



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:23 AM UTC

PDB ID : 2DER / pdb\_00002der  
Title : Cocrystal structure of an RNA sulfuration enzyme MnmA and tRNA-Glu in the initial tRNA binding state  
Authors : Numata, T.; Ikeuchi, Y.; Fukai, S.; Suzuki, T.; Nureki, O.  
Deposited on : 2006-02-17  
Resolution : 3.10 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

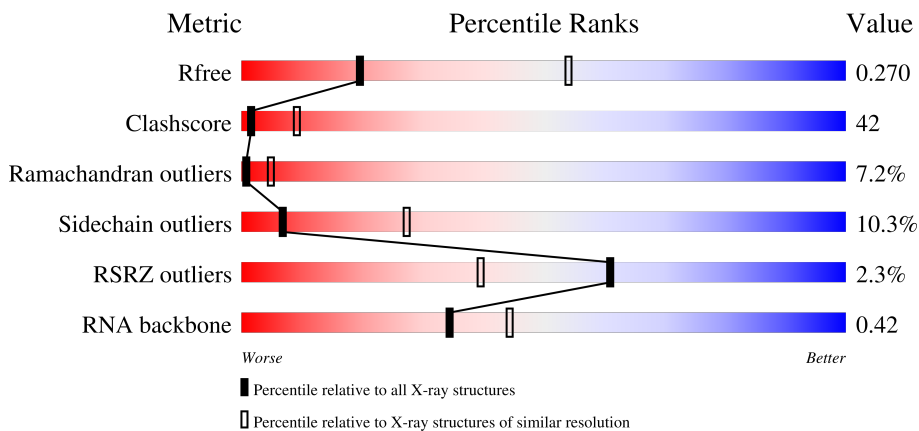
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

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



| Metric                | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|--------------------------|--|
| $R_{free}$            | 180053                   | 1456 (3.10-3.10)                                   |
| Clashscore            | 190562                   | 1539 (3.10-3.10)                                   |
| Ramachandran outliers | 187476                   | 1467 (3.10-3.10)                                   |
| Sidechain outliers    | 187428                   | 1467 (3.10-3.10)                                   |
| RSRZ outliers         | 180081                   | 1456 (3.10-3.10)                                   |
| RNA backbone          | 3983                     | 1022 (3.32-2.88)                                   |

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   | C     | 76     | 3% (Poor fit)<br>17% (0 outliers)   46% (1 outlier)   26% (2 outliers)   8% (3+ outliers)    |
| 1   | D     | 76     | 21% (0 outliers)   43% (1 outlier)   21% (2 outliers)   8% (3+ outliers)   7% (Not modelled) |
| 2   | A     | 380    | % (Poor fit)<br>33% (0 outliers)   47% (1 outlier)   11% (2 outliers)   8% (3+ outliers)     |
| 2   | B     | 380    | 4% (Poor fit)<br>29% (0 outliers)   54% (1 outlier)   10% (2 outliers)   6% (3+ outliers)    |

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:

| <b>Mol</b> | <b>Type</b> | <b>Chain</b> | <b>Res</b> | <b>Chirality</b> | <b>Geometry</b> | <b>Clashes</b> | <b>Electron density</b> |
|------------|-------------|--------------|------------|------------------|-----------------|----------------|-------------------------|
| 3          | PO4         | A            | 1002       | -                | -               | X              | -                       |

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 8675 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 tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
|     |       |          | Total | C   | N   | O   | P  |         |         |       |
| 1   | C     | 74       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1573  | 701 | 279 | 519 | 74 |         |         |       |
| 1   | D     | 71       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1509  | 673 | 269 | 496 | 71 |         |         |       |

- Molecule 2 is a protein called tRNA-specific 2-thiouridylase mnmA.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
|     |       |          | Total | C    | N   | O   | S  |         |         |       |
| 2   | A     | 348      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2733  | 1735 | 463 | 524 | 11 |         |         |       |
| 2   | B     | 359      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2815  | 1786 | 477 | 540 | 12 |         |         |       |

There are 24 discrepancies between the modelled and reference sequences:

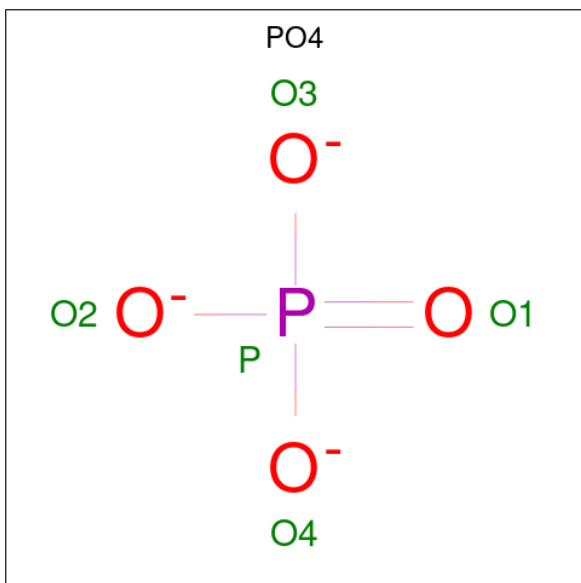
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -11     | MET      | -      | expression tag | UNP P25745 |
| A     | -10     | ARG      | -      | expression tag | UNP P25745 |
| A     | -9      | GLY      | -      | expression tag | UNP P25745 |
| A     | -8      | SER      | -      | expression tag | UNP P25745 |
| A     | -7      | HIS      | -      | expression tag | UNP P25745 |
| A     | -6      | HIS      | -      | expression tag | UNP P25745 |
| A     | -5      | HIS      | -      | expression tag | UNP P25745 |
| A     | -4      | HIS      | -      | expression tag | UNP P25745 |
| A     | -3      | HIS      | -      | expression tag | UNP P25745 |
| A     | -2      | HIS      | -      | expression tag | UNP P25745 |
| A     | -1      | GLY      | -      | expression tag | UNP P25745 |
| A     | 0       | SER      | -      | expression tag | UNP P25745 |
| B     | -11     | MET      | -      | expression tag | UNP P25745 |
| B     | -10     | ARG      | -      | expression tag | UNP P25745 |
| B     | -9      | GLY      | -      | expression tag | UNP P25745 |
| B     | -8      | SER      | -      | expression tag | UNP P25745 |
| B     | -7      | HIS      | -      | expression tag | UNP P25745 |

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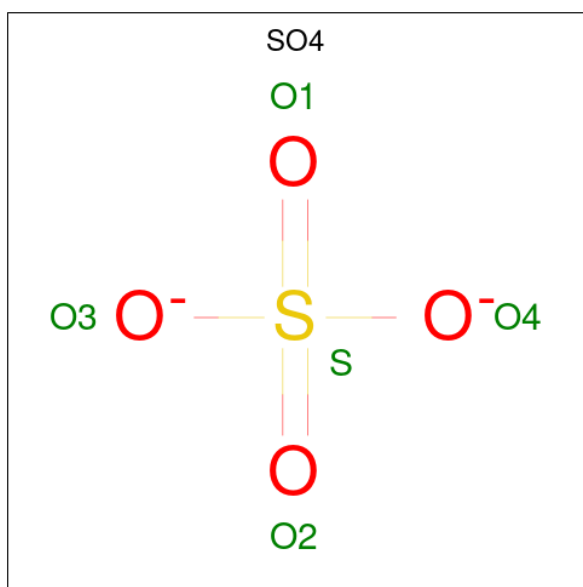
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| B     | -6      | HIS      | -      | expression tag | UNP P25745 |
| B     | -5      | HIS      | -      | expression tag | UNP P25745 |
| B     | -4      | HIS      | -      | expression tag | UNP P25745 |
| B     | -3      | HIS      | -      | expression tag | UNP P25745 |
| B     | -2      | HIS      | -      | expression tag | UNP P25745 |
| B     | -1      | GLY      | -      | expression tag | UNP P25745 |
| B     | 0       | SER      | -      | expression tag | UNP P25745 |

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).



| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 3   | C     | 1        | Total O P<br>5 4 1 | 0       | 0       |
| 3   | A     | 1        | Total O P<br>5 4 1 | 0       | 0       |
| 3   | B     | 1        | Total O P<br>5 4 1 | 0       | 0       |
| 3   | B     | 1        | Total O P<br>5 4 1 | 0       | 0       |

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



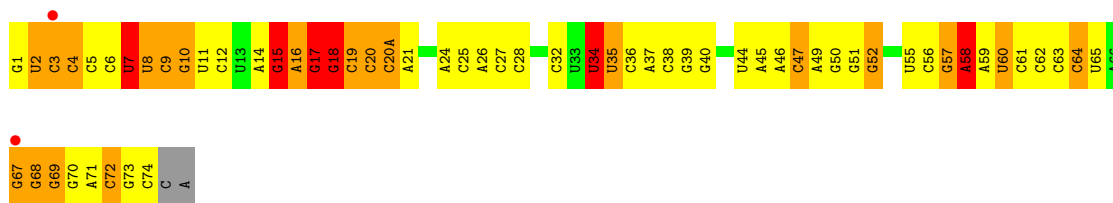
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

### 3 Residue-property plots [i](#)

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.

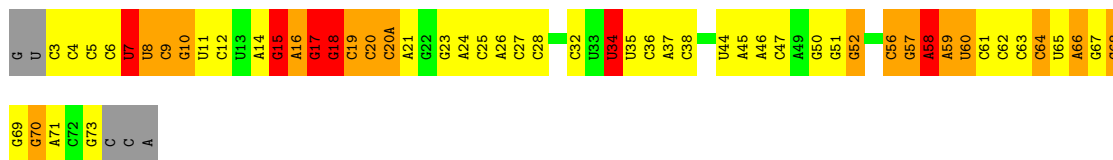
- Molecule 1: tRNA

Chain C: 3% 17% 46% 26% 8%



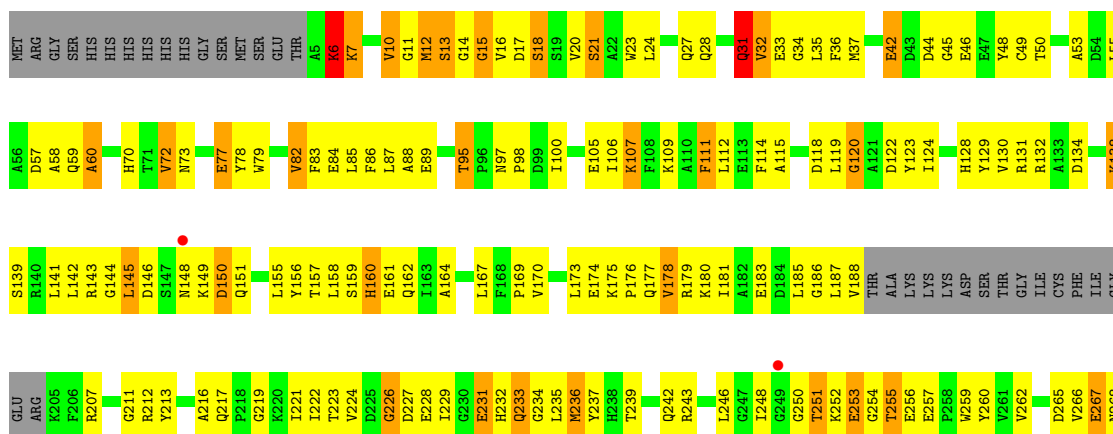
- Molecule 1: tRNA

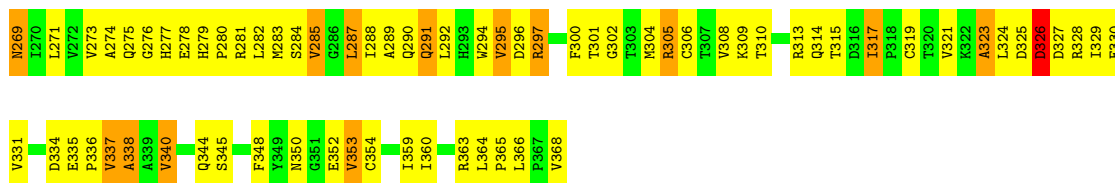
Chain D: 21% 43% 21% 8% 7%



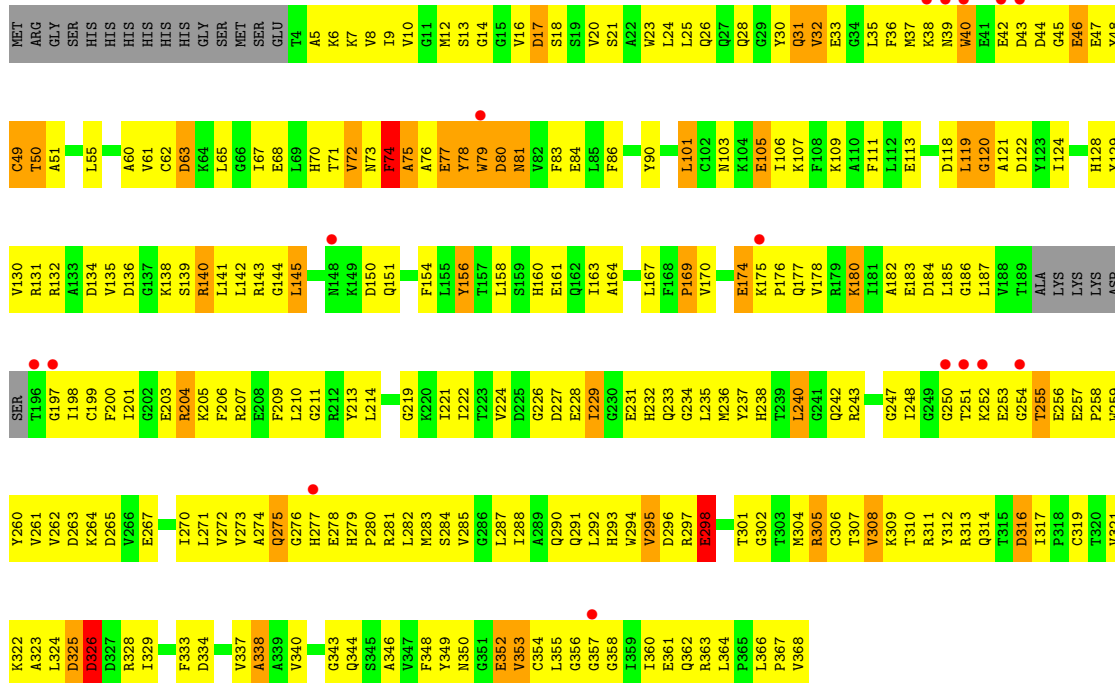
- Molecule 2: tRNA-specific 2-thiouridylase mmmA

