



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 12:15 am BST

PDB ID : 1XMQ  
Title : Crystal Structure of t6A37-ASLLysUUU AAA-mRNA Bound to the Decoding Center  
Authors : Murphy, F.V.; Ramakrishnan, V.; Malkiewicz, A.; Agris, P.F.  
Deposited on : 2004-10-04  
Resolution : 3.00 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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
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

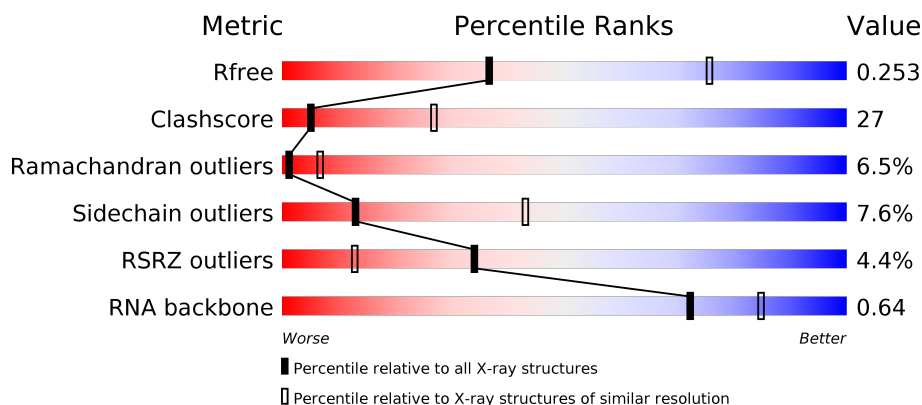
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


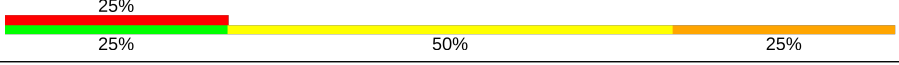
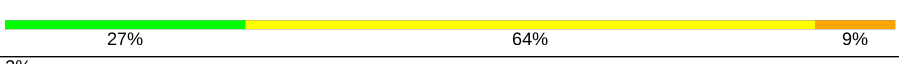

The reported resolution of this entry is 3.00 Å.

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                      | 2092 (3.00-3.00)                                      |
| Clashscore            | 141614                      | 2416 (3.00-3.00)                                      |
| Ramachandran outliers | 138981                      | 2333 (3.00-3.00)                                      |
| Sidechain outliers    | 138945                      | 2336 (3.00-3.00)                                      |
| RSRZ outliers         | 127900                      | 1990 (3.00-3.00)                                      |
| RNA backbone          | 3102                        | 1173 (3.30-2.70)                                      |

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

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | A     | 1522   |  |
| 2   | W     | 4      |  |
| 3   | X     | 11     |  |
| 4   | B     | 256    |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 5   | C     | 239    |                  |
| 6   | D     | 209    |                  |
| 7   | E     | 162    |                  |
| 8   | F     | 101    |                  |
| 9   | G     | 156    |                  |
| 10  | H     | 138    |                  |
| 11  | I     | 128    |                  |
| 12  | J     | 105    |                  |
| 13  | K     | 129    |                  |
| 14  | L     | 135    |                  |
| 15  | M     | 126    |                  |
| 16  | N     | 61     |                  |
| 17  | O     | 89     |                  |
| 18  | P     | 88     |                  |
| 19  | Q     | 105    |                  |
| 20  | R     | 88     |                  |
| 21  | S     | 93     |                  |
| 22  | T     | 106    |                  |
| 23  | V     | 27     |                  |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 25  | MG   | A     | 1608 | -         | -        | -       | X                |
| 25  | MG   | A     | 1613 | -         | -        | -       | X                |
| 25  | MG   | A     | 1627 | -         | -        | -       | X                |
| 25  | MG   | A     | 493  | -         | -        | -       | X                |
| 3   | T6A  | X     | 37   | X         | -        | -       | -                |

## 2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 52081 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16s ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1   | A     | 1507     | Total | C     | N    | O     | P    | 22      | 0       | 0     |
|     |       |          | 32380 | 14414 | 5990 | 10470 | 1506 |         |         |       |

- Molecule 2 is a RNA chain called A-Site Messenger RNA.

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 2   | W     | 4        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 85    | 40 | 20 | 22 | 3 |         |         |       |

- Molecule 3 is a RNA chain called Anticodon RNA.

| Mol | Chain | Residues | Atoms |     |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 3   | X     | 11       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 236   | 108 | 37 | 81 | 10 |         |         |       |

- Molecule 4 is a protein called 30S Ribosomal Protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | B     | 234      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1900  | 1213 | 341 | 341 | 5 |         |         |       |

- Molecule 5 is a protein called 30S Ribosomal Protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5   | C     | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1612  | 1016 | 314 | 281 | 1 |         |         |       |

- Molecule 6 is a protein called 30S Ribosomal Protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 6   | D     | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1703  | 1066 | 339 | 291 | 7 |         |         |       |

- Molecule 7 is a protein called 30S Ribosomal Protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | E     | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1146  | 724 | 217 | 201 | 4 |         |         |       |

- Molecule 8 is a protein called 30S Ribosomal Protein S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | F     | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 843   | 531 | 155 | 154 | 3 |         |         |       |

- Molecule 9 is a protein called 30S Ribosomal Protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9   | G     | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1257  | 781 | 252 | 218 | 6 |         |         |       |

- Molecule 10 is a protein called 30S Ribosomal Protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | H     | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1116  | 705 | 215 | 193 | 3 |         |         |       |

- Molecule 11 is a protein called 30S Ribosomal Protein S9.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 11  | I     | 127      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1011  | 639 | 198 | 174 |         |         |       |

- Molecule 12 is a protein called 30S Ribosomal Protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | J     | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 792   | 498 | 156 | 137 | 1 |         |         |       |

- Molecule 13 is a protein called 30S Ribosomal Protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | K     | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 885   | 549 | 168 | 165 | 3 |         |         |       |

- Molecule 14 is a protein called 30S Ribosomal Protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14  | L     | 124      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 970   | 611 | 195 | 163 | 1 |         |         |       |

- Molecule 15 is a protein called 30S Ribosomal Protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15  | M     | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 997   | 617 | 207 | 171 | 2 |         |         |       |

- Molecule 16 is a protein called 30S Ribosomal Protein S14.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 16  | N     | 60       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 492   | 312 | 104 | 72 | 4 |         |         |       |

- Molecule 17 is a protein called 30S Ribosomal Protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17  | O     | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 734   | 459 | 147 | 126 | 2 |         |         |       |

- Molecule 18 is a protein called 30S Ribosomal Protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 18  | P     | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 700   | 443 | 139 | 117 | 1 |         |         |       |

- Molecule 19 is a protein called 30S Ribosomal Protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | Q     | 104      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 857   | 547 | 161 | 147 | 2 |         |         |       |

- Molecule 20 is a protein called 30S Ribosomal Protein S18.

| Mol | Chain | Residues | Atoms |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 20  | R     | 73       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 597   | 380 | 118 | 99 |         |         |       |

- Molecule 21 is a protein called 30S Ribosomal Protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 21  | S     | 80       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 647   | 414 | 119 | 112 | 2 |         |         |       |

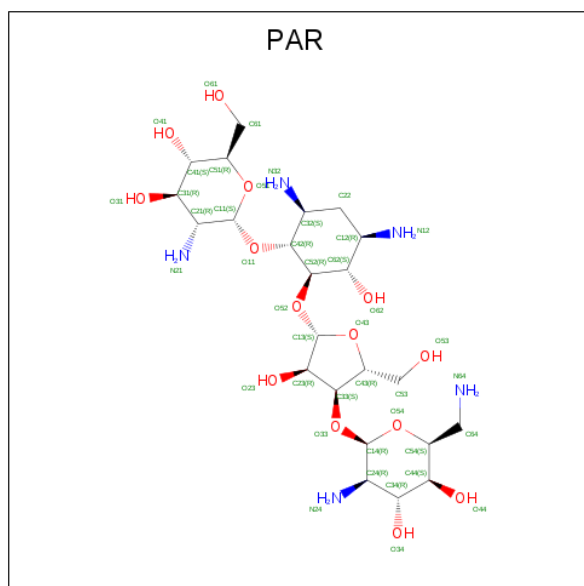
- Molecule 22 is a protein called 30S Ribosomal Protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 22  | T     | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 762   | 469 | 162 | 129 | 2 |         |         |       |

- Molecule 23 is a protein called 30S Ribosomal Protein Thx.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 23  | V     | 24       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 208   | 128 | 50 | 30 |         |         |       |

- Molecule 24 is PAROMOMYCIN (three-letter code: PAR) (formula:  $C_{23}H_{45}N_5O_{14}$ ).



| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---------|---------|
| 24  | A     | 1        | Total | C  | N | O  | 0       | 0       |
|     |       |          | 42    | 23 | 5 | 14 |         |         |

- Molecule 25 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 25  | X     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

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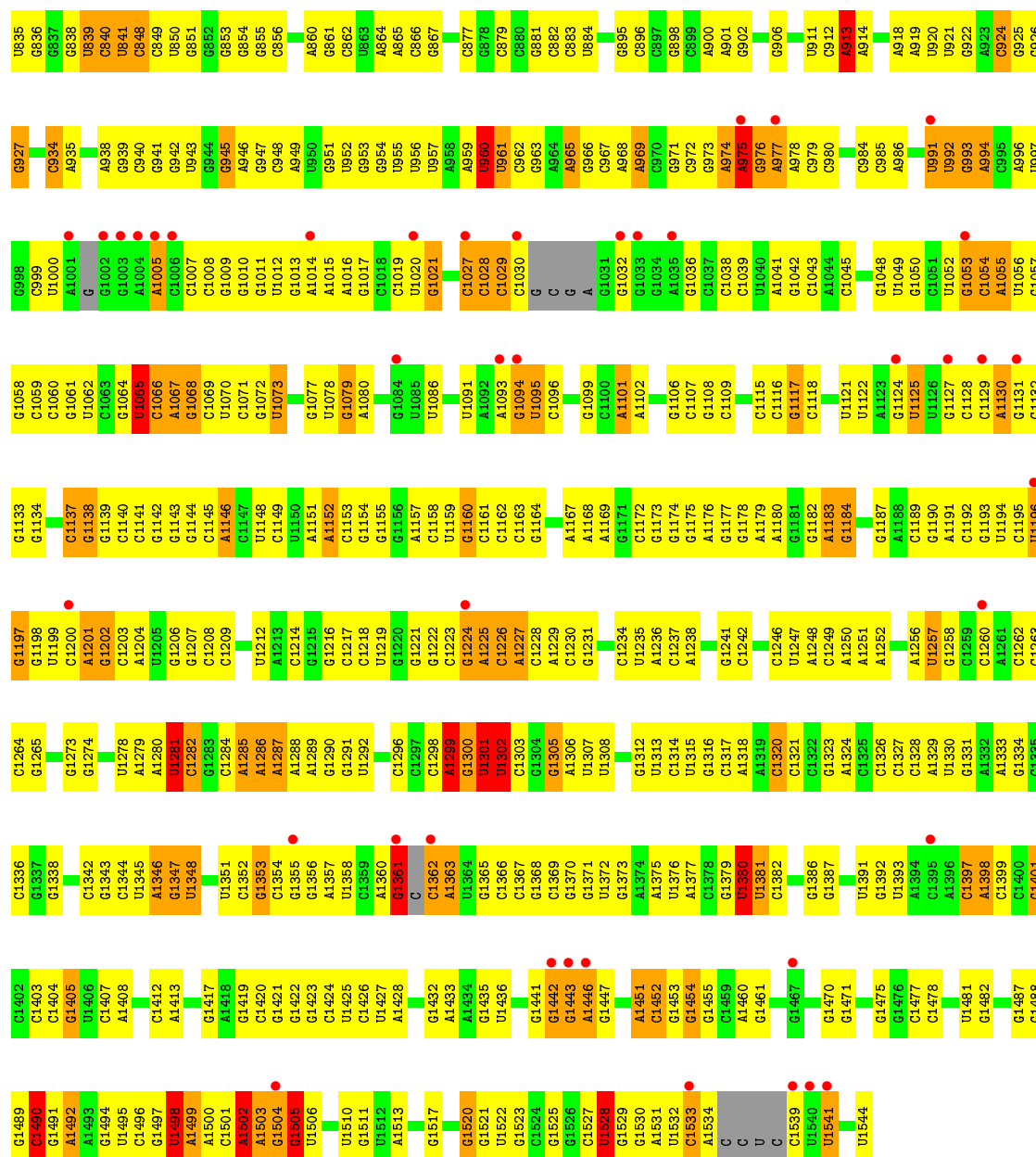
| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 25  | A     | 104      | Total<br>104 | Mg<br>104 | 0       | 0       |
| 25  | N     | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 26  | D     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 26  | N     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |







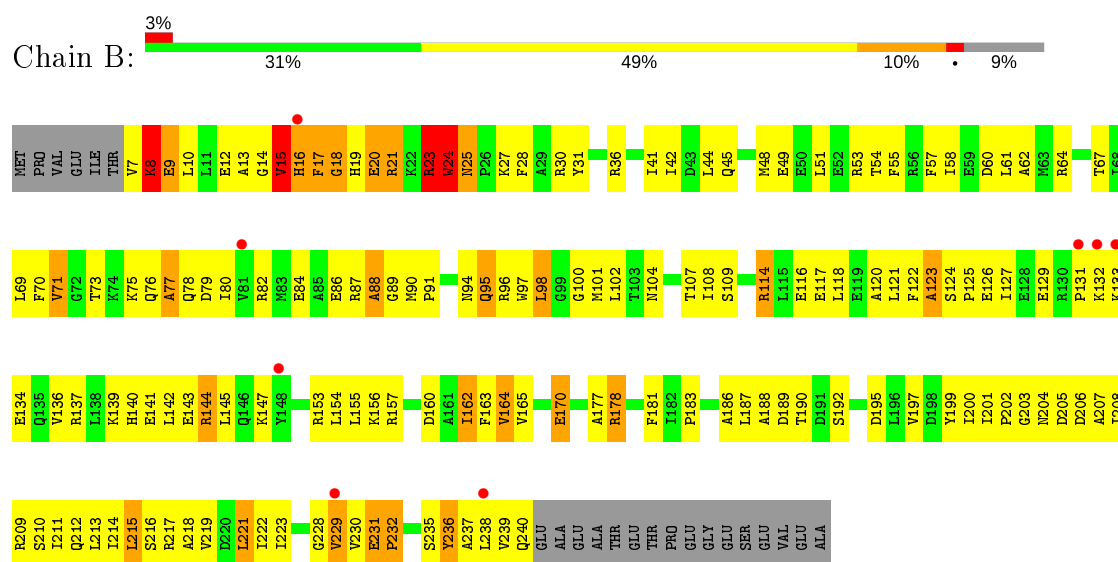
- Molecule 2: A-Site Messenger RNA



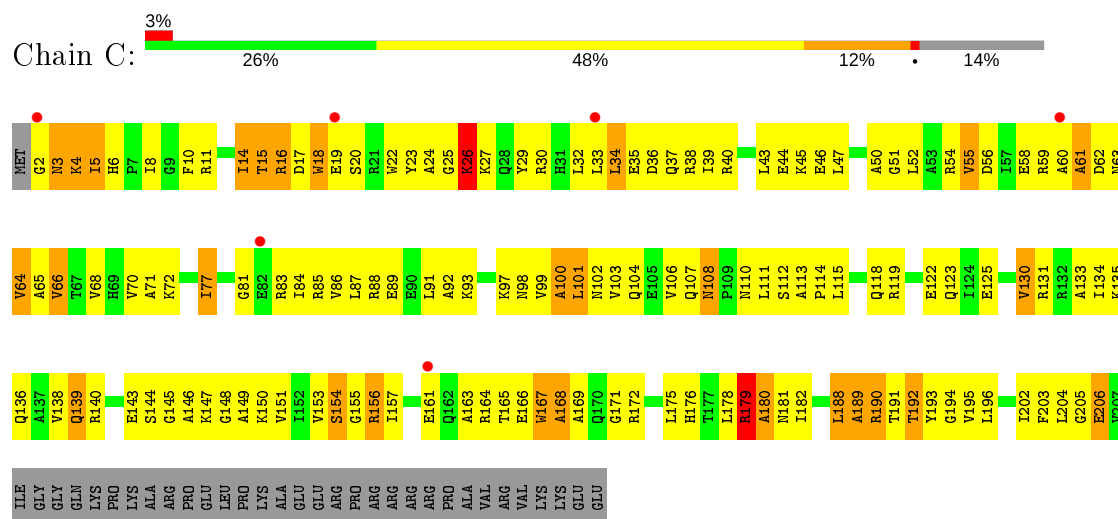
- Molecule 3: Anticodon RNA



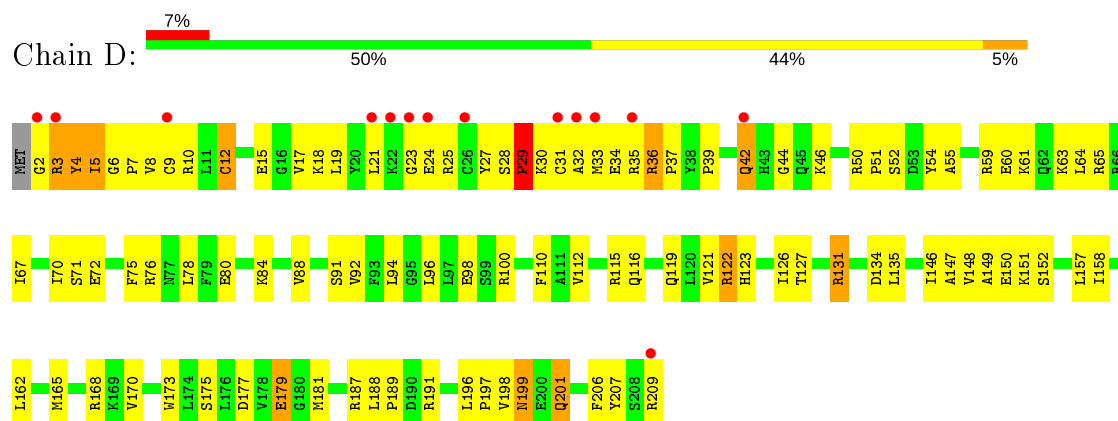
- Molecule 4: 30S Ribosomal Protein S2



- Molecule 5: 30S Ribosomal Protein S3

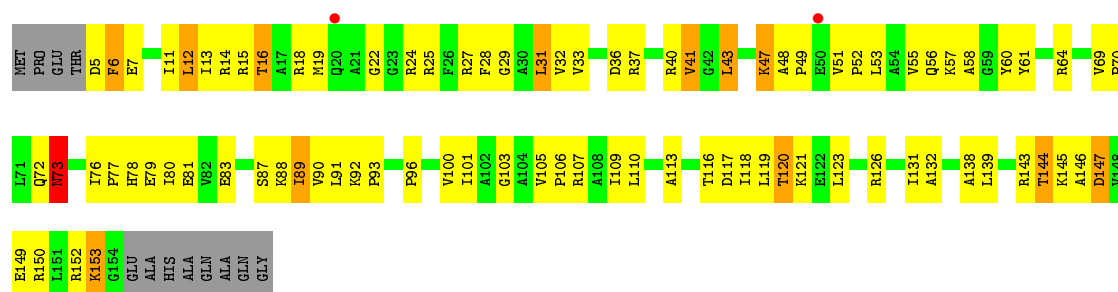


- Molecule 6: 30S Ribosomal Protein S4



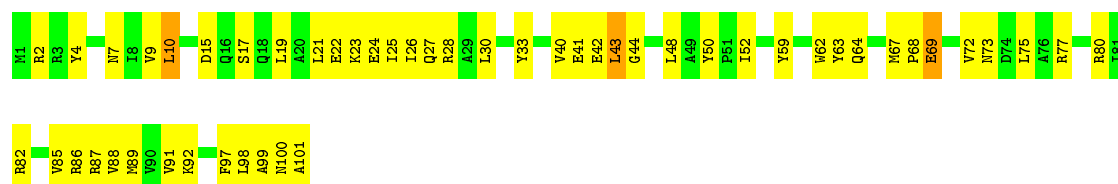
- Molecule 7: 30S Ribosomal Protein S5





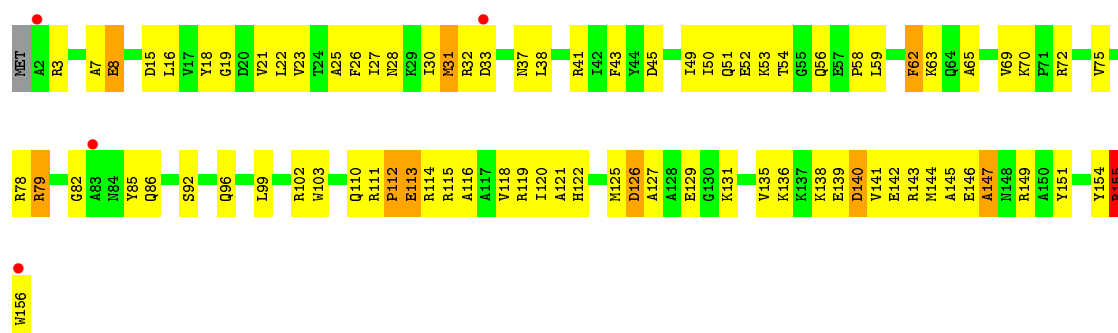
• Molecule 8: 30S Ribosomal Protein S6

Chain F: 50% 48%



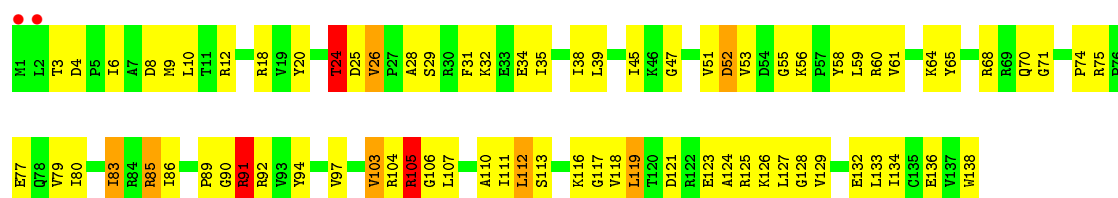
• Molecule 9: 30S Ribosomal Protein S7

Chain G: 46% 47% 3% 6%



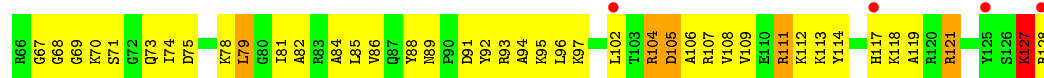
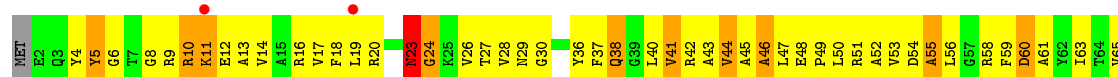
• Molecule 10: 30S Ribosomal Protein S8

Chain H: 45% 48% 5%

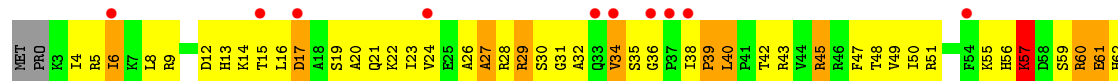


• Molecule 11: 30S Ribosomal Protein S9

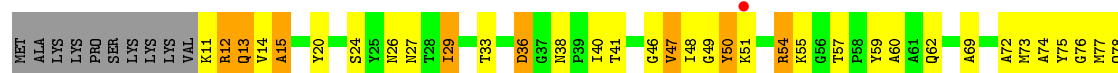
Chain I: 30% 56% 12%



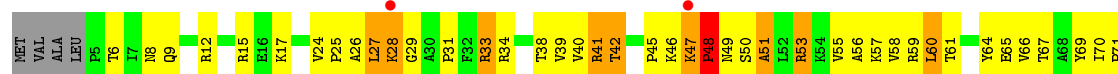
• Molecule 12: 30S Ribosomal Protein S10



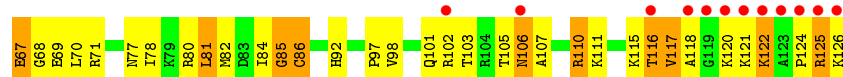
• Molecule 13: 30S Ribosomal Protein S11



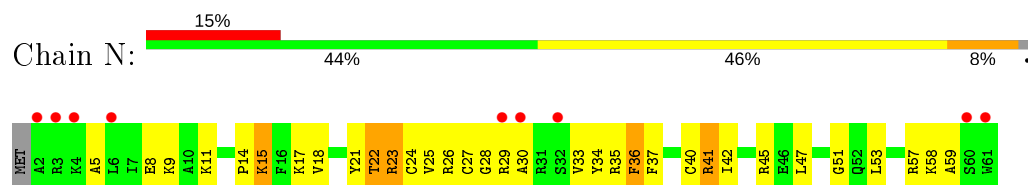
• Molecule 14: 30S Ribosomal Protein S12



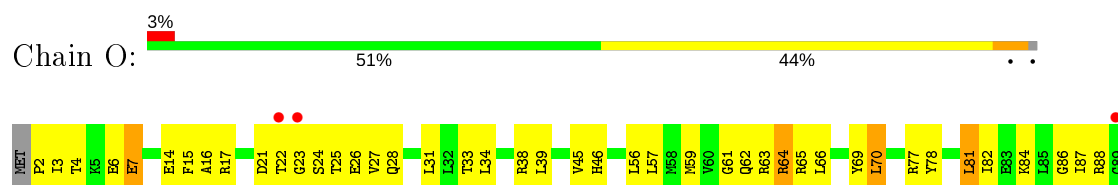
• Molecule 15: 30S Ribosomal Protein S13



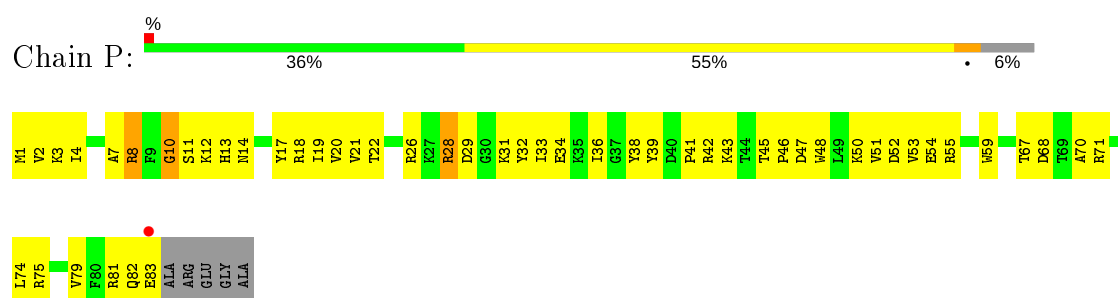
- Molecule 16: 30S Ribosomal Protein S14



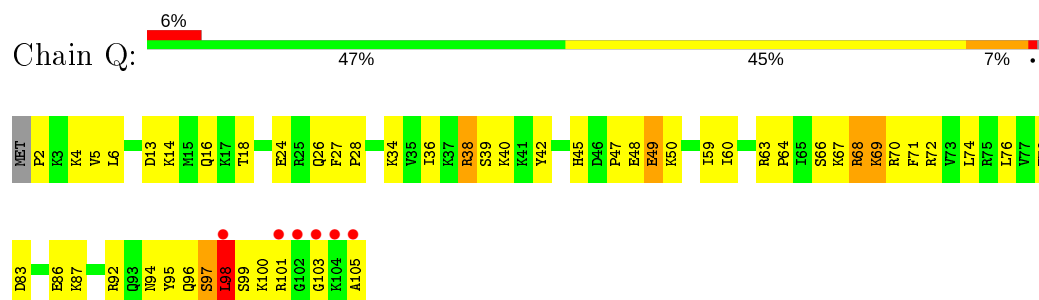
- Molecule 17: 30S Ribosomal Protein S15



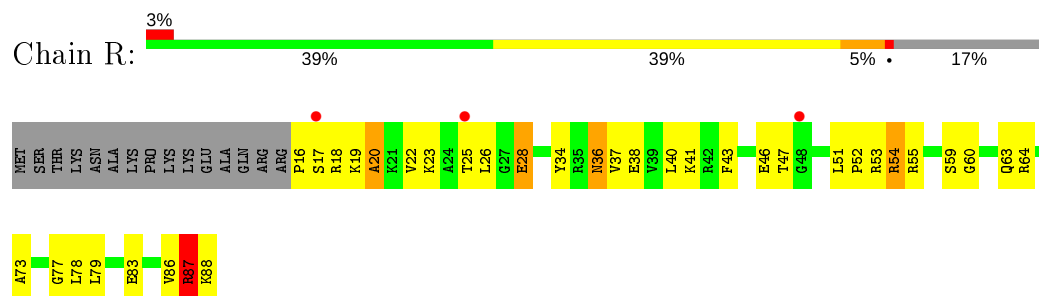
- Molecule 18: 30S Ribosomal Protein S16



- Molecule 19: 30S Ribosomal Protein S17

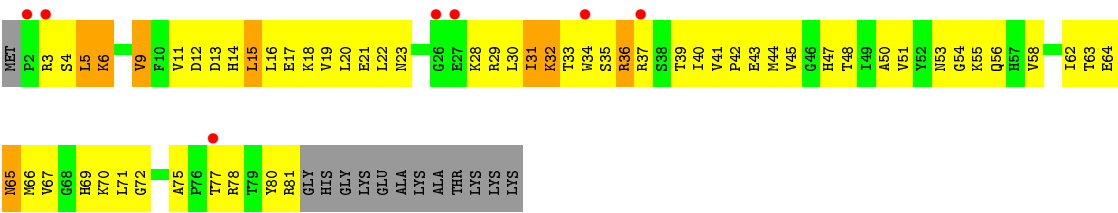


- Molecule 20: 30S Ribosomal Protein S18

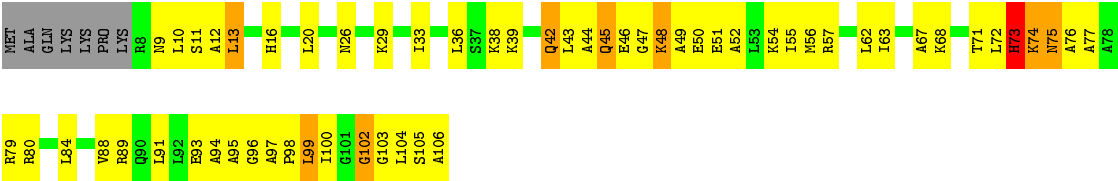
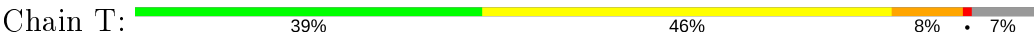


- Molecule 21: 30S Ribosomal Protein S19

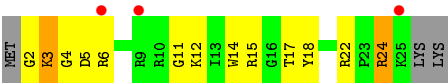




● Molecule 22: 30S Ribosomal Protein S20



● Molecule 23: 30S Ribosomal Protein Thx



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 41 21 2   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 400.72Å 400.72Å 175.09Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 99.00 – 3.00<br>283.35 – 2.99                               | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | (Not available) (99.00-3.00)<br>93.1 (283.35-2.99)          | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | 0.14  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.80 (at 3.01Å)   | Xtriage          |
| Refinement program  | CNS   | Depositor        |
| R, $R_{free}$   | 0.222 , 0.236<br>0.215 , 0.253                              | Depositor<br>DCC |
| $R_{free}$ test set   | 13422 reflections (5.08%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 70.2  | Xtriage          |
| Anisotropy  | 0.240   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 71.3   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.90  | EDS              |
| Total number of atoms   | 52081   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 77.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.35% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, T6A, PAR

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

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # $ Z  > 5$    | RMSZ        | # $ Z  > 5$     |
| 1   | A     | 0.49         | 1/36244 (0.0%) | 0.74        | 41/56567 (0.1%) |
| 2   | W     | 0.44         | 0/96           | 0.86        | 1/148 (0.7%)    |
| 3   | X     | 0.44         | 0/226          | 0.78        | 0/349           |
| 4   | B     | 0.32         | 0/1935         | 0.60        | 0/2609          |
| 5   | C     | 0.35         | 0/1636         | 0.63        | 0/2205          |
| 6   | D     | 0.36         | 0/1733         | 0.61        | 1/2318 (0.0%)   |
| 7   | E     | 0.42         | 0/1162         | 0.67        | 0/1564          |
| 8   | F     | 0.30         | 0/856          | 0.59        | 0/1154          |
| 9   | G     | 0.32         | 0/1276         | 0.59        | 0/1709          |
| 10  | H     | 0.40         | 0/1136         | 0.73        | 0/1527          |
| 11  | I     | 0.33         | 0/1029         | 0.61        | 0/1378          |
| 12  | J     | 0.35         | 0/805          | 0.63        | 0/1082          |
| 13  | K     | 0.37         | 0/900          | 0.63        | 0/1213          |
| 14  | L     | 0.42         | 0/986          | 0.75        | 0/1320          |
| 15  | M     | 0.32         | 0/1008         | 0.62        | 0/1347          |
| 16  | N     | 0.36         | 0/501          | 0.64        | 0/664           |
| 17  | O     | 0.33         | 0/745          | 0.60        | 0/992           |
| 18  | P     | 0.45         | 0/716          | 0.72        | 0/963           |
| 19  | Q     | 0.43         | 0/870          | 0.75        | 0/1159          |
| 20  | R     | 0.32         | 0/603          | 0.60        | 0/799           |
| 21  | S     | 0.30         | 0/661          | 0.64        | 0/890           |
| 22  | T     | 0.38         | 0/764          | 0.75        | 1/1006 (0.1%)   |
| 23  | V     | 0.43         | 0/212          | 0.64        | 0/277           |
| All | All   | 0.45         | 1/56100 (0.0%) | 0.71        | 44/83240 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 4                   | 40                  |
| 3   | X     | 1                   | 0                   |
| All | All   | 5                   | 40                  |

All (1) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 1   | A     | 1361 | G    | C3'-O3' | 5.66 | 1.50        | 1.42     |

All (44) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 281  | G    | C2'-C3'-O3' | 10.04 | 131.59      | 109.50   |
| 1   | A     | 1498 | U    | C2'-C3'-O3' | 9.79  | 131.04      | 109.50   |
| 1   | A     | 243  | A    | C2'-C3'-O3' | 9.48  | 130.35      | 109.50   |
| 1   | A     | 1302 | U    | C2'-C3'-O3' | 9.13  | 129.59      | 109.50   |
| 1   | A     | 366  | C    | C2'-C3'-O3' | 9.11  | 129.55      | 109.50   |
| 1   | A     | 328  | C    | C2'-C3'-O3' | 9.02  | 129.33      | 109.50   |
| 1   | A     | 181  | G    | C2'-C3'-O3' | 8.93  | 129.15      | 109.50   |
| 1   | A     | 1528 | U    | C2'-C3'-O3' | 8.56  | 128.33      | 109.50   |
| 1   | A     | 965  | A    | C2'-C3'-O3' | 8.31  | 127.78      | 109.50   |
| 1   | A     | 792  | A    | C2'-C3'-O3' | 8.28  | 127.72      | 109.50   |
| 1   | A     | 484  | G    | C2'-C3'-O3' | 8.24  | 127.63      | 109.50   |
| 1   | A     | 559  | A    | C2'-C3'-O3' | 8.22  | 127.58      | 109.50   |
| 1   | A     | 812  | C    | C2'-C3'-O3' | 8.17  | 127.47      | 109.50   |
| 1   | A     | 266  | G    | C2'-C3'-O3' | 7.81  | 126.67      | 109.50   |
| 1   | A     | 575  | G    | C2'-C3'-O3' | 7.79  | 126.63      | 109.50   |
| 1   | A     | 1505 | G    | C2'-C3'-O3' | 7.49  | 125.97      | 109.50   |
| 1   | A     | 913  | A    | C2'-C3'-O3' | 7.38  | 125.75      | 109.50   |
| 1   | A     | 60   | A    | C2'-C3'-O3' | 7.14  | 125.21      | 109.50   |
| 1   | A     | 115  | G    | C2'-C3'-O3' | 6.96  | 124.83      | 113.70   |
| 1   | A     | 1490 | C    | C5'-C4'-O4' | -6.84 | 100.89      | 109.10   |
| 1   | A     | 372  | C    | C2'-C3'-O3' | 6.49  | 124.08      | 113.70   |
| 1   | A     | 353  | A    | C5'-C4'-O4' | -6.38 | 101.44      | 109.10   |
| 1   | A     | 1346 | A    | C2'-C3'-O3' | 6.34  | 123.84      | 113.70   |
| 6   | D     | 12   | CYS  | CA-CB-SG    | 6.29  | 125.31      | 114.00   |
| 1   | A     | 1502 | A    | N9-C1'-C2'  | 6.28  | 122.17      | 114.00   |
| 1   | A     | 509  | A    | C2'-C3'-O3' | 6.27  | 123.74      | 113.70   |
| 1   | A     | 497  | A    | C2'-C3'-O3' | 6.09  | 123.44      | 113.70   |
| 1   | A     | 1528 | U    | C4'-C3'-O3' | 5.88  | 124.75      | 113.00   |
| 1   | A     | 1299 | A    | N9-C1'-C2'  | 5.87  | 121.63      | 114.00   |
| 1   | A     | 760  | G    | N9-C1'-C2'  | -5.79 | 105.63      | 112.00   |
| 1   | A     | 533  | A    | C2'-C3'-O3' | 5.79  | 122.96      | 113.70   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 22  | T     | 13     | LEU  | N-CA-C      | -5.73 | 95.52       | 111.00   |
| 1   | A     | 190(K) | G    | N9-C1'-C2'  | -5.68 | 105.75      | 112.00   |
| 1   | A     | 328    | C    | O4'-C1'-N1  | -5.68 | 103.66      | 108.20   |
| 1   | A     | 1503   | A    | C2'-C3'-O3' | 5.65  | 122.74      | 113.70   |
| 1   | A     | 115    | G    | N9-C1'-C2'  | 5.50  | 121.15      | 114.00   |
| 2   | W     | 1      | A    | O5'-C5'-C4' | 5.32  | 121.81      | 111.70   |
| 1   | A     | 389    | A    | C5'-C4'-C3' | 5.32  | 124.51      | 116.00   |
| 1   | A     | 108    | G    | O4'-C1'-N9  | 5.28  | 112.42      | 108.20   |
| 1   | A     | 960    | U    | C2'-C3'-O3' | 5.26  | 122.11      | 113.70   |
| 1   | A     | 1065   | U    | C1'-O4'-C4' | -5.20 | 105.74      | 109.90   |
| 1   | A     | 1380   | U    | C2'-C3'-O3' | 5.08  | 121.83      | 113.70   |
| 1   | A     | 58     | C    | N1-C1'-C2'  | -5.04 | 106.45      | 112.00   |
| 1   | A     | 366    | C    | C4'-C3'-O3' | 5.03  | 123.06      | 113.00   |

All (5) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 1   | A     | 243  | A    | C3'  |
| 1   | A     | 281  | G    | C3'  |
| 1   | A     | 366  | C    | C3'  |
| 1   | A     | 1528 | U    | C3'  |
| 3   | X     | 37   | T6A  | C14  |

All (40) planarity outliers are listed below:

| Mol | Chain | Res    | Type | Group     |
|-----|-------|--------|------|-----------|
| 1   | A     | 1013   | G    | Sidechain |
| 1   | A     | 1048   | G    | Sidechain |
| 1   | A     | 106    | C    | Sidechain |
| 1   | A     | 1073   | U    | Sidechain |
| 1   | A     | 1077   | G    | Sidechain |
| 1   | A     | 1079   | G    | Sidechain |
| 1   | A     | 1281   | U    | Sidechain |
| 1   | A     | 1299   | A    | Sidechain |
| 1   | A     | 1301   | U    | Sidechain |
| 1   | A     | 1361   | G    | Sidechain |
| 1   | A     | 1405   | G    | Sidechain |
| 1   | A     | 1454   | G    | Sidechain |
| 1   | A     | 1490   | C    | Sidechain |
| 1   | A     | 1492   | A    | Sidechain |
| 1   | A     | 1498   | U    | Sidechain |
| 1   | A     | 190(K) | G    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 195 | A    | Sidechain |
| 1   | A     | 250 | A    | Sidechain |
| 1   | A     | 290 | C    | Sidechain |
| 1   | A     | 291 | C    | Sidechain |
| 1   | A     | 380 | G    | Sidechain |
| 1   | A     | 387 | U    | Sidechain |
| 1   | A     | 481 | G    | Sidechain |
| 1   | A     | 51  | A    | Sidechain |
| 1   | A     | 521 | G    | Sidechain |
| 1   | A     | 528 | C    | Sidechain |
| 1   | A     | 529 | G    | Sidechain |
| 1   | A     | 561 | U    | Sidechain |
| 1   | A     | 573 | A    | Sidechain |
| 1   | A     | 58  | C    | Sidechain |
| 1   | A     | 580 | U    | Sidechain |
| 1   | A     | 587 | G    | Sidechain |
| 1   | A     | 664 | G    | Sidechain |
| 1   | A     | 682 | G    | Sidechain |
| 1   | A     | 727 | G    | Sidechain |
| 1   | A     | 748 | C    | Sidechain |
| 1   | A     | 879 | C    | Sidechain |
| 1   | A     | 898 | G    | Sidechain |
| 1   | A     | 924 | C    | Sidechain |
| 1   | A     | 975 | A    | Sidechain |

## 5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 32380 | 0        | 16346    | 879     | 0            |
| 2   | W     | 85    | 0        | 46       | 4       | 0            |
| 3   | X     | 236   | 0        | 122      | 13      | 0            |
| 4   | B     | 1900  | 0        | 1951     | 183     | 0            |
| 5   | C     | 1612  | 0        | 1677     | 194     | 0            |
| 6   | D     | 1703  | 0        | 1764     | 111     | 0            |
| 7   | E     | 1146  | 0        | 1207     | 99      | 0            |
| 8   | F     | 843   | 0        | 857      | 56      | 0            |
| 9   | G     | 1257  | 0        | 1296     | 88      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 10  | H     | 1116  | 0        | 1177     | 86      | 0            |
| 11  | I     | 1011  | 0        | 1043     | 115     | 0            |
| 12  | J     | 792   | 0        | 835      | 119     | 0            |
| 13  | K     | 885   | 0        | 904      | 66      | 0            |
| 14  | L     | 970   | 0        | 1057     | 107     | 0            |
| 15  | M     | 997   | 0        | 1072     | 95      | 0            |
| 16  | N     | 492   | 0        | 529      | 43      | 0            |
| 17  | O     | 734   | 0        | 771      | 38      | 0            |
| 18  | P     | 700   | 0        | 720      | 55      | 0            |
| 19  | Q     | 857   | 0        | 930      | 57      | 0            |
| 20  | R     | 597   | 0        | 668      | 58      | 0            |
| 21  | S     | 647   | 0        | 673      | 91      | 0            |
| 22  | T     | 762   | 0        | 856      | 58      | 0            |
| 23  | V     | 208   | 0        | 221      | 18      | 0            |
| 24  | A     | 42    | 0        | 45       | 2       | 0            |
| 25  | A     | 104   | 0        | 0        | 0       | 0            |
| 25  | N     | 1     | 0        | 0        | 0       | 0            |
| 25  | X     | 2     | 0        | 0        | 0       | 0            |
| 26  | D     | 1     | 0        | 0        | 0       | 0            |
| 26  | N     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 52081 | 0        | 36767    | 2401    | 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 27.

