



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 07:54 AM GMT

PDB ID : 1HNZ  
Title : STRUCTURE OF THE THERMUS THERMOPHILUS 30S RIBOSOMAL  
SUBUNIT IN COMPLEX WITH HYGROMYCIN B  
Authors : Brodersen, D.E.; Clemons Jr., W.M.; Carter, A.P.; Morgan-Warren, R.; Wim-  
berly, B.T.; Ramakrishnan, V.  
Deposited on : 2000-12-08  
Resolution : 3.30 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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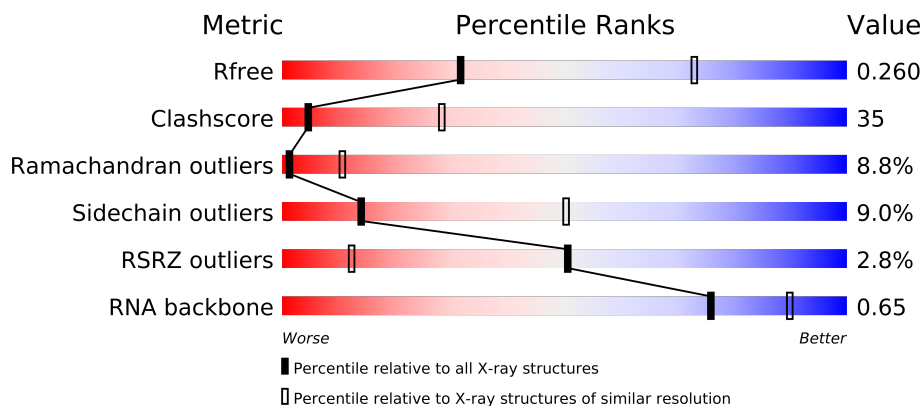
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.30 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.





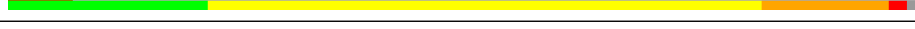
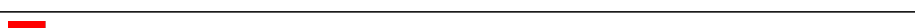
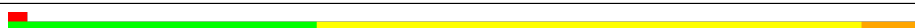
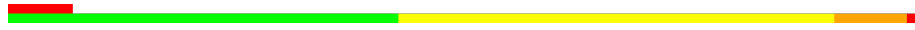
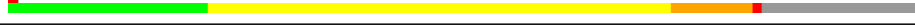
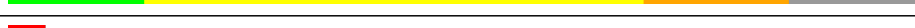



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 66092                       | 1341 (3.40-3.20)                                      |
| Clashscore            | 79885                       | 1696 (3.40-3.20)                                      |
| Ramachandran outliers | 78287                       | 1664 (3.40-3.20)                                      |
| Sidechain outliers    | 78261                       | 1662 (3.40-3.20)                                      |
| RSRZ outliers         | 66119                       | 1342 (3.40-3.20)                                      |
| RNA backbone          | 1838                        | 1042 (3.90-2.70)                                      |

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 1522   |                  |
| 2   | X     | 6      |                  |
| 3   | B     | 256    |                  |
| 4   | C     | 239    |                  |
| 5   | D     | 209    |                  |
| 6   | E     | 162    |                  |
| 7   | F     | 101    |                  |
| 8   | G     | 156    |                  |
| 9   | H     | 138    |                  |
| 10  | I     | 128    |                  |
| 11  | J     | 105    |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 12  | K     | 129    |  |
| 13  | L     | 135    |  |
| 14  | M     | 126    |  |
| 15  | N     | 61     |  |
| 16  | O     | 89     |  |
| 17  | P     | 88     |  |
| 18  | Q     | 105    |  |
| 19  | R     | 88     |  |
| 20  | S     | 93     |  |
| 21  | T     | 106    |  |
| 22  | V     | 26     |  |

## 2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 51906 atoms, of which 0 are hydrogen and 0 are deuterium.

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     |
|     |       |          | 32391 | 14418 | 6002 | 10465 | 1506 |         |         |       |

- Molecule 2 is a RNA chain called FRAGMENT OF MESSENGER RNA.

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 2   | X     | 6        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 117   | 54 | 14 | 44 | 5 |         |         |       |

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | B     | 234      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1900  | 1213 | 341 | 341 | 5 |         |         |       |

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | C     | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1612  | 1016 | 314 | 281 | 1 |         |         |       |

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5   | D     | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1703  | 1066 | 339 | 291 | 7 |         |         |       |

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | E     | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1146  | 724 | 217 | 201 | 4 |         |         |       |

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | F     | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 843   | 531 | 155 | 154 | 3 |         |         |       |

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | G     | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1257  | 781 | 252 | 218 | 6 |         |         |       |

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9   | H     | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1116  | 705 | 215 | 193 | 3 |         |         |       |

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | I     | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1011  | 639 | 198 | 174 |   |         |         |       |

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | J     | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 792   | 498 | 156 | 137 | 1 |         |         |       |

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | K     | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 885   | 549 | 168 | 165 | 3 |         |         |       |

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | L     | 124      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 970   | 611 | 195 | 163 | 1 |         |         |       |

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14  | M     | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 997   | 617 | 207 | 171 | 2 |         |         |       |

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S14.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 15  | N     | 60       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 492   | 312 | 104 | 72 | 4 |         |         |       |

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | O     | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 734   | 459 | 147 | 126 | 2 |         |         |       |

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17  | P     | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 735   | 462 | 147 | 125 | 1 |         |         |       |

