



# Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 09:59 pm BST

PDB ID : 2GIC  
Title : Crystal Structure of a vesicular stomatitis virus nucleocapsid-RNA complex  
Authors : Green, T.J.; Zhang, X.; Wertz, G.W.; Luo, M.  
Deposited on : 2006-03-28  
Resolution : 2.92 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.

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

|                                |   |  |
|--------------------------------|---|--|
| MolProbity                     | : | 4.02b-467  |
| Xtriage (Phenix)               | : | 1.13   |
| EDS                            | : | 2.11   |
| Percentile statistics          | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac                         | : | 5.8.0158   |
| CCP4                           | : | 7.0.044 (Gargrove)   |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)  |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)  |
| Validation Pipeline (wwPDB-VP) | : | 2.11   |

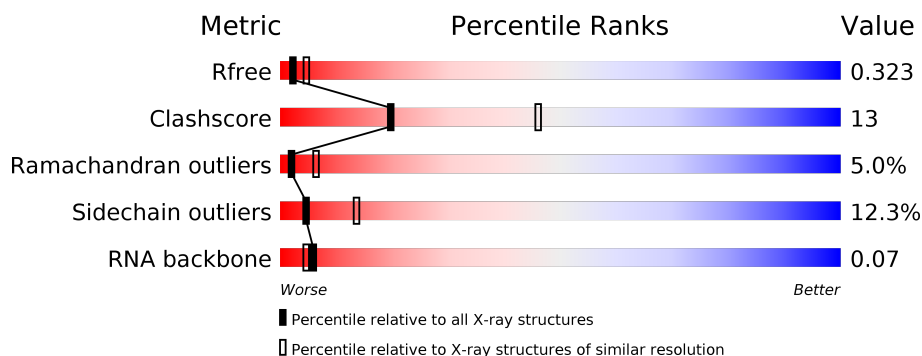
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.92 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 2307 (2.94-2.90)                                      |
| Clashscore            | 141614                      | 2531 (2.94-2.90)                                      |
| Ramachandran outliers | 138981                      | 2462 (2.94-2.90)                                      |
| Sidechain outliers    | 138945                      | 2464 (2.94-2.90)                                      |
| RNA backbone          | 3102                        | 1001 (3.18-2.66)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | R     | 45     | 9% 29% 51% 11%   |
| 2   | A     | 422    | 70% 24% 5%       |
| 2   | B     | 422    | 67% 25% 7% .     |
| 2   | C     | 422    | 68% 23% 6% ..    |
| 2   | D     | 422    | 70% 24% 5% .     |
| 2   | E     | 422    | 68% 26% 5%       |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17432 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.

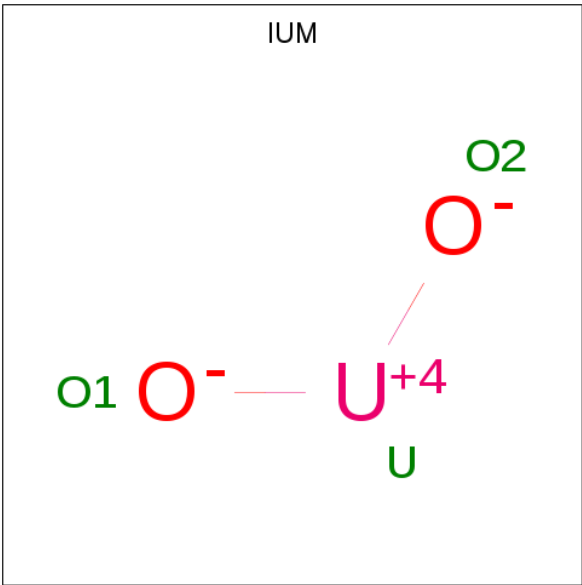
- Molecule 1 is a RNA chain called 45-MER.

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 1   | R     | 45       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 900   | 405 | 90 | 360 | 45 |         |         |       |

- Molecule 2 is a protein called Nucleocapsid protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | A     | 421      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3327  | 2118 | 558 | 633 | 18 |         |         |       |
| 2   | B     | 415      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3290  | 2097 | 552 | 623 | 18 |         |         |       |
| 2   | C     | 413      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3275  | 2089 | 550 | 618 | 18 |         |         |       |
| 2   | D     | 416      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3298  | 2103 | 553 | 624 | 18 |         |         |       |
| 2   | E     | 421      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3327  | 2118 | 558 | 633 | 18 |         |         |       |

- Molecule 3 is URANYL (VI) ION (three-letter code: IUM) (formula: O<sub>2</sub>U).



| Mol | Chain | Residues | Atoms          | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 3   | A     | 1        | Total U<br>1 1 | 0       | 0       |
| 3   | A     | 1        | Total U<br>1 1 | 0       | 0       |
| 3   | A     | 1        | Total U<br>1 1 | 0       | 0       |
| 3   | A     | 1        | Total U<br>1 1 | 0       | 0       |
| 3   | B     | 1        | Total U<br>1 1 | 0       | 0       |
| 3   | B     | 1        | Total U<br>1 1 | 0       | 0       |
| 3   | B     | 1        | Total U<br>1 1 | 0       | 0       |
| 3   | C     | 1        | Total U<br>1 1 | 0       | 0       |
| 3   | C     | 1        | Total U<br>1 1 | 0       | 0       |
| 3   | C     | 1        | Total U<br>1 1 | 0       | 0       |
| 3   | D     | 1        | Total U<br>1 1 | 0       | 0       |
| 3   | D     | 1        | Total U<br>1 1 | 0       | 0       |
| 3   | E     | 1        | Total U<br>1 1 | 0       | 0       |
| 3   | E     | 1        | Total U<br>1 1 | 0       | 0       |

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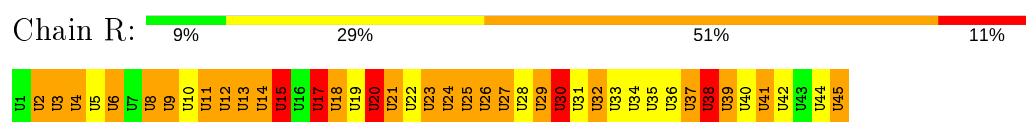
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| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 3   | E     | 1        | Total | U | 0       | 0       |
|     |       |          | 1     | 1 |         |         |