All (2401) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:972:C:H4'    | 12:J:57:LYS:HG2  | 1.31                     | 1.08              |
| 4:B:84:GLU:HB3   | 4:B:219:VAL:HG21 | 1.35                     | 1.06              |
| 19:Q:98:LEU:HD12 | 19:Q:98:LEU:H    | 1.20                     | 1.05              |
| 21:S:33:THR:HG22 | 21:S:35:SER:H    | 1.16                     | 1.04              |
| 1:A:1490:C:H5'   | 1:A:1490:C:H6    | 1.18                     | 1.04              |
| 21:S:55:LYS:HG2  | 21:S:56:GLN:HE21 | 1.19                     | 1.03              |
| 5:C:3:ASN:N      | 5:C:3:ASN:HD22   | 1.56                     | 1.01              |
| 1:A:243:A:H4'    | 1:A:244:U:H5'    | 1.43                     | 1.00              |
| 1:A:189:G:O2'    | 1:A:190:C:H5''   | 1.60                     | 1.00              |
| 21:S:28:LYS:HG2  | 21:S:29:ARG:H    | 1.25                     | 0.99              |
| 5:C:26:LYS:H     | 5:C:26:LYS:HD3   | 1.27                     | 0.99              |
| 1:A:1226:C:H4'   | 1:A:1227:A:OP1   | 1.62                     | 0.98              |
| 18:P:28:ARG:HH11 | 18:P:28:ARG:HG2  | 1.30                     | 0.96              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 12:J:32:ALA:HB2  | 12:J:76:ASN:HD22 | 1.29                     | 0.96              |
| 4:B:18:GLY:HA2   | 4:B:41:ILE:HA    | 1.45                     | 0.96              |
| 6:D:36:ARG:H     | 6:D:37:PRO:HD3   | 1.27                     | 0.95              |
| 12:J:90:LEU:H    | 12:J:91:PRO:HD2  | 1.32                     | 0.95              |
| 1:A:664:G:H22    | 1:A:741:G:H1     | 1.11                     | 0.95              |
| 1:A:1190:G:OP1   | 5:C:4:LYS:HA     | 1.67                     | 0.94              |
| 20:R:47:THR:HA   | 20:R:83:GLU:HB2  | 1.46                     | 0.94              |
| 1:A:1502:A:H2    | 1:A:1505:G:H1    | 1.11                     | 0.94              |
| 12:J:4:ILE:HD12  | 12:J:74:ILE:HB   | 1.50                     | 0.94              |
| 14:L:41:ARG:HG2  | 14:L:42:THR:H    | 1.28                     | 0.93              |
| 12:J:49:VAL:O    | 12:J:60:ARG:HA   | 1.68                     | 0.93              |
| 14:L:47:LYS:HB3  | 14:L:48:PRO:CD   | 1.97                     | 0.93              |
| 8:F:100:ASN:HD22 | 20:R:23:LYS:HG2  | 1.35                     | 0.91              |
| 14:L:75:HIS:HD2  | 14:L:77:LEU:H    | 1.18                     | 0.91              |
| 1:A:1158:C:H5''  | 4:B:133:LYS:HE3  | 1.52                     | 0.91              |
| 13:K:84:VAL:HG23 | 13:K:110:ASP:HA  | 1.50                     | 0.91              |
| 12:J:45:ARG:HB3  | 12:J:45:ARG:HH11 | 1.35                     | 0.90              |
| 7:E:80:ILE:HD12  | 7:E:138:ALA:HB1  | 1.54                     | 0.90              |
| 12:J:31:GLY:HA2  | 12:J:78:ASN:ND2  | 1.87                     | 0.90              |
| 15:M:37:THR:HG23 | 15:M:55:ARG:HD2  | 1.53                     | 0.90              |
| 15:M:17:VAL:O    | 15:M:20:THR:HB   | 1.72                     | 0.89              |
| 12:J:5:ARG:H     | 12:J:100:THR:HA  | 1.36                     | 0.89              |
| 5:C:188:LEU:HD13 | 5:C:189:ALA:H    | 1.38                     | 0.88              |
| 12:J:6:ILE:HG23  | 12:J:98:ILE:HG12 | 1.56                     | 0.88              |
| 22:T:39:LYS:HD2  | 22:T:55:ILE:HD13 | 1.54                     | 0.87              |
| 6:D:98:GLU:HG2   | 6:D:189:PRO:HG3  | 1.57                     | 0.87              |
| 3:X:37:T6A:H8    | 3:X:37:T6A:H5'   | 1.39                     | 0.86              |
| 12:J:34:VAL:HG22 | 12:J:74:ILE:HG23 | 1.57                     | 0.86              |
| 6:D:36:ARG:N     | 6:D:37:PRO:HD3   | 1.91                     | 0.86              |
| 13:K:54:ARG:O    | 13:K:57:THR:HG22 | 1.76                     | 0.85              |
| 1:A:1489:G:C2'   | 1:A:1490:C:H5''  | 2.06                     | 0.85              |
| 4:B:77:ALA:HB2   | 4:B:211:ILE:HD13 | 1.58                     | 0.85              |
| 1:A:1489:G:H2'   | 1:A:1490:C:H5''  | 1.58                     | 0.85              |
| 14:L:53:ARG:HG2  | 14:L:93:LEU:HD11 | 1.59                     | 0.84              |
| 1:A:1305:G:O2'   | 1:A:1306:A:H8    | 1.59                     | 0.84              |
| 5:C:191:THR:HG21 | 5:C:193:TYR:CZ   | 2.12                     | 0.84              |
| 1:A:1490:C:C6    | 1:A:1490:C:H5'   | 2.10                     | 0.84              |
| 5:C:34:LEU:HD12  | 16:N:25:VAL:HG21 | 1.57                     | 0.84              |
| 1:A:939:G:H5''   | 9:G:102:ARG:NH2  | 1.93                     | 0.84              |
| 22:T:50:GLU:HG2  | 22:T:54:LYS:HE3  | 1.60                     | 0.83              |
| 9:G:155:ARG:CZ   | 9:G:155:ARG:HA   | 2.08                     | 0.83              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 15:M:120:LYS:HE2 | 15:M:122:LYS:HB3 | 1.59                     | 0.83              |
| 1:A:1223:C:P     | 21:S:78:ARG:HH12 | 2.01                     | 0.82              |
| 5:C:3:ASN:N      | 5:C:3:ASN:ND2    | 2.24                     | 0.82              |
| 8:F:7:ASN:HB2    | 8:F:89:MET:HB3   | 1.60                     | 0.82              |
| 10:H:10:LEU:HD22 | 10:H:83:ILE:HD11 | 1.61                     | 0.82              |
| 23:V:6:ARG:HG3   | 23:V:15:ARG:NH1  | 1.94                     | 0.82              |
| 14:L:126:LYS:H   | 14:L:126:LYS:CD  | 1.90                     | 0.82              |
| 13:K:54:ARG:NH1  | 13:K:54:ARG:HB3  | 1.94                     | 0.82              |
| 5:C:119:ARG:HG2  | 5:C:140:ARG:HH12 | 1.44                     | 0.82              |
| 15:M:65:LYS:HE3  | 15:M:69:GLU:HG2  | 1.62                     | 0.82              |
| 1:A:1305:G:HO2'  | 1:A:1306:A:H8    | 0.87                     | 0.82              |
| 9:G:54:THR:HG22  | 9:G:56:GLN:H     | 1.43                     | 0.82              |
| 7:E:79:GLU:HG3   | 7:E:93:PRO:HD2   | 1.62                     | 0.82              |
| 15:M:10:PRO:HB2  | 15:M:18:ALA:HB1  | 1.60                     | 0.81              |
| 4:B:71:VAL:HG23  | 4:B:164:VAL:HA   | 1.59                     | 0.81              |
| 16:N:57:ARG:HG2  | 16:N:58:LYS:H    | 1.43                     | 0.81              |
| 3:X:37:T6A:H153  | 3:X:38:A:H2      | 1.46                     | 0.81              |
| 1:A:371:G:O2'    | 1:A:372:C:H5'    | 1.80                     | 0.81              |
| 1:A:877:C:O2     | 10:H:3:THR:HG21  | 1.80                     | 0.81              |
| 7:E:51:VAL:HB    | 7:E:52:PRO:HD3   | 1.63                     | 0.81              |
| 4:B:124:SER:HB2  | 4:B:125:PRO:HD2  | 1.63                     | 0.80              |
| 12:J:90:LEU:H    | 12:J:91:PRO:CD   | 1.94                     | 0.80              |
| 4:B:102:LEU:HD21 | 4:B:162:ILE:HD11 | 1.63                     | 0.80              |
| 1:A:579:G:H5'    | 1:A:728:A:H1'    | 1.63                     | 0.80              |
| 1:A:216:G:H2'    | 1:A:217:C:C6     | 2.17                     | 0.80              |
| 11:I:46:ALA:HB2  | 11:I:74:ILE:HG23 | 1.62                     | 0.80              |
| 14:L:47:LYS:HB3  | 14:L:48:PRO:HD3  | 1.60                     | 0.80              |
| 1:A:1124:G:H3'   | 1:A:1145:C:N4    | 1.96                     | 0.80              |
| 1:A:250:A:H4'    | 1:A:251:G:O5'    | 1.79                     | 0.80              |
| 1:A:266:G:H5''   | 1:A:268:C:H41    | 1.46                     | 0.79              |
| 5:C:14:ILE:HG22  | 5:C:15:THR:H     | 1.45                     | 0.79              |
| 7:E:60:TYR:HE1   | 7:E:64:ARG:HH21  | 1.30                     | 0.79              |
| 15:M:3:ARG:HG2   | 15:M:9:ILE:HG13  | 1.64                     | 0.79              |
| 20:R:68:LYS:O    | 20:R:72:ARG:HG3  | 1.83                     | 0.79              |
| 7:E:41:VAL:HG22  | 7:E:113:ALA:HA   | 1.64                     | 0.79              |
| 4:B:12:GLU:OE2   | 4:B:213:LEU:HD11 | 1.82                     | 0.79              |
| 5:C:64:VAL:HB    | 5:C:99:VAL:HG21  | 1.65                     | 0.79              |
| 19:Q:101:ARG:HE  | 19:Q:101:ARG:HA  | 1.46                     | 0.79              |
| 17:O:17:ARG:HH11 | 17:O:17:ARG:HG3  | 1.48                     | 0.79              |
| 5:C:14:ILE:HG22  | 5:C:15:THR:N     | 1.98                     | 0.78              |
| 20:R:55:ARG:HB3  | 20:R:55:ARG:NH1  | 1.98                     | 0.78              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:C:77:ILE:HA    | 5:C:84:ILE:HB     | 1.65                     | 0.78              |
| 21:S:30:LEU:HD23 | 21:S:31:ILE:N     | 1.98                     | 0.78              |
| 1:A:1054:C:O2    | 1:A:1196:U:H2'    | 1.81                     | 0.78              |
| 4:B:17:PHE:HB3   | 4:B:44:LEU:HD21   | 1.63                     | 0.78              |
| 23:V:6:ARG:HG3   | 23:V:15:ARG:HH12  | 1.48                     | 0.78              |
| 11:I:70:LYS:O    | 11:I:74:ILE:HG13  | 1.82                     | 0.78              |
| 12:J:49:VAL:CG2  | 16:N:41:ARG:HB2   | 2.14                     | 0.78              |
| 19:Q:59:ILE:HG22 | 19:Q:71:PHE:CD1   | 2.18                     | 0.78              |
| 20:R:38:GLU:HA   | 20:R:41:LYS:HE2   | 1.63                     | 0.78              |
| 1:A:946:A:H2'    | 1:A:947:G:C8      | 2.19                     | 0.78              |
| 1:A:1148:U:H4'   | 11:I:14:VAL:HG11  | 1.64                     | 0.78              |
| 18:P:28:ARG:HG2  | 18:P:29:ASP:OD2   | 1.84                     | 0.78              |
| 1:A:975:A:H5'    | 1:A:975:A:H8      | 1.48                     | 0.77              |
| 14:L:75:HIS:CD2  | 14:L:77:LEU:H     | 2.03                     | 0.77              |
| 11:I:65:VAL:HG21 | 11:I:73:GLN:HB3   | 1.64                     | 0.77              |
| 6:D:151:LYS:H    | 6:D:151:LYS:HD2   | 1.46                     | 0.76              |
| 10:H:51:VAL:HG12 | 10:H:52:ASP:H     | 1.50                     | 0.76              |
| 22:T:36:LEU:HD12 | 22:T:62:LEU:HD12  | 1.65                     | 0.76              |
| 1:A:1367:C:H5'   | 12:J:60:ARG:NH1   | 2.01                     | 0.76              |
| 1:A:1151:A:HO2'  | 1:A:1152:A:H8     | 1.32                     | 0.76              |
| 14:L:57:LYS:HD3  | 14:L:67:THR:HG22  | 1.66                     | 0.76              |
| 15:M:63:THR:HG23 | 15:M:64:TRP:N     | 2.01                     | 0.76              |
| 19:Q:27:PHE:HB2  | 19:Q:28:PRO:HD2   | 1.67                     | 0.76              |
| 22:T:89:ARG:HG3  | 22:T:104:LEU:HD13 | 1.68                     | 0.76              |
| 5:C:91:LEU:HD23  | 5:C:92:ALA:N      | 2.01                     | 0.75              |
| 12:J:45:ARG:NH1  | 12:J:45:ARG:HB3   | 2.01                     | 0.75              |
| 11:I:6:GLY:N     | 11:I:84:ALA:HB2   | 2.01                     | 0.75              |
| 1:A:1016:A:H2'   | 1:A:1017:G:O4'    | 1.85                     | 0.75              |
| 1:A:328:C:O2     | 1:A:328:C:H2'     | 1.85                     | 0.75              |
| 7:E:105:VAL:HB   | 7:E:106:PRO:HD3   | 1.69                     | 0.75              |
| 15:M:49:THR:HB   | 15:M:52:GLU:HG3   | 1.68                     | 0.75              |
| 20:R:54:ARG:HD3  | 20:R:55:ARG:HG2   | 1.67                     | 0.75              |
| 1:A:1168:A:H2'   | 1:A:1169:A:C8     | 2.21                     | 0.74              |
| 22:T:57:ARG:NH1  | 22:T:102:GLY:HA3  | 2.02                     | 0.74              |
| 1:A:1281:U:H5'   | 1:A:1282:C:H5     | 1.50                     | 0.74              |
| 5:C:193:TYR:HE1  | 5:C:196:LEU:HD21  | 1.51                     | 0.74              |
| 5:C:64:VAL:HG12  | 5:C:65:ALA:H      | 1.52                     | 0.74              |
| 21:S:51:VAL:O    | 21:S:58:VAL:HG22  | 1.87                     | 0.74              |
| 1:A:1250:A:H4'   | 11:I:68:GLY:H     | 1.49                     | 0.74              |
| 8:F:10:LEU:HD12  | 8:F:59:TYR:HB3    | 1.69                     | 0.74              |
| 7:E:144:THR:HB   | 7:E:147:ASP:OD1   | 1.88                     | 0.74              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 10:H:9:MET:HG3   | 10:H:26:VAL:HG21  | 1.67                     | 0.74              |
| 18:P:67:THR:HG22 | 18:P:68:ASP:N     | 2.00                     | 0.74              |
| 8:F:101:ALA:HB2  | 20:R:28:GLU:HG3   | 1.67                     | 0.74              |
| 12:J:38:ILE:HB   | 12:J:71:LEU:CB    | 2.17                     | 0.74              |
| 1:A:1029:C:H2'   | 1:A:1030:C:O4'    | 1.87                     | 0.74              |
| 4:B:178:ARG:HG3  | 4:B:178:ARG:HH11  | 1.51                     | 0.74              |
| 18:P:20:VAL:HG11 | 18:P:32:TYR:CB    | 2.18                     | 0.74              |
| 4:B:15:VAL:HG11  | 4:B:209:ARG:HG3   | 1.68                     | 0.74              |
| 14:L:46:LYS:HD2  | 14:L:47:LYS:H     | 1.52                     | 0.74              |
| 1:A:1132:C:H2'   | 1:A:1133:G:H8     | 1.51                     | 0.73              |
| 5:C:64:VAL:HB    | 5:C:99:VAL:CG2    | 2.18                     | 0.73              |
| 4:B:218:ALA:O    | 4:B:222:ILE:HG13  | 1.87                     | 0.73              |
| 6:D:36:ARG:H     | 6:D:37:PRO:CD     | 2.01                     | 0.73              |
| 7:E:11:ILE:HB    | 7:E:31:LEU:HB3    | 1.70                     | 0.73              |
| 10:H:9:MET:SD    | 10:H:32:LYS:HG2   | 2.28                     | 0.73              |
| 3:X:37:T6A:H153  | 3:X:38:A:C2       | 2.24                     | 0.73              |
| 1:A:687:A:H4'    | 1:A:688:G:O5'     | 1.88                     | 0.73              |
| 4:B:114:ARG:NH1  | 4:B:118:LEU:HD21  | 2.03                     | 0.73              |
| 4:B:69:LEU:HD12  | 4:B:155:LEU:HD11  | 1.69                     | 0.73              |
| 21:S:33:THR:HG22 | 21:S:35:SER:N     | 2.00                     | 0.73              |
| 11:I:106:ALA:O   | 11:I:108:VAL:HG23 | 1.89                     | 0.73              |
| 12:J:49:VAL:HG23 | 16:N:41:ARG:HB2   | 1.70                     | 0.73              |
| 14:L:70:ILE:HD13 | 14:L:77:LEU:HD12  | 1.70                     | 0.73              |
| 10:H:121:ASP:HB2 | 10:H:125:ARG:HH21 | 1.53                     | 0.73              |
| 12:J:5:ARG:N     | 12:J:100:THR:HA   | 2.04                     | 0.73              |
| 21:S:15:LEU:HA   | 21:S:18:LYS:HB3   | 1.71                     | 0.73              |
| 1:A:969:A:H61    | 15:M:126:LYS:CB   | 2.01                     | 0.72              |
| 7:E:11:ILE:HG22  | 7:E:12:LEU:HD12   | 1.70                     | 0.72              |
| 4:B:143:GLU:O    | 4:B:147:LYS:HG3   | 1.88                     | 0.72              |
| 4:B:231:GLU:HB2  | 4:B:232:PRO:HD2   | 1.71                     | 0.72              |
| 1:A:1117:G:H4'   | 11:I:104:ARG:NH1  | 2.04                     | 0.72              |
| 1:A:1305:G:N2    | 1:A:1331:G:O2'    | 2.21                     | 0.72              |
| 1:A:1152:A:H5''  | 12:J:13:HIS:CD2   | 2.24                     | 0.72              |
| 11:I:97:LYS:HG2  | 11:I:102:LEU:HD12 | 1.70                     | 0.72              |
| 1:A:1238:A:H5'   | 1:A:1336:C:H41    | 1.53                     | 0.72              |
| 1:A:686:U:HO2'   | 1:A:687:A:H8      | 1.38                     | 0.72              |
| 8:F:86:ARG:O     | 8:F:87:ARG:HG2    | 1.89                     | 0.72              |
| 18:P:38:TYR:CE2  | 18:P:50:LYS:HD3   | 2.24                     | 0.72              |
| 1:A:344:A:H4'    | 1:A:345:C:OP2     | 1.89                     | 0.72              |
| 1:A:840:C:H5''   | 1:A:841:U:OP1     | 1.89                     | 0.72              |
| 11:I:118:LYS:O   | 11:I:119:ALA:HB3  | 1.89                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 12:J:38:ILE:HB   | 12:J:71:LEU:HB2  | 1.71                     | 0.72              |
| 1:A:1106:G:H5''  | 5:C:172:ARG:HG2  | 1.71                     | 0.71              |
| 4:B:8:LYS:CD     | 4:B:9:GLU:H      | 2.02                     | 0.71              |
| 13:K:54:ARG:HB3  | 13:K:54:ARG:HH11 | 1.52                     | 0.71              |
| 1:A:1417:G:H2'   | 1:A:1482:G:H22   | 1.55                     | 0.71              |
| 15:M:15:VAL:HG23 | 15:M:43:THR:O    | 1.90                     | 0.71              |
| 5:C:8:ILE:HG23   | 5:C:16:ARG:HG2   | 1.71                     | 0.71              |
| 6:D:119:GLN:HG2  | 6:D:123:HIS:CD2  | 2.25                     | 0.71              |
| 1:A:112:G:H4'    | 1:A:389:A:H5''   | 1.72                     | 0.71              |
| 15:M:49:THR:HG22 | 15:M:51:ALA:N    | 2.06                     | 0.71              |
| 1:A:1130:A:OP2   | 1:A:1131:G:H5''  | 1.91                     | 0.71              |
| 1:A:1241:G:H2'   | 1:A:1242:C:C6    | 2.26                     | 0.70              |
| 1:A:1497:G:O2'   | 1:A:1498:U:H5'   | 1.91                     | 0.70              |
| 1:A:518:C:HO2'   | 14:L:50:SER:HB3  | 1.56                     | 0.70              |
| 1:A:677:U:H3     | 1:A:713:G:H22    | 1.39                     | 0.70              |
| 5:C:123:GLN:NE2  | 5:C:140:ARG:HH22 | 1.89                     | 0.70              |
| 6:D:199:ASN:HD21 | 6:D:201:GLN:HB2  | 1.54                     | 0.70              |
| 15:M:54:VAL:O    | 15:M:58:GLU:HG2  | 1.90                     | 0.70              |
| 5:C:52:LEU:H     | 5:C:52:LEU:HD23  | 1.57                     | 0.70              |
| 6:D:110:PHE:HD1  | 6:D:162:LEU:HD21 | 1.56                     | 0.70              |
| 7:E:120:THR:HG23 | 7:E:121:LYS:N    | 2.05                     | 0.70              |
| 1:A:1489:G:H2'   | 1:A:1490:C:C5'   | 2.21                     | 0.70              |
| 14:L:89:ARG:NH2  | 14:L:97:ARG:HH11 | 1.89                     | 0.70              |
| 4:B:51:LEU:HD22  | 4:B:55:PHE:HE1   | 1.56                     | 0.70              |
| 4:B:18:GLY:H     | 4:B:41:ILE:HG23  | 1.56                     | 0.70              |
| 7:E:76:ILE:HG23  | 7:E:77:PRO:HD2   | 1.72                     | 0.70              |
| 1:A:1145:C:H5'   | 1:A:1146:A:OP1   | 1.91                     | 0.70              |
| 1:A:180:U:H2'    | 1:A:181:G:H5'    | 1.74                     | 0.70              |
| 20:R:17:SER:HB2  | 20:R:54:ARG:NH2  | 2.07                     | 0.70              |
| 1:A:818:G:O2'    | 1:A:819:A:H5''   | 1.92                     | 0.70              |
| 1:A:975:A:H5'    | 1:A:975:A:C8     | 2.25                     | 0.70              |
| 5:C:36:ASP:HB3   | 5:C:40:ARG:HH12  | 1.56                     | 0.70              |
| 7:E:57:LYS:HG2   | 7:E:61:TYR:CE2   | 2.26                     | 0.70              |
| 8:F:2:ARG:CZ     | 8:F:69:GLU:HG2   | 2.21                     | 0.70              |
| 21:S:17:GLU:HA   | 21:S:20:LEU:HG   | 1.74                     | 0.70              |
| 4:B:8:LYS:HD3    | 4:B:9:GLU:H      | 1.56                     | 0.70              |
| 1:A:1250:A:H4'   | 11:I:68:GLY:N    | 2.06                     | 0.70              |
| 7:E:76:ILE:HG22  | 7:E:78:HIS:H     | 1.55                     | 0.70              |
| 1:A:1064:G:H4'   | 1:A:1065:U:H5''  | 1.72                     | 0.70              |
| 4:B:71:VAL:CG2   | 4:B:164:VAL:HG23 | 2.21                     | 0.70              |
| 7:E:92:LYS:HB3   | 7:E:119:LEU:HB2  | 1.73                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 12:J:5:ARG:HA    | 12:J:73:ASP:OD1  | 1.91                     | 0.70              |
| 15:M:49:THR:HG22 | 15:M:51:ALA:H    | 1.57                     | 0.70              |
| 11:I:8:GLY:HA2   | 11:I:79:LEU:HD13 | 1.73                     | 0.69              |
| 21:S:17:GLU:O    | 21:S:21:GLU:HG3  | 1.92                     | 0.69              |
| 1:A:1356:G:H2'   | 1:A:1357:A:C8    | 2.27                     | 0.69              |
| 1:A:243:A:C4'    | 1:A:244:U:H5'    | 2.20                     | 0.69              |
| 4:B:97:TRP:HZ2   | 4:B:102:LEU:HD13 | 1.57                     | 0.69              |
| 1:A:524:G:H2'    | 1:A:525:C:C6     | 2.28                     | 0.69              |
| 4:B:98:LEU:O     | 4:B:101:MET:HG3  | 1.92                     | 0.69              |
| 5:C:70:VAL:HG12  | 5:C:71:ALA:N     | 2.07                     | 0.69              |
| 14:L:60:LEU:HD11 | 14:L:85:ILE:HD12 | 1.74                     | 0.69              |
| 1:A:1256:A:H5'   | 1:A:1258:G:H1'   | 1.74                     | 0.69              |
| 5:C:190:ARG:HG2  | 5:C:190:ARG:HH11 | 1.57                     | 0.69              |
| 1:A:518:C:O2'    | 14:L:50:SER:HB3  | 1.93                     | 0.69              |
| 6:D:146:ILE:HD12 | 6:D:146:ILE:N    | 2.06                     | 0.69              |
| 1:A:243:A:H4'    | 1:A:244:U:C5'    | 2.21                     | 0.69              |
| 5:C:15:THR:O     | 5:C:16:ARG:HB2   | 1.91                     | 0.69              |
| 11:I:111:ARG:HD3 | 11:I:112:LYS:N   | 2.07                     | 0.69              |
| 12:J:94:VAL:HG12 | 12:J:95:GLU:N    | 2.07                     | 0.69              |
| 4:B:231:GLU:HB2  | 4:B:232:PRO:CD   | 2.22                     | 0.69              |
| 5:C:178:LEU:O    | 5:C:179:ARG:HB3  | 1.93                     | 0.69              |
| 1:A:1435:G:H2'   | 1:A:1436:U:C6    | 2.27                     | 0.69              |
| 6:D:78:LEU:HD22  | 6:D:96:LEU:HB3   | 1.73                     | 0.69              |
| 14:L:41:ARG:HG2  | 14:L:42:THR:N    | 2.06                     | 0.69              |
| 14:L:59:ARG:HD3  | 14:L:65:GLU:HG3  | 1.72                     | 0.69              |
| 1:A:235:C:H5'    | 19:Q:70:ARG:HG2  | 1.73                     | 0.69              |
| 8:F:4:TYR:CE2    | 8:F:72:VAL:HG21  | 2.28                     | 0.69              |
| 18:P:26:ARG:HD3  | 18:P:31:LYS:H    | 1.58                     | 0.69              |
| 1:A:865:A:H5'    | 1:A:1078:U:O4    | 1.93                     | 0.69              |
| 5:C:2:GLY:C      | 5:C:3:ASN:HD22   | 1.95                     | 0.69              |
| 18:P:74:LEU:O    | 18:P:79:VAL:HG23 | 1.93                     | 0.69              |
| 15:M:9:ILE:N     | 15:M:9:ILE:HD12  | 2.07                     | 0.68              |
| 1:A:1072:G:H2'   | 1:A:1073:U:C6    | 2.28                     | 0.68              |
| 1:A:673:G:H2'    | 1:A:674:G:C8     | 2.28                     | 0.68              |
| 15:M:22:ILE:HD12 | 15:M:25:ILE:HD12 | 1.73                     | 0.68              |
| 1:A:1281:U:H5'   | 1:A:1282:C:C5    | 2.28                     | 0.68              |
| 1:A:972:C:H4'    | 12:J:57:LYS:CG   | 2.18                     | 0.68              |
| 13:K:126:ARG:O   | 13:K:127:LYS:HB2 | 1.94                     | 0.68              |
| 12:J:90:LEU:N    | 12:J:91:PRO:HD2  | 2.08                     | 0.68              |
| 1:A:382:A:H2'    | 1:A:383:A:C8     | 2.29                     | 0.68              |
| 13:K:77:MET:HE1  | 13:K:80:VAL:HG12 | 1.75                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1116:C:H2'   | 1:A:1117:G:H5''  | 1.74                     | 0.68              |
| 1:A:113:G:H1'    | 1:A:354:G:H5'    | 1.76                     | 0.68              |
| 5:C:23:TYR:CD2   | 5:C:24:ALA:N     | 2.61                     | 0.68              |
| 5:C:26:LYS:CD    | 5:C:26:LYS:H     | 2.05                     | 0.68              |
| 1:A:1195:C:H3'   | 1:A:1196:U:C5'   | 2.22                     | 0.68              |
| 14:L:47:LYS:CB   | 14:L:48:PRO:HD3  | 2.22                     | 0.68              |
| 1:A:1366:C:H2'   | 1:A:1367:C:H6    | 1.57                     | 0.68              |
| 17:O:24:SER:OG   | 17:O:27:VAL:HG23 | 1.93                     | 0.68              |
| 21:S:62:ILE:HD12 | 21:S:66:MET:HG3  | 1.76                     | 0.68              |
| 5:C:112:SER:HB3  | 5:C:115:LEU:HD12 | 1.76                     | 0.68              |
| 5:C:91:LEU:HD11  | 5:C:99:VAL:HG13  | 1.75                     | 0.68              |
| 1:A:1137:C:H4'   | 1:A:1138:G:C2    | 2.28                     | 0.68              |
| 1:A:1510:U:H2'   | 1:A:1511:G:C8    | 2.29                     | 0.68              |
| 4:B:142:LEU:HD23 | 4:B:142:LEU:O    | 1.94                     | 0.68              |
| 12:J:34:VAL:HG12 | 12:J:36:GLY:H    | 1.58                     | 0.68              |
| 5:C:110:ASN:ND2  | 5:C:140:ARG:HB3  | 2.08                     | 0.67              |
| 1:A:1121:U:H2'   | 1:A:1122:U:H6    | 1.59                     | 0.67              |
| 19:Q:67:LYS:HA   | 19:Q:70:ARG:HH12 | 1.58                     | 0.67              |
| 1:A:1182:G:O2'   | 1:A:1183:A:H5''  | 1.95                     | 0.67              |
| 1:A:1391:U:H2'   | 1:A:1392:G:C8    | 2.29                     | 0.67              |
| 11:I:8:GLY:HA3   | 11:I:79:LEU:HB3  | 1.75                     | 0.67              |
| 12:J:35:SER:HB2  | 12:J:72:VAL:O    | 1.94                     | 0.67              |
| 23:V:24:ARG:N    | 23:V:24:ARG:HD3  | 2.09                     | 0.67              |
| 1:A:353:A:H5'    | 1:A:353:A:C8     | 2.30                     | 0.67              |
| 18:P:28:ARG:HG2  | 18:P:28:ARG:NH1  | 2.04                     | 0.67              |
| 9:G:15:ASP:HB3   | 9:G:19:GLY:N     | 2.08                     | 0.67              |
| 1:A:1224:G:H1    | 1:A:1362:C:H42   | 1.42                     | 0.67              |
| 1:A:853:G:O2'    | 1:A:854:G:H5'    | 1.94                     | 0.67              |
| 4:B:116:GLU:HG2  | 4:B:153:ARG:NH2  | 2.09                     | 0.67              |
| 21:S:33:THR:HG22 | 21:S:34:TRP:H    | 1.58                     | 0.67              |
| 9:G:50:ILE:O     | 9:G:54:THR:HB    | 1.95                     | 0.67              |
| 11:I:48:GLU:N    | 11:I:49:PRO:HD2  | 2.10                     | 0.67              |
| 12:J:32:ALA:HB2  | 12:J:76:ASN:ND2  | 2.06                     | 0.67              |
| 13:K:47:VAL:O    | 13:K:47:VAL:HG12 | 1.94                     | 0.67              |
| 1:A:1132:C:H2'   | 1:A:1133:G:C8    | 2.29                     | 0.67              |
| 1:A:254:G:OP1    | 19:Q:67:LYS:O    | 2.11                     | 0.67              |
| 7:E:80:ILE:HD11  | 7:E:91:LEU:HD12  | 1.77                     | 0.67              |
| 9:G:146:GLU:HG2  | 9:G:149:ARG:HH21 | 1.60                     | 0.67              |
| 14:L:27:LEU:O    | 14:L:29:GLY:N    | 2.28                     | 0.67              |
| 1:A:1427:U:H2'   | 1:A:1428:A:H8    | 1.58                     | 0.66              |
| 16:N:29:ARG:HH11 | 16:N:29:ARG:HG2  | 1.60                     | 0.66              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:X:37:T6A:C8    | 3:X:37:T6A:H5'    | 2.28                     | 0.66              |
| 1:A:992:U:H4'    | 1:A:993:G:O5'     | 1.94                     | 0.66              |
| 12:J:4:ILE:O     | 12:J:73:ASP:HA    | 1.96                     | 0.66              |
| 21:S:50:ALA:HA   | 21:S:58:VAL:O     | 1.95                     | 0.66              |
| 1:A:1417:G:H2'   | 1:A:1482:G:N2     | 2.10                     | 0.66              |
| 1:A:538:G:H5''   | 14:L:114:LYS:HG3  | 1.76                     | 0.66              |
| 5:C:64:VAL:HB    | 5:C:99:VAL:CB     | 2.26                     | 0.66              |
| 1:A:1305:G:H5'   | 23:V:4:GLY:HA3    | 1.75                     | 0.66              |
| 4:B:118:LEU:HB3  | 4:B:142:LEU:HD12  | 1.77                     | 0.66              |
| 1:A:1196:U:H5''  | 1:A:1197:G:H5'    | 1.77                     | 0.66              |
| 1:A:1208:C:H2'   | 1:A:1209:C:H6     | 1.61                     | 0.66              |
| 1:A:190(L):U:O2' | 1:A:191:G:H5'     | 1.95                     | 0.66              |
| 11:I:47:LEU:C    | 11:I:49:PRO:HD2   | 2.15                     | 0.66              |
| 14:L:25:PRO:C    | 14:L:27:LEU:H     | 1.99                     | 0.66              |
| 1:A:1320:C:O2    | 21:S:72:GLY:HA3   | 1.96                     | 0.66              |
| 15:M:82:MET:HE3  | 15:M:92:HIS:HB3   | 1.77                     | 0.66              |
| 1:A:1502:A:H2    | 1:A:1505:G:N1     | 1.88                     | 0.66              |
| 1:A:969:A:H61    | 15:M:126:LYS:HB2  | 1.60                     | 0.66              |
| 6:D:110:PHE:CD1  | 6:D:162:LEU:HD21  | 2.31                     | 0.66              |
| 6:D:151:LYS:N    | 6:D:151:LYS:HD2   | 2.11                     | 0.66              |
| 19:Q:101:ARG:NE  | 19:Q:101:ARG:HA   | 2.11                     | 0.66              |
| 1:A:216:G:H2'    | 1:A:217:C:H6      | 1.60                     | 0.65              |
| 1:A:835:U:OP1    | 20:R:64:ARG:NH2   | 2.27                     | 0.65              |
| 1:A:954:G:H2'    | 1:A:955:U:C6      | 2.31                     | 0.65              |
| 4:B:101:MET:HA   | 4:B:108:ILE:HD12  | 1.78                     | 0.65              |
| 5:C:191:THR:HB   | 5:C:194:GLY:O     | 1.96                     | 0.65              |
| 6:D:131:ARG:H    | 6:D:131:ARG:HD2   | 1.61                     | 0.65              |
| 6:D:162:LEU:HD12 | 6:D:181:MET:CE    | 2.26                     | 0.65              |
| 6:D:8:VAL:HG13   | 6:D:21:LEU:HD13   | 1.78                     | 0.65              |
| 1:A:1038:C:H2'   | 1:A:1039:C:C6     | 2.32                     | 0.65              |
| 1:A:112:G:H21    | 1:A:354:G:H5'     | 1.61                     | 0.65              |
| 1:A:19:C:H2'     | 1:A:20:U:H6       | 1.61                     | 0.65              |
| 13:K:80:VAL:HG13 | 13:K:103:LEU:HD21 | 1.77                     | 0.65              |
| 1:A:314:C:O2'    | 1:A:315:A:H5'     | 1.96                     | 0.65              |
| 5:C:77:ILE:HD13  | 5:C:84:ILE:HD12   | 1.79                     | 0.65              |
| 6:D:25:ARG:C     | 6:D:27:TYR:H      | 2.00                     | 0.65              |
| 1:A:1343:G:H2'   | 1:A:1344:C:C6     | 2.32                     | 0.65              |
| 20:R:86:VAL:O    | 20:R:87:ARG:HB2   | 1.96                     | 0.65              |
| 5:C:10:PHE:CE2   | 5:C:178:LEU:HD13  | 2.32                     | 0.65              |
| 1:A:738:C:P      | 8:F:92:LYS:HE3    | 2.36                     | 0.65              |
| 21:S:33:THR:HG22 | 21:S:34:TRP:N     | 2.11                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1251:A:H2'   | 1:A:1252:A:C8    | 2.31                     | 0.65              |
| 11:I:44:VAL:HG12 | 11:I:51:ARG:HH12 | 1.60                     | 0.65              |
| 15:M:50:GLU:O    | 15:M:54:VAL:HG23 | 1.96                     | 0.65              |
| 21:S:28:LYS:HG2  | 21:S:29:ARG:N    | 2.04                     | 0.65              |
| 1:A:1320:C:N3    | 21:S:36:ARG:HG3  | 2.12                     | 0.65              |
| 1:A:1086:U:H3    | 1:A:1099:G:H22   | 1.44                     | 0.65              |
| 1:A:115:G:H1'    | 1:A:116:A:N7     | 2.11                     | 0.65              |
| 1:A:1201:A:H4'   | 1:A:1202:G:O5'   | 1.97                     | 0.65              |
| 4:B:197:VAL:HB   | 4:B:200:ILE:HG12 | 1.77                     | 0.65              |
| 9:G:38:LEU:HA    | 9:G:41:ARG:HG3   | 1.78                     | 0.65              |
| 1:A:1223:C:P     | 21:S:78:ARG:NH1  | 2.69                     | 0.65              |
| 1:A:1392:G:H21   | 1:A:1502:A:H8    | 1.45                     | 0.65              |
| 1:A:1368:G:O2'   | 1:A:1369:C:H5'   | 1.97                     | 0.64              |
| 8:F:21:LEU:O     | 8:F:24:GLU:HB3   | 1.97                     | 0.64              |
| 15:M:65:LYS:CE   | 15:M:69:GLU:HG2  | 2.26                     | 0.64              |
| 17:O:70:LEU:HD12 | 17:O:78:TYR:HB2  | 1.78                     | 0.64              |
| 1:A:1053:G:C4'   | 1:A:1054:C:H5'   | 2.27                     | 0.64              |
| 1:A:1427:U:H2'   | 1:A:1428:A:C8    | 2.32                     | 0.64              |
| 6:D:8:VAL:HG21   | 6:D:115:ARG:CZ   | 2.27                     | 0.64              |
| 9:G:70:LYS:HB3   | 9:G:96:GLN:HG2   | 1.78                     | 0.64              |
| 4:B:12:GLU:C     | 4:B:14:GLY:H     | 1.98                     | 0.64              |
| 1:A:1116:C:C2'   | 1:A:1117:G:H5''  | 2.26                     | 0.64              |
| 1:A:1355:G:H2'   | 1:A:1356:G:C8    | 2.33                     | 0.64              |
| 1:A:518:C:H5''   | 1:A:519:C:C6     | 2.32                     | 0.64              |
| 1:A:714:G:H2'    | 1:A:715:A:C8     | 2.32                     | 0.64              |
| 1:A:1367:C:H5'   | 12:J:60:ARG:HH12 | 1.63                     | 0.64              |
| 1:A:686:U:O2'    | 1:A:687:A:H8     | 1.78                     | 0.64              |
| 4:B:28:PHE:CD2   | 4:B:190:THR:HA   | 2.33                     | 0.64              |
| 1:A:1366:C:H2'   | 1:A:1367:C:C6    | 2.32                     | 0.64              |
| 14:L:89:ARG:HG2  | 14:L:97:ARG:HA   | 1.80                     | 0.64              |
| 20:R:36:ASN:HD21 | 20:R:38:GLU:HG2  | 1.62                     | 0.64              |
| 1:A:1117:G:H5'   | 1:A:1117:G:H8    | 1.63                     | 0.64              |
| 1:A:1286:A:H2'   | 1:A:1287:A:H4'   | 1.79                     | 0.64              |
| 14:L:126:LYS:HD2 | 14:L:126:LYS:H   | 1.62                     | 0.64              |
| 15:M:62:ASN:O    | 15:M:63:THR:HB   | 1.98                     | 0.64              |
| 16:N:9:LYS:HD3   | 16:N:9:LYS:C     | 2.17                     | 0.64              |
| 17:O:16:ALA:HB1  | 17:O:21:ASP:HB3  | 1.80                     | 0.64              |
| 1:A:939:G:H2'    | 1:A:940:C:C6     | 2.33                     | 0.64              |
| 4:B:91:PRO:HG3   | 4:B:154:LEU:HB2  | 1.79                     | 0.64              |
| 4:B:71:VAL:O     | 4:B:165:VAL:HG23 | 1.98                     | 0.64              |
| 5:C:154:SER:OG   | 5:C:155:GLY:N    | 2.28                     | 0.64              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1228:C:H4'   | 15:M:116:THR:HA   | 1.79                     | 0.64              |
| 1:A:166:G:O2'    | 1:A:167:G:H5'     | 1.97                     | 0.64              |
| 1:A:1305:G:C5'   | 23:V:4:GLY:HA3    | 2.27                     | 0.64              |
| 4:B:98:LEU:N     | 4:B:98:LEU:HD23   | 2.13                     | 0.64              |
| 5:C:188:LEU:CD1  | 5:C:189:ALA:H     | 2.10                     | 0.64              |
| 1:A:912:C:O2'    | 1:A:913:A:H5'     | 1.98                     | 0.63              |
| 1:A:1117:G:H4'   | 11:I:104:ARG:HH11 | 1.62                     | 0.63              |
| 12:J:4:ILE:HA    | 12:J:100:THR:HA   | 1.78                     | 0.63              |
| 14:L:47:LYS:CB   | 14:L:48:PRO:CD    | 2.73                     | 0.63              |
| 6:D:76:ARG:HH11  | 6:D:76:ARG:HG2    | 1.64                     | 0.63              |
| 21:S:5:LEU:O     | 21:S:6:LYS:HB2    | 1.98                     | 0.63              |
| 1:A:35:G:H2'     | 1:A:36:C:C6       | 2.33                     | 0.63              |
| 1:A:382:A:H2'    | 1:A:383:A:H8      | 1.64                     | 0.63              |
| 1:A:975:A:O5'    | 1:A:976:G:H5'     | 1.98                     | 0.63              |
| 5:C:108:ASN:HD22 | 5:C:111:LEU:HG    | 1.64                     | 0.63              |
| 6:D:30:LYS:C     | 6:D:32:ALA:H      | 2.00                     | 0.63              |
| 1:A:1187:G:OP1   | 11:I:113:LYS:HE2  | 1.98                     | 0.63              |
| 22:T:51:GLU:HA   | 22:T:54:LYS:HD2   | 1.81                     | 0.63              |
| 1:A:1285:A:H4'   | 1:A:1286:A:O5'    | 1.98                     | 0.63              |
| 1:A:1347:G:N2    | 1:A:1373:G:H2'    | 2.14                     | 0.63              |
| 1:A:1355:G:H2'   | 1:A:1356:G:H8     | 1.63                     | 0.63              |
| 8:F:80:ARG:NH1   | 8:F:88:VAL:HB     | 2.13                     | 0.63              |
| 7:E:144:THR:HG22 | 7:E:146:ALA:H     | 1.63                     | 0.63              |
| 7:E:78:HIS:HD2   | 10:H:107:LEU:HD12 | 1.61                     | 0.63              |
| 10:H:29:SER:OG   | 10:H:32:LYS:HB2   | 1.99                     | 0.63              |
| 1:A:1490:C:C5'   | 1:A:1490:C:H6     | 2.03                     | 0.63              |
| 9:G:99:LEU:HD22  | 9:G:103:TRP:CZ2   | 2.34                     | 0.63              |
| 1:A:949:A:H62    | 15:M:106:ASN:HD21 | 1.47                     | 0.63              |
| 1:A:1189:C:P     | 12:J:51:ARG:HH22  | 2.21                     | 0.63              |
| 1:A:838:G:H2'    | 1:A:839:U:H5''    | 1.81                     | 0.63              |
| 1:A:1053:G:C3'   | 1:A:1054:C:H5'    | 2.28                     | 0.63              |
| 1:A:266:G:C8     | 1:A:266:G:H5'     | 2.34                     | 0.63              |
| 1:A:662:G:H2'    | 1:A:663:A:C8      | 2.33                     | 0.63              |
| 12:J:84:GLN:O    | 12:J:88:LEU:HD12  | 1.98                     | 0.63              |
| 14:L:24:VAL:HG13 | 14:L:98:TYR:HE2   | 1.62                     | 0.63              |
| 5:C:155:GLY:CA   | 5:C:164:ARG:H     | 2.12                     | 0.62              |
| 20:R:36:ASN:ND2  | 20:R:38:GLU:HG2   | 2.14                     | 0.62              |
| 6:D:199:ASN:C    | 6:D:199:ASN:HD22  | 2.02                     | 0.62              |
| 6:D:28:SER:O     | 6:D:30:LYS:N      | 2.32                     | 0.62              |
| 11:I:44:VAL:HG12 | 11:I:51:ARG:NH1   | 2.14                     | 0.62              |
| 11:I:92:TYR:O    | 11:I:96:LEU:HD13  | 1.99                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1015:A:H2'   | 1:A:1016:A:C8    | 2.34                     | 0.62              |
| 5:C:191:THR:HG21 | 5:C:193:TYR:CE1  | 2.33                     | 0.62              |
| 7:E:110:LEU:HD13 | 7:E:118:ILE:HD13 | 1.81                     | 0.62              |
| 12:J:5:ARG:HD2   | 12:J:99:LYS:HB2  | 1.80                     | 0.62              |
| 18:P:11:SER:OG   | 18:P:14:ASN:HB3  | 1.99                     | 0.62              |
| 19:Q:68:ARG:N    | 19:Q:70:ARG:NH1  | 2.48                     | 0.62              |
| 3:X:36:U:H2'     | 3:X:37:T6A:H5''  | 1.81                     | 0.62              |
| 5:C:191:THR:HG22 | 5:C:192:THR:N    | 2.14                     | 0.62              |
| 7:E:15:ARG:O     | 7:E:16:THR:O     | 2.18                     | 0.62              |
| 17:O:25:THR:HG21 | 17:O:70:LEU:HD23 | 1.81                     | 0.62              |
| 1:A:1351:U:O2'   | 1:A:1352:C:H5'   | 2.00                     | 0.62              |
| 1:A:781:A:H2'    | 1:A:782:A:H5'    | 1.82                     | 0.62              |
| 14:L:27:LEU:C    | 14:L:29:GLY:H    | 2.02                     | 0.62              |
| 22:T:45:GLN:O    | 22:T:45:GLN:HG2  | 1.99                     | 0.62              |
| 1:A:1291:G:H4'   | 11:I:38:GLN:O    | 2.00                     | 0.62              |
| 4:B:95:GLN:O     | 4:B:96:ARG:HD2   | 1.99                     | 0.62              |
| 5:C:119:ARG:CG   | 5:C:140:ARG:HH12 | 2.13                     | 0.62              |
| 5:C:148:GLY:HA3  | 5:C:172:ARG:O    | 1.99                     | 0.62              |
| 7:E:96:PRO:HA    | 7:E:117:ASP:OD2  | 1.99                     | 0.62              |
| 21:S:55:LYS:HG2  | 21:S:56:GLN:NE2  | 2.04                     | 0.62              |
| 1:A:419:C:C6     | 1:A:425:G:N2     | 2.68                     | 0.62              |
| 7:E:36:ASP:OD2   | 7:E:40:ARG:HB2   | 2.00                     | 0.62              |
| 13:K:14:VAL:HG21 | 13:K:40:ILE:HD11 | 1.81                     | 0.62              |
| 13:K:57:THR:HG23 | 13:K:60:ALA:H    | 1.65                     | 0.62              |
| 14:L:55:VAL:HG12 | 14:L:56:ALA:N    | 2.14                     | 0.62              |
| 17:O:56:LEU:HA   | 17:O:59:MET:HE2  | 1.82                     | 0.62              |
| 22:T:10:LEU:O    | 22:T:13:LEU:HD12 | 2.00                     | 0.62              |
| 3:X:36:U:C2'     | 3:X:37:T6A:H5''  | 2.29                     | 0.62              |
| 1:A:1057:G:O2'   | 1:A:1058:G:H5'   | 1.99                     | 0.61              |
| 1:A:109:A:H2'    | 1:A:326:G:N2     | 2.15                     | 0.61              |
| 5:C:118:GLN:O    | 5:C:122:GLU:HG3  | 2.00                     | 0.61              |
| 1:A:1195:C:H3'   | 1:A:1196:U:H5'   | 1.80                     | 0.61              |
| 13:K:54:ARG:CB   | 13:K:54:ARG:HH11 | 2.12                     | 0.61              |
| 19:Q:68:ARG:H    | 19:Q:70:ARG:NH1  | 1.98                     | 0.61              |
| 1:A:474:G:H5''   | 18:P:81:ARG:NH1  | 2.15                     | 0.61              |
| 6:D:162:LEU:HD12 | 6:D:181:MET:HE1  | 1.82                     | 0.61              |
| 20:R:53:ARG:HH11 | 20:R:59:SER:HA   | 1.64                     | 0.61              |
| 4:B:178:ARG:NH1  | 4:B:178:ARG:HG3  | 2.10                     | 0.61              |
| 5:C:60:ALA:O     | 5:C:61:ALA:HB2   | 2.00                     | 0.61              |
| 5:C:70:VAL:HG12  | 5:C:71:ALA:H     | 1.63                     | 0.61              |
| 7:E:80:ILE:HG13  | 7:E:91:LEU:HB2   | 1.82                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1161:C:H2'   | 1:A:1162:C:H6    | 1.64                     | 0.61              |
| 6:D:127:THR:CG2  | 6:D:147:ALA:HB3  | 2.29                     | 0.61              |
| 6:D:35:ARG:O     | 6:D:36:ARG:HB2   | 1.99                     | 0.61              |
| 21:S:43:GLU:CD   | 21:S:43:GLU:H    | 2.04                     | 0.61              |
| 22:T:89:ARG:HH22 | 22:T:106:ALA:HA  | 1.66                     | 0.61              |
| 1:A:918:A:H2'    | 1:A:919:A:C8     | 2.35                     | 0.61              |
| 6:D:151:LYS:H    | 6:D:151:LYS:CD   | 2.13                     | 0.61              |
| 7:E:41:VAL:HG21  | 7:E:113:ALA:HB2  | 1.81                     | 0.61              |
| 12:J:12:ASP:HB3  | 12:J:15:THR:HG22 | 1.81                     | 0.61              |
| 8:F:100:ASN:HA   | 20:R:23:LYS:HE2  | 1.82                     | 0.61              |
| 15:M:63:THR:HG23 | 15:M:64:TRP:H    | 1.65                     | 0.61              |
| 1:A:376:G:OP2    | 18:P:67:THR:HG21 | 2.00                     | 0.61              |
| 1:A:299:G:H2'    | 1:A:300:A:C8     | 2.35                     | 0.61              |
| 7:E:18:ARG:HH21  | 7:E:25:ARG:HB3   | 1.64                     | 0.61              |
| 4:B:139:LYS:O    | 4:B:143:GLU:HG2  | 2.00                     | 0.61              |
| 5:C:190:ARG:NH1  | 5:C:190:ARG:HG2  | 2.15                     | 0.61              |
| 4:B:69:LEU:HD23  | 4:B:70:PHE:N     | 2.16                     | 0.61              |
| 5:C:91:LEU:HD21  | 5:C:99:VAL:CG1   | 2.31                     | 0.61              |
| 18:P:34:GLU:OE2  | 18:P:55:ARG:HD3  | 2.01                     | 0.61              |
| 1:A:1061:G:O2'   | 1:A:1062:U:H5'   | 2.00                     | 0.60              |
| 1:A:666:G:H5'    | 1:A:726:C:H1'    | 1.83                     | 0.60              |
| 4:B:79:ASP:HB3   | 4:B:238:LEU:HD13 | 1.81                     | 0.60              |
| 18:P:67:THR:CG2  | 18:P:68:ASP:N    | 2.63                     | 0.60              |
| 3:X:36:U:H2'     | 3:X:37:T6A:C5'   | 2.31                     | 0.60              |
| 1:A:1443:G:H5''  | 1:A:1446:A:H5'   | 1.82                     | 0.60              |
| 1:A:371:G:C2'    | 1:A:372:C:H5'    | 2.31                     | 0.60              |
| 4:B:51:LEU:HD22  | 4:B:55:PHE:CE1   | 2.35                     | 0.60              |
| 7:E:5:ASP:CG     | 7:E:6:PHE:H      | 2.04                     | 0.60              |
| 1:A:1005:A:H5'   | 1:A:1038:C:H1'   | 1.83                     | 0.60              |
| 6:D:8:VAL:HG21   | 6:D:115:ARG:NH1  | 2.17                     | 0.60              |
| 14:L:110:VAL:H   | 14:L:122:THR:CG2 | 2.13                     | 0.60              |
| 15:M:5:ALA:HB3   | 15:M:8:GLU:HG3   | 1.83                     | 0.60              |
| 22:T:39:LYS:HD2  | 22:T:55:ILE:CD1  | 2.28                     | 0.60              |
| 4:B:23:ARG:HH11  | 4:B:24:TRP:HA    | 1.66                     | 0.60              |
| 11:I:36:TYR:HD2  | 11:I:37:PHE:CE2  | 2.20                     | 0.60              |
| 14:L:89:ARG:CZ   | 14:L:97:ARG:HD2  | 2.32                     | 0.60              |
| 1:A:1068:G:H8    | 1:A:1068:G:OP2   | 1.83                     | 0.60              |
| 4:B:144:ARG:HA   | 4:B:147:LYS:HD2  | 1.84                     | 0.60              |
| 4:B:164:VAL:HG12 | 4:B:186:ALA:HB2  | 1.84                     | 0.60              |
| 5:C:10:PHE:CZ    | 5:C:178:LEU:HD13 | 2.37                     | 0.60              |
| 5:C:26:LYS:N     | 5:C:26:LYS:HD3   | 2.08                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:C:35:GLU:CD    | 5:C:59:ARG:HH22  | 2.05                     | 0.60              |
| 6:D:7:PRO:HB2    | 6:D:10:ARG:HD2   | 1.83                     | 0.60              |
| 9:G:155:ARG:O    | 9:G:156:TRP:HB3  | 2.02                     | 0.60              |
| 10:H:6:ILE:O     | 10:H:10:LEU:HG   | 2.01                     | 0.60              |
| 22:T:67:ALA:HB2  | 22:T:77:ALA:HB2  | 1.83                     | 0.60              |
| 1:A:1425:U:H2'   | 1:A:1426:C:C6    | 2.37                     | 0.60              |
| 1:A:448:A:OP2    | 1:A:485:G:N2     | 2.35                     | 0.60              |
| 6:D:50:ARG:HD2   | 6:D:51:PRO:O     | 2.02                     | 0.60              |
| 15:M:78:ILE:HA   | 15:M:81:LEU:CD2  | 2.31                     | 0.60              |
| 1:A:748:C:O2'    | 1:A:749:C:C6     | 2.55                     | 0.60              |
| 9:G:113:GLU:HG2  | 9:G:119:ARG:HG2  | 1.83                     | 0.60              |
| 9:G:144:MET:O    | 9:G:147:ALA:HB3  | 2.02                     | 0.60              |
| 12:J:42:THR:HG23 | 12:J:67:THR:O    | 2.00                     | 0.60              |
| 13:K:101:SER:C   | 13:K:103:LEU:H   | 2.04                     | 0.60              |
| 14:L:60:LEU:N    | 14:L:64:TYR:O    | 2.34                     | 0.60              |
| 1:A:1178:G:N2    | 1:A:1180:A:H3'   | 2.17                     | 0.60              |
| 1:A:975:A:H4'    | 1:A:976:G:H5'    | 1.84                     | 0.60              |
| 5:C:119:ARG:HG2  | 5:C:140:ARG:NH1  | 2.15                     | 0.60              |
| 8:F:10:LEU:CD1   | 8:F:59:TYR:HB3   | 2.31                     | 0.60              |
| 12:J:49:VAL:HG22 | 16:N:41:ARG:HD2  | 1.84                     | 0.60              |
| 1:A:1225:A:N3    | 1:A:1225:A:H2'   | 2.17                     | 0.60              |
| 1:A:397:A:H5'    | 1:A:398:C:OP1    | 2.01                     | 0.60              |
| 1:A:580:U:H2'    | 1:A:581:G:O4'    | 2.02                     | 0.60              |
| 1:A:839:U:O2     | 1:A:839:U:H2'    | 2.00                     | 0.60              |
| 9:G:22:LEU:HG    | 9:G:62:PHE:HE2   | 1.67                     | 0.60              |
| 9:G:3:ARG:HG3    | 9:G:3:ARG:HH11   | 1.66                     | 0.60              |
| 1:A:112:G:N2     | 1:A:354:G:H5'    | 2.17                     | 0.59              |
| 5:C:43:LEU:HD22  | 5:C:68:VAL:HG21  | 1.84                     | 0.59              |
| 9:G:139:GLU:O    | 9:G:143:ARG:HG3  | 2.01                     | 0.59              |
| 14:L:85:ILE:HG23 | 14:L:98:TYR:HB3  | 1.84                     | 0.59              |
| 12:J:14:LYS:C    | 12:J:16:LEU:H    | 2.06                     | 0.59              |
| 1:A:1124:G:H4'   | 12:J:38:ILE:HG12 | 1.83                     | 0.59              |
| 1:A:1133:G:H2'   | 1:A:1134:G:H8    | 1.66                     | 0.59              |
| 1:A:1497:G:C2'   | 1:A:1498:U:H5'   | 2.32                     | 0.59              |
| 1:A:130:A:OP2    | 1:A:190(E):U:H2' | 2.01                     | 0.59              |
| 1:A:478:A:O2'    | 1:A:479:C:H5'    | 2.02                     | 0.59              |
| 1:A:948:C:O2'    | 1:A:949:A:H5'    | 2.03                     | 0.59              |
| 1:A:1115:C:H2'   | 1:A:1116:C:H6    | 1.67                     | 0.59              |
| 1:A:986:A:H1'    | 21:S:54:GLY:O    | 2.01                     | 0.59              |
| 11:I:5:TYR:HA    | 11:I:17:VAL:O    | 2.01                     | 0.59              |
| 1:A:1320:C:OP1   | 21:S:70:LYS:HE3  | 2.02                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:C:155:GLY:HA3  | 5:C:164:ARG:H    | 1.68                     | 0.59              |
| 1:A:620:C:N1     | 6:D:135:LEU:HD13 | 2.17                     | 0.59              |
| 12:J:71:LEU:O    | 12:J:72:VAL:HB   | 2.03                     | 0.59              |
| 18:P:20:VAL:CG1  | 18:P:32:TYR:HB2  | 2.32                     | 0.59              |
| 1:A:1347:G:O2'   | 1:A:1348:U:P     | 2.60                     | 0.59              |
| 1:A:975:A:H4'    | 1:A:976:G:C5'    | 2.32                     | 0.59              |
| 1:A:975:A:H4'    | 1:A:976:G:O5'    | 2.03                     | 0.59              |
| 7:E:144:THR:HG22 | 7:E:146:ALA:N    | 2.18                     | 0.59              |
| 10:H:55:GLY:O    | 10:H:56:LYS:HD2  | 2.02                     | 0.59              |
| 1:A:130:A:C8     | 19:Q:63:ARG:HG3  | 2.38                     | 0.59              |
| 1:A:1369:C:H2'   | 1:A:1370:G:C8    | 2.37                     | 0.59              |
| 1:A:627:G:O2'    | 1:A:628:G:H5'    | 2.02                     | 0.59              |
| 1:A:1206:G:H4'   | 5:C:192:THR:O    | 2.03                     | 0.59              |
| 18:P:21:VAL:HG21 | 18:P:59:TRP:CD1  | 2.38                     | 0.59              |
| 4:B:209:ARG:HE   | 4:B:239:VAL:HG11 | 1.67                     | 0.59              |
| 4:B:219:VAL:O    | 4:B:223:ILE:HG13 | 2.03                     | 0.59              |
| 4:B:80:ILE:HD13  | 4:B:212:GLN:HB2  | 1.84                     | 0.59              |
| 6:D:19:LEU:HD22  | 6:D:67:ILE:HG12  | 1.84                     | 0.59              |
| 5:C:34:LEU:HD23  | 5:C:34:LEU:C     | 2.24                     | 0.59              |
| 6:D:63:LYS:HD2   | 6:D:198:VAL:HG22 | 1.84                     | 0.59              |
| 7:E:79:GLU:HG3   | 7:E:93:PRO:CD    | 2.32                     | 0.59              |
| 1:A:190(L):U:O2  | 22:T:105:SER:HB2 | 2.03                     | 0.59              |
| 1:A:1247:U:O2'   | 1:A:1248:A:H5'   | 2.02                     | 0.59              |
| 1:A:991:U:O2'    | 1:A:992:U:H5'    | 2.02                     | 0.59              |
| 4:B:141:GLU:O    | 4:B:145:LEU:HG   | 2.02                     | 0.59              |
| 4:B:7:VAL:HG11   | 4:B:221:LEU:HD23 | 1.84                     | 0.59              |
| 10:H:119:LEU:HB2 | 10:H:123:GLU:HB2 | 1.83                     | 0.59              |
| 4:B:88:ALA:HB1   | 4:B:90:MET:HG2   | 1.85                     | 0.58              |
| 7:E:24:ARG:HH11  | 7:E:24:ARG:HG2   | 1.68                     | 0.58              |
| 14:L:27:LEU:C    | 14:L:29:GLY:N    | 2.53                     | 0.58              |
| 15:M:37:THR:HG22 | 15:M:39:ILE:HG13 | 1.85                     | 0.58              |
| 15:M:63:THR:CG2  | 15:M:64:TRP:N    | 2.66                     | 0.58              |
| 23:V:3:LYS:HB3   | 23:V:14:TRP:CG   | 2.38                     | 0.58              |
| 21:S:20:LEU:HD12 | 21:S:21:GLU:N    | 2.18                     | 0.58              |
| 21:S:3:ARG:HH22  | 21:S:69:HIS:HE1  | 1.51                     | 0.58              |
| 1:A:357:G:O2'    | 1:A:358:U:H5'    | 2.03                     | 0.58              |
| 4:B:97:TRP:CZ2   | 4:B:101:MET:HB2  | 2.38                     | 0.58              |
| 5:C:155:GLY:O    | 5:C:156:ARG:HB2  | 2.02                     | 0.58              |
| 10:H:103:VAL:CG2 | 10:H:110:ALA:HB2 | 2.33                     | 0.58              |
| 1:A:523:A:H61    | 14:L:92:ASP:HB2  | 1.67                     | 0.58              |
| 1:A:760:G:H1     | 19:Q:105:ALA:HA  | 1.67                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:R:46:GLU:CD    | 20:R:46:GLU:H     | 2.07                     | 0.58              |
| 1:A:501:C:H2'     | 1:A:502:G:H8      | 1.67                     | 0.58              |
| 1:A:977:A:H2'     | 1:A:978:A:H5''    | 1.86                     | 0.58              |
| 23:V:24:ARG:HD3   | 23:V:24:ARG:H     | 1.69                     | 0.58              |
| 5:C:108:ASN:ND2   | 5:C:111:LEU:HG    | 2.19                     | 0.58              |
| 1:A:1201:A:O2'    | 1:A:1202:G:OP2    | 2.22                     | 0.58              |
| 1:A:135:C:O2      | 18:P:1:MET:HB2    | 2.03                     | 0.58              |
| 1:A:1397:C:H4'    | 1:A:1398:A:OP2    | 2.04                     | 0.58              |
| 1:A:129(A):G:O2'  | 1:A:190(E):U:H2'  | 2.03                     | 0.58              |
| 1:A:352:C:H4'     | 1:A:354:G:OP1     | 2.04                     | 0.58              |
| 4:B:188:ALA:HB1   | 4:B:192:SER:OG    | 2.03                     | 0.58              |
| 4:B:71:VAL:HG23   | 4:B:164:VAL:CA    | 2.32                     | 0.58              |
| 5:C:107:GLN:O     | 5:C:108:ASN:HB3   | 2.03                     | 0.58              |
| 12:J:82:ILE:O     | 12:J:86:MET:HB2   | 2.03                     | 0.58              |
| 20:R:37:VAL:O     | 20:R:41:LYS:HG3   | 2.03                     | 0.58              |
| 1:A:1095:U:H2'    | 1:A:1096:C:C6     | 2.38                     | 0.58              |
| 1:A:1148:U:H2'    | 1:A:1149:C:O4'    | 2.04                     | 0.58              |
| 1:A:353:A:H5'     | 1:A:353:A:H8      | 1.69                     | 0.58              |
| 22:T:73:HIS:O     | 22:T:74:LYS:HB2   | 2.02                     | 0.58              |
| 1:A:1420:C:H2'    | 1:A:1421:G:H8     | 1.68                     | 0.58              |
| 1:A:959:A:H3'     | 1:A:960:U:H5''    | 1.85                     | 0.58              |
| 9:G:38:LEU:HD12   | 9:G:38:LEU:C      | 2.24                     | 0.58              |
| 10:H:112:LEU:HD23 | 10:H:112:LEU:N    | 2.19                     | 0.58              |
| 1:A:706:A:O2'     | 13:K:29:ILE:HD11  | 2.03                     | 0.58              |
| 4:B:84:GLU:HB3    | 4:B:219:VAL:CG2   | 2.23                     | 0.58              |
| 1:A:1057:G:H5''   | 5:C:154:SER:CB    | 2.34                     | 0.58              |
| 5:C:22:TRP:CG     | 5:C:59:ARG:HD2    | 2.39                     | 0.58              |
| 4:B:17:PHE:CD1    | 4:B:18:GLY:N      | 2.72                     | 0.58              |
| 9:G:37:ASN:HD21   | 11:I:41:VAL:HG23  | 1.69                     | 0.58              |
| 13:K:84:VAL:HG23  | 13:K:110:ASP:CA   | 2.29                     | 0.58              |
| 15:M:5:ALA:HB2    | 15:M:22:ILE:HD13  | 1.85                     | 0.58              |
| 22:T:50:GLU:HG3   | 22:T:100:ILE:HG13 | 1.84                     | 0.58              |
| 1:A:1121:U:H2'    | 1:A:1122:U:C6     | 2.38                     | 0.57              |
| 1:A:1392:G:O2'    | 1:A:1502:A:H5''   | 2.03                     | 0.57              |
| 1:A:1443:G:H5''   | 1:A:1446:A:C5'    | 2.34                     | 0.57              |
| 4:B:17:PHE:HD1    | 4:B:18:GLY:N      | 2.01                     | 0.57              |
| 10:H:113:SER:HB2  | 10:H:134:ILE:HD11 | 1.85                     | 0.57              |
| 15:M:78:ILE:O     | 15:M:81:LEU:HD23  | 2.03                     | 0.57              |
| 19:Q:48:GLU:O     | 19:Q:49:GLU:C     | 2.41                     | 0.57              |
| 1:A:1312:G:O2'    | 1:A:1313:U:H5'    | 2.05                     | 0.57              |
| 1:A:405:U:H3'     | 1:A:406:G:H5'     | 1.86                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:C:64:VAL:HB     | 5:C:99:VAL:HB     | 1.86                     | 0.57              |
| 1:A:1152:A:H5'    | 12:J:13:HIS:HD2   | 1.69                     | 0.57              |
| 14:L:41:ARG:HB3   | 14:L:41:ARG:NH1   | 2.19                     | 0.57              |
| 1:A:1193:G:O2'    | 1:A:1194:U:H5'    | 2.04                     | 0.57              |
| 11:I:24:GLY:HA2   | 11:I:59:PHE:O     | 2.05                     | 0.57              |
| 12:J:24:VAL:O     | 12:J:28:ARG:HG3   | 2.04                     | 0.57              |
| 1:A:127:G:HO2'    | 19:Q:2:PRO:N      | 2.03                     | 0.57              |
| 19:Q:45:HIS:CD2   | 19:Q:47:PRO:HG3   | 2.38                     | 0.57              |
| 1:A:1347:G:H2'    | 1:A:1373:G:H1     | 1.69                     | 0.57              |
| 1:A:287:U:O2'     | 1:A:288:A:H5'     | 2.04                     | 0.57              |
| 7:E:88:LYS:NZ     | 7:E:123:LEU:HD12  | 2.18                     | 0.57              |
| 17:O:33:THR:HG23  | 17:O:63:ARG:HH12  | 1.70                     | 0.57              |
| 19:Q:5:VAL:O      | 19:Q:6:LEU:HD23   | 2.04                     | 0.57              |
| 1:A:1160:G:O2'    | 1:A:1161:C:H5'    | 2.04                     | 0.57              |
| 1:A:1197:G:O2'    | 1:A:1198:G:H5'    | 2.04                     | 0.57              |
| 1:A:1525:G:P      | 13:K:120:ARG:HH22 | 2.27                     | 0.57              |
| 1:A:262:A:H5'     | 22:T:74:LYS:HD3   | 1.86                     | 0.57              |
| 5:C:134:ILE:HG23  | 5:C:151:VAL:HB    | 1.87                     | 0.57              |
| 12:J:4:ILE:HG13   | 12:J:74:ILE:O     | 2.05                     | 0.57              |
| 14:L:110:VAL:O    | 14:L:113:ARG:HB2  | 2.04                     | 0.57              |
| 14:L:71:PRO:O     | 14:L:102:ARG:HD2  | 2.03                     | 0.57              |
| 18:P:51:VAL:HG12  | 18:P:52:ASP:N     | 2.18                     | 0.57              |
| 1:A:384:G:H2'     | 1:A:385:C:C6      | 2.39                     | 0.57              |
| 5:C:34:LEU:HD12   | 16:N:25:VAL:CG2   | 2.33                     | 0.57              |
| 1:A:653:A:C8      | 10:H:56:LYS:HG2   | 2.40                     | 0.57              |
| 14:L:46:LYS:CD    | 14:L:47:LYS:H     | 2.17                     | 0.57              |
| 1:A:17:U:H2'      | 1:A:18:C:C6       | 2.39                     | 0.57              |
| 1:A:353:A:H8      | 1:A:353:A:C5'     | 2.17                     | 0.57              |
| 8:F:44:GLY:HA2    | 8:F:59:TYR:CE1    | 2.40                     | 0.57              |
| 19:Q:68:ARG:O     | 19:Q:69:LYS:HB2   | 2.04                     | 0.57              |
| 20:R:55:ARG:HB3   | 20:R:55:ARG:HH11  | 1.69                     | 0.57              |
| 1:A:1053:G:HO2'   | 1:A:1199:U:H5     | 1.52                     | 0.57              |
| 10:H:112:LEU:HD23 | 10:H:112:LEU:H    | 1.68                     | 0.57              |
| 21:S:15:LEU:O     | 21:S:19:VAL:HG12  | 2.05                     | 0.57              |
| 1:A:1056:U:H5'    | 5:C:163:ALA:HB2   | 1.87                     | 0.57              |
| 1:A:586:C:O2'     | 1:A:587:G:H5'     | 2.04                     | 0.57              |
| 9:G:155:ARG:HA    | 9:G:155:ARG:NH1   | 2.20                     | 0.57              |
| 1:A:1128:C:H4'    | 11:I:16:ARG:HH12  | 1.69                     | 0.57              |
| 1:A:353:A:C5'     | 1:A:353:A:C8      | 2.88                     | 0.57              |
| 1:A:528:C:H5'     | 1:A:535:A:C6      | 2.40                     | 0.57              |
| 11:I:11:LYS:O     | 11:I:11:LYS:HG2   | 2.05                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 12:J:30:SER:OG   | 12:J:81:THR:HA   | 2.05                     | 0.57              |
| 16:N:14:PRO:O    | 16:N:15:LYS:CB   | 2.53                     | 0.57              |
| 21:S:28:LYS:CG   | 21:S:29:ARG:H    | 2.09                     | 0.57              |
| 1:A:190(F):G:H4' | 1:A:190(G):G:OP2 | 2.03                     | 0.56              |
| 4:B:14:GLY:O     | 4:B:15:VAL:HG13  | 2.04                     | 0.56              |
| 5:C:91:LEU:HD21  | 5:C:99:VAL:HG12  | 1.86                     | 0.56              |
| 6:D:24:GLU:HG2   | 6:D:25:ARG:H     | 1.70                     | 0.56              |
| 9:G:26:PHE:CE2   | 9:G:30:ILE:HD11  | 2.39                     | 0.56              |
| 11:I:8:GLY:CA    | 11:I:79:LEU:HB3  | 2.35                     | 0.56              |
| 4:B:116:GLU:HG2  | 4:B:153:ARG:CZ   | 2.34                     | 0.56              |
| 4:B:69:LEU:CD1   | 4:B:155:LEU:HD11 | 2.35                     | 0.56              |
| 5:C:134:ILE:HG22 | 5:C:168:ALA:HB3  | 1.85                     | 0.56              |
| 5:C:89:GLU:O     | 5:C:93:LYS:HB2   | 2.05                     | 0.56              |
| 6:D:177:ASP:OD1  | 6:D:179:GLU:HB2  | 2.05                     | 0.56              |
| 21:S:5:LEU:O     | 21:S:6:LYS:CB    | 2.53                     | 0.56              |
| 4:B:139:LYS:O    | 4:B:139:LYS:HD3  | 2.05                     | 0.56              |
| 4:B:181:PHE:HD2  | 10:H:70:GLN:HB3  | 1.70                     | 0.56              |
| 1:A:335:C:H2'    | 1:A:336:C:H6     | 1.70                     | 0.56              |
| 4:B:15:VAL:HG11  | 4:B:209:ARG:CG   | 2.35                     | 0.56              |
| 4:B:97:TRP:CH2   | 4:B:101:MET:HB2  | 2.40                     | 0.56              |
| 10:H:4:ASP:OD2   | 10:H:85:ARG:NH1  | 2.38                     | 0.56              |
| 10:H:28:ALA:HB2  | 10:H:59:LEU:HG   | 1.87                     | 0.56              |
| 11:I:127:LYS:HE3 | 11:I:127:LYS:H   | 1.70                     | 0.56              |
| 14:L:39:VAL:HG12 | 14:L:40:VAL:N    | 2.20                     | 0.56              |
| 12:J:47:PHE:CZ   | 16:N:37:PHE:HE1  | 2.23                     | 0.56              |
| 19:Q:40:LYS:HD3  | 19:Q:42:TYR:CZ   | 2.40                     | 0.56              |
| 1:A:390:C:H2'    | 1:A:391:G:C8     | 2.40                     | 0.56              |
| 5:C:18:TRP:HE3   | 5:C:18:TRP:H     | 1.54                     | 0.56              |
| 5:C:70:VAL:HG12  | 5:C:72:LYS:H     | 1.70                     | 0.56              |
| 12:J:9:ARG:HB3   | 12:J:9:ARG:NH1   | 2.21                     | 0.56              |
| 19:Q:80:GLY:O    | 19:Q:81:ARG:HB3  | 2.05                     | 0.56              |
| 21:S:30:LEU:HD23 | 21:S:31:ILE:H    | 1.67                     | 0.56              |
| 21:S:31:ILE:O    | 21:S:32:LYS:HB3  | 2.04                     | 0.56              |
| 1:A:1066:C:O2'   | 1:A:1067:A:H5'   | 2.06                     | 0.56              |
| 1:A:149:A:H2'    | 1:A:150:C:C6     | 2.40                     | 0.56              |
| 1:A:67:C:H2'     | 1:A:68:G:C8      | 2.41                     | 0.56              |
| 1:A:750:G:N3     | 17:O:23:GLY:HA3  | 2.19                     | 0.56              |
| 4:B:121:LEU:O    | 4:B:127:ILE:HG23 | 2.05                     | 0.56              |
| 1:A:1292:U:P     | 9:G:41:ARG:HH22  | 2.28                     | 0.56              |
| 9:G:79:ARG:NH1   | 9:G:82:GLY:H     | 2.03                     | 0.56              |
| 1:A:1305:G:OP2   | 1:A:1305:G:C8    | 2.58                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:87:ARG:O     | 4:B:88:ALA:HB2   | 2.06                     | 0.56              |
| 1:A:974:A:OP2    | 16:N:41:ARG:NH1  | 2.38                     | 0.56              |
| 1:A:1154:G:H2'   | 1:A:1155:G:H8    | 1.70                     | 0.56              |
| 1:A:1281:U:H4'   | 1:A:1282:C:OP2   | 2.06                     | 0.56              |
| 1:A:1316:G:N2    | 1:A:1318:A:H3'   | 2.21                     | 0.56              |
| 10:H:51:VAL:HG12 | 10:H:52:ASP:N    | 2.19                     | 0.56              |
| 13:K:121:PRO:HG2 | 13:K:126:ARG:HG3 | 1.87                     | 0.56              |
| 21:S:15:LEU:HD12 | 21:S:16:LEU:H    | 1.71                     | 0.56              |
| 5:C:51:GLY:O     | 5:C:70:VAL:HG13  | 2.05                     | 0.56              |
| 10:H:34:GLU:HA   | 10:H:34:GLU:OE2  | 2.06                     | 0.56              |
| 4:B:178:ARG:NH2  | 10:H:68:ARG:HH22 | 2.04                     | 0.56              |
| 1:A:1392:G:N2    | 1:A:1502:A:H8    | 2.04                     | 0.56              |
| 1:A:1521:G:H2'   | 1:A:1522:U:C6    | 2.41                     | 0.56              |
| 1:A:370:C:O2'    | 1:A:371:G:H5'    | 2.05                     | 0.56              |
| 1:A:954:G:H2'    | 1:A:955:U:H6     | 1.69                     | 0.56              |
| 4:B:88:ALA:CB    | 4:B:90:MET:HG2   | 2.36                     | 0.56              |
| 5:C:99:VAL:CG2   | 5:C:100:ALA:N    | 2.68                     | 0.56              |
| 5:C:130:VAL:HG21 | 5:C:157:ILE:HG23 | 1.87                     | 0.56              |
| 12:J:39:PRO:O    | 12:J:40:LEU:HB2  | 2.05                     | 0.56              |
| 4:B:221:LEU:O    | 4:B:221:LEU:HD13 | 2.05                     | 0.56              |
| 11:I:51:ARG:HG2  | 11:I:56:LEU:HD12 | 1.87                     | 0.56              |
| 11:I:53:VAL:HG21 | 11:I:85:LEU:HD21 | 1.88                     | 0.56              |
| 12:J:49:VAL:O    | 12:J:60:ARG:O    | 2.23                     | 0.56              |
| 14:L:46:LYS:CG   | 14:L:47:LYS:N    | 2.70                     | 0.56              |
| 1:A:1176:A:H2'   | 1:A:1177:G:C8    | 2.42                     | 0.55              |
| 1:A:157:G:O2'    | 1:A:158:G:H5'    | 2.06                     | 0.55              |
| 4:B:62:ALA:C     | 4:B:64:ARG:H     | 2.08                     | 0.55              |
| 1:A:1052:U:H2'   | 1:A:1055:A:OP1   | 2.07                     | 0.55              |
| 1:A:269:C:H2'    | 1:A:270:A:C8     | 2.41                     | 0.55              |
| 1:A:421:U:H5''   | 1:A:423:G:N2     | 2.20                     | 0.55              |
| 5:C:14:ILE:HG22  | 5:C:15:THR:HG23  | 1.88                     | 0.55              |
| 10:H:64:LYS:HG2  | 10:H:79:VAL:HG21 | 1.89                     | 0.55              |
| 12:J:38:ILE:HB   | 12:J:71:LEU:HB3  | 1.89                     | 0.55              |
| 13:K:110:ASP:HB2 | 20:R:88:LYS:HZ2  | 1.70                     | 0.55              |
| 14:L:34:ARG:O    | 14:L:61:THR:HG23 | 2.05                     | 0.55              |
| 17:O:33:THR:HG23 | 17:O:63:ARG:NH1  | 2.21                     | 0.55              |
| 1:A:1054:C:OP1   | 1:A:1197:G:OP1   | 2.24                     | 0.55              |
| 1:A:1392:G:O2'   | 1:A:1393:U:H5'   | 2.06                     | 0.55              |
| 1:A:1425:U:H3    | 1:A:1475:G:H1    | 1.53                     | 0.55              |
| 4:B:78:GLN:HA    | 4:B:94:ASN:OD1   | 2.06                     | 0.55              |
| 1:A:1057:G:H5''  | 5:C:154:SER:HB2  | 1.87                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 13:K:72:ALA:HB1  | 13:K:77:MET:HG3  | 1.87                     | 0.55              |
| 21:S:36:ARG:HA   | 21:S:71:LEU:HB2  | 1.88                     | 0.55              |
| 23:V:12:LYS:HB3  | 23:V:22:ARG:HD2  | 1.89                     | 0.55              |
| 1:A:328:C:O2     | 1:A:328:C:C2'    | 2.53                     | 0.55              |
| 5:C:107:GLN:H    | 5:C:107:GLN:CD   | 2.10                     | 0.55              |
| 11:I:20:ARG:O    | 11:I:60:ASP:N    | 2.39                     | 0.55              |
| 5:C:40:ARG:HB3   | 5:C:44:GLU:OE2   | 2.06                     | 0.55              |
| 16:N:29:ARG:NH1  | 16:N:29:ARG:HG2  | 2.22                     | 0.55              |
| 16:N:29:ARG:HB3  | 16:N:40:CYS:HB3  | 1.88                     | 0.55              |
| 20:R:43:PHE:HA   | 20:R:51:LEU:HD12 | 1.88                     | 0.55              |
| 22:T:73:HIS:O    | 22:T:74:LYS:CB   | 2.54                     | 0.55              |
| 1:A:1106:G:OP1   | 5:C:172:ARG:HD3  | 2.06                     | 0.55              |
| 1:A:559:A:P      | 7:E:126:ARG:HH22 | 2.30                     | 0.55              |
| 1:A:683:G:H21    | 13:K:38:ASN:ND2  | 2.04                     | 0.55              |
| 1:A:718:G:C8     | 13:K:116:HIS:HB3 | 2.41                     | 0.55              |
| 1:A:738:C:OP2    | 8:F:92:LYS:HE3   | 2.07                     | 0.55              |
| 8:F:19:LEU:O     | 8:F:23:LYS:HG3   | 2.07                     | 0.55              |
| 9:G:122:HIS:HD2  | 9:G:125:MET:HE3  | 1.72                     | 0.55              |
| 12:J:4:ILE:HA    | 12:J:100:THR:CA  | 2.37                     | 0.55              |
| 12:J:8:LEU:HB2   | 12:J:70:ARG:HB2  | 1.87                     | 0.55              |
| 15:M:85:GLY:O    | 15:M:86:CYS:O    | 2.24                     | 0.55              |
| 18:P:20:VAL:HG11 | 18:P:32:TYR:HB3  | 1.87                     | 0.55              |
| 1:A:1116:C:H2'   | 1:A:1117:G:C5'   | 2.37                     | 0.55              |
| 1:A:683:G:H21    | 13:K:38:ASN:HD22 | 1.54                     | 0.55              |
| 4:B:97:TRP:CZ2   | 4:B:102:LEU:HD13 | 2.39                     | 0.55              |
| 8:F:2:ARG:NH1    | 8:F:69:GLU:HB3   | 2.21                     | 0.55              |
| 10:H:45:ILE:HG13 | 10:H:47:GLY:H    | 1.70                     | 0.55              |
| 11:I:118:LYS:O   | 11:I:119:ALA:CB  | 2.53                     | 0.55              |
| 14:L:24:VAL:HG12 | 14:L:24:VAL:O    | 2.05                     | 0.55              |
| 14:L:41:ARG:HB3  | 14:L:41:ARG:HH11 | 1.71                     | 0.55              |
| 14:L:46:LYS:HE3  | 14:L:47:LYS:HB2  | 1.89                     | 0.55              |
| 15:M:63:THR:CG2  | 15:M:64:TRP:H    | 2.20                     | 0.55              |
| 17:O:17:ARG:HG3  | 17:O:17:ARG:NH1  | 2.20                     | 0.55              |
| 20:R:87:ARG:HG2  | 20:R:87:ARG:HH11 | 1.72                     | 0.55              |
| 4:B:16:HIS:NE2   | 4:B:214:ILE:HG12 | 2.22                     | 0.55              |
| 18:P:67:THR:CG2  | 18:P:68:ASP:H    | 2.20                     | 0.55              |
| 1:A:1218:C:H2'   | 1:A:1219:U:C6    | 2.42                     | 0.55              |
| 1:A:1481:U:O2'   | 1:A:1482:G:H5'   | 2.06                     | 0.55              |
| 7:E:43:LEU:HD11  | 7:E:132:ALA:HB1  | 1.88                     | 0.55              |
| 9:G:78:ARG:HB2   | 9:G:156:TRP:HZ3  | 1.72                     | 0.55              |
| 11:I:89:ASN:HD21 | 11:I:91:ASP:HB2  | 1.71                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 16:N:23:ARG:NH1  | 16:N:30:ALA:HB2  | 2.22                     | 0.55              |
| 22:T:44:ALA:C    | 22:T:46:GLU:H    | 2.10                     | 0.55              |
| 1:A:1151:A:O2'   | 1:A:1152:A:H8    | 1.89                     | 0.55              |
| 1:A:1208:C:H2'   | 1:A:1209:C:C6    | 2.40                     | 0.55              |
| 5:C:123:GLN:HE22 | 5:C:140:ARG:NH2  | 2.04                     | 0.55              |
| 5:C:36:ASP:HB3   | 5:C:40:ARG:NH1   | 2.21                     | 0.55              |
| 6:D:92:VAL:O     | 6:D:96:LEU:HD13  | 2.07                     | 0.55              |
| 9:G:15:ASP:HB3   | 9:G:19:GLY:H     | 1.72                     | 0.55              |
| 12:J:4:ILE:HA    | 12:J:100:THR:CB  | 2.37                     | 0.55              |
| 14:L:126:LYS:H   | 14:L:126:LYS:CE  | 2.20                     | 0.55              |
| 14:L:41:ARG:HH12 | 14:L:57:LYS:HZ3  | 1.55                     | 0.55              |
| 16:N:24:CYS:HB3  | 16:N:28:GLY:H    | 1.71                     | 0.55              |
| 20:R:43:PHE:C    | 20:R:51:LEU:HD12 | 2.28                     | 0.55              |
| 1:A:1343:G:H2'   | 1:A:1344:C:H6    | 1.70                     | 0.54              |
| 1:A:961:U:O2'    | 1:A:962:C:H5'    | 2.07                     | 0.54              |
| 6:D:173:TRP:CD2  | 6:D:189:PRO:HB3  | 2.42                     | 0.54              |