Chain A: 33% 47% 11% 8%





• Molecule 2: tRNA-specific 2-thiouridylase mmmA



## 4 Data and refinement statistics i

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | C 1 2 1   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 225.39Å 175.84Å 52.97Å<br>90.00° 101.62° 90.00°             | Depositor        |
| Resolution (Å)  | 46.75 – 3.10<br>46.75 – 3.10                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 83.9 (46.75-3.10)<br>90.1 (46.75-3.10)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.12  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 0.96 (at 3.01Å)   | Xtrriage         |
| Refinement program  | CNS   | Depositor        |
| R, $R_{free}$   | 0.219 , 0.269<br>0.225 , 0.270                              | Depositor<br>DCC |
| $R_{free}$ test set   | 2924 reflections (4.74%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 57.3  | Xtrriage         |
| Anisotropy  | 0.120   | Xtrriage         |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 74.8   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$ | Xtrriage         |
| Estimated twinning fraction   | 0.055 for -h-2*1,-k,l                                       | Xtrriage         |
| $F_o, F_c$ correlation  | 0.91  | EDS              |
| Total number of atoms   | 8675  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 65.0  | wwPDB-VP         |

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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: SO4, PO4

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   | C     | 0.39         | 0/1755  | 0.85        | 7/2731 (0.3%)   |
| 1   | D     | 0.38         | 0/1684  | 0.86        | 7/2622 (0.3%)   |
| 2   | A     | 0.57         | 0/2790  | 1.06        | 18/3777 (0.5%)  |
| 2   | B     | 0.50         | 0/2873  | 1.02        | 21/3889 (0.5%)  |
| All | All   | 0.48         | 0/9102  | 0.97        | 53/13019 (0.4%) |

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   | C     | 0                   | 2                   |
| 1   | D     | 0                   | 2                   |
| All | All   | 0                   | 4                   |

There are no bond length outliers.

All (53) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 1   | D     | 34  | U    | C2'-C3'-O3' | 11.99  | 127.48      | 109.50   |
| 1   | C     | 34  | U    | C2'-C3'-O3' | 11.82  | 127.23      | 109.50   |
| 2   | A     | 45  | GLY  | N-CA-C      | -11.05 | 102.52      | 114.67   |
| 2   | A     | 14  | GLY  | N-CA-C      | -8.96  | 102.79      | 115.43   |
| 1   | D     | 34  | U    | C4'-C3'-O3' | 8.37   | 121.96      | 109.40   |
| 1   | C     | 34  | U    | C4'-C3'-O3' | 7.70   | 120.94      | 109.40   |
| 2   | A     | 77  | GLU  | N-CA-C      | -7.23  | 103.40      | 111.28   |
| 2   | B     | 14  | GLY  | N-CA-C      | -7.20  | 105.28      | 115.43   |
| 2   | B     | 105 | GLU  | N-CA-C      | 7.19   | 120.17      | 111.40   |
| 2   | B     | 340 | VAL  | N-CA-C      | -7.02  | 100.52      | 109.30   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | A     | 31  | GLN  | N-CA-C      | -6.96 | 95.75       | 107.99   |
| 1   | C     | 18  | G    | N9-C1'-C2'  | 6.77  | 124.15      | 114.00   |
| 1   | D     | 18  | G    | N9-C1'-C2'  | 6.70  | 124.05      | 114.00   |
| 2   | A     | 13  | SER  | N-CA-C      | -6.65 | 105.20      | 113.38   |
| 2   | B     | 50  | THR  | N-CA-C      | -6.60 | 105.30      | 113.15   |
| 2   | A     | 282 | LEU  | N-CA-C      | -6.47 | 105.69      | 113.97   |
| 1   | D     | 15  | G    | C2'-C3'-O3' | 6.21  | 118.82      | 109.50   |
| 2   | B     | 31  | GLN  | N-CA-C      | -6.17 | 97.13       | 107.99   |
| 1   | C     | 7   | U    | C2'-C3'-O3' | 6.12  | 118.68      | 109.50   |
| 2   | A     | 353 | VAL  | N-CA-C      | 6.07  | 117.52      | 108.23   |
| 2   | B     | 282 | LEU  | N-CA-C      | -6.01 | 106.11      | 113.50   |
| 1   | D     | 58  | A    | N9-C1'-C2'  | 5.97  | 120.95      | 112.00   |
| 2   | B     | 235 | LEU  | N-CA-C      | -5.94 | 106.36      | 113.97   |
| 1   | C     | 15  | G    | C2'-C3'-O3' | 5.90  | 118.35      | 109.50   |
| 2   | B     | 325 | ASP  | N-CA-C      | 5.87  | 115.59      | 107.73   |
| 1   | D     | 58  | A    | C4'-C3'-O3' | -5.84 | 104.24      | 113.00   |
| 2   | B     | 32  | VAL  | N-CA-C      | 5.76  | 115.90      | 107.37   |
| 1   | D     | 7   | U    | C2'-C3'-O3' | 5.60  | 117.90      | 109.50   |
| 1   | C     | 58  | A    | N9-C1'-C2'  | 5.51  | 120.26      | 112.00   |
| 2   | A     | 291 | GLN  | N-CA-C      | -5.49 | 103.70      | 111.56   |
| 2   | A     | 235 | LEU  | N-CA-C      | -5.47 | 106.60      | 113.72   |
| 2   | A     | 354 | CYS  | N-CA-C      | -5.42 | 100.96      | 109.25   |
| 2   | B     | 298 | GLU  | CA-C-N      | 5.38  | 125.39      | 119.90   |
| 2   | B     | 298 | GLU  | C-N-CA      | 5.38  | 125.39      | 119.90   |
| 2   | A     | 233 | GLN  | N-CA-C      | -5.34 | 102.10      | 113.20   |
| 2   | A     | 18  | SER  | N-CA-C      | -5.28 | 105.19      | 111.69   |
| 2   | A     | 300 | PHE  | N-CA-C      | 5.28  | 117.33      | 108.73   |
| 2   | A     | 340 | VAL  | N-CA-C      | -5.25 | 101.90      | 108.84   |
| 2   | B     | 352 | GLU  | N-CA-C      | -5.25 | 106.55      | 113.17   |
| 2   | B     | 174 | GLU  | N-CA-C      | -5.23 | 100.00      | 108.52   |
| 2   | B     | 291 | GLN  | N-CA-C      | -5.14 | 104.32      | 111.52   |
| 1   | C     | 47  | C    | N1-C1'-C2'  | 5.14  | 121.71      | 114.00   |
| 2   | B     | 343 | GLY  | N-CA-C      | -5.13 | 107.46      | 114.64   |
| 2   | B     | 63  | ASP  | N-CA-C      | -5.11 | 104.68      | 112.04   |
| 2   | B     | 334 | ASP  | N-CA-C      | -5.09 | 107.20      | 113.41   |
| 2   | B     | 13  | SER  | N-CA-C      | -5.08 | 107.13      | 113.38   |
| 2   | A     | 95  | THR  | CA-C-N      | 5.08  | 125.06      | 120.03   |
| 2   | A     | 95  | THR  | C-N-CA      | 5.08  | 125.06      | 120.03   |
| 2   | A     | 255 | THR  | N-CA-C      | -5.07 | 106.18      | 112.47   |
| 2   | A     | 6   | LYS  | N-CA-C      | 5.02  | 121.50      | 110.80   |
| 2   | B     | 364 | LEU  | CA-C-N      | 5.01  | 126.11      | 119.84   |
| 2   | B     | 364 | LEU  | C-N-CA      | 5.01  | 126.11      | 119.84   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2   | B     | 353 | VAL  | N-CA-C | 5.01 | 115.30      | 107.99   |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | C     | 17  | G    | Sidechain |
| 1   | C     | 18  | G    | Sidechain |
| 1   | D     | 17  | G    | Sidechain |
| 1   | D     | 18  | 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   | C     | 1573  | 0        | 802      | 86      | 0            |
| 1   | D     | 1509  | 0        | 770      | 77      | 0            |
| 2   | A     | 2733  | 0        | 2670     | 239     | 0            |
| 2   | B     | 2815  | 0        | 2750     | 270     | 0            |
| 3   | A     | 5     | 0        | 0        | 3       | 0            |
| 3   | B     | 10    | 0        | 0        | 0       | 0            |
| 3   | C     | 5     | 0        | 0        | 0       | 0            |
| 4   | A     | 15    | 0        | 0        | 0       | 0            |
| 4   | B     | 10    | 0        | 0        | 0       | 0            |
| All | All   | 8675  | 0        | 6992     | 660     | 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 42.