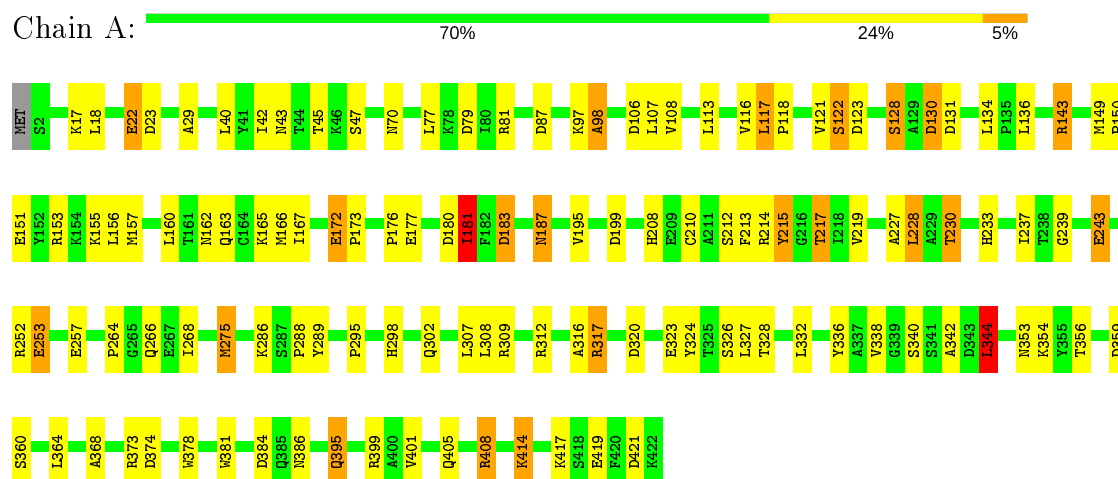
### 3 Residue-property plots

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

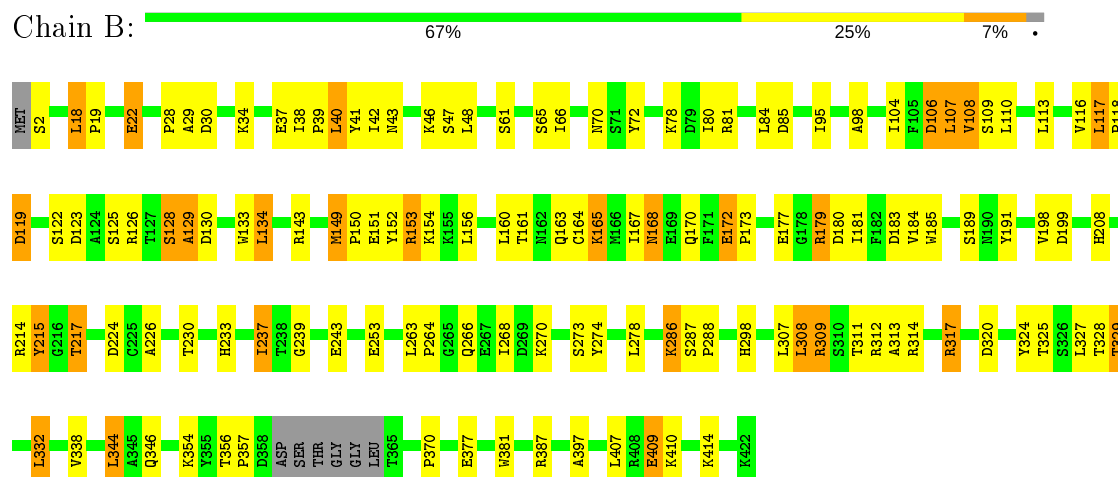
- Molecule 1: 45-MER



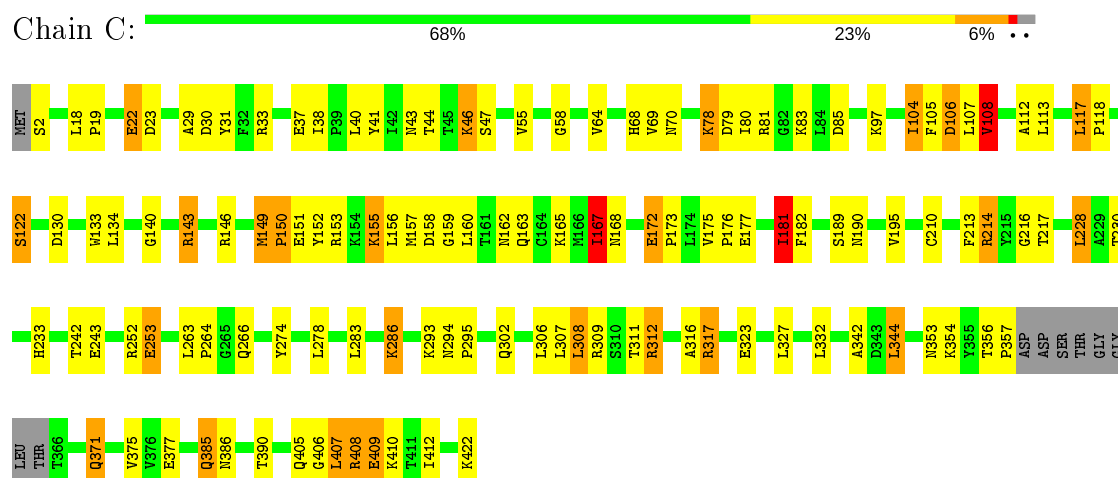
- Molecule 2: Nucleocapsid protein



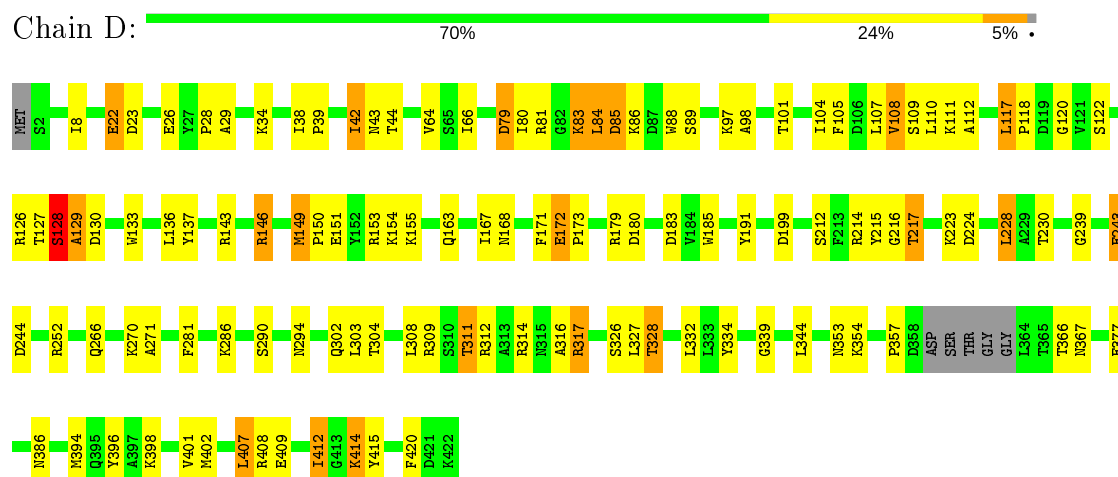
- Molecule 2: Nucleocapsid protein



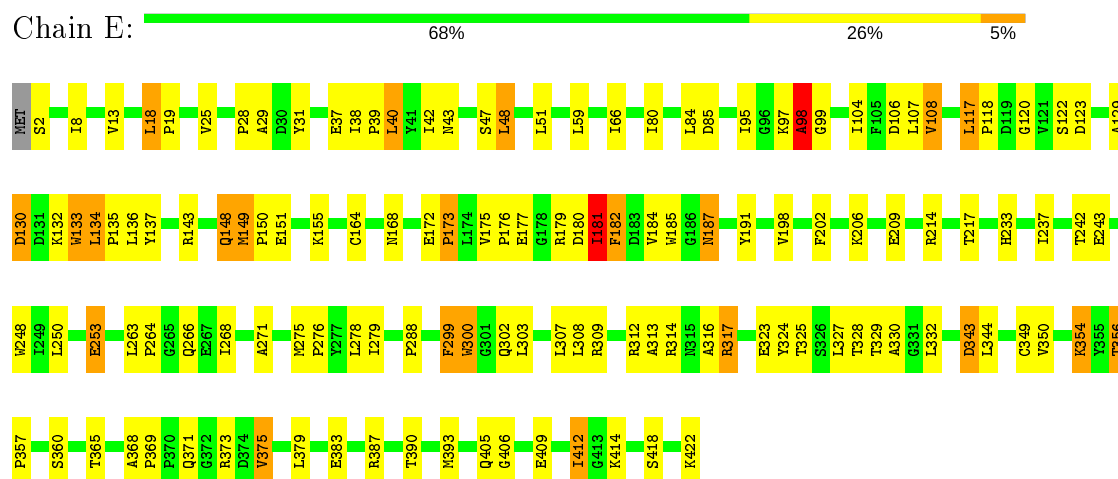
- Molecule 2: Nucleocapsid protein



- Molecule 2: Nucleocapsid protein



- Molecule 2: Nucleocapsid protein



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 2   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 166.16 Å   236.32 Å   75.65 Å<br>90.00°   90.00°   90.00°   | Depositor        |
| Resolution (Å)  | 44.86 – 2.92<br>44.84 – 2.92                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 91.9 (44.86-2.92)<br>90.5 (44.84-2.92)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 4.95 (at 2.90 Å)  | Xtriage          |
| Refinement program  | REFMAC 5.2.0005   | Depositor        |
| R, $R_{free}$   | 0.255   ,   0.306<br>0.270   ,   0.323                      | Depositor<br>DCC |
| $R_{free}$ test set   | 3262 reflections (5.05%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 73.1  | Xtriage          |
| Anisotropy  | 0.676   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.29 , 33.2   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.87  | EDS              |
| Total number of atoms   | 17432   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 28.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IUM

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   | R     | 0.93         | 0/989       | 1.56        | 10/1526 (0.7%)  |
| 2   | A     | 0.39         | 0/3403      | 0.54        | 0/4607          |
| 2   | B     | 0.40         | 0/3365      | 0.55        | 0/4554          |
| 2   | C     | 0.39         | 0/3350      | 0.56        | 0/4533          |
| 2   | D     | 0.39         | 0/3373      | 0.56        | 0/4565          |
| 2   | E     | 0.40         | 0/3403      | 0.54        | 0/4607          |
| All | All   | 0.44         | 0/17883     | 0.66        | 10/24392 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | B     | 0                   | 1                   |
| 2   | E     | 0                   | 1                   |
| All | All   | 0                   | 2                   |

There are no bond length outliers.

All (10) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | R     | 20  | U    | P-O3'-C3'   | 8.96  | 130.45      | 119.70   |
| 1   | R     | 9   | U    | O4'-C1'-N1  | 6.62  | 113.50      | 108.20   |
| 1   | R     | 9   | U    | O4'-C4'-C3' | -6.12 | 97.88       | 104.00   |
| 1   | R     | 34  | U    | O4'-C1'-N1  | 5.87  | 112.90      | 108.20   |
| 1   | R     | 15  | U    | C2-N1-C1'   | 5.75  | 124.61      | 117.70   |
| 1   | R     | 17  | U    | P-O3'-C3'   | 5.33  | 126.10      | 119.70   |
| 1   | R     | 32  | U    | C3'-C2'-C1' | 5.22  | 105.68      | 101.50   |
| 1   | R     | 37  | U    | O4'-C1'-N1  | 5.11  | 112.29      | 108.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | R     | 38  | U    | P-O3'-C3'   | 5.09  | 125.81      | 119.70   |
| 1   | R     | 30  | U    | C4'-C3'-C2' | -5.07 | 97.53       | 102.60   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 2   | B     | 106 | ASP  | Peptide |
| 2   | E     | 98  | ALA  | Peptide |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | R     | 900   | 0        | 451      | 62      | 0            |
| 2   | A     | 3327  | 0        | 3287     | 87      | 0            |
| 2   | B     | 3290  | 0        | 3253     | 105     | 0            |
| 2   | C     | 3275  | 0        | 3242     | 81      | 0            |
| 2   | D     | 3298  | 0        | 3264     | 75      | 0            |
| 2   | E     | 3327  | 0        | 3287     | 92      | 0            |
| 3   | A     | 4     | 0        | 0        | 0       | 0            |
| 3   | B     | 3     | 0        | 0        | 0       | 0            |
| 3   | C     | 3     | 0        | 0        | 0       | 0            |
| 3   | D     | 2     | 0        | 0        | 0       | 0            |
| 3   | E     | 3     | 0        | 0        | 0       | 0            |
| All | All   | 17432 | 0        | 16784    | 435     | 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 13.