| 9:G:114:ARG:HH11 | 9:G:114:ARG:HG2  | 1.72                     | 0.54              |
| 12:J:59:SER:O    | 12:J:60:ARG:HB2  | 2.07                     | 0.54              |
| 12:J:4:ILE:CD1   | 12:J:74:ILE:HB   | 2.29                     | 0.54              |
| 5:C:33:LEU:HD11  | 16:N:53:LEU:HD23 | 1.89                     | 0.54              |
| 1:A:1157:A:H4'   | 1:A:1158:C:O5'   | 2.07                     | 0.54              |
| 1:A:1285:A:H8    | 1:A:1285:A:OP1   | 1.90                     | 0.54              |
| 1:A:485:G:HO2'   | 1:A:486:U:H5     | 1.55                     | 0.54              |
| 5:C:110:ASN:HD22 | 5:C:140:ARG:HB3  | 1.72                     | 0.54              |
| 5:C:156:ARG:NH2  | 5:C:161:GLU:HA   | 2.22                     | 0.54              |
| 5:C:86:VAL:O     | 5:C:89:GLU:HB3   | 2.07                     | 0.54              |
| 6:D:64:LEU:HD12  | 6:D:75:PHE:HZ    | 1.71                     | 0.54              |
| 22:T:56:MET:HE1  | 22:T:104:LEU:HG  | 1.90                     | 0.54              |
| 23:V:24:ARG:N    | 23:V:24:ARG:CD   | 2.69                     | 0.54              |
| 1:A:1250:A:H2'   | 1:A:1251:A:C8    | 2.43                     | 0.54              |
| 1:A:556:C:O2'    | 1:A:557:G:H5'    | 2.07                     | 0.54              |
| 1:A:722:A:H4'    | 1:A:723:U:C4     | 2.43                     | 0.54              |
| 7:E:103:GLY:O    | 7:E:106:PRO:HD2  | 2.08                     | 0.54              |
| 1:A:877:C:H1'    | 10:H:3:THR:CG2   | 2.38                     | 0.54              |
| 14:L:75:HIS:HD2  | 14:L:77:LEU:N    | 1.98                     | 0.54              |
| 18:P:19:ILE:HG22 | 18:P:36:ILE:HG13 | 1.88                     | 0.54              |
| 1:A:107:G:C2'    | 1:A:108:G:H5'    | 2.38                     | 0.54              |
| 1:A:1241:G:H2'   | 1:A:1242:C:H6    | 1.68                     | 0.54              |
| 1:A:190(I):G:O2' | 1:A:190(J):U:H5' | 2.07                     | 0.54              |
| 1:A:538:G:H5''   | 14:L:114:LYS:CG  | 2.37                     | 0.54              |
| 1:A:639:G:O2'    | 1:A:640:A:H5'    | 2.07                     | 0.54              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:740:U:O2'     | 1:A:741:G:H5'    | 2.07                     | 0.54              |
| 4:B:230:VAL:HG12  | 4:B:231:GLU:N    | 2.23                     | 0.54              |
| 5:C:70:VAL:O      | 5:C:106:VAL:HG23 | 2.07                     | 0.54              |
| 6:D:127:THR:HG22  | 6:D:147:ALA:HB3  | 1.88                     | 0.54              |
| 7:E:72:GLN:O      | 7:E:73:ASN:HB3   | 2.08                     | 0.54              |
| 11:I:108:VAL:HG12 | 11:I:109:VAL:N   | 2.23                     | 0.54              |
| 19:Q:4:LYS:HE3    | 19:Q:6:LEU:HD21  | 1.89                     | 0.54              |
| 1:A:151:A:H2'     | 1:A:152:A:O4'    | 2.08                     | 0.54              |
| 1:A:653:A:OP1     | 10:H:56:LYS:NZ   | 2.40                     | 0.54              |
| 4:B:10:LEU:HD23   | 4:B:48:MET:CE    | 2.37                     | 0.54              |
| 7:E:15:ARG:O      | 7:E:27:ARG:O     | 2.26                     | 0.54              |
| 11:I:23:ASN:HD22  | 11:I:23:ASN:C    | 2.10                     | 0.54              |
| 14:L:55:VAL:HG12  | 14:L:56:ALA:H    | 1.71                     | 0.54              |
| 17:O:70:LEU:HD12  | 17:O:78:TYR:CA   | 2.36                     | 0.54              |
| 20:R:53:ARG:C     | 20:R:55:ARG:H    | 2.11                     | 0.54              |
| 15:M:84:ILE:HG21  | 21:S:65:ASN:HD22 | 1.72                     | 0.54              |
| 1:A:1223:C:OP1    | 1:A:1224:G:H3'   | 2.08                     | 0.54              |
| 1:A:539:A:H2'     | 1:A:540:G:C8     | 2.42                     | 0.54              |
| 1:A:60:A:H4'      | 1:A:61:G:O5'     | 2.06                     | 0.54              |
| 1:A:743:U:H2'     | 1:A:744:C:C6     | 2.43                     | 0.54              |
| 1:A:861:G:O2'     | 1:A:862:C:H5'    | 2.08                     | 0.54              |
| 5:C:134:ILE:HD11  | 5:C:153:VAL:CG2  | 2.38                     | 0.54              |
| 6:D:149:ALA:HB3   | 6:D:152:SER:HB2  | 1.90                     | 0.54              |
| 7:E:87:SER:HB3    | 7:E:131:ILE:HD13 | 1.90                     | 0.54              |
| 9:G:85:TYR:HD1    | 9:G:154:TYR:HE1  | 1.54                     | 0.54              |
| 17:O:78:TYR:CZ    | 17:O:82:ILE:HD11 | 2.43                     | 0.54              |
| 21:S:77:THR:HG22  | 21:S:78:ARG:N    | 2.21                     | 0.54              |
| 1:A:1236:A:OP1    | 23:V:2:GLY:HA3   | 2.08                     | 0.54              |
| 13:K:126:ARG:HB3  | 13:K:126:ARG:NH1 | 2.22                     | 0.54              |
| 14:L:60:LEU:CD2   | 14:L:66:VAL:HG22 | 2.38                     | 0.54              |
| 1:A:1118:C:H1'    | 1:A:1179:A:C4    | 2.43                     | 0.54              |
| 1:A:1381:U:O2'    | 1:A:1382:C:H5'   | 2.08                     | 0.54              |
| 1:A:955:U:O2'     | 1:A:956:U:H5'    | 2.08                     | 0.54              |
| 4:B:25:ASN:HD22   | 4:B:27:LYS:H     | 1.55                     | 0.54              |
| 7:E:13:ILE:HA     | 7:E:29:GLY:O     | 2.08                     | 0.54              |
| 9:G:122:HIS:HD2   | 9:G:125:MET:CE   | 2.20                     | 0.54              |
| 14:L:111:LYS:O    | 14:L:112:ASP:HB2 | 2.08                     | 0.54              |
| 16:N:9:LYS:HG3    | 16:N:21:TYR:O    | 2.08                     | 0.54              |
| 1:A:1007:C:H2'    | 1:A:1008:C:H6    | 1.72                     | 0.54              |
| 1:A:1101:A:H4'    | 1:A:1102:A:O5'   | 2.08                     | 0.54              |
| 1:A:346:G:C2'     | 1:A:347:G:H5'    | 2.38                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:D:5:ILE:HG22   | 6:D:5:ILE:O      | 2.06                     | 0.54              |
| 8:F:2:ARG:NE     | 8:F:69:GLU:HG2   | 2.23                     | 0.54              |
| 8:F:62:TRP:CE3   | 8:F:62:TRP:O     | 2.61                     | 0.54              |
| 1:A:1250:A:H5''  | 11:I:68:GLY:N    | 2.23                     | 0.54              |
| 14:L:119:LYS:O   | 14:L:120:TYR:HB2 | 2.08                     | 0.54              |
| 1:A:191:G:N3     | 22:T:105:SER:HB3 | 2.23                     | 0.54              |
| 1:A:1064:G:H4'   | 1:A:1065:U:C5'   | 2.37                     | 0.54              |
| 1:A:1453:G:H2'   | 1:A:1454:G:O4'   | 2.08                     | 0.54              |
| 4:B:19:HIS:ND1   | 4:B:204:ASN:ND2  | 2.56                     | 0.54              |
| 9:G:23:VAL:HG13  | 9:G:43:PHE:CE2   | 2.42                     | 0.54              |
| 11:I:28:VAL:O    | 11:I:29:ASN:HB2  | 2.07                     | 0.54              |
| 9:G:37:ASN:ND2   | 11:I:41:VAL:HG23 | 2.23                     | 0.54              |
| 11:I:71:SER:HA   | 11:I:74:ILE:HD12 | 1.89                     | 0.54              |
| 12:J:22:LYS:HE2  | 12:J:90:LEU:HB2  | 1.90                     | 0.54              |
| 21:S:20:LEU:HA   | 21:S:23:ASN:ND2  | 2.22                     | 0.54              |
| 1:A:112:G:H5'    | 1:A:389:A:H4'    | 1.90                     | 0.53              |
| 1:A:1520:G:O2'   | 1:A:1521:G:H5'   | 2.08                     | 0.53              |
| 1:A:190(L):U:C2  | 22:T:105:SER:HB2 | 2.43                     | 0.53              |
| 1:A:542:G:H2'    | 1:A:543:C:H6     | 1.72                     | 0.53              |
| 8:F:4:TYR:CE2    | 8:F:72:VAL:CG2   | 2.91                     | 0.53              |
| 1:A:738:C:OP1    | 8:F:92:LYS:HE3   | 2.08                     | 0.53              |
| 13:K:91:ARG:O    | 13:K:95:ILE:HG13 | 2.08                     | 0.53              |
| 18:P:26:ARG:HD3  | 18:P:31:LYS:N    | 2.22                     | 0.53              |
| 1:A:1314:C:OP2   | 21:S:6:LYS:HG2   | 2.08                     | 0.53              |
| 1:A:19:C:H2'     | 1:A:20:U:C6      | 2.43                     | 0.53              |
| 6:D:61:LYS:HD3   | 6:D:206:PHE:CD2  | 2.44                     | 0.53              |
| 7:E:60:TYR:HE1   | 7:E:64:ARG:NH2   | 2.03                     | 0.53              |
| 9:G:112:PRO:O    | 9:G:113:GLU:C    | 2.46                     | 0.53              |
| 9:G:3:ARG:HG3    | 9:G:3:ARG:NH1    | 2.23                     | 0.53              |
| 21:S:31:ILE:O    | 21:S:32:LYS:CB   | 2.55                     | 0.53              |
| 1:A:1054:C:O2'   | 1:A:1055:A:H5''  | 2.09                     | 0.53              |
| 1:A:1065:U:H4'   | 1:A:1066:C:O5'   | 2.07                     | 0.53              |
| 1:A:769:G:H4'    | 1:A:1513:A:H4'   | 1.91                     | 0.53              |
| 10:H:121:ASP:HB2 | 10:H:125:ARG:NH2 | 2.23                     | 0.53              |
| 14:L:47:LYS:CG   | 14:L:48:PRO:HD3  | 2.39                     | 0.53              |
| 17:O:14:GLU:HG3  | 17:O:15:PHE:CD1  | 2.43                     | 0.53              |
| 20:R:18:ARG:C    | 20:R:19:LYS:HD2  | 2.28                     | 0.53              |
| 1:A:1495:U:H2'   | 1:A:1496:C:H6    | 1.73                     | 0.53              |
| 6:D:30:LYS:C     | 6:D:32:ALA:N     | 2.61                     | 0.53              |
| 10:H:86:ILE:HD12 | 10:H:133:LEU:CD2 | 2.39                     | 0.53              |
| 15:M:40:ASN:HD22 | 15:M:41:PRO:CD   | 2.21                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 15:M:65:LYS:HE3  | 15:M:69:GLU:CG    | 2.37                     | 0.53              |
| 20:R:86:VAL:O    | 20:R:87:ARG:CB    | 2.56                     | 0.53              |
| 1:A:1038:C:H2'   | 1:A:1039:C:H6     | 1.74                     | 0.53              |
| 1:A:203:U:H5'    | 1:A:216:G:N2      | 2.24                     | 0.53              |
| 6:D:199:ASN:C    | 6:D:199:ASN:ND2   | 2.62                     | 0.53              |
| 19:Q:94:ASN:O    | 19:Q:97:SER:HB3   | 2.09                     | 0.53              |
| 1:A:1250:A:H5'   | 11:I:68:GLY:O     | 2.08                     | 0.53              |
| 9:G:120:ILE:H    | 9:G:120:ILE:HD12  | 1.73                     | 0.53              |
| 14:L:110:VAL:H   | 14:L:122:THR:HG22 | 1.72                     | 0.53              |
| 1:A:881:G:P      | 14:L:12:ARG:HH22  | 2.32                     | 0.53              |
| 14:L:24:VAL:HG13 | 14:L:98:TYR:CE2   | 2.41                     | 0.53              |
| 1:A:1424:C:O2'   | 1:A:1425:U:H5'    | 2.09                     | 0.53              |
| 1:A:264:U:H4'    | 19:Q:63:ARG:HD3   | 1.89                     | 0.53              |
| 1:A:502:G:H4'    | 1:A:550:G:H4'     | 1.90                     | 0.53              |
| 1:A:810:C:H2'    | 1:A:811:C:H6      | 1.73                     | 0.53              |
| 9:G:115:ARG:HB2  | 9:G:118:VAL:HG23  | 1.90                     | 0.53              |
| 9:G:116:ALA:O    | 9:G:120:ILE:HD12  | 2.09                     | 0.53              |
| 14:L:40:VAL:O    | 14:L:40:VAL:HG12  | 2.09                     | 0.53              |
| 20:R:19:LYS:HD2  | 20:R:19:LYS:N     | 2.24                     | 0.53              |
| 1:A:1128:C:H4'   | 11:I:16:ARG:NH1   | 2.24                     | 0.53              |
| 1:A:1501:C:OP2   | 1:A:1504:G:H2'    | 2.09                     | 0.53              |
| 1:A:540:G:H21    | 6:D:42:GLN:NE2    | 2.07                     | 0.53              |
| 1:A:537:G:OP1    | 14:L:113:ARG:NH2  | 2.41                     | 0.53              |
| 18:P:22:THR:HA   | 18:P:33:ILE:HD12  | 1.91                     | 0.53              |
| 1:A:1305:G:H5''  | 23:V:4:GLY:C      | 2.29                     | 0.53              |
| 1:A:426:G:H2'    | 1:A:427:U:C6      | 2.43                     | 0.53              |
| 4:B:134:GLU:HA   | 4:B:137:ARG:HG3   | 1.90                     | 0.53              |
| 4:B:16:HIS:NE2   | 4:B:214:ILE:CG1   | 2.71                     | 0.53              |
| 4:B:75:LYS:HE3   | 4:B:78:GLN:NE2    | 2.24                     | 0.53              |
| 5:C:87:LEU:C     | 5:C:89:GLU:H      | 2.12                     | 0.53              |
| 11:I:4:TYR:CE2   | 11:I:88:TYR:HA    | 2.44                     | 0.53              |
| 19:Q:79:SER:O    | 19:Q:80:GLY:O     | 2.27                     | 0.53              |
| 21:S:63:THR:HG22 | 21:S:64:GLU:N     | 2.23                     | 0.53              |
| 1:A:723:U:H5''   | 1:A:724:G:OP2     | 2.09                     | 0.53              |
| 1:A:968:A:H4'    | 1:A:969:A:OP2     | 2.09                     | 0.53              |
| 13:K:84:VAL:HG11 | 13:K:95:ILE:HD11  | 1.90                     | 0.53              |
| 14:L:24:VAL:O    | 14:L:26:ALA:N     | 2.35                     | 0.53              |
| 19:Q:66:SER:OG   | 19:Q:69:LYS:HB3   | 2.09                     | 0.53              |
| 19:Q:76:LEU:HD23 | 19:Q:76:LEU:C     | 2.29                     | 0.53              |
| 1:A:530:G:O6     | 2:W:3:A:H1'       | 2.09                     | 0.53              |
| 1:A:1262:C:O2'   | 1:A:1263:C:H5'    | 2.09                     | 0.52              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:1300:G:O2'  | 1:A:1301:U:P     | 2.67                     | 0.52              |
| 1:A:701:C:H5'   | 1:A:703:G:O4'    | 2.09                     | 0.52              |
| 1:A:984:C:H2'   | 1:A:985:C:H6     | 1.74                     | 0.52              |
| 5:C:14:ILE:O    | 5:C:16:ARG:N     | 2.42                     | 0.52              |
| 7:E:147:ASP:OD1 | 7:E:147:ASP:N    | 2.41                     | 0.52              |
| 16:N:57:ARG:HG2 | 16:N:58:LYS:N    | 2.20                     | 0.52              |
| 1:A:1278:U:H5'' | 1:A:1279:A:O4'   | 2.09                     | 0.52              |
| 1:A:265:G:H2'   | 1:A:267:C:H5     | 1.73                     | 0.52              |
| 1:A:945:G:C2    | 1:A:946:A:C8     | 2.96                     | 0.52              |
| 5:C:148:GLY:O   | 5:C:149:ALA:HB2  | 2.09                     | 0.52              |
| 9:G:75:VAL:HG21 | 9:G:86:GLN:HB3   | 1.91                     | 0.52              |
| 12:J:94:VAL:CG1 | 12:J:95:GLU:N    | 2.71                     | 0.52              |
| 17:O:4:THR:OG1  | 17:O:7:GLU:HB2   | 2.10                     | 0.52              |
| 1:A:401:C:H1'   | 1:A:622:A:H1'    | 1.92                     | 0.52              |
| 4:B:51:LEU:CD2  | 4:B:55:PHE:HE1   | 2.23                     | 0.52              |
| 5:C:205:GLY:O   | 5:C:206:GLU:HB2  | 2.09                     | 0.52              |
| 6:D:64:LEU:HD12 | 6:D:75:PHE:CZ    | 2.45                     | 0.52              |
| 7:E:32:VAL:HG23 | 7:E:58:ALA:HB1   | 1.92                     | 0.52              |
| 9:G:79:ARG:HH12 | 9:G:82:GLY:HA2   | 1.75                     | 0.52              |
| 4:B:178:ARG:NH2 | 10:H:68:ARG:NH2  | 2.57                     | 0.52              |
| 1:A:1056:U:H5'  | 5:C:163:ALA:CB   | 2.40                     | 0.52              |
| 1:A:337:C:H2'   | 1:A:338:A:C8     | 2.44                     | 0.52              |
| 1:A:376:G:P     | 18:P:67:THR:HG21 | 2.49                     | 0.52              |
| 6:D:70:ILE:HD11 | 6:D:100:ARG:HD2  | 1.90                     | 0.52              |
| 9:G:78:ARG:HH11 | 9:G:154:TYR:HB3  | 1.75                     | 0.52              |
| 9:G:79:ARG:HH11 | 9:G:82:GLY:H     | 1.57                     | 0.52              |
| 19:Q:78:GLU:O   | 19:Q:78:GLU:HG3  | 2.09                     | 0.52              |
| 1:A:428:G:OP2   | 6:D:7:PRO:HG3    | 2.09                     | 0.52              |
| 4:B:45:GLN:O    | 4:B:49:GLU:HG3   | 2.09                     | 0.52              |
| 5:C:110:ASN:O   | 5:C:111:LEU:HD23 | 2.10                     | 0.52              |
| 5:C:22:TRP:CZ3  | 5:C:32:LEU:HB2   | 2.45                     | 0.52              |
| 9:G:140:ASP:HA  | 9:G:143:ARG:HD2  | 1.91                     | 0.52              |
| 11:I:36:TYR:CD2 | 11:I:37:PHE:CE2  | 2.98                     | 0.52              |
| 11:I:48:GLU:HA  | 11:I:51:ARG:HD2  | 1.92                     | 0.52              |
| 19:Q:81:ARG:O   | 19:Q:81:ARG:HG3  | 2.08                     | 0.52              |
| 22:T:76:ALA:O   | 22:T:80:ARG:HG2  | 2.09                     | 0.52              |
| 1:A:1347:G:C6   | 11:I:107:ARG:NH2 | 2.78                     | 0.52              |
| 1:A:748:C:H6    | 1:A:748:C:OP2    | 1.92                     | 0.52              |
| 9:G:110:GLN:OE1 | 9:G:110:GLN:HA   | 2.09                     | 0.52              |
| 12:J:49:VAL:O   | 12:J:60:ARG:CA   | 2.50                     | 0.52              |
| 12:J:5:ARG:HB3  | 12:J:99:LYS:C    | 2.29                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 12:J:50:ILE:HB   | 16:N:41:ARG:NE   | 2.25                     | 0.52              |
| 18:P:45:THR:HB   | 18:P:46:PRO:HD2  | 1.92                     | 0.52              |
| 1:A:1333:A:H2'   | 1:A:1334:G:O4'   | 2.10                     | 0.52              |
| 1:A:1347:G:H2'   | 1:A:1373:G:N1    | 2.25                     | 0.52              |
| 1:A:676:A:H1'    | 13:K:115:PRO:HB3 | 1.92                     | 0.52              |
| 1:A:992:U:O2'    | 1:A:993:G:OP2    | 2.24                     | 0.52              |
| 5:C:44:GLU:C     | 5:C:46:GLU:H     | 2.12                     | 0.52              |
| 14:L:125:PRO:HA  | 14:L:126:LYS:HE3 | 1.92                     | 0.52              |
| 18:P:67:THR:HG22 | 18:P:68:ASP:H    | 1.69                     | 0.52              |
| 22:T:47:GLY:O    | 22:T:49:ALA:N    | 2.42                     | 0.52              |
| 1:A:973:G:H3'    | 1:A:974:A:H5''   | 1.92                     | 0.52              |
| 1:A:1108:G:H5'   | 1:A:1191:A:H4'   | 1.92                     | 0.52              |
| 1:A:131:C:H2'    | 1:A:132:C:H6     | 1.75                     | 0.52              |
| 1:A:1372:U:O2'   | 1:A:1373:G:H5'   | 2.10                     | 0.52              |
| 1:A:346:G:H2'    | 1:A:347:G:H5'    | 1.92                     | 0.52              |
| 5:C:107:GLN:NE2  | 5:C:107:GLN:H    | 2.07                     | 0.52              |
| 10:H:123:GLU:O   | 10:H:126:LYS:HB3 | 2.09                     | 0.52              |
| 1:A:1343:G:H1'   | 11:I:121:ARG:NH1 | 2.25                     | 0.52              |
| 15:M:3:ARG:HA    | 15:M:8:GLU:O     | 2.09                     | 0.52              |
| 18:P:51:VAL:CG1  | 18:P:52:ASP:N    | 2.73                     | 0.52              |
| 21:S:53:ASN:HD21 | 21:S:58:VAL:HG13 | 1.75                     | 0.52              |
| 1:A:1353:G:OP1   | 23:V:3:LYS:HE2   | 2.09                     | 0.52              |
| 1:A:1161:C:H2'   | 1:A:1162:C:C6    | 2.44                     | 0.52              |
| 1:A:1347:G:C2'   | 1:A:1348:U:OP2   | 2.58                     | 0.52              |
| 5:C:11:ARG:HG3   | 5:C:178:LEU:HD12 | 1.91                     | 0.52              |
| 9:G:111:ARG:HB3  | 9:G:113:GLU:OE2  | 2.10                     | 0.52              |
| 14:L:46:LYS:CG   | 14:L:47:LYS:H    | 2.23                     | 0.52              |
| 15:M:97:PRO:HB2  | 15:M:101:GLN:OE1 | 2.10                     | 0.52              |
| 1:A:267:C:P      | 19:Q:67:LYS:HB2  | 2.50                     | 0.52              |
| 21:S:39:THR:HG22 | 21:S:40:ILE:O    | 2.09                     | 0.52              |
| 1:A:1532:U:O2'   | 1:A:1533:C:H5'   | 2.10                     | 0.51              |
| 1:A:176:C:H2'    | 1:A:177:C:H6     | 1.74                     | 0.51              |
| 4:B:14:GLY:C     | 4:B:15:VAL:HG22  | 2.30                     | 0.51              |
| 4:B:54:THR:O     | 4:B:57:PHE:HB3   | 2.09                     | 0.51              |
| 4:B:8:LYS:CD     | 4:B:9:GLU:N      | 2.71                     | 0.51              |
| 15:M:4:ILE:HG22  | 15:M:5:ALA:N     | 2.25                     | 0.51              |
| 21:S:32:LYS:HA   | 21:S:50:ALA:O    | 2.09                     | 0.51              |
| 21:S:40:ILE:HG21 | 21:S:62:ILE:HD13 | 1.91                     | 0.51              |
| 22:T:57:ARG:HH11 | 22:T:102:GLY:HA3 | 1.75                     | 0.51              |
| 3:X:30:G:H2'     | 3:X:30:G:N3      | 2.25                     | 0.51              |
| 1:A:131:C:H2'    | 1:A:132:C:C6     | 2.46                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1525:G:OP1    | 13:K:120:ARG:NH2  | 2.43                     | 0.51              |
| 1:A:179:A:H2'     | 1:A:180:U:C6      | 2.46                     | 0.51              |
| 1:A:657:G:H4'     | 17:O:28:GLN:HG2   | 1.92                     | 0.51              |
| 5:C:191:THR:CG2   | 5:C:192:THR:N     | 2.73                     | 0.51              |
| 6:D:170:VAL:HG11  | 6:D:175:SER:HA    | 1.91                     | 0.51              |
| 7:E:57:LYS:HG2    | 7:E:61:TYR:HE2    | 1.71                     | 0.51              |
| 13:K:91:ARG:HH11  | 20:R:88:LYS:NZ    | 2.08                     | 0.51              |
| 21:S:30:LEU:O     | 21:S:31:ILE:HD13  | 2.11                     | 0.51              |
| 22:T:29:LYS:O     | 22:T:33:ILE:HG13  | 2.10                     | 0.51              |
| 1:A:1042:G:O2'    | 1:A:1043:C:H5'    | 2.09                     | 0.51              |
| 1:A:528:C:H5'     | 1:A:535:A:N6      | 2.26                     | 0.51              |
| 1:A:975:A:C5'     | 1:A:976:G:H5'     | 2.40                     | 0.51              |
| 7:E:33:VAL:HG11   | 7:E:109:ILE:HA    | 1.92                     | 0.51              |
| 8:F:4:TYR:CZ      | 8:F:72:VAL:HG21   | 2.45                     | 0.51              |
| 1:A:1250:A:H4'    | 11:I:68:GLY:CA    | 2.40                     | 0.51              |
| 1:A:748:C:O2'     | 1:A:749:C:H6      | 1.92                     | 0.51              |
| 7:E:51:VAL:O      | 7:E:55:VAL:HG23   | 2.11                     | 0.51              |
| 10:H:103:VAL:HG21 | 10:H:110:ALA:HB2  | 1.91                     | 0.51              |
| 10:H:65:TYR:HA    | 10:H:79:VAL:HG23  | 1.92                     | 0.51              |
| 12:J:19:SER:OG    | 12:J:91:PRO:HB3   | 2.11                     | 0.51              |
| 15:M:110:ARG:HG2  | 15:M:110:ARG:HH11 | 1.76                     | 0.51              |
| 17:O:66:LEU:O     | 17:O:69:TYR:HB3   | 2.10                     | 0.51              |
| 1:A:1320:C:H41    | 21:S:37:ARG:HH11  | 1.59                     | 0.51              |
| 1:A:258:G:O2'     | 1:A:259:G:H5'     | 2.11                     | 0.51              |
| 1:A:920:U:H2'     | 1:A:921:U:C6      | 2.46                     | 0.51              |
| 6:D:8:VAL:C       | 6:D:10:ARG:H      | 2.13                     | 0.51              |
| 7:E:110:LEU:HD13  | 7:E:118:ILE:HG21  | 1.93                     | 0.51              |
| 7:E:83:GLU:HG2    | 7:E:88:LYS:HD2    | 1.93                     | 0.51              |
| 12:J:5:ARG:O      | 12:J:98:ILE:HA    | 2.10                     | 0.51              |
| 14:L:126:LYS:HD2  | 14:L:126:LYS:N    | 2.26                     | 0.51              |
| 14:L:85:ILE:CG2   | 14:L:98:TYR:HB3   | 2.40                     | 0.51              |
| 15:M:62:ASN:O     | 15:M:63:THR:CB    | 2.59                     | 0.51              |
| 22:T:100:ILE:C    | 22:T:102:GLY:N    | 2.63                     | 0.51              |
| 22:T:56:MET:HE3   | 22:T:88:VAL:HG11  | 1.93                     | 0.51              |
| 4:B:118:LEU:CB    | 4:B:142:LEU:HD12  | 2.41                     | 0.51              |
| 1:A:1206:G:H1'    | 5:C:193:TYR:O     | 2.11                     | 0.51              |
| 6:D:17:VAL:HG12   | 6:D:18:LYS:N      | 2.25                     | 0.51              |
| 1:A:689:C:P       | 13:K:46:GLY:HA3   | 2.50                     | 0.51              |
| 14:L:46:LYS:O     | 14:L:47:LYS:C     | 2.49                     | 0.51              |
| 15:M:5:ALA:CB     | 15:M:22:ILE:HD13  | 2.41                     | 0.51              |
| 16:N:27:CYS:SG    | 16:N:29:ARG:HB2   | 2.50                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 22:T:57:ARG:NH2  | 22:T:100:ILE:HG21 | 2.25                     | 0.51              |
| 1:A:195:A:H4'    | 22:T:68:LYS:HE2   | 1.91                     | 0.51              |
| 22:T:94:ALA:O    | 22:T:95:ALA:HB3   | 2.09                     | 0.51              |
| 1:A:1028:C:H2'   | 1:A:1029:C:C6     | 2.45                     | 0.51              |
| 1:A:1140:C:H2'   | 1:A:1141:C:C6     | 2.46                     | 0.51              |
| 1:A:1221:G:H4'   | 21:S:53:ASN:O     | 2.11                     | 0.51              |
| 1:A:1327:C:O2'   | 1:A:1328:C:H5'    | 2.11                     | 0.51              |
| 1:A:622:A:H2'    | 1:A:623:C:H5'     | 1.93                     | 0.51              |
| 1:A:969:A:H61    | 15:M:126:LYS:HB3  | 1.74                     | 0.51              |
| 4:B:25:ASN:C     | 4:B:25:ASN:HD22   | 2.13                     | 0.51              |
| 4:B:42:ILE:HD12  | 4:B:203:GLY:HA2   | 1.92                     | 0.51              |
| 5:C:60:ALA:O     | 5:C:61:ALA:CB     | 2.57                     | 0.51              |
| 11:I:55:ALA:O    | 11:I:56:LEU:HB3   | 2.10                     | 0.51              |
| 1:A:818:G:C2'    | 1:A:819:A:H5''    | 2.40                     | 0.51              |
| 4:B:21:ARG:HH11  | 4:B:21:ARG:HG3    | 1.75                     | 0.51              |
| 4:B:84:GLU:OE1   | 4:B:216:SER:HA    | 2.11                     | 0.51              |
| 5:C:10:PHE:O     | 5:C:178:LEU:HD11  | 2.11                     | 0.51              |
| 5:C:87:LEU:C     | 5:C:89:GLU:N      | 2.63                     | 0.51              |
| 1:A:620:C:C1'    | 6:D:135:LEU:HD13  | 2.41                     | 0.51              |
| 6:D:32:ALA:C     | 6:D:34:GLU:H      | 2.15                     | 0.51              |
| 6:D:61:LYS:HD2   | 6:D:207:TYR:OH    | 2.11                     | 0.51              |
| 7:E:100:VAL:O    | 7:E:107:ARG:NH2   | 2.43                     | 0.51              |
| 12:J:80:LYS:HA   | 12:J:83:GLU:OE2   | 2.10                     | 0.51              |
| 13:K:91:ARG:HH11 | 20:R:88:LYS:HZ3   | 1.58                     | 0.51              |
| 16:N:36:PHE:O    | 16:N:36:PHE:CD1   | 2.63                     | 0.51              |
| 18:P:4:ILE:HG23  | 18:P:36:ILE:HD11  | 1.92                     | 0.51              |
| 1:A:1306:A:N6    | 1:A:1331:G:H1'    | 2.25                     | 0.51              |
| 1:A:403:C:O3'    | 6:D:122:ARG:HD2   | 2.11                     | 0.51              |
| 1:A:501:C:H2'    | 1:A:502:G:C8      | 2.45                     | 0.51              |
| 5:C:134:ILE:CG2  | 5:C:168:ALA:HB3   | 2.41                     | 0.51              |
| 6:D:29:PRO:C     | 6:D:30:LYS:HG3    | 2.31                     | 0.51              |
| 7:E:12:LEU:HD13  | 7:E:31:LEU:HB2    | 1.92                     | 0.51              |
| 8:F:99:ALA:O     | 8:F:100:ASN:HB3   | 2.11                     | 0.51              |
| 10:H:51:VAL:HG11 | 10:H:60:ARG:NH1   | 2.26                     | 0.51              |
| 15:M:34:LEU:HD13 | 15:M:41:PRO:HA    | 1.93                     | 0.51              |
| 1:A:377:G:OP1    | 18:P:3:LYS:HD3    | 2.10                     | 0.51              |
| 1:A:1221:G:O3'   | 21:S:77:THR:HG21  | 2.10                     | 0.51              |
| 22:T:10:LEU:O    | 22:T:12:ALA:N     | 2.43                     | 0.51              |
| 23:V:5:ASP:O     | 23:V:11:GLY:HA3   | 2.10                     | 0.51              |
| 1:A:1041:A:H2'   | 1:A:1042:G:H8     | 1.76                     | 0.51              |
| 1:A:1256:A:O3'   | 1:A:1257:U:H4'    | 2.11                     | 0.51              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:883:C:O2'   | 1:A:884:U:H5'    | 2.11                     | 0.51              |
| 4:B:189:ASP:OD1 | 4:B:205:ASP:HB3  | 2.11                     | 0.51              |
| 5:C:154:SER:O   | 5:C:165:THR:HA   | 2.10                     | 0.51              |
| 1:A:539:A:H2'   | 1:A:540:G:H8     | 1.75                     | 0.50              |
| 11:I:8:GLY:HA2  | 11:I:79:LEU:CD1  | 2.40                     | 0.50              |
| 1:A:1300:G:HO2' | 1:A:1301:U:H6    | 1.54                     | 0.50              |
| 4:B:211:ILE:O   | 4:B:215:LEU:HB2  | 2.10                     | 0.50              |
| 4:B:23:ARG:HD3  | 4:B:24:TRP:N     | 2.26                     | 0.50              |
| 11:I:46:ALA:HB2 | 11:I:74:ILE:CG2  | 2.38                     | 0.50              |
| 11:I:75:ASP:O   | 11:I:78:LYS:HB3  | 2.11                     | 0.50              |
| 12:J:31:GLY:HA2 | 12:J:78:ASN:HD22 | 1.70                     | 0.50              |
| 22:T:67:ALA:O   | 22:T:73:HIS:ND1  | 2.44                     | 0.50              |
| 1:A:244:U:O4    | 1:A:906:G:H1'    | 2.11                     | 0.50              |
| 1:A:279:A:H5''  | 1:A:280:C:H3'    | 1.91                     | 0.50              |
| 1:A:332:G:O2'   | 1:A:333:G:H5'    | 2.11                     | 0.50              |
| 4:B:77:ALA:HB2  | 4:B:211:ILE:CD1  | 2.35                     | 0.50              |
| 5:C:179:ARG:HD3 | 5:C:206:GLU:HG2  | 1.92                     | 0.50              |
| 7:E:41:VAL:HG21 | 7:E:113:ALA:CB   | 2.42                     | 0.50              |
| 7:E:81:GLU:HG2  | 7:E:90:VAL:HG22  | 1.92                     | 0.50              |
| 12:J:5:ARG:HB3  | 12:J:99:LYS:O    | 2.12                     | 0.50              |
| 14:L:50:SER:O   | 14:L:51:ALA:HB2  | 2.10                     | 0.50              |
| 1:A:1053:G:H4'  | 1:A:1054:C:H5'   | 1.94                     | 0.50              |
| 1:A:384:G:H2'   | 1:A:385:C:H6     | 1.75                     | 0.50              |
| 1:A:392:G:H2'   | 1:A:393:A:C8     | 2.46                     | 0.50              |
| 1:A:407:G:H2'   | 1:A:408:A:C8     | 2.46                     | 0.50              |
| 1:A:665:A:N3    | 1:A:732:C:H2'    | 2.27                     | 0.50              |
| 4:B:80:ILE:HD11 | 4:B:208:ILE:CG2  | 2.41                     | 0.50              |
| 9:G:23:VAL:O    | 9:G:27:ILE:HG13  | 2.11                     | 0.50              |
| 11:I:93:ARG:O   | 11:I:95:LYS:N    | 2.45                     | 0.50              |
| 12:J:89:ASP:HB2 | 12:J:91:PRO:HD2  | 1.91                     | 0.50              |
| 1:A:1128:C:H5'  | 11:I:16:ARG:NH2  | 2.27                     | 0.50              |
| 1:A:1451:A:O2'  | 1:A:1452:C:OP1   | 2.30                     | 0.50              |
| 1:A:474:G:H2'   | 1:A:475:G:H8     | 1.76                     | 0.50              |
| 1:A:560:U:H5'   | 1:A:566:G:N2     | 2.27                     | 0.50              |
| 4:B:12:GLU:C    | 4:B:14:GLY:N     | 2.63                     | 0.50              |
| 4:B:235:SER:C   | 4:B:237:ALA:H    | 2.14                     | 0.50              |
| 7:E:121:LYS:HE3 | 7:E:123:LEU:CD2  | 2.42                     | 0.50              |
| 19:Q:66:SER:O   | 19:Q:70:ARG:NH1  | 2.45                     | 0.50              |
| 1:A:547:A:H4'   | 1:A:548:G:O5'    | 2.11                     | 0.50              |
| 1:A:624:C:H2'   | 1:A:625:G:H8     | 1.77                     | 0.50              |
| 4:B:13:ALA:HA   | 4:B:17:PHE:HD2   | 1.74                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:D:70:ILE:HD11  | 6:D:100:ARG:CD   | 2.42                     | 0.50              |
| 6:D:70:ILE:HG22  | 6:D:71:SER:O     | 2.12                     | 0.50              |
| 8:F:101:ALA:HA   | 20:R:28:GLU:CD   | 2.31                     | 0.50              |
| 8:F:19:LEU:HD23  | 8:F:19:LEU:C     | 2.31                     | 0.50              |
| 8:F:30:LEU:HD23  | 8:F:75:LEU:HD21  | 1.92                     | 0.50              |
| 11:I:117:HIS:C   | 11:I:118:LYS:HG3 | 2.32                     | 0.50              |
| 14:L:27:LEU:HG   | 14:L:28:LYS:H    | 1.77                     | 0.50              |
| 17:O:87:ILE:HG22 | 17:O:88:ARG:N    | 2.26                     | 0.50              |
| 1:A:1222:G:P     | 21:S:77:THR:HG21 | 2.52                     | 0.50              |
| 1:A:1386:G:O2'   | 1:A:1387:G:H5'   | 2.12                     | 0.50              |
| 1:A:560:U:O2'    | 1:A:561:U:OP2    | 2.24                     | 0.50              |
| 4:B:80:ILE:HD11  | 4:B:208:ILE:HG22 | 1.94                     | 0.50              |
| 5:C:70:VAL:CG1   | 5:C:71:ALA:N     | 2.74                     | 0.50              |
| 11:I:26:VAL:HG13 | 11:I:61:ALA:HB3  | 1.93                     | 0.50              |
| 14:L:114:LYS:NZ  | 14:L:125:PRO:HG3 | 2.26                     | 0.50              |
| 15:M:5:ALA:O     | 15:M:6:GLY:C     | 2.50                     | 0.50              |
| 1:A:532:A:H2     | 1:A:1207:G:H4'   | 1.76                     | 0.50              |
| 5:C:55:VAL:HG12  | 5:C:55:VAL:O     | 2.11                     | 0.50              |
| 5:C:84:ILE:O     | 5:C:88:ARG:HG3   | 2.11                     | 0.50              |
| 8:F:73:ASN:O     | 8:F:77:ARG:HG3   | 2.11                     | 0.50              |
| 9:G:32:ARG:O     | 9:G:33:ASP:HB2   | 2.11                     | 0.50              |
| 12:J:55:LYS:HG3  | 12:J:56:HIS:N    | 2.27                     | 0.50              |
| 12:J:79:ARG:HG2  | 12:J:79:ARG:HH11 | 1.75                     | 0.50              |
| 18:P:45:THR:C    | 18:P:47:ASP:H    | 2.15                     | 0.50              |
| 21:S:17:GLU:HA   | 21:S:20:LEU:CG   | 2.40                     | 0.50              |
| 1:A:586:C:O3'    | 10:H:89:PRO:HB2  | 2.12                     | 0.50              |
| 7:E:41:VAL:CG2   | 7:E:113:ALA:HA   | 2.38                     | 0.50              |
| 7:E:37:ARG:HG2   | 7:E:37:ARG:HH11  | 1.77                     | 0.50              |
| 7:E:53:LEU:O     | 7:E:57:LYS:HB2   | 2.12                     | 0.50              |
| 15:M:3:ARG:HG2   | 15:M:9:ILE:CG1   | 2.37                     | 0.50              |
| 15:M:82:MET:HE3  | 15:M:92:HIS:CB   | 2.41                     | 0.50              |
| 1:A:1316:G:H5''  | 16:N:17:LYS:HD2  | 1.94                     | 0.49              |
| 1:A:1404:C:H2'   | 1:A:1405:G:C8    | 2.47                     | 0.49              |
| 10:H:60:ARG:NH1  | 10:H:60:ARG:HG3  | 2.27                     | 0.49              |
| 12:J:80:LYS:O    | 12:J:83:GLU:HB2  | 2.12                     | 0.49              |
| 1:A:141:A:O2'    | 1:A:142:G:H5'    | 2.12                     | 0.49              |
| 1:A:552:U:O2     | 14:L:31:PRO:HB3  | 2.12                     | 0.49              |
| 6:D:187:ARG:HG3  | 6:D:188:LEU:N    | 2.27                     | 0.49              |
| 6:D:199:ASN:ND2  | 6:D:201:GLN:H    | 2.09                     | 0.49              |
| 8:F:22:GLU:OE1   | 8:F:25:ILE:HD12  | 2.12                     | 0.49              |
| 10:H:68:ARG:HH11 | 10:H:68:ARG:HG2  | 1.76                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 10:H:6:ILE:HD12  | 10:H:35:ILE:HD12 | 1.93                     | 0.49              |
| 15:M:44:ARG:HB3  | 15:M:46:LYS:HG3  | 1.94                     | 0.49              |
| 1:A:1143:G:H2'   | 1:A:1144:G:C8    | 2.48                     | 0.49              |
| 1:A:407:G:H2'    | 1:A:408:A:H8     | 1.77                     | 0.49              |
| 1:A:41:G:H2'     | 1:A:42:G:C8      | 2.47                     | 0.49              |
| 4:B:10:LEU:HD23  | 4:B:48:MET:HE1   | 1.94                     | 0.49              |
| 7:E:6:PHE:HE2    | 7:E:36:ASP:HB3   | 1.77                     | 0.49              |
| 17:O:82:ILE:HD13 | 17:O:88:ARG:HG3  | 1.94                     | 0.49              |
| 18:P:8:ARG:HB2   | 18:P:28:ARG:NH1  | 2.27                     | 0.49              |
| 18:P:31:LYS:HB3  | 18:P:31:LYS:NZ   | 2.27                     | 0.49              |
| 1:A:1412:C:H2'   | 1:A:1413:A:C8    | 2.48                     | 0.49              |
| 1:A:57:G:H2'     | 1:A:58:C:C6      | 2.46                     | 0.49              |
| 1:A:782:A:H2'    | 1:A:783:C:O4'    | 2.12                     | 0.49              |
| 6:D:6:GLY:O      | 6:D:8:VAL:HG23   | 2.11                     | 0.49              |
| 9:G:136:LYS:O    | 9:G:139:GLU:N    | 2.45                     | 0.49              |
| 10:H:20:TYR:CE2  | 10:H:75:ARG:HD2  | 2.48                     | 0.49              |
| 16:N:9:LYS:HE2   | 16:N:22:THR:O    | 2.12                     | 0.49              |
| 19:Q:45:HIS:HB3  | 19:Q:72:ARG:HG2  | 1.93                     | 0.49              |
| 21:S:53:ASN:N    | 21:S:53:ASN:HD22 | 2.07                     | 0.49              |
| 1:A:1196:U:H5''  | 1:A:1197:G:C5'   | 2.40                     | 0.49              |
| 1:A:1317:C:OP1   | 16:N:17:LYS:HG2  | 2.12                     | 0.49              |
| 1:A:375:U:O2     | 18:P:28:ARG:NE   | 2.39                     | 0.49              |
| 1:A:530:G:H1'    | 3:X:35:U:O2'     | 2.12                     | 0.49              |
| 1:A:794:A:H2'    | 1:A:795:C:C6     | 2.47                     | 0.49              |
| 4:B:18:GLY:CA    | 4:B:41:ILE:HA    | 2.32                     | 0.49              |
| 5:C:58:GLU:O     | 5:C:64:VAL:HA    | 2.12                     | 0.49              |
| 5:C:70:VAL:CG1   | 5:C:71:ALA:H     | 2.26                     | 0.49              |
| 6:D:196:LEU:CD2  | 6:D:197:PRO:HD2  | 2.43                     | 0.49              |
| 1:A:1080:A:O3'   | 7:E:16:THR:OG1   | 2.30                     | 0.49              |
| 9:G:122:HIS:HA   | 9:G:125:MET:HE3  | 1.94                     | 0.49              |
| 11:I:10:ARG:HD2  | 11:I:105:ASP:HB3 | 1.95                     | 0.49              |
| 12:J:45:ARG:O    | 12:J:64:GLU:HA   | 2.13                     | 0.49              |
| 1:A:1296:C:H5''  | 15:M:14:ARG:HD2  | 1.94                     | 0.49              |
| 1:A:1027:C:H3'   | 1:A:1028:C:H5''  | 1.92                     | 0.49              |
| 1:A:518:C:H2'    | 1:A:530:G:C2     | 2.47                     | 0.49              |
| 4:B:178:ARG:O    | 10:H:71:GLY:HA2  | 2.11                     | 0.49              |
| 11:I:10:ARG:HG2  | 11:I:75:ASP:HB2  | 1.94                     | 0.49              |
| 18:P:20:VAL:CG1  | 18:P:21:VAL:N    | 2.76                     | 0.49              |
| 20:R:47:THR:HG23 | 20:R:83:GLU:O    | 2.12                     | 0.49              |
| 1:A:26:A:N6      | 1:A:558:G:H1'    | 2.27                     | 0.49              |
| 1:A:513:C:H2'    | 1:A:514:C:H6     | 1.78                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:838:G:C2'     | 1:A:839:U:H5''    | 2.42                     | 0.49              |
| 5:C:77:ILE:CD1    | 5:C:84:ILE:HD12   | 2.43                     | 0.49              |
| 1:A:8:A:N6        | 6:D:209:ARG:HB2   | 2.27                     | 0.49              |
| 6:D:55:ALA:O      | 6:D:59:ARG:HG2    | 2.12                     | 0.49              |
| 8:F:19:LEU:O      | 8:F:19:LEU:HD23   | 2.12                     | 0.49              |
| 10:H:119:LEU:HD12 | 10:H:124:ALA:N    | 2.27                     | 0.49              |
| 11:I:28:VAL:HG22  | 11:I:63:ILE:HB    | 1.95                     | 0.49              |
| 13:K:49:GLY:O     | 13:K:50:TYR:C     | 2.50                     | 0.49              |
| 14:L:41:ARG:CG    | 14:L:42:THR:H     | 2.11                     | 0.49              |
| 1:A:1360:A:H2'    | 1:A:1361:G:C8     | 2.48                     | 0.49              |
| 5:C:139:GLN:O     | 5:C:143:GLU:N     | 2.46                     | 0.49              |
| 5:C:52:LEU:H      | 5:C:52:LEU:CD2    | 2.23                     | 0.49              |
| 7:E:80:ILE:CD1    | 7:E:91:LEU:HD12   | 2.41                     | 0.49              |
| 15:M:36:LYS:HD2   | 15:M:59:TYR:OH    | 2.12                     | 0.49              |
| 17:O:22:THR:O     | 17:O:27:VAL:HG11  | 2.13                     | 0.49              |
| 19:Q:68:ARG:O     | 19:Q:68:ARG:CG    | 2.61                     | 0.49              |
| 1:A:1019:C:H2'    | 1:A:1020:U:C6     | 2.48                     | 0.49              |
| 1:A:83:U:H2'      | 1:A:84:U:C6       | 2.48                     | 0.49              |
| 4:B:235:SER:C     | 4:B:237:ALA:N     | 2.65                     | 0.49              |
| 4:B:73:THR:HG23   | 4:B:95:GLN:O      | 2.13                     | 0.49              |
| 5:C:191:THR:HG21  | 5:C:193:TYR:CE2   | 2.46                     | 0.49              |
| 7:E:93:PRO:HG2    | 10:H:105:ARG:HH21 | 1.78                     | 0.49              |
| 9:G:58:PRO:HG2    | 9:G:59:LEU:H      | 1.78                     | 0.49              |
| 12:J:51:ARG:HG3   | 12:J:59:SER:HB3   | 1.94                     | 0.49              |
| 1:A:707:C:H4'     | 13:K:20:TYR:CD1   | 2.48                     | 0.49              |
| 15:M:40:ASN:HD22  | 15:M:41:PRO:N     | 2.11                     | 0.49              |
| 4:B:137:ARG:HH11  | 4:B:137:ARG:HB3   | 1.78                     | 0.49              |
| 5:C:30:ARG:HG2    | 5:C:30:ARG:NH1    | 2.26                     | 0.49              |
| 1:A:972:C:C4'     | 12:J:57:LYS:HG2   | 2.23                     | 0.49              |
| 15:M:98:VAL:O     | 15:M:98:VAL:HG12  | 2.13                     | 0.49              |
| 16:N:9:LYS:HD3    | 16:N:9:LYS:O      | 2.12                     | 0.49              |
| 18:P:42:ARG:O     | 18:P:43:LYS:C     | 2.50                     | 0.49              |
| 19:Q:67:LYS:CA    | 19:Q:70:ARG:HH12  | 2.24                     | 0.49              |
| 21:S:15:LEU:O     | 21:S:19:VAL:N     | 2.45                     | 0.49              |
| 2:W:3:A:C2'       | 2:W:4:A:H5'       | 2.42                     | 0.49              |
| 1:A:1130:A:OP2    | 1:A:1130:A:H3'    | 2.12                     | 0.48              |
| 1:A:1342:C:O2'    | 1:A:1343:G:H5'    | 2.13                     | 0.48              |
| 1:A:532:A:H5''    | 5:C:161:GLU:OE1   | 2.13                     | 0.48              |
| 4:B:164:VAL:HG21  | 4:B:170:GLU:HB3   | 1.94                     | 0.48              |
| 5:C:99:VAL:HG22   | 5:C:100:ALA:N     | 2.28                     | 0.48              |
| 7:E:72:GLN:O      | 7:E:73:ASN:CB     | 2.61                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 11:I:19:LEU:HB3  | 11:I:59:PHE:CD2  | 2.48                     | 0.48              |
| 1:A:1460:A:H2'   | 1:A:1461:G:O4'   | 2.13                     | 0.48              |
| 1:A:163:C:O2'    | 1:A:164:U:H5'    | 2.13                     | 0.48              |
| 1:A:662:G:O2'    | 1:A:836:G:H5'    | 2.13                     | 0.48              |
| 1:A:865:A:H2'    | 1:A:866:C:C6     | 2.48                     | 0.48              |
| 1:A:996:A:H2'    | 1:A:997:U:C6     | 2.48                     | 0.48              |
| 4:B:23:ARG:O     | 4:B:24:TRP:O     | 2.31                     | 0.48              |
| 5:C:34:LEU:HD11  | 5:C:38:ARG:NH2   | 2.29                     | 0.48              |
| 6:D:72:GLU:HA    | 6:D:72:GLU:OE2   | 2.13                     | 0.48              |
| 9:G:125:MET:O    | 9:G:129:GLU:HG2  | 2.13                     | 0.48              |
| 9:G:78:ARG:HB2   | 9:G:156:TRP:CZ3  | 2.48                     | 0.48              |
| 1:A:1291:G:O2'   | 11:I:38:GLN:HB3  | 2.13                     | 0.48              |
| 21:S:20:LEU:HA   | 21:S:23:ASN:HD22 | 1.79                     | 0.48              |
| 1:A:84:U:H2'     | 1:A:88:A:C8      | 2.49                     | 0.48              |
| 1:A:924:C:H5'    | 1:A:1399:C:OP2   | 2.13                     | 0.48              |
| 6:D:148:VAL:HG11 | 6:D:158:ILE:HD13 | 1.95                     | 0.48              |
| 6:D:7:PRO:HG2    | 6:D:10:ARG:HD2   | 1.94                     | 0.48              |
| 7:E:37:ARG:NH1   | 7:E:37:ARG:HG2   | 2.28                     | 0.48              |
| 10:H:10:LEU:CD2  | 10:H:83:ILE:HD11 | 2.37                     | 0.48              |
| 16:N:35:ARG:C    | 16:N:37:PHE:H    | 2.16                     | 0.48              |
| 18:P:39:TYR:CE2  | 18:P:41:PRO:HG3  | 2.47                     | 0.48              |
| 20:R:87:ARG:O    | 20:R:88:LYS:HB3  | 2.13                     | 0.48              |
| 21:S:4:SER:O     | 21:S:5:LEU:HG    | 2.13                     | 0.48              |
| 1:A:1194:U:H2'   | 1:A:1195:C:C6    | 2.48                     | 0.48              |
| 1:A:1425:U:H2'   | 1:A:1426:C:H6    | 1.76                     | 0.48              |
| 1:A:399:G:H2'    | 1:A:400:C:C6     | 2.48                     | 0.48              |
| 1:A:403:C:O2'    | 1:A:404:U:H5'    | 2.12                     | 0.48              |
| 1:A:41:G:H2'     | 1:A:42:G:H8      | 1.77                     | 0.48              |
| 1:A:498:U:O2'    | 1:A:499:A:H5'    | 2.13                     | 0.48              |
| 1:A:942:G:H2'    | 1:A:943:U:H6     | 1.77                     | 0.48              |
| 5:C:150:LYS:HB2  | 5:C:169:ALA:HB2  | 1.95                     | 0.48              |
| 1:A:542:G:OP1    | 6:D:10:ARG:NH2   | 2.46                     | 0.48              |
| 7:E:13:ILE:O     | 7:E:13:ILE:HG13  | 2.13                     | 0.48              |
| 7:E:15:ARG:O     | 7:E:15:ARG:HD2   | 2.14                     | 0.48              |
| 15:M:40:ASN:HD22 | 15:M:40:ASN:C    | 2.15                     | 0.48              |
| 17:O:14:GLU:HG3  | 17:O:15:PHE:CE1  | 2.48                     | 0.48              |
| 17:O:25:THR:CG2  | 17:O:70:LEU:HD23 | 2.42                     | 0.48              |
| 1:A:1060:C:O2'   | 1:A:1061:G:H5'   | 2.14                     | 0.48              |
| 1:A:1137:C:H4'   | 1:A:1138:G:N1    | 2.27                     | 0.48              |
| 1:A:337:C:H2'    | 1:A:338:A:H8     | 1.78                     | 0.48              |
| 1:A:112:G:H21    | 1:A:354:G:C5'    | 2.24                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:575:G:OP1    | 1:A:575:G:H4'    | 2.13                     | 0.48              |
| 1:A:840:C:H4'    | 1:A:841:U:O5'    | 2.13                     | 0.48              |
| 4:B:100:GLY:O    | 4:B:104:ASN:N    | 2.41                     | 0.48              |
| 7:E:11:ILE:HG12  | 7:E:33:VAL:HG23  | 1.95                     | 0.48              |
| 16:N:14:PRO:O    | 16:N:15:LYS:HB2  | 2.14                     | 0.48              |
| 17:O:2:PRO:C     | 17:O:3:ILE:HD12  | 2.33                     | 0.48              |
| 20:R:25:THR:O    | 20:R:26:LEU:HB2  | 2.13                     | 0.48              |
| 1:A:192:U:H1'    | 22:T:103:GLY:HA2 | 1.95                     | 0.48              |
| 1:A:1343:G:O2'   | 1:A:1344:C:H5'   | 2.14                     | 0.48              |
| 4:B:17:PHE:O     | 4:B:18:GLY:C     | 2.51                     | 0.48              |
| 5:C:195:VAL:C    | 5:C:196:LEU:HD22 | 2.34                     | 0.48              |
| 14:L:53:ARG:CG   | 14:L:69:TYR:HE1  | 2.26                     | 0.48              |
| 15:M:2:ALA:HB3   | 15:M:53:VAL:HG11 | 1.95                     | 0.48              |
| 23:V:2:GLY:O     | 23:V:4:GLY:N     | 2.47                     | 0.48              |
| 1:A:1053:G:O2'   | 1:A:1199:U:H5    | 1.96                     | 0.48              |
| 1:A:1238:A:H5'   | 1:A:1336:C:N4    | 2.26                     | 0.48              |
| 1:A:481:G:O2'    | 1:A:482:A:N7     | 2.34                     | 0.48              |
| 1:A:74:C:C2'     | 1:A:75:G:H5'     | 2.42                     | 0.48              |
| 5:C:108:ASN:C    | 5:C:110:ASN:H    | 2.17                     | 0.48              |
| 5:C:39:ILE:HG22  | 5:C:40:ARG:N     | 2.28                     | 0.48              |
| 9:G:135:VAL:O    | 9:G:139:GLU:HG3  | 2.13                     | 0.48              |
| 10:H:60:ARG:HG3  | 10:H:60:ARG:HH11 | 1.79                     | 0.48              |
| 11:I:93:ARG:C    | 11:I:95:LYS:H    | 2.17                     | 0.48              |
| 14:L:117:ARG:NH2 | 14:L:124:LYS:HA  | 2.29                     | 0.48              |
| 17:O:3:ILE:HD11  | 17:O:38:ARG:HG3  | 1.96                     | 0.48              |
| 17:O:87:ILE:HG22 | 17:O:88:ARG:HG2  | 1.95                     | 0.48              |
| 21:S:19:VAL:HG13 | 21:S:20:LEU:N    | 2.29                     | 0.48              |
| 22:T:72:LEU:HD13 | 22:T:77:ALA:HA   | 1.96                     | 0.48              |
| 1:A:107:G:H2'    | 1:A:108:G:H5'    | 1.96                     | 0.48              |
| 1:A:136:C:H2'    | 1:A:137:C:H6     | 1.79                     | 0.48              |
| 1:A:975:A:C4'    | 1:A:976:G:H5'    | 2.42                     | 0.48              |
| 4:B:124:SER:HB2  | 4:B:125:PRO:CD   | 2.40                     | 0.48              |
| 5:C:150:LYS:HB3  | 5:C:169:ALA:CB   | 2.44                     | 0.48              |
| 5:C:50:ALA:HB1   | 5:C:70:VAL:HG11  | 1.96                     | 0.48              |
| 12:J:64:GLU:HG2  | 16:N:59:ALA:HB2  | 1.95                     | 0.48              |
| 15:M:14:ARG:NH1  | 15:M:16:ASP:OD1  | 2.47                     | 0.48              |
| 15:M:78:ILE:HA   | 15:M:81:LEU:HD21 | 1.95                     | 0.48              |
| 21:S:71:LEU:N    | 21:S:71:LEU:HD12 | 2.29                     | 0.48              |
| 1:A:1152:A:H2'   | 1:A:1153:C:C6    | 2.49                     | 0.48              |
| 1:A:1251:A:H2'   | 1:A:1252:A:H8    | 1.79                     | 0.48              |
| 1:A:255:G:H1'    | 19:Q:16:GLN:NE2  | 2.28                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:939:G:H5'    | 9:G:102:ARG:HH22  | 1.74                     | 0.48              |
| 4:B:15:VAL:HG21  | 4:B:213:LEU:HD13  | 1.95                     | 0.48              |
| 4:B:30:ARG:HG2   | 4:B:31:TYR:CD1    | 2.48                     | 0.48              |
| 9:G:92:SER:O     | 9:G:96:GLN:HB2    | 2.14                     | 0.48              |
| 13:K:51:LYS:O    | 13:K:51:LYS:HD3   | 2.14                     | 0.48              |
| 1:A:1195:C:H2'   | 1:A:1197:G:H5'    | 1.96                     | 0.48              |
| 1:A:262:A:C6     | 1:A:263:A:C6      | 3.01                     | 0.48              |
| 1:A:393:A:O2'    | 1:A:394:G:H5'     | 2.14                     | 0.48              |
| 1:A:485:G:O2'    | 1:A:486:U:H5      | 1.95                     | 0.48              |
| 1:A:828:A:H2'    | 1:A:829:G:O4'     | 2.13                     | 0.48              |
| 5:C:30:ARG:HH11  | 5:C:30:ARG:HG2    | 1.78                     | 0.48              |
| 6:D:126:ILE:HG22 | 6:D:127:THR:N     | 2.28                     | 0.48              |
| 6:D:30:LYS:O     | 6:D:32:ALA:N      | 2.47                     | 0.48              |
| 6:D:80:GLU:O     | 6:D:84:LYS:HG3    | 2.14                     | 0.48              |
| 10:H:86:ILE:HD12 | 10:H:133:LEU:HD22 | 1.96                     | 0.48              |
| 12:J:72:VAL:HG12 | 12:J:73:ASP:N     | 2.29                     | 0.48              |
| 18:P:20:VAL:CG1  | 18:P:32:TYR:CB    | 2.85                     | 0.48              |
| 21:S:80:TYR:O    | 21:S:81:ARG:HB3   | 2.14                     | 0.48              |
| 1:A:1010:G:H2'   | 1:A:1011:G:H8     | 1.79                     | 0.47              |
| 1:A:849:C:O2'    | 1:A:850:U:H5'     | 2.13                     | 0.47              |
| 1:A:895:G:H2'    | 1:A:896:C:C6      | 2.48                     | 0.47              |
| 4:B:178:ARG:HH22 | 10:H:74:PRO:HB3   | 1.79                     | 0.47              |
| 12:J:5:ARG:CD    | 12:J:99:LYS:HB2   | 2.43                     | 0.47              |
| 12:J:61:GLU:OE1  | 16:N:45:ARG:NH1   | 2.40                     | 0.47              |
| 14:L:8:ASN:O     | 14:L:12:ARG:HG3   | 2.14                     | 0.47              |
| 22:T:50:GLU:HB2  | 22:T:99:LEU:HD12  | 1.96                     | 0.47              |
| 1:A:1007:C:H2'   | 1:A:1008:C:C6     | 2.48                     | 0.47              |
| 1:A:1041:A:H2'   | 1:A:1042:G:C8     | 2.49                     | 0.47              |
| 1:A:1470:G:O2'   | 1:A:1471:G:H5'    | 2.14                     | 0.47              |
| 1:A:102:G:N3     | 1:A:151:A:H2      | 2.12                     | 0.47              |
| 1:A:339:C:H2'    | 1:A:340:U:H6      | 1.80                     | 0.47              |
| 1:A:339:C:H2'    | 1:A:340:U:C6      | 2.49                     | 0.47              |
| 1:A:448:A:H2'    | 1:A:449:C:C6      | 2.48                     | 0.47              |
| 1:A:953:G:O2'    | 1:A:954:G:H5'     | 2.13                     | 0.47              |
| 6:D:157:LEU:HD23 | 6:D:157:LEU:O     | 2.14                     | 0.47              |
| 8:F:91:VAL:HG13  | 20:R:72:ARG:HH22  | 1.79                     | 0.47              |
| 10:H:111:ILE:O   | 10:H:134:ILE:HB   | 2.14                     | 0.47              |
| 1:A:1363:A:H1'   | 1:A:1365:G:N7     | 2.28                     | 0.47              |
| 1:A:180:U:C2'    | 1:A:181:G:H5'     | 2.43                     | 0.47              |
| 1:A:485:G:O2'    | 1:A:486:U:C5      | 2.68                     | 0.47              |
| 1:A:895:G:H2'    | 1:A:896:C:H6      | 1.79                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:913:A:OP2     | 14:L:91:LYS:HE3   | 2.14                     | 0.47              |
| 6:D:36:ARG:N      | 6:D:37:PRO:CD     | 2.66                     | 0.47              |
| 14:L:33:ARG:HD2   | 14:L:33:ARG:HA    | 1.51                     | 0.47              |
| 17:O:70:LEU:HD12  | 17:O:78:TYR:CB    | 2.41                     | 0.47              |
| 17:O:87:ILE:O     | 17:O:88:ARG:HB2   | 2.13                     | 0.47              |
| 1:A:1285:A:C8     | 1:A:1285:A:OP1    | 2.67                     | 0.47              |
| 1:A:1372:U:H2'    | 1:A:1373:G:O4'    | 2.14                     | 0.47              |
| 1:A:67:C:O2'      | 1:A:171:A:H1'     | 2.14                     | 0.47              |
| 1:A:186:C:H2'     | 1:A:187:C:C6      | 2.48                     | 0.47              |
| 1:A:864:A:H2'     | 1:A:865:A:C8      | 2.50                     | 0.47              |
| 1:A:974:A:OP2     | 16:N:29:ARG:NH2   | 2.47                     | 0.47              |
| 4:B:82:ARG:O      | 4:B:86:GLU:HG3    | 2.15                     | 0.47              |
| 9:G:115:ARG:HB2   | 9:G:118:VAL:CG2   | 2.43                     | 0.47              |
| 13:K:29:ILE:C     | 13:K:29:ILE:HD12  | 2.35                     | 0.47              |
| 19:Q:59:ILE:CG2   | 19:Q:71:PHE:CD1   | 2.94                     | 0.47              |
| 20:R:22:VAL:O     | 20:R:22:VAL:HG12  | 2.14                     | 0.47              |
| 21:S:33:THR:CG2   | 21:S:35:SER:H     | 2.07                     | 0.47              |
| 1:A:818:G:C3'     | 1:A:819:A:H5''    | 2.44                     | 0.47              |
| 4:B:16:HIS:CE1    | 4:B:214:ILE:HG12  | 2.49                     | 0.47              |
| 5:C:131:ARG:O     | 5:C:135:LYS:HB2   | 2.14                     | 0.47              |
| 5:C:123:GLN:HE22  | 5:C:140:ARG:HH22  | 1.57                     | 0.47              |
| 6:D:149:ALA:O     | 6:D:152:SER:N     | 2.37                     | 0.47              |
| 10:H:119:LEU:HD12 | 10:H:124:ALA:CA   | 2.45                     | 0.47              |
| 11:I:10:ARG:HE    | 11:I:105:ASP:HB3  | 1.80                     | 0.47              |
| 13:K:103:LEU:HD23 | 13:K:104:GLN:N    | 2.30                     | 0.47              |
| 13:K:13:GLN:HA    | 13:K:75:TYR:O     | 2.15                     | 0.47              |
| 13:K:15:ALA:O     | 13:K:77:MET:HA    | 2.14                     | 0.47              |
| 14:L:56:ALA:O     | 14:L:67:THR:HA    | 2.15                     | 0.47              |
| 15:M:80:ARG:C     | 15:M:82:MET:H     | 2.18                     | 0.47              |
| 8:F:50:TYR:CE1    | 20:R:77:GLY:HA2   | 2.49                     | 0.47              |
| 1:A:1289:A:H2'    | 1:A:1290:G:H5'    | 1.97                     | 0.47              |
| 1:A:1392:G:N2     | 1:A:1502:A:C8     | 2.81                     | 0.47              |
| 1:A:1405:G:P      | 24:A:1545:PAR:O34 | 2.73                     | 0.47              |
| 1:A:270:A:H2'     | 1:A:271:C:C6      | 2.50                     | 0.47              |
| 1:A:302:G:H5''    | 14:L:17:LYS:NZ    | 2.29                     | 0.47              |
| 1:A:820:U:H4'     | 1:A:821:G:OP2     | 2.15                     | 0.47              |
| 1:A:900:A:H2'     | 1:A:901:A:C8      | 2.50                     | 0.47              |
| 1:A:946:A:H2'     | 1:A:947:G:H8      | 1.76                     | 0.47              |
| 4:B:23:ARG:HH11   | 4:B:24:TRP:CA     | 2.27                     | 0.47              |
| 8:F:2:ARG:CD      | 8:F:69:GLU:HG2    | 2.45                     | 0.47              |
| 9:G:126:ASP:OD1   | 9:G:131:LYS:HE3   | 2.15                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:H:119:LEU:HD12 | 10:H:124:ALA:HA   | 1.97                     | 0.47              |
| 12:J:60:ARG:O     | 12:J:61:GLU:O     | 2.33                     | 0.47              |
| 15:M:118:ALA:HB1  | 15:M:121:LYS:NZ   | 2.30                     | 0.47              |
| 15:M:40:ASN:HD22  | 15:M:41:PRO:HD2   | 1.78                     | 0.47              |
| 18:P:17:TYR:HE1   | 18:P:41:PRO:HG2   | 1.79                     | 0.47              |
| 20:R:53:ARG:HG2   | 20:R:63:GLN:OE1   | 2.14                     | 0.47              |
| 1:A:1320:C:C2     | 21:S:72:GLY:HA3   | 2.49                     | 0.47              |
| 1:A:1305:G:H22    | 1:A:1331:G:H2'    | 1.79                     | 0.47              |
| 1:A:975:A:O2'     | 1:A:976:G:OP2     | 2.25                     | 0.47              |
| 4:B:23:ARG:NH1    | 4:B:24:TRP:HA     | 2.30                     | 0.47              |
| 6:D:64:LEU:HB2    | 6:D:198:VAL:HG11  | 1.95                     | 0.47              |
| 11:I:23:ASN:ND2   | 11:I:23:ASN:C     | 2.68                     | 0.47              |
| 12:J:94:VAL:HG12  | 12:J:95:GLU:H     | 1.79                     | 0.47              |
| 17:O:21:ASP:OD2   | 17:O:24:SER:HB3   | 2.15                     | 0.47              |
| 18:P:71:ARG:HD3   | 18:P:75:ARG:HH21  | 1.80                     | 0.47              |
| 21:S:64:GLU:OE2   | 21:S:67:VAL:HG21  | 2.15                     | 0.47              |
| 22:T:77:ALA:O     | 22:T:80:ARG:HB2   | 2.14                     | 0.47              |
| 1:A:1133:G:H2'    | 1:A:1134:G:C8     | 2.47                     | 0.47              |
| 1:A:1229:A:N6     | 15:M:105:THR:HG22 | 2.29                     | 0.47              |
| 1:A:383:A:H2'     | 1:A:384:G:H5'     | 1.97                     | 0.47              |
| 1:A:961:U:C2'     | 1:A:962:C:H5'     | 2.44                     | 0.47              |
| 4:B:164:VAL:HG12  | 4:B:186:ALA:CB    | 2.44                     | 0.47              |
| 5:C:147:LYS:HE2   | 5:C:205:GLY:N     | 2.30                     | 0.47              |
| 5:C:150:LYS:CB    | 5:C:169:ALA:HB2   | 2.45                     | 0.47              |
| 8:F:23:LYS:O      | 8:F:27:GLN:HG2    | 2.14                     | 0.47              |
| 8:F:33:TYR:HB2    | 8:F:75:LEU:HD23   | 1.96                     | 0.47              |
| 11:I:82:ALA:O     | 11:I:86:VAL:HG23  | 2.15                     | 0.47              |
| 13:K:115:PRO:C    | 13:K:117:ASN:H    | 2.18                     | 0.47              |
| 21:S:12:ASP:HB3   | 21:S:14:HIS:CD2   | 2.49                     | 0.47              |
| 1:A:291:C:O2'     | 1:A:292:G:H5'     | 2.15                     | 0.47              |
| 1:A:32:A:H2'      | 1:A:33:A:C8       | 2.49                     | 0.47              |
| 1:A:344:A:O2'     | 1:A:345:C:OP1     | 2.31                     | 0.47              |
| 1:A:611:A:H2      | 1:A:630:G:N2      | 2.13                     | 0.47              |
| 1:A:1109:C:OP2    | 5:C:176:HIS:CD2   | 2.68                     | 0.47              |
| 9:G:121:ALA:HB1   | 9:G:125:MET:HE2   | 1.96                     | 0.47              |
| 11:I:44:VAL:HG12  | 11:I:51:ARG:HH22  | 1.80                     | 0.47              |
| 1:A:1011:G:C2'    | 1:A:1012:U:H5'    | 2.44                     | 0.47              |
| 1:A:190:C:O4'     | 1:A:190:C:O2      | 2.33                     | 0.47              |
| 1:A:335:C:H2'     | 1:A:336:C:C6      | 2.49                     | 0.47              |
| 4:B:101:MET:CA    | 4:B:108:ILE:HD12  | 2.44                     | 0.47              |
| 4:B:178:ARG:NH2   | 10:H:74:PRO:HG3   | 2.30                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:B:228:GLY:O    | 4:B:229:VAL:C     | 2.53                     | 0.47              |
| 5:C:47:LEU:N     | 5:C:47:LEU:HD12   | 2.29                     | 0.47              |
| 7:E:149:GLU:O    | 7:E:153:LYS:HG2   | 2.15                     | 0.47              |
| 9:G:138:LYS:HE2  | 9:G:142:GLU:OE1   | 2.14                     | 0.47              |
| 12:J:30:SER:HB2  | 12:J:81:THR:N     | 2.30                     | 0.47              |
| 13:K:82:VAL:HG23 | 13:K:105:VAL:HG13 | 1.97                     | 0.47              |
| 14:L:26:ALA:O    | 14:L:27:LEU:O     | 2.33                     | 0.47              |
| 1:A:1066:C:C2'   | 1:A:1067:A:H5'    | 2.45                     | 0.47              |
| 1:A:1505:G:H2'   | 1:A:1541:U:OP2    | 2.14                     | 0.47              |
| 1:A:405:U:O4     | 6:D:2:GLY:HA3     | 2.15                     | 0.47              |
| 4:B:12:GLU:CD    | 4:B:213:LEU:HD11  | 2.35                     | 0.47              |
| 1:A:521:G:OP1    | 14:L:73:GLU:O     | 2.33                     | 0.47              |
| 15:M:67:GLU:HB3  | 15:M:68:GLY:H     | 1.52                     | 0.47              |
| 1:A:1069:C:O2'   | 1:A:1192:C:H1'    | 2.15                     | 0.46              |
| 1:A:1176:A:H2'   | 1:A:1177:G:H8     | 1.78                     | 0.46              |
| 1:A:674:G:H2'    | 1:A:675:A:H8      | 1.79                     | 0.46              |
| 4:B:187:LEU:HD12 | 4:B:201:ILE:O     | 2.15                     | 0.46              |
| 7:E:11:ILE:CG2   | 7:E:12:LEU:HD12   | 2.44                     | 0.46              |
| 8:F:40:VAL:CG2   | 8:F:41:GLU:N      | 2.79                     | 0.46              |
| 8:F:44:GLY:O     | 8:F:59:TYR:HA     | 2.16                     | 0.46              |
| 10:H:118:VAL:C   | 10:H:119:LEU:HD23 | 2.34                     | 0.46              |
| 11:I:48:GLU:N    | 11:I:49:PRO:CD    | 2.78                     | 0.46              |
| 22:T:100:ILE:O   | 22:T:102:GLY:N    | 2.48                     | 0.46              |
| 1:A:1038:C:H2'   | 1:A:1039:C:C5     | 2.50                     | 0.46              |
| 1:A:1499:A:O2'   | 1:A:1500:A:H5'    | 2.14                     | 0.46              |
| 1:A:722:A:N3     | 1:A:722:A:H3'     | 2.29                     | 0.46              |
| 5:C:61:ALA:C     | 5:C:63:ASN:H      | 2.19                     | 0.46              |
| 5:C:43:LEU:CD2   | 5:C:68:VAL:HG21   | 2.45                     | 0.46              |
| 1:A:921:U:O2     | 7:E:19:MET:HB2    | 2.14                     | 0.46              |
| 8:F:26:ILE:HG21  | 8:F:63:TYR:HE2    | 1.79                     | 0.46              |
| 10:H:90:GLY:O    | 10:H:91:ARG:HB2   | 2.15                     | 0.46              |
| 11:I:44:VAL:HG12 | 11:I:51:ARG:NH2   | 2.29                     | 0.46              |
| 1:A:1128:C:H42   | 1:A:1143:G:H1     | 1.64                     | 0.46              |
| 1:A:1326:C:OP1   | 23:V:12:LYS:NZ    | 2.45                     | 0.46              |
| 1:A:1521:G:H2'   | 1:A:1522:U:H6     | 1.79                     | 0.46              |
| 5:C:25:GLY:C     | 5:C:27:LYS:H      | 2.19                     | 0.46              |
| 5:C:43:LEU:O     | 5:C:47:LEU:HB2    | 2.16                     | 0.46              |
| 6:D:4:TYR:O      | 6:D:5:ILE:HB      | 2.15                     | 0.46              |
| 1:A:8:A:H5'      | 7:E:101:ILE:HG22  | 1.96                     | 0.46              |
| 11:I:5:TYR:CD1   | 11:I:5:TYR:C      | 2.89                     | 0.46              |
| 13:K:33:THR:HB   | 13:K:38:ASN:C     | 2.36                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 15:M:33:ALA:HA   | 15:M:59:TYR:CE2  | 2.51                     | 0.46              |
| 1:A:1313:U:O4    | 21:S:4:SER:HB2   | 2.15                     | 0.46              |
| 1:A:1124:G:H3'   | 1:A:1145:C:C4    | 2.49                     | 0.46              |
| 1:A:1141:C:H2'   | 1:A:1142:G:H8    | 1.81                     | 0.46              |
| 1:A:190(J):U:O2' | 1:A:190(K):G:H5' | 2.16                     | 0.46              |
| 1:A:200:G:H2'    | 1:A:201:C:O4'    | 2.15                     | 0.46              |
| 1:A:252:U:H2'    | 1:A:253:U:C6     | 2.50                     | 0.46              |
| 1:A:647:C:O2'    | 1:A:648:A:H5'    | 2.14                     | 0.46              |
| 1:A:833:U:H2'    | 1:A:834:C:C6     | 2.50                     | 0.46              |
| 5:C:155:GLY:HA2  | 5:C:164:ARG:H    | 1.80                     | 0.46              |
| 8:F:4:TYR:HD1    | 8:F:92:LYS:HA    | 1.80                     | 0.46              |
| 12:J:26:ALA:HB1  | 12:J:84:GLN:CB   | 2.45                     | 0.46              |
| 1:A:1203:C:O2'   | 1:A:1204:A:H5'   | 2.16                     | 0.46              |
| 1:A:692:U:H2'    | 1:A:694:A:OP2    | 2.16                     | 0.46              |
| 5:C:111:LEU:HD21 | 5:C:144:SER:O    | 2.15                     | 0.46              |
| 5:C:18:TRP:HB3   | 16:N:51:GLY:O    | 2.16                     | 0.46              |
| 5:C:84:ILE:O     | 5:C:84:ILE:HG12  | 2.15                     | 0.46              |
| 6:D:91:SER:O     | 6:D:94:LEU:N     | 2.49                     | 0.46              |
| 7:E:48:ALA:HB1   | 7:E:49:PRO:HD2   | 1.97                     | 0.46              |
| 8:F:9:VAL:HB     | 8:F:87:ARG:HB2   | 1.96                     | 0.46              |
| 11:I:27:THR:HG23 | 11:I:30:GLY:O    | 2.15                     | 0.46              |
| 12:J:12:ASP:HB3  | 12:J:15:THR:CG2  | 2.45                     | 0.46              |
| 12:J:26:ALA:HB1  | 12:J:84:GLN:HB3  | 1.97                     | 0.46              |
| 12:J:8:LEU:HD23  | 12:J:96:ILE:HG12 | 1.97                     | 0.46              |
| 15:M:107:ALA:O   | 15:M:111:LYS:HG3 | 2.15                     | 0.46              |
| 16:N:23:ARG:HG3  | 16:N:23:ARG:HH11 | 1.80                     | 0.46              |
| 22:T:50:GLU:HB2  | 22:T:99:LEU:CD1  | 2.46                     | 0.46              |
| 1:A:1544:U:O3'   | 2:W:1:A:O5'      | 2.31                     | 0.46              |
| 1:A:1365:G:C6    | 1:A:1366:C:C4    | 3.04                     | 0.46              |
| 1:A:333:G:H4'    | 22:T:16:HIS:CD2  | 2.51                     | 0.46              |
| 1:A:392:G:H2'    | 1:A:393:A:H8     | 1.81                     | 0.46              |
| 1:A:97:G:H2'     | 1:A:98:U:O4'     | 2.16                     | 0.46              |
| 4:B:136:VAL:HG12 | 4:B:140:HIS:CD2  | 2.50                     | 0.46              |
| 5:C:103:VAL:HG12 | 5:C:104:GLN:N    | 2.29                     | 0.46              |
| 9:G:15:ASP:OD2   | 9:G:16:LEU:N     | 2.48                     | 0.46              |
| 11:I:10:ARG:O    | 11:I:11:LYS:C    | 2.53                     | 0.46              |
| 15:M:121:LYS:O   | 15:M:122:LYS:HB2 | 2.16                     | 0.46              |
| 15:M:124:PRO:HB3 | 15:M:126:LYS:HE3 | 1.97                     | 0.46              |
| 15:M:65:LYS:HE3  | 15:M:69:GLU:OE2  | 2.15                     | 0.46              |
| 1:A:1263:C:H2'   | 1:A:1264:C:C6    | 2.50                     | 0.46              |
| 1:A:1287:A:H2'   | 1:A:1288:A:C8    | 2.51                     | 0.46              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:1307:U:H2'    | 1:A:1308:U:C6    | 2.51                     | 0.46              |
| 1:A:204:U:H5'     | 1:A:216:G:OP1    | 2.15                     | 0.46              |
| 1:A:939:G:H5''    | 9:G:102:ARG:CZ   | 2.45                     | 0.46              |
| 4:B:16:HIS:HA     | 4:B:204:ASN:OD1  | 2.16                     | 0.46              |
| 4:B:60:ASP:O      | 4:B:64:ARG:HB2   | 2.15                     | 0.46              |
| 4:B:7:VAL:CG1     | 4:B:221:LEU:HD23 | 2.46                     | 0.46              |
| 5:C:134:ILE:O     | 5:C:138:VAL:HG23 | 2.16                     | 0.46              |
| 6:D:65:ARG:HG3    | 6:D:75:PHE:CD1   | 2.51                     | 0.46              |
| 7:E:18:ARG:HE     | 7:E:25:ARG:HB2   | 1.81                     | 0.46              |
| 12:J:14:LYS:C     | 12:J:16:LEU:N    | 2.68                     | 0.46              |
| 16:N:26:ARG:NH1   | 16:N:47:LEU:HG   | 2.31                     | 0.46              |
| 18:P:1:MET:HE3    | 18:P:3:LYS:HE3   | 1.98                     | 0.46              |
| 18:P:53:VAL:HG23  | 18:P:54:GLU:N    | 2.30                     | 0.46              |
| 19:Q:48:GLU:O     | 19:Q:50:LYS:N    | 2.49                     | 0.46              |
| 22:T:67:ALA:HA    | 22:T:73:HIS:H    | 1.80                     | 0.46              |
| 22:T:96:GLY:O     | 22:T:97:ALA:HB3  | 2.16                     | 0.46              |
| 1:A:1260:C:O5'    | 1:A:1284:C:H4'   | 2.15                     | 0.46              |
| 1:A:1305:G:N2     | 1:A:1331:G:C2'   | 2.78                     | 0.46              |
| 1:A:1376:U:H2'    | 1:A:1377:A:C8    | 2.50                     | 0.46              |
| 1:A:415:A:H3'     | 1:A:416:G:H5''   | 1.97                     | 0.46              |
| 7:E:32:VAL:HG23   | 7:E:58:ALA:CB    | 2.45                     | 0.46              |
| 11:I:28:VAL:HA    | 11:I:63:ILE:O    | 2.15                     | 0.46              |
| 13:K:15:ALA:O     | 13:K:78:GLN:N    | 2.48                     | 0.46              |
| 1:A:1054:C:C2'    | 1:A:1055:A:H5''  | 2.46                     | 0.46              |
| 1:A:1422:G:O2'    | 1:A:1423:G:H5'   | 2.16                     | 0.46              |
| 1:A:555:C:H2'     | 1:A:556:C:C6     | 2.51                     | 0.46              |
| 4:B:126:GLU:HA    | 4:B:129:GLU:OE1  | 2.16                     | 0.46              |
| 4:B:25:ASN:ND2    | 4:B:27:LYS:H     | 2.14                     | 0.46              |
| 4:B:17:PHE:CB     | 4:B:44:LEU:HD21  | 2.41                     | 0.46              |
| 6:D:191:ARG:O     | 6:D:191:ARG:HD2  | 2.16                     | 0.46              |
| 7:E:11:ILE:HG21   | 7:E:31:LEU:HD12  | 1.97                     | 0.46              |
| 10:H:97:VAL:HG21  | 10:H:128:GLY:HA2 | 1.98                     | 0.46              |
| 10:H:20:TYR:HE2   | 10:H:75:ARG:HD2  | 1.79                     | 0.46              |
| 13:K:126:ARG:HH11 | 13:K:126:ARG:HB3 | 1.80                     | 0.46              |
| 15:M:37:THR:O     | 15:M:55:ARG:NH1  | 2.43                     | 0.46              |
| 1:A:1202:G:C2'    | 1:A:1203:C:H5'   | 2.45                     | 0.46              |
| 1:A:1248:A:H1'    | 11:I:70:LYS:NZ   | 2.30                     | 0.46              |
| 1:A:960:U:O2      | 1:A:960:U:H2'    | 2.16                     | 0.46              |
| 4:B:213:LEU:HD23  | 4:B:213:LEU:C    | 2.36                     | 0.46              |
| 5:C:191:THR:HG22  | 5:C:193:TYR:H    | 1.81                     | 0.46              |
| 7:E:89:ILE:HD13   | 7:E:90:VAL:H     | 1.81                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:H:107:LEU:N    | 10:H:107:LEU:HD23 | 2.30                     | 0.46              |
| 13:K:12:ARG:O     | 13:K:13:GLN:O     | 2.32                     | 0.46              |
| 21:S:22:LEU:HD22  | 21:S:28:LYS:HB2   | 1.98                     | 0.46              |