All (660) 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:C:56:C:H2'    | 1:C:57:G:H5''   | 1.32                     | 1.06              |
| 1:D:56:C:H2'    | 1:D:57:G:H5''   | 1.33                     | 1.04              |
| 2:A:35:LEU:HD11 | 2:A:72:VAL:HG23 | 1.40                     | 1.03              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:51:G:H2'     | 1:D:52:G:H5''    | 1.45                     | 0.98              |
| 1:C:51:G:H2'     | 1:C:52:G:H5''    | 1.49                     | 0.95              |
| 1:D:24:A:O2'     | 2:B:256:GLU:HB3  | 1.67                     | 0.93              |
| 2:B:254:GLY:HA2  | 2:B:259:TRP:HH2  | 1.32                     | 0.92              |
| 1:C:56:C:C2'     | 1:C:57:G:H5''    | 2.00                     | 0.92              |
| 2:B:35:LEU:HD11  | 2:B:72:VAL:HG22  | 1.53                     | 0.90              |
| 2:A:274:ALA:HB1  | 2:A:279:HIS:ND1  | 1.87                     | 0.90              |
| 2:B:310:THR:HB   | 2:B:314:GLN:HE22 | 1.35                     | 0.90              |
| 1:D:19:C:OP2     | 1:D:20:C:H3'     | 1.70                     | 0.89              |
| 2:B:283:MET:HE1  | 2:B:338:ALA:HA   | 1.55                     | 0.89              |
| 1:D:56:C:C2'     | 1:D:57:G:H5''    | 2.02                     | 0.88              |
| 2:B:38:LYS:NZ    | 2:B:71:THR:HB    | 1.88                     | 0.88              |
| 1:C:1:G:H1'      | 1:C:73:G:H22     | 1.39                     | 0.88              |
| 2:A:17:ASP:O     | 2:A:21:SER:HB2   | 1.74                     | 0.86              |
| 1:D:9:C:O2'      | 1:D:45:A:H2'     | 1.77                     | 0.85              |
| 1:D:57:G:H5'     | 1:D:57:G:H8      | 1.40                     | 0.84              |
| 2:A:287:LEU:HD12 | 2:A:331:VAL:HB   | 1.57                     | 0.84              |
| 2:B:321:VAL:HG12 | 2:B:329:ILE:HD11 | 1.59                     | 0.84              |
| 1:C:57:G:H8      | 1:C:57:G:H5'     | 1.41                     | 0.84              |
| 2:B:259:TRP:CZ3  | 2:B:275:GLN:HB3  | 2.14                     | 0.83              |
| 2:A:251:THR:HG22 | 2:A:252:LYS:N    | 1.92                     | 0.83              |
| 2:A:251:THR:HG22 | 2:A:252:LYS:H    | 1.42                     | 0.82              |
| 1:C:9:C:O2'      | 1:C:45:A:H2'     | 1.79                     | 0.82              |
| 2:B:40:TRP:HB2   | 2:B:205:LYS:HE2  | 1.62                     | 0.81              |
| 2:B:197:GLY:O    | 2:B:201:ILE:HG12 | 1.81                     | 0.81              |
| 1:D:57:G:H5'     | 1:D:57:G:C8      | 2.16                     | 0.81              |
| 1:D:51:G:C2'     | 1:D:52:G:H5''    | 2.10                     | 0.81              |
| 2:A:262:VAL:HG13 | 2:A:281:ARG:O    | 1.80                     | 0.81              |
| 1:C:19:C:OP2     | 1:C:20:C:H3'     | 1.81                     | 0.80              |
| 1:C:25:C:H5'     | 2:A:256:GLU:O    | 1.82                     | 0.80              |
| 1:D:60:U:H5''    | 1:D:61:C:OP2     | 1.82                     | 0.80              |
| 2:A:138:LYS:HD2  | 2:A:160:HIS:HB2  | 1.63                     | 0.80              |
| 1:D:5:C:H42      | 1:D:68:G:H1      | 1.28                     | 0.79              |
| 1:C:6:C:H2'      | 1:C:6:C:O2       | 1.82                     | 0.79              |
| 2:A:219:GLY:H    | 2:A:232:HIS:HB2  | 1.48                     | 0.79              |
| 2:A:143:ARG:HA   | 2:A:150:ASP:OD2  | 1.83                     | 0.79              |
| 2:B:74:PHE:HD1   | 2:B:78:TYR:HB2   | 1.46                     | 0.79              |
| 2:B:284:SER:OG   | 2:B:363:ARG:HD2  | 1.82                     | 0.79              |
| 1:C:51:G:C2'     | 1:C:52:G:H5''    | 2.13                     | 0.78              |
| 1:D:9:C:H5'      | 1:D:10:G:OP2     | 1.83                     | 0.78              |
| 1:C:57:G:H5'     | 1:C:57:G:C8      | 2.19                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:60:U:H5'     | 1:C:61:C:OP2     | 1.85                     | 0.76              |
| 2:A:173:LEU:HB3  | 2:A:177:GLN:NE2  | 2.01                     | 0.76              |
| 2:A:308:VAL:HG23 | 2:A:319:CYS:SG   | 2.25                     | 0.76              |
| 2:B:262:VAL:HG11 | 2:B:281:ARG:HB3  | 1.68                     | 0.75              |
| 2:A:128:HIS:CD2  | 2:A:155:LEU:HD21 | 2.22                     | 0.75              |
| 1:C:17:G:H2'     | 1:C:57:G:H22     | 1.52                     | 0.74              |
| 2:B:131:ARG:NE   | 2:B:144:GLY:HA2  | 2.02                     | 0.74              |
| 2:B:48:TYR:HB3   | 2:B:204:ARG:HH22 | 1.51                     | 0.74              |
| 2:A:174:GLU:C    | 2:A:176:PRO:HD2  | 2.12                     | 0.74              |
| 2:B:103:ASN:OD1  | 2:B:107:LYS:HD2  | 1.88                     | 0.74              |
| 2:B:252:LYS:O    | 2:B:252:LYS:HD3  | 1.87                     | 0.74              |
| 1:C:17:G:H2'     | 1:C:57:G:N2      | 2.03                     | 0.74              |
| 2:A:37:MET:SD    | 2:A:111:PHE:HD1  | 2.11                     | 0.73              |
| 1:C:14:A:H2'     | 1:C:15:G:O4'     | 1.89                     | 0.72              |
| 2:A:265:ASP:CG   | 2:A:268:ASN:HD22 | 1.95                     | 0.72              |
| 1:D:5:C:N4       | 1:D:68:G:H1      | 1.87                     | 0.72              |
| 2:A:287:LEU:HD22 | 2:A:360:ILE:HG12 | 1.72                     | 0.72              |
| 1:C:9:C:H5'      | 1:C:10:G:OP2     | 1.89                     | 0.72              |
| 2:A:308:VAL:HG22 | 2:A:348:PHE:CD2  | 2.24                     | 0.72              |
| 2:B:74:PHE:CD1   | 2:B:78:TYR:HB2   | 2.24                     | 0.72              |
| 1:D:68:G:H2'     | 1:D:69:G:H8      | 1.55                     | 0.71              |
| 2:A:6:LYS:HA     | 2:A:122:ASP:OD2  | 1.91                     | 0.70              |
| 2:B:308:VAL:HG12 | 2:B:309:LYS:H    | 1.56                     | 0.70              |
| 1:D:24:A:H2'     | 1:D:25:C:C6      | 2.26                     | 0.70              |
| 2:B:254:GLY:HA2  | 2:B:259:TRP:CH2  | 2.22                     | 0.70              |
| 2:B:75:ALA:HB3   | 2:B:77:GLU:HG3   | 1.73                     | 0.69              |
| 2:B:38:LYS:HZ2   | 2:B:71:THR:HB    | 1.57                     | 0.69              |
| 2:A:222:ILE:CG2  | 2:A:226:GLY:HA2  | 2.23                     | 0.69              |
| 1:D:21:A:H61     | 1:D:46:A:H2'     | 1.58                     | 0.69              |
| 1:D:25:C:H5'     | 2:B:256:GLU:O    | 1.92                     | 0.69              |
| 2:A:7:LYS:HD2    | 2:A:120:GLY:O    | 1.92                     | 0.69              |
| 2:A:287:LEU:CD1  | 2:A:331:VAL:HB   | 2.22                     | 0.69              |
| 2:B:232:HIS:O    | 2:B:233:GLN:HB2  | 1.91                     | 0.69              |
| 2:B:325:ASP:HB3  | 2:B:326:ASP:OD1  | 1.93                     | 0.69              |
| 2:A:279:HIS:HD2  | 2:A:280:PRO:N    | 1.89                     | 0.68              |
| 1:C:34:U:H2'     | 1:C:34:U:O2      | 1.94                     | 0.68              |
| 2:B:243:ARG:HE   | 2:B:258:PRO:CB   | 2.07                     | 0.68              |
| 2:A:236:MET:HG2  | 2:A:237:TYR:CD1  | 2.28                     | 0.68              |
| 2:A:276:GLY:C    | 2:A:278:GLU:H    | 1.99                     | 0.68              |
| 2:A:337:VAL:CG1  | 2:A:340:VAL:HG23 | 2.24                     | 0.68              |
| 2:A:324:LEU:HD13 | 2:A:330:GLU:HB2  | 1.74                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:75:ALA:C     | 2:B:77:GLU:H     | 2.02                     | 0.68              |
| 2:B:283:MET:HE2  | 2:B:283:MET:HA   | 1.76                     | 0.68              |
| 1:C:20:C:H1'     | 1:C:21:A:O4'     | 1.94                     | 0.68              |
| 2:A:308:VAL:HG12 | 2:A:309:LYS:N    | 2.08                     | 0.67              |
| 1:C:24:A:O2'     | 2:A:256:GLU:HB3  | 1.94                     | 0.67              |
| 2:A:143:ARG:HG3  | 2:A:352:GLU:HA   | 1.77                     | 0.67              |
| 2:A:243:ARG:HB2  | 2:A:260:TYR:CE1  | 2.29                     | 0.67              |
| 2:A:321:VAL:HG11 | 2:A:329:ILE:HD11 | 1.75                     | 0.67              |
| 1:D:17:G:H2'     | 1:D:57:G:N2      | 2.10                     | 0.67              |
| 2:B:366:LEU:HD12 | 2:B:367:PRO:HD2  | 1.76                     | 0.67              |
| 1:D:34:U:H2'     | 1:D:34:U:O2      | 1.95                     | 0.67              |
| 2:A:224:VAL:HG21 | 2:A:279:HIS:CE1  | 2.31                     | 0.66              |
| 2:A:224:VAL:HG21 | 2:A:279:HIS:HE1  | 1.59                     | 0.66              |
| 1:C:9:C:HO2'     | 1:C:45:A:H2'     | 1.60                     | 0.66              |
| 2:A:123:TYR:C    | 2:A:124:ILE:HD12 | 2.21                     | 0.66              |
| 2:A:254:GLY:HA2  | 2:A:275:GLN:OE1  | 1.94                     | 0.66              |
| 2:B:45:GLY:C     | 2:B:47:GLU:H     | 2.01                     | 0.66              |
| 2:A:232:HIS:HB3  | 2:A:234:GLY:H    | 1.60                     | 0.66              |
| 2:B:174:GLU:C    | 2:B:176:PRO:HD2  | 2.20                     | 0.66              |
| 2:B:322:LYS:O    | 2:B:329:ILE:HD12 | 1.94                     | 0.66              |
| 2:A:363:ARG:HD2  | 2:A:365:PRO:HG3  | 1.76                     | 0.66              |
| 1:C:21:A:H61     | 1:C:46:A:H2'     | 1.61                     | 0.65              |
| 1:C:16:A:O2'     | 1:C:60:U:O2'     | 2.15                     | 0.65              |
| 2:A:105:GLU:O    | 2:A:109:LYS:HB3  | 1.97                     | 0.65              |
| 2:A:130:VAL:HG11 | 2:A:141:LEU:HD11 | 1.77                     | 0.65              |
| 2:A:222:ILE:HG23 | 2:A:226:GLY:HA2  | 1.77                     | 0.65              |
| 2:A:42:GLU:CD    | 2:A:42:GLU:H     | 2.04                     | 0.65              |
| 2:A:290:GLN:HG3  | 2:A:291:GLN:HG3  | 1.78                     | 0.65              |
| 2:B:224:VAL:HG13 | 2:B:281:ARG:NH1  | 2.12                     | 0.64              |
| 1:C:57:G:H8      | 1:C:57:G:C5'     | 2.10                     | 0.64              |
| 1:C:2:U:H5''     | 1:C:3:C:C5       | 2.32                     | 0.64              |
| 2:B:279:HIS:CD2  | 2:B:281:ARG:HB2  | 2.31                     | 0.64              |
| 1:D:17:G:H2'     | 1:D:57:G:H22     | 1.62                     | 0.64              |
| 1:D:57:G:H8      | 1:D:57:G:C5'     | 2.08                     | 0.64              |
| 2:A:289:ALA:HB3  | 2:A:329:ILE:CG2  | 2.28                     | 0.64              |
| 2:B:38:LYS:HZ1   | 2:B:71:THR:HB    | 1.59                     | 0.64              |
| 2:B:26:GLN:HB3   | 2:B:32:VAL:HG11  | 1.80                     | 0.64              |
| 2:B:243:ARG:HE   | 2:B:258:PRO:HB2  | 1.62                     | 0.64              |
| 2:A:310:THR:HB   | 2:A:314:GLN:OE1  | 1.98                     | 0.64              |
| 2:A:207:ARG:HE   | 2:A:237:TYR:HD2  | 1.46                     | 0.63              |
| 1:D:20:C:H1'     | 1:D:21:A:O4'     | 1.97                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:363:ARG:O    | 2:A:365:PRO:HD3  | 1.98                     | 0.63              |
| 2:B:219:GLY:H    | 2:B:232:HIS:HB2  | 1.63                     | 0.63              |
| 2:A:12:MET:HE1   | 2:A:34:GLY:HA3   | 1.81                     | 0.63              |
| 1:C:51:G:C3'     | 1:C:52:G:H5''    | 2.29                     | 0.63              |
| 1:C:56:C:C3'     | 1:C:57:G:H5''    | 2.27                     | 0.63              |
| 1:D:11:U:H2'     | 1:D:12:C:C6      | 2.34                     | 0.63              |
| 2:A:48:TYR:C     | 2:A:50:THR:H     | 2.07                     | 0.63              |
| 2:A:146:ASP:OD1  | 2:A:174:GLU:HG2  | 1.99                     | 0.63              |
| 1:D:51:G:C3'     | 1:D:52:G:H5''    | 2.29                     | 0.63              |
| 2:A:279:HIS:CD2  | 2:A:281:ARG:H    | 2.17                     | 0.62              |
| 2:B:74:PHE:C     | 2:B:76:ALA:H     | 2.07                     | 0.62              |
| 2:B:214:LEU:CD2  | 2:B:236:MET:HE1  | 2.29                     | 0.62              |
| 2:A:321:VAL:CG1  | 2:A:329:ILE:HD11 | 2.29                     | 0.62              |
| 2:B:288:ILE:HG22 | 2:B:361:GLU:HG2  | 1.80                     | 0.62              |
| 1:D:56:C:C3'     | 1:D:57:G:H5''    | 2.28                     | 0.62              |
| 1:C:61:C:H2'     | 1:C:62:C:C6      | 2.35                     | 0.62              |
| 1:D:6:C:H2'      | 1:D:7:U:C6       | 2.35                     | 0.62              |
| 2:A:10:VAL:O     | 2:A:12:MET:HE2   | 1.99                     | 0.62              |
| 2:A:131:ARG:CD   | 2:A:144:GLY:HA2  | 2.30                     | 0.62              |
| 1:D:24:A:H2'     | 1:D:25:C:H6      | 1.65                     | 0.62              |
| 2:B:304:MET:HE2  | 2:B:306:CYS:HB3  | 1.80                     | 0.61              |
| 1:C:6:C:H2'      | 1:C:7:U:H5'      | 1.81                     | 0.61              |
| 2:B:154:PHE:HE1  | 2:B:312:TYR:CG   | 2.18                     | 0.61              |
| 2:B:292:LEU:HD23 | 2:B:358:GLY:HA3  | 1.82                     | 0.61              |
| 1:C:6:C:O2       | 1:C:6:C:C2'      | 2.48                     | 0.61              |
| 1:C:16:A:H4'     | 1:C:16:A:OP1     | 2.01                     | 0.61              |
| 2:A:174:GLU:HB3  | 2:A:176:PRO:HD2  | 1.83                     | 0.61              |
| 2:B:86:PHE:HE1   | 2:B:210:LEU:HD11 | 1.65                     | 0.61              |
| 2:A:287:LEU:C    | 2:A:288:ILE:HD12 | 2.25                     | 0.61              |
| 2:A:236:MET:HG2  | 2:A:237:TYR:HD1  | 1.65                     | 0.61              |
| 2:A:252:LYS:O    | 2:A:253:GLU:HB3  | 2.00                     | 0.61              |
| 1:C:20:C:H5'     | 1:C:20(A):C:OP1  | 2.01                     | 0.60              |
| 2:A:111:PHE:C    | 2:A:111:PHE:CD2  | 2.80                     | 0.60              |
| 2:A:111:PHE:C    | 2:A:111:PHE:HD2  | 2.09                     | 0.60              |
| 2:B:46:GLU:O     | 2:B:47:GLU:HB2   | 2.02                     | 0.60              |
| 1:D:11:U:H2'     | 1:D:12:C:H6      | 1.66                     | 0.60              |
| 2:B:43:ASP:CG    | 2:B:44:ASP:H     | 2.08                     | 0.60              |
| 1:D:16:A:H4'     | 1:D:16:A:OP1     | 2.01                     | 0.59              |
