      | 113.00   |
| 1   | A     | 301 | U    | P-O3'-C3'   | -5.41 | 112.08      | 120.20   |
| 1   | A     | 63  | A    | OP1-P-O3'   | -5.41 | 91.77       | 108.00   |
| 1   | A     | 59  | U    | OP1-P-O3'   | -5.40 | 91.80       | 108.00   |
| 1   | A     | 14  | G    | C3'-C2'-O2' | 5.38  | 118.77      | 110.70   |
| 1   | A     | 113 | G    | P-O3'-C3'   | -5.38 | 112.13      | 120.20   |
| 1   | A     | 39  | C    | C1'-C2'-O2' | -5.37 | 100.34      | 108.40   |
| 1   | A     | 24  | U    | O3'-P-O5'   | -5.37 | 95.94       | 104.00   |
| 1   | A     | 85  | C    | C1'-C2'-O2' | -5.37 | 100.35      | 108.40   |
| 1   | A     | 53  | C    | P-O3'-C3'   | -5.37 | 112.15      | 120.20   |
| 1   | A     | 80  | G    | O3'-P-O5'   | 5.37  | 112.05      | 104.00   |
| 1   | A     | 360 | C    | O3'-P-O5'   | 5.36  | 112.04      | 104.00   |
| 1   | A     | 9   | G    | C1'-C2'-O2' | 5.36  | 116.44      | 108.40   |
| 1   | A     | 32  | G    | C4'-C3'-O3' | -5.36 | 104.96      | 113.00   |
| 1   | A     | 86  | C    | C3'-C2'-O2' | 5.36  | 118.74      | 110.70   |
| 1   | A     | 49  | A    | C1'-C2'-O2' | -5.36 | 100.37      | 108.40   |
| 1   | A     | 172 | U    | P-O3'-C3'   | -5.34 | 112.18      | 120.20   |
| 1   | A     | 356 | A    | O3'-P-O5'   | -5.34 | 95.98       | 104.00   |
| 1   | A     | 223 | A    | P-O3'-C3'   | -5.34 | 112.19      | 120.20   |
| 1   | A     | 8   | C    | C2'-C3'-O3' | -5.33 | 105.71      | 113.70   |
| 1   | A     | 276 | A    | C3'-C2'-O2' | 5.32  | 118.68      | 110.70   |
| 1   | A     | 276 | A    | O4'-C4'-C3' | -5.31 | 98.69       | 104.00   |
| 1   | A     | 103 | U    | P-O3'-C3'   | 5.30  | 128.16      | 120.20   |
| 1   | A     | 131 | C    | C3'-C2'-O2' | 5.30  | 118.65      | 110.70   |
| 1   | A     | 164 | U    | C3'-C2'-O2' | 5.30  | 118.65      | 110.70   |
| 1   | A     | 357 | C    | O3'-P-O5'   | -5.29 | 96.07       | 104.00   |
| 1   | A     | 109 | A    | O5'-P-OP1   | -5.29 | 92.14       | 108.00   |
| 1   | A     | 335 | G    | C1'-C2'-O2' | 5.28  | 116.32      | 108.40   |
| 1   | A     | 212 | G    | P-O3'-C3'   | -5.27 | 112.29      | 120.20   |
| 1   | A     | 60  | A    | O3'-P-O5'   | 5.27  | 111.90      | 104.00   |
| 1   | A     | 3   | G    | C3'-C2'-O2' | 5.26  | 118.59      | 110.70   |
| 1   | A     | 188 | A    | C1'-C2'-O2' | -5.25 | 100.52      | 108.40   |
| 1   | A     | 125 | U    | P-O3'-C3'   | -5.24 | 112.34      | 120.20   |
| 1   | A     | 287 | A    | C3'-C2'-O2' | 5.24  | 118.56      | 110.70   |
| 1   | A     | 236 | G    | C4'-C3'-O3' | -5.23 | 105.16      | 113.00   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 328 | C    | O3'-P-O5'   | -5.22 | 96.17       | 104.00   |
| 1   | A     | 28  | G    | O5'-P-OP2   | 5.22  | 123.66      | 108.00   |
| 1   | A     | 119 | C    | P-O3'-C3'   | -5.22 | 112.37      | 120.20   |
| 1   | A     | 25  | A    | P-O5'-C5'   | -5.21 | 113.08      | 120.90   |
| 1   | A     | 318 | A    | P-O3'-C3'   | -5.21 | 112.39      | 120.20   |
| 1   | A     | 93  | A    | OP1-P-O3'   | -5.20 | 92.39       | 108.00   |
| 1   | A     | 91  | C    | O5'-P-OP1   | -5.20 | 92.40       | 108.00   |
| 1   | A     | 11  | C    | C2'-C3'-O3' | -5.20 | 105.90      | 113.70   |
| 1   | A     | 359 | G    | C4'-C3'-O3' | -5.19 | 105.21      | 113.00   |
| 1   | A     | 366 | A    | P-O3'-C3'   | -5.19 | 112.41      | 120.20   |
| 1   | A     | 170 | G    | P-O5'-C5'   | -5.19 | 113.12      | 120.90   |
| 1   | A     | 356 | A    | C4'-C3'-O3' | -5.17 | 105.24      | 113.00   |
| 1   | A     | 111 | G    | C4'-C3'-O3' | -5.17 | 105.25      | 113.00   |
| 1   | A     | 250 | C    | C2'-C3'-O3' | -5.16 | 105.96      | 113.70   |
| 1   | A     | 97  | G    | O4'-C4'-C3' | -5.16 | 98.84       | 104.00   |
| 1   | A     | 171 | A    | C2'-C3'-O3' | -5.14 | 105.99      | 113.70   |
| 1   | A     | 232 | G    | P-O3'-C3'   | -5.14 | 112.49      | 120.20   |
| 1   | A     | 92  | G    | N9-C1'-C2'  | 5.13  | 119.69      | 112.00   |
| 1   | A     | 122 | A    | C1'-C2'-O2' | -5.13 | 100.71      | 108.40   |
| 1   | A     | 98  | G    | P-O3'-C3'   | -5.13 | 112.51      | 120.20   |
| 1   | A     | 60  | A    | OP2-P-O3'   | 5.12  | 123.36      | 108.00   |
| 1   | A     | 227 | A    | O3'-P-O5'   | -5.11 | 96.33       | 104.00   |
| 1   | A     | 115 | A    | C1'-C2'-O2' | 5.10  | 116.04      | 108.40   |
| 1   | A     | 199 | U    | C1'-C2'-O2' | -5.09 | 100.76      | 108.40   |
| 1   | A     | 117 | G    | OP1-P-O3'   | -5.08 | 92.77       | 108.00   |
| 1   | A     | 320 | G    | C4'-C3'-O3' | -5.07 | 105.40      | 113.00   |
| 1   | A     | 62  | C    | C2'-C3'-O3' | -5.06 | 106.10      | 113.70   |
| 1   | A     | 202 | U    | P-O3'-C3'   | -5.06 | 112.61      | 120.20   |
| 1   | A     | 260 | A    | C2'-C3'-O3' | -5.05 | 101.92      | 109.50   |
| 1   | A     | 387 | U    | P-O3'-C3'   | -5.05 | 112.63      | 120.20   |
| 1   | A     | 9   | G    | P-O3'-C3'   | -5.04 | 112.65      | 120.20   |
| 1   | A     | 127 | C    | C2'-C3'-O3' | -5.04 | 106.15      | 113.70   |
| 1   | A     | 258 | U    | P-O3'-C3'   | -5.02 | 112.67      | 120.20   |
| 1   | A     | 366 | A    | O4'-C4'-C3' | -5.01 | 98.98       | 104.00   |
| 1   | A     | 94  | C    | O3'-P-O5'   | 5.01  | 111.51      | 104.00   |
| 1   | A     | 61  | A    | P-O5'-C5'   | -5.00 | 113.40      | 120.90   |