| 1:A:1399:C:C2     | 1:A:1502:A:N6     | 2.84                     | 0.45              |
| 1:A:190(K):G:HO2' | 1:A:190(L):U:H6   | 1.59                     | 0.45              |
| 1:A:959:A:H2'     | 1:A:960:U:O4'     | 2.16                     | 0.45              |
| 4:B:76:GLN:HA     | 4:B:76:GLN:OE1    | 2.15                     | 0.45              |
| 5:C:172:ARG:NH2   | 5:C:203:PHE:HE2   | 2.14                     | 0.45              |
| 5:C:175:LEU:HD23  | 5:C:182:ILE:HD13  | 1.99                     | 0.45              |
| 6:D:7:PRO:CB      | 6:D:10:ARG:HD2    | 2.46                     | 0.45              |
| 7:E:69:VAL:HG22   | 7:E:139:LEU:HB3   | 1.97                     | 0.45              |
| 7:E:93:PRO:HG2    | 10:H:105:ARG:NH2  | 2.31                     | 0.45              |
| 9:G:16:LEU:N      | 9:G:16:LEU:HD22   | 2.31                     | 0.45              |
| 12:J:21:GLN:O     | 12:J:21:GLN:HG2   | 2.16                     | 0.45              |
| 12:J:26:ALA:O     | 12:J:27:ALA:HB2   | 2.16                     | 0.45              |
| 13:K:124:LYS:HD3  | 13:K:125:PHE:CE1  | 2.51                     | 0.45              |
| 18:P:7:ALA:O      | 18:P:17:TYR:HA    | 2.16                     | 0.45              |
| 1:A:1305:G:O2'    | 1:A:1306:A:C8     | 2.47                     | 0.45              |
| 1:A:363:A:H62     | 14:L:28:LYS:HE3   | 1.82                     | 0.45              |
| 1:A:406:G:H2'     | 1:A:407:G:H8      | 1.81                     | 0.45              |
| 1:A:686:U:O2'     | 1:A:687:A:C8      | 2.57                     | 0.45              |
| 1:A:7:G:H21       | 7:E:121:LYS:HG2   | 1.82                     | 0.45              |
| 1:A:840:C:H5'     | 1:A:848:C:O2      | 2.16                     | 0.45              |
| 4:B:9:GLU:OE2     | 4:B:12:GLU:HA     | 2.16                     | 0.45              |
| 4:B:95:GLN:HG3    | 4:B:147:LYS:O     | 2.16                     | 0.45              |
| 5:C:113:ALA:HB3   | 5:C:114:PRO:HD3   | 1.98                     | 0.45              |
| 5:C:155:GLY:O     | 5:C:156:ARG:CB    | 2.64                     | 0.45              |
| 6:D:25:ARG:C      | 6:D:27:TYR:N      | 2.68                     | 0.45              |
| 7:E:7:GLU:OE2     | 7:E:37:ARG:NE     | 2.47                     | 0.45              |
| 8:F:40:VAL:HG22   | 8:F:41:GLU:N      | 2.31                     | 0.45              |
| 8:F:41:GLU:O      | 8:F:43:LEU:N      | 2.49                     | 0.45              |
| 12:J:16:LEU:O     | 12:J:17:ASP:C     | 2.55                     | 0.45              |
| 1:A:302:G:H5''    | 14:L:17:LYS:HZ1   | 1.81                     | 0.45              |
| 21:S:62:ILE:HD12  | 21:S:66:MET:CG    | 2.45                     | 0.45              |
| 1:A:1071:C:H2'    | 1:A:1072:G:H8     | 1.82                     | 0.45              |
| 1:A:1142:G:H2'    | 1:A:1143:G:O4'    | 2.15                     | 0.45              |
| 1:A:1305:G:OP2    | 1:A:1305:G:H8     | 2.00                     | 0.45              |
| 1:A:1323:G:H2'    | 1:A:1324:A:C8     | 2.51                     | 0.45              |
| 1:A:149:A:H2'     | 1:A:150:C:H6      | 1.82                     | 0.45              |
| 1:A:178:C:O2'     | 1:A:179:A:H5'     | 2.16                     | 0.45              |
| 4:B:206:ASP:O     | 4:B:207:ALA:HB3   | 2.17                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:C:23:TYR:CG    | 5:C:24:ALA:N      | 2.84                     | 0.45              |
| 5:C:64:VAL:HG12  | 5:C:65:ALA:N      | 2.28                     | 0.45              |
| 7:E:11:ILE:HD11  | 7:E:33:VAL:HG21   | 1.98                     | 0.45              |
| 10:H:53:VAL:C    | 10:H:55:GLY:N     | 2.70                     | 0.45              |
| 12:J:60:ARG:HH11 | 12:J:60:ARG:HG2   | 1.81                     | 0.45              |
| 12:J:71:LEU:O    | 12:J:72:VAL:CB    | 2.64                     | 0.45              |
| 13:K:51:LYS:O    | 13:K:55:LYS:HE2   | 2.16                     | 0.45              |
| 15:M:8:GLU:C     | 15:M:9:ILE:HD12   | 2.36                     | 0.45              |
| 20:R:55:ARG:HB3  | 20:R:55:ARG:CZ    | 2.45                     | 0.45              |
| 21:S:62:ILE:CD1  | 21:S:66:MET:HG3   | 2.46                     | 0.45              |
| 1:A:105:G:H2'    | 1:A:106:C:C6      | 2.51                     | 0.45              |
| 1:A:1061:G:C2'   | 1:A:1062:U:H5'    | 2.47                     | 0.45              |
| 1:A:1182:G:C2'   | 1:A:1183:A:OP2    | 2.64                     | 0.45              |
| 1:A:1407:C:O2'   | 1:A:1408:A:H5'    | 2.16                     | 0.45              |
| 1:A:830:G:O2'    | 1:A:831:U:H5'     | 2.16                     | 0.45              |
| 5:C:6:HIS:HD2    | 5:C:8:ILE:H       | 1.65                     | 0.45              |
| 6:D:3:ARG:NH1    | 6:D:70:ILE:HA     | 2.31                     | 0.45              |
| 13:K:33:THR:HB   | 13:K:38:ASN:O     | 2.17                     | 0.45              |
| 21:S:71:LEU:H    | 21:S:71:LEU:HD12  | 1.82                     | 0.45              |
| 1:A:1072:G:H2'   | 1:A:1073:U:H6     | 1.77                     | 0.45              |
| 1:A:1117:G:O3'   | 11:I:104:ARG:HD2  | 2.16                     | 0.45              |
| 1:A:173:U:H6     | 1:A:198:G:HO2'    | 1.63                     | 0.45              |
| 1:A:860:A:H2'    | 1:A:861:G:O4'     | 2.17                     | 0.45              |
| 6:D:187:ARG:HG3  | 6:D:188:LEU:H     | 1.81                     | 0.45              |
| 14:L:83:VAL:HG11 | 14:L:100:ILE:HD13 | 1.98                     | 0.45              |
| 17:O:3:ILE:O     | 17:O:3:ILE:HG22   | 2.15                     | 0.45              |
| 1:A:671:G:H2'    | 1:A:672:U:C6      | 2.52                     | 0.45              |
| 1:A:810:C:H2'    | 1:A:811:C:C6      | 2.50                     | 0.45              |
| 1:A:942:G:H2'    | 1:A:943:U:C6      | 2.51                     | 0.45              |
| 4:B:204:ASN:HB2  | 4:B:210:SER:OG    | 2.15                     | 0.45              |
| 4:B:215:LEU:O    | 4:B:219:VAL:HG23  | 2.17                     | 0.45              |
| 9:G:78:ARG:NH1   | 9:G:154:TYR:HB3   | 2.31                     | 0.45              |
| 11:I:13:ALA:CB   | 11:I:67:GLY:O     | 2.65                     | 0.45              |
| 12:J:9:ARG:CB    | 12:J:9:ARG:NH1    | 2.80                     | 0.45              |
| 15:M:84:ILE:O    | 15:M:85:GLY:C     | 2.55                     | 0.45              |
| 17:O:26:GLU:HA   | 17:O:81:LEU:HD11  | 1.98                     | 0.45              |
| 18:P:18:ARG:NH1  | 18:P:32:TYR:OH    | 2.49                     | 0.45              |
| 20:R:38:GLU:OE1  | 20:R:38:GLU:N     | 2.38                     | 0.45              |
| 20:R:87:ARG:O    | 20:R:88:LYS:CB    | 2.64                     | 0.45              |
| 22:T:26:ASN:OD1  | 22:T:71:THR:HA    | 2.16                     | 0.45              |
| 1:A:1127:G:N2    | 1:A:1146:A:H62    | 2.14                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1296:C:H5'   | 1:A:1302:U:O4     | 2.16                     | 0.45              |
| 1:A:1251:A:H1'   | 1:A:1369:C:O2'    | 2.17                     | 0.45              |
| 1:A:1370:G:O2'   | 1:A:1371:G:H5'    | 2.16                     | 0.45              |
| 1:A:1413:A:C2    | 1:A:1488:G:C2     | 3.05                     | 0.45              |
| 1:A:457:C:H2'    | 1:A:458:C:H6      | 1.81                     | 0.45              |
| 1:A:474:G:H2'    | 1:A:475:G:C8      | 2.52                     | 0.45              |
| 1:A:791:G:H2'    | 1:A:792:A:C5'     | 2.47                     | 0.45              |
| 4:B:36:ARG:HD2   | 4:B:41:ILE:CD1    | 2.47                     | 0.45              |
| 9:G:120:ILE:N    | 9:G:120:ILE:HD12  | 2.31                     | 0.45              |
| 12:J:45:ARG:CB   | 12:J:45:ARG:HH11  | 2.18                     | 0.45              |
| 14:L:114:LYS:HA  | 14:L:114:LYS:HE2  | 1.98                     | 0.45              |
| 1:A:953:G:H1'    | 15:M:125:ARG:HA   | 1.99                     | 0.45              |
| 18:P:43:LYS:HA   | 18:P:48:TRP:HB3   | 1.99                     | 0.45              |
| 19:Q:98:LEU:CD1  | 19:Q:98:LEU:H     | 2.00                     | 0.45              |
| 22:T:48:LYS:O    | 22:T:52:ALA:HB2   | 2.17                     | 0.45              |
| 3:X:34:U:H2'     | 3:X:35:U:C6       | 2.51                     | 0.45              |
| 1:A:1183:A:O2'   | 1:A:1184:G:P      | 2.75                     | 0.45              |
| 1:A:176:C:O2'    | 1:A:177:C:H5'     | 2.17                     | 0.45              |
| 1:A:692:U:O2     | 1:A:695:A:H8      | 1.99                     | 0.45              |
| 4:B:27:LYS:HD3   | 4:B:195:ASP:OD2   | 2.17                     | 0.45              |
| 5:C:108:ASN:OD1  | 5:C:110:ASN:HB2   | 2.17                     | 0.45              |
| 7:E:69:VAL:HG21  | 7:E:139:LEU:HD13  | 1.99                     | 0.45              |
| 10:H:117:GLY:O   | 10:H:119:LEU:HD23 | 2.17                     | 0.45              |
| 18:P:20:VAL:HG12 | 18:P:21:VAL:N     | 2.31                     | 0.45              |
| 21:S:15:LEU:HD12 | 21:S:16:LEU:N     | 2.32                     | 0.45              |
| 1:A:255:G:O6     | 1:A:266:G:O6      | 2.35                     | 0.45              |
| 1:A:28:G:O2'     | 1:A:296:U:OP1     | 2.35                     | 0.45              |
| 1:A:701:C:H5''   | 1:A:702:A:H3'     | 1.99                     | 0.45              |
| 1:A:706:A:H1'    | 13:K:29:ILE:HD11  | 1.99                     | 0.45              |
| 4:B:54:THR:O     | 4:B:58:ILE:HG13   | 2.16                     | 0.45              |
| 5:C:167:TRP:O    | 5:C:168:ALA:HB3   | 2.17                     | 0.45              |
| 7:E:144:THR:CG2  | 7:E:145:LYS:N     | 2.80                     | 0.45              |
| 9:G:122:HIS:O    | 9:G:126:ASP:HB2   | 2.17                     | 0.45              |
| 9:G:22:LEU:O     | 9:G:25:ALA:HB3    | 2.17                     | 0.45              |
| 11:I:9:ARG:HD3   | 11:I:14:VAL:HG22  | 1.98                     | 0.45              |
| 19:Q:86:GLU:O    | 19:Q:87:LYS:C     | 2.54                     | 0.45              |
| 1:A:1108:G:H4'   | 1:A:1191:A:O4'    | 2.16                     | 0.45              |
| 1:A:248:C:O2'    | 1:A:249:U:H5'     | 2.15                     | 0.45              |
| 1:A:412:A:H1'    | 1:A:413:G:C2      | 2.52                     | 0.45              |
| 4:B:213:LEU:O    | 4:B:217:ARG:HG2   | 2.16                     | 0.45              |
| 4:B:51:LEU:O     | 4:B:55:PHE:HD1    | 2.00                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:C:136:GLN:O    | 5:C:139:GLN:N     | 2.50                     | 0.45              |
| 5:C:6:HIS:CD2    | 5:C:8:ILE:HB      | 2.52                     | 0.45              |
| 8:F:91:VAL:CG1   | 20:R:72:ARG:NH2   | 2.79                     | 0.45              |
| 9:G:85:TYR:CD1   | 9:G:154:TYR:HE1   | 2.33                     | 0.45              |
| 10:H:8:ASP:O     | 10:H:12:ARG:HG3   | 2.17                     | 0.45              |
| 11:I:44:VAL:O    | 11:I:51:ARG:NH2   | 2.49                     | 0.45              |
| 13:K:121:PRO:HG2 | 13:K:126:ARG:CG   | 2.47                     | 0.45              |
| 14:L:115:LYS:C   | 14:L:117:ARG:H    | 2.20                     | 0.45              |
| 14:L:110:VAL:O   | 14:L:122:THR:HG21 | 2.17                     | 0.45              |
| 12:J:49:VAL:HG21 | 16:N:41:ARG:O     | 2.17                     | 0.45              |
| 19:Q:24:GLU:OE1  | 19:Q:39:SER:HB3   | 2.16                     | 0.45              |
| 22:T:74:LYS:HB3  | 22:T:74:LYS:HE3   | 1.61                     | 0.45              |
| 1:A:1423:G:H2'   | 1:A:1424:C:C6     | 2.53                     | 0.44              |
| 1:A:251:G:H4'    | 1:A:252:U:O5'     | 2.17                     | 0.44              |
| 4:B:71:VAL:HG21  | 4:B:164:VAL:HG23  | 1.96                     | 0.44              |
| 5:C:157:ILE:HG21 | 5:C:164:ARG:NH2   | 2.31                     | 0.44              |
| 6:D:24:GLU:HG2   | 6:D:25:ARG:N      | 2.31                     | 0.44              |
| 8:F:67:MET:HB2   | 8:F:68:PRO:CD     | 2.47                     | 0.44              |
| 10:H:4:ASP:C     | 10:H:4:ASP:OD1    | 2.55                     | 0.44              |
| 11:I:10:ARG:HH11 | 11:I:10:ARG:CG    | 2.30                     | 0.44              |
| 11:I:13:ALA:HB1  | 11:I:67:GLY:O     | 2.17                     | 0.44              |
| 12:J:15:THR:O    | 12:J:16:LEU:HD23  | 2.17                     | 0.44              |
| 14:L:102:ARG:HB2 | 14:L:120:TYR:HA   | 1.99                     | 0.44              |
| 14:L:119:LYS:O   | 14:L:120:TYR:CB   | 2.65                     | 0.44              |
| 19:Q:27:PHE:CE1  | 19:Q:36:ILE:HD11  | 2.52                     | 0.44              |
| 1:A:1125:U:P     | 1:A:1145:C:H42    | 2.40                     | 0.44              |
| 1:A:1154:G:O2'   | 1:A:1155:G:H5'    | 2.17                     | 0.44              |
| 1:A:1420:C:H2'   | 1:A:1421:G:C8     | 2.50                     | 0.44              |
| 1:A:21:G:H2'     | 1:A:22:G:C8       | 2.53                     | 0.44              |
| 1:A:738:C:OP2    | 8:F:92:LYS:CE     | 2.65                     | 0.44              |
| 1:A:925:G:C6     | 1:A:927:G:N7      | 2.85                     | 0.44              |
| 1:A:1056:U:C5'   | 5:C:163:ALA:HB2   | 2.46                     | 0.44              |
| 6:D:39:PRO:O     | 6:D:44:GLY:HA3    | 2.16                     | 0.44              |
| 8:F:28:ARG:HG3   | 8:F:28:ARG:NH1    | 2.33                     | 0.44              |
| 9:G:65:ALA:HB1   | 9:G:127:ALA:HB3   | 1.99                     | 0.44              |
| 10:H:10:LEU:HD12 | 10:H:85:ARG:HG2   | 1.99                     | 0.44              |
| 11:I:69:GLY:O    | 11:I:73:GLN:HG3   | 2.17                     | 0.44              |
| 1:A:716:A:N3     | 13:K:117:ASN:O    | 2.50                     | 0.44              |
| 16:N:36:PHE:HD1  | 16:N:37:PHE:CE1   | 2.36                     | 0.44              |
| 17:O:62:GLN:OE1  | 17:O:65:ARG:NH2   | 2.50                     | 0.44              |
| 18:P:43:LYS:HB3  | 18:P:48:TRP:CD1   | 2.52                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 19:Q:97:SER:HA   | 19:Q:103:GLY:H   | 1.82                     | 0.44              |
| 21:S:62:ILE:HD12 | 21:S:63:THR:H    | 1.82                     | 0.44              |
| 1:A:1174:G:O2'   | 1:A:1175:G:H5'   | 2.18                     | 0.44              |
| 1:A:1197:G:OP1   | 1:A:1197:G:H3'   | 2.18                     | 0.44              |
| 1:A:190(K):G:O2' | 1:A:190(L):U:P   | 2.75                     | 0.44              |
| 1:A:222:U:H2'    | 1:A:223:U:C6     | 2.52                     | 0.44              |
| 1:A:113:G:C1'    | 1:A:354:G:H5'    | 2.47                     | 0.44              |
| 1:A:586:C:C2'    | 1:A:587:G:H5'    | 2.47                     | 0.44              |
| 5:C:134:ILE:HG22 | 5:C:168:ALA:CB   | 2.48                     | 0.44              |
| 7:E:152:ARG:NH2  | 10:H:107:LEU:O   | 2.50                     | 0.44              |
| 9:G:45:ASP:O     | 9:G:49:ILE:HG13  | 2.17                     | 0.44              |
| 10:H:104:ARG:NH2 | 10:H:138:TRP:CH2 | 2.85                     | 0.44              |
| 14:L:83:VAL:HG13 | 14:L:84:LEU:N    | 2.32                     | 0.44              |
| 15:M:5:ALA:O     | 15:M:7:VAL:N     | 2.50                     | 0.44              |
| 15:M:77:ASN:O    | 15:M:80:ARG:HB3  | 2.17                     | 0.44              |
| 16:N:41:ARG:HG3  | 16:N:42:ILE:N    | 2.32                     | 0.44              |
| 19:Q:59:ILE:HG23 | 19:Q:71:PHE:HB3  | 1.99                     | 0.44              |
| 1:A:1172:C:H2'   | 1:A:1173:G:C8    | 2.52                     | 0.44              |
| 1:A:1477:C:H2'   | 1:A:1478:C:C6    | 2.53                     | 0.44              |
| 6:D:31:CYS:O     | 6:D:32:ALA:HB3   | 2.18                     | 0.44              |
| 6:D:8:VAL:HG13   | 6:D:21:LEU:CD1   | 2.47                     | 0.44              |
| 7:E:12:LEU:C     | 7:E:12:LEU:HD22  | 2.37                     | 0.44              |
| 1:A:1128:C:C4'   | 11:I:16:ARG:HH12 | 2.30                     | 0.44              |
| 12:J:29:ARG:NH1  | 12:J:84:GLN:OE1  | 2.50                     | 0.44              |
| 12:J:75:ILE:O    | 12:J:76:ASN:HB2  | 2.17                     | 0.44              |
| 5:C:33:LEU:CD1   | 16:N:53:LEU:HD23 | 2.47                     | 0.44              |
| 20:R:87:ARG:HG2  | 20:R:87:ARG:NH1  | 2.32                     | 0.44              |
| 1:A:1091:U:O2    | 1:A:1093:A:C8    | 2.70                     | 0.44              |
| 1:A:1141:C:O2'   | 1:A:1142:G:H5'   | 2.17                     | 0.44              |
| 1:A:217:C:H2'    | 1:A:218:C:C6     | 2.52                     | 0.44              |
| 1:A:56:U:H2'     | 1:A:57:G:C8      | 2.53                     | 0.44              |
| 1:A:652:U:C4     | 1:A:752:G:N3     | 2.85                     | 0.44              |
| 1:A:934:C:C4     | 1:A:1345:U:C5    | 3.05                     | 0.44              |
| 4:B:62:ALA:C     | 4:B:64:ARG:N     | 2.71                     | 0.44              |
| 6:D:8:VAL:C      | 6:D:10:ARG:N     | 2.70                     | 0.44              |
| 11:I:10:ARG:HH11 | 11:I:10:ARG:HG2  | 1.83                     | 0.44              |
| 11:I:42:ARG:O    | 11:I:43:ALA:C    | 2.56                     | 0.44              |
| 19:Q:67:LYS:O    | 19:Q:68:ARG:HB3  | 2.17                     | 0.44              |
| 8:F:91:VAL:CG1   | 20:R:72:ARG:HH22 | 2.30                     | 0.44              |
| 21:S:32:LYS:O    | 21:S:32:LYS:HG3  | 2.17                     | 0.44              |
| 21:S:33:THR:CG2  | 21:S:34:TRP:H    | 2.28                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 21:S:64:GLU:O    | 21:S:67:VAL:HG23 | 2.17                     | 0.44              |
| 1:A:1454:G:H2'   | 1:A:1455:G:H8    | 1.82                     | 0.44              |
| 1:A:242:C:H2'    | 1:A:243:A:H5'    | 2.00                     | 0.44              |
| 1:A:390:C:H2'    | 1:A:391:G:H8     | 1.78                     | 0.44              |
| 1:A:839:U:C2'    | 1:A:839:U:O2     | 2.64                     | 0.44              |
| 4:B:53:ARG:NH1   | 4:B:199:TYR:CD2  | 2.85                     | 0.44              |
| 5:C:19:GLU:O     | 5:C:40:ARG:NH2   | 2.51                     | 0.44              |
| 12:J:48:THR:HG1  | 12:J:62:HIS:CD2  | 2.35                     | 0.44              |
| 14:L:28:LYS:O    | 14:L:28:LYS:HG2  | 2.17                     | 0.44              |
| 15:M:33:ALA:O    | 15:M:37:THR:HB   | 2.18                     | 0.44              |
| 21:S:13:ASP:O    | 21:S:14:HIS:C    | 2.56                     | 0.44              |
| 21:S:80:TYR:CD2  | 21:S:81:ARG:HB2  | 2.53                     | 0.44              |
| 1:A:1014:A:H2'   | 1:A:1015:A:C8    | 2.53                     | 0.44              |
| 4:B:122:PHE:O    | 4:B:123:ALA:HB2  | 2.18                     | 0.44              |
| 5:C:180:ALA:CB   | 5:C:182:ILE:HG13 | 2.48                     | 0.44              |
| 6:D:127:THR:HG21 | 6:D:147:ALA:HB3  | 2.00                     | 0.44              |
| 8:F:15:ASP:OD1   | 8:F:17:SER:HB2   | 2.18                     | 0.44              |
| 9:G:141:VAL:O    | 9:G:144:MET:N    | 2.50                     | 0.44              |
| 12:J:20:ALA:C    | 12:J:22:LYS:H    | 2.21                     | 0.44              |
| 13:K:101:SER:C   | 13:K:103:LEU:N   | 2.70                     | 0.44              |
| 14:L:41:ARG:HG2  | 14:L:42:THR:O    | 2.17                     | 0.44              |
| 16:N:11:LYS:HB2  | 16:N:11:LYS:HE3  | 1.83                     | 0.44              |
| 17:O:45:VAL:HG12 | 17:O:46:HIS:H    | 1.82                     | 0.44              |
| 17:O:17:ARG:NH1  | 17:O:77:ARG:NH1  | 2.66                     | 0.44              |
| 21:S:53:ASN:N    | 21:S:53:ASN:ND2  | 2.66                     | 0.44              |
| 1:A:674:G:H2'    | 1:A:675:A:C8     | 2.53                     | 0.44              |
| 1:A:832:C:O2'    | 1:A:833:U:H5'    | 2.17                     | 0.44              |
| 5:C:107:GLN:O    | 5:C:108:ASN:CB   | 2.66                     | 0.44              |
| 9:G:8:GLU:OE1    | 9:G:8:GLU:O      | 2.36                     | 0.44              |
| 10:H:51:VAL:HG21 | 10:H:60:ARG:HH11 | 1.83                     | 0.44              |
| 12:J:23:ILE:HG21 | 12:J:72:VAL:HG11 | 1.99                     | 0.44              |
| 12:J:60:ARG:O    | 12:J:61:GLU:HB3  | 2.18                     | 0.44              |
| 13:K:69:ALA:O    | 13:K:73:MET:HG2  | 2.17                     | 0.44              |
| 14:L:41:ARG:HH22 | 14:L:57:LYS:NZ   | 2.15                     | 0.44              |
| 14:L:6:THR:OG1   | 14:L:9:GLN:HG3   | 2.18                     | 0.44              |
| 19:Q:95:TYR:HA   | 19:Q:98:LEU:HD13 | 1.98                     | 0.44              |
| 15:M:84:ILE:CG2  | 21:S:65:ASN:HD22 | 2.29                     | 0.44              |
| 22:T:50:GLU:O    | 22:T:54:LYS:HG3  | 2.18                     | 0.44              |
| 1:A:1053:G:C3'   | 1:A:1054:C:C5'   | 2.94                     | 0.44              |
| 1:A:1202:G:H2'   | 1:A:1203:C:H5'   | 1.99                     | 0.44              |
| 1:A:1234:C:O2'   | 1:A:1235:U:H5'   | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1354:C:O2'   | 1:A:1355:G:H5'   | 2.17                     | 0.44              |
| 1:A:865:A:O2'    | 1:A:866:C:H5'    | 2.17                     | 0.44              |
| 4:B:162:ILE:HD12 | 4:B:177:ALA:HB2  | 2.00                     | 0.44              |
| 5:C:61:ALA:O     | 5:C:62:ASP:HB2   | 2.17                     | 0.44              |
| 6:D:7:PRO:CG     | 6:D:10:ARG:HD2   | 2.48                     | 0.44              |
| 8:F:82:ARG:HE    | 8:F:82:ARG:HA    | 1.83                     | 0.44              |
| 1:A:1375:A:P     | 9:G:28:ASN:HD22  | 2.40                     | 0.44              |
| 11:I:19:LEU:HB3  | 11:I:59:PHE:HD2  | 1.83                     | 0.44              |
| 19:Q:95:TYR:HA   | 19:Q:98:LEU:CD1  | 2.48                     | 0.44              |
| 1:A:584:G:H2'    | 1:A:585:G:C8     | 2.53                     | 0.43              |
| 1:A:609:A:C2'    | 1:A:610:G:H5'    | 2.48                     | 0.43              |
| 4:B:102:LEU:CD1  | 4:B:102:LEU:N    | 2.81                     | 0.43              |
| 4:B:118:LEU:C    | 4:B:120:ALA:N    | 2.70                     | 0.43              |
| 4:B:200:ILE:HG22 | 4:B:202:PRO:HD3  | 1.99                     | 0.43              |
| 4:B:70:PHE:CD2   | 4:B:215:LEU:HD21 | 2.53                     | 0.43              |
| 8:F:82:ARG:HB2   | 8:F:85:VAL:CG2   | 2.48                     | 0.43              |
| 12:J:85:LEU:O    | 12:J:87:THR:N    | 2.50                     | 0.43              |
| 13:K:51:LYS:C    | 13:K:51:LYS:HD3  | 2.38                     | 0.43              |
| 14:L:53:ARG:HG3  | 14:L:69:TYR:HE1  | 1.82                     | 0.43              |
| 14:L:89:ARG:NH2  | 14:L:97:ARG:HD2  | 2.33                     | 0.43              |
| 20:R:53:ARG:NH1  | 20:R:60:GLY:N    | 2.65                     | 0.43              |
| 2:W:3:A:O2'      | 2:W:4:A:H5'      | 2.18                     | 0.43              |
| 1:A:1152:A:O2'   | 1:A:1153:C:H5'   | 2.18                     | 0.43              |
| 1:A:1313:U:O4    | 21:S:4:SER:CB    | 2.67                     | 0.43              |
| 1:A:334:C:H2'    | 1:A:335:C:C6     | 2.53                     | 0.43              |
| 4:B:132:LYS:O    | 4:B:136:VAL:HG23 | 2.17                     | 0.43              |
| 4:B:19:HIS:CD2   | 4:B:204:ASN:HA   | 2.53                     | 0.43              |
| 5:C:3:ASN:C      | 5:C:4:LYS:HG2    | 2.38                     | 0.43              |
| 7:E:28:PHE:O     | 7:E:47:LYS:HA    | 2.18                     | 0.43              |
| 11:I:112:LYS:HD3 | 11:I:112:LYS:O   | 2.17                     | 0.43              |
| 1:A:1061:G:H1'   | 12:J:56:HIS:CE1  | 2.53                     | 0.43              |
| 12:J:94:VAL:HG12 | 12:J:95:GLU:O    | 2.18                     | 0.43              |
| 19:Q:27:PHE:HB2  | 19:Q:28:PRO:CD   | 2.44                     | 0.43              |
| 20:R:34:TYR:HA   | 20:R:69:THR:HG23 | 1.99                     | 0.43              |
| 1:A:1300:G:O2'   | 1:A:1301:U:H6    | 2.01                     | 0.43              |
| 1:A:1330:U:OP1   | 15:M:23:TYR:O    | 2.35                     | 0.43              |
| 1:A:22:G:H2'     | 1:A:23:C:C6      | 2.53                     | 0.43              |
| 1:A:757:U:H2'    | 1:A:758:G:O4'    | 2.17                     | 0.43              |
| 4:B:8:LYS:HD2    | 4:B:9:GLU:N      | 2.34                     | 0.43              |
| 5:C:172:ARG:NH2  | 5:C:203:PHE:CE2  | 2.86                     | 0.43              |
| 5:C:4:LYS:HB3    | 5:C:4:LYS:HE2    | 1.85                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 7:E:144:THR:CG2   | 7:E:146:ALA:H    | 2.31                     | 0.43              |
| 8:F:10:LEU:HD12   | 8:F:59:TYR:O     | 2.19                     | 0.43              |
| 11:I:53:VAL:O     | 11:I:54:ASP:HB2  | 2.18                     | 0.43              |
| 1:A:528:C:H41     | 14:L:49:ASN:ND2  | 2.17                     | 0.43              |
| 15:M:58:GLU:OE2   | 15:M:58:GLU:HA   | 2.17                     | 0.43              |
| 19:Q:26:GLN:O     | 19:Q:27:PHE:HB3  | 2.18                     | 0.43              |
| 22:T:63:ILE:HD13  | 22:T:80:ARG:HB3  | 2.01                     | 0.43              |
| 3:X:36:U:H2'      | 3:X:37:T6A:H5'   | 2.00                     | 0.43              |
| 1:A:1320:C:O2'    | 1:A:1321:C:H5'   | 2.18                     | 0.43              |
| 5:C:91:LEU:CD2    | 5:C:92:ALA:N     | 2.76                     | 0.43              |
| 6:D:196:LEU:HD23  | 6:D:197:PRO:HD2  | 2.00                     | 0.43              |
| 15:M:110:ARG:HH11 | 15:M:110:ARG:CG  | 2.30                     | 0.43              |
| 15:M:121:LYS:N    | 15:M:121:LYS:HD2 | 2.32                     | 0.43              |
| 19:Q:6:LEU:O      | 19:Q:59:ILE:N    | 2.47                     | 0.43              |
| 19:Q:80:GLY:O     | 19:Q:81:ARG:CB   | 2.66                     | 0.43              |
| 1:A:1320:C:N4     | 21:S:37:ARG:HD3  | 2.33                     | 0.43              |
| 3:X:31:A:H2'      | 3:X:32:C:C6      | 2.53                     | 0.43              |
| 1:A:1301:U:O2'    | 1:A:1302:U:OP1   | 2.34                     | 0.43              |
| 1:A:513:C:H2'     | 1:A:514:C:C6     | 2.54                     | 0.43              |
| 1:A:780:A:O2'     | 1:A:781:A:H5''   | 2.19                     | 0.43              |
| 1:A:662:G:O2'     | 1:A:836:G:C5'    | 2.67                     | 0.43              |
| 5:C:178:LEU:O     | 5:C:179:ARG:CB   | 2.63                     | 0.43              |
| 8:F:2:ARG:NH1     | 8:F:69:GLU:HG2   | 2.32                     | 0.43              |
| 16:N:8:GLU:O      | 16:N:11:LYS:HB3  | 2.19                     | 0.43              |
| 17:O:14:GLU:OE1   | 17:O:84:LYS:HE2  | 2.19                     | 0.43              |
| 20:R:37:VAL:HG22  | 20:R:78:LEU:HB3  | 1.99                     | 0.43              |
| 1:A:1318:A:O2'    | 21:S:37:ARG:HB3  | 2.19                     | 0.43              |
| 1:A:1182:G:H5'    | 1:A:1184:G:H5'   | 2.00                     | 0.43              |
| 1:A:1236:A:H2'    | 1:A:1237:C:C6    | 2.53                     | 0.43              |
| 1:A:1286:A:H2'    | 1:A:1287:A:O5'   | 2.19                     | 0.43              |
| 1:A:562:C:H1'     | 14:L:15:ARG:HB3  | 1.99                     | 0.43              |
| 1:A:74:C:H2'      | 1:A:75:G:H5'     | 2.01                     | 0.43              |
| 1:A:824:C:H2'     | 1:A:825:G:H8     | 1.82                     | 0.43              |
| 4:B:212:GLN:NE2   | 4:B:216:SER:HB3  | 2.33                     | 0.43              |
| 5:C:5:ILE:O       | 5:C:5:ILE:HD12   | 2.19                     | 0.43              |
| 8:F:64:GLN:HG2    | 8:F:64:GLN:O     | 2.17                     | 0.43              |
| 7:E:79:GLU:O      | 10:H:104:ARG:CZ  | 2.67                     | 0.43              |
| 11:I:44:VAL:HG12  | 11:I:51:ARG:CZ   | 2.49                     | 0.43              |
| 12:J:60:ARG:N     | 12:J:60:ARG:HD2  | 2.34                     | 0.43              |
| 1:A:1305:G:H22    | 1:A:1331:G:C2'   | 2.30                     | 0.43              |
| 1:A:272:C:O2'     | 1:A:273:A:H5'    | 2.19                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:687:A:HO2'   | 1:A:688:G:P       | 2.42                     | 0.43              |
| 6:D:31:CYS:C     | 6:D:33:MET:H      | 2.21                     | 0.43              |
| 9:G:3:ARG:CG     | 9:G:3:ARG:HH11    | 2.31                     | 0.43              |
| 11:I:49:PRO:O    | 11:I:52:ALA:HB3   | 2.19                     | 0.43              |
| 12:J:42:THR:HG22 | 12:J:43:ARG:N     | 2.34                     | 0.43              |
| 15:M:11:ARG:HG2  | 15:M:12:ASN:N     | 2.33                     | 0.43              |
| 18:P:67:THR:N    | 18:P:70:ALA:HB3   | 2.34                     | 0.43              |
| 19:Q:100:LYS:O   | 19:Q:101:ARG:NE   | 2.52                     | 0.43              |
| 23:V:15:ARG:O    | 23:V:17:THR:HG23  | 2.19                     | 0.43              |
| 1:A:999:C:H2'    | 1:A:1000:U:C6     | 2.53                     | 0.43              |
| 1:A:1201:A:H4'   | 1:A:1202:G:C5'    | 2.48                     | 0.43              |
| 1:A:1273:G:H2'   | 1:A:1274:G:O4'    | 2.19                     | 0.43              |
| 1:A:136:C:H2'    | 1:A:137:C:C6      | 2.54                     | 0.43              |
| 1:A:232:G:H1'    | 1:A:262:A:N1      | 2.34                     | 0.43              |
| 5:C:167:TRP:HB3  | 5:C:168:ALA:H     | 1.37                     | 0.43              |
| 7:E:51:VAL:CB    | 7:E:52:PRO:HD3    | 2.43                     | 0.43              |
| 9:G:151:TYR:N    | 9:G:151:TYR:CD1   | 2.87                     | 0.43              |
| 10:H:38:ILE:CD1  | 10:H:118:VAL:HG12 | 2.48                     | 0.43              |
| 13:K:126:ARG:O   | 13:K:127:LYS:CB   | 2.65                     | 0.43              |
| 13:K:36:ASP:C    | 13:K:36:ASP:OD2   | 2.57                     | 0.43              |
| 14:L:126:LYS:H   | 14:L:126:LYS:HE3  | 1.84                     | 0.43              |
| 20:R:55:ARG:HH11 | 20:R:55:ARG:CB    | 2.29                     | 0.43              |
| 20:R:73:ALA:HB3  | 20:R:79:LEU:HD12  | 2.01                     | 0.43              |
| 22:T:45:GLN:HB2  | 22:T:91:LEU:HD13  | 2.01                     | 0.43              |
| 1:A:119:A:H4'    | 1:A:120:A:O5'     | 2.19                     | 0.43              |
| 1:A:1489:G:C2'   | 1:A:1490:C:C5'    | 2.85                     | 0.43              |
| 1:A:285:G:O2'    | 1:A:286:G:H5'     | 2.18                     | 0.43              |
| 1:A:123:C:OP1    | 1:A:312:C:H5'     | 2.18                     | 0.43              |
| 5:C:91:LEU:HD21  | 5:C:99:VAL:HG13   | 1.99                     | 0.43              |
| 6:D:6:GLY:O      | 6:D:7:PRO:C       | 2.57                     | 0.43              |
| 7:E:6:PHE:CE2    | 7:E:36:ASP:HB3    | 2.53                     | 0.43              |
| 11:I:114:TYR:CE1 | 12:J:59:SER:O     | 2.72                     | 0.43              |
| 17:O:26:GLU:N    | 17:O:26:GLU:OE2   | 2.51                     | 0.43              |
| 1:A:1054:C:N4    | 3:X:34:U:C1'      | 2.82                     | 0.43              |
| 1:A:1167:A:H2'   | 1:A:1168:A:C8     | 2.54                     | 0.43              |
| 1:A:1399:C:C2    | 1:A:1401:G:C5     | 3.07                     | 0.43              |
| 1:A:1424:C:C2'   | 1:A:1425:U:H5'    | 2.49                     | 0.43              |
| 1:A:265:G:H2'    | 1:A:267:C:C5      | 2.53                     | 0.43              |
| 1:A:343:U:H2'    | 1:A:345:C:C5      | 2.54                     | 0.43              |
| 1:A:603:U:H2'    | 1:A:604:G:H8      | 1.84                     | 0.43              |
| 1:A:939:G:H2'    | 1:A:940:C:H6      | 1.81                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:B:160:ASP:O    | 4:B:183:PRO:HD2   | 2.19                     | 0.43              |
| 5:C:139:GLN:HE21 | 5:C:139:GLN:CA    | 2.30                     | 0.43              |
| 8:F:10:LEU:HD11  | 8:F:59:TYR:HD2    | 1.84                     | 0.43              |
| 9:G:26:PHE:O     | 9:G:30:ILE:HG13   | 2.19                     | 0.43              |
| 1:A:598:U:H4'    | 10:H:94:TYR:CD1   | 2.54                     | 0.43              |
| 11:I:127:LYS:HA  | 11:I:127:LYS:HE3  | 2.01                     | 0.43              |
| 12:J:94:VAL:CG1  | 12:J:95:GLU:H     | 2.32                     | 0.43              |
| 13:K:46:GLY:C    | 13:K:48:ILE:H     | 2.22                     | 0.43              |
| 17:O:57:LEU:HA   | 17:O:57:LEU:HD12  | 1.73                     | 0.43              |
| 21:S:42:PRO:O    | 21:S:45:VAL:HG23  | 2.19                     | 0.43              |
| 1:A:1128:C:HO2'  | 1:A:1130:A:H8     | 1.62                     | 0.42              |
| 1:A:113:G:H1'    | 1:A:354:G:C5'     | 2.46                     | 0.42              |
| 1:A:1495:U:H2'   | 1:A:1496:C:C6     | 2.53                     | 0.42              |
| 1:A:1499:A:H1'   | 1:A:1520:G:H5'    | 2.01                     | 0.42              |
| 1:A:261:U:O2     | 1:A:263:A:C8      | 2.72                     | 0.42              |
| 1:A:463:A:O2'    | 1:A:474:G:H5'     | 2.18                     | 0.42              |
| 1:A:731:G:H5'    | 1:A:766:A:H4'     | 2.00                     | 0.42              |
| 1:A:951:G:O2'    | 1:A:952:U:H5'     | 2.19                     | 0.42              |
| 10:H:31:PHE:HZ   | 10:H:134:ILE:CD1  | 2.32                     | 0.42              |
| 10:H:56:LYS:O    | 10:H:58:TYR:HD1   | 2.02                     | 0.42              |
| 7:E:143:ARG:NH1  | 10:H:77:GLU:OE2   | 2.52                     | 0.42              |
| 12:J:23:ILE:N    | 12:J:23:ILE:HD12  | 2.34                     | 0.42              |
| 13:K:59:TYR:O    | 13:K:62:GLN:HB3   | 2.18                     | 0.42              |
| 15:M:32:GLU:OE1  | 15:M:64:TRP:HZ2   | 2.01                     | 0.42              |
| 21:S:41:VAL:HB   | 21:S:43:GLU:OE2   | 2.19                     | 0.42              |
| 21:S:58:VAL:HG23 | 21:S:58:VAL:O     | 2.19                     | 0.42              |
| 22:T:54:LYS:HG3  | 22:T:100:ILE:HD12 | 2.01                     | 0.42              |
| 22:T:50:GLU:H    | 22:T:99:LEU:HD12  | 1.83                     | 0.42              |
| 1:A:1153:C:H2'   | 1:A:1154:G:H8     | 1.84                     | 0.42              |
| 1:A:1202:G:H2'   | 1:A:1203:C:C5'    | 2.49                     | 0.42              |
| 1:A:1206:G:C6    | 1:A:1207:G:C5     | 3.08                     | 0.42              |
| 1:A:1226:C:OP2   | 15:M:103:THR:HG21 | 2.19                     | 0.42              |
| 1:A:1246:C:O2'   | 1:A:1247:U:H5'    | 2.19                     | 0.42              |
| 1:A:1250:A:C5'   | 11:I:68:GLY:N     | 2.82                     | 0.42              |
| 1:A:129(A):G:O2' | 1:A:130:A:OP2     | 2.36                     | 0.42              |
| 1:A:327:A:O3'    | 1:A:328:C:H4'     | 2.19                     | 0.42              |
| 4:B:209:ARG:NH2  | 4:B:236:TYR:HE2   | 2.17                     | 0.42              |
| 5:C:123:GLN:NE2  | 5:C:140:ARG:NH2   | 2.59                     | 0.42              |
| 9:G:52:GLU:O     | 9:G:54:THR:N      | 2.52                     | 0.42              |
| 12:J:9:ARG:HH11  | 12:J:9:ARG:CB     | 2.32                     | 0.42              |
| 14:L:41:ARG:CB   | 14:L:41:ARG:NH1   | 2.82                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:106:C:O2      | 1:A:379:C:H4'    | 2.20                     | 0.42              |
| 1:A:1380:U:O2'    | 1:A:1381:U:P     | 2.77                     | 0.42              |
| 1:A:413:G:O2'     | 1:A:416:G:O6     | 2.36                     | 0.42              |
| 1:A:437:U:C2'     | 1:A:438:G:H5'    | 2.49                     | 0.42              |
| 4:B:10:LEU:HD23   | 4:B:48:MET:HE2   | 2.01                     | 0.42              |
| 4:B:223:ILE:HG21  | 4:B:230:VAL:HG21 | 2.02                     | 0.42              |
| 4:B:23:ARG:HD3    | 4:B:23:ARG:C     | 2.39                     | 0.42              |
| 5:C:180:ALA:O     | 5:C:181:ASN:C    | 2.56                     | 0.42              |
| 6:D:32:ALA:C      | 6:D:34:GLU:N     | 2.72                     | 0.42              |
| 1:A:1250:A:C4'    | 11:I:68:GLY:H    | 2.24                     | 0.42              |
| 1:A:1367:C:H4'    | 12:J:48:THR:HG21 | 2.01                     | 0.42              |
| 14:L:28:LYS:O     | 14:L:29:GLY:C    | 2.58                     | 0.42              |
| 14:L:38:THR:HG22  | 14:L:39:VAL:HG23 | 2.01                     | 0.42              |
| 15:M:49:THR:CG2   | 15:M:51:ALA:HB3  | 2.49                     | 0.42              |
| 16:N:23:ARG:HG3   | 16:N:23:ARG:NH1  | 2.34                     | 0.42              |
| 18:P:10:GLY:HA3   | 18:P:14:ASN:O    | 2.20                     | 0.42              |
| 21:S:9:VAL:HG12   | 21:S:9:VAL:O     | 2.18                     | 0.42              |
| 1:A:1009:G:N1     | 1:A:1021:G:N2    | 2.67                     | 0.42              |
| 1:A:1011:G:H2'    | 1:A:1012:U:H5'   | 2.01                     | 0.42              |
| 1:A:416:G:C8      | 1:A:418:C:N4     | 2.87                     | 0.42              |
| 1:A:635:G:O2'     | 1:A:636:U:H5'    | 2.19                     | 0.42              |
| 1:A:957:U:H3      | 1:A:960:U:C5'    | 2.32                     | 0.42              |
| 5:C:119:ARG:O     | 5:C:122:GLU:HB2  | 2.18                     | 0.42              |
| 5:C:133:ALA:O     | 5:C:136:GLN:HB2  | 2.20                     | 0.42              |
| 5:C:139:GLN:O     | 5:C:143:GLU:HB2  | 2.20                     | 0.42              |
| 6:D:60:GLU:HA     | 6:D:60:GLU:OE1   | 2.20                     | 0.42              |
| 6:D:70:ILE:HG22   | 6:D:71:SER:N     | 2.34                     | 0.42              |
| 7:E:69:VAL:HA     | 7:E:70:PRO:HD3   | 1.75                     | 0.42              |
| 10:H:86:ILE:HD11  | 10:H:136:GLU:HB2 | 2.00                     | 0.42              |
| 11:I:10:ARG:CD    | 11:I:105:ASP:HB3 | 2.49                     | 0.42              |
| 11:I:128:ARG:OXT  | 11:I:128:ARG:HG2 | 2.18                     | 0.42              |
| 15:M:117:VAL:HG12 | 15:M:118:ALA:N   | 2.34                     | 0.42              |
| 19:Q:27:PHE:CZ    | 19:Q:36:ILE:HD11 | 2.54                     | 0.42              |
| 21:S:36:ARG:NH2   | 21:S:75:ALA:HB3  | 2.34                     | 0.42              |
| 1:A:1027:C:N4     | 1:A:1029:C:H41   | 2.17                     | 0.42              |
| 1:A:1230:C:O2'    | 1:A:1231:G:H5'   | 2.20                     | 0.42              |
| 1:A:976:G:C8      | 1:A:1358:U:O2    | 2.73                     | 0.42              |
| 1:A:1441:G:H4'    | 1:A:1442:G:C5    | 2.55                     | 0.42              |
| 1:A:191:G:C4      | 22:T:105:SER:HB3 | 2.53                     | 0.42              |
| 1:A:51:A:H4'      | 1:A:52:G:C5'     | 2.50                     | 0.42              |
| 1:A:731:G:OP1     | 1:A:766:A:H1'    | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:818:G:H3'    | 1:A:819:A:C5'    | 2.50                     | 0.42              |
| 4:B:71:VAL:HG23  | 4:B:164:VAL:HG23 | 2.00                     | 0.42              |
| 6:D:8:VAL:HG11   | 6:D:21:LEU:CB    | 2.50                     | 0.42              |
| 6:D:8:VAL:HG11   | 6:D:21:LEU:HB3   | 2.01                     | 0.42              |
| 9:G:78:ARG:HD2   | 9:G:156:TRP:HE3  | 1.84                     | 0.42              |
| 11:I:112:LYS:HD3 | 11:I:112:LYS:C   | 2.40                     | 0.42              |
| 12:J:26:ALA:HA   | 12:J:84:GLN:OE1  | 2.19                     | 0.42              |
| 13:K:47:VAL:O    | 13:K:47:VAL:CG1  | 2.62                     | 0.42              |
| 22:T:93:GLU:OE2  | 22:T:93:GLU:HA   | 2.19                     | 0.42              |
| 1:A:1522:U:O2'   | 1:A:1523:G:H5'   | 2.19                     | 0.42              |
| 4:B:53:ARG:NH1   | 4:B:199:TYR:HD2  | 2.18                     | 0.42              |
| 5:C:172:ARG:HB3  | 5:C:172:ARG:HH11 | 1.84                     | 0.42              |
| 9:G:145:ALA:O    | 9:G:146:GLU:C    | 2.55                     | 0.42              |
| 5:C:23:TYR:OH    | 12:J:9:ARG:HD3   | 2.20                     | 0.42              |
| 14:L:89:ARG:HG2  | 14:L:97:ARG:CA   | 2.47                     | 0.42              |
| 15:M:71:ARG:HG2  | 15:M:71:ARG:HH11 | 1.84                     | 0.42              |
| 19:Q:82:MET:O    | 19:Q:83:ASP:C    | 2.57                     | 0.42              |
| 1:A:1222:G:OP1   | 21:S:77:THR:HG21 | 2.19                     | 0.42              |
| 23:V:2:GLY:C     | 23:V:4:GLY:N     | 2.72                     | 0.42              |
| 1:A:1070:U:O2'   | 1:A:1071:C:H5'   | 2.19                     | 0.42              |
| 1:A:1227:A:H3'   | 1:A:1227:A:H8    | 1.85                     | 0.42              |
| 1:A:1527:C:O2'   | 1:A:1528:U:H5'   | 2.19                     | 0.42              |
| 1:A:287:U:C2'    | 1:A:288:A:H5'    | 2.50                     | 0.42              |
| 1:A:614:A:C2     | 1:A:627:G:C2     | 3.08                     | 0.42              |
| 4:B:142:LEU:HD23 | 4:B:142:LEU:C    | 2.40                     | 0.42              |
| 4:B:144:ARG:HA   | 4:B:147:LYS:CD   | 2.49                     | 0.42              |
| 4:B:206:ASP:CG   | 4:B:207:ALA:H    | 2.22                     | 0.42              |
| 4:B:223:ILE:CD1  | 4:B:230:VAL:HG21 | 2.50                     | 0.42              |
| 6:D:162:LEU:HD12 | 6:D:181:MET:SD   | 2.58                     | 0.42              |
| 7:E:15:ARG:O     | 7:E:16:THR:HG22  | 2.20                     | 0.42              |
| 11:I:17:VAL:HG11 | 11:I:81:ILE:HA   | 2.01                     | 0.42              |
| 12:J:22:LYS:HE2  | 12:J:90:LEU:HD12 | 2.00                     | 0.42              |
| 21:S:13:ASP:O    | 21:S:17:GLU:HG2  | 2.20                     | 0.42              |
| 21:S:63:THR:HG22 | 21:S:64:GLU:H    | 1.84                     | 0.42              |
| 22:T:36:LEU:HA   | 22:T:39:LYS:HB2  | 2.02                     | 0.42              |
| 22:T:91:LEU:C    | 22:T:93:GLU:H    | 2.22                     | 0.42              |
| 1:A:280:C:O2     | 19:Q:38:ARG:HG3  | 2.20                     | 0.42              |
| 1:A:502:G:H2'    | 1:A:503:C:C6     | 2.55                     | 0.42              |
| 1:A:61:G:H2'     | 1:A:62:U:O4'     | 2.19                     | 0.42              |
| 5:C:125:GLU:HG2  | 5:C:190:ARG:O    | 2.19                     | 0.42              |
| 5:C:14:ILE:CG2   | 5:C:15:THR:H     | 2.09                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 9:G:116:ALA:HA   | 9:G:119:ARG:CZ    | 2.50                     | 0.42              |
| 9:G:21:VAL:HG23  | 9:G:22:LEU:N      | 2.35                     | 0.42              |
| 11:I:44:VAL:CG1  | 11:I:51:ARG:HH22  | 2.32                     | 0.42              |
| 11:I:50:LEU:O    | 11:I:53:VAL:HG22  | 2.20                     | 0.42              |
| 11:I:58:ARG:HG3  | 11:I:58:ARG:HH11  | 1.84                     | 0.42              |
| 12:J:51:ARG:CZ   | 12:J:61:GLU:HB2   | 2.49                     | 0.42              |
| 13:K:78:GLN:O    | 13:K:103:LEU:HD23 | 2.20                     | 0.42              |
| 16:N:34:TYR:HD1  | 16:N:34:TYR:H     | 1.66                     | 0.42              |
| 18:P:4:ILE:HA    | 18:P:20:VAL:O     | 2.20                     | 0.42              |
| 18:P:28:ARG:NH1  | 18:P:29:ASP:OD2   | 2.49                     | 0.42              |
| 1:A:1196:U:OP1   | 1:A:1197:G:H5'    | 2.20                     | 0.42              |
| 1:A:959:A:C2     | 1:A:1222:G:O4'    | 2.73                     | 0.42              |
| 1:A:1296:C:H4'   | 1:A:1302:U:C5     | 2.55                     | 0.42              |
| 1:A:818:G:C3'    | 1:A:819:A:C5'     | 2.97                     | 0.42              |
| 1:A:882:C:O2'    | 1:A:883:C:H5'     | 2.20                     | 0.42              |
| 4:B:88:ALA:C     | 4:B:90:MET:N      | 2.72                     | 0.42              |
| 5:C:17:ASP:O     | 5:C:54:ARG:NH2    | 2.53                     | 0.42              |
| 5:C:20:SER:HB3   | 5:C:22:TRP:NE1    | 2.35                     | 0.42              |
| 5:C:25:GLY:O     | 5:C:27:LYS:N      | 2.53                     | 0.42              |
| 6:D:12:CYS:SG    | 6:D:19:LEU:O      | 2.78                     | 0.42              |
| 1:A:559:A:OP1    | 7:E:126:ARG:NH2   | 2.52                     | 0.42              |
| 12:J:99:LYS:O    | 12:J:100:THR:O    | 2.38                     | 0.42              |
| 13:K:49:GLY:O    | 13:K:50:TYR:O     | 2.38                     | 0.42              |
| 13:K:69:ALA:O    | 13:K:72:ALA:HB3   | 2.20                     | 0.42              |
| 1:A:1058:G:O2'   | 1:A:1059:C:H5'    | 2.20                     | 0.42              |
| 1:A:1109:C:P     | 5:C:176:HIS:CD2   | 3.12                     | 0.42              |
| 1:A:1298:C:H4'   | 1:A:1299:A:O4'    | 2.20                     | 0.42              |
| 1:A:1237:C:H4'   | 1:A:1334:G:N2     | 2.35                     | 0.42              |
| 1:A:1454:G:O2'   | 1:A:1455:G:H5'    | 2.20                     | 0.42              |
| 1:A:406:G:H2'    | 1:A:407:G:C8      | 2.55                     | 0.42              |
| 1:A:58:C:O2'     | 1:A:59:A:H5'      | 2.20                     | 0.42              |
| 1:A:940:C:H2'    | 1:A:941:G:C8      | 2.55                     | 0.42              |
| 4:B:88:ALA:C     | 4:B:90:MET:H      | 2.23                     | 0.42              |
| 10:H:116:LYS:HD2 | 10:H:129:VAL:HG21 | 2.02                     | 0.42              |
| 11:I:10:ARG:NE   | 11:I:105:ASP:HB3  | 2.35                     | 0.42              |
| 11:I:127:LYS:HE3 | 11:I:127:LYS:N    | 2.33                     | 0.42              |
| 11:I:4:TYR:CZ    | 11:I:88:TYR:HD1   | 2.38                     | 0.42              |
| 11:I:18:PHE:O    | 11:I:61:ALA:HA    | 2.20                     | 0.42              |
| 14:L:47:LYS:HG2  | 14:L:48:PRO:HD3   | 2.02                     | 0.42              |
| 1:A:1117:G:H5'   | 1:A:1117:G:C8     | 2.50                     | 0.41              |
| 1:A:1229:A:H2'   | 1:A:1230:C:C6     | 2.55                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:193:C:H2'    | 1:A:194:C:C6      | 2.55                     | 0.41              |
| 1:A:373:A:H1'    | 1:A:481:G:O2'     | 2.20                     | 0.41              |
| 1:A:382:A:C2     | 1:A:383:A:C4      | 3.08                     | 0.41              |
| 1:A:463:A:C2'    | 1:A:474:G:H5'     | 2.50                     | 0.41              |
| 1:A:664:G:OP1    | 20:R:64:ARG:HD2   | 2.20                     | 0.41              |
| 1:A:834:C:H2'    | 1:A:835:U:H6      | 1.84                     | 0.41              |
| 1:A:976:G:N7     | 1:A:1358:U:C2     | 2.88                     | 0.41              |
| 4:B:107:THR:C    | 4:B:109:SER:N     | 2.74                     | 0.41              |
| 4:B:219:VAL:C    | 4:B:221:LEU:N     | 2.74                     | 0.41              |
| 5:C:36:ASP:O     | 5:C:39:ILE:HB     | 2.20                     | 0.41              |
| 7:E:12:LEU:CD1   | 7:E:31:LEU:HB2    | 2.50                     | 0.41              |
| 7:E:78:HIS:CD2   | 10:H:107:LEU:HD12 | 2.49                     | 0.41              |
| 10:H:31:PHE:CZ   | 10:H:134:ILE:HD13 | 2.55                     | 0.41              |
| 12:J:9:ARG:HB3   | 12:J:9:ARG:CZ     | 2.50                     | 0.41              |
| 14:L:114:LYS:HZ3 | 14:L:125:PRO:HG3  | 1.85                     | 0.41              |
| 14:L:47:LYS:HB3  | 14:L:48:PRO:HD2   | 1.92                     | 0.41              |
| 1:A:375:U:O2'    | 18:P:28:ARG:HD2   | 2.20                     | 0.41              |
| 22:T:76:ALA:HA   | 22:T:79:ARG:NH1   | 2.34                     | 0.41              |
| 1:A:1163:C:H2'   | 1:A:1164:G:H8     | 1.85                     | 0.41              |
| 1:A:1423:G:H2'   | 1:A:1424:C:H6     | 1.85                     | 0.41              |
| 1:A:1531:A:O5'   | 1:A:1531:A:H8     | 2.02                     | 0.41              |
| 1:A:490:G:O2'    | 1:A:491:G:H5'     | 2.20                     | 0.41              |
| 1:A:653:A:P      | 10:H:56:LYS:NZ    | 2.93                     | 0.41              |
| 1:A:692:U:O2     | 1:A:695:A:C8      | 2.73                     | 0.41              |
| 1:A:779:C:H2'    | 1:A:780:A:O4'     | 2.20                     | 0.41              |
| 4:B:141:GLU:O    | 4:B:144:ARG:HG3   | 2.20                     | 0.41              |
| 5:C:193:TYR:CE1  | 5:C:196:LEU:HD21  | 2.42                     | 0.41              |
| 6:D:199:ASN:HD22 | 6:D:201:GLN:H     | 1.68                     | 0.41              |
| 6:D:60:GLU:OE2   | 6:D:199:ASN:HB3   | 2.20                     | 0.41              |
| 9:G:141:VAL:O    | 9:G:144:MET:HB2   | 2.20                     | 0.41              |
| 10:H:104:ARG:HG2 | 10:H:104:ARG:HH11 | 1.85                     | 0.41              |
| 11:I:40:LEU:O    | 11:I:41:VAL:C     | 2.58                     | 0.41              |
| 15:M:59:TYR:O    | 15:M:63:THR:CG2   | 2.69                     | 0.41              |
| 15:M:9:ILE:N     | 15:M:9:ILE:CD1    | 2.77                     | 0.41              |
| 18:P:20:VAL:HG11 | 18:P:32:TYR:CG    | 2.55                     | 0.41              |
| 20:R:16:PRO:O    | 20:R:17:SER:HB3   | 2.19                     | 0.41              |
| 20:R:19:LYS:O    | 20:R:20:ALA:HB2   | 2.19                     | 0.41              |
| 20:R:34:TYR:HA   | 20:R:69:THR:CG2   | 2.50                     | 0.41              |
| 20:R:36:ASN:O    | 20:R:40:LEU:HG    | 2.20                     | 0.41              |
| 20:R:43:PHE:CA   | 20:R:51:LEU:HD12  | 2.50                     | 0.41              |
| 13:K:91:ARG:NH1  | 20:R:88:LYS:NZ    | 2.67                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:1127:G:H21    | 1:A:1146:A:H62   | 1.69                     | 0.41              |
| 1:A:1229:A:C2     | 1:A:1230:C:C4    | 3.08                     | 0.41              |
| 1:A:640:A:O2'     | 1:A:641:U:H5'    | 2.20                     | 0.41              |
| 1:A:866:C:H2'     | 1:A:867:G:O5'    | 2.20                     | 0.41              |
| 4:B:20:GLU:HB2    | 4:B:190:THR:HB   | 2.02                     | 0.41              |
| 1:A:1060:C:H5     | 5:C:2:GLY:HA3    | 1.84                     | 0.41              |
| 7:E:88:LYS:HZ3    | 7:E:123:LEU:HD12 | 1.83                     | 0.41              |
| 9:G:26:PHE:HB2    | 9:G:62:PHE:HZ    | 1.85                     | 0.41              |
| 13:K:79:SER:OG    | 13:K:106:LYS:HG2 | 2.20                     | 0.41              |
| 15:M:20:THR:C     | 15:M:22:ILE:H    | 2.24                     | 0.41              |
| 17:O:2:PRO:O      | 17:O:3:ILE:HD12  | 2.19                     | 0.41              |
| 17:O:87:ILE:CG2   | 17:O:88:ARG:N    | 2.83                     | 0.41              |
| 19:Q:63:ARG:HG2   | 19:Q:64:PRO:HD2  | 2.02                     | 0.41              |
| 22:T:74:LYS:HB3   | 22:T:75:ASN:H    | 1.56                     | 0.41              |
| 1:A:1055:A:C2     | 1:A:1056:U:H1'   | 2.55                     | 0.41              |
| 1:A:1172:C:H2'    | 1:A:1173:G:H8    | 1.84                     | 0.41              |
| 1:A:217:C:H2'     | 1:A:218:C:H6     | 1.86                     | 0.41              |
| 1:A:269:C:H2'     | 1:A:270:A:H8     | 1.84                     | 0.41              |
| 1:A:53:A:N6       | 1:A:54:C:C4      | 2.87                     | 0.41              |
| 1:A:556:C:C2'     | 1:A:557:G:H5'    | 2.51                     | 0.41              |
| 1:A:609:A:H2'     | 1:A:610:G:H5'    | 2.03                     | 0.41              |
| 1:A:791:G:H2'     | 1:A:792:A:H5'    | 2.01                     | 0.41              |
| 1:A:959:A:H5''    | 1:A:960:U:OP2    | 2.20                     | 0.41              |
| 7:E:18:ARG:NH2    | 7:E:25:ARG:HB3   | 2.33                     | 0.41              |
| 10:H:127:LEU:HD23 | 10:H:127:LEU:N   | 2.34                     | 0.41              |
| 10:H:53:VAL:C     | 10:H:55:GLY:H    | 2.22                     | 0.41              |
| 1:A:1370:G:H5''   | 11:I:12:GLU:OE1  | 2.20                     | 0.41              |
| 11:I:97:LYS:HG2   | 11:I:102:LEU:CD1 | 2.44                     | 0.41              |
| 13:K:40:ILE:O     | 13:K:41:THR:HG23 | 2.21                     | 0.41              |
| 15:M:118:ALA:HB1  | 15:M:121:LYS:HZ1 | 1.83                     | 0.41              |
| 16:N:17:LYS:HG3   | 16:N:18:VAL:N    | 2.36                     | 0.41              |
| 22:T:42:GLN:HA    | 22:T:42:GLN:OE1  | 2.21                     | 0.41              |
| 1:A:109:A:H2'     | 1:A:326:G:H21    | 1.84                     | 0.41              |
| 1:A:1107:C:C4     | 1:A:1108:G:C8    | 3.07                     | 0.41              |
| 1:A:112:G:H4'     | 1:A:389:A:C5'    | 2.46                     | 0.41              |
| 1:A:518:C:HO2'    | 14:L:50:SER:CB   | 2.30                     | 0.41              |
| 1:A:57:G:H2'      | 1:A:58:C:H6      | 1.85                     | 0.41              |
| 1:A:877:C:H1'     | 10:H:3:THR:HG23  | 2.02                     | 0.41              |
| 1:A:976:G:C8      | 1:A:1358:U:C2    | 3.09                     | 0.41              |
| 4:B:67:THR:N      | 4:B:160:ASP:OD2  | 2.48                     | 0.41              |
| 4:B:228:GLY:O     | 4:B:229:VAL:O    | 2.39                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:C:139:GLN:NE2  | 5:C:139:GLN:CA    | 2.84                     | 0.41              |
| 5:C:38:ARG:HH11  | 5:C:38:ARG:HG3    | 1.86                     | 0.41              |
| 5:C:65:ALA:O     | 5:C:66:VAL:HB     | 2.20                     | 0.41              |
| 6:D:121:VAL:O    | 6:D:134:ASP:HA    | 2.21                     | 0.41              |
| 6:D:146:ILE:N    | 6:D:146:ILE:CD1   | 2.77                     | 0.41              |
| 7:E:15:ARG:HG2   | 7:E:28:PHE:CE2    | 2.56                     | 0.41              |
| 7:E:40:ARG:HG2   | 7:E:40:ARG:HH11   | 1.84                     | 0.41              |
| 9:G:51:GLN:HA    | 9:G:51:GLN:OE1    | 2.21                     | 0.41              |
| 11:I:50:LEU:HG   | 11:I:81:ILE:HG21  | 2.02                     | 0.41              |
| 11:I:93:ARG:C    | 11:I:95:LYS:N     | 2.74                     | 0.41              |
| 15:M:125:ARG:C   | 15:M:125:ARG:HD2  | 2.41                     | 0.41              |
| 19:Q:5:VAL:HA    | 19:Q:59:ILE:O     | 2.20                     | 0.41              |
| 22:T:43:LEU:CD1  | 22:T:55:ILE:HD12  | 2.50                     | 0.41              |
| 1:A:1355:G:O2'   | 1:A:1356:G:H5'    | 2.20                     | 0.41              |
| 1:A:967:C:O3'    | 11:I:128:ARG:CZ   | 2.68                     | 0.41              |
| 6:D:52:SER:C     | 6:D:54:TYR:N      | 2.71                     | 0.41              |
| 1:A:559:A:P      | 7:E:126:ARG:NH2   | 2.94                     | 0.41              |
| 9:G:126:ASP:CG   | 9:G:131:LYS:HE3   | 2.40                     | 0.41              |
| 9:G:62:PHE:O     | 9:G:63:LYS:C      | 2.58                     | 0.41              |
| 10:H:10:LEU:HD12 | 10:H:85:ARG:CG    | 2.50                     | 0.41              |
| 1:A:1347:G:N7    | 11:I:10:ARG:NH2   | 2.69                     | 0.41              |
| 11:I:127:LYS:HE3 | 11:I:127:LYS:CA   | 2.51                     | 0.41              |
| 12:J:32:ALA:C    | 12:J:34:VAL:H     | 2.23                     | 0.41              |
| 13:K:26:ASN:O    | 13:K:27:ASN:HB2   | 2.20                     | 0.41              |
| 13:K:89:ALA:C    | 13:K:91:ARG:H     | 2.24                     | 0.41              |
| 15:M:40:ASN:ND2  | 15:M:40:ASN:C     | 2.74                     | 0.41              |
| 15:M:15:VAL:HG21 | 15:M:48:LEU:HD21  | 2.01                     | 0.41              |
| 20:R:54:ARG:H    | 20:R:54:ARG:HG3   | 1.71                     | 0.41              |
| 21:S:31:ILE:O    | 21:S:32:LYS:HG2   | 2.21                     | 0.41              |
| 1:A:1182:G:HO2'  | 1:A:1183:A:H5''   | 1.84                     | 0.41              |
| 1:A:994:A:N7     | 1:A:1216:G:H4'    | 2.36                     | 0.41              |
| 1:A:1300:G:C2'   | 1:A:1301:U:OP2    | 2.69                     | 0.41              |
| 1:A:1315:U:H2'   | 1:A:1316:G:O4'    | 2.20                     | 0.41              |
| 1:A:1432:G:HO2'  | 1:A:1433:A:H8     | 1.69                     | 0.41              |
| 1:A:1491:G:N7    | 24:A:1545:PAR:O53 | 2.50                     | 0.41              |
| 1:A:404:U:H2'    | 1:A:405:U:C6      | 2.56                     | 0.41              |
| 1:A:824:C:H2'    | 1:A:825:G:C8      | 2.56                     | 0.41              |
| 1:A:911:U:H2'    | 1:A:912:C:C6      | 2.55                     | 0.41              |
| 1:A:979:C:OP2    | 1:A:980:C:H5      | 2.03                     | 0.41              |
| 4:B:19:HIS:CG    | 4:B:204:ASN:HA    | 2.55                     | 0.41              |
| 10:H:126:LYS:HG2 | 10:H:127:LEU:HD23 | 2.02                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 15:M:11:ARG:HA   | 15:M:45:VAL:HB    | 2.02                     | 0.41              |
| 15:M:80:ARG:C    | 15:M:82:MET:N     | 2.73                     | 0.41              |
| 18:P:82:GLN:O    | 18:P:83:GLU:C     | 2.59                     | 0.41              |
| 20:R:37:VAL:CG2  | 20:R:78:LEU:HB3   | 2.51                     | 0.41              |
| 1:A:1305:G:N2    | 1:A:1331:G:HO2'   | 2.17                     | 0.41              |
| 1:A:1320:C:O2    | 21:S:36:ARG:NH1   | 2.54                     | 0.41              |
| 1:A:1435:G:H2'   | 1:A:1436:U:H6     | 1.82                     | 0.41              |
| 1:A:1497:G:H2'   | 1:A:1498:U:H5'    | 2.03                     | 0.41              |
| 1:A:1521:G:O2'   | 1:A:1522:U:H5'    | 2.20                     | 0.41              |
| 1:A:437:U:O2'    | 1:A:438:G:H5'     | 2.19                     | 0.41              |
| 1:A:443:C:H2'    | 1:A:444:C:H6      | 1.86                     | 0.41              |
| 4:B:239:VAL:HG12 | 4:B:240:GLN:NE2   | 2.35                     | 0.41              |
| 6:D:112:VAL:HG22 | 6:D:116:GLN:OE1   | 2.20                     | 0.41              |
| 6:D:76:ARG:NH1   | 6:D:76:ARG:HG2    | 2.31                     | 0.41              |
| 1:A:1194:U:H4'   | 7:E:22:GLY:HA2    | 2.03                     | 0.41              |
| 8:F:26:ILE:O     | 8:F:30:LEU:HG     | 2.20                     | 0.41              |
| 1:A:1249:C:O2'   | 11:I:73:GLN:NE2   | 2.53                     | 0.41              |
| 11:I:78:LYS:HE2  | 11:I:78:LYS:HB3   | 1.92                     | 0.41              |
| 13:K:74:ALA:C    | 13:K:76:GLY:H     | 2.24                     | 0.41              |
| 14:L:83:VAL:HG13 | 14:L:100:ILE:HG23 | 2.02                     | 0.41              |
| 14:L:58:VAL:N    | 14:L:66:VAL:O     | 2.52                     | 0.41              |
| 15:M:15:VAL:O    | 15:M:19:LEU:HG    | 2.20                     | 0.41              |
| 15:M:24:GLY:HA3  | 15:M:66:LEU:HD22  | 2.03                     | 0.41              |
| 22:T:16:HIS:CE1  | 22:T:20:LEU:HD11  | 2.55                     | 0.41              |
| 1:A:1216:G:O2'   | 1:A:1217:C:H5'    | 2.20                     | 0.41              |
| 1:A:1264:C:O2'   | 1:A:1265:G:H5'    | 2.21                     | 0.41              |
| 1:A:1347:G:O2'   | 1:A:1348:U:OP2    | 2.38                     | 0.41              |
| 1:A:1419:G:O2'   | 1:A:1420:C:H5'    | 2.21                     | 0.41              |
| 1:A:240:C:H2'    | 1:A:241:C:H6      | 1.85                     | 0.41              |
| 1:A:286:G:O2'    | 1:A:287:U:H5'     | 2.21                     | 0.41              |
| 1:A:6:G:H4'      | 1:A:298:A:H4'     | 2.01                     | 0.41              |
| 1:A:558:G:H2'    | 1:A:559:A:C2      | 2.55                     | 0.41              |
| 1:A:832:C:H2'    | 1:A:833:U:O4'     | 2.20                     | 0.41              |
| 5:C:35:GLU:OE1   | 5:C:97:LYS:HE3    | 2.20                     | 0.41              |
| 6:D:17:VAL:CG1   | 6:D:18:LYS:N      | 2.84                     | 0.41              |
| 7:E:87:SER:HB3   | 7:E:131:ILE:CD1   | 2.50                     | 0.41              |
| 8:F:48:LEU:CD1   | 8:F:52:ILE:HB     | 2.51                     | 0.41              |
| 11:I:11:LYS:O    | 11:I:12:GLU:HB3   | 2.21                     | 0.41              |
| 15:M:44:ARG:HB3  | 15:M:46:LYS:CG    | 2.51                     | 0.41              |
| 18:P:12:LYS:O    | 18:P:13:HIS:HB2   | 2.20                     | 0.41              |
| 20:R:47:THR:CG2  | 20:R:83:GLU:H     | 2.34                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 21:S:30:LEU:HA   | 21:S:48:THR:O    | 2.20                     | 0.41              |
| 1:A:1194:U:O2'   | 1:A:1195:C:H5'   | 2.20                     | 0.41              |
| 1:A:1202:G:O2'   | 1:A:1203:C:H5'   | 2.21                     | 0.41              |
| 1:A:279:A:C5'    | 1:A:280:C:H3'    | 2.51                     | 0.41              |
| 1:A:623:C:O2'    | 1:A:624:C:H5'    | 2.21                     | 0.41              |
| 1:A:708:C:O2'    | 1:A:709:G:H5'    | 2.20                     | 0.41              |
| 5:C:83:ARG:O     | 5:C:85:ARG:N     | 2.53                     | 0.41              |
| 10:H:104:ARG:O   | 10:H:106:GLY:N   | 2.54                     | 0.41              |
| 14:L:45:PRO:HD3  | 14:L:51:ALA:O    | 2.20                     | 0.41              |
| 22:T:38:LYS:O    | 22:T:39:LYS:C    | 2.59                     | 0.41              |
| 1:A:1014:A:C2    | 1:A:1219:U:H1'   | 2.56                     | 0.41              |
| 1:A:1184:G:H3'   | 1:A:1184:G:OP1   | 2.21                     | 0.41              |
| 1:A:1403:C:H6    | 1:A:1403:C:O5'   | 2.03                     | 0.41              |
| 1:A:502:G:H2'    | 1:A:503:C:O4'    | 2.21                     | 0.41              |
| 1:A:744:C:H2'    | 1:A:745:C:C6     | 2.55                     | 0.41              |
| 1:A:834:C:H2'    | 1:A:835:U:C6     | 2.56                     | 0.41              |
| 1:A:839:U:H5'    | 1:A:840:C:H5     | 1.86                     | 0.41              |
| 1:A:918:A:H2'    | 1:A:919:A:O4'    | 2.21                     | 0.41              |
| 4:B:178:ARG:HH22 | 10:H:74:PRO:CB   | 2.33                     | 0.41              |
| 4:B:7:VAL:O      | 4:B:7:VAL:HG23   | 2.21                     | 0.41              |
| 5:C:145:GLY:O    | 5:C:146:ALA:HB3  | 2.20                     | 0.41              |
| 7:E:76:ILE:CG2   | 7:E:77:PRO:HD2   | 2.45                     | 0.41              |
| 9:G:37:ASN:O     | 9:G:41:ARG:HG3   | 2.21                     | 0.41              |
| 15:M:13:LYS:O    | 15:M:45:VAL:HG23 | 2.21                     | 0.41              |
| 19:Q:18:THR:HG23 | 19:Q:69:LYS:HE3  | 2.02                     | 0.41              |
| 21:S:42:PRO:C    | 21:S:44:MET:H    | 2.23                     | 0.41              |
| 1:A:1152:A:H5''  | 12:J:13:HIS:HB2  | 2.03                     | 0.40              |
| 1:A:1347:G:H2'   | 1:A:1373:G:C6    | 2.56                     | 0.40              |
| 1:A:1427:U:O2'   | 1:A:1428:A:H5'   | 2.21                     | 0.40              |
| 1:A:158:G:N2     | 1:A:164:U:H1'    | 2.36                     | 0.40              |
| 1:A:509:A:H2'    | 1:A:510:A:C8     | 2.56                     | 0.40              |
| 1:A:532:A:C2'    | 1:A:533:A:OP1    | 2.69                     | 0.40              |
| 4:B:144:ARG:HD2  | 4:B:145:LEU:HD23 | 2.02                     | 0.40              |
| 4:B:80:ILE:CD1   | 4:B:212:GLN:HB2  | 2.51                     | 0.40              |
| 9:G:155:ARG:HA   | 9:G:155:ARG:NE   | 2.33                     | 0.40              |
| 10:H:80:ILE:HG22 | 10:H:80:ILE:O    | 2.19                     | 0.40              |
| 19:Q:13:ASP:O    | 19:Q:13:ASP:OD2  | 2.38                     | 0.40              |
| 21:S:36:ARG:NH2  | 21:S:75:ALA:O    | 2.48                     | 0.40              |
| 1:A:1286:A:H2    | 23:V:18:TYR:HH   | 1.66                     | 0.40              |
| 1:A:1094:G:OP2   | 1:A:1095:U:H5    | 2.04                     | 0.40              |
| 1:A:1053:G:O6    | 1:A:1199:U:H2'   | 2.22                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1329:A:O2'   | 1:A:1330:U:H5'   | 2.20                     | 0.40              |
| 1:A:173:U:H5''   | 1:A:197:A:O4'    | 2.22                     | 0.40              |
| 1:A:938:A:C6     | 1:A:939:G:C5     | 3.09                     | 0.40              |
| 4:B:89:GLY:O     | 4:B:154:LEU:HD13 | 2.21                     | 0.40              |
| 5:C:100:ALA:O    | 5:C:101:LEU:HB2  | 2.21                     | 0.40              |
| 5:C:179:ARG:HG2  | 5:C:180:ALA:N    | 2.29                     | 0.40              |
| 6:D:149:ALA:O    | 6:D:150:GLU:C    | 2.59                     | 0.40              |
| 6:D:50:ARG:HA    | 6:D:51:PRO:HD3   | 1.89                     | 0.40              |
| 9:G:15:ASP:OD1   | 9:G:18:TYR:HD1   | 2.03                     | 0.40              |
| 12:J:47:PHE:HB2  | 12:J:63:PHE:HB2  | 2.04                     | 0.40              |
| 18:P:43:LYS:HA   | 18:P:48:TRP:CB   | 2.51                     | 0.40              |
| 1:A:450:G:N7     | 1:A:481:G:C6     | 2.90                     | 0.40              |
| 1:A:713:G:H2'    | 1:A:714:G:C8     | 2.56                     | 0.40              |
| 1:A:947:G:H2'    | 1:A:948:C:O4'    | 2.21                     | 0.40              |
| 6:D:165:MET:SD   | 6:D:168:ARG:HD2  | 2.61                     | 0.40              |
| 8:F:97:PHE:O     | 8:F:98:LEU:C     | 2.59                     | 0.40              |
| 9:G:121:ALA:O    | 9:G:125:MET:HG3  | 2.21                     | 0.40              |
| 9:G:31:MET:HG2   | 9:G:32:ARG:N     | 2.36                     | 0.40              |
| 12:J:22:LYS:CE   | 12:J:90:LEU:HD12 | 2.51                     | 0.40              |
| 21:S:44:MET:O    | 21:S:62:ILE:HG21 | 2.21                     | 0.40              |
| 21:S:47:HIS:O    | 21:S:62:ILE:HG22 | 2.21                     | 0.40              |
| 1:A:1029:C:H2'   | 1:A:1030:C:C6    | 2.56                     | 0.40              |
| 1:A:836:G:C6     | 1:A:851:G:C6     | 3.10                     | 0.40              |
| 1:A:855:G:C6     | 1:A:856:C:C4     | 3.09                     | 0.40              |
| 1:A:962:C:H2'    | 1:A:963:G:O4'    | 2.21                     | 0.40              |
| 4:B:117:GLU:O    | 4:B:117:GLU:HG2  | 2.21                     | 0.40              |
| 5:C:113:ALA:HB2  | 5:C:202:ILE:HG13 | 2.04                     | 0.40              |
| 6:D:152:SER:O    | 6:D:158:ILE:HD12 | 2.22                     | 0.40              |
| 8:F:28:ARG:HG3   | 8:F:28:ARG:HH11  | 1.85                     | 0.40              |
| 10:H:24:THR:HG23 | 10:H:61:VAL:HB   | 2.03                     | 0.40              |
| 10:H:35:ILE:O    | 10:H:39:LEU:HD23 | 2.20                     | 0.40              |
| 10:H:94:TYR:CE2  | 10:H:132:GLU:HG3 | 2.57                     | 0.40              |
| 13:K:11:LYS:O    | 13:K:12:ARG:HB2  | 2.22                     | 0.40              |
| 14:L:24:VAL:HG12 | 14:L:26:ALA:HB2  | 2.03                     | 0.40              |
| 14:L:89:ARG:NE   | 14:L:97:ARG:HD2  | 2.36                     | 0.40              |
| 1:A:1216:G:H5''  | 16:N:5:ALA:HB2   | 2.02                     | 0.40              |
| 17:O:61:GLY:O    | 17:O:64:ARG:HG2  | 2.22                     | 0.40              |
| 1:A:463:A:O4'    | 18:P:82:GLN:NE2  | 2.55                     | 0.40              |
| 20:R:51:LEU:HA   | 20:R:52:PRO:HD3  | 1.84                     | 0.40              |
| 20:R:59:SER:O    | 20:R:60:GLY:C    | 2.59                     | 0.40              |
| 1:A:1061:G:H1'   | 12:J:56:HIS:HE1  | 1.87                     | 0.40              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:109:A:H5'    | 1:A:110:C:C5    | 2.56                     | 0.40              |
| 1:A:321:A:O2'    | 1:A:322:C:H5'   | 2.21                     | 0.40              |
| 1:A:434:U:H2'    | 1:A:435:C:C6    | 2.56                     | 0.40              |
| 4:B:24:TRP:CD1   | 4:B:24:TRP:N    | 2.89                     | 0.40              |
| 4:B:57:PHE:CZ    | 4:B:61:LEU:HD11 | 2.57                     | 0.40              |
| 1:A:1079:G:O3'   | 7:E:14:ARG:NH2  | 2.55                     | 0.40              |
| 9:G:69:VAL:O     | 9:G:69:VAL:HG12 | 2.20                     | 0.40              |
| 9:G:72:ARG:HA    | 9:G:96:GLN:HE21 | 1.87                     | 0.40              |
| 12:J:75:ILE:HG22 | 12:J:76:ASN:ND2 | 2.36                     | 0.40              |
| 19:Q:92:ARG:O    | 19:Q:95:TYR:HB2 | 2.22                     | 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 |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 4   | B     | 232/256 (91%) | 176 (76%) | 40 (17%) | 16 (7%)  | 1           | 6  |
| 5   | C     | 204/239 (85%) | 131 (64%) | 46 (22%) | 27 (13%) | 0           | 1  |
| 6   | D     | 206/209 (99%) | 168 (82%) | 28 (14%) | 10 (5%)  | 2           | 13 |
| 7   | E     | 148/162 (91%) | 140 (95%) | 5 (3%)   | 3 (2%)   | 7           | 34 |
| 8   | F     | 99/101 (98%)  | 80 (81%)  | 18 (18%) | 1 (1%)   | 15          | 53 |
| 9   | G     | 153/156 (98%) | 122 (80%) | 24 (16%) | 7 (5%)   | 2           | 14 |
| 10  | H     | 136/138 (99%) | 116 (85%) | 15 (11%) | 5 (4%)   | 3           | 19 |
| 11  | I     | 125/128 (98%) | 94 (75%)  | 19 (15%) | 12 (10%) | 0           | 3  |
| 12  | J     | 96/105 (91%)  | 60 (62%)  | 25 (26%) | 11 (12%) | 0           | 2  |
| 13  | K     | 117/129 (91%) | 88 (75%)  | 23 (20%) | 6 (5%)   | 2           | 12 |
| 14  | L     | 122/135 (90%) | 97 (80%)  | 16 (13%) | 9 (7%)   | 1           | 5  |
| 15  | M     | 123/126 (98%) | 88 (72%)  | 22 (18%) | 13 (11%) | 0           | 2  |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 16  | N     | 58/61 (95%)     | 44 (76%)   | 10 (17%)  | 4 (7%)   | 1           | 6  |
| 17  | O     | 86/89 (97%)     | 77 (90%)   | 8 (9%)    | 1 (1%)   | 13          | 48 |
| 18  | P     | 81/88 (92%)     | 69 (85%)   | 11 (14%)  | 1 (1%)   | 13          | 48 |
| 19  | Q     | 102/105 (97%)   | 85 (83%)   | 9 (9%)    | 8 (8%)   | 1           | 4  |
| 20  | R     | 71/88 (81%)     | 53 (75%)   | 16 (22%)  | 2 (3%)   | 5           | 25 |
| 21  | S     | 78/93 (84%)     | 60 (77%)   | 12 (15%)  | 6 (8%)   | 1           | 5  |
| 22  | T     | 97/106 (92%)    | 68 (70%)   | 20 (21%)  | 9 (9%)   | 0           | 3  |
| 23  | V     | 22/27 (82%)     | 16 (73%)   | 5 (23%)   | 1 (4%)   | 2           | 14 |
| All | All   | 2356/2541 (93%) | 1832 (78%) | 372 (16%) | 152 (6%) | 1           | 7  |