| 2:B:290:GLN:HE21 | 2:B:328:ARG:CD   | 2.15                     | 0.59              |
| 1:C:18:G:H5''    | 1:C:19:C:H5      | 1.67                     | 0.59              |
| 2:A:143:ARG:HG3  | 2:A:352:GLU:OE1  | 2.02                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:48:TYR:HB3   | 2:B:204:ARG:NH2  | 2.16                     | 0.59              |
| 2:A:279:HIS:HD2  | 2:A:280:PRO:CD   | 2.15                     | 0.59              |
| 1:C:73:G:H2'     | 1:D:73:G:O6      | 2.02                     | 0.59              |
| 2:A:276:GLY:O    | 2:A:278:GLU:N    | 2.35                     | 0.59              |
| 2:B:290:GLN:NE2  | 2:B:328:ARG:HD3  | 2.18                     | 0.59              |
| 2:A:279:HIS:CD2  | 2:A:280:PRO:HD2  | 2.37                     | 0.59              |
| 2:A:7:LYS:HE3    | 2:A:31:GLN:HE22  | 1.66                     | 0.59              |
| 2:B:262:VAL:CG1  | 2:B:281:ARG:HB3  | 2.33                     | 0.59              |
| 2:B:276:GLY:C    | 2:B:278:GLU:H    | 2.10                     | 0.59              |
| 2:B:304:MET:HE1  | 2:B:355:LEU:CD1  | 2.33                     | 0.59              |
| 2:A:160:HIS:CD2  | 2:A:161:GLU:H    | 2.21                     | 0.59              |
| 2:B:35:LEU:HD23  | 2:B:111:PHE:CE1  | 2.37                     | 0.58              |
| 2:A:7:LYS:HA     | 2:A:31:GLN:O     | 2.04                     | 0.58              |
| 1:C:24:A:H2'     | 1:C:25:C:C6      | 2.39                     | 0.58              |
| 2:A:289:ALA:HB3  | 2:A:329:ILE:HG21 | 1.84                     | 0.58              |
| 2:B:366:LEU:CD1  | 2:B:367:PRO:HD2  | 2.34                     | 0.58              |
| 2:A:129:TYR:HB3  | 2:A:151:GLN:HG3  | 1.85                     | 0.58              |
| 2:A:129:TYR:HD1  | 2:A:175:LYS:HZ3  | 1.51                     | 0.58              |
| 2:A:279:HIS:CD2  | 2:A:280:PRO:N    | 2.71                     | 0.58              |
| 2:B:174:GLU:H    | 2:B:177:GLN:NE2  | 2.00                     | 0.58              |
| 2:B:307:THR:HG21 | 2:B:316:ASP:HB3  | 1.85                     | 0.58              |
| 2:A:274:ALA:CB   | 2:A:279:HIS:ND1  | 2.66                     | 0.58              |
| 2:A:289:ALA:O    | 2:A:329:ILE:HG22 | 2.04                     | 0.58              |
| 2:B:106:ILE:HG22 | 2:B:107:LYS:N    | 2.18                     | 0.58              |
| 2:B:23:TRP:CE2   | 2:B:185:LEU:HD11 | 2.38                     | 0.58              |
| 2:B:46:GLU:H     | 2:B:46:GLU:CD    | 2.12                     | 0.58              |
| 2:B:243:ARG:HH21 | 2:B:258:PRO:HG3  | 1.69                     | 0.58              |
| 2:B:304:MET:HE1  | 2:B:355:LEU:HD13 | 1.85                     | 0.58              |
| 1:C:68:G:N3      | 1:C:68:G:H2'     | 2.17                     | 0.57              |
| 2:A:207:ARG:NE   | 2:A:237:TYR:HD2  | 2.02                     | 0.57              |
| 2:B:198:ILE:C    | 2:B:200:PHE:H    | 2.12                     | 0.57              |
| 2:A:15:GLY:O     | 2:A:188:VAL:HG21 | 2.04                     | 0.57              |
| 2:B:20:VAL:O     | 2:B:24:LEU:HG    | 2.03                     | 0.57              |
| 2:B:214:LEU:HD23 | 2:B:236:MET:HE1  | 1.84                     | 0.57              |
| 2:B:26:GLN:HB3   | 2:B:32:VAL:CG1   | 2.35                     | 0.57              |
| 2:B:43:ASP:OD1   | 2:B:204:ARG:NH1  | 2.38                     | 0.57              |
| 2:A:44:ASP:HB3   | 2:A:46:GLU:HG2   | 1.86                     | 0.57              |
| 2:B:38:LYS:HB2   | 2:B:73:ASN:HA    | 1.86                     | 0.57              |
| 2:B:107:LYS:O    | 2:B:111:PHE:HB3  | 2.05                     | 0.57              |
| 2:A:231:GLU:CD   | 2:A:231:GLU:H    | 2.11                     | 0.57              |
| 2:A:276:GLY:C    | 2:A:278:GLU:N    | 2.60                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:262:VAL:HG11 | 2:A:281:ARG:HB3  | 1.87                     | 0.57              |
| 2:A:325:ASP:HB2  | 2:A:326:ASP:OD1  | 2.05                     | 0.57              |
| 2:B:261:VAL:HG13 | 2:B:271:LEU:HD21 | 1.87                     | 0.57              |
| 1:C:67:G:C2      | 1:C:68:G:N7      | 2.73                     | 0.57              |
| 2:A:232:HIS:NE2  | 2:A:271:LEU:HB2  | 2.19                     | 0.57              |
| 2:B:61:VAL:O     | 2:B:65:LEU:HD13  | 2.04                     | 0.57              |
| 1:C:37:A:C2'     | 1:C:38:C:H5'     | 2.35                     | 0.56              |
| 2:A:85:LEU:HD22  | 2:B:324:LEU:O    | 2.05                     | 0.56              |
| 1:C:15:G:O2'     | 1:C:16:A:P       | 2.63                     | 0.56              |
| 2:A:175:LYS:N    | 2:A:176:PRO:HD2  | 2.20                     | 0.56              |
| 2:B:40:TRP:CB    | 2:B:205:LYS:HE2  | 2.33                     | 0.56              |
| 2:B:263:ASP:OD1  | 2:B:264:LYS:N    | 2.38                     | 0.56              |
| 1:C:56:C:H2'     | 1:C:57:G:C5'     | 2.21                     | 0.56              |
| 2:B:311:ARG:H    | 2:B:314:GLN:NE2  | 2.03                     | 0.56              |
| 2:A:305:ARG:CG   | 2:A:305:ARG:HH11 | 2.16                     | 0.56              |
| 1:C:11:U:H2'     | 1:C:12:C:C6      | 2.41                     | 0.56              |
| 2:A:95:THR:HG22  | 2:A:344:GLN:HE21 | 1.69                     | 0.56              |
| 2:B:10:VAL:O     | 2:B:10:VAL:HG13  | 2.05                     | 0.56              |
| 2:B:47:GLU:O     | 2:B:48:TYR:C     | 2.48                     | 0.56              |
| 2:B:296:ASP:OD2  | 2:B:296:ASP:C    | 2.48                     | 0.56              |
| 1:D:9:C:HO2'     | 1:D:45:A:H2'     | 1.69                     | 0.56              |
| 2:A:350:ASN:CG   | 2:A:350:ASN:O    | 2.48                     | 0.56              |
| 2:B:138:LYS:HE2  | 2:B:160:HIS:CD2  | 2.41                     | 0.56              |
| 1:D:14:A:H2'     | 1:D:15:G:O4'     | 2.06                     | 0.56              |
| 2:A:138:LYS:HG3  | 2:A:160:HIS:ND1  | 2.21                     | 0.56              |
| 2:A:134:ASP:HA   | 2:A:139:SER:HA   | 1.87                     | 0.56              |
| 2:B:86:PHE:CE1   | 2:B:210:LEU:HD11 | 2.41                     | 0.56              |
| 2:A:118:ASP:C    | 2:A:120:GLY:H    | 2.14                     | 0.55              |
| 1:C:73:G:H2'     | 1:D:73:G:C6      | 2.42                     | 0.55              |
| 1:D:51:G:H2'     | 1:D:52:G:C5'     | 2.28                     | 0.55              |
| 2:A:129:TYR:CD1  | 2:A:175:LYS:HG3  | 2.42                     | 0.55              |
| 2:A:254:GLY:C    | 2:A:256:GLU:N    | 2.61                     | 0.55              |
| 1:C:9:C:O2'      | 1:C:45:A:C2'     | 2.53                     | 0.55              |
| 2:B:236:MET:HG3  | 2:B:237:TYR:CD2  | 2.41                     | 0.55              |
| 1:C:37:A:H2'     | 1:C:38:C:H5'     | 1.87                     | 0.55              |
| 2:A:243:ARG:HB2  | 2:A:260:TYR:HE1  | 1.68                     | 0.55              |
| 1:C:51:G:H2'     | 1:C:52:G:C5'     | 2.32                     | 0.55              |
| 1:D:15:G:O2'     | 1:D:16:A:P       | 2.64                     | 0.55              |
| 2:B:140:ARG:CB   | 2:B:140:ARG:HH11 | 2.19                     | 0.55              |
| 2:A:337:VAL:HG12 | 2:A:340:VAL:HG23 | 1.89                     | 0.54              |
| 2:B:129:TYR:CE2  | 2:B:145:LEU:O    | 2.61                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:23:TRP:O     | 2:A:27:GLN:HG2   | 2.07                     | 0.54              |
| 2:B:131:ARG:CD   | 2:B:144:GLY:HA2  | 2.38                     | 0.54              |
| 2:A:227:ASP:O    | 2:A:228:GLU:C    | 2.51                     | 0.54              |
| 2:B:308:VAL:HG12 | 2:B:309:LYS:N    | 2.23                     | 0.54              |
| 2:A:232:HIS:O    | 2:A:233:GLN:HB2  | 2.08                     | 0.54              |
| 2:A:308:VAL:HG12 | 2:A:309:LYS:H    | 1.70                     | 0.54              |
| 2:A:324:LEU:HD23 | 2:A:328:ARG:CD   | 2.38                     | 0.54              |
| 1:D:8:U:H5'      | 1:D:9:C:OP2      | 2.08                     | 0.54              |
| 1:D:9:C:O2'      | 1:D:45:A:C2'     | 2.54                     | 0.54              |
| 2:A:10:VAL:HG22  | 2:A:12:MET:HE2   | 1.89                     | 0.54              |
| 2:A:216:ALA:HB1  | 2:A:233:GLN:O    | 2.07                     | 0.54              |
| 1:D:63:C:H2'     | 1:D:64:C:C6      | 2.43                     | 0.54              |
| 2:B:40:TRP:CG    | 2:B:205:LYS:HG3  | 2.43                     | 0.54              |
| 2:B:232:HIS:O    | 2:B:233:GLN:CB   | 2.56                     | 0.53              |
| 2:A:53:ALA:O     | 2:A:57:ASP:OD2   | 2.26                     | 0.53              |
| 2:A:24:LEU:O     | 2:A:28:GLN:HG3   | 2.08                     | 0.53              |
| 2:A:251:THR:CG2  | 2:A:252:LYS:H    | 2.09                     | 0.53              |
| 2:A:305:ARG:HH11 | 2:A:305:ARG:HG2  | 1.74                     | 0.53              |
| 2:B:9:ILE:CD1    | 2:B:119:LEU:HB3  | 2.39                     | 0.53              |
| 2:B:290:GLN:HE21 | 2:B:328:ARG:HG2  | 1.74                     | 0.53              |
| 2:A:305:ARG:NH2  | 2:A:334:ASP:OD2  | 2.41                     | 0.53              |
| 2:A:155:LEU:HB3  | 2:A:158:LEU:HD22 | 1.91                     | 0.53              |
| 2:A:159:SER:OG   | 2:A:162:GLN:HG3  | 2.08                     | 0.53              |
| 2:A:118:ASP:O    | 2:A:120:GLY:N    | 2.42                     | 0.53              |
| 2:B:296:ASP:O    | 2:B:298:GLU:N    | 2.42                     | 0.53              |
| 2:A:217:GLN:HB3  | 2:B:368:VAL:HG12 | 1.90                     | 0.53              |
| 2:B:140:ARG:HH11 | 2:B:140:ARG:HB2  | 1.74                     | 0.53              |
| 1:D:69:G:H2'     | 1:D:70:G:H5'     | 1.91                     | 0.53              |
| 2:B:276:GLY:O    | 2:B:278:GLU:N    | 2.42                     | 0.53              |
| 2:B:227:ASP:O    | 2:B:228:GLU:C    | 2.51                     | 0.53              |
| 2:B:254:GLY:CA   | 2:B:259:TRP:HH2  | 2.12                     | 0.53              |
| 2:B:49:CYS:C     | 2:B:51:ALA:H     | 2.17                     | 0.52              |
| 2:B:150:ASP:OD2  | 2:B:151:GLN:N    | 2.41                     | 0.52              |
| 2:B:183:GLU:C    | 2:B:185:LEU:H    | 2.15                     | 0.52              |
| 2:A:131:ARG:HD3  | 2:A:144:GLY:HA2  | 1.90                     | 0.52              |
| 2:B:143:ARG:HH21 | 2:B:349:TYR:HB3  | 1.75                     | 0.52              |
| 2:B:294:TRP:O    | 2:B:296:ASP:N    | 2.43                     | 0.52              |
| 1:D:15:G:O3'     | 1:D:16:A:O4'     | 2.28                     | 0.52              |
| 1:D:16:A:N3      | 1:D:16:A:H2'     | 2.24                     | 0.52              |
| 2:B:283:MET:CE   | 2:B:338:ALA:HA   | 2.32                     | 0.52              |
| 1:C:7:U:O4       | 1:C:49:A:N6      | 2.43                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:254:GLY:C    | 2:A:256:GLU:H    | 2.17                     | 0.52              |
| 2:A:279:HIS:HD2  | 2:A:280:PRO:HD2  | 1.75                     | 0.52              |
| 2:A:294:TRP:O    | 2:A:297:ARG:N    | 2.39                     | 0.52              |
| 2:B:9:ILE:HD11   | 2:B:119:LEU:HB3  | 1.91                     | 0.52              |
| 2:B:142:LEU:HA   | 2:B:352:GLU:O    | 2.10                     | 0.52              |
| 1:D:59:A:H2'     | 1:D:60:U:O4'     | 2.09                     | 0.52              |
| 2:A:48:TYR:O     | 2:A:50:THR:N     | 2.43                     | 0.52              |
| 1:D:18:G:H5''    | 1:D:19:C:H5      | 1.74                     | 0.52              |
| 2:A:131:ARG:HG3  | 2:A:144:GLY:HA2  | 1.92                     | 0.52              |
| 1:D:20:C:H5'     | 1:D:20(A):C:OP1  | 2.09                     | 0.52              |
| 2:A:37:MET:CE    | 2:A:111:PHE:HD1  | 2.23                     | 0.52              |
| 1:D:8:U:H2'      | 1:D:46:A:N3      | 2.25                     | 0.52              |
| 1:D:44:U:H2'     | 1:D:45:A:O4'     | 2.10                     | 0.52              |
| 2:A:20:VAL:O     | 2:A:24:LEU:HG    | 2.10                     | 0.52              |
| 2:A:251:THR:CG2  | 2:A:252:LYS:N    | 2.61                     | 0.52              |
| 2:B:75:ALA:C     | 2:B:77:GLU:N     | 2.68                     | 0.52              |
| 2:A:129:TYR:CE1  | 2:A:175:LYS:HG3  | 2.45                     | 0.51              |
| 2:B:17:ASP:O     | 2:B:21:SER:HB2   | 2.10                     | 0.51              |
| 2:B:296:ASP:OD2  | 2:B:298:GLU:HB2  | 2.10                     | 0.51              |
| 2:A:159:SER:O    | 2:A:162:GLN:N    | 2.40                     | 0.51              |
| 1:C:25:C:O2'     | 2:A:248:ILE:O    | 2.27                     | 0.51              |
| 1:D:16:A:O2'     | 1:D:60:U:O2'     | 2.27                     | 0.51              |
| 1:D:23:G:O2'     | 1:D:24:A:H5'     | 2.11                     | 0.51              |
| 2:A:77:GLU:OE1   | 2:A:77:GLU:N     | 2.38                     | 0.51              |
| 1:D:58:A:O2'     | 1:D:60:U:OP2     | 2.28                     | 0.51              |
| 2:A:17:ASP:OD1   | 2:A:178:VAL:HG11 | 2.10                     | 0.51              |
| 2:B:366:LEU:CG   | 2:B:367:PRO:HD2  | 2.41                     | 0.51              |
| 2:B:229:ILE:HG12 | 2:B:229:ILE:O    | 2.09                     | 0.51              |
| 2:B:45:GLY:C     | 2:B:47:GLU:N     | 2.68                     | 0.51              |
| 1:D:57:G:C8      | 1:D:57:G:C5'     | 2.88                     | 0.51              |
| 2:A:279:HIS:CD2  | 2:A:280:PRO:CD   | 2.94                     | 0.51              |
| 2:A:308:VAL:CG1  | 2:A:309:LYS:N    | 2.73                     | 0.51              |
| 2:B:86:PHE:CG    | 2:B:206:PHE:HD2  | 2.28                     | 0.51              |
| 1:D:56:C:H2'     | 1:D:57:G:C5'     | 2.23                     | 0.51              |
| 2:A:180:LYS:O    | 2:A:181:ILE:C    | 2.54                     | 0.51              |
| 2:A:267:GLU:CD   | 2:A:267:GLU:H    | 2.19                     | 0.51              |
| 2:A:97:ASN:HD22  | 2:A:97:ASN:C     | 2.18                     | 0.50              |
| 2:B:305:ARG:HH11 | 2:B:305:ARG:CG   | 2.24                     | 0.50              |
| 2:B:337:VAL:CG1  | 2:B:338:ALA:N    | 2.74                     | 0.50              |