There are no chirality outliers.

There are no planarity outliers.



## 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     | 8412  | 0        | 4224     | 261     | 0            |
| 2   | A     | 31    | 0        | 0        | 0       | 0            |
| 3   | A     | 14    | 0        | 0        | 4       | 0            |
| 4   | A     | 14    | 0        | 26       | 1       | 0            |
| 5   | A     | 35    | 0        | 31       | 5       | 0            |
| 6   | A     | 31    | 0        | 0        | 1       | 0            |
| All | All   | 8537  | 0        | 4281     | 262     | 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 21.

All (262) 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:39:C:H2'  | 1:A:40:C:H5''  | 1.26                     | 1.13              |
| 1:A:334:U:H6  | 1:A:334:U:H5'  | 1.18                     | 1.05              |
| 1:A:334:U:H6  | 1:A:334:U:C5'  | 1.69                     | 1.04              |
| 1:A:39:C:C2'  | 1:A:40:C:H5''  | 1.89                     | 1.02              |
| 1:A:139:C:H2' | 1:A:140:A:H8   | 1.25                     | 0.99              |
| 1:A:334:U:H5' | 1:A:334:U:C6   | 1.99                     | 0.96              |
| 1:A:165:C:H42 | 1:A:212:G:H1   | 1.11                     | 0.94              |
| 1:A:2:U:H4'   | 1:A:3:G:OP2    | 1.69                     | 0.92              |
| 1:A:60:A:C2'  | 1:A:61:A:H5'   | 2.00                     | 0.91              |
| 1:A:352:U:O2' | 1:A:353:U:H5'  | 1.69                     | 0.91              |
| 1:A:40:C:H6   | 1:A:40:C:H5'   | 1.35                     | 0.90              |
| 1:A:116:C:OP1 | 5:A:450:EPE:C5 | 2.23                     | 0.87              |
| 1:A:316:G:C2  | 1:A:317:G:H1'  | 2.10                     | 0.86              |
| 1:A:139:C:H2' | 1:A:140:A:C8   | 2.11                     | 0.85              |
| 1:A:338:G:H2' | 1:A:339:U:O5'  | 1.78                     | 0.83              |
| 1:A:39:C:H2'  | 1:A:40:C:C5'   | 2.08                     | 0.82              |
| 1:A:221:U:H3' | 1:A:222:A:H5'' | 1.61                     | 0.81              |
| 1:A:83:G:N3   | 1:A:83:G:H2'   | 1.96                     | 0.81              |
| 1:A:62:C:O2'  | 1:A:63:A:H5'   | 1.79                     | 0.81              |
| 1:A:167:A:C2' | 1:A:168:U:H5'  | 2.12                     | 0.80              |
| 1:A:60:A:H2'  | 1:A:61:A:H5'   | 1.64                     | 0.80              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 3:A:441:NH4:N  | 6:A:530:HOH:O   | 2.16                     | 0.79              |
| 1:A:167:A:H5'' | 1:A:167:A:H8    | 1.51                     | 0.76              |
| 1:A:334:U:C5'  | 1:A:334:U:C6    | 2.60                     | 0.75              |
| 1:A:63:A:O2'   | 1:A:64:G:H5'    | 1.86                     | 0.75              |
| 1:A:138:A:OP1  | 1:A:139:C:C5    | 2.40                     | 0.75              |
| 1:A:306:U:H3   | 1:A:313:A:N6    | 1.84                     | 0.75              |
| 1:A:190:C:H5'' | 1:A:190:C:H6    | 1.52                     | 0.74              |
| 1:A:325:G:O2'  | 1:A:326:A:OP2   | 2.05                     | 0.73              |
| 1:A:40:C:H5'   | 1:A:40:C:C6     | 2.22                     | 0.73              |
| 1:A:114:G:C6   | 1:A:115:A:C2    | 2.78                     | 0.72              |
| 1:A:88:U:C2'   | 1:A:89:G:H5'    | 2.20                     | 0.71              |
| 1:A:27:A:H2'   | 1:A:28:G:O4'    | 1.91                     | 0.71              |
| 1:A:206:A:O2'  | 1:A:207:A:H5''  | 1.91                     | 0.70              |
| 1:A:48:G:N2    | 1:A:59:U:C5     | 2.60                     | 0.70              |
| 1:A:148:C:H5'' | 1:A:148:C:H6    | 1.57                     | 0.70              |
| 1:A:361:C:H2'  | 1:A:362:G:H8    | 1.55                     | 0.70              |
| 1:A:387:U:C2'  | 1:A:388:G:H5'   | 2.21                     | 0.70              |
| 1:A:28:G:N2    | 1:A:40:C:O2     | 2.20                     | 0.70              |
| 1:A:164:U:H3   | 1:A:213:G:H1    | 1.41                     | 0.69              |
| 1:A:151:A:H5'' | 1:A:153:G:H5'   | 1.74                     | 0.69              |
| 1:A:107:G:N3   | 1:A:107:G:H2'   | 2.08                     | 0.69              |
| 1:A:167:A:H2'  | 1:A:168:U:H5'   | 1.75                     | 0.69              |
| 1:A:116:C:OP1  | 5:A:450:EPE:H52 | 1.93                     | 0.68              |
| 1:A:387:U:O2'  | 1:A:388:G:H5'   | 1.93                     | 0.68              |
| 1:A:60:A:O2'   | 1:A:61:A:H5'    | 1.93                     | 0.68              |
| 1:A:116:C:OP1  | 5:A:450:EPE:H51 | 1.94                     | 0.67              |