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 18  | Q     | 104      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 857   | 547 | 161 | 147 | 2 |         |         |       |

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S18.

| Mol | Chain | Residues | Atoms |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 19  | R     | 73       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 597   | 380 | 118 | 99 |         |         |       |

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20  | S     | 80       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 647   | 414 | 119 | 112 | 2 |         |         |       |

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 21  | T     | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 762   | 469 | 162 | 129 | 2 |         |         |       |

- Molecule 22 is a protein called 30S RIBOSOMAL PROTEIN THX.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 22  | V     | 24       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 208   | 128 | 50 | 30 |         |         |       |

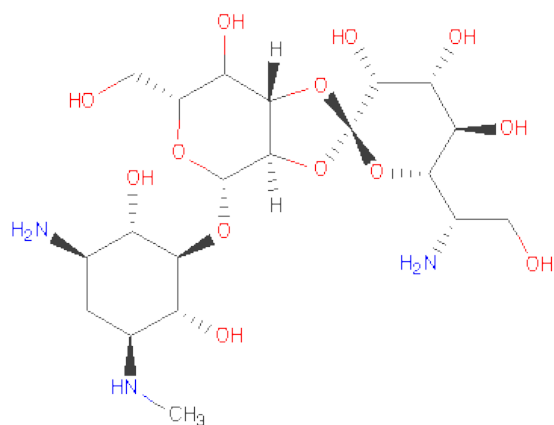
- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 23  | H     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 23  | A     | 94       | Total | Mg | 0       | 0       |
|     |       |          | 94    | 94 |         |         |
| 23  | D     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 24 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 24  | D     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 24  | N     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 25 is HYGROMYCIN B (three-letter code: HYG) (formula: C<sub>20</sub>H<sub>37</sub>N<sub>3</sub>O<sub>13</sub>).



| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---------|---------|
|     |       |          | Total | C  | N | O  |         |         |
| 25  | A     | 1        | 36    | 20 | 3 | 13 | 0       | 0       |