All (152) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | B     | 8   | LYS  |
| 4   | B     | 15  | VAL  |
| 4   | B     | 16  | HIS  |
| 4   | B     | 24  | TRP  |
| 4   | B     | 123 | ALA  |
| 4   | B     | 229 | VAL  |
| 4   | B     | 232 | PRO  |
| 5   | C     | 4   | LYS  |
| 5   | C     | 15  | THR  |
| 5   | C     | 61  | ALA  |
| 5   | C     | 100 | ALA  |
| 5   | C     | 101 | LEU  |
| 5   | C     | 156 | ARG  |
| 5   | C     | 179 | ARG  |
| 5   | C     | 206 | GLU  |
| 6   | D     | 3   | ARG  |
| 6   | D     | 29  | PRO  |
| 6   | D     | 36  | ARG  |
| 6   | D     | 88  | VAL  |
| 7   | E     | 16  | THR  |
| 10  | H     | 91  | ARG  |
| 11  | I     | 23  | ASN  |
| 11  | I     | 41  | VAL  |
| 11  | I     | 55  | ALA  |
| 11  | I     | 127 | LYS  |
| 12  | J     | 27  | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | J     | 72  | VAL  |
| 12  | J     | 90  | LEU  |
| 13  | K     | 12  | ARG  |
| 13  | K     | 13  | GLN  |
| 13  | K     | 50  | TYR  |
| 14  | L     | 27  | LEU  |
| 14  | L     | 28  | LYS  |
| 14  | L     | 47  | LYS  |
| 15  | M     | 63  | THR  |
| 15  | M     | 86  | CYS  |
| 15  | M     | 122 | LYS  |
| 16  | N     | 22  | THR  |
| 19  | Q     | 69  | LYS  |
| 19  | Q     | 80  | GLY  |
| 19  | Q     | 81  | ARG  |
| 20  | R     | 87  | ARG  |
| 21  | S     | 5   | LEU  |
| 21  | S     | 6   | LYS  |
| 21  | S     | 32  | LYS  |
| 22  | T     | 74  | LYS  |
| 22  | T     | 99  | LEU  |
| 4   | B     | 18  | GLY  |
| 4   | B     | 21  | ARG  |
| 4   | B     | 23  | ARG  |
| 4   | B     | 88  | ALA  |
| 5   | C     | 16  | ARG  |
| 5   | C     | 26  | LYS  |
| 5   | C     | 154 | SER  |
| 5   | C     | 171 | GLY  |
| 5   | C     | 180 | ALA  |
| 6   | D     | 42  | GLN  |
| 6   | D     | 179 | GLU  |
| 8   | F     | 42  | GLU  |
| 9   | G     | 147 | ALA  |
| 10  | H     | 24  | THR  |
| 10  | H     | 105 | ARG  |
| 11  | I     | 38  | GLN  |
| 11  | I     | 94  | ALA  |
| 12  | J     | 34  | VAL  |
| 12  | J     | 61  | GLU  |
| 12  | J     | 73  | ASP  |
| 13  | K     | 128 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | L     | 41  | ARG  |
| 14  | L     | 80  | HIS  |
| 15  | M     | 6   | GLY  |
| 15  | M     | 106 | ASN  |
| 16  | N     | 15  | LYS  |
| 16  | N     | 36  | PHE  |
| 18  | P     | 10  | GLY  |
| 19  | Q     | 49  | GLU  |
| 19  | Q     | 97  | SER  |
| 19  | Q     | 99  | SER  |
| 20  | R     | 20  | ALA  |
| 21  | S     | 9   | VAL  |
| 22  | T     | 9   | ASN  |
| 22  | T     | 11  | SER  |
| 4   | B     | 17  | PHE  |
| 4   | B     | 20  | GLU  |
| 4   | B     | 131 | PRO  |
| 5   | C     | 14  | ILE  |
| 5   | C     | 45  | LYS  |
| 5   | C     | 81  | GLY  |
| 5   | C     | 98  | ASN  |
| 5   | C     | 102 | ASN  |
| 5   | C     | 189 | ALA  |
| 7   | E     | 153 | LYS  |
| 9   | G     | 7   | ALA  |
| 9   | G     | 62  | PHE  |
| 11  | I     | 11  | LYS  |
| 11  | I     | 45  | ALA  |
| 11  | I     | 46  | ALA  |
| 11  | I     | 105 | ASP  |
| 12  | J     | 89  | ASP  |
| 13  | K     | 15  | ALA  |
| 14  | L     | 48  | PRO  |
| 15  | M     | 67  | GLU  |
| 15  | M     | 116 | THR  |
| 22  | T     | 48  | LYS  |
| 22  | T     | 73  | HIS  |
| 22  | T     | 98  | PRO  |
| 22  | T     | 102 | GLY  |
| 23  | V     | 3   | LYS  |
| 4   | B     | 77  | ALA  |
| 5   | C     | 55  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | C     | 64  | VAL  |
| 5   | C     | 108 | ASN  |
| 6   | D     | 4   | TYR  |
| 6   | D     | 46  | LYS  |
| 10  | H     | 83  | ILE  |
| 11  | I     | 24  | GLY  |
| 12  | J     | 17  | ASP  |
| 12  | J     | 57  | LYS  |
| 15  | M     | 37  | THR  |
| 19  | Q     | 14  | LYS  |
| 19  | Q     | 98  | LEU  |
| 21  | S     | 31  | ILE  |
| 22  | T     | 45  | GLN  |
| 5   | C     | 29  | TYR  |
| 5   | C     | 66  | VAL  |
| 6   | D     | 23  | GLY  |
| 7   | E     | 73  | ASN  |
| 9   | G     | 53  | LYS  |
| 9   | G     | 112 | PRO  |
| 9   | G     | 155 | ARG  |
| 12  | J     | 40  | LEU  |
| 14  | L     | 51  | ALA  |
| 14  | L     | 116 | SER  |
| 4   | B     | 95  | GLN  |
| 5   | C     | 168 | ALA  |
| 9   | G     | 113 | GLU  |
| 14  | L     | 79  | GLU  |
| 15  | M     | 21  | TYR  |
| 15  | M     | 36  | LYS  |
| 16  | N     | 23  | ARG  |
| 5   | C     | 77  | ILE  |
| 10  | H     | 103 | VAL  |
| 13  | K     | 47  | VAL  |
| 15  | M     | 4   | ILE  |
| 15  | M     | 117 | VAL  |
| 6   | D     | 5   | ILE  |
| 11  | I     | 44  | VAL  |
| 12  | J     | 39  | PRO  |
| 15  | M     | 85  | GLY  |
| 21  | S     | 11  | VAL  |
| 17  | O     | 86  | GLY  |
| 5   | C     | 130 | 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 |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 4   | B     | 202/220 (92%)   | 181 (90%)  | 21 (10%) | 7           | 27 |
| 5   | C     | 160/188 (85%)   | 145 (91%)  | 15 (9%)  | 8           | 32 |
| 6   | D     | 180/181 (99%)   | 173 (96%)  | 7 (4%)   | 32          | 69 |
| 7   | E     | 115/123 (94%)   | 101 (88%)  | 14 (12%) | 5           | 21 |
| 8   | F     | 90/90 (100%)    | 87 (97%)   | 3 (3%)   | 38          | 73 |
| 9   | G     | 126/127 (99%)   | 120 (95%)  | 6 (5%)   | 25          | 62 |
| 10  | H     | 119/119 (100%)  | 108 (91%)  | 11 (9%)  | 9           | 34 |
| 11  | I     | 98/99 (99%)     | 89 (91%)   | 9 (9%)   | 9           | 34 |
| 12  | J     | 87/92 (95%)     | 79 (91%)   | 8 (9%)   | 9           | 34 |
| 13  | K     | 90/99 (91%)     | 83 (92%)   | 7 (8%)   | 12          | 42 |
| 14  | L     | 104/111 (94%)   | 94 (90%)   | 10 (10%) | 8           | 32 |
| 15  | M     | 100/101 (99%)   | 91 (91%)   | 9 (9%)   | 9           | 35 |
| 16  | N     | 49/50 (98%)     | 47 (96%)   | 2 (4%)   | 30          | 67 |
| 17  | O     | 79/80 (99%)     | 71 (90%)   | 8 (10%)  | 7           | 29 |
| 18  | P     | 72/74 (97%)     | 69 (96%)   | 3 (4%)   | 30          | 66 |
| 19  | Q     | 96/97 (99%)     | 89 (93%)   | 7 (7%)   | 14          | 44 |
| 20  | R     | 64/77 (83%)     | 60 (94%)   | 4 (6%)   | 18          | 51 |
| 21  | S     | 71/80 (89%)     | 68 (96%)   | 3 (4%)   | 30          | 66 |
| 22  | T     | 75/82 (92%)     | 71 (95%)   | 4 (5%)   | 22          | 58 |
| 23  | V     | 19/22 (86%)     | 18 (95%)   | 1 (5%)   | 22          | 58 |
| All | All   | 1996/2112 (94%) | 1844 (92%) | 152 (8%) | 13          | 43 |