| 1:A:222:A:H4'  | 1:A:222:A:OP1   | 1.94                     | 0.67              |
| 1:A:338:G:C2'  | 1:A:339:U:O5'   | 2.42                     | 0.66              |
| 1:A:88:U:H2'   | 1:A:89:G:H5'    | 1.77                     | 0.66              |
| 1:A:117:G:N7   | 5:A:450:EPE:S   | 2.68                     | 0.66              |
| 1:A:49:A:C4    | 1:A:60:A:C2     | 2.84                     | 0.66              |
| 1:A:65:U:H5''  | 1:A:66:U:O5'    | 1.96                     | 0.65              |
| 1:A:49:A:C6    | 1:A:60:A:N3     | 2.65                     | 0.65              |
| 1:A:49:A:C5    | 1:A:60:A:C2     | 2.85                     | 0.65              |
| 1:A:219:A:H2'  | 1:A:220:G:H8    | 1.62                     | 0.65              |
| 1:A:316:G:N2   | 1:A:317:G:H1'   | 2.12                     | 0.65              |
| 1:A:146:U:H2'  | 1:A:147:U:C6    | 2.31                     | 0.64              |
| 1:A:63:A:H2'   | 1:A:64:G:H8     | 1.63                     | 0.64              |
| 1:A:111:G:OP1  | 3:A:445:NH4:N   | 2.30                     | 0.64              |
| 1:A:362:G:H2'  | 1:A:363:U:C6    | 2.33                     | 0.64              |
| 1:A:142:G:N2   | 1:A:144:A:H3'   | 2.13                     | 0.64              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:A:116:C:OP2  | 5:A:450:EPE:O2S | 2.16                     | 0.63              |
| 1:A:306:U:O5'  | 1:A:306:U:H6    | 1.82                     | 0.63              |
| 1:A:213:G:H2'  | 1:A:214:U:C6    | 2.35                     | 0.62              |
| 1:A:40:C:H6    | 1:A:40:C:C5'    | 2.11                     | 0.62              |
| 1:A:65:U:H5''  | 1:A:66:U:C5'    | 2.30                     | 0.62              |
| 1:A:361:C:H2'  | 1:A:362:G:C8    | 2.34                     | 0.62              |
| 1:A:61:A:H2'   | 1:A:62:C:C6     | 2.36                     | 0.61              |
| 1:A:299:A:O4'  | 1:A:301:U:C6    | 2.54                     | 0.61              |
| 1:A:352:U:HO2' | 1:A:353:U:H5'   | 1.66                     | 0.60              |
| 1:A:48:G:C2    | 1:A:59:U:C5     | 2.90                     | 0.60              |
| 1:A:61:A:H2'   | 1:A:62:C:H6     | 1.65                     | 0.60              |
| 1:A:309:U:O2'  | 1:A:310:C:OP2   | 2.18                     | 0.60              |
| 1:A:389:U:H5'  | 1:A:389:U:C6    | 2.36                     | 0.60              |
| 1:A:339:U:H2'  | 1:A:341:C:C4    | 2.36                     | 0.60              |
| 1:A:287:A:H8   | 1:A:287:A:OP2   | 1.85                     | 0.59              |
| 1:A:333:A:O2'  | 1:A:334:U:OP2   | 2.19                     | 0.59              |
| 1:A:170:G:O2'  | 1:A:171:A:H5'   | 2.03                     | 0.59              |
| 1:A:355:A:H2'  | 1:A:356:A:O4'   | 2.03                     | 0.58              |
| 1:A:104:G:H5'' | 1:A:105:A:H5'   | 1.84                     | 0.58              |
| 1:A:360:C:H2'  | 1:A:361:C:C6    | 2.39                     | 0.58              |
| 1:A:219:A:H2'  | 1:A:220:G:C8    | 2.39                     | 0.58              |
| 1:A:314:G:H2'  | 1:A:315:G:H8    | 1.68                     | 0.58              |
| 1:A:291:G:O2'  | 1:A:292:A:OP2   | 2.21                     | 0.58              |
| 1:A:221:U:H3'  | 1:A:222:A:C5'   | 2.29                     | 0.58              |
| 1:A:190:C:H5'' | 1:A:190:C:C6    | 2.37                     | 0.57              |
| 1:A:40:C:H2'   | 1:A:41:G:O4'    | 2.04                     | 0.57              |
| 1:A:306:U:H3   | 1:A:313:A:H61   | 1.53                     | 0.57              |
| 1:A:349:A:O5'  | 1:A:349:A:H8    | 1.86                     | 0.57              |
| 1:A:180:C:C2'  | 1:A:181:A:H5''  | 2.34                     | 0.57              |
| 1:A:2:U:H5''   | 1:A:2:U:H6      | 1.70                     | 0.57              |
| 1:A:180:C:C3'  | 1:A:181:A:H5''  | 2.34                     | 0.57              |
| 1:A:95:A:H2'   | 1:A:96:U:C6     | 2.40                     | 0.56              |
| 1:A:95:A:H2'   | 1:A:96:U:H6     | 1.71                     | 0.56              |
| 1:A:238:U:H5'  | 1:A:238:U:C6    | 2.41                     | 0.56              |
| 1:A:174:A:H4'  | 1:A:238:U:O2'   | 2.06                     | 0.56              |
| 1:A:311:G:N3   | 1:A:311:G:H2'   | 2.19                     | 0.56              |
| 1:A:341:C:H4'  | 1:A:342:G:O5'   | 2.06                     | 0.56              |
| 1:A:55:G:N2    | 1:A:202:U:C2    | 2.73                     | 0.56              |
| 1:A:238:U:H5'  | 1:A:238:U:H6    | 1.71                     | 0.55              |
| 1:A:350:G:O5'  | 1:A:350:G:H8    | 1.90                     | 0.55              |
| 1:A:308:U:O2'  | 1:A:310:C:N4    | 2.38                     | 0.55              |