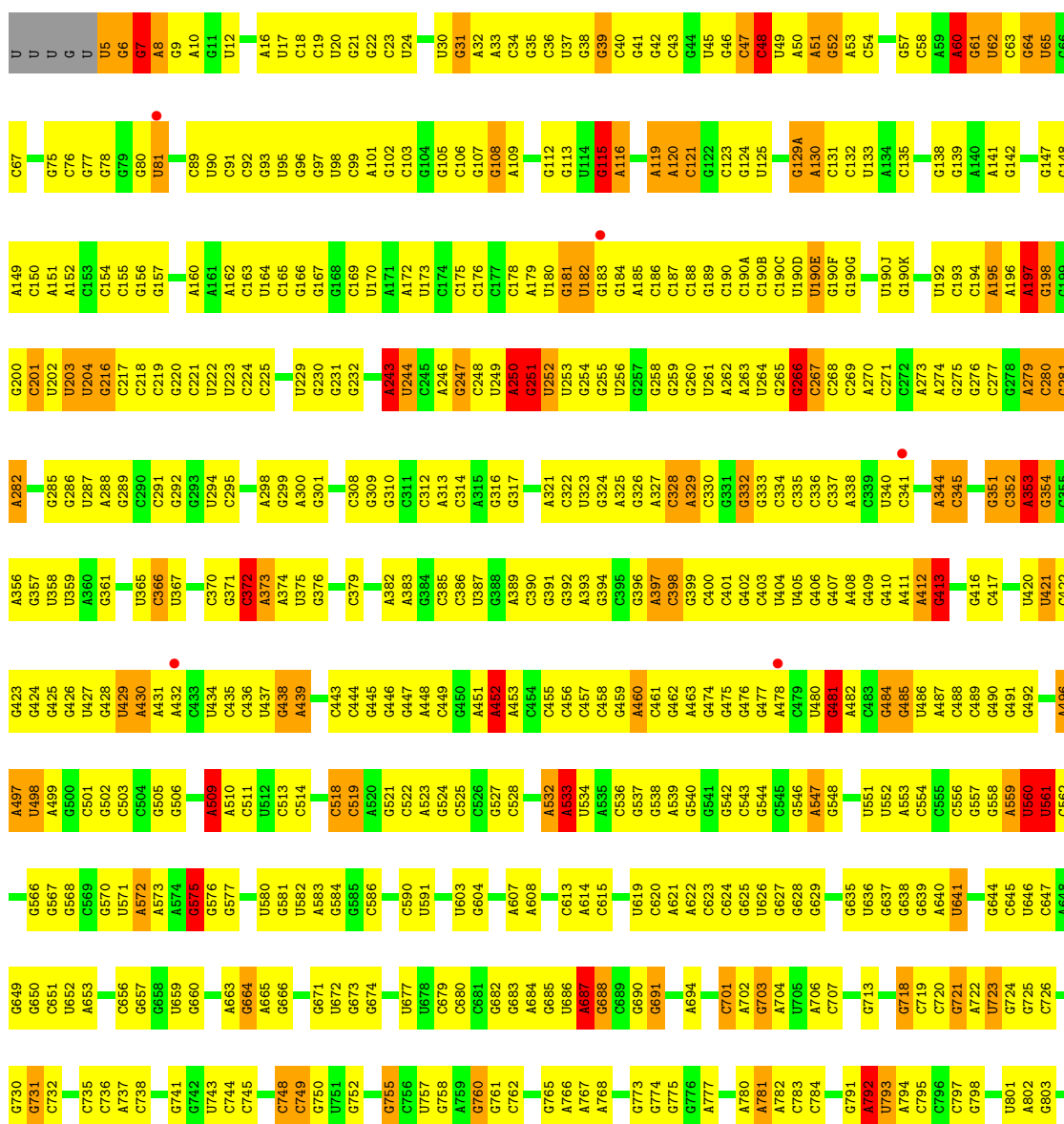


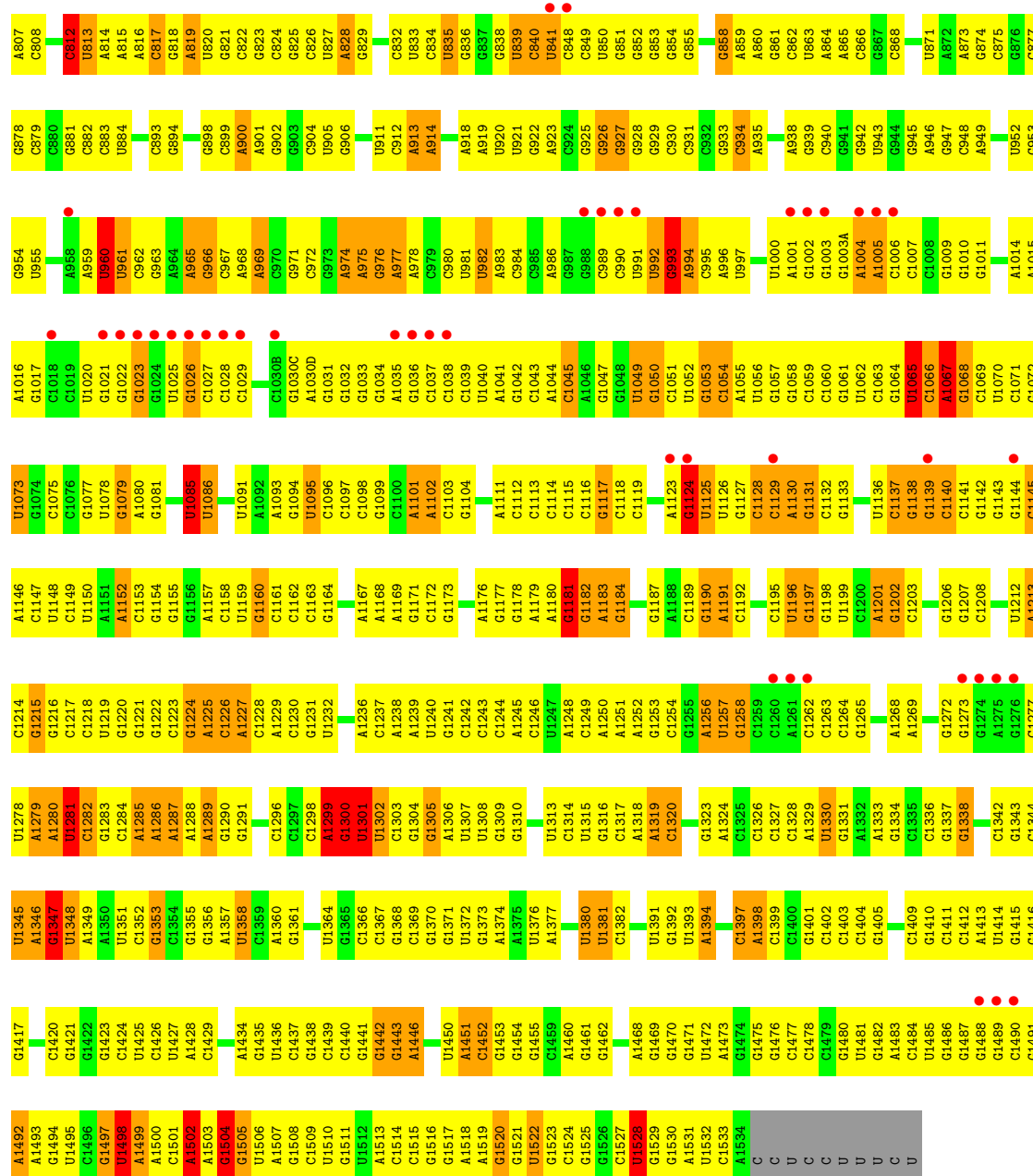
### 3 Residue-property plots

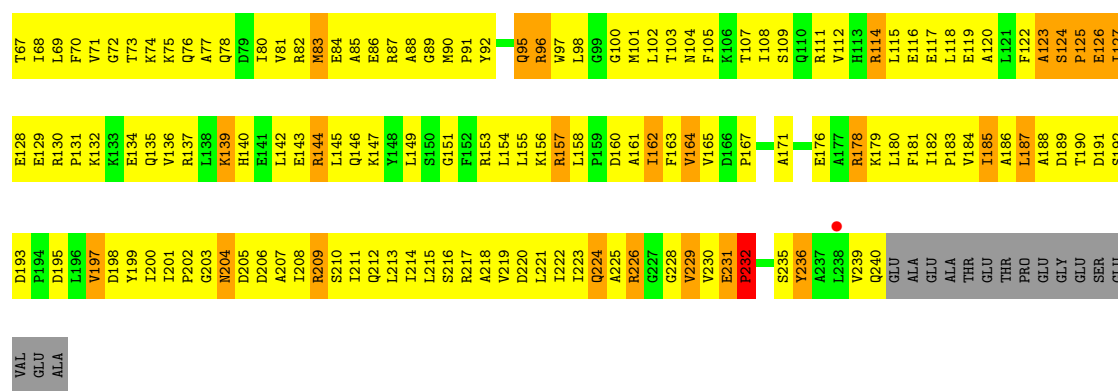
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