| 2:A:305:ARG:CG   | 2:A:305:ARG:NH1  | 2.74                     | 0.50              |
| 2:A:290:GLN:O    | 2:A:291:GLN:HB2  | 2.11                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:73:ASN:O     | 2:B:74:PHE:O     | 2.29                     | 0.50              |
| 1:D:52:G:O6      | 1:D:62:C:N3      | 2.44                     | 0.50              |
| 2:B:175:LYS:N    | 2:B:176:PRO:HD2  | 2.26                     | 0.50              |
| 1:C:73:G:H5'     | 1:C:74:C:O5'     | 2.11                     | 0.50              |
| 2:A:129:TYR:HD1  | 2:A:175:LYS:NZ   | 2.09                     | 0.50              |
| 2:A:285:VAL:HG23 | 2:A:364:LEU:O    | 2.11                     | 0.50              |
| 2:B:74:PHE:C     | 2:B:76:ALA:N     | 2.70                     | 0.50              |
| 2:B:222:ILE:HD13 | 2:B:270:ILE:HG21 | 1.93                     | 0.50              |
| 1:C:52:G:O6      | 1:C:62:C:N3      | 2.44                     | 0.50              |
| 2:B:81:ASN:H     | 2:B:81:ASN:ND2   | 2.10                     | 0.50              |
| 2:B:276:GLY:C    | 2:B:278:GLU:N    | 2.69                     | 0.50              |
| 2:B:350:ASN:HB2  | 2:B:355:LEU:HD21 | 1.94                     | 0.50              |
| 2:B:25:LEU:O     | 2:B:28:GLN:HB3   | 2.12                     | 0.50              |
| 2:B:73:ASN:O     | 2:B:74:PHE:C     | 2.54                     | 0.50              |
| 1:D:61:C:H2'     | 1:D:62:C:C6      | 2.47                     | 0.50              |
| 1:C:65:U:H6      | 1:C:65:U:O5'     | 1.95                     | 0.50              |
| 2:B:204:ARG:HB3  | 2:B:204:ARG:HH11 | 1.76                     | 0.50              |
| 2:B:209:PHE:C    | 2:B:211:GLY:N    | 2.69                     | 0.50              |
| 2:B:307:THR:HG21 | 2:B:316:ASP:OD2  | 2.11                     | 0.50              |
| 2:B:9:ILE:HD13   | 2:B:119:LEU:HD13 | 1.93                     | 0.49              |
| 2:B:37:MET:HE1   | 2:B:107:LYS:HG2  | 1.94                     | 0.49              |
| 2:B:134:ASP:HA   | 2:B:139:SER:HA   | 1.93                     | 0.49              |
| 1:C:8:U:H5'      | 1:C:9:C:OP2      | 2.11                     | 0.49              |
| 2:B:48:TYR:C     | 2:B:50:THR:H     | 2.20                     | 0.49              |
| 2:B:71:THR:O     | 2:B:72:VAL:HG13  | 2.13                     | 0.49              |
| 1:D:6:C:H2'      | 1:D:7:U:H6       | 1.75                     | 0.49              |
| 2:A:13:SER:OG    | 3:A:1002:PO4:O2  | 2.30                     | 0.49              |
| 1:D:34:U:O2      | 1:D:34:U:C2'     | 2.58                     | 0.49              |
| 2:A:246:LEU:HD13 | 2:A:273:VAL:HG11 | 1.95                     | 0.49              |
| 1:D:50:G:H2'     | 1:D:51:G:C8      | 2.48                     | 0.49              |
| 2:B:279:HIS:ND1  | 2:B:280:PRO:HD2  | 2.27                     | 0.49              |
| 2:B:290:GLN:NE2  | 2:B:328:ARG:CD   | 2.75                     | 0.49              |
| 2:B:311:ARG:O    | 2:B:314:GLN:HB3  | 2.12                     | 0.49              |
| 1:C:68:G:N2      | 1:C:69:G:C8      | 2.81                     | 0.49              |
| 2:B:224:VAL:HG23 | 2:B:273:VAL:O    | 2.12                     | 0.49              |
| 1:C:15:G:HO2'    | 1:C:16:A:P       | 2.35                     | 0.49              |
| 1:D:8:U:C5'      | 1:D:9:C:OP2      | 2.61                     | 0.49              |
| 2:A:185:LEU:O    | 2:A:186:GLY:C    | 2.55                     | 0.49              |
| 2:A:33:GLU:OE1   | 2:A:70:HIS:HE1   | 1.95                     | 0.48              |
| 2:A:144:GLY:O    | 2:A:145:LEU:C    | 2.56                     | 0.48              |
| 2:B:304:MET:HE2  | 2:B:306:CYS:SG   | 2.52                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:348:PHE:N    | 2:A:348:PHE:CD1  | 2.81                     | 0.48              |
| 2:B:74:PHE:O     | 2:B:76:ALA:N     | 2.39                     | 0.48              |
| 1:C:72:C:H2'     | 1:C:73:G:O4'     | 2.13                     | 0.48              |
| 1:D:50:G:H2'     | 1:D:51:G:H8      | 1.78                     | 0.48              |
| 2:A:304:MET:HE2  | 2:A:306:CYS:HB3  | 1.95                     | 0.48              |
| 2:B:305:ARG:HH11 | 2:B:305:ARG:HG2  | 1.78                     | 0.48              |
| 2:B:283:MET:HB2  | 2:B:366:LEU:HD22 | 1.94                     | 0.48              |
| 1:D:9:C:C5'      | 1:D:10:G:OP2     | 2.58                     | 0.48              |
| 2:B:183:GLU:C    | 2:B:185:LEU:N    | 2.70                     | 0.48              |
| 2:B:103:ASN:HA   | 2:B:107:LYS:HB2  | 1.94                     | 0.48              |
| 1:D:37:A:C2'     | 1:D:38:C:H5'     | 2.44                     | 0.48              |
| 2:A:36:PHE:CE1   | 2:A:55:LEU:HA    | 2.48                     | 0.48              |
| 2:A:145:LEU:O    | 2:A:146:ASP:HB2  | 2.13                     | 0.48              |
| 2:B:154:PHE:HE1  | 2:B:312:TYR:CD2  | 2.31                     | 0.48              |
| 2:A:265:ASP:OD1  | 2:A:268:ASN:ND2  | 2.38                     | 0.48              |
| 2:B:45:GLY:O     | 2:B:47:GLU:N     | 2.37                     | 0.48              |
| 2:B:130:VAL:HG21 | 2:B:141:LEU:HD11 | 1.95                     | 0.48              |
| 2:B:271:LEU:HD23 | 2:B:271:LEU:C    | 2.38                     | 0.48              |
| 2:B:337:VAL:HG12 | 2:B:338:ALA:N    | 2.29                     | 0.48              |
| 1:C:8:U:C5'      | 1:C:9:C:OP2      | 2.62                     | 0.48              |
| 1:D:11:U:C2      | 1:D:12:C:C5      | 3.01                     | 0.48              |
| 2:B:35:LEU:HD23  | 2:B:111:PHE:HE1  | 1.78                     | 0.48              |
| 2:B:274:ALA:HB1  | 2:B:279:HIS:CD2  | 2.49                     | 0.48              |
| 1:C:58:A:HO2'    | 1:C:59:A:H3'     | 1.78                     | 0.47              |
| 1:C:15:G:O3'     | 1:C:16:A:O4'     | 2.32                     | 0.47              |
| 1:C:57:G:C8      | 1:C:57:G:C5'     | 2.91                     | 0.47              |
| 2:B:118:ASP:C    | 2:B:120:GLY:H    | 2.21                     | 0.47              |
| 2:B:271:LEU:HD23 | 2:B:272:VAL:O    | 2.13                     | 0.47              |
| 2:B:304:MET:HE2  | 2:B:306:CYS:CB   | 2.44                     | 0.47              |
| 2:B:325:ASP:O    | 2:B:326:ASP:C    | 2.57                     | 0.47              |
| 2:B:132:ARG:NH1  | 2:B:164:ALA:O    | 2.46                     | 0.47              |
| 2:B:198:ILE:C    | 2:B:200:PHE:N    | 2.71                     | 0.47              |
| 2:B:308:VAL:CG2  | 2:B:319:CYS:SG   | 3.02                     | 0.47              |
| 2:B:312:TYR:CZ   | 2:B:313:ARG:HD3  | 2.49                     | 0.47              |
| 2:B:78:TYR:HA    | 2:B:106:ILE:HD11 | 1.97                     | 0.47              |
| 2:B:83:PHE:HA    | 2:B:206:PHE:CE2  | 2.49                     | 0.47              |
| 2:B:243:ARG:HH21 | 2:B:258:PRO:CG   | 2.27                     | 0.47              |
| 1:C:2:U:N3       | 1:C:72:C:N4      | 2.63                     | 0.47              |
| 1:C:19:C:OP2     | 1:C:20:C:H5''    | 2.15                     | 0.47              |
| 2:A:88:ALA:CB    | 2:B:324:LEU:HD11 | 2.45                     | 0.47              |
| 2:A:325:ASP:O    | 2:A:326:ASP:C    | 2.56                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:337:VAL:HG13 | 2:A:338:ALA:N    | 2.30                     | 0.47              |
| 2:A:150:ASP:C    | 2:A:150:ASP:OD1  | 2.58                     | 0.47              |
| 2:A:279:HIS:CD2  | 2:A:279:HIS:C    | 2.92                     | 0.47              |
| 2:B:344:GLN:O    | 2:B:360:ILE:HG13 | 2.15                     | 0.47              |
| 1:D:69:G:H2'     | 1:D:70:G:C5'     | 2.44                     | 0.47              |
| 2:A:132:ARG:NH1  | 2:A:164:ALA:O    | 2.47                     | 0.47              |
| 2:B:158:LEU:O    | 2:B:295:VAL:HG12 | 2.14                     | 0.47              |
| 1:C:34:U:O2      | 1:C:34:U:C2'     | 2.58                     | 0.47              |
| 2:A:72:VAL:HG12  | 2:A:73:ASN:H     | 1.80                     | 0.47              |
| 2:A:308:VAL:CG1  | 2:A:309:LYS:H    | 2.27                     | 0.47              |
| 2:B:81:ASN:H     | 2:B:81:ASN:HD22  | 1.62                     | 0.47              |
| 2:B:298:GLU:OE1  | 2:B:298:GLU:HA   | 2.15                     | 0.46              |
| 2:A:287:LEU:CD2  | 2:A:360:ILE:HG12 | 2.43                     | 0.46              |
| 2:A:325:ASP:OD2  | 2:A:326:ASP:OD1  | 2.33                     | 0.46              |
| 2:B:74:PHE:HD2   | 2:B:74:PHE:N     | 2.13                     | 0.46              |
| 1:C:3:C:H5''     | 1:C:4:C:OP1      | 2.15                     | 0.46              |
| 2:A:252:LYS:O    | 2:A:252:LYS:HG3  | 2.15                     | 0.46              |
| 2:B:254:GLY:CA   | 2:B:259:TRP:CH2  | 2.95                     | 0.46              |
| 2:A:23:TRP:CE2   | 2:A:185:LEU:HD11 | 2.49                     | 0.46              |
| 2:A:48:TYR:C     | 2:A:50:THR:N     | 2.72                     | 0.46              |
| 2:A:100:ILE:HD12 | 2:A:156:TYR:CE2  | 2.51                     | 0.46              |
| 2:A:221:ILE:HG13 | 2:A:231:GLU:O    | 2.16                     | 0.46              |
| 2:A:23:TRP:CD2   | 2:A:185:LEU:HD11 | 2.51                     | 0.46              |
| 2:A:129:TYR:HE1  | 2:A:175:LYS:CB   | 2.29                     | 0.46              |
| 2:A:265:ASP:O    | 2:A:269:ASN:N    | 2.48                     | 0.46              |
| 2:B:74:PHE:N     | 2:B:74:PHE:CD2   | 2.83                     | 0.46              |
| 2:A:83:PHE:CE1   | 2:A:87:LEU:HD11  | 2.51                     | 0.46              |
| 2:A:185:LEU:O    | 2:A:187:LEU:HG   | 2.16                     | 0.46              |
| 2:A:368:VAL:OXT  | 2:A:368:VAL:HG13 | 2.14                     | 0.46              |
| 2:B:366:LEU:HG   | 2:B:367:PRO:HD2  | 1.97                     | 0.46              |
| 1:C:6:C:N4       | 1:C:67:G:H1      | 2.14                     | 0.46              |
| 2:B:290:GLN:HE21 | 2:B:328:ARG:CG   | 2.29                     | 0.46              |
| 2:B:293:HIS:O    | 2:B:356:GLY:HA3  | 2.15                     | 0.46              |
| 1:C:2:U:H2'      | 1:C:3:C:OP1      | 2.16                     | 0.46              |
| 2:A:138:LYS:HA   | 2:A:138:LYS:HD3  | 1.60                     | 0.46              |
| 2:A:158:LEU:HA   | 2:A:162:GLN:OE1  | 2.16                     | 0.46              |
| 2:B:35:LEU:HD21  | 2:B:72:VAL:HG21  | 1.97                     | 0.46              |
| 2:B:81:ASN:ND2   | 2:B:81:ASN:N     | 2.61                     | 0.46              |
| 2:B:287:LEU:HD23 | 2:B:333:PHE:HZ   | 1.80                     | 0.46              |
| 2:A:118:ASP:C    | 2:A:120:GLY:N    | 2.74                     | 0.45              |
| 2:B:279:HIS:HD2  | 2:B:281:ARG:HB2  | 1.79                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:43:ASP:CG    | 2:B:44:ASP:N     | 2.75                     | 0.45              |
| 2:B:255:THR:C    | 2:B:257:GLU:H    | 2.25                     | 0.45              |
| 2:B:322:LYS:HB2  | 2:B:322:LYS:HE3  | 1.71                     | 0.45              |
| 1:D:7:U:O2'      | 1:D:8:U:OP1      | 2.31                     | 0.45              |
| 1:D:51:G:N2      | 1:D:63:C:O2      | 2.38                     | 0.45              |
| 2:A:86:PHE:CD1   | 2:A:98:PRO:HB3   | 2.52                     | 0.45              |
| 2:A:232:HIS:NE2  | 2:A:271:LEU:CB   | 2.78                     | 0.45              |
| 2:B:86:PHE:CZ    | 2:B:90:TYR:HE1   | 2.34                     | 0.45              |
| 2:B:240:LEU:N    | 2:B:240:LEU:HD23 | 2.32                     | 0.45              |
| 1:C:59:A:H2'     | 1:C:60:U:O4'     | 2.16                     | 0.45              |
| 1:D:37:A:H2'     | 1:D:38:C:H5'     | 1.98                     | 0.45              |
| 2:A:284:SER:O    | 2:A:336:PRO:HA   | 2.16                     | 0.45              |
| 2:B:275:GLN:HE21 | 2:B:275:GLN:C    | 2.24                     | 0.45              |
| 2:A:7:LYS:HE3    | 2:A:31:GLN:NE2   | 2.30                     | 0.45              |
| 2:A:324:LEU:C    | 2:A:325:ASP:OD1  | 2.60                     | 0.45              |
| 1:D:6:C:O2'      | 1:D:7:U:H5'      | 2.17                     | 0.45              |
| 2:A:105:GLU:HA   | 2:A:105:GLU:OE1  | 2.16                     | 0.45              |
| 2:B:154:PHE:CE1  | 2:B:312:TYR:CG   | 3.03                     | 0.45              |
| 2:B:287:LEU:HD23 | 2:B:333:PHE:CZ   | 2.52                     | 0.45              |
| 2:B:324:LEU:O    | 2:B:325:ASP:CG   | 2.60                     | 0.45              |
| 2:A:10:VAL:O     | 2:A:10:VAL:HG22  | 2.17                     | 0.45              |
| 2:A:44:ASP:C     | 2:A:46:GLU:N     | 2.70                     | 0.45              |
| 2:A:254:GLY:HA2  | 2:A:275:GLN:CD   | 2.40                     | 0.45              |
| 2:B:301:THR:HG22 | 2:B:302:GLY:N    | 2.31                     | 0.45              |
| 2:B:312:TYR:CD1  | 2:B:313:ARG:HG2  | 2.51                     | 0.45              |
| 2:A:11:GLY:HA3   | 2:A:111:PHE:HE1  | 1.82                     | 0.45              |
| 2:A:78:TYR:CE1   | 2:A:82:VAL:HG21  | 2.51                     | 0.45              |
| 1:C:63:C:H2'     | 1:C:64:C:C6      | 2.52                     | 0.45              |
| 2:A:317:ILE:O    | 2:A:317:ILE:CG1  | 2.65                     | 0.45              |
| 2:B:144:GLY:O    | 2:B:145:LEU:O    | 2.35                     | 0.45              |
| 2:B:183:GLU:O    | 2:B:185:LEU:N    | 2.50                     | 0.45              |
| 1:D:38:C:H3'     | 1:D:38:C:O2      | 2.16                     | 0.45              |
| 2:A:79:TRP:O     | 2:A:84:GLU:HG2   | 2.17                     | 0.45              |
| 2:A:359:ILE:N    | 2:A:359:ILE:HD12 | 2.31                     | 0.45              |
| 2:B:222:ILE:O    | 2:B:272:VAL:HA   | 2.17                     | 0.45              |
| 1:D:15:G:HO2'    | 1:D:16:A:P       | 2.40                     | 0.44              |
| 2:B:174:GLU:HB2  | 2:B:177:GLN:HE21 | 1.80                     | 0.44              |
| 1:D:65:U:H2'     | 1:D:66:A:O4'     | 2.18                     | 0.44              |
| 2:A:144:GLY:O    | 2:A:145:LEU:O    | 2.35                     | 0.44              |
| 2:B:236:MET:HG3  | 2:B:237:TYR:HD2  | 1.82                     | 0.44              |