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| Atom-1         | Atom-2        | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|---------------|--------------------------|-------------------|
| 1:A:387:U:H2'  | 1:A:388:G:H5' | 1.88                     | 0.55              |
| 1:A:181:A:OP1  | 1:A:181:A:C8  | 2.60                     | 0.55              |
| 1:A:152:U:H4'  | 1:A:153:G:OP2 | 2.07                     | 0.55              |
| 1:A:276:A:H2'  | 1:A:277:A:O4' | 2.07                     | 0.55              |
| 1:A:7:C:H2'    | 1:A:8:C:H6    | 1.70                     | 0.55              |
| 1:A:238:U:H6   | 1:A:238:U:C5' | 2.20                     | 0.55              |
| 1:A:107:G:N3   | 1:A:107:G:C2' | 2.69                     | 0.54              |
| 1:A:122:A:O4'  | 1:A:247:A:H4' | 2.08                     | 0.54              |
| 1:A:358:C:OP2  | 3:A:439:NH4:N | 2.40                     | 0.54              |
| 1:A:140:A:H3'  | 1:A:141:C:H6  | 1.71                     | 0.54              |
| 1:A:32:G:N2    | 1:A:34:G:H3'  | 2.22                     | 0.54              |
| 1:A:49:A:C6    | 1:A:60:A:C2   | 2.95                     | 0.54              |
| 1:A:167:A:H5'' | 1:A:167:A:C8  | 2.38                     | 0.54              |
| 1:A:83:G:N3    | 1:A:83:G:C2'  | 2.70                     | 0.54              |
| 1:A:57:A:C2    | 1:A:200:U:C2  | 2.95                     | 0.54              |
| 1:A:100:A:H2'  | 1:A:101:U:O4' | 2.08                     | 0.54              |
| 1:A:334:U:C6   | 1:A:334:U:C4' | 2.92                     | 0.53              |
| 1:A:7:C:H2'    | 1:A:8:C:C6    | 2.43                     | 0.53              |
| 1:A:88:U:O2'   | 1:A:89:G:H5'  | 2.08                     | 0.53              |
| 1:A:66:U:H2'   | 1:A:67:A:C8   | 2.44                     | 0.53              |
| 1:A:45:U:H2'   | 1:A:46:G:C8   | 2.44                     | 0.53              |
| 1:A:63:A:H2'   | 1:A:64:G:C8   | 2.43                     | 0.53              |
| 1:A:85:C:C2    | 1:A:99:A:C2   | 2.97                     | 0.53              |
| 1:A:128:G:O2'  | 1:A:192:A:N3  | 2.37                     | 0.52              |
| 1:A:283:A:H2'  | 1:A:284:G:O4' | 2.09                     | 0.52              |
| 1:A:296:C:H2'  | 1:A:297:A:C8  | 2.45                     | 0.52              |
| 1:A:369:G:H5'' | 1:A:370:A:OP1 | 2.10                     | 0.51              |
| 1:A:254:A:H2'  | 1:A:255:U:C6  | 2.45                     | 0.51              |
| 1:A:302:A:C2   | 1:A:318:A:C4  | 2.98                     | 0.51              |
| 1:A:165:C:N4   | 1:A:212:G:H1  | 1.94                     | 0.51              |
| 1:A:195:U:C2'  | 1:A:196:C:H5' | 2.41                     | 0.51              |
| 1:A:49:A:C2    | 1:A:60:A:C2   | 2.98                     | 0.50              |
| 1:A:148:C:H5'' | 1:A:148:C:C6  | 2.42                     | 0.50              |
| 1:A:45:U:H2'   | 1:A:46:G:H8   | 1.75                     | 0.50              |
| 1:A:121:A:C8   | 1:A:248:G:H1' | 2.47                     | 0.50              |
| 1:A:328:C:H2'  | 1:A:329:A:C8  | 2.46                     | 0.50              |
| 1:A:169:G:C6   | 1:A:170:G:C5  | 2.98                     | 0.50              |
| 1:A:302:A:H2'  | 1:A:303:C:O4' | 2.12                     | 0.50              |
| 1:A:35:A:O2'   | 1:A:37:U:OP2  | 2.29                     | 0.50              |
| 1:A:388:G:O2'  | 1:A:389:U:OP2 | 2.29                     | 0.50              |
| 1:A:-2:G:C8    | 1:A:-2:G:H5'' | 2.45                     | 0.50              |