#### • Molecule 1: 16S RIBOSOMAL RNA

Chain A: 

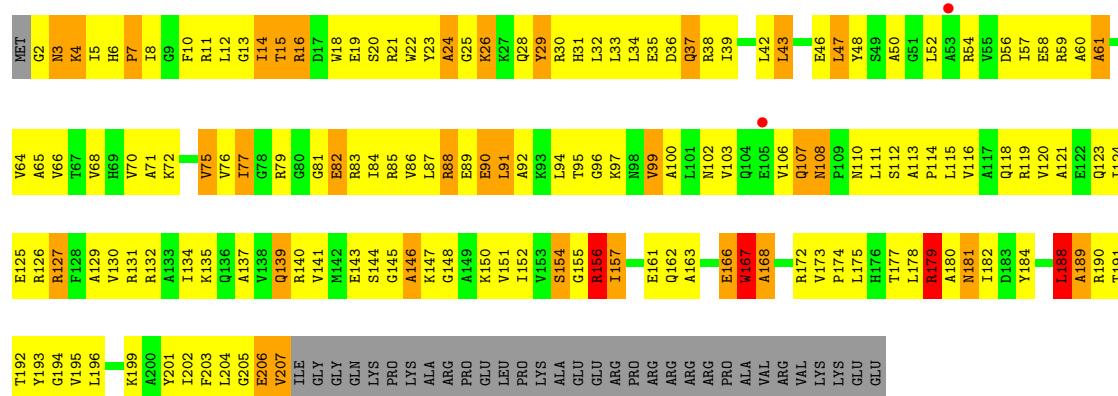






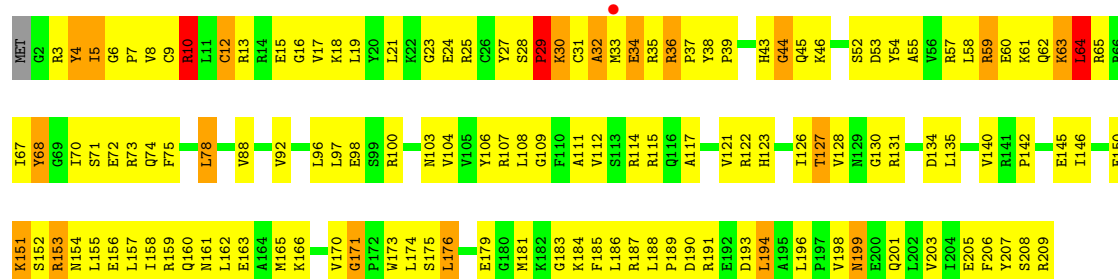
• Molecule 4: 30S RIBOSOMAL PROTEIN S3

Chain C:



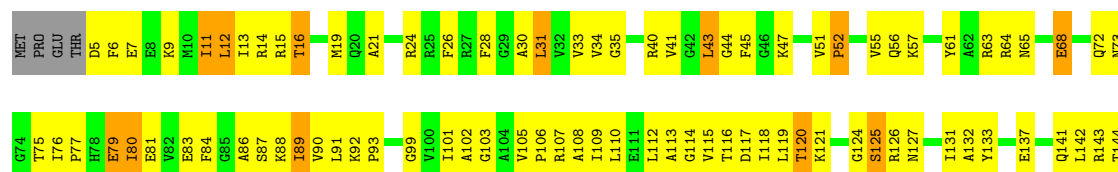
• Molecule 5: 30S RIBOSOMAL PROTEIN S4

Chain D:



• Molecule 6: 30S RIBOSOMAL PROTEIN S5

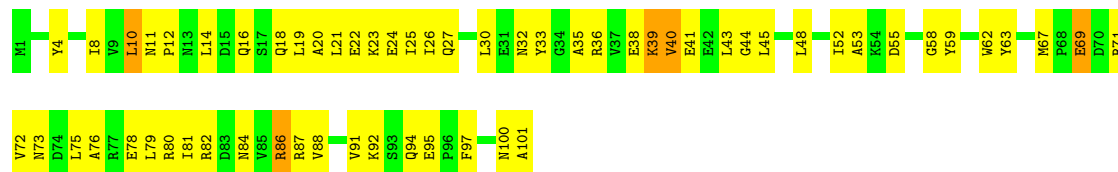
Chain E:





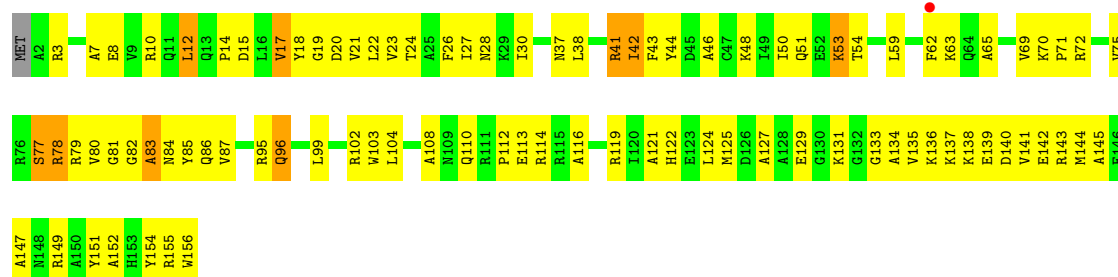
• Molecule 7: 30S RIBOSOMAL PROTEIN S6

Chain F:



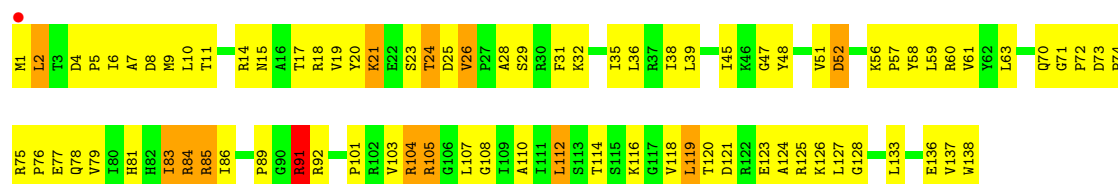
• Molecule 8: 30S RIBOSOMAL PROTEIN S7

Chain G:



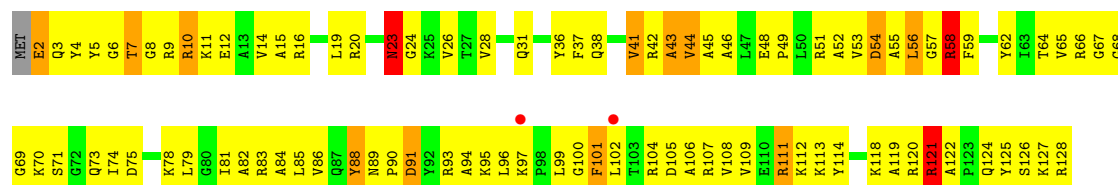
• Molecule 9: 30S RIBOSOMAL PROTEIN S8

Chain H:



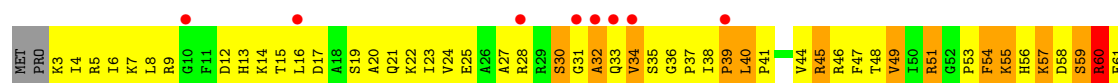
• Molecule 10: 30S RIBOSOMAL PROTEIN S9

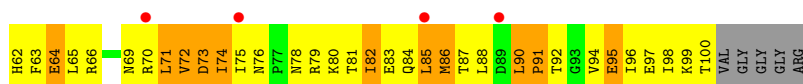
Chain I:



• Molecule 11: 30S RIBOSOMAL PROTEIN S10

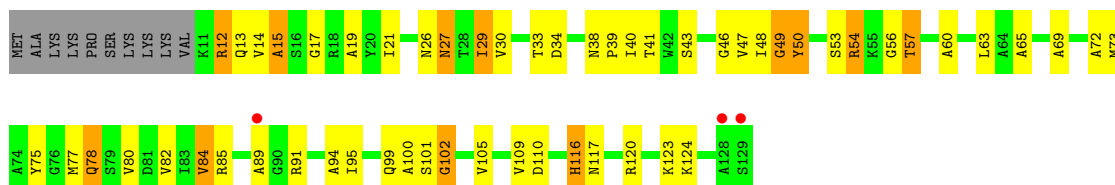
Chain J:





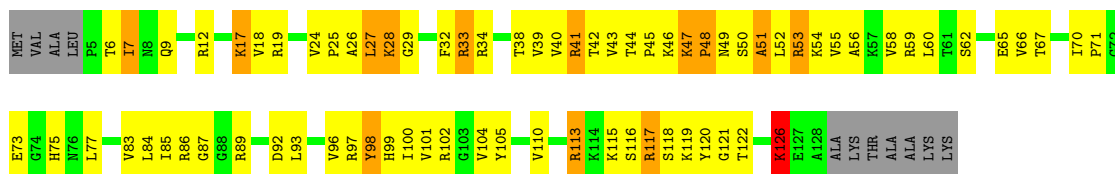
• Molecule 12: 30S RIBOSOMAL PROTEIN S11

Chain K:



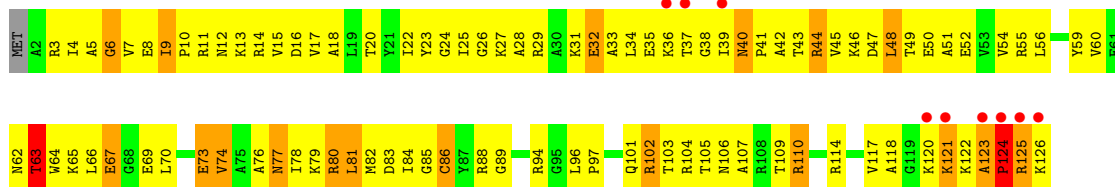
• Molecule 13: 30S RIBOSOMAL PROTEIN S12

Chain L:



• Molecule 14: 30S RIBOSOMAL PROTEIN S13

Chain M:



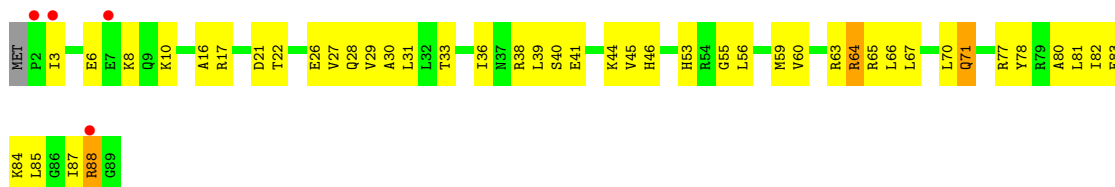
• Molecule 15: 30S RIBOSOMAL PROTEIN S14