All (435) 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) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:A:143:ARG:HD2 | 2:A:155:LYS:CE  | 1.44                     | 1.45              |
| 2:A:143:ARG:CD  | 2:A:155:LYS:HE2 | 1.52                     | 1.36              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:109:SER:O    | 2:B:110:LEU:HD23 | 1.31                     | 1.22              |
| 2:D:107:LEU:O    | 2:D:108:VAL:HG22 | 1.42                     | 1.18              |
| 2:B:107:LEU:N    | 2:B:107:LEU:HD23 | 1.56                     | 1.16              |
| 2:B:37:GLU:HB2   | 2:B:108:VAL:CG2  | 1.76                     | 1.14              |
| 2:B:117:LEU:HB2  | 2:B:118:PRO:HD3  | 1.30                     | 1.11              |
| 2:C:143:ARG:HH11 | 2:C:155:LYS:HD3  | 1.17                     | 1.08              |
| 1:R:22:U:H2'     | 2:B:317:ARG:HE   | 1.21                     | 1.06              |
| 2:B:37:GLU:HB2   | 2:B:108:VAL:HG21 | 1.34                     | 1.05              |
| 2:C:214:ARG:HA   | 2:C:217:THR:HG22 | 1.36                     | 1.03              |
| 2:B:106:ASP:C    | 2:B:107:LEU:HD23 | 1.79                     | 1.01              |
| 2:A:143:ARG:HD2  | 2:A:155:LYS:HE3  | 1.41                     | 0.98              |
| 2:D:143:ARG:HE   | 2:D:155:LYS:HE3  | 1.27                     | 0.96              |
| 2:A:117:LEU:HB3  | 2:A:118:PRO:HD3  | 1.46                     | 0.94              |
| 2:E:133:TRP:CD1  | 2:E:134:LEU:N    | 2.36                     | 0.94              |
| 2:D:117:LEU:HB2  | 2:D:118:PRO:HD3  | 1.48                     | 0.93              |
| 2:B:172:GLU:HB3  | 2:B:173:PRO:HD3  | 1.49                     | 0.93              |
| 2:B:107:LEU:N    | 2:B:107:LEU:CD2  | 2.31                     | 0.92              |
| 2:E:129:ALA:HB1  | 2:E:133:TRP:HE1  | 1.33                     | 0.91              |
| 2:A:143:ARG:HD2  | 2:A:155:LYS:HE2  | 0.92                     | 0.90              |
| 2:B:37:GLU:HB2   | 2:B:108:VAL:HG22 | 1.56                     | 0.88              |
| 2:D:214:ARG:HA   | 2:D:217:THR:HG22 | 1.54                     | 0.88              |
| 2:B:320:ASP:HB3  | 2:C:312:ARG:NH2  | 1.89                     | 0.88              |
| 2:B:109:SER:O    | 2:B:110:LEU:CD2  | 2.21                     | 0.87              |
| 2:A:324:TYR:O    | 2:A:328:THR:HG23 | 1.76                     | 0.86              |
| 2:C:117:LEU:HB2  | 2:C:118:PRO:HD3  | 1.59                     | 0.85              |
| 2:D:146:ARG:HH11 | 2:D:223:LYS:HE2  | 1.40                     | 0.85              |
| 2:B:107:LEU:HD13 | 2:B:274:TYR:OH   | 1.77                     | 0.84              |
| 2:B:117:LEU:HB2  | 2:B:118:PRO:CD   | 2.07                     | 0.83              |
| 2:C:2:SER:HB3    | 2:D:243:GLU:HG3  | 1.58                     | 0.83              |
| 2:E:117:LEU:HB2  | 2:E:118:PRO:HD3  | 1.60                     | 0.82              |
| 1:R:11:U:H3'     | 1:R:12:U:H5''    | 1.62                     | 0.81              |
| 2:B:37:GLU:CB    | 2:B:108:VAL:HG21 | 2.09                     | 0.81              |
| 2:A:143:ARG:CG   | 2:A:155:LYS:HE2  | 2.09                     | 0.81              |
| 2:B:164:CYS:HA   | 2:B:168:ASN:H    | 1.46                     | 0.81              |
| 2:D:83:LYS:HG3   | 2:D:101:THR:HG22 | 1.64                     | 0.79              |
| 2:D:143:ARG:HE   | 2:D:155:LYS:CE   | 1.97                     | 0.78              |
| 2:E:324:TYR:O    | 2:E:328:THR:HG23 | 1.84                     | 0.78              |
| 2:B:106:ASP:C    | 2:B:107:LEU:CD2  | 2.53                     | 0.77              |
| 2:A:323:GLU:OE1  | 2:B:239:GLY:HA3  | 1.84                     | 0.77              |
| 2:C:143:ARG:NH1  | 2:C:155:LYS:HD3  | 1.97                     | 0.77              |
| 2:D:107:LEU:O    | 2:D:108:VAL:CG2  | 2.30                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:253:GLU:CD   | 2:A:253:GLU:H    | 1.88                     | 0.76              |
| 2:B:320:ASP:HB3  | 2:C:312:ARG:HH22 | 1.47                     | 0.76              |
| 2:C:253:GLU:CD   | 2:C:253:GLU:H    | 1.89                     | 0.76              |
| 2:A:215:TYR:HD2  | 2:A:215:TYR:N    | 1.83                     | 0.75              |
| 2:D:143:ARG:NE   | 2:D:155:LYS:HE3  | 1.99                     | 0.74              |
| 2:A:354:LYS:HD2  | 2:E:379:LEU:HB3  | 1.68                     | 0.74              |
| 2:A:214:ARG:HA   | 2:A:217:THR:HG22 | 1.68                     | 0.74              |
| 2:A:215:TYR:CD2  | 2:A:215:TYR:N    | 2.55                     | 0.74              |
| 2:C:117:LEU:CB   | 2:C:118:PRO:HD3  | 2.17                     | 0.74              |
| 2:E:133:TRP:O    | 2:E:136:LEU:N    | 2.20                     | 0.74              |
| 2:D:107:LEU:C    | 2:D:108:VAL:HG22 | 2.06                     | 0.74              |
| 2:D:146:ARG:HH11 | 2:D:223:LYS:CE   | 2.01                     | 0.73              |
| 1:R:3:U:H2'      | 1:R:4:U:H4'      | 1.70                     | 0.73              |
| 2:A:215:TYR:H    | 2:A:215:TYR:HD2  | 1.36                     | 0.73              |
| 2:E:37:GLU:HB2   | 2:E:108:VAL:HG21 | 1.68                     | 0.73              |
| 1:R:38:U:H3'     | 1:R:39:U:H5''    | 1.69                     | 0.73              |
| 2:C:44:THR:OG1   | 2:C:46:LYS:HE3   | 1.90                     | 0.71              |
| 2:C:172:GLU:H    | 2:C:173:PRO:HD2  | 1.55                     | 0.71              |
| 2:E:129:ALA:HB1  | 2:E:133:TRP:NE1  | 2.04                     | 0.71              |
| 2:E:133:TRP:HD1  | 2:E:133:TRP:H    | 1.35                     | 0.71              |
| 2:A:399:ARG:HB3  | 2:E:422:LYS:NZ   | 2.06                     | 0.70              |
| 1:R:23:U:H5'     | 2:B:317:ARG:HH21 | 1.56                     | 0.70              |
| 2:B:214:ARG:HA   | 2:B:217:THR:HG22 | 1.74                     | 0.70              |
| 1:R:44:U:H5''    | 2:E:143:ARG:NH2  | 2.07                     | 0.70              |
| 1:R:15:U:C4      | 2:C:408:ARG:HD3  | 2.28                     | 0.69              |
| 2:E:356:THR:HG23 | 2:E:357:PRO:HD3  | 1.72                     | 0.69              |
| 2:C:214:ARG:HA   | 2:C:217:THR:CG2  | 2.20                     | 0.68              |
| 2:C:37:GLU:HB2   | 2:C:108:VAL:HG21 | 1.76                     | 0.68              |
| 1:R:23:U:H5'     | 2:B:317:ARG:NH2  | 2.09                     | 0.68              |
| 2:E:253:GLU:CD   | 2:E:253:GLU:H    | 1.98                     | 0.67              |
| 1:R:44:U:C2'     | 1:R:45:U:H5''    | 2.24                     | 0.66              |
| 2:B:356:THR:HG23 | 2:B:357:PRO:HD3  | 1.77                     | 0.66              |
| 2:C:172:GLU:H    | 2:C:173:PRO:CD   | 2.08                     | 0.66              |
| 2:E:133:TRP:CG   | 2:E:134:LEU:N    | 2.64                     | 0.66              |
| 1:R:12:U:OP2     | 2:C:286:LYS:NZ   | 2.28                     | 0.66              |
| 2:E:354:LYS:HE3  | 2:E:356:THR:HA   | 1.76                     | 0.66              |
| 1:R:29:U:OP1     | 2:A:286:LYS:NZ   | 2.25                     | 0.65              |
| 2:A:399:ARG:HB3  | 2:E:422:LYS:HZ2  | 1.62                     | 0.65              |
| 2:D:66:ILE:HD13  | 2:D:185:TRP:CD1  | 2.31                     | 0.65              |
| 1:R:44:U:C3'     | 1:R:45:U:H5''    | 2.27                     | 0.64              |
| 2:D:107:LEU:C    | 2:D:108:VAL:CG2  | 2.66                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:364:LEU:HB3  | 2:A:368:ALA:HB2  | 1.80                     | 0.64              |
| 2:C:323:GLU:CD   | 2:D:239:GLY:HA3  | 2.18                     | 0.64              |
| 1:R:13:U:H3'     | 2:C:317:ARG:HH21 | 1.62                     | 0.64              |
| 2:D:28:PRO:HG2   | 2:D:266:GLN:HE21 | 1.62                     | 0.64              |
| 2:C:233:HIS:CE1  | 2:C:312:ARG:HE   | 2.16                     | 0.64              |
| 2:B:179:ARG:HA   | 2:B:183:ASP:CG   | 2.18                     | 0.64              |
| 1:R:6:U:C6       | 1:R:6:U:H5''     | 2.32                     | 0.63              |
| 2:E:40:LEU:HD22  | 2:E:42:ILE:HG13  | 1.80                     | 0.63              |
| 2:E:379:LEU:O    | 2:E:383:GLU:HG2  | 1.99                     | 0.63              |
| 1:R:6:U:O4'      | 2:D:149:MET:HG3  | 1.99                     | 0.63              |
| 2:B:28:PRO:HG2   | 2:B:266:GLN:HE21 | 1.64                     | 0.63              |
| 2:A:143:ARG:CD   | 2:A:155:LYS:CE   | 2.32                     | 0.62              |
| 1:R:15:U:H5'     | 2:C:408:ARG:HH22 | 1.64                     | 0.62              |
| 2:E:317:ARG:H    | 2:E:317:ARG:NE   | 1.97                     | 0.62              |
| 2:B:325:THR:O    | 2:B:329:THR:HG22 | 2.00                     | 0.62              |
| 1:R:15:U:H5''    | 2:C:408:ARG:HH12 | 1.64                     | 0.62              |
| 2:C:79:ASP:C     | 2:C:81:ARG:H     | 2.03                     | 0.62              |
| 1:R:2:U:H3'      | 1:R:3:U:H5''     | 1.79                     | 0.62              |
| 2:A:253:GLU:O    | 2:A:257:GLU:HG3  | 2.00                     | 0.62              |
| 2:A:42:ILE:HG21  | 2:A:70:ASN:HB3   | 1.80                     | 0.62              |
| 1:R:44:U:H2'     | 1:R:45:U:H5''    | 1.82                     | 0.61              |
| 2:D:29:ALA:H     | 2:D:266:GLN:HE22 | 1.47                     | 0.61              |
| 2:E:104:ILE:HD11 | 2:E:198:VAL:HG22 | 1.81                     | 0.61              |
| 2:E:133:TRP:HD1  | 2:E:134:LEU:H    | 1.42                     | 0.61              |
| 2:C:143:ARG:HH11 | 2:C:155:LYS:CD   | 2.05                     | 0.61              |
| 2:E:302:GLN:HG2  | 2:E:316:ALA:CB   | 2.31                     | 0.61              |
| 1:R:44:U:OP2     | 2:E:155:LYS:NZ   | 2.33                     | 0.61              |
| 1:R:41:U:O5'     | 2:E:317:ARG:NH2  | 2.34                     | 0.60              |
| 2:B:149:MET:O    | 2:B:151:GLU:N    | 2.33                     | 0.60              |
| 1:R:17:U:H5''    | 2:C:143:ARG:HH12 | 1.65                     | 0.60              |
| 2:B:29:ALA:H     | 2:B:266:GLN:HE22 | 1.47                     | 0.60              |
| 2:A:395:GLN:HA   | 2:A:395:GLN:HE21 | 1.65                     | 0.60              |
| 2:C:149:MET:HB2  | 2:C:150:PRO:HD2  | 1.84                     | 0.60              |
| 2:D:143:ARG:HD2  | 2:D:216:GLY:HA2  | 1.83                     | 0.60              |
| 2:B:298:HIS:NE2  | 2:B:317:ARG:NH1  | 2.50                     | 0.59              |
| 2:D:146:ARG:NH1  | 2:D:223:LYS:NZ   | 2.51                     | 0.59              |
| 2:E:350:VAL:HG12 | 2:E:350:VAL:O    | 2.03                     | 0.59              |
| 2:E:151:GLU:CD   | 2:E:155:LYS:HD2  | 2.22                     | 0.58              |
| 2:E:97:LYS:O     | 2:E:98:ALA:C     | 2.40                     | 0.58              |
| 2:A:136:LEU:HD22 | 2:A:163:GLN:HE21 | 1.68                     | 0.58              |
| 2:D:89:SER:O     | 2:D:270:LYS:NZ   | 2.35                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:128:SER:OG   | 2:D:129:ALA:N    | 2.36                     | 0.58              |
| 2:A:253:GLU:N    | 2:A:253:GLU:CD   | 2.56                     | 0.58              |
| 1:R:17:U:H3'     | 2:C:143:ARG:HH22 | 1.68                     | 0.58              |
| 2:A:317:ARG:CZ   | 2:A:317:ARG:H    | 2.16                     | 0.58              |
| 2:B:230:THR:HG21 | 2:B:298:HIS:CE1  | 2.38                     | 0.58              |
| 2:C:385:GLN:HG2  | 2:C:390:THR:HG22 | 1.84                     | 0.58              |
| 2:B:233:HIS:CE1  | 2:B:312:ARG:HD2  | 2.39                     | 0.58              |
| 1:R:3:U:H4'      | 2:D:224:ASP:HB3  | 1.86                     | 0.58              |
| 2:D:303:LEU:HA   | 2:D:412:ILE:HD13 | 1.86                     | 0.58              |
| 1:R:17:U:H2'     | 1:R:18:U:H5''    | 1.85                     | 0.58              |
| 2:B:172:GLU:HB3  | 2:B:173:PRO:CD   | 2.29                     | 0.58              |
| 2:B:106:ASP:O    | 2:B:107:LEU:HD22 | 2.05                     | 0.57              |
| 2:D:38:ILE:O     | 2:D:38:ILE:HG13  | 2.04                     | 0.57              |
| 2:D:407:LEU:HD13 | 2:D:414:LYS:HA   | 1.86                     | 0.57              |
| 2:A:165:LYS:HA   | 2:E:184:VAL:HG22 | 1.86                     | 0.57              |
| 2:C:155:LYS:HA   | 2:C:155:LYS:HE3  | 1.87                     | 0.57              |
| 2:E:390:THR:OG1  | 2:E:393:MET:HG2  | 2.04                     | 0.57              |
| 2:B:317:ARG:CZ   | 2:B:317:ARG:H    | 2.18                     | 0.57              |
| 2:C:55:VAL:HG12  | 2:C:69:VAL:HG12  | 1.87                     | 0.57              |
| 2:D:143:ARG:CD   | 2:D:216:GLY:HA2  | 2.35                     | 0.56              |
| 1:R:20:U:OP1     | 2:B:286:LYS:NZ   | 2.30                     | 0.56              |
| 2:B:104:ILE:HD11 | 2:B:198:VAL:HG22 | 1.87                     | 0.56              |