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| Atom-1         | Atom-2        | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|---------------|--------------------------|-------------------|
| 1:A:300:G:O2'  | 1:A:301:U:P   | 2.70                     | 0.50              |
| 1:A:91:C:N3    | 1:A:274:G:O2' | 2.45                     | 0.50              |
| 1:A:320:G:O2'  | 1:A:321:G:H5' | 2.11                     | 0.50              |
| 1:A:59:U:O5'   | 1:A:59:U:H6   | 1.94                     | 0.49              |
| 1:A:327:A:C5   | 1:A:328:C:C5  | 3.00                     | 0.49              |
| 1:A:90:G:H5''  | 1:A:91:C:OP2  | 2.12                     | 0.49              |
| 1:A:154:A:N6   | 1:A:155:G:N3  | 2.60                     | 0.49              |
| 1:A:167:A:O2'  | 1:A:168:U:H5' | 2.12                     | 0.49              |
| 1:A:146:U:H2'  | 1:A:147:U:H6  | 1.72                     | 0.49              |
| 1:A:139:C:C2'  | 1:A:140:A:O5' | 2.60                     | 0.49              |
| 1:A:207:A:OP1  | 1:A:207:A:H3' | 2.13                     | 0.49              |
| 1:A:290:A:C2   | 1:A:291:G:O6  | 2.66                     | 0.49              |
| 1:A:370:A:C4   | 1:A:371:A:C8  | 3.01                     | 0.49              |
| 1:A:325:G:O2'  | 1:A:326:A:P   | 2.71                     | 0.49              |
| 1:A:169:G:H2'  | 1:A:170:G:O4' | 2.13                     | 0.48              |
| 1:A:156:G:H2'  | 1:A:157:C:O4' | 2.13                     | 0.48              |
| 1:A:328:C:H2'  | 1:A:329:A:H8  | 1.79                     | 0.48              |
| 1:A:74:C:H6    | 1:A:74:C:O5'  | 1.97                     | 0.48              |
| 1:A:243:G:H5'' | 1:A:244:G:OP2 | 2.14                     | 0.48              |
| 1:A:52:G:C2    | 1:A:205:C:O2  | 2.67                     | 0.48              |
| 1:A:351:C:C2'  | 1:A:352:U:H5' | 2.44                     | 0.48              |
| 1:A:32:G:N1    | 1:A:35:A:OP2  | 2.43                     | 0.47              |
| 1:A:333:A:HO2' | 1:A:334:U:P   | 2.36                     | 0.47              |
| 1:A:325:G:HO2' | 1:A:326:A:P   | 2.34                     | 0.47              |
| 1:A:200:U:H2'  | 1:A:201:C:H6  | 1.79                     | 0.47              |
| 1:A:307:G:H2'  | 1:A:307:G:N3  | 2.29                     | 0.47              |
| 1:A:195:U:H5'' | 1:A:195:U:H6  | 1.80                     | 0.47              |
| 1:A:279:C:H2'  | 1:A:280:A:O4' | 2.14                     | 0.47              |
| 1:A:296:C:H2'  | 1:A:297:A:H8  | 1.78                     | 0.47              |
| 1:A:121:A:N7   | 1:A:248:G:H1' | 2.29                     | 0.47              |
| 1:A:197:C:N3   | 1:A:198:U:C5  | 2.83                     | 0.47              |
| 1:A:194:G:H1'  | 1:A:240:A:O2' | 2.16                     | 0.46              |
| 1:A:72:A:N6    | 1:A:115:A:H4' | 2.31                     | 0.46              |
| 1:A:192:A:H2'  | 1:A:193:A:C8  | 2.51                     | 0.46              |
| 1:A:61:A:O2'   | 1:A:62:C:H5'  | 2.16                     | 0.46              |
| 1:A:68:G:C5    | 1:A:120:A:C2  | 3.04                     | 0.46              |
| 1:A:256:U:H2'  | 1:A:257:C:C6  | 2.51                     | 0.46              |
| 1:A:290:A:O5'  | 1:A:290:A:H8  | 1.99                     | 0.46              |
| 1:A:306:U:C2   | 1:A:307:G:C8  | 3.04                     | 0.46              |
| 1:A:251:U:H2'  | 1:A:252:G:C8  | 2.52                     | 0.45              |
| 1:A:314:G:H2'  | 1:A:315:G:C8  | 2.49                     | 0.45              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:A:368:C:C2   | 1:A:374:G:N2    | 2.85                     | 0.45              |
| 1:A:91:C:H2'   | 1:A:92:G:O4'    | 2.17                     | 0.45              |
| 1:A:94:C:O2    | 1:A:94:C:H2'    | 2.16                     | 0.45              |
| 1:A:116:C:H6   | 1:A:116:C:O5'   | 2.00                     | 0.45              |
| 1:A:139:C:H2'  | 1:A:140:A:O5'   | 2.16                     | 0.44              |
| 1:A:257:C:H2'  | 1:A:258:U:O4'   | 2.17                     | 0.44              |
| 1:A:57:A:C2    | 1:A:200:U:N3    | 2.84                     | 0.44              |
| 1:A:147:U:H2'  | 1:A:148:C:C6    | 2.51                     | 0.44              |
| 1:A:165:C:H5'' | 1:A:165:C:H6    | 1.82                     | 0.44              |
| 1:A:183:A:H2'  | 1:A:184:A:H8    | 1.82                     | 0.44              |
| 1:A:279:C:H6   | 1:A:279:C:O5'   | 2.01                     | 0.44              |
| 1:A:387:U:H2'  | 1:A:388:G:C5'   | 2.48                     | 0.44              |
| 1:A:73:A:H2'   | 1:A:74:C:O4'    | 2.17                     | 0.44              |
| 1:A:76:C:H2'   | 1:A:77:A:O4'    | 2.18                     | 0.44              |
| 1:A:24:U:C2    | 1:A:248:G:N2    | 2.86                     | 0.44              |
| 1:A:201:C:O2   | 1:A:201:C:H2'   | 2.18                     | 0.44              |
| 1:A:49:A:C5    | 1:A:199:U:C5    | 3.06                     | 0.44              |
| 1:A:51:G:OP2   | 1:A:51:G:H8     | 2.01                     | 0.44              |
| 1:A:60:A:C3'   | 1:A:61:A:H5'    | 2.47                     | 0.44              |
| 1:A:64:G:H2'   | 1:A:65:U:H6     | 1.82                     | 0.44              |
| 1:A:162:U:H3'  | 1:A:163:A:H5''  | 2.00                     | 0.43              |
| 1:A:352:U:H2'  | 1:A:353:U:H6    | 1.83                     | 0.43              |
| 1:A:147:U:H2'  | 1:A:148:C:H6    | 1.83                     | 0.43              |
| 1:A:352:U:H2'  | 1:A:353:U:C6    | 2.52                     | 0.43              |
| 1:A:254:A:H2'  | 1:A:255:U:H6    | 1.83                     | 0.43              |
| 1:A:321:G:H2'  | 1:A:322:A:O4'   | 2.19                     | 0.43              |
| 1:A:324:G:C6   | 1:A:325:G:N1    | 2.87                     | 0.43              |
| 1:A:181:A:H2'  | 1:A:182:U:H6    | 1.84                     | 0.43              |
| 1:A:170:G:C6   | 1:A:171:A:N7    | 2.87                     | 0.43              |
| 1:A:355:A:N6   | 1:A:388:G:H1'   | 2.34                     | 0.43              |
| 1:A:78:A:H2'   | 1:A:79:G:O4'    | 2.19                     | 0.42              |
| 1:A:351:C:O2'  | 1:A:352:U:H5'   | 2.19                     | 0.42              |
| 1:A:181:A:H2'  | 1:A:182:U:C6    | 2.55                     | 0.42              |
| 1:A:333:A:N9   | 1:A:335:G:N7    | 2.67                     | 0.42              |
| 1:A:335:G:O5'  | 1:A:335:G:H8    | 2.02                     | 0.42              |
| 1:A:138:A:N1   | 1:A:224:A:O2'   | 2.47                     | 0.42              |
| 1:A:58:G:O6    | 4:A:446:SPM:H82 | 2.20                     | 0.42              |
| 1:A:64:G:H2'   | 1:A:65:U:C6     | 2.55                     | 0.42              |
| 1:A:137:A:H4'  | 1:A:138:A:O5'   | 2.19                     | 0.42              |
| 1:A:183:A:O2'  | 1:A:369:G:N2    | 2.51                     | 0.42              |
| 1:A:122:A:H2'  | 1:A:123:C:O4'   | 2.19                     | 0.42              |