Chain N:



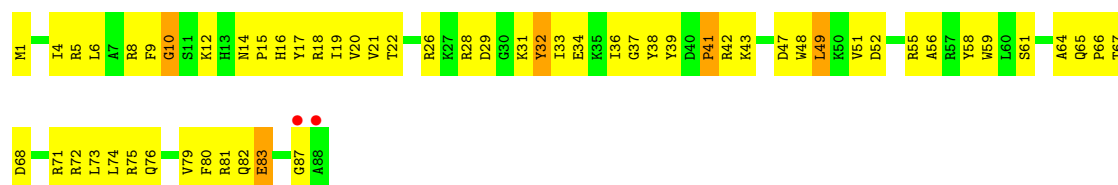
• Molecule 16: 30S RIBOSOMAL PROTEIN S15

Chain O:



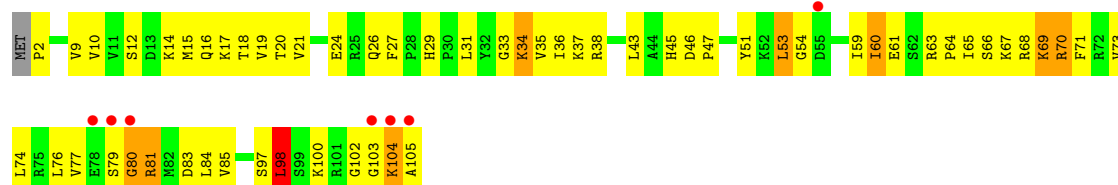
• Molecule 17: 30S RIBOSOMAL PROTEIN S16

Chain P:



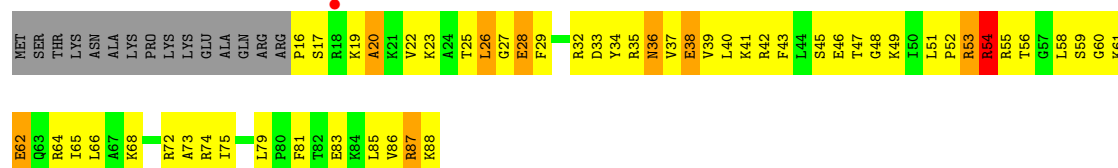
• Molecule 18: 30S RIBOSOMAL PROTEIN S17

Chain Q:



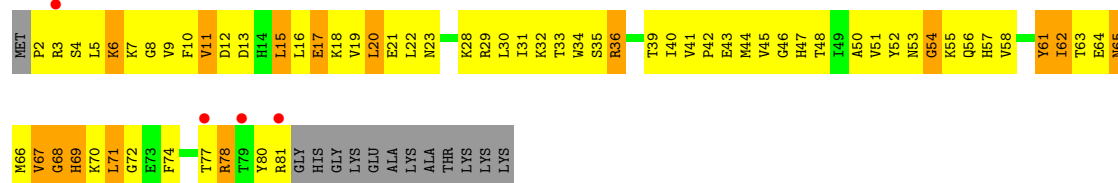
• Molecule 19: 30S RIBOSOMAL PROTEIN S18

Chain R:



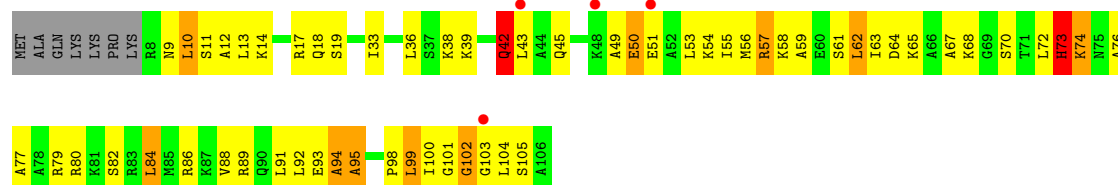
• Molecule 20: 30S RIBOSOMAL PROTEIN S19

Chain S:



• Molecule 21: 30S RIBOSOMAL PROTEIN S20

Chain T:



• Molecule 22: 30S RIBOSOMAL PROTEIN THX

Chain V:



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 41 21 2   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 402.06Å 402.06Å 175.26Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 50.00 – 3.30<br>49.87 – 3.08                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 88.0 (50.00-3.30)<br>83.0 (49.87-3.08)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | 0.16  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.88 (at 3.07Å)   | Xtriage          |
| Refinement program  | CNS   | Depositor        |
| R, $R_{free}$   | 0.218 , 0.261<br>0.219 , 0.260                              | Depositor<br>DCC |
| $R_{free}$ test set   | 10985 reflections (5.34%)                                   | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 88.1  | Xtriage          |
| Anisotropy  | 0.284   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.27 , 56.1   | EDS              |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| L-test for twinning   | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Outliers  | 1 of 216718 reflections (0.000%)                            | Xtriage          |
| $F_o, F_c$ correlation  | 0.90  | EDS              |
| Total number of atoms   | 51906   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 94.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.46% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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     | 0.51         | 1/36259 (0.0%) | 0.75        | 43/56593 (0.1%) |
| 2   | X     | 0.54         | 0/128          | 0.66        | 0/196           |
| 3   | B     | 0.38         | 0/1935         | 0.68        | 0/2609          |
| 4   | C     | 0.38         | 0/1636         | 0.68        | 0/2205          |
| 5   | D     | 0.40         | 0/1733         | 0.68        | 1/2318 (0.0%)   |
| 6   | E     | 0.47         | 0/1162         | 0.78        | 0/1564          |
| 7   | F     | 0.34         | 0/856          | 0.64        | 0/1154          |
| 8   | G     | 0.36         | 0/1276         | 0.61        | 0/1709          |
| 9   | H     | 0.44         | 0/1136         | 0.76        | 0/1527          |
| 10  | I     | 0.37         | 0/1029         | 0.67        | 0/1378          |
| 11  | J     | 0.37         | 0/805          | 0.69        | 0/1082          |
| 12  | K     | 0.38         | 0/900          | 0.71        | 0/1213          |
| 13  | L     | 0.42         | 0/986          | 0.74        | 0/1320          |
| 14  | M     | 0.36         | 0/1008         | 0.70        | 0/1347          |
| 15  | N     | 0.42         | 0/501          | 0.79        | 0/664           |
| 16  | O     | 0.36         | 0/745          | 0.62        | 0/992           |
| 17  | P     | 0.43         | 0/751          | 0.76        | 0/1008          |
| 18  | Q     | 0.46         | 0/870          | 0.77        | 0/1159          |
| 19  | R     | 0.38         | 0/603          | 0.66        | 0/799           |
| 20  | S     | 0.37         | 0/661          | 0.77        | 1/890 (0.1%)    |
| 21  | T     | 0.39         | 0/764          | 0.74        | 0/1006          |
| 22  | V     | 0.49         | 0/212          | 0.72        | 0/277           |
| All | All   | 0.47         | 1/55956 (0.0%) | 0.74        | 45/83010 (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     | 3                   | 39                  |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 9   | H     | 0                   | 1                   |
| All | All   | 3                   | 40                  |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | A     | 121 | C    | N1-C2 | 5.29 | 1.45        | 1.40     |

All (45) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 1498 | U    | C2'-C3'-O3' | 10.50 | 132.60      | 109.50   |
| 1   | A     | 559  | A    | C2'-C3'-O3' | 9.09  | 129.51      | 109.50   |
| 1   | A     | 181  | G    | C2'-C3'-O3' | 8.86  | 128.99      | 109.50   |
| 1   | A     | 1528 | U    | C2'-C3'-O3' | 8.80  | 128.87      | 109.50   |
| 1   | A     | 575  | G    | C2'-C3'-O3' | 8.13  | 127.38      | 109.50   |
| 1   | A     | 108  | G    | O4'-C1'-N9  | 8.08  | 114.66      | 108.20   |
| 1   | A     | 60   | A    | C2'-C3'-O3' | 8.08  | 127.27      | 109.50   |
| 1   | A     | 366  | C    | C2'-C3'-O3' | 7.92  | 126.94      | 109.50   |
| 1   | A     | 792  | A    | C2'-C3'-O3' | 7.90  | 126.88      | 109.50   |
| 1   | A     | 7    | G    | C2'-C3'-O3' | 7.66  | 126.35      | 109.50   |
| 1   | A     | 197  | A    | N9-C1'-C2'  | 7.08  | 123.21      | 114.00   |
| 1   | A     | 266  | G    | C2'-C3'-O3' | 6.90  | 124.74      | 113.70   |
| 1   | A     | 372  | C    | C2'-C3'-O3' | 6.72  | 124.45      | 113.70   |
| 1   | A     | 48   | C    | C2'-C3'-O3' | 6.71  | 124.43      | 113.70   |
| 1   | A     | 1299 | A    | N9-C1'-C2'  | 6.52  | 122.48      | 114.00   |
| 1   | A     | 1504 | G    | C2'-C3'-O3' | 6.51  | 124.12      | 113.70   |
| 1   | A     | 1124 | G    | N9-C1'-C2'  | 6.42  | 122.34      | 114.00   |
| 1   | A     | 509  | A    | C2'-C3'-O3' | 6.26  | 123.72      | 113.70   |
| 1   | A     | 243  | A    | C2'-C3'-O3' | 6.05  | 123.38      | 113.70   |
| 5   | D     | 12   | CYS  | CA-CB-SG    | 6.03  | 124.85      | 114.00   |
| 1   | A     | 960  | U    | C2'-C3'-O3' | 6.02  | 123.34      | 113.70   |
| 1   | A     | 353  | A    | C5'-C4'-O4' | -6.01 | 101.88      | 109.10   |
| 1   | A     | 115  | G    | C2'-C3'-O3' | 5.92  | 123.18      | 113.70   |
| 1   | A     | 993  | G    | N9-C1'-C2'  | 5.92  | 121.70      | 114.00   |
| 1   | A     | 1502 | A    | N9-C1'-C2'  | 5.88  | 121.64      | 114.00   |
| 1   | A     | 1065 | U    | C1'-O4'-C4' | -5.82 | 105.24      | 109.90   |
| 1   | A     | 115  | G    | N9-C1'-C2'  | 5.76  | 121.49      | 114.00   |
| 1   | A     | 533  | A    | C2'-C3'-O3' | 5.74  | 122.88      | 113.70   |
| 1   | A     | 687  | A    | C2'-C3'-O3' | 5.66  | 122.76      | 113.70   |
| 1   | A     | 266  | G    | O4'-C1'-N9  | -5.63 | 103.70      | 108.20   |
| 1   | A     | 484  | G    | C2'-C3'-O3' | 5.59  | 122.64      | 113.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 20  | S     | 54   | GLY  | N-CA-C      | -5.57 | 99.18       | 113.10   |
| 1   | A     | 1067 | A    | C2'-C3'-O3' | 5.54  | 122.56      | 113.70   |
| 1   | A     | 533  | A    | N9-C1'-C2'  | 5.44  | 121.07      | 114.00   |
| 1   | A     | 243  | A    | N9-C1'-C2'  | 5.35  | 120.95      | 114.00   |
| 1   | A     | 1528 | U    | C4'-C3'-O3' | 5.33  | 123.67      | 113.00   |
| 1   | A     | 1300 | G    | N9-C1'-C2'  | 5.32  | 120.91      | 114.00   |
| 1   | A     | 1347 | G    | OP2-P-O3'   | 5.29  | 116.83      | 105.20   |
| 1   | A     | 266  | G    | N9-C1'-C2'  | 5.28  | 120.87      | 114.00   |
| 1   | A     | 1347 | G    | N9-C1'-C2'  | 5.24  | 120.81      | 114.00   |
| 1   | A     | 452  | A    | N9-C1'-C2'  | 5.23  | 120.79      | 114.00   |
| 1   | A     | 1181 | G    | N9-C1'-C2'  | 5.21  | 120.77      | 114.00   |
| 1   | A     | 760  | G    | N9-C1'-C2'  | -5.16 | 106.32      | 112.00   |
| 1   | A     | 560  | U    | C2'-C3'-O3' | 5.10  | 121.86      | 113.70   |
| 1   | A     | 812  | C    | OP2-P-O3'   | 5.03  | 116.27      | 105.20   |