All (152) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | B     | 8   | LYS  |
| 4   | B     | 9   | GLU  |
| 4   | B     | 15  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | B     | 23  | ARG  |
| 4   | B     | 24  | TRP  |
| 4   | B     | 25  | ASN  |
| 4   | B     | 71  | VAL  |
| 4   | B     | 98  | LEU  |
| 4   | B     | 114 | ARG  |
| 4   | B     | 144 | ARG  |
| 4   | B     | 156 | LYS  |
| 4   | B     | 157 | ARG  |
| 4   | B     | 162 | ILE  |
| 4   | B     | 163 | PHE  |
| 4   | B     | 164 | VAL  |
| 4   | B     | 170 | GLU  |
| 4   | B     | 178 | ARG  |
| 4   | B     | 215 | LEU  |
| 4   | B     | 221 | LEU  |
| 4   | B     | 231 | GLU  |
| 4   | B     | 236 | TYR  |
| 5   | C     | 3   | ASN  |
| 5   | C     | 5   | ILE  |
| 5   | C     | 18  | TRP  |
| 5   | C     | 26  | LYS  |
| 5   | C     | 34  | LEU  |
| 5   | C     | 37  | GLN  |
| 5   | C     | 56  | ASP  |
| 5   | C     | 139 | GLN  |
| 5   | C     | 166 | GLU  |
| 5   | C     | 167 | TRP  |
| 5   | C     | 179 | ARG  |
| 5   | C     | 188 | LEU  |
| 5   | C     | 190 | ARG  |
| 5   | C     | 192 | THR  |
| 5   | C     | 204 | LEU  |
| 6   | D     | 9   | CYS  |
| 6   | D     | 15  | GLU  |
| 6   | D     | 29  | PRO  |
| 6   | D     | 122 | ARG  |
| 6   | D     | 131 | ARG  |
| 6   | D     | 199 | ASN  |
| 6   | D     | 201 | GLN  |
| 7   | E     | 6   | PHE  |
| 7   | E     | 12  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | E     | 31  | LEU  |
| 7   | E     | 41  | VAL  |
| 7   | E     | 43  | LEU  |
| 7   | E     | 47  | LYS  |
| 7   | E     | 56  | GLN  |
| 7   | E     | 73  | ASN  |
| 7   | E     | 89  | ILE  |
| 7   | E     | 116 | THR  |
| 7   | E     | 120 | THR  |
| 7   | E     | 144 | THR  |
| 7   | E     | 147 | ASP  |
| 7   | E     | 150 | ARG  |
| 8   | F     | 10  | LEU  |
| 8   | F     | 43  | LEU  |
| 8   | F     | 69  | GLU  |
| 9   | G     | 8   | GLU  |
| 9   | G     | 31  | MET  |
| 9   | G     | 79  | ARG  |
| 9   | G     | 126 | ASP  |
| 9   | G     | 140 | ASP  |
| 9   | G     | 155 | ARG  |
| 10  | H     | 18  | ARG  |
| 10  | H     | 24  | THR  |
| 10  | H     | 25  | ASP  |
| 10  | H     | 26  | VAL  |
| 10  | H     | 52  | ASP  |
| 10  | H     | 85  | ARG  |
| 10  | H     | 91  | ARG  |
| 10  | H     | 92  | ARG  |
| 10  | H     | 105 | ARG  |
| 10  | H     | 112 | LEU  |
| 10  | H     | 119 | LEU  |
| 11  | I     | 5   | TYR  |
| 11  | I     | 10  | ARG  |
| 11  | I     | 23  | ASN  |
| 11  | I     | 60  | ASP  |
| 11  | I     | 79  | LEU  |
| 11  | I     | 104 | ARG  |
| 11  | I     | 111 | ARG  |
| 11  | I     | 121 | ARG  |
| 11  | I     | 127 | LYS  |
| 12  | J     | 6   | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | J     | 29  | ARG  |
| 12  | J     | 45  | ARG  |
| 12  | J     | 57  | LYS  |
| 12  | J     | 60  | ARG  |
| 12  | J     | 71  | LEU  |
| 12  | J     | 80  | LYS  |
| 12  | J     | 83  | GLU  |
| 13  | K     | 24  | SER  |
| 13  | K     | 29  | ILE  |
| 13  | K     | 36  | ASP  |
| 13  | K     | 54  | ARG  |
| 13  | K     | 84  | VAL  |
| 13  | K     | 92  | GLU  |
| 13  | K     | 114 | VAL  |
| 14  | L     | 33  | ARG  |
| 14  | L     | 42  | THR  |
| 14  | L     | 48  | PRO  |
| 14  | L     | 53  | ARG  |
| 14  | L     | 60  | LEU  |
| 14  | L     | 80  | HIS  |
| 14  | L     | 81  | SER  |
| 14  | L     | 86  | ARG  |
| 14  | L     | 113 | ARG  |
| 14  | L     | 126 | LYS  |
| 15  | M     | 20  | THR  |
| 15  | M     | 40  | ASN  |
| 15  | M     | 56  | LEU  |
| 15  | M     | 70  | LEU  |
| 15  | M     | 81  | LEU  |
| 15  | M     | 102 | ARG  |
| 15  | M     | 110 | ARG  |
| 15  | M     | 115 | LYS  |
| 15  | M     | 125 | ARG  |
| 16  | N     | 33  | VAL  |
| 16  | N     | 41  | ARG  |
| 17  | O     | 6   | GLU  |
| 17  | O     | 7   | GLU  |
| 17  | O     | 31  | LEU  |
| 17  | O     | 34  | LEU  |
| 17  | O     | 39  | LEU  |
| 17  | O     | 64  | ARG  |
| 17  | O     | 70  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | O     | 81  | LEU  |
| 18  | P     | 2   | VAL  |
| 18  | P     | 8   | ARG  |
| 18  | P     | 28  | ARG  |
| 19  | Q     | 34  | LYS  |
| 19  | Q     | 38  | ARG  |
| 19  | Q     | 60  | ILE  |
| 19  | Q     | 68  | ARG  |
| 19  | Q     | 74  | LEU  |
| 19  | Q     | 96  | GLN  |
| 19  | Q     | 98  | LEU  |
| 20  | R     | 28  | GLU  |
| 20  | R     | 36  | ASN  |
| 20  | R     | 54  | ARG  |
| 20  | R     | 87  | ARG  |
| 21  | S     | 15  | LEU  |
| 21  | S     | 36  | ARG  |
| 21  | S     | 65  | ASN  |
| 22  | T     | 42  | GLN  |
| 22  | T     | 73  | HIS  |
| 22  | T     | 75  | ASN  |
| 22  | T     | 84  | LEU  |
| 23  | V     | 24  | ARG  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | B     | 25  | ASN  |
| 4   | B     | 40  | HIS  |
| 4   | B     | 78  | GLN  |
| 4   | B     | 212 | GLN  |
| 4   | B     | 240 | GLN  |
| 5   | C     | 3   | ASN  |
| 5   | C     | 6   | HIS  |
| 5   | C     | 69  | HIS  |
| 5   | C     | 107 | GLN  |
| 5   | C     | 108 | ASN  |
| 5   | C     | 110 | ASN  |
| 5   | C     | 123 | GLN  |
| 5   | C     | 139 | GLN  |
| 5   | C     | 176 | HIS  |
| 6   | D     | 42  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | D     | 62  | GLN  |
| 6   | D     | 119 | GLN  |
| 6   | D     | 160 | GLN  |
| 6   | D     | 199 | ASN  |
| 7   | E     | 73  | ASN  |
| 8   | F     | 16  | GLN  |
| 8   | F     | 18  | GLN  |
| 8   | F     | 27  | GLN  |
| 8   | F     | 32  | ASN  |
| 8   | F     | 57  | GLN  |
| 8   | F     | 64  | GLN  |
| 8   | F     | 100 | ASN  |
| 9   | G     | 37  | ASN  |
| 9   | G     | 68  | ASN  |
| 9   | G     | 96  | GLN  |
| 9   | G     | 106 | GLN  |
| 10  | H     | 82  | HIS  |
| 11  | I     | 23  | ASN  |
| 11  | I     | 73  | GLN  |
| 11  | I     | 89  | ASN  |
| 12  | J     | 56  | HIS  |
| 12  | J     | 76  | ASN  |
| 12  | J     | 78  | ASN  |
| 13  | K     | 38  | ASN  |
| 13  | K     | 62  | GLN  |
| 14  | L     | 49  | ASN  |
| 14  | L     | 75  | HIS  |
| 15  | M     | 12  | ASN  |
| 15  | M     | 40  | ASN  |
| 15  | M     | 62  | ASN  |
| 15  | M     | 106 | ASN  |
| 17  | O     | 13  | GLN  |
| 17  | O     | 37  | ASN  |
| 17  | O     | 71  | GLN  |
| 18  | P     | 82  | GLN  |
| 19  | Q     | 16  | GLN  |
| 20  | R     | 36  | ASN  |
| 21  | S     | 14  | HIS  |
| 21  | S     | 23  | ASN  |
| 21  | S     | 53  | ASN  |
| 21  | S     | 56  | GLN  |
| 21  | S     | 69  | HIS  |