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| Atom-1         | Atom-2        | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|---------------|--------------------------|-------------------|
| 1:A:130:U:H2'  | 1:A:131:C:C6  | 2.54                     | 0.42              |
| 1:A:238:U:C6   | 1:A:238:U:C5' | 3.00                     | 0.42              |
| 1:A:48:G:H2'   | 1:A:58:G:N2   | 2.35                     | 0.42              |
| 1:A:49:A:C6    | 1:A:60:A:C4   | 3.07                     | 0.42              |
| 1:A:28:G:O6    | 3:A:435:NH4:N | 2.52                     | 0.42              |
| 1:A:154:A:N6   | 1:A:155:G:C2  | 2.88                     | 0.41              |
| 1:A:379:U:O5'  | 1:A:379:U:H6  | 2.03                     | 0.41              |
| 1:A:389:U:H5'  | 1:A:389:U:H6  | 1.83                     | 0.41              |
| 1:A:49:A:N1    | 1:A:60:A:N3   | 2.68                     | 0.41              |
| 1:A:-2:G:H2'   | 1:A:-2:G:N3   | 2.36                     | 0.41              |
| 1:A:120:A:OP1  | 1:A:237:A:O2' | 2.36                     | 0.41              |
| 1:A:174:A:N7   | 1:A:191:A:H2  | 2.18                     | 0.41              |
| 1:A:300:G:HO2' | 1:A:301:U:P   | 2.44                     | 0.41              |
| 1:A:164:U:H3   | 1:A:213:G:H22 | 1.66                     | 0.41              |
| 1:A:196:C:H2'  | 1:A:197:C:H6  | 1.85                     | 0.41              |
| 1:A:300:G:C4   | 1:A:317:G:C6  | 3.08                     | 0.41              |
| 1:A:333:A:N1   | 1:A:349:A:C6  | 2.88                     | 0.41              |
| 1:A:2:U:C4'    | 1:A:3:G:OP2   | 2.55                     | 0.41              |
| 1:A:3:G:N3     | 1:A:3:G:H2'   | 2.36                     | 0.41              |
| 1:A:114:G:C6   | 1:A:115:A:N1  | 2.88                     | 0.41              |
| 1:A:38:C:H2'   | 1:A:39:C:H6   | 1.84                     | 0.41              |
| 1:A:313:A:H2'  | 1:A:314:G:O4' | 2.21                     | 0.41              |
| 1:A:108:G:O2'  | 1:A:261:C:H3' | 2.21                     | 0.41              |
| 1:A:141:C:O2'  | 1:A:385:G:OP1 | 2.32                     | 0.41              |
| 1:A:156:G:C2   | 1:A:157:C:H1' | 2.55                     | 0.41              |
| 1:A:64:G:C2'   | 1:A:65:U:O5'  | 2.69                     | 0.41              |
| 1:A:62:C:H2'   | 1:A:63:A:H8   | 1.86                     | 0.40              |
| 1:A:138:A:H5'  | 1:A:139:C:H5' | 2.03                     | 0.40              |
| 1:A:87:G:H2'   | 1:A:88:U:H5'  | 2.03                     | 0.40              |
| 1:A:159:A:H2'  | 1:A:160:G:C5' | 2.50                     | 0.40              |
| 1:A:23:C:C2    | 1:A:249:A:C2  | 3.09                     | 0.40              |
| 1:A:151:A:C5'  | 1:A:153:G:H5' | 2.49                     | 0.40              |
| 1:A:324:G:O5'  | 1:A:324:G:H8  | 2.03                     | 0.40              |
| 1:A:57:A:N6    | 1:A:58:G:N2   | 2.70                     | 0.40              |
| 1:A:196:C:C2   | 1:A:197:C:C5  | 3.09                     | 0.40              |
| 1:A:334:U:H2'  | 1:A:335:G:H5' | 2.03                     | 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     | 391/393 (99%) | 137 (35%)         | 31 (7%)         |

All (137) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | -1  | G    |
| 1   | A     | 0   | G    |
| 1   | A     | 1   | G    |
| 1   | A     | 2   | U    |
| 1   | A     | 13  | U    |
| 1   | A     | 16  | G    |
| 1   | A     | 23  | C    |
| 1   | A     | 25  | A    |
| 1   | A     | 26  | U    |
| 1   | A     | 28  | G    |
| 1   | A     | 29  | G    |
| 1   | A     | 37  | U    |
| 1   | A     | 38  | C    |
| 1   | A     | 40  | C    |
| 1   | A     | 41  | G    |
| 1   | A     | 42  | A    |
| 1   | A     | 43  | A    |
| 1   | A     | 49  | A    |
| 1   | A     | 50  | A    |
| 1   | A     | 51  | G    |
| 1   | A     | 55  | G    |
| 1   | A     | 60  | A    |
| 1   | A     | 61  | A    |
| 1   | A     | 63  | A    |
| 1   | A     | 65  | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 66  | U    |
| 1   | A     | 78  | A    |
| 1   | A     | 82  | U    |
| 1   | A     | 83  | G    |
| 1   | A     | 84  | U    |
| 1   | A     | 86  | C    |
| 1   | A     | 89  | G    |
| 1   | A     | 90  | G    |
| 1   | A     | 93  | A    |
| 1   | A     | 97  | G    |
| 1   | A     | 105 | A    |
| 1   | A     | 106 | A    |
| 1   | A     | 108 | G    |
| 1   | A     | 111 | G    |
| 1   | A     | 113 | G    |
| 1   | A     | 115 | A    |
| 1   | A     | 134 | A    |
| 1   | A     | 137 | A    |
| 1   | A     | 138 | A    |
| 1   | A     | 139 | C    |
| 1   | A     | 140 | A    |
| 1   | A     | 145 | C    |
| 1   | A     | 146 | U    |
| 1   | A     | 148 | C    |
| 1   | A     | 151 | A    |
| 1   | A     | 152 | U    |
| 1   | A     | 153 | G    |
| 1   | A     | 158 | U    |
| 1   | A     | 160 | G    |
| 1   | A     | 161 | G    |
| 1   | A     | 163 | A    |
| 1   | A     | 164 | U    |
| 1   | A     | 165 | C    |
| 1   | A     | 167 | A    |
| 1   | A     | 168 | U    |
| 1   | A     | 169 | G    |
| 1   | A     | 174 | A    |
| 1   | A     | 180 | C    |
| 1   | A     | 181 | A    |
| 1   | A     | 190 | C    |
| 1   | A     | 196 | C    |
| 1   | A     | 197 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 198 | U    |
| 1   | A     | 199 | U    |
| 1   | A     | 201 | C    |
| 1   | A     | 202 | U    |
| 1   | A     | 203 | G    |
| 1   | A     | 206 | A    |
| 1   | A     | 207 | A    |
| 1   | A     | 208 | A    |
| 1   | A     | 213 | G    |
| 1   | A     | 217 | A    |
| 1   | A     | 218 | G    |
| 1   | A     | 221 | U    |
| 1   | A     | 222 | A    |
| 1   | A     | 223 | A    |
| 1   | A     | 224 | A    |
| 1   | A     | 237 | A    |
| 1   | A     | 238 | U    |
| 1   | A     | 243 | G    |
| 1   | A     | 245 | A    |
| 1   | A     | 246 | A    |
| 1   | A     | 247 | A    |
| 1   | A     | 258 | U    |
| 1   | A     | 260 | A    |
| 1   | A     | 261 | C    |
| 1   | A     | 269 | G    |
| 1   | A     | 271 | U    |
| 1   | A     | 273 | U    |
| 1   | A     | 279 | C    |
| 1   | A     | 285 | U    |
| 1   | A     | 287 | A    |
| 1   | A     | 290 | A    |
| 1   | A     | 291 | G    |
| 1   | A     | 292 | A    |
| 1   | A     | 297 | A    |
| 1   | A     | 298 | U    |
| 1   | A     | 300 | G    |
| 1   | A     | 301 | U    |
| 1   | A     | 303 | C    |
| 1   | A     | 308 | U    |
| 1   | A     | 309 | U    |
| 1   | A     | 310 | C    |
| 1   | A     | 311 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 312 | C    |
| 1   | A     | 313 | A    |
| 1   | A     | 316 | G    |
| 1   | A     | 318 | A    |
| 1   | A     | 320 | G    |
| 1   | A     | 321 | G    |
| 1   | A     | 322 | A    |
| 1   | A     | 326 | A    |
| 1   | A     | 332 | U    |
| 1   | A     | 333 | A    |
| 1   | A     | 334 | U    |
| 1   | A     | 335 | G    |
| 1   | A     | 337 | C    |
| 1   | A     | 339 | U    |
| 1   | A     | 340 | U    |
| 1   | A     | 341 | C    |
| 1   | A     | 342 | G    |
| 1   | A     | 343 | C    |
| 1   | A     | 352 | U    |
| 1   | A     | 355 | A    |
| 1   | A     | 361 | C    |
| 1   | A     | 369 | G    |
| 1   | A     | 370 | A    |
| 1   | A     | 372 | C    |
| 1   | A     | 377 | C    |
| 1   | A     | 378 | G    |
| 1   | A     | 384 | U    |
| 1   | A     | 389 | U    |