| 2:B:368:VAL:OXT  | 2:B:368:VAL:HG13 | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:25:C:C4      | 1:D:26:A:N7      | 2.86                     | 0.44              |
| 1:D:38:C:O2      | 1:D:38:C:O5'     | 2.35                     | 0.44              |
| 2:A:148:ASN:ND2  | 2:A:148:ASN:O    | 2.50                     | 0.44              |
| 2:A:232:HIS:O    | 2:A:233:GLN:CB   | 2.65                     | 0.44              |
| 2:B:33:GLU:CD    | 2:B:70:HIS:HE1   | 2.25                     | 0.44              |
| 2:B:46:GLU:O     | 2:B:47:GLU:CB    | 2.65                     | 0.44              |
| 2:B:243:ARG:HB2  | 2:B:260:TYR:CE2  | 2.52                     | 0.44              |
| 1:C:55:U:H5'     | 1:C:55:U:H6      | 1.81                     | 0.44              |
| 2:A:59:GLN:O     | 2:A:60:ALA:C     | 2.59                     | 0.44              |
| 2:B:79:TRP:O     | 2:B:80:ASP:C     | 2.60                     | 0.44              |
| 1:C:50:G:H2'     | 1:C:51:G:C8      | 2.53                     | 0.44              |
| 2:A:288:ILE:HD12 | 2:A:288:ILE:N    | 2.33                     | 0.44              |
| 2:A:35:LEU:HD11  | 2:A:72:VAL:CG2   | 2.29                     | 0.44              |
| 2:A:89:GLU:CD    | 2:B:328:ARG:HH21 | 2.22                     | 0.44              |
| 1:C:50:G:H2'     | 1:C:51:G:H8      | 1.82                     | 0.44              |
| 1:D:27:C:H2'     | 1:D:28:C:C6      | 2.52                     | 0.44              |
| 2:A:12:MET:CE    | 2:A:34:GLY:HA3   | 2.47                     | 0.44              |
| 2:B:214:LEU:HD21 | 2:B:236:MET:HE1  | 2.00                     | 0.44              |
| 2:B:324:LEU:HD12 | 2:B:324:LEU:HA   | 1.87                     | 0.44              |
| 2:A:12:MET:HE1   | 2:A:34:GLY:CA    | 2.46                     | 0.43              |
| 2:B:135:VAL:O    | 2:B:136:ASP:HB3  | 2.17                     | 0.43              |
| 2:B:222:ILE:HG23 | 2:B:270:ILE:HG23 | 2.00                     | 0.43              |
| 2:A:131:ARG:CG   | 2:A:144:GLY:HA2  | 2.48                     | 0.43              |
| 2:B:209:PHE:C    | 2:B:211:GLY:H    | 2.25                     | 0.43              |
| 2:B:238:HIS:HA   | 2:B:242:GLN:NE2  | 2.32                     | 0.43              |
| 2:A:16:VAL:HG22  | 2:A:188:VAL:HB   | 1.99                     | 0.43              |
| 2:B:107:LYS:HE2  | 2:B:199:CYS:SG   | 2.58                     | 0.43              |
| 2:B:129:TYR:HE2  | 2:B:145:LEU:O    | 2.01                     | 0.43              |
| 2:B:243:ARG:NH2  | 2:B:258:PRO:HG3  | 2.33                     | 0.43              |
| 2:B:265:ASP:OD2  | 2:B:267:GLU:HB2  | 2.18                     | 0.43              |
| 2:B:275:GLN:CD   | 2:B:275:GLN:N    | 2.77                     | 0.43              |
| 1:D:8:U:O2       | 1:D:21:A:H2      | 2.01                     | 0.43              |
| 2:A:124:ILE:HD12 | 2:A:124:ILE:N    | 2.32                     | 0.43              |
| 2:A:156:TYR:CE2  | 2:A:345:SER:HB3  | 2.54                     | 0.43              |
| 2:A:337:VAL:HG11 | 2:A:340:VAL:CG2  | 2.49                     | 0.43              |
| 2:B:128:HIS:O    | 2:B:170:VAL:HG23 | 2.17                     | 0.43              |
| 2:B:305:ARG:CG   | 2:B:305:ARG:NH1  | 2.81                     | 0.43              |
| 2:B:307:THR:HG21 | 2:B:316:ASP:CB   | 2.48                     | 0.43              |
| 1:C:62:C:H6      | 1:C:62:C:O5'     | 2.02                     | 0.43              |
| 2:A:72:VAL:HG12  | 2:A:73:ASN:N     | 2.33                     | 0.43              |
| 2:A:294:TRP:O    | 2:A:296:ASP:N    | 2.52                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:112:LEU:HD12 | 2:A:124:ILE:HG12 | 2.01                     | 0.43              |
| 2:A:302:GLY:H    | 2:A:323:ALA:HB3  | 1.84                     | 0.43              |
| 2:B:101:LEU:O    | 2:B:105:GLU:HB2  | 2.18                     | 0.43              |
| 2:B:118:ASP:O    | 2:B:120:GLY:N    | 2.52                     | 0.43              |
| 2:B:247:GLY:O    | 2:B:248:ILE:HD12 | 2.19                     | 0.43              |
| 2:B:254:GLY:C    | 2:B:255:THR:OG1  | 2.61                     | 0.43              |
| 1:C:20:C:C4'     | 1:C:20(A):C:OP1  | 2.67                     | 0.43              |
| 2:A:337:VAL:HG11 | 2:A:340:VAL:HG23 | 1.98                     | 0.43              |
| 2:B:9:ILE:HD12   | 2:B:121:ALA:HB2  | 2.01                     | 0.43              |
| 2:B:203:GLU:O    | 2:B:207:ARG:HG2  | 2.19                     | 0.43              |
| 2:B:307:THR:O    | 2:B:348:PHE:HA   | 2.18                     | 0.43              |
| 2:B:323:ALA:HA   | 2:B:329:ILE:HD13 | 2.00                     | 0.43              |
| 2:A:138:LYS:HD2  | 2:A:160:HIS:CB   | 2.40                     | 0.43              |
| 2:B:141:LEU:HB2  | 2:B:163:ILE:CD1  | 2.48                     | 0.43              |
| 2:B:221:ILE:HG13 | 2:B:231:GLU:O    | 2.18                     | 0.43              |
| 2:B:275:GLN:O    | 2:B:275:GLN:NE2  | 2.43                     | 0.43              |
| 2:B:46:GLU:CD    | 2:B:46:GLU:N     | 2.76                     | 0.43              |
| 1:C:44:U:H2'     | 1:C:45:A:O4'     | 2.18                     | 0.43              |
| 2:A:37:MET:SD    | 2:A:111:PHE:CD1  | 3.01                     | 0.43              |
| 2:A:138:LYS:HE3  | 2:A:160:HIS:ND1  | 2.34                     | 0.43              |
| 2:A:363:ARG:C    | 2:A:365:PRO:HD3  | 2.44                     | 0.43              |
| 2:B:198:ILE:HG23 | 2:B:199:CYS:N    | 2.34                     | 0.43              |
| 2:B:309:LYS:NZ   | 2:B:316:ASP:OD1  | 2.49                     | 0.43              |
| 2:A:128:HIS:NE2  | 2:A:155:LEU:HD21 | 2.34                     | 0.42              |
| 2:A:239:THR:HG22 | 2:A:242:GLN:OE1  | 2.19                     | 0.42              |
| 2:A:308:VAL:HG22 | 2:A:348:PHE:CE2  | 2.54                     | 0.42              |
| 2:A:324:LEU:HD23 | 2:A:328:ARG:HG2  | 2.00                     | 0.42              |
| 2:B:12:MET:SD    | 2:B:62:CYS:SG    | 3.17                     | 0.42              |
| 2:B:36:PHE:CG    | 2:B:55:LEU:HD13  | 2.53                     | 0.42              |
| 2:B:283:MET:HE2  | 2:B:283:MET:CA   | 2.47                     | 0.42              |
| 1:D:32:C:O5'     | 1:D:32:C:H6      | 2.02                     | 0.42              |
| 1:C:32:C:H6      | 1:C:32:C:O5'     | 2.03                     | 0.42              |
| 1:D:56:C:H6      | 1:D:56:C:O5'     | 2.02                     | 0.42              |
| 2:A:55:LEU:O     | 2:A:58:ALA:HB3   | 2.19                     | 0.42              |
| 2:A:85:LEU:O     | 2:A:86:PHE:C     | 2.62                     | 0.42              |
| 2:A:142:LEU:CD2  | 2:A:353:VAL:HG22 | 2.49                     | 0.42              |
| 1:C:52:G:N2      | 1:C:63:C:H1'     | 2.34                     | 0.42              |
| 1:C:73:G:H4'     | 1:C:74:C:H5''    | 2.01                     | 0.42              |
| 2:A:12:MET:HE3   | 2:A:12:MET:HB2   | 1.70                     | 0.42              |
| 2:A:32:VAL:O     | 2:A:32:VAL:HG22  | 2.19                     | 0.42              |
| 2:A:248:ILE:HG21 | 2:A:259:TRP:CE2  | 2.54                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:7:LYS:HA     | 2:B:31:GLN:O     | 2.19                     | 0.42              |
| 2:B:224:VAL:O    | 2:B:224:VAL:HG12 | 2.18                     | 0.42              |
| 2:A:222:ILE:HG22 | 2:A:223:THR:O    | 2.19                     | 0.42              |
| 2:B:32:VAL:O     | 2:B:32:VAL:HG13  | 2.19                     | 0.42              |
| 2:A:88:ALA:HB1   | 2:B:324:LEU:HD11 | 2.02                     | 0.42              |
| 2:B:5:ALA:O      | 2:B:6:LYS:C      | 2.62                     | 0.42              |
| 2:B:141:LEU:HD23 | 2:B:354:CYS:HB3  | 2.01                     | 0.42              |
| 2:B:237:TYR:CD2  | 2:B:237:TYR:N    | 2.87                     | 0.42              |
| 1:C:35:U:H2'     | 1:C:36:C:C6      | 2.54                     | 0.42              |
| 1:D:3:C:O2       | 1:D:71:A:H3'     | 2.20                     | 0.42              |
| 2:A:323:ALA:O    | 2:A:324:LEU:C    | 2.63                     | 0.42              |
| 2:B:60:ALA:O     | 2:B:63:ASP:HB2   | 2.20                     | 0.42              |
| 2:B:221:ILE:HG22 | 2:B:229:ILE:CG2  | 2.50                     | 0.42              |
| 1:C:20:C:H4'     | 1:C:20(A):C:OP1  | 2.20                     | 0.42              |
| 2:A:160:HIS:HD2  | 2:A:161:GLU:H    | 1.67                     | 0.42              |
| 2:A:324:LEU:HA   | 2:A:324:LEU:HD12 | 1.80                     | 0.42              |
| 2:B:18:SER:O     | 2:B:21:SER:HB3   | 2.20                     | 0.42              |
| 2:B:174:GLU:CB   | 2:B:177:GLN:HE21 | 2.32                     | 0.42              |
| 2:A:301:THR:HA   | 2:A:323:ALA:CB   | 2.49                     | 0.42              |
| 1:C:3:C:O5'      | 1:C:3:C:H6       | 2.03                     | 0.41              |
| 2:B:9:ILE:O      | 2:B:124:ILE:HA   | 2.20                     | 0.41              |
| 2:B:210:LEU:O    | 2:B:214:LEU:O    | 2.38                     | 0.41              |
| 1:C:16:A:N3      | 1:C:16:A:H2'     | 2.35                     | 0.41              |
| 2:A:243:ARG:HB2  | 2:A:260:TYR:CD1  | 2.54                     | 0.41              |
| 2:B:42:GLU:OE2   | 2:B:47:GLU:HG2   | 2.20                     | 0.41              |
| 2:B:76:ALA:O     | 2:B:80:ASP:OD1   | 2.38                     | 0.41              |
| 2:B:83:PHE:O     | 2:B:84:GLU:C     | 2.61                     | 0.41              |
| 2:B:304:MET:CE   | 2:B:306:CYS:HB3  | 2.49                     | 0.41              |
| 2:B:73:ASN:ND2   | 2:B:74:PHE:CD2   | 2.88                     | 0.41              |
| 1:C:20:C:C5'     | 1:C:20(A):C:OP1  | 2.68                     | 0.41              |
| 1:C:39:G:O2'     | 1:C:40:G:H5'     | 2.20                     | 0.41              |
| 2:A:142:LEU:HD23 | 2:A:353:VAL:HA   | 2.02                     | 0.41              |
| 2:A:257:GLU:H    | 2:A:257:GLU:HG2  | 1.67                     | 0.41              |
| 2:B:304:MET:HG2  | 2:B:321:VAL:HB   | 2.02                     | 0.41              |
| 1:C:9:C:C5'      | 1:C:10:G:OP2     | 2.63                     | 0.41              |
| 1:C:27:C:H2'     | 1:C:28:C:C6      | 2.55                     | 0.41              |
| 2:A:179:ARG:O    | 2:A:183:GLU:HG3  | 2.21                     | 0.41              |
| 2:A:292:LEU:HG   | 2:A:327:ASP:O    | 2.20                     | 0.41              |
| 2:B:8:VAL:HG12   | 2:B:30:TYR:HB3   | 2.02                     | 0.41              |
| 2:B:175:LYS:O    | 2:B:176:PRO:C    | 2.62                     | 0.41              |
| 2:B:232:HIS:HB3  | 2:B:234:GLY:H    | 1.85                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:36:C:O5'     | 1:D:36:C:H6      | 2.04                     | 0.41              |
| 2:A:211:GLY:C    | 2:A:213:TYR:H    | 2.28                     | 0.41              |
| 2:B:118:ASP:C    | 2:B:120:GLY:N    | 2.79                     | 0.41              |
| 2:B:185:LEU:O    | 2:B:186:GLY:C    | 2.63                     | 0.41              |
| 1:C:25:C:C4      | 1:C:26:A:N7      | 2.88                     | 0.41              |
| 2:B:35:LEU:HD23  | 2:B:111:PHE:CD1  | 2.56                     | 0.41              |
| 2:B:346:ALA:O    | 2:B:357:GLY:HA3  | 2.20                     | 0.41              |
| 2:A:15:GLY:HA3   | 3:A:1002:PO4:O2  | 2.20                     | 0.41              |
| 2:B:32:VAL:O     | 2:B:67:ILE:HG23  | 2.21                     | 0.41              |
| 2:B:75:ALA:O     | 2:B:77:GLU:N     | 2.54                     | 0.41              |
| 2:B:156:TYR:CD1  | 2:B:156:TYR:C    | 2.99                     | 0.41              |
| 2:A:129:TYR:CE2  | 2:A:145:LEU:O    | 2.74                     | 0.41              |
| 2:A:142:LEU:HD21 | 2:A:353:VAL:HG22 | 2.01                     | 0.41              |
| 2:A:149:LYS:HB3  | 2:A:175:LYS:HD2  | 2.03                     | 0.41              |
| 2:A:174:GLU:C    | 2:A:176:PRO:CD   | 2.89                     | 0.41              |
| 2:A:279:HIS:HA   | 2:A:280:PRO:HD3  | 1.95                     | 0.41              |
| 2:B:237:TYR:HD2  | 2:B:237:TYR:N    | 2.18                     | 0.41              |
| 2:B:361:GLU:HG3  | 2:B:362:GLN:N    | 2.33                     | 0.41              |
| 2:A:18:SER:HB3   | 3:A:1002:PO4:O2  | 2.20                     | 0.41              |
| 2:A:231:GLU:CD   | 2:A:231:GLU:N    | 2.77                     | 0.41              |
| 2:A:283:MET:HB2  | 2:A:366:LEU:CD1  | 2.51                     | 0.41              |
| 2:B:368:VAL:OXT  | 2:B:368:VAL:CG1  | 2.70                     | 0.41              |
| 1:C:58:A:O2'     | 1:C:59:A:H3'     | 2.21                     | 0.40              |
| 2:B:86:PHE:CE1   | 2:B:206:PHE:HB3  | 2.55                     | 0.40              |
| 2:B:182:ALA:O    | 2:B:187:LEU:HB2  | 2.22                     | 0.40              |
| 1:C:5:C:C2       | 1:C:6:C:H6       | 2.39                     | 0.40              |
| 2:A:294:TRP:O    | 2:A:295:VAL:C    | 2.63                     | 0.40              |
| 2:B:78:TYR:O     | 2:B:79:TRP:C     | 2.65                     | 0.40              |
| 2:B:86:PHE:HE1   | 2:B:210:LEU:CD1  | 2.31                     | 0.40              |
| 2:B:169:PRO:HG2  | 2:B:170:VAL:H    | 1.87                     | 0.40              |
| 2:B:180:LYS:O    | 2:B:183:GLU:N    | 2.53                     | 0.40              |
| 2:A:324:LEU:HD23 | 2:A:328:ARG:CG   | 2.52                     | 0.40              |
| 2:B:48:TYR:O     | 2:B:50:THR:N     | 2.55                     | 0.40              |
| 2:B:50:THR:HG22  | 2:B:50:THR:O     | 2.22                     | 0.40              |
| 2:B:238:HIS:HA   | 2:B:242:GLN:HE22 | 1.87                     | 0.40              |
| 2:A:180:LYS:O    | 2:A:183:GLU:N    | 2.49                     | 0.40              |
| 2:A:212:ARG:HG2  | 2:A:212:ARG:NH1  | 2.37                     | 0.40              |
| 2:B:17:ASP:OD1   | 2:B:175:LYS:NZ   | 2.54                     | 0.40              |
| 2:B:174:GLU:O    | 2:B:175:LYS:C    | 2.64                     | 0.40              |
| 1:C:2:U:H5''     | 1:C:3:C:C4       | 2.56                     | 0.40              |
| 2:B:274:ALA:CB   | 2:B:279:HIS:CD2  | 3.04                     | 0.40              |