| 2:C:143:ARG:HG2  | 2:C:216:GLY:HA2  | 1.87                     | 0.56              |
| 2:C:302:GLN:HG2  | 2:C:316:ALA:CB   | 2.35                     | 0.56              |
| 2:E:278:LEU:HD12 | 2:E:279:ILE:HG12 | 1.87                     | 0.56              |
| 1:R:24:U:H5'     | 1:R:24:U:H6      | 1.70                     | 0.56              |
| 2:A:17:LYS:HG3   | 2:B:268:ILE:HD11 | 1.87                     | 0.56              |
| 2:A:187:ASN:N    | 2:A:187:ASN:HD22 | 2.02                     | 0.56              |
| 2:C:155:LYS:O    | 2:C:155:LYS:HG3  | 2.05                     | 0.56              |
| 2:A:342:ALA:N    | 2:E:387:ARG:HH12 | 2.04                     | 0.56              |
| 2:B:38:ILE:HD11  | 2:B:107:LEU:HD12 | 1.87                     | 0.56              |
| 2:C:157:MET:HG3  | 2:C:158:ASP:H    | 1.71                     | 0.56              |
| 2:B:37:GLU:OE2   | 2:B:108:VAL:HG11 | 2.06                     | 0.56              |
| 2:B:226:ALA:O    | 2:B:230:THR:HG23 | 2.06                     | 0.56              |
| 2:B:253:GLU:H    | 2:B:253:GLU:CD   | 2.09                     | 0.56              |
| 2:C:41:TYR:HB2   | 2:C:190:ASN:HD21 | 1.69                     | 0.56              |
| 2:D:212:SER:O    | 2:D:215:TYR:HD1  | 1.90                     | 0.55              |
| 2:A:336:TYR:O    | 2:A:340:SER:HB2  | 2.07                     | 0.55              |
| 2:C:149:MET:O    | 2:C:151:GLU:N    | 2.38                     | 0.55              |
| 2:C:253:GLU:CD   | 2:C:253:GLU:N    | 2.60                     | 0.55              |
| 2:E:133:TRP:N    | 2:E:133:TRP:CD1  | 2.67                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:3:U:C2'      | 1:R:4:U:H4'      | 2.36                     | 0.55              |
| 2:A:130:ASP:CG   | 2:A:131:ASP:H    | 2.09                     | 0.55              |
| 2:A:233:HIS:CE1  | 2:A:312:ARG:HD2  | 2.42                     | 0.55              |
| 2:E:202:PHE:HB2  | 2:E:214:ARG:HD3  | 1.89                     | 0.55              |
| 1:R:22:U:H2'     | 2:B:317:ARG:NE   | 2.06                     | 0.55              |
| 2:B:106:ASP:O    | 2:B:107:LEU:CD2  | 2.54                     | 0.55              |
| 2:D:136:LEU:HD22 | 2:D:163:GLN:HG3  | 1.89                     | 0.54              |
| 2:D:328:THR:HG21 | 2:D:415:TYR:HE1  | 1.71                     | 0.54              |
| 2:B:356:THR:CG2  | 2:B:357:PRO:HD3  | 2.37                     | 0.54              |
| 2:C:146:ARG:HD3  | 2:C:146:ARG:O    | 2.08                     | 0.54              |
| 2:E:130:ASP:C    | 2:E:132:LYS:H    | 2.10                     | 0.54              |
| 1:R:18:U:H4'     | 1:R:18:U:OP1     | 2.08                     | 0.54              |
| 2:A:257:GLU:OE1  | 2:A:295:PRO:HD2  | 2.08                     | 0.54              |
| 2:B:118:PRO:O    | 2:B:119:ASP:HB2  | 2.08                     | 0.53              |
| 2:B:324:TYR:O    | 2:B:328:THR:HG22 | 2.07                     | 0.53              |
| 2:E:268:ILE:HG22 | 2:E:275:MET:HG3  | 1.89                     | 0.53              |
| 2:A:117:LEU:HB3  | 2:A:118:PRO:CD   | 2.29                     | 0.53              |
| 1:R:6:U:H6       | 1:R:6:U:H5''     | 1.72                     | 0.53              |
| 2:A:149:MET:O    | 2:A:151:GLU:N    | 2.41                     | 0.53              |
| 2:B:317:ARG:NH1  | 2:B:317:ARG:H    | 2.06                     | 0.53              |
| 2:E:97:LYS:O     | 2:E:99:GLY:N     | 2.42                     | 0.53              |
| 2:D:179:ARG:HA   | 2:D:183:ASP:CG   | 2.29                     | 0.53              |
| 2:A:302:GLN:HG2  | 2:A:316:ALA:CB   | 2.39                     | 0.53              |
| 2:C:29:ALA:H     | 2:C:266:GLN:HE22 | 1.57                     | 0.53              |
| 1:R:30:U:H2'     | 1:R:31:U:O4'     | 2.09                     | 0.53              |
| 2:C:38:ILE:O     | 2:C:38:ILE:HG13  | 2.08                     | 0.53              |
| 2:E:149:MET:O    | 2:E:151:GLU:N    | 2.38                     | 0.53              |
| 2:C:210:CYS:HB3  | 2:C:213:PHE:CE1  | 2.44                     | 0.52              |
| 2:E:133:TRP:O    | 2:E:134:LEU:C    | 2.48                     | 0.52              |
| 2:E:129:ALA:O    | 2:E:133:TRP:CD1  | 2.62                     | 0.52              |
| 1:R:41:U:C4      | 2:E:312:ARG:HG3  | 2.44                     | 0.52              |
| 2:A:149:MET:C    | 2:A:151:GLU:H    | 2.13                     | 0.52              |
| 2:A:23:ASP:HB2   | 2:A:286:LYS:NZ   | 2.24                     | 0.52              |
| 2:B:66:ILE:HD13  | 2:B:185:TRP:CD1  | 2.44                     | 0.52              |
| 2:D:304:THR:HG21 | 2:D:334:TYR:CD2  | 2.45                     | 0.52              |
| 1:R:14:U:H5''    | 2:C:317:ARG:HH22 | 1.74                     | 0.52              |
| 2:E:151:GLU:OE2  | 2:E:155:LYS:HD2  | 2.09                     | 0.52              |
| 2:B:320:ASP:CB   | 2:C:312:ARG:HH22 | 2.22                     | 0.52              |
| 2:D:43:ASN:HB2   | 2:D:112:ALA:N    | 2.25                     | 0.52              |
| 1:R:4:U:OP2      | 2:D:290:SER:HB2  | 2.10                     | 0.52              |
| 2:D:107:LEU:HD11 | 2:D:281:PHE:CZ   | 2.45                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:317:ARG:H    | 2:D:317:ARG:NE   | 2.08                     | 0.52              |
| 2:A:298:HIS:NE2  | 2:A:317:ARG:NH1  | 2.58                     | 0.51              |
| 2:A:29:ALA:H     | 2:A:266:GLN:HE22 | 1.57                     | 0.51              |
| 2:E:233:HIS:O    | 2:E:237:ILE:HG12 | 2.11                     | 0.51              |
| 1:R:4:U:C6       | 2:D:317:ARG:HG3  | 2.44                     | 0.51              |
| 1:R:8:U:P        | 2:D:155:LYS:NZ   | 2.83                     | 0.51              |
| 2:D:105:PHE:C    | 2:D:107:LEU:H    | 2.14                     | 0.51              |
| 1:R:26:U:H5''    | 2:B:143:ARG:HH21 | 1.76                     | 0.51              |
| 2:B:104:ILE:HD11 | 2:B:198:VAL:HA   | 1.92                     | 0.51              |
| 2:B:66:ILE:HD13  | 2:B:185:TRP:CG   | 2.46                     | 0.51              |
| 2:D:149:MET:O    | 2:D:151:GLU:N    | 2.44                     | 0.51              |
| 2:D:107:LEU:CD1  | 2:D:281:PHE:CZ   | 2.93                     | 0.51              |
| 2:A:143:ARG:HG3  | 2:A:155:LYS:HE2  | 1.92                     | 0.51              |
| 1:R:23:U:C5'     | 2:B:317:ARG:NH2  | 2.74                     | 0.50              |
| 2:C:133:TRP:HB3  | 2:C:167:ILE:HD12 | 1.92                     | 0.50              |
| 1:R:44:U:H5''    | 2:E:143:ARG:HH22 | 1.76                     | 0.50              |
| 2:B:270:LYS:HE3  | 2:B:273:SER:HB2  | 1.93                     | 0.50              |
| 2:B:160:LEU:HD12 | 2:B:161:THR:HG23 | 1.94                     | 0.50              |
| 2:D:146:ARG:NH1  | 2:D:223:LYS:CE   | 2.74                     | 0.50              |
| 2:E:343:ASP:OD2  | 2:E:373:ARG:NH2  | 2.45                     | 0.50              |
| 2:A:166:MET:C    | 2:A:167:ILE:HG13 | 2.32                     | 0.50              |
| 2:A:143:ARG:HD3  | 2:A:219:VAL:HG11 | 1.94                     | 0.50              |
| 1:R:13:U:H3'     | 2:C:317:ARG:NH2  | 2.25                     | 0.50              |
| 2:D:117:LEU:HB2  | 2:D:118:PRO:CD   | 2.32                     | 0.50              |
| 2:A:324:TYR:HD1  | 2:B:237:ILE:HD11 | 1.76                     | 0.50              |
| 2:B:65:SER:HB2   | 2:B:117:LEU:HD11 | 1.94                     | 0.50              |
| 2:D:133:TRP:HB3  | 2:D:167:ILE:HD13 | 1.94                     | 0.50              |
| 2:A:214:ARG:HA   | 2:A:217:THR:CG2  | 2.38                     | 0.49              |
| 2:A:106:ASP:C    | 2:A:107:LEU:HD12 | 2.33                     | 0.49              |
| 2:C:149:MET:C    | 2:C:151:GLU:H    | 2.14                     | 0.49              |
| 2:E:253:GLU:CD   | 2:E:253:GLU:N    | 2.65                     | 0.49              |
| 2:C:106:ASP:C    | 2:C:107:LEU:HD12 | 2.33                     | 0.49              |
| 2:A:143:ARG:HH11 | 2:A:155:LYS:HE3  | 1.77                     | 0.49              |
| 2:D:328:THR:HG21 | 2:D:415:TYR:CE1  | 2.46                     | 0.49              |
| 2:E:66:ILE:HD13  | 2:E:185:TRP:CD1  | 2.47                     | 0.49              |
| 2:A:77:LEU:C     | 2:A:79:ASP:H     | 2.16                     | 0.49              |
| 2:A:136:LEU:HD21 | 2:A:162:ASN:HD22 | 1.77                     | 0.49              |
| 2:B:38:ILE:HG13  | 2:B:38:ILE:O     | 2.13                     | 0.48              |
| 2:A:320:ASP:HA   | 2:A:324:TYR:OH   | 2.14                     | 0.48              |
| 2:A:338:VAL:HG13 | 2:A:373:ARG:NH1  | 2.28                     | 0.48              |
| 2:B:109:SER:C    | 2:B:110:LEU:HD23 | 2.24                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:107:LEU:CD1  | 2:B:274:TYR:HE2  | 2.26                     | 0.48              |
| 2:B:107:LEU:HD23 | 2:B:107:LEU:H    | 1.66                     | 0.48              |
| 2:D:172:GLU:HB3  | 2:D:173:PRO:HD3  | 1.96                     | 0.48              |
| 1:R:6:U:H3'      | 2:D:408:ARG:HH22 | 1.79                     | 0.48              |
| 2:D:109:SER:O    | 2:D:110:LEU:HD23 | 2.14                     | 0.47              |
| 2:A:210:CYS:HB3  | 2:A:213:PHE:CE1  | 2.49                     | 0.47              |
| 2:C:117:LEU:CB   | 2:C:118:PRO:CD   | 2.90                     | 0.47              |
| 2:E:29:ALA:H     | 2:E:266:GLN:HE22 | 1.62                     | 0.47              |
| 2:C:43:ASN:CG    | 2:C:112:ALA:HB3  | 2.35                     | 0.47              |
| 1:R:4:U:H3'      | 2:D:317:ARG:NE   | 2.28                     | 0.47              |
| 2:C:342:ALA:HB1  | 2:C:344:LEU:HD23 | 1.96                     | 0.47              |
| 2:D:149:MET:C    | 2:D:151:GLU:H    | 2.18                     | 0.47              |
| 1:R:27:U:O2'     | 1:R:29:U:OP2     | 2.32                     | 0.47              |
| 2:A:166:MET:H    | 2:E:184:VAL:HG13 | 1.80                     | 0.47              |
| 2:B:149:MET:C    | 2:B:151:GLU:H    | 2.18                     | 0.47              |
| 2:A:414:LYS:HA   | 2:A:414:LYS:HE3  | 1.95                     | 0.47              |
| 1:R:2:U:OP1      | 2:D:286:LYS:NZ   | 2.34                     | 0.47              |
| 2:A:81:ARG:HD2   | 2:A:208:HIS:HE2  | 1.80                     | 0.47              |
| 2:B:172:GLU:CB   | 2:B:173:PRO:HD3  | 2.33                     | 0.47              |
| 2:B:107:LEU:CD1  | 2:B:274:TYR:CE2  | 2.98                     | 0.47              |
| 2:B:66:ILE:O     | 2:B:70:ASN:ND2   | 2.48                     | 0.47              |
| 2:B:184:VAL:HG13 | 2:C:165:LYS:HA   | 1.96                     | 0.47              |
| 2:C:19:PRO:HD3   | 2:D:228:LEU:HD22 | 1.97                     | 0.47              |
| 2:A:42:ILE:CG2   | 2:A:70:ASN:HB3   | 2.45                     | 0.46              |
| 2:B:107:LEU:HD13 | 2:B:274:TYR:CZ   | 2.50                     | 0.46              |
| 2:E:117:LEU:CB   | 2:E:118:PRO:HD3  | 2.36                     | 0.46              |
| 2:E:250:LEU:HD22 | 2:E:379:LEU:HD21 | 1.98                     | 0.46              |
| 2:E:368:ALA:HB1  | 2:E:369:PRO:HD2  | 1.96                     | 0.46              |
| 2:B:41:TYR:HA    | 2:B:110:LEU:O    | 2.15                     | 0.46              |
| 2:B:332:LEU:HD21 | 2:B:397:ALA:HB2  | 1.98                     | 0.46              |
| 2:E:325:THR:O    | 2:E:329:THR:HG22 | 2.15                     | 0.46              |
| 2:A:268:ILE:HG22 | 2:A:275:MET:SD   | 2.56                     | 0.46              |
| 2:D:66:ILE:HD11  | 2:D:191:TYR:HB2  | 1.97                     | 0.46              |
| 2:D:84:LEU:HD11  | 2:D:88:TRP:HB2   | 1.96                     | 0.46              |
| 2:A:419:GLU:OE1  | 2:B:309:ARG:NH1  | 2.48                     | 0.46              |
| 1:R:23:U:C5'     | 2:B:317:ARG:HH21 | 2.26                     | 0.46              |
| 2:B:409:GLU:OE2  | 2:B:409:GLU:N    | 2.48                     | 0.46              |
| 2:D:339:GLY:HA3  | 2:D:396:TYR:OH   | 2.16                     | 0.46              |
| 1:R:8:U:OP1      | 2:D:154:LYS:NZ   | 2.46                     | 0.46              |
| 2:B:152:TYR:HD1  | 2:B:153:ARG:H    | 1.63                     | 0.46              |
| 2:B:199:ASP:OD1  | 2:B:214:ARG:HD2  | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:293:LYS:C    | 2:C:295:PRO:HD3  | 2.36                     | 0.46              |
| 2:D:199:ASP:OD1  | 2:D:217:THR:HG23 | 2.16                     | 0.46              |
| 2:E:130:ASP:O    | 2:E:132:LYS:N    | 2.49                     | 0.46              |
| 2:B:317:ARG:HG2  | 2:B:317:ARG:O    | 2.16                     | 0.46              |
| 2:B:72:TYR:CE1   | 2:B:134:LEU:HD12 | 2.51                     | 0.46              |
| 2:C:79:ASP:C     | 2:C:81:ARG:N     | 2.68                     | 0.46              |