All (31) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 40  | C    |
| 1   | A     | 50  | A    |
| 1   | A     | 55  | G    |
| 1   | A     | 59  | U    |
| 1   | A     | 82  | U    |
| 1   | A     | 83  | G    |
| 1   | A     | 105 | A    |
| 1   | A     | 115 | A    |
| 1   | A     | 137 | A    |
| 1   | A     | 152 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 168 | U    |
| 1   | A     | 174 | A    |
| 1   | A     | 198 | U    |
| 1   | A     | 206 | A    |
| 1   | A     | 207 | A    |
| 1   | A     | 237 | A    |
| 1   | A     | 289 | C    |
| 1   | A     | 291 | G    |
| 1   | A     | 297 | A    |
| 1   | A     | 300 | G    |
| 1   | A     | 308 | U    |
| 1   | A     | 310 | C    |
| 1   | A     | 311 | G    |
| 1   | A     | 320 | G    |
| 1   | A     | 325 | G    |
| 1   | A     | 333 | A    |
| 1   | A     | 334 | U    |
| 1   | A     | 341 | C    |
| 1   | A     | 366 | A    |
| 1   | A     | 369 | G    |
| 1   | A     | 389 | U    |

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 50 ligands modelled in this entry, 31 are monoatomic and 14 are modelled with single atom - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 4   | SPM  | A     | 446 | -    | 13,13,13     | 0.59 | 0           | 12,12,12    | 1.13 | 1 (8%)      |
| 5   | EPE  | A     | 448 | -    | 12,12,15     | 2.16 | 3 (25%)     | 15,16,20    | 1.90 | 2 (13%)     |
| 5   | EPE  | A     | 449 | -    | 0,3,15       | -    | -           | 0,3,20      | -    | -           |
| 5   | EPE  | A     | 450 | -    | 15,15,15     | 2.14 | 2 (13%)     | 19,20,20    | 1.25 | 2 (10%)     |
| 5   | EPE  | A     | 447 | -    | 0,3,15       | -    | -           | 0,3,20      | -    | -           |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 5   | EPE  | A     | 448 | -    | -       | 5/6/14/19  | 1/1/1/1 |
| 5   | EPE  | A     | 450 | -    | -       | 6/9/19/19  | 0/1/1/1 |
| 4   | SPM  | A     | 446 | -    | -       | 6/11/11/11 | -       |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 5   | A     | 450 | EPE  | C10-S | -6.51 | 1.68        | 1.77     |
| 5   | A     | 448 | EPE  | C10-S | -5.65 | 1.69        | 1.77     |
| 5   | A     | 450 | EPE  | O3S-S | 4.83  | 1.65        | 1.47     |
| 5   | A     | 448 | EPE  | O3S-S | 4.07  | 1.62        | 1.47     |
| 5   | A     | 448 | EPE  | C9-N1 | 2.08  | 1.52        | 1.47     |

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 5   | A     | 448 | EPE  | O3S-S-C10 | 5.57  | 116.91      | 106.00   |
| 5   | A     | 450 | EPE  | O1S-S-C10 | 2.62  | 110.69      | 106.73   |
| 5   | A     | 450 | EPE  | O2S-S-C10 | 2.35  | 110.28      | 106.73   |
| 5   | A     | 448 | EPE  | O3S-S-O1S | -2.25 | 105.77      | 111.40   |
| 4   | A     | 446 | SPM  | C6-N5-C4  | 2.01  | 122.93      | 113.40   |

There are no chirality outliers.

All (17) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 5   | A     | 448 | EPE  | C10-C9-N1-C2    |
| 5   | A     | 448 | EPE  | C9-C10-S-O1S    |
| 5   | A     | 448 | EPE  | C9-C10-S-O3S    |
| 4   | A     | 446 | SPM  | C7-C8-C9-N10    |
| 4   | A     | 446 | SPM  | N5-C6-C7-C8     |
| 4   | A     | 446 | SPM  | C2-C3-C4-N5     |
| 4   | A     | 446 | SPM  | C8-C9-N10-C11   |
| 5   | A     | 448 | EPE  | C10-C9-N1-C6    |
| 5   | A     | 450 | EPE  | C10-C9-N1-C6    |
| 5   | A     | 448 | EPE  | C9-C10-S-O2S    |
| 5   | A     | 450 | EPE  | C9-C10-S-O2S    |
| 5   | A     | 450 | EPE  | C10-C9-N1-C2    |
| 4   | A     | 446 | SPM  | C3-C4-N5-C6     |
| 5   | A     | 450 | EPE  | C9-C10-S-O3S    |
| 4   | A     | 446 | SPM  | C11-C12-C13-N14 |
| 5   | A     | 450 | EPE  | C8-C7-N4-C3     |
| 5   | A     | 450 | EPE  | C8-C7-N4-C5     |

All (1) ring outliers are listed below:

| Mol | Chain | Res | Type | Atoms             |
|-----|-------|-----|------|-------------------|
| 5   | A     | 448 | EPE  | C2-C3-C5-C6-N1-N4 |

2 monomers are involved in 6 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | A     | 446 | SPM  | 1       | 0            |
| 5   | A     | 450 | EPE  | 5       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 393/393 (100%) | -0.05  | 16 (4%) 41 34 | 45, 92, 218, 309      | 0     |