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| Atom-1        | Atom-2        | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|---------------|--------------------------|-------------------|
| 2:B:312:TYR:C | 2:B:314:GLN:H | 2.30                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |   |
|-----|-------|---------------|-----------|----------|----------|-------------|---|
| 2   | A     | 344/380 (90%) | 275 (80%) | 44 (13%) | 25 (7%)  | 1           | 5 |
| 2   | B     | 355/380 (93%) | 275 (78%) | 55 (16%) | 25 (7%)  | 1           | 5 |
| All | All   | 699/760 (92%) | 550 (79%) | 99 (14%) | 50 (7%)  | 1           | 5 |

All (50) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | A     | 49  | CYS  |
| 2   | A     | 145 | LEU  |
| 2   | A     | 326 | ASP  |
| 2   | A     | 338 | ALA  |
| 2   | B     | 74  | PHE  |
| 2   | B     | 80  | ASP  |
| 2   | B     | 145 | LEU  |
| 2   | B     | 213 | TYR  |
| 2   | B     | 297 | ARG  |
| 2   | B     | 338 | ALA  |
| 2   | A     | 6   | LYS  |
| 2   | A     | 107 | LYS  |
| 2   | A     | 119 | LEU  |
| 2   | A     | 178 | VAL  |
| 2   | A     | 226 | GLY  |
| 2   | A     | 229 | ILE  |
| 2   | A     | 250 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | A     | 253 | GLU  |
| 2   | A     | 277 | HIS  |
| 2   | A     | 295 | VAL  |
| 2   | A     | 297 | ARG  |
| 2   | B     | 40  | TRP  |
| 2   | B     | 46  | GLU  |
| 2   | B     | 49  | CYS  |
| 2   | B     | 119 | LEU  |
| 2   | B     | 120 | GLY  |
| 2   | B     | 178 | VAL  |
| 2   | B     | 229 | ILE  |
| 2   | B     | 253 | GLU  |
| 2   | B     | 277 | HIS  |
| 2   | B     | 295 | VAL  |
| 2   | B     | 326 | ASP  |
| 2   | A     | 42  | GLU  |
| 2   | A     | 114 | PHE  |
| 2   | A     | 120 | GLY  |
| 2   | A     | 323 | ALA  |
| 2   | B     | 77  | GLU  |
| 2   | B     | 184 | ASP  |
| 2   | A     | 60  | ALA  |
| 2   | A     | 115 | ALA  |
| 2   | B     | 75  | ALA  |
| 2   | B     | 226 | GLY  |
| 2   | A     | 169 | PRO  |
| 2   | B     | 78  | TYR  |
| 2   | B     | 109 | LYS  |
| 2   | B     | 169 | PRO  |
| 2   | A     | 251 | THR  |
| 2   | A     | 15  | GLY  |
| 2   | A     | 106 | ILE  |
| 2   | B     | 250 | GLY  |