| 2:A:43:ASN:ND2   | 2:A:45:THR:OG1   | 2.48                     | 0.45              |
| 2:B:133:TRP:HB3  | 2:B:167:ILE:HG21 | 1.99                     | 0.45              |
| 2:B:81:ARG:HD3   | 2:B:208:HIS:HE2  | 1.82                     | 0.45              |
| 2:D:317:ARG:H    | 2:D:317:ARG:CD   | 2.28                     | 0.45              |
| 2:E:175:VAL:HB   | 2:E:176:PRO:HD2  | 1.98                     | 0.45              |
| 2:C:172:GLU:N    | 2:C:173:PRO:HD2  | 2.27                     | 0.45              |
| 2:A:374:ASP:O    | 2:A:378:TRP:HD1  | 1.98                     | 0.45              |
| 2:E:263:LEU:HA   | 2:E:264:PRO:HD3  | 1.83                     | 0.45              |
| 2:B:18:LEU:HD21  | 2:C:242:THR:HG22 | 1.97                     | 0.45              |
| 1:R:11:U:H3'     | 1:R:12:U:C5'     | 2.42                     | 0.45              |
| 2:C:31:TYR:CD2   | 2:C:283:LEU:HA   | 2.51                     | 0.45              |
| 2:E:129:ALA:O    | 2:E:133:TRP:HD1  | 1.99                     | 0.45              |
| 2:B:37:GLU:CG    | 2:B:108:VAL:HG21 | 2.46                     | 0.45              |
| 2:E:233:HIS:HB2  | 2:E:312:ARG:CZ   | 2.47                     | 0.45              |
| 1:R:31:U:H3'     | 2:A:317:ARG:NE   | 2.30                     | 0.45              |
| 2:A:354:LYS:HE3  | 2:A:356:THR:HA   | 1.99                     | 0.45              |
| 2:B:128:SER:O    | 2:B:130:ASP:N    | 2.49                     | 0.45              |
| 2:B:81:ARG:HD3   | 2:B:208:HIS:CE1  | 2.52                     | 0.45              |
| 2:C:41:TYR:HB2   | 2:C:190:ASN:ND2  | 2.31                     | 0.45              |
| 2:B:253:GLU:CD   | 2:B:253:GLU:N    | 2.70                     | 0.45              |
| 2:C:140:GLY:HA2  | 2:C:216:GLY:HA3  | 1.97                     | 0.45              |
| 2:E:299:PHE:HE1  | 2:E:328:THR:HG22 | 1.82                     | 0.45              |
| 2:C:104:ILE:HD12 | 2:C:104:ILE:N    | 2.32                     | 0.45              |
| 2:A:228:LEU:HD12 | 2:E:19:PRO:HD3   | 1.98                     | 0.45              |
| 2:B:152:TYR:HD1  | 2:B:153:ARG:N    | 2.14                     | 0.45              |
| 2:B:287:SER:HA   | 2:B:288:PRO:HD3  | 1.88                     | 0.45              |
| 2:D:146:ARG:NH1  | 2:D:223:LYS:HE2  | 2.20                     | 0.45              |
| 2:B:66:ILE:HD11  | 2:B:191:TYR:HB2  | 1.99                     | 0.44              |
| 2:C:68:HIS:HE1   | 2:C:117:LEU:H    | 1.66                     | 0.44              |
| 1:R:14:U:C5'     | 2:C:317:ARG:HH22 | 2.30                     | 0.44              |
| 2:B:308:LEU:O    | 2:B:309:ARG:HB2  | 2.16                     | 0.44              |
| 2:C:405:GLN:O    | 2:C:407:LEU:HG   | 2.16                     | 0.44              |
| 2:A:417:LYS:HE2  | 2:A:421:ASP:OD2  | 2.18                     | 0.44              |
| 2:B:123:ASP:C    | 2:B:125:SER:H    | 2.21                     | 0.44              |
| 2:B:38:ILE:H     | 2:B:108:VAL:HG23 | 1.82                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:317:ARG:NH1  | 2:C:317:ARG:H    | 2.16                     | 0.44              |
| 2:B:128:SER:O    | 2:B:129:ALA:C    | 2.56                     | 0.44              |
| 2:D:117:LEU:CB   | 2:D:118:PRO:HD3  | 2.34                     | 0.44              |
| 1:R:2:U:H3'      | 1:R:3:U:C5'      | 2.46                     | 0.44              |
| 2:B:346:GLN:O    | 2:E:8:ILE:HD11   | 2.18                     | 0.44              |
| 2:E:48:LEU:HA    | 2:E:51:LEU:HD12  | 2.00                     | 0.44              |
| 2:C:306:LEU:HD22 | 2:C:412:ILE:HD12 | 1.99                     | 0.44              |
| 2:A:122:SER:OG   | 2:A:123:ASP:N    | 2.50                     | 0.43              |
| 2:B:215:TYR:N    | 2:B:215:TYR:CD2  | 2.86                     | 0.43              |
| 2:C:308:LEU:O    | 2:C:309:ARG:HB2  | 2.17                     | 0.43              |
| 2:E:172:GLU:H    | 2:E:173:PRO:CD   | 2.31                     | 0.43              |
| 2:D:28:PRO:HG2   | 2:D:266:GLN:NE2  | 2.31                     | 0.43              |
| 2:E:172:GLU:H    | 2:E:173:PRO:HD2  | 1.84                     | 0.43              |
| 2:E:148:GLN:HG2  | 2:E:179:ARG:HD2  | 2.00                     | 0.43              |
| 2:E:149:MET:C    | 2:E:151:GLU:H    | 2.21                     | 0.43              |
| 2:D:214:ARG:HA   | 2:D:217:THR:CG2  | 2.37                     | 0.43              |
| 2:C:263:LEU:HA   | 2:C:264:PRO:HD3  | 1.84                     | 0.43              |
| 2:D:302:GLN:HG2  | 2:D:316:ALA:CB   | 2.48                     | 0.43              |
| 1:R:14:U:O5'     | 2:C:317:ARG:NH2  | 2.51                     | 0.43              |
| 2:A:227:ALA:HA   | 2:A:230:THR:HG23 | 2.01                     | 0.43              |
| 2:E:172:GLU:N    | 2:E:173:PRO:CD   | 2.81                     | 0.43              |
| 2:E:66:ILE:HD11  | 2:E:191:TYR:HB2  | 2.00                     | 0.43              |
| 2:E:28:PRO:O     | 2:E:31:TYR:HB3   | 2.19                     | 0.43              |
| 2:E:59:LEU:HD11  | 2:E:137:TYR:CE2  | 2.53                     | 0.43              |
| 2:E:233:HIS:HB2  | 2:E:312:ARG:NH1  | 2.34                     | 0.43              |
| 1:R:17:U:C5'     | 2:C:155:LYS:HZ3  | 2.32                     | 0.43              |
| 2:A:228:LEU:HD23 | 2:A:289:TYR:HB3  | 2.00                     | 0.43              |
| 2:E:25:VAL:HG11  | 2:E:288:PRO:HA   | 2.01                     | 0.43              |
| 2:E:303:LEU:HA   | 2:E:412:ILE:HD13 | 2.00                     | 0.43              |
| 2:A:288:PRO:HG2  | 2:A:289:TYR:CE2  | 2.53                     | 0.43              |
| 2:E:181:ILE:HB   | 2:E:182:PHE:H    | 1.72                     | 0.43              |
| 2:D:85:ASP:OD1   | 2:D:86:LYS:HE3   | 2.19                     | 0.42              |
| 2:C:107:LEU:HD23 | 2:C:274:TYR:HE2  | 1.84                     | 0.42              |
| 2:E:38:ILE:HA    | 2:E:39:PRO:HD3   | 1.84                     | 0.42              |
| 2:A:408:ARG:H    | 2:A:408:ARG:HG2  | 1.65                     | 0.42              |
| 2:A:212:SER:O    | 2:A:215:TYR:CD2  | 2.72                     | 0.42              |
| 2:D:303:LEU:HD22 | 2:D:328:THR:HG22 | 2.01                     | 0.42              |
| 1:R:12:U:P       | 2:C:286:LYS:HZ3  | 2.43                     | 0.42              |
| 2:E:248:TRP:CD1  | 2:E:375:VAL:HG22 | 2.55                     | 0.42              |
| 2:E:38:ILE:HD11  | 2:E:107:LEU:HB3  | 2.01                     | 0.42              |
| 2:B:152:TYR:CD1  | 2:B:153:ARG:N    | 2.88                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:19:PRO:HD3   | 2:C:228:LEU:HD22 | 2.02                     | 0.42              |
| 2:B:263:LEU:HA   | 2:B:264:PRO:HD3  | 1.82                     | 0.42              |
| 2:D:137:TYR:OH   | 2:D:173:PRO:HD3  | 2.20                     | 0.42              |
| 2:E:302:GLN:HG3  | 2:E:313:ALA:HB1  | 2.00                     | 0.42              |
| 2:A:344:LEU:HD21 | 2:E:330:ALA:HB2  | 2.01                     | 0.42              |
| 2:A:181:ILE:N    | 2:A:183:ASP:OD1  | 2.53                     | 0.42              |
| 2:A:199:ASP:OD1  | 2:A:217:THR:HG23 | 2.19                     | 0.42              |
| 2:A:239:GLY:HA3  | 2:E:323:GLU:CD   | 2.40                     | 0.42              |
| 2:B:81:ARG:HD3   | 2:B:208:HIS:NE2  | 2.34                     | 0.42              |
| 1:R:21:U:H4'     | 2:B:224:ASP:CG   | 2.40                     | 0.42              |
| 2:C:105:PHE:C    | 2:C:107:LEU:H    | 2.22                     | 0.42              |
| 2:E:409:GLU:HA   | 2:E:414:LYS:HD2  | 2.01                     | 0.42              |
| 2:E:172:GLU:N    | 2:E:173:PRO:HD2  | 2.34                     | 0.42              |
| 1:R:27:U:H4'     | 1:R:29:U:C5      | 2.54                     | 0.42              |
| 2:C:78:LYS:HD3   | 2:C:78:LYS:HA    | 1.81                     | 0.42              |
| 2:C:409:GLU:O    | 2:C:410:LYS:HB2  | 2.19                     | 0.41              |
| 2:D:398:LYS:O    | 2:D:402:MET:HG2  | 2.20                     | 0.41              |
| 2:A:172:GLU:CB   | 2:A:173:PRO:HD3  | 2.50                     | 0.41              |
| 2:B:40:LEU:HD13  | 2:B:42:ILE:HD11  | 2.02                     | 0.41              |
| 1:R:23:U:H2'     | 1:R:25:U:H5''    | 2.02                     | 0.41              |
| 2:D:43:ASN:ND2   | 2:D:111:LYS:HD3  | 2.35                     | 0.41              |
| 2:A:342:ALA:H    | 2:E:387:ARG:HH12 | 1.68                     | 0.41              |
| 2:A:381:TRP:O    | 2:A:384:ASP:HB2  | 2.20                     | 0.41              |
| 2:B:370:PRO:HD3  | 2:B:381:TRP:CG   | 2.56                     | 0.41              |
| 2:D:290:SER:O    | 2:D:294:ASN:ND2  | 2.50                     | 0.41              |
| 2:D:79:ASP:HB2   | 2:D:81:ARG:HG3   | 2.02                     | 0.41              |
| 2:A:342:ALA:HB2  | 2:E:329:THR:HG21 | 2.02                     | 0.41              |
| 1:R:8:U:P        | 2:D:155:LYS:HZ1  | 2.42                     | 0.41              |
| 1:R:31:U:H2'     | 2:A:317:ARG:HE   | 1.84                     | 0.41              |
| 2:E:187:ASN:HD22 | 2:E:187:ASN:HA   | 1.70                     | 0.41              |
| 2:E:275:MET:HB3  | 2:E:276:PRO:HD3  | 2.01                     | 0.41              |
| 2:A:97:LYS:O     | 2:A:98:ALA:C     | 2.59                     | 0.41              |
| 2:C:175:VAL:O    | 2:C:181:ILE:HG12 | 2.20                     | 0.41              |
| 2:C:293:LYS:HA   | 2:C:293:LYS:HD2  | 1.91                     | 0.41              |
| 2:E:130:ASP:C    | 2:E:132:LYS:N    | 2.73                     | 0.41              |
| 2:E:214:ARG:HA   | 2:E:217:THR:OG1  | 2.21                     | 0.41              |
| 2:B:128:SER:C    | 2:B:130:ASP:N    | 2.70                     | 0.41              |
| 2:C:294:ASN:N    | 2:C:295:PRO:HD3  | 2.36                     | 0.41              |
| 2:E:133:TRP:O    | 2:E:135:PRO:N    | 2.54                     | 0.41              |
| 2:A:149:MET:C    | 2:A:151:GLU:N    | 2.75                     | 0.41              |
| 2:A:199:ASP:OD1  | 2:A:214:ARG:NE   | 2.52                     | 0.41              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:A:243:GLU:HG3  | 2:E:2:SER:HB3   | 2.02                     | 0.41              |
| 2:A:401:VAL:HG23 | 2:A:421:ASP:HB2 | 2.03                     | 0.41              |
| 2:A:128:SER:C    | 2:A:130:ASP:H   | 2.23                     | 0.41              |
| 2:D:311:THR:O    | 2:D:314:ARG:HG2 | 2.21                     | 0.41              |
| 2:B:81:ARG:HB3   | 2:B:208:HIS:HE2 | 1.87                     | 0.40              |
| 2:E:18:LEU:HB2   | 2:E:19:PRO:HD2  | 2.03                     | 0.40              |
| 2:E:299:PHE:O    | 2:E:300:TRP:C   | 2.59                     | 0.40              |
| 2:B:28:PRO:HG2   | 2:B:266:GLN:NE2 | 2.34                     | 0.40              |
| 2:B:313:ALA:O    | 2:B:314:ARG:C   | 2.58                     | 0.40              |
| 2:B:38:ILE:HA    | 2:B:39:PRO:HD3  | 1.88                     | 0.40              |
| 2:C:181:ILE:HB   | 2:C:182:PHE:H   | 1.51                     | 0.40              |
| 2:D:401:VAL:HG21 | 2:D:420:PHE:HB2 | 2.03                     | 0.40              |
| 2:E:302:GLN:HG3  | 2:E:313:ALA:CB  | 2.51                     | 0.40              |
| 2:A:395:GLN:HA   | 2:A:395:GLN:NE2 | 2.35                     | 0.40              |
| 2:D:43:ASN:HD22  | 2:D:111:LYS:HD3 | 1.85                     | 0.40              |
| 1:R:13:U:H5'     | 1:R:14:U:OP2    | 2.21                     | 0.40              |
| 1:R:35:U:OP2     | 2:A:155:LYS:NZ  | 2.41                     | 0.40              |
| 2:C:22:GLU:HB3   | 2:C:23:ASP:H    | 1.55                     | 0.40              |
| 2:C:356:THR:N    | 2:C:357:PRO:HD3 | 2.36                     | 0.40              |
| 2:D:38:ILE:HA    | 2:D:39:PRO:HD3  | 1.91                     | 0.40              |
| 1:R:20:U:H2'     | 1:R:21:U:O4'    | 2.21                     | 0.40              |
| 2:B:118:PRO:O    | 2:B:119:ASP:CB  | 2.70                     | 0.40              |
| 2:C:58:GLY:HA3   | 2:C:64:VAL:HB   | 2.03                     | 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     | 419/422 (99%) | 354 (84%) | 46 (11%) | 19 (4%)  | <a href="#">2</a> <a href="#">8</a> |
| 2   | B     | 411/422 (97%) | 344 (84%) | 45 (11%) | 22 (5%)  | <a href="#">2</a> <a href="#">5</a> |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |   |
|-----|-------|-----------------|------------|-----------|----------|-------------|---|
| 2   | C     | 409/422 (97%)   | 340 (83%)  | 49 (12%)  | 20 (5%)  | 2           | 7 |
| 2   | D     | 412/422 (98%)   | 343 (83%)  | 48 (12%)  | 21 (5%)  | 2           | 6 |
| 2   | E     | 419/422 (99%)   | 349 (83%)  | 48 (12%)  | 22 (5%)  | 2           | 5 |
| All | All   | 2070/2110 (98%) | 1730 (84%) | 236 (11%) | 104 (5%) | 2           | 6 |