All (16) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 226 | G    | 5.2  |
| 1   | A     | 225 | U    | 4.6  |
| 1   | A     | 157 | C    | 3.6  |
| 1   | A     | 389 | U    | 2.7  |
| 1   | A     | 156 | G    | 2.7  |
| 1   | A     | 261 | C    | 2.7  |
| 1   | A     | 236 | G    | 2.5  |
| 1   | A     | 237 | A    | 2.4  |
| 1   | A     | 337 | C    | 2.3  |
| 1   | A     | 342 | G    | 2.3  |
| 1   | A     | 390 | G    | 2.3  |
| 1   | A     | 0   | G    | 2.1  |
| 1   | A     | 328 | C    | 2.1  |
| 1   | A     | 138 | A    | 2.0  |
| 1   | A     | 183 | A    | 2.0  |
| 1   | A     | -2  | G    | 2.0  |

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

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

| Mol | Type | Chain | Res | Atoms | RSCC  | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|-------|------|----------------------------|-------|
| 3   | NH4  | A     | 445 | 1/1   | -0.23 | 0.70 | 24,24,24,24                | 1     |
| 3   | NH4  | A     | 444 | 1/1   | 0.43  | 0.62 | 30,30,30,30                | 1     |
| 3   | NH4  | A     | 443 | 1/1   | 0.45  | 0.57 | 33,33,33,33                | 1     |
| 3   | NH4  | A     | 439 | 1/1   | 0.52  | 0.40 | 30,30,30,30                | 1     |
| 5   | EPE  | A     | 447 | 4/15  | 0.61  | 0.16 | 92,95,101,112              | 4     |
| 3   | NH4  | A     | 437 | 1/1   | 0.65  | 0.28 | 24,24,24,24                | 1     |
| 2   | MG   | A     | 425 | 1/1   | 0.67  | 0.16 | 141,141,141,141            | 0     |
| 2   | MG   | A     | 424 | 1/1   | 0.74  | 0.23 | 85,85,85,85                | 0     |
| 3   | NH4  | A     | 442 | 1/1   | 0.77  | 0.62 | 48,48,48,48                | 1     |
| 5   | EPE  | A     | 449 | 4/15  | 0.77  | 0.31 | 56,57,62,77                | 4     |
| 3   | NH4  | A     | 441 | 1/1   | 0.79  | 0.18 | 66,66,66,66                | 0     |
| 5   | EPE  | A     | 450 | 15/15 | 0.80  | 0.17 | 72,122,145,148             | 15    |
| 2   | MG   | A     | 410 | 1/1   | 0.84  | 0.30 | 72,72,72,72                | 0     |
| 2   | MG   | A     | 430 | 1/1   | 0.86  | 0.21 | 61,61,61,61                | 0     |
| 2   | MG   | A     | 431 | 1/1   | 0.88  | 0.14 | 94,94,94,94                | 0     |
| 3   | NH4  | A     | 434 | 1/1   | 0.88  | 0.12 | 87,87,87,87                | 0     |
| 2   | MG   | A     | 421 | 1/1   | 0.88  | 0.68 | 94,94,94,94                | 0     |
| 2   | MG   | A     | 404 | 1/1   | 0.88  | 0.20 | 97,97,97,97                | 0     |
| 2   | MG   | A     | 401 | 1/1   | 0.89  | 0.21 | 74,74,74,74                | 0     |
| 2   | MG   | A     | 415 | 1/1   | 0.89  | 0.25 | 59,59,59,59                | 0     |
| 2   | MG   | A     | 429 | 1/1   | 0.89  | 0.47 | 86,86,86,86                | 0     |
| 3   | NH4  | A     | 440 | 1/1   | 0.89  | 0.19 | 62,62,62,62                | 0     |
| 2   | MG   | A     | 409 | 1/1   | 0.89  | 0.29 | 70,70,70,70                | 0     |
| 2   | MG   | A     | 422 | 1/1   | 0.89  | 0.42 | 96,96,96,96                | 0     |
| 2   | MG   | A     | 405 | 1/1   | 0.90  | 0.07 | 90,90,90,90                | 0     |
| 5   | EPE  | A     | 448 | 12/15 | 0.90  | 0.29 | 54,67,79,80                | 12    |
| 2   | MG   | A     | 423 | 1/1   | 0.90  | 0.25 | 78,78,78,78                | 0     |
| 2   | MG   | A     | 427 | 1/1   | 0.90  | 0.09 | 67,67,67,67                | 0     |
| 2   | MG   | A     | 411 | 1/1   | 0.91  | 0.20 | 75,75,75,75                | 0     |
| 2   | MG   | A     | 414 | 1/1   | 0.92  | 0.30 | 85,85,85,85                | 0     |
| 2   | MG   | A     | 406 | 1/1   | 0.92  | 0.28 | 92,92,92,92                | 0     |
| 3   | NH4  | A     | 436 | 1/1   | 0.92  | 0.30 | 53,53,53,53                | 0     |
| 4   | SPM  | A     | 446 | 14/14 | 0.93  | 0.26 | 28,64,73,76                | 14    |
| 3   | NH4  | A     | 432 | 1/1   | 0.93  | 0.14 | 57,57,57,57                | 0     |
| 2   | MG   | A     | 428 | 1/1   | 0.93  | 0.27 | 75,75,75,75                | 0     |
| 3   | NH4  | A     | 435 | 1/1   | 0.93  | 0.19 | 33,33,33,33                | 0     |
| 2   | MG   | A     | 412 | 1/1   | 0.93  | 0.08 | 70,70,70,70                | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | MG   | A     | 413 | 1/1   | 0.94 | 0.15 | 72,72,72,72                 | 0     |
| 2   | MG   | A     | 418 | 1/1   | 0.94 | 0.16 | 47,47,47,47                 | 0     |
| 2   | MG   | A     | 420 | 1/1   | 0.94 | 0.22 | 75,75,75,75                 | 0     |
| 2   | MG   | A     | 426 | 1/1   | 0.95 | 0.10 | 92,92,92,92                 | 0     |
| 3   | NH4  | A     | 433 | 1/1   | 0.95 | 0.17 | 56,56,56,56                 | 0     |
| 3   | NH4  | A     | 438 | 1/1   | 0.95 | 0.24 | 47,47,47,47                 | 0     |
| 2   | MG   | A     | 417 | 1/1   | 0.95 | 0.10 | 103,103,103,103             | 0     |
| 2   | MG   | A     | 416 | 1/1   | 0.95 | 0.16 | 62,62,62,62                 | 0     |
| 2   | MG   | A     | 408 | 1/1   | 0.96 | 0.13 | 55,55,55,55                 | 0     |
| 2   | MG   | A     | 419 | 1/1   | 0.96 | 0.04 | 80,80,80,80                 | 0     |
| 2   | MG   | A     | 403 | 1/1   | 0.96 | 0.12 | 78,78,78,78                 | 0     |
| 2   | MG   | A     | 407 | 1/1   | 0.97 | 0.11 | 56,56,56,56                 | 0     |
| 2   | MG   | A     | 402 | 1/1   | 0.99 | 0.09 | 70,70,70,70                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.