### 5.3.2 Protein sidechains [i](#)

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 2   | A     | 288/315 (91%) | 257 (89%) | 31 (11%) | 6           | 25 |
| 2   | B     | 297/315 (94%) | 268 (90%) | 29 (10%) | 7           | 29 |
| All | All   | 585/630 (93%) | 525 (90%) | 60 (10%) | 7           | 27 |

All (60) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | A     | 7   | LYS  |
| 2   | A     | 10  | VAL  |
| 2   | A     | 12  | MET  |
| 2   | A     | 21  | SER  |
| 2   | A     | 31  | GLN  |
| 2   | A     | 32  | VAL  |
| 2   | A     | 72  | VAL  |
| 2   | A     | 82  | VAL  |
| 2   | A     | 107 | LYS  |
| 2   | A     | 111 | PHE  |
| 2   | A     | 138 | LYS  |
| 2   | A     | 150 | ASP  |
| 2   | A     | 157 | THR  |
| 2   | A     | 160 | HIS  |
| 2   | A     | 167 | LEU  |
| 2   | A     | 170 | VAL  |
| 2   | A     | 231 | GLU  |
| 2   | A     | 236 | MET  |
| 2   | A     | 255 | THR  |
| 2   | A     | 266 | VAL  |
| 2   | A     | 267 | GLU  |
| 2   | A     | 269 | ASN  |
| 2   | A     | 285 | VAL  |
| 2   | A     | 287 | LEU  |
| 2   | A     | 305 | ARG  |
| 2   | A     | 313 | ARG  |
| 2   | A     | 315 | THR  |
| 2   | A     | 317 | ILE  |
| 2   | A     | 326 | ASP  |
| 2   | A     | 335 | GLU  |
| 2   | A     | 337 | VAL  |
| 2   | B     | 16  | VAL  |
| 2   | B     | 17  | ASP  |
| 2   | B     | 39  | ASN  |
| 2   | B     | 68  | GLU  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 2          | B            | 72         | VAL         |
| 2          | B            | 74         | PHE         |
| 2          | B            | 79         | TRP         |
| 2          | B            | 81         | ASN         |
| 2          | B            | 101        | LEU         |
| 2          | B            | 113        | GLU         |
| 2          | B            | 122        | ASP         |
| 2          | B            | 140        | ARG         |
| 2          | B            | 156        | TYR         |
| 2          | B            | 161        | GLU         |
| 2          | B            | 167        | LEU         |
| 2          | B            | 180        | LYS         |
| 2          | B            | 204        | ARG         |
| 2          | B            | 240        | LEU         |
| 2          | B            | 251        | THR         |
| 2          | B            | 255        | THR         |
| 2          | B            | 275        | GLN         |
| 2          | B            | 285        | VAL         |
| 2          | B            | 298        | GLU         |
| 2          | B            | 305        | ARG         |
| 2          | B            | 308        | VAL         |
| 2          | B            | 316        | ASP         |
| 2          | B            | 317        | ILE         |
| 2          | B            | 326        | ASP         |
| 2          | B            | 353        | VAL         |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 2          | A            | 26         | GLN         |
| 2          | A            | 31         | GLN         |
| 2          | A            | 59         | GLN         |
| 2          | A            | 70         | HIS         |
| 2          | A            | 97         | ASN         |
| 2          | A            | 148        | ASN         |
| 2          | A            | 177        | GLN         |
| 2          | A            | 268        | ASN         |
| 2          | A            | 269        | ASN         |
| 2          | A            | 279        | HIS         |
| 2          | B            | 70         | HIS         |
| 2          | B            | 73         | ASN         |
| 2          | B            | 81         | ASN         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 177 | GLN  |
| 2   | B     | 242 | GLN  |
| 2   | B     | 269 | ASN  |
| 2   | B     | 275 | GLN  |
| 2   | B     | 279 | HIS  |
| 2   | B     | 290 | GLN  |
| 2   | B     | 314 | GLN  |
| 2   | B     | 362 | GLN  |

### 5.3.3 RNA [i](#)

| Mol | Chain | Analysed      | Backbone Outliers | Pucker Outliers |
|-----|-------|---------------|-------------------|-----------------|
| 1   | C     | 73/76 (96%)   | 24 (32%)          | 9 (12%)         |
| 1   | D     | 70/76 (92%)   | 21 (30%)          | 10 (14%)        |
| All | All   | 143/152 (94%) | 45 (31%)          | 19 (13%)        |

All (45) RNA backbone outliers are listed below:

| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | C     | 2     | U    |
| 1   | C     | 3     | C    |
| 1   | C     | 4     | C    |
| 1   | C     | 8     | U    |
| 1   | C     | 9     | C    |
| 1   | C     | 10    | G    |
| 1   | C     | 16    | A    |
| 1   | C     | 17    | G    |
| 1   | C     | 18    | G    |
| 1   | C     | 19    | C    |
| 1   | C     | 20    | C    |
| 1   | C     | 20(A) | C    |
| 1   | C     | 34    | U    |
| 1   | C     | 35    | U    |
| 1   | C     | 52    | G    |
| 1   | C     | 57    | G    |
| 1   | C     | 58    | A    |
| 1   | C     | 64    | C    |
| 1   | C     | 67    | G    |
| 1   | C     | 68    | G    |
| 1   | C     | 69    | G    |
| 1   | C     | 70    | G    |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | C     | 71    | A    |
| 1   | C     | 72    | C    |
| 1   | D     | 4     | C    |
| 1   | D     | 8     | U    |
| 1   | D     | 9     | C    |
| 1   | D     | 10    | G    |
| 1   | D     | 16    | A    |
| 1   | D     | 17    | G    |
| 1   | D     | 18    | G    |
| 1   | D     | 19    | C    |
| 1   | D     | 20    | C    |
| 1   | D     | 20(A) | C    |
| 1   | D     | 34    | U    |
| 1   | D     | 35    | U    |
| 1   | D     | 52    | G    |
| 1   | D     | 57    | G    |
| 1   | D     | 58    | A    |
| 1   | D     | 59    | A    |
| 1   | D     | 64    | C    |
| 1   | D     | 66    | A    |
| 1   | D     | 67    | G    |
| 1   | D     | 68    | G    |
| 1   | D     | 70    | G    |

All (19) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 7   | U    |
| 1   | C     | 9   | C    |
| 1   | C     | 15  | G    |
| 1   | C     | 18  | G    |
| 1   | C     | 20  | C    |
| 1   | C     | 34  | U    |
| 1   | C     | 47  | C    |
| 1   | C     | 57  | G    |
| 1   | C     | 60  | U    |
| 1   | D     | 7   | U    |
| 1   | D     | 9   | C    |
| 1   | D     | 15  | G    |
| 1   | D     | 18  | G    |
| 1   | D     | 20  | C    |
| 1   | D     | 34  | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 47  | C    |
| 1   | D     | 56  | C    |
| 1   | D     | 57  | G    |
| 1   | D     | 60  | 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](#)

9 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | PO4  | C     | 1004 | -    | 4,4,4        | 1.65 | 0        | 6,6,6       | 0.47 | 0        |
| 4   | SO4  | B     | 2004 | -    | 4,4,4        | 0.37 | 0        | 6,6,6       | 0.10 | 0        |
| 3   | PO4  | B     | 1001 | -    | 4,4,4        | 1.80 | 1 (25%)  | 6,6,6       | 0.46 | 0        |
| 4   | SO4  | A     | 2003 | -    | 4,4,4        | 0.36 | 0        | 6,6,6       | 0.09 | 0        |
| 4   | SO4  | B     | 2002 | -    | 4,4,4        | 0.36 | 0        | 6,6,6       | 0.15 | 0        |
| 4   | SO4  | A     | 2005 | -    | 4,4,4        | 0.35 | 0        | 6,6,6       | 0.12 | 0        |
| 3   | PO4  | A     | 1002 | -    | 4,4,4        | 1.65 | 0        | 6,6,6       | 0.47 | 0        |
| 3   | PO4  | B     | 1003 | -    | 4,4,4        | 1.71 | 1 (25%)  | 6,6,6       | 0.46 | 0        |
| 4   | SO4  | A     | 2001 | -    | 4,4,4        | 0.40 | 0        | 6,6,6       | 0.20 | 0        |

All (2) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3   | B     | 1001 | PO4  | P-O4  | -2.11 | 1.48        | 1.54     |
| 3   | B     | 1003 | PO4  | P-O3  | -2.05 | 1.48        | 1.54     |

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | A     | 1002 | PO4  | 3       | 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

### 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, 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   | C     | 74/76 (97%)   | 0.30   | 2 (2%) 56 35  | 32, 71, 172, 188      | 0     |
| 1   | D     | 71/76 (93%)   | 0.09   | 0 100 100     | 42, 73, 145, 185      | 0     |
| 2   | A     | 348/380 (91%) | -0.25  | 2 (0%) 85 70  | 11, 43, 80, 104       | 0     |
| 2   | B     | 359/380 (94%) | 0.04   | 16 (4%) 38 20 | 19, 57, 110, 166      | 0     |
| All | All   | 852/912 (93%) | -0.05  | 20 (2%) 61 39 | 11, 53, 111, 188      | 0     |

All (20) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | B     | 196 | THR  | 5.1  |
| 2   | B     | 40  | TRP  | 4.1  |
| 2   | A     | 249 | GLY  | 3.5  |
| 2   | B     | 250 | GLY  | 2.7  |
| 2   | B     | 254 | GLY  | 2.7  |
| 2   | B     | 357 | GLY  | 2.6  |
| 2   | B     | 39  | ASN  | 2.6  |
| 2   | B     | 251 | THR  | 2.6  |
| 2   | B     | 148 | ASN  | 2.6  |
| 1   | C     | 67  | G    | 2.5  |
| 2   | B     | 42  | GLU  | 2.5  |
| 2   | B     | 79  | TRP  | 2.3  |
| 1   | C     | 3   | C    | 2.3  |
| 2   | B     | 38  | LYS  | 2.3  |
| 2   | A     | 148 | ASN  | 2.3  |
| 2   | B     | 252 | LYS  | 2.3  |
| 2   | B     | 277 | HIS  | 2.2  |
| 2   | B     | 43  | ASP  | 2.1  |
| 2   | B     | 175 | LYS  | 2.1  |
| 2   | B     | 197 | GLY  | 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 [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 3   | PO4  | C     | 1004 | 5/5   | 0.67 | 0.14 | 141,149,151,152             | 0     |
| 4   | SO4  | B     | 2004 | 5/5   | 0.70 | 0.10 | 116,118,120,120             | 0     |
| 4   | SO4  | A     | 2003 | 5/5   | 0.76 | 0.12 | 140,141,143,144             | 0     |
| 4   | SO4  | B     | 2002 | 5/5   | 0.77 | 0.10 | 130,131,134,134             | 0     |
| 4   | SO4  | A     | 2001 | 5/5   | 0.80 | 0.11 | 82,90,97,102                | 0     |
| 4   | SO4  | A     | 2005 | 5/5   | 0.90 | 0.12 | 89,92,93,99                 | 0     |
| 3   | PO4  | B     | 1003 | 5/5   | 0.94 | 0.07 | 72,73,78,81                 | 0     |
| 3   | PO4  | A     | 1002 | 5/5   | 0.96 | 0.07 | 53,54,63,69                 | 0     |
| 3   | PO4  | B     | 1001 | 5/5   | 0.96 | 0.06 | 47,56,64,68                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.