All (104) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | A     | 47  | SER  |
| 2   | A     | 98  | ALA  |
| 2   | A     | 113 | LEU  |
| 2   | A     | 172 | GLU  |
| 2   | B     | 98  | ALA  |
| 2   | B     | 117 | LEU  |
| 2   | B     | 122 | SER  |
| 2   | B     | 128 | SER  |
| 2   | B     | 150 | PRO  |
| 2   | B     | 168 | ASN  |
| 2   | C     | 113 | LEU  |
| 2   | C     | 117 | LEU  |
| 2   | C     | 122 | SER  |
| 2   | C     | 172 | GLU  |
| 2   | C     | 181 | ILE  |
| 2   | D     | 98  | ALA  |
| 2   | D     | 122 | SER  |
| 2   | D     | 357 | PRO  |
| 2   | E     | 98  | ALA  |
| 2   | A     | 150 | PRO  |
| 2   | A     | 181 | ILE  |
| 2   | A     | 344 | LEU  |
| 2   | B     | 22  | GLU  |
| 2   | B     | 47  | SER  |
| 2   | B     | 119 | ASP  |
| 2   | B     | 129 | ALA  |
| 2   | B     | 172 | GLU  |
| 2   | B     | 177 | GLU  |
| 2   | B     | 344 | LEU  |
| 2   | C     | 130 | ASP  |
| 2   | C     | 150 | PRO  |
| 2   | C     | 344 | LEU  |
| 2   | C     | 371 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 120 | GLY  |
| 2   | D     | 130 | ASP  |
| 2   | D     | 168 | ASN  |
| 2   | D     | 344 | LEU  |
| 2   | D     | 366 | THR  |
| 2   | D     | 386 | ASN  |
| 2   | E     | 47  | SER  |
| 2   | E     | 120 | GLY  |
| 2   | E     | 122 | SER  |
| 2   | E     | 177 | GLU  |
| 2   | E     | 343 | ASP  |
| 2   | E     | 344 | LEU  |
| 2   | E     | 360 | SER  |
| 2   | E     | 371 | GLN  |
| 2   | E     | 406 | GLY  |
| 2   | A     | 22  | GLU  |
| 2   | A     | 176 | PRO  |
| 2   | A     | 180 | ASP  |
| 2   | A     | 386 | ASN  |
| 2   | B     | 43  | ASN  |
| 2   | B     | 61  | SER  |
| 2   | B     | 113 | LEU  |
| 2   | B     | 170 | GLN  |
| 2   | B     | 180 | ASP  |
| 2   | D     | 79  | ASP  |
| 2   | D     | 127 | THR  |
| 2   | D     | 150 | PRO  |
| 2   | D     | 172 | GLU  |
| 2   | D     | 180 | ASP  |
| 2   | E     | 150 | PRO  |
| 2   | E     | 299 | PHE  |
| 2   | E     | 300 | TRP  |
| 2   | A     | 117 | LEU  |
| 2   | A     | 122 | SER  |
| 2   | A     | 130 | ASP  |
| 2   | B     | 165 | LYS  |
| 2   | C     | 22  | GLU  |
| 2   | C     | 168 | ASN  |
| 2   | C     | 176 | PRO  |
| 2   | C     | 386 | ASN  |
| 2   | C     | 406 | GLY  |
| 2   | D     | 22  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 129 | ALA  |
| 2   | E     | 108 | VAL  |
| 2   | E     | 164 | CYS  |
| 2   | E     | 168 | ASN  |
| 2   | E     | 365 | THR  |
| 2   | A     | 128 | SER  |
| 2   | A     | 360 | SER  |
| 2   | C     | 47  | SER  |
| 2   | C     | 83  | LYS  |
| 2   | C     | 108 | VAL  |
| 2   | C     | 159 | GLY  |
| 2   | D     | 117 | LEU  |
| 2   | D     | 128 | SER  |
| 2   | D     | 271 | ALA  |
| 2   | E     | 173 | PRO  |
| 2   | E     | 271 | ALA  |
| 2   | B     | 179 | ARG  |
| 2   | B     | 309 | ARG  |
| 2   | C     | 167 | ILE  |
| 2   | E     | 80  | ILE  |
| 2   | E     | 117 | LEU  |
| 2   | A     | 121 | VAL  |
| 2   | A     | 264 | PRO  |
| 2   | C     | 80  | ILE  |
| 2   | E     | 181 | ILE  |
| 2   | B     | 80  | ILE  |
| 2   | D     | 42  | ILE  |
| 2   | D     | 80  | ILE  |
| 2   | A     | 108 | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2   | A     | 362/363 (100%) | 323 (89%) | 39 (11%) | 6           | 19 |
| 2   | B     | 358/363 (99%)  | 311 (87%) | 47 (13%) | 4           | 12 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 2   | C     | 356/363 (98%)   | 303 (85%)  | 53 (15%)  | 3           | 8  |
| 2   | D     | 359/363 (99%)   | 315 (88%)  | 44 (12%)  | 4           | 13 |
| 2   | E     | 362/363 (100%)  | 324 (90%)  | 38 (10%)  | 7           | 20 |
| All | All   | 1797/1815 (99%) | 1576 (88%) | 221 (12%) | 4           | 13 |