## 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | A     | 1506/1522 (98%) | 241 (16%)         | 69 (4%)         |
| 2   | W     | 3/4 (75%)       | 0                 | 0               |
| 3   | X     | 10/11 (90%)     | 1 (10%)           | 1 (10%)         |
| All | All   | 1519/1537 (98%) | 242 (15%)         | 70 (4%)         |

All (242) RNA backbone outliers are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 8      | A    |
| 1   | A     | 9      | G    |
| 1   | A     | 31     | G    |
| 1   | A     | 32     | A    |
| 1   | A     | 39     | G    |
| 1   | A     | 47     | C    |
| 1   | A     | 49     | U    |
| 1   | A     | 50     | A    |
| 1   | A     | 51     | A    |
| 1   | A     | 52     | G    |
| 1   | A     | 60     | A    |
| 1   | A     | 61     | G    |
| 1   | A     | 101    | A    |
| 1   | A     | 116    | A    |
| 1   | A     | 120    | A    |
| 1   | A     | 121    | C    |
| 1   | A     | 129(A) | G    |
| 1   | A     | 130    | A    |
| 1   | A     | 131    | C    |
| 1   | A     | 144    | G    |
| 1   | A     | 163    | C    |
| 1   | A     | 182    | U    |
| 1   | A     | 189    | G    |
| 1   | A     | 190    | C    |
| 1   | A     | 190(A) | C    |
| 1   | A     | 190(D) | U    |
| 1   | A     | 190(E) | U    |
| 1   | A     | 190(F) | G    |
| 1   | A     | 190(L) | U    |
| 1   | A     | 195    | A    |
| 1   | A     | 197    | A    |
| 1   | A     | 201    | C    |
| 1   | A     | 202    | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 204 | U    |
| 1   | A     | 216 | G    |
| 1   | A     | 244 | U    |
| 1   | A     | 247 | G    |
| 1   | A     | 251 | G    |
| 1   | A     | 252 | U    |
| 1   | A     | 266 | G    |
| 1   | A     | 267 | C    |
| 1   | A     | 280 | C    |
| 1   | A     | 282 | A    |
| 1   | A     | 289 | G    |
| 1   | A     | 328 | C    |
| 1   | A     | 329 | A    |
| 1   | A     | 332 | G    |
| 1   | A     | 344 | A    |
| 1   | A     | 345 | C    |
| 1   | A     | 351 | G    |
| 1   | A     | 352 | C    |
| 1   | A     | 353 | A    |
| 1   | A     | 354 | G    |
| 1   | A     | 367 | U    |
| 1   | A     | 373 | A    |
| 1   | A     | 397 | A    |
| 1   | A     | 398 | C    |
| 1   | A     | 411 | A    |
| 1   | A     | 413 | G    |
| 1   | A     | 414 | A    |
| 1   | A     | 416 | G    |
| 1   | A     | 417 | C    |
| 1   | A     | 420 | U    |
| 1   | A     | 421 | U    |
| 1   | A     | 422 | C    |
| 1   | A     | 423 | G    |
| 1   | A     | 424 | G    |
| 1   | A     | 425 | G    |
| 1   | A     | 429 | U    |
| 1   | A     | 430 | A    |
| 1   | A     | 439 | A    |
| 1   | A     | 448 | A    |
| 1   | A     | 452 | A    |
| 1   | A     | 461 | C    |
| 1   | A     | 462 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 481 | G    |
| 1   | A     | 482 | A    |
| 1   | A     | 484 | G    |
| 1   | A     | 485 | G    |
| 1   | A     | 497 | A    |
| 1   | A     | 498 | U    |
| 1   | A     | 509 | A    |
| 1   | A     | 510 | A    |
| 1   | A     | 511 | C    |
| 1   | A     | 518 | C    |
| 1   | A     | 519 | C    |
| 1   | A     | 527 | G    |
| 1   | A     | 531 | U    |
| 1   | A     | 532 | A    |
| 1   | A     | 533 | A    |
| 1   | A     | 534 | U    |
| 1   | A     | 547 | A    |
| 1   | A     | 559 | A    |
| 1   | A     | 560 | U    |
| 1   | A     | 561 | U    |
| 1   | A     | 562 | C    |
| 1   | A     | 572 | A    |
| 1   | A     | 573 | A    |
| 1   | A     | 575 | G    |
| 1   | A     | 576 | G    |
| 1   | A     | 577 | G    |
| 1   | A     | 596 | C    |
| 1   | A     | 653 | A    |
| 1   | A     | 665 | A    |
| 1   | A     | 666 | G    |
| 1   | A     | 686 | U    |
| 1   | A     | 687 | A    |
| 1   | A     | 688 | G    |
| 1   | A     | 695 | A    |
| 1   | A     | 702 | A    |
| 1   | A     | 703 | G    |
| 1   | A     | 718 | G    |
| 1   | A     | 723 | U    |
| 1   | A     | 731 | G    |
| 1   | A     | 733 | A    |
| 1   | A     | 748 | C    |
| 1   | A     | 755 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 777  | A    |
| 1   | A     | 781  | A    |
| 1   | A     | 782  | A    |
| 1   | A     | 793  | U    |
| 1   | A     | 794  | A    |
| 1   | A     | 813  | U    |
| 1   | A     | 817  | C    |
| 1   | A     | 819  | A    |
| 1   | A     | 828  | A    |
| 1   | A     | 839  | U    |
| 1   | A     | 840  | C    |
| 1   | A     | 841  | U    |
| 1   | A     | 848  | C    |
| 1   | A     | 902  | G    |
| 1   | A     | 914  | A    |
| 1   | A     | 922  | G    |
| 1   | A     | 926  | G    |
| 1   | A     | 927  | G    |
| 1   | A     | 934  | C    |
| 1   | A     | 935  | A    |
| 1   | A     | 945  | G    |
| 1   | A     | 960  | U    |
| 1   | A     | 961  | U    |
| 1   | A     | 966  | G    |
| 1   | A     | 969  | A    |
| 1   | A     | 971  | G    |
| 1   | A     | 974  | A    |
| 1   | A     | 975  | A    |
| 1   | A     | 976  | G    |
| 1   | A     | 977  | A    |
| 1   | A     | 991  | U    |
| 1   | A     | 992  | U    |
| 1   | A     | 993  | G    |
| 1   | A     | 994  | A    |
| 1   | A     | 1005 | A    |
| 1   | A     | 1021 | G    |
| 1   | A     | 1027 | C    |
| 1   | A     | 1028 | C    |
| 1   | A     | 1029 | C    |
| 1   | A     | 1032 | G    |
| 1   | A     | 1036 | G    |
| 1   | A     | 1045 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1050 | G    |
| 1   | A     | 1053 | G    |
| 1   | A     | 1054 | C    |
| 1   | A     | 1055 | A    |
| 1   | A     | 1065 | U    |
| 1   | A     | 1066 | C    |
| 1   | A     | 1068 | G    |
| 1   | A     | 1094 | G    |
| 1   | A     | 1095 | U    |
| 1   | A     | 1101 | A    |
| 1   | A     | 1117 | G    |
| 1   | A     | 1125 | U    |
| 1   | A     | 1129 | C    |
| 1   | A     | 1130 | A    |
| 1   | A     | 1137 | C    |
| 1   | A     | 1138 | G    |
| 1   | A     | 1139 | G    |
| 1   | A     | 1146 | A    |
| 1   | A     | 1152 | A    |
| 1   | A     | 1159 | U    |
| 1   | A     | 1160 | G    |
| 1   | A     | 1183 | A    |
| 1   | A     | 1184 | G    |
| 1   | A     | 1196 | U    |
| 1   | A     | 1197 | G    |
| 1   | A     | 1200 | C    |
| 1   | A     | 1201 | A    |
| 1   | A     | 1202 | G    |
| 1   | A     | 1212 | U    |
| 1   | A     | 1214 | C    |
| 1   | A     | 1224 | G    |
| 1   | A     | 1225 | A    |
| 1   | A     | 1226 | C    |
| 1   | A     | 1227 | A    |
| 1   | A     | 1257 | U    |
| 1   | A     | 1280 | A    |
| 1   | A     | 1281 | U    |
| 1   | A     | 1282 | C    |
| 1   | A     | 1285 | A    |
| 1   | A     | 1286 | A    |
| 1   | A     | 1287 | A    |
| 1   | A     | 1300 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1301 | U    |
| 1   | A     | 1302 | U    |
| 1   | A     | 1303 | C    |
| 1   | A     | 1305 | G    |
| 1   | A     | 1320 | C    |
| 1   | A     | 1338 | G    |
| 1   | A     | 1346 | A    |
| 1   | A     | 1347 | G    |
| 1   | A     | 1348 | U    |
| 1   | A     | 1353 | G    |
| 1   | A     | 1361 | G    |
| 1   | A     | 1362 | C    |
| 1   | A     | 1363 | A    |
| 1   | A     | 1379 | G    |
| 1   | A     | 1381 | U    |
| 1   | A     | 1398 | A    |
| 1   | A     | 1401 | G    |
| 1   | A     | 1442 | G    |
| 1   | A     | 1443 | G    |
| 1   | A     | 1446 | A    |
| 1   | A     | 1447 | G    |
| 1   | A     | 1452 | C    |
| 1   | A     | 1487 | G    |
| 1   | A     | 1490 | C    |
| 1   | A     | 1492 | A    |
| 1   | A     | 1494 | G    |
| 1   | A     | 1499 | A    |
| 1   | A     | 1502 | A    |
| 1   | A     | 1503 | A    |
| 1   | A     | 1504 | G    |
| 1   | A     | 1505 | G    |
| 1   | A     | 1506 | U    |
| 1   | A     | 1517 | G    |
| 1   | A     | 1520 | G    |
| 1   | A     | 1529 | G    |
| 1   | A     | 1530 | G    |
| 1   | A     | 1533 | C    |
| 1   | A     | 1534 | A    |
| 1   | A     | 1539 | C    |
| 1   | A     | 1541 | U    |
| 3   | X     | 37   | T6A  |