All (221) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | A     | 18  | LEU  |
| 2   | A     | 22  | GLU  |
| 2   | A     | 40  | LEU  |
| 2   | A     | 87  | ASP  |
| 2   | A     | 116 | VAL  |
| 2   | A     | 134 | LEU  |
| 2   | A     | 143 | ARG  |
| 2   | A     | 153 | ARG  |
| 2   | A     | 156 | LEU  |
| 2   | A     | 157 | MET  |
| 2   | A     | 160 | LEU  |
| 2   | A     | 177 | GLU  |
| 2   | A     | 181 | ILE  |
| 2   | A     | 183 | ASP  |
| 2   | A     | 187 | ASN  |
| 2   | A     | 195 | VAL  |
| 2   | A     | 215 | TYR  |
| 2   | A     | 217 | THR  |
| 2   | A     | 228 | LEU  |
| 2   | A     | 230 | THR  |
| 2   | A     | 237 | ILE  |
| 2   | A     | 243 | GLU  |
| 2   | A     | 252 | ARG  |
| 2   | A     | 253 | GLU  |
| 2   | A     | 275 | MET  |
| 2   | A     | 307 | LEU  |
| 2   | A     | 308 | LEU  |
| 2   | A     | 309 | ARG  |
| 2   | A     | 317 | ARG  |
| 2   | A     | 326 | SER  |
| 2   | A     | 327 | LEU  |
| 2   | A     | 332 | LEU  |
| 2   | A     | 344 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | A     | 353 | ASN  |
| 2   | A     | 359 | ASP  |
| 2   | A     | 395 | GLN  |
| 2   | A     | 405 | GLN  |
| 2   | A     | 408 | ARG  |
| 2   | A     | 414 | LYS  |
| 2   | B     | 2   | SER  |
| 2   | B     | 18  | LEU  |
| 2   | B     | 22  | GLU  |
| 2   | B     | 30  | ASP  |
| 2   | B     | 34  | LYS  |
| 2   | B     | 40  | LEU  |
| 2   | B     | 46  | LYS  |
| 2   | B     | 48  | LEU  |
| 2   | B     | 78  | LYS  |
| 2   | B     | 84  | LEU  |
| 2   | B     | 85  | ASP  |
| 2   | B     | 95  | ILE  |
| 2   | B     | 107 | LEU  |
| 2   | B     | 108 | VAL  |
| 2   | B     | 116 | VAL  |
| 2   | B     | 126 | ARG  |
| 2   | B     | 134 | LEU  |
| 2   | B     | 149 | MET  |
| 2   | B     | 153 | ARG  |
| 2   | B     | 154 | LYS  |
| 2   | B     | 156 | LEU  |
| 2   | B     | 163 | GLN  |
| 2   | B     | 165 | LYS  |
| 2   | B     | 181 | ILE  |
| 2   | B     | 189 | SER  |
| 2   | B     | 215 | TYR  |
| 2   | B     | 217 | THR  |
| 2   | B     | 237 | ILE  |
| 2   | B     | 243 | GLU  |
| 2   | B     | 278 | LEU  |
| 2   | B     | 286 | LYS  |
| 2   | B     | 307 | LEU  |
| 2   | B     | 308 | LEU  |
| 2   | B     | 311 | THR  |
| 2   | B     | 317 | ARG  |
| 2   | B     | 327 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 329 | THR  |
| 2   | B     | 332 | LEU  |
| 2   | B     | 338 | VAL  |
| 2   | B     | 344 | LEU  |
| 2   | B     | 354 | LYS  |
| 2   | B     | 377 | GLU  |
| 2   | B     | 387 | ARG  |
| 2   | B     | 407 | LEU  |
| 2   | B     | 409 | GLU  |
| 2   | B     | 410 | LYS  |
| 2   | B     | 414 | LYS  |
| 2   | C     | 18  | LEU  |
| 2   | C     | 30  | ASP  |
| 2   | C     | 33  | ARG  |
| 2   | C     | 40  | LEU  |
| 2   | C     | 46  | LYS  |
| 2   | C     | 70  | ASN  |
| 2   | C     | 78  | LYS  |
| 2   | C     | 85  | ASP  |
| 2   | C     | 97  | LYS  |
| 2   | C     | 104 | ILE  |
| 2   | C     | 106 | ASP  |
| 2   | C     | 108 | VAL  |
| 2   | C     | 122 | SER  |
| 2   | C     | 134 | LEU  |
| 2   | C     | 143 | ARG  |
| 2   | C     | 149 | MET  |
| 2   | C     | 152 | TYR  |
| 2   | C     | 153 | ARG  |
| 2   | C     | 155 | LYS  |
| 2   | C     | 156 | LEU  |
| 2   | C     | 160 | LEU  |
| 2   | C     | 162 | ASN  |
| 2   | C     | 163 | GLN  |
| 2   | C     | 167 | ILE  |
| 2   | C     | 177 | GLU  |
| 2   | C     | 181 | ILE  |
| 2   | C     | 189 | SER  |
| 2   | C     | 195 | VAL  |
| 2   | C     | 214 | ARG  |
| 2   | C     | 228 | LEU  |
| 2   | C     | 230 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 243 | GLU  |
| 2   | C     | 252 | ARG  |
| 2   | C     | 253 | GLU  |
| 2   | C     | 278 | LEU  |
| 2   | C     | 286 | LYS  |
| 2   | C     | 307 | LEU  |
| 2   | C     | 308 | LEU  |
| 2   | C     | 311 | THR  |
| 2   | C     | 312 | ARG  |
| 2   | C     | 317 | ARG  |
| 2   | C     | 327 | LEU  |
| 2   | C     | 332 | LEU  |
| 2   | C     | 353 | ASN  |
| 2   | C     | 354 | LYS  |
| 2   | C     | 371 | GLN  |
| 2   | C     | 375 | VAL  |
| 2   | C     | 377 | GLU  |
| 2   | C     | 385 | GLN  |
| 2   | C     | 407 | LEU  |
| 2   | C     | 408 | ARG  |
| 2   | C     | 409 | GLU  |
| 2   | C     | 422 | LYS  |
| 2   | D     | 8   | ILE  |
| 2   | D     | 22  | GLU  |
| 2   | D     | 23  | ASP  |
| 2   | D     | 26  | GLU  |
| 2   | D     | 34  | LYS  |
| 2   | D     | 42  | ILE  |
| 2   | D     | 44  | THR  |
| 2   | D     | 64  | VAL  |
| 2   | D     | 83  | LYS  |
| 2   | D     | 84  | LEU  |
| 2   | D     | 85  | ASP  |
| 2   | D     | 97  | LYS  |
| 2   | D     | 104 | ILE  |
| 2   | D     | 108 | VAL  |
| 2   | D     | 126 | ARG  |
| 2   | D     | 128 | SER  |
| 2   | D     | 146 | ARG  |
| 2   | D     | 149 | MET  |
| 2   | D     | 153 | ARG  |
| 2   | D     | 171 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 217 | THR  |
| 2   | D     | 228 | LEU  |
| 2   | D     | 230 | THR  |
| 2   | D     | 243 | GLU  |
| 2   | D     | 244 | ASP  |
| 2   | D     | 252 | ARG  |
| 2   | D     | 308 | LEU  |
| 2   | D     | 309 | ARG  |
| 2   | D     | 311 | THR  |
| 2   | D     | 312 | ARG  |
| 2   | D     | 317 | ARG  |
| 2   | D     | 326 | SER  |
| 2   | D     | 327 | LEU  |
| 2   | D     | 328 | THR  |
| 2   | D     | 332 | LEU  |
| 2   | D     | 353 | ASN  |
| 2   | D     | 354 | LYS  |
| 2   | D     | 367 | ASN  |
| 2   | D     | 377 | GLU  |
| 2   | D     | 394 | MET  |
| 2   | D     | 407 | LEU  |
| 2   | D     | 409 | GLU  |
| 2   | D     | 412 | ILE  |
| 2   | D     | 414 | LYS  |
| 2   | E     | 13  | VAL  |
| 2   | E     | 18  | LEU  |
| 2   | E     | 40  | LEU  |
| 2   | E     | 43  | ASN  |
| 2   | E     | 48  | LEU  |
| 2   | E     | 84  | LEU  |
| 2   | E     | 85  | ASP  |
| 2   | E     | 95  | ILE  |
| 2   | E     | 106 | ASP  |
| 2   | E     | 123 | ASP  |
| 2   | E     | 130 | ASP  |
| 2   | E     | 133 | TRP  |
| 2   | E     | 134 | LEU  |
| 2   | E     | 148 | GLN  |
| 2   | E     | 149 | MET  |
| 2   | E     | 180 | ASP  |
| 2   | E     | 181 | ILE  |
| 2   | E     | 182 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | E     | 187 | ASN  |
| 2   | E     | 206 | LYS  |
| 2   | E     | 209 | GLU  |
| 2   | E     | 242 | THR  |
| 2   | E     | 243 | GLU  |
| 2   | E     | 253 | GLU  |
| 2   | E     | 307 | LEU  |
| 2   | E     | 308 | LEU  |
| 2   | E     | 309 | ARG  |
| 2   | E     | 314 | ARG  |
| 2   | E     | 317 | ARG  |
| 2   | E     | 327 | LEU  |
| 2   | E     | 332 | LEU  |
| 2   | E     | 349 | CYS  |
| 2   | E     | 354 | LYS  |
| 2   | E     | 356 | THR  |
| 2   | E     | 375 | VAL  |
| 2   | E     | 405 | GLN  |
| 2   | E     | 412 | ILE  |
| 2   | E     | 418 | SER  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | A     | 43  | ASN  |
| 2   | A     | 68  | HIS  |
| 2   | A     | 70  | ASN  |
| 2   | A     | 162 | ASN  |
| 2   | A     | 163 | GLN  |
| 2   | A     | 187 | ASN  |
| 2   | A     | 260 | GLN  |
| 2   | A     | 266 | GLN  |
| 2   | A     | 347 | GLN  |
| 2   | A     | 395 | GLN  |
| 2   | B     | 70  | ASN  |
| 2   | B     | 163 | GLN  |
| 2   | B     | 266 | GLN  |
| 2   | B     | 347 | GLN  |
| 2   | B     | 385 | GLN  |
| 2   | C     | 63  | ASN  |
| 2   | C     | 68  | HIS  |
| 2   | C     | 70  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 168 | ASN  |
| 2   | C     | 266 | GLN  |
| 2   | D     | 43  | ASN  |
| 2   | D     | 57  | GLN  |
| 2   | D     | 63  | ASN  |
| 2   | D     | 68  | HIS  |
| 2   | D     | 70  | ASN  |
| 2   | D     | 163 | GLN  |
| 2   | D     | 203 | HIS  |
| 2   | D     | 266 | GLN  |
| 2   | D     | 347 | GLN  |
| 2   | D     | 371 | GLN  |
| 2   | D     | 395 | GLN  |
| 2   | E     | 70  | ASN  |
| 2   | E     | 187 | ASN  |
| 2   | E     | 266 | GLN  |
| 2   | E     | 315 | ASN  |
| 2   | E     | 347 | GLN  |
| 2   | E     | 395 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed    | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------|-------------------|-----------------|
| 1   | R     | 44/45 (97%) | 35 (79%)          | 8 (18%)         |

All (35) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | R     | 2   | U    |
| 1   | R     | 3   | U    |
| 1   | R     | 4   | U    |
| 1   | R     | 5   | U    |
| 1   | R     | 6   | U    |
| 1   | R     | 8   | U    |
| 1   | R     | 9   | U    |
| 1   | R     | 10  | U    |
| 1   | R     | 11  | U    |
| 1   | R     | 12  | U    |
| 1   | R     | 13  | U    |
| 1   | R     | 14  | U    |
| 1   | R     | 15  | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | R     | 17  | U    |
| 1   | R     | 18  | U    |
| 1   | R     | 19  | U    |
| 1   | R     | 21  | U    |
| 1   | R     | 23  | U    |
| 1   | R     | 24  | U    |
| 1   | R     | 25  | U    |
| 1   | R     | 26  | U    |
| 1   | R     | 27  | U    |
| 1   | R     | 28  | U    |
| 1   | R     | 29  | U    |
| 1   | R     | 30  | U    |
| 1   | R     | 32  | U    |
| 1   | R     | 33  | U    |
| 1   | R     | 36  | U    |
| 1   | R     | 37  | U    |
| 1   | R     | 38  | U    |
| 1   | R     | 39  | U    |
| 1   | R     | 40  | U    |
| 1   | R     | 41  | U    |
| 1   | R     | 42  | U    |
| 1   | R     | 45  | U    |

All (8) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | R     | 4   | U    |
| 1   | R     | 5   | U    |
| 1   | R     | 6   | U    |
| 1   | R     | 12  | U    |
| 1   | R     | 14  | U    |
| 1   | R     | 20  | U    |
| 1   | R     | 32  | U    |
| 1   | R     | 39  | U    |

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

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



## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 15 are modelled with single atom - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.