All (70) RNA pucker outliers are listed below:



| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 7      | G    |
| 1   | A     | 30     | U    |
| 1   | A     | 48     | C    |
| 1   | A     | 51     | A    |
| 1   | A     | 60     | A    |
| 1   | A     | 115    | G    |
| 1   | A     | 119    | A    |
| 1   | A     | 129(A) | G    |
| 1   | A     | 181    | G    |
| 1   | A     | 243    | A    |
| 1   | A     | 250    | A    |
| 1   | A     | 251    | G    |
| 1   | A     | 266    | G    |
| 1   | A     | 279    | A    |
| 1   | A     | 281    | G    |
| 1   | A     | 328    | C    |
| 1   | A     | 344    | A    |
| 1   | A     | 353    | A    |
| 1   | A     | 366    | C    |
| 1   | A     | 372    | C    |
| 1   | A     | 428    | G    |
| 1   | A     | 429    | U    |
| 1   | A     | 484    | G    |
| 1   | A     | 496    | A    |
| 1   | A     | 497    | A    |
| 1   | A     | 509    | A    |
| 1   | A     | 518    | C    |
| 1   | A     | 533    | A    |
| 1   | A     | 559    | A    |
| 1   | A     | 560    | U    |
| 1   | A     | 575    | G    |
| 1   | A     | 687    | A    |
| 1   | A     | 701    | C    |
| 1   | A     | 792    | A    |
| 1   | A     | 812    | C    |
| 1   | A     | 819    | A    |
| 1   | A     | 840    | C    |
| 1   | A     | 913    | A    |
| 1   | A     | 945    | G    |
| 1   | A     | 960    | U    |
| 1   | A     | 965    | A    |
| 1   | A     | 975    | A    |
| 1   | A     | 992    | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 993  | G    |
| 1   | A     | 1049 | U    |
| 1   | A     | 1065 | U    |
| 1   | A     | 1067 | A    |
| 1   | A     | 1117 | G    |
| 1   | A     | 1183 | A    |
| 1   | A     | 1196 | U    |
| 1   | A     | 1201 | A    |
| 1   | A     | 1224 | G    |
| 1   | A     | 1226 | C    |
| 1   | A     | 1281 | U    |
| 1   | A     | 1285 | A    |
| 1   | A     | 1300 | G    |
| 1   | A     | 1301 | U    |
| 1   | A     | 1302 | U    |
| 1   | A     | 1346 | A    |
| 1   | A     | 1347 | G    |
| 1   | A     | 1380 | U    |
| 1   | A     | 1397 | C    |
| 1   | A     | 1451 | A    |
| 1   | A     | 1490 | C    |
| 1   | A     | 1498 | U    |
| 1   | A     | 1503 | A    |
| 1   | A     | 1504 | G    |
| 1   | A     | 1505 | G    |
| 1   | A     | 1528 | U    |
| 3   | X     | 37   | T6A  |

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | T6A  | X     | 37  | 3    | 24,34,35     | 1.24 | 3 (12%)  | 24,49,52    | 4.20 | 8 (33%)  |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals  | Torsions   | Rings   |
|-----|------|-------|-----|------|----------|------------|---------|
| 3   | T6A  | X     | 37  | 3    | 1/1/9/11 | 5/15/41/42 | 0/3/3/3 |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | X     | 37  | T6A  | C15-C14 | -3.14 | 1.42        | 1.51     |
| 3   | X     | 37  | T6A  | O14-C14 | -2.86 | 1.35        | 1.43     |
| 3   | X     | 37  | T6A  | C12-N11 | -2.47 | 1.41        | 1.46     |

All (8) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | X     | 37  | T6A  | O14-C14-C15 | 12.08 | 145.52      | 109.74   |
| 3   | X     | 37  | T6A  | C12-N11-C10 | 11.64 | 135.18      | 122.75   |
| 3   | X     | 37  | T6A  | O14-C14-C12 | -7.17 | 94.80       | 109.14   |
| 3   | X     | 37  | T6A  | N6-C10-N11  | 6.18  | 122.40      | 113.76   |
| 3   | X     | 37  | T6A  | O10-C10-N6  | -4.41 | 116.16      | 123.62   |
| 3   | X     | 37  | T6A  | C15-C14-C12 | 3.62  | 119.62      | 112.30   |
| 3   | X     | 37  | T6A  | C2-N1-C6    | 2.84  | 119.03      | 116.59   |
| 3   | X     | 37  | T6A  | O4'-C4'-C5' | -2.21 | 102.10      | 109.37   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 3   | X     | 37  | T6A  | C14  |

All (5) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | X     | 37  | T6A  | C13-C12-N11-C10 |
| 3   | X     | 37  | T6A  | N11-C12-C14-O14 |
| 3   | X     | 37  | T6A  | C13-C12-C14-O14 |
| 3   | X     | 37  | T6A  | O4'-C4'-C5'-O5' |
| 3   | X     | 37  | T6A  | C14-C12-N11-C10 |

There are no ring outliers.

1 monomer is involved in 8 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | X     | 37  | T6A  | 8       | 0            |

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 110 ligands modelled in this entry, 109 are monoatomic - leaving 1 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 24  | PAR  | A     | 1545 | 1    | 45,45,45     | 1.53 | 7 (15%)  | 64,67,67    | 1.27 | 6 (9%)   |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 24  | PAR  | A     | 1545 | 1    | -       | 4/18/94/94 | 0/4/4/4 |

All (7) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 24  | A     | 1545 | PAR  | C24-N24 | 4.14 | 1.53        | 1.47     |
| 24  | A     | 1545 | PAR  | O54-C14 | 3.80 | 1.51        | 1.41     |
| 24  | A     | 1545 | PAR  | C64-C54 | 3.43 | 1.56        | 1.52     |
| 24  | A     | 1545 | PAR  | C11-C21 | 3.12 | 1.58        | 1.52     |
| 24  | A     | 1545 | PAR  | C44-C34 | 2.23 | 1.58        | 1.52     |
| 24  | A     | 1545 | PAR  | O51-C11 | 2.17 | 1.47        | 1.41     |
| 24  | A     | 1545 | PAR  | O51-C51 | 2.16 | 1.49        | 1.44     |

All (6) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | A     | 1545 | PAR  | C14-O54-C54 | 3.72  | 120.99      | 113.69   |
| 24  | A     | 1545 | PAR  | O33-C14-C24 | 3.16  | 113.65      | 108.22   |
| 24  | A     | 1545 | PAR  | O54-C54-C64 | 2.86  | 111.33      | 106.01   |
| 24  | A     | 1545 | PAR  | O11-C11-C21 | 2.80  | 113.04      | 108.22   |
| 24  | A     | 1545 | PAR  | O52-C13-C23 | 2.31  | 112.74      | 107.96   |
| 24  | A     | 1545 | PAR  | O52-C13-O43 | -2.22 | 109.03      | 111.43   |

There are no chirality outliers.

All (4) torsion outliers are listed below:

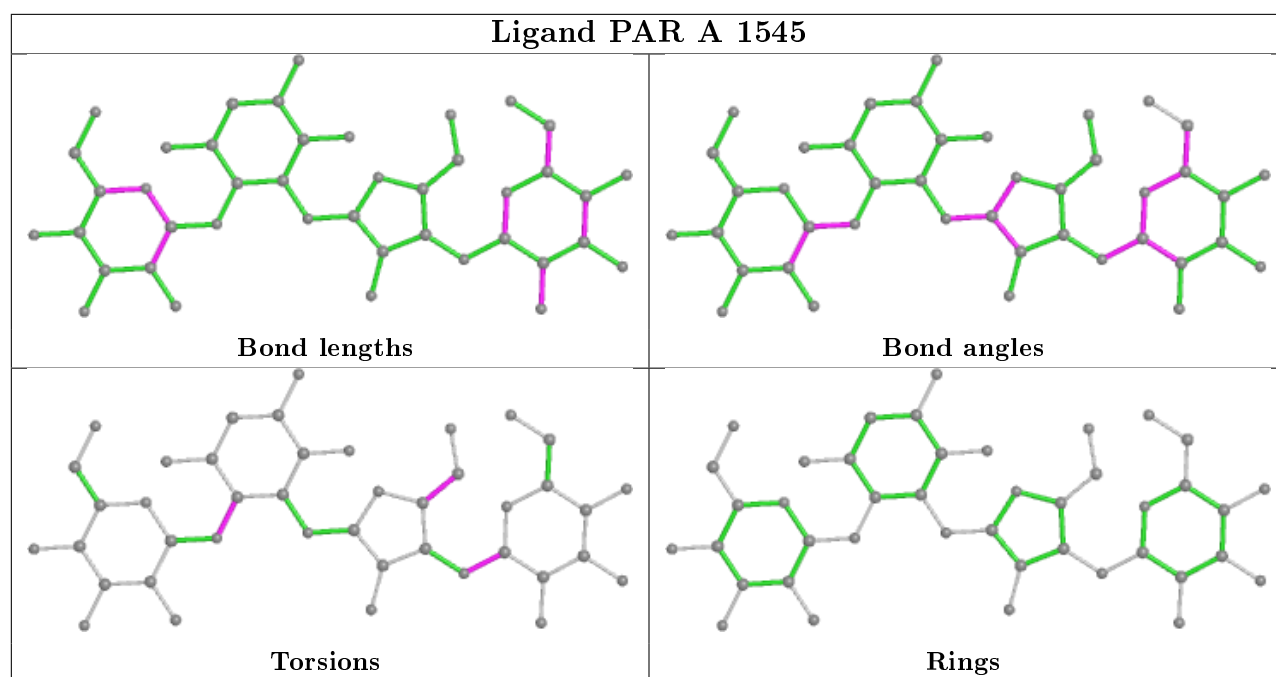
| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 24  | A     | 1545 | PAR  | C33-C43-C53-O53 |
| 24  | A     | 1545 | PAR  | O43-C43-C53-O53 |
| 24  | A     | 1545 | PAR  | C24-C14-O33-C33 |
| 24  | A     | 1545 | PAR  | C52-C42-O11-C11 |

There are no ring outliers.

1 monomer is involved in 2 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 24  | A     | 1545 | PAR  | 2       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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   | A     | 1506/1522 (98%) | 0.96   | 65 (4%)  | 35  | 13  | 29, 61, 149, 201      | 0     |
| 2   | W     | 4/4 (100%)      | 1.16   | 1 (25%)  | 0   | 0   | 49, 53, 55, 127       | 0     |
| 3   | X     | 10/11 (90%)     | 0.49   | 0        | 100 | 100 | 63, 79, 146, 163      | 0     |
| 4   | B     | 234/256 (91%)   | 0.27   | 8 (3%)   | 45  | 19  | 38, 106, 176, 201     | 0     |
| 5   | C     | 206/239 (86%)   | 0.31   | 6 (2%)   | 51  | 23  | 41, 91, 159, 197      | 0     |
| 6   | D     | 208/209 (99%)   | 0.46   | 14 (6%)  | 17  | 5   | 41, 72, 143, 200      | 0     |
| 7   | E     | 150/162 (92%)   | 0.34   | 2 (1%)   | 77  | 51  | 33, 56, 107, 187      | 0     |
| 8   | F     | 101/101 (100%)  | 0.05   | 0        | 100 | 100 | 51, 99, 138, 167      | 0     |
| 9   | G     | 155/156 (99%)   | 0.24   | 4 (2%)   | 56  | 27  | 34, 82, 151, 191      | 0     |
| 10  | H     | 138/138 (100%)  | 0.29   | 2 (1%)   | 75  | 49  | 32, 53, 99, 163       | 0     |
| 11  | I     | 127/128 (99%)   | 0.45   | 6 (4%)   | 31  | 11  | 43, 96, 148, 200      | 0     |
| 12  | J     | 98/105 (93%)    | 0.86   | 12 (12%) | 4   | 1   | 47, 127, 197, 201     | 0     |
| 13  | K     | 119/129 (92%)   | 0.35   | 2 (1%)   | 70  | 41  | 37, 67, 120, 182      | 0     |
| 14  | L     | 124/135 (91%)   | 0.45   | 5 (4%)   | 38  | 15  | 31, 56, 135, 175      | 0     |
| 15  | M     | 125/126 (99%)   | 1.03   | 13 (10%) | 6   | 2   | 47, 83, 165, 201      | 0     |
| 16  | N     | 60/61 (98%)     | 0.86   | 9 (15%)  | 2   | 1   | 50, 81, 133, 200      | 0     |
| 17  | O     | 88/89 (98%)     | 0.31   | 3 (3%)   | 45  | 19  | 39, 74, 135, 195      | 0     |
| 18  | P     | 83/88 (94%)     | 0.38   | 1 (1%)   | 79  | 54  | 36, 52, 94, 174       | 0     |
| 19  | Q     | 104/105 (99%)   | 0.64   | 6 (5%)   | 23  | 7   | 29, 57, 139, 201      | 0     |
| 20  | R     | 73/88 (82%)     | 0.28   | 3 (4%)   | 37  | 14  | 50, 74, 161, 193      | 0     |
| 21  | S     | 80/93 (86%)     | 0.67   | 7 (8%)   | 10  | 3   | 55, 105, 165, 201     | 0     |
| 22  | T     | 99/106 (93%)    | 0.28   | 0        | 100 | 100 | 28, 59, 118, 175      | 0     |
| 23  | V     | 24/27 (88%)     | 0.95   | 3 (12%)  | 3   | 1   | 39, 67, 122, 166      | 0     |
| All | All   | 3916/4078 (96%) | 0.63   | 172 (4%) | 34  | 13  | 28, 70, 158, 201      | 0     |

All (172) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 15  | M     | 123  | ALA  | 17.9 |
| 1   | A     | 1539 | C    | 13.4 |
| 15  | M     | 126  | LYS  | 12.6 |
| 15  | M     | 124  | PRO  | 12.6 |
| 1   | A     | 424  | G    | 11.9 |
| 21  | S     | 3    | ARG  | 11.1 |
| 15  | M     | 125  | ARG  | 10.6 |
| 1   | A     | 190  | C    | 9.7  |
| 1   | A     | 423  | G    | 9.4  |
| 15  | M     | 119  | GLY  | 9.3  |
| 19  | Q     | 105  | ALA  | 9.0  |
| 1   | A     | 1129 | C    | 8.8  |
| 15  | M     | 120  | LYS  | 8.6  |
| 1   | A     | 415  | A    | 8.0  |
| 1   | A     | 417  | C    | 7.9  |
| 6   | D     | 23   | GLY  | 7.9  |
| 19  | Q     | 103  | GLY  | 7.4  |
| 11  | I     | 128  | ARG  | 7.1  |
| 19  | Q     | 104  | LYS  | 7.0  |
| 1   | A     | 1541 | U    | 7.0  |
| 1   | A     | 419  | C    | 6.9  |
| 19  | Q     | 102  | GLY  | 6.9  |
| 1   | A     | 412  | A    | 6.8  |
| 1   | A     | 1035 | A    | 6.1  |
| 6   | D     | 35   | ARG  | 5.8  |
| 1   | A     | 414  | A    | 5.8  |
| 1   | A     | 1540 | U    | 5.7  |
| 12  | J     | 17   | ASP  | 5.7  |
| 4   | B     | 132  | LYS  | 5.6  |
| 6   | D     | 209  | ARG  | 5.5  |
| 1   | A     | 1446 | A    | 4.7  |
| 9   | G     | 2    | ALA  | 4.7  |
| 1   | A     | 1361 | G    | 4.6  |
| 15  | M     | 122  | LYS  | 4.6  |
| 1   | A     | 1033 | G    | 4.6  |
| 12  | J     | 33   | GLN  | 4.5  |
| 16  | N     | 2    | ALA  | 4.3  |
| 15  | M     | 102  | ARG  | 4.3  |
| 1   | A     | 1005 | A    | 4.2  |
| 1   | A     | 416  | G    | 4.1  |
| 15  | M     | 106  | ASN  | 4.1  |
| 1   | A     | 1027 | C    | 4.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 16  | N     | 30   | ALA  | 4.0  |
| 1   | A     | 421  | U    | 3.9  |
| 1   | A     | 420  | U    | 3.9  |
| 1   | A     | 1124 | G    | 3.9  |
| 10  | H     | 1    | MET  | 3.8  |
| 13  | K     | 129  | SER  | 3.8  |
| 21  | S     | 37   | ARG  | 3.7  |
| 14  | L     | 28   | LYS  | 3.7  |
| 1   | A     | 422  | C    | 3.6  |
| 19  | Q     | 101  | ARG  | 3.5  |
| 23  | V     | 6    | ARG  | 3.5  |
| 4   | B     | 238  | LEU  | 3.4  |
| 12  | J     | 70   | ARG  | 3.4  |
| 15  | M     | 118  | ALA  | 3.4  |
| 16  | N     | 6    | LEU  | 3.4  |
| 20  | R     | 17   | SER  | 3.3  |
| 1   | A     | 1094 | G    | 3.3  |
| 5   | C     | 82   | GLU  | 3.3  |
| 17  | O     | 23   | GLY  | 3.2  |
| 14  | L     | 73   | GLU  | 3.2  |
| 10  | H     | 2    | LEU  | 3.2  |
| 12  | J     | 37   | PRO  | 3.2  |
| 11  | I     | 102  | LEU  | 3.2  |
| 12  | J     | 34   | VAL  | 3.1  |
| 16  | N     | 3    | ARG  | 3.1  |
| 2   | W     | 4    | A    | 3.1  |
| 1   | A     | 1362 | C    | 3.0  |
| 14  | L     | 115  | LYS  | 3.0  |
| 5   | C     | 2    | GLY  | 3.0  |
| 12  | J     | 36   | GLY  | 3.0  |
| 14  | L     | 89   | ARG  | 3.0  |
| 12  | J     | 54   | PHE  | 3.0  |
| 12  | J     | 89   | ASP  | 2.9  |
| 6   | D     | 21   | LEU  | 2.9  |
| 15  | M     | 7    | VAL  | 2.9  |
| 18  | P     | 83   | GLU  | 2.9  |
| 21  | S     | 77   | THR  | 2.9  |
| 6   | D     | 24   | GLU  | 2.9  |
| 21  | S     | 2    | PRO  | 2.9  |
| 6   | D     | 33   | MET  | 2.8  |
| 6   | D     | 2    | GLY  | 2.8  |
| 6   | D     | 3    | ARG  | 2.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 7   | E     | 20   | GLN  | 2.8  |
| 23  | V     | 25   | LYS  | 2.8  |
| 1   | A     | 1030 | C    | 2.7  |
| 15  | M     | 116  | THR  | 2.7  |
| 1   | A     | 373  | A    | 2.7  |
| 1   | A     | 418  | C    | 2.7  |
| 11  | I     | 19   | LEU  | 2.7  |
| 4   | B     | 131  | PRO  | 2.7  |
| 1   | A     | 1006 | C    | 2.6  |
| 1   | A     | 1020 | U    | 2.6  |
| 1   | A     | 1533 | C    | 2.6  |
| 1   | A     | 425  | G    | 2.6  |
| 1   | A     | 1004 | A    | 2.6  |
| 21  | S     | 34   | TRP  | 2.6  |
| 7   | E     | 50   | GLU  | 2.6  |
| 5   | C     | 161  | GLU  | 2.5  |
| 1   | A     | 1032 | G    | 2.5  |
| 6   | D     | 32   | ALA  | 2.5  |
| 16  | N     | 61   | TRP  | 2.5  |
| 1   | A     | 1200 | C    | 2.5  |
| 16  | N     | 32   | SER  | 2.5  |
| 1   | A     | 1002 | G    | 2.4  |
| 1   | A     | 266  | G    | 2.4  |
| 1   | A     | 202  | U    | 2.4  |
| 1   | A     | 630  | G    | 2.4  |
| 12  | J     | 15   | THR  | 2.4  |
| 17  | O     | 22   | THR  | 2.4  |
| 4   | B     | 16   | HIS  | 2.3  |
| 6   | D     | 22   | LYS  | 2.3  |
| 16  | N     | 60   | SER  | 2.3  |
| 5   | C     | 60   | ALA  | 2.3  |
| 21  | S     | 26   | GLY  | 2.3  |
| 1   | A     | 426  | G    | 2.3  |
| 1   | A     | 1504 | G    | 2.3  |
| 6   | D     | 31   | CYS  | 2.3  |
| 4   | B     | 81   | VAL  | 2.3  |
| 1   | A     | 1224 | G    | 2.3  |
| 1   | A     | 1355 | G    | 2.3  |
| 1   | A     | 1003 | G    | 2.2  |
| 1   | A     | 1127 | G    | 2.2  |
| 1   | A     | 991  | U    | 2.2  |
| 19  | Q     | 98   | LEU  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 4   | B     | 229  | VAL  | 2.2  |
| 1   | A     | 1196 | U    | 2.2  |
| 1   | A     | 1467 | G    | 2.2  |
| 14  | L     | 47   | LYS  | 2.2  |
| 1   | A     | 631  | G    | 2.2  |
| 1   | A     | 1443 | G    | 2.2  |
| 13  | K     | 51   | LYS  | 2.2  |
| 16  | N     | 4    | LYS  | 2.2  |
| 1   | A     | 1442 | G    | 2.2  |
| 1   | A     | 977  | A    | 2.2  |
| 16  | N     | 29   | ARG  | 2.2  |
| 5   | C     | 19   | GLU  | 2.2  |
| 9   | G     | 156  | TRP  | 2.2  |
| 1   | A     | 723  | U    | 2.2  |
| 23  | V     | 9    | ARG  | 2.2  |
| 9   | G     | 33   | ASP  | 2.1  |
| 11  | I     | 11   | LYS  | 2.1  |
| 20  | R     | 48   | GLY  | 2.1  |
| 1   | A     | 1395 | C    | 2.1  |
| 9   | G     | 83   | ALA  | 2.1  |
| 1   | A     | 481  | G    | 2.1  |
| 1   | A     | 1131 | G    | 2.1  |
| 21  | S     | 27   | GLU  | 2.1  |
| 6   | D     | 9    | CYS  | 2.1  |
| 1   | A     | 975  | A    | 2.1  |
| 1   | A     | 1084 | G    | 2.1  |
| 15  | M     | 121  | LYS  | 2.1  |
| 12  | J     | 24   | VAL  | 2.1  |
| 1   | A     | 1093 | A    | 2.1  |
| 1   | A     | 548  | G    | 2.1  |
| 1   | A     | 1053 | G    | 2.1  |
| 6   | D     | 42   | GLN  | 2.1  |
| 11  | I     | 117  | HIS  | 2.1  |
| 20  | R     | 25   | THR  | 2.1  |
| 1   | A     | 1014 | A    | 2.1  |
| 12  | J     | 6    | ILE  | 2.1  |
| 1   | A     | 1260 | C    | 2.1  |
| 6   | D     | 26   | CYS  | 2.0  |
| 12  | J     | 38   | ILE  | 2.0  |
| 4   | B     | 133  | LYS  | 2.0  |
| 1   | A     | 1001 | A    | 2.0  |
| 4   | B     | 148  | TYR  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 17  | O     | 89  | GLY  | 2.0  |
| 5   | C     | 33  | LEU  | 2.0  |
| 1   | A     | 411 | A    | 2.0  |
| 11  | I     | 125 | TYR  | 2.0  |

## 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 3   | T6A  | X     | 37  | 32/33 | 0.92 | 0.28 | 67,76,76,76                | 0     |

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 25  | MG   | A     | 1608 | 1/1   | 0.34 | 0.58 | 29,29,29,29                | 1     |
| 25  | MG   | A     | 1548 | 1/1   | 0.53 | 0.32 | 29,29,29,29                | 1     |
| 25  | MG   | A     | 1607 | 1/1   | 0.58 | 0.32 | 29,29,29,29                | 1     |
| 25  | MG   | A     | 1602 | 1/1   | 0.64 | 0.18 | 29,29,29,29                | 1     |
| 25  | MG   | A     | 1614 | 1/1   | 0.68 | 0.23 | 29,29,29,29                | 0     |
| 25  | MG   | A     | 1613 | 1/1   | 0.68 | 0.48 | 29,29,29,29                | 1     |
| 25  | MG   | A     | 1630 | 1/1   | 0.69 | 0.33 | 29,29,29,29                | 1     |
| 25  | MG   | N     | 423  | 1/1   | 0.69 | 0.24 | 29,29,29,29                | 1     |
| 25  | MG   | A     | 1595 | 1/1   | 0.69 | 0.34 | 29,29,29,29                | 1     |
| 25  | MG   | A     | 1620 | 1/1   | 0.70 | 0.34 | 29,29,29,29                | 1     |
| 25  | MG   | A     | 493  | 1/1   | 0.70 | 0.69 | 29,29,29,29                | 1     |
| 25  | MG   | A     | 441  | 1/1   | 0.72 | 0.24 | 29,29,29,29                | 1     |
| 25  | MG   | A     | 1575 | 1/1   | 0.73 | 0.29 | 29,29,29,29                | 1     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 25  | MG   | A     | 1562 | 1/1   | 0.73 | 0.39 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1585 | 1/1   | 0.74 | 0.39 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 470  | 1/1   | 0.75 | 0.21 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1627 | 1/1   | 0.77 | 0.42 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1628 | 1/1   | 0.78 | 0.33 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 467  | 1/1   | 0.78 | 0.27 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1633 | 1/1   | 0.79 | 0.33 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1554 | 1/1   | 0.79 | 0.23 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 87   | 1/1   | 0.80 | 0.38 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1601 | 1/1   | 0.81 | 0.09 | 29,29,29,29                 | 0     |
| 25  | MG   | A     | 1634 | 1/1   | 0.81 | 0.41 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1597 | 1/1   | 0.81 | 0.13 | 29,29,29,29                 | 0     |
| 25  | MG   | A     | 1610 | 1/1   | 0.82 | 0.41 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1632 | 1/1   | 0.82 | 0.43 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1564 | 1/1   | 0.83 | 0.23 | 29,29,29,29                 | 0     |
| 25  | MG   | A     | 214  | 1/1   | 0.83 | 0.24 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 471  | 1/1   | 0.84 | 0.31 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1603 | 1/1   | 0.84 | 0.43 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1596 | 1/1   | 0.84 | 0.23 | 29,29,29,29                 | 0     |
| 25  | MG   | A     | 1594 | 1/1   | 0.85 | 0.29 | 29,29,29,29                 | 1     |
| 25  | MG   | X     | 500  | 1/1   | 0.85 | 0.44 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1565 | 1/1   | 0.85 | 0.40 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1600 | 1/1   | 0.86 | 0.21 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 210  | 1/1   | 0.87 | 0.16 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 71   | 1/1   | 0.87 | 0.34 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1635 | 1/1   | 0.87 | 0.22 | 29,29,29,29                 | 0     |
| 25  | MG   | X     | 502  | 1/1   | 0.87 | 0.39 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1591 | 1/1   | 0.87 | 0.26 | 29,29,29,29                 | 0     |
| 25  | MG   | A     | 1615 | 1/1   | 0.87 | 0.17 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1584 | 1/1   | 0.88 | 0.27 | 29,29,29,29                 | 0     |
| 25  | MG   | A     | 1571 | 1/1   | 0.88 | 0.21 | 29,29,29,29                 | 0     |
| 25  | MG   | A     | 1558 | 1/1   | 0.89 | 0.14 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1611 | 1/1   | 0.89 | 0.19 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1559 | 1/1   | 0.89 | 0.27 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1578 | 1/1   | 0.89 | 0.16 | 29,29,29,29                 | 0     |
| 25  | MG   | A     | 1624 | 1/1   | 0.89 | 0.35 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1612 | 1/1   | 0.90 | 0.24 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1547 | 1/1   | 0.90 | 0.35 | 29,29,29,29                 | 0     |
| 25  | MG   | A     | 1616 | 1/1   | 0.90 | 0.15 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1563 | 1/1   | 0.90 | 0.34 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1569 | 1/1   | 0.90 | 0.33 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1568 | 1/1   | 0.91 | 0.21 | 29,29,29,29                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 25  | MG   | A     | 469  | 1/1   | 0.91 | 0.27 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1592 | 1/1   | 0.91 | 0.23 | 29,29,29,29                 | 0     |
| 25  | MG   | A     | 1631 | 1/1   | 0.91 | 0.15 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 473  | 1/1   | 0.91 | 0.29 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 211  | 1/1   | 0.91 | 0.33 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1619 | 1/1   | 0.91 | 0.16 | 29,29,29,29                 | 0     |
| 25  | MG   | A     | 1572 | 1/1   | 0.91 | 0.14 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1583 | 1/1   | 0.92 | 0.25 | 29,29,29,29                 | 0     |
| 25  | MG   | A     | 1546 | 1/1   | 0.92 | 0.26 | 29,29,29,29                 | 0     |
| 25  | MG   | A     | 1622 | 1/1   | 0.92 | 0.23 | 29,29,29,29                 | 1     |
| 24  | PAR  | A     | 1545 | 42/42 | 0.92 | 0.30 | 28,28,28,28                 | 0     |
| 25  | MG   | A     | 1580 | 1/1   | 0.92 | 0.34 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1621 | 1/1   | 0.93 | 0.37 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1623 | 1/1   | 0.93 | 0.24 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1581 | 1/1   | 0.93 | 0.34 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1617 | 1/1   | 0.93 | 0.16 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1599 | 1/1   | 0.93 | 0.24 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1593 | 1/1   | 0.93 | 0.27 | 29,29,29,29                 | 0     |
| 25  | MG   | A     | 1551 | 1/1   | 0.93 | 0.28 | 29,29,29,29                 | 0     |
| 25  | MG   | A     | 1574 | 1/1   | 0.93 | 0.30 | 29,29,29,29                 | 0     |
| 25  | MG   | A     | 1577 | 1/1   | 0.93 | 0.14 | 29,29,29,29                 | 0     |
| 25  | MG   | A     | 1586 | 1/1   | 0.94 | 0.29 | 29,29,29,29                 | 0     |
| 25  | MG   | A     | 1550 | 1/1   | 0.94 | 0.26 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1556 | 1/1   | 0.94 | 0.34 | 29,29,29,29                 | 0     |
| 25  | MG   | A     | 466  | 1/1   | 0.94 | 0.29 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1557 | 1/1   | 0.94 | 0.32 | 29,29,29,29                 | 0     |
| 25  | MG   | A     | 1549 | 1/1   | 0.94 | 0.28 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1604 | 1/1   | 0.95 | 0.25 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1561 | 1/1   | 0.95 | 0.10 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1629 | 1/1   | 0.95 | 0.24 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 86   | 1/1   | 0.95 | 0.22 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1553 | 1/1   | 0.95 | 0.36 | 29,29,29,29                 | 0     |
| 25  | MG   | A     | 1582 | 1/1   | 0.95 | 0.20 | 29,29,29,29                 | 0     |
| 25  | MG   | A     | 1609 | 1/1   | 0.95 | 0.29 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1566 | 1/1   | 0.96 | 0.37 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1576 | 1/1   | 0.96 | 0.31 | 29,29,29,29                 | 0     |
| 25  | MG   | A     | 1560 | 1/1   | 0.96 | 0.25 | 29,29,29,29                 | 0     |
| 25  | MG   | A     | 1552 | 1/1   | 0.96 | 0.29 | 29,29,29,29                 | 0     |
| 25  | MG   | A     | 1573 | 1/1   | 0.96 | 0.32 | 29,29,29,29                 | 0     |
| 25  | MG   | A     | 1618 | 1/1   | 0.96 | 0.18 | 29,29,29,29                 | 0     |
| 25  | MG   | A     | 1579 | 1/1   | 0.96 | 0.23 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1598 | 1/1   | 0.96 | 0.26 | 29,29,29,29                 | 0     |

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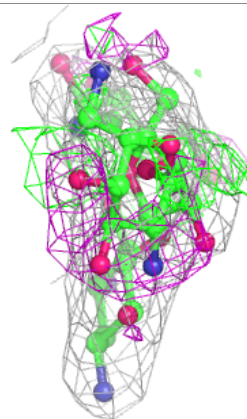
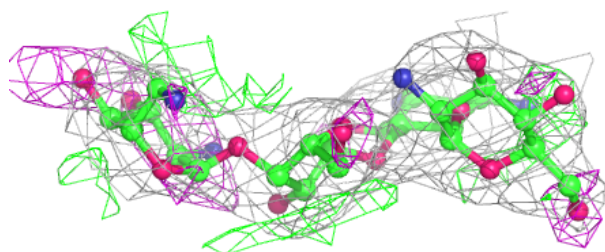
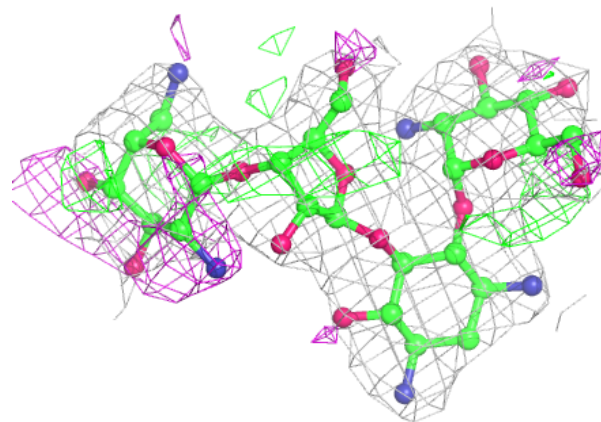
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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 25  | MG   | A     | 1606 | 1/1   | 0.97 | 0.18 | 29,29,29,29                 | 0     |
| 25  | MG   | A     | 1570 | 1/1   | 0.97 | 0.19 | 29,29,29,29                 | 0     |
| 25  | MG   | A     | 1555 | 1/1   | 0.97 | 0.28 | 29,29,29,29                 | 0     |
| 25  | MG   | A     | 1587 | 1/1   | 0.97 | 0.32 | 29,29,29,29                 | 0     |
| 26  | ZN   | D     | 306  | 1/1   | 0.97 | 0.39 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1590 | 1/1   | 0.98 | 0.23 | 29,29,29,29                 | 0     |
| 25  | MG   | A     | 1625 | 1/1   | 0.98 | 0.22 | 29,29,29,29                 | 0     |
| 25  | MG   | A     | 1589 | 1/1   | 0.98 | 0.34 | 29,29,29,29                 | 0     |
| 25  | MG   | A     | 1626 | 1/1   | 0.98 | 0.17 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1605 | 1/1   | 0.98 | 0.25 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1567 | 1/1   | 0.98 | 0.37 | 29,29,29,29                 | 1     |
| 26  | ZN   | N     | 307  | 1/1   | 0.98 | 0.24 | 29,29,29,29                 | 1     |
| 25  | MG   | A     | 1588 | 1/1   | 0.98 | 0.30 | 29,29,29,29                 | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

#### Electron density around PAR A 1545:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.