All (3) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 1   | A     | 181  | G    | C3'  |
| 1   | A     | 1498 | U    | C3'  |
| 1   | A     | 1528 | U    | C3'  |

All (40) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | A     | 1073 | U    | Sidechain |
| 1   | A     | 1077 | G    | Sidechain |
| 1   | A     | 1079 | G    | Sidechain |
| 1   | A     | 1085 | U    | Sidechain |
| 1   | A     | 1181 | G    | Sidechain |
| 1   | A     | 12   | U    | Sidechain |
| 1   | A     | 1281 | U    | Sidechain |
| 1   | A     | 1289 | A    | Sidechain |
| 1   | A     | 1299 | A    | Sidechain |
| 1   | A     | 1301 | U    | Sidechain |
| 1   | A     | 1330 | U    | Sidechain |
| 1   | A     | 1345 | U    | Sidechain |
| 1   | A     | 1358 | U    | Sidechain |
| 1   | A     | 1401 | G    | Sidechain |
| 1   | A     | 1434 | A    | Sidechain |
| 1   | A     | 1522 | U    | Sidechain |
| 1   | A     | 197  | A    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 250 | A    | Sidechain |
| 1   | A     | 251 | G    | Sidechain |
| 1   | A     | 263 | A    | Sidechain |
| 1   | A     | 266 | G    | Sidechain |
| 1   | A     | 413 | G    | Sidechain |
| 1   | A     | 452 | A    | Sidechain |
| 1   | A     | 481 | G    | Sidechain |
| 1   | A     | 561 | U    | Sidechain |
| 1   | A     | 572 | A    | Sidechain |
| 1   | A     | 575 | G    | Sidechain |
| 1   | A     | 641 | U    | Sidechain |
| 1   | A     | 664 | G    | Sidechain |
| 1   | A     | 691 | G    | Sidechain |
| 1   | A     | 773 | G    | Sidechain |
| 1   | A     | 835 | U    | Sidechain |
| 1   | A     | 868 | C    | Sidechain |
| 1   | A     | 871 | U    | Sidechain |
| 1   | A     | 873 | A    | Sidechain |
| 1   | A     | 879 | C    | Sidechain |
| 1   | A     | 898 | G    | Sidechain |
| 1   | A     | 900 | A    | Sidechain |
| 1   | A     | 982 | U    | Sidechain |
| 9   | H     | 58  | TYR  | Sidechain |

## 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 32391 | 0        | 16349    | 1226    | 0            |
| 2   | X     | 117   | 0        | 64       | 0       | 0            |
| 3   | B     | 1900  | 0        | 1951     | 256     | 1            |
| 4   | C     | 1612  | 0        | 1677     | 235     | 0            |
| 5   | D     | 1703  | 0        | 1763     | 180     | 0            |
| 6   | E     | 1146  | 0        | 1207     | 110     | 0            |
| 7   | F     | 843   | 0        | 857      | 69      | 0            |
| 8   | G     | 1257  | 0        | 1296     | 96      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 9   | H     | 1116  | 0        | 1177     | 99      | 0            |
| 10  | I     | 1011  | 0        | 1043     | 138     | 0            |
| 11  | J     | 792   | 0        | 835      | 149     | 0            |
| 12  | K     | 885   | 0        | 904      | 62      | 0            |
| 13  | L     | 970   | 0        | 1057     | 114     | 0            |
| 14  | M     | 997   | 0        | 1072     | 124     | 0            |
| 15  | N     | 492   | 0        | 529      | 71      | 0            |
| 16  | O     | 734   | 0        | 771      | 62      | 0            |
| 17  | P     | 735   | 0        | 752      | 62      | 0            |
| 18  | Q     | 857   | 0        | 930      | 76      | 0            |
| 19  | R     | 597   | 0        | 668      | 82      | 0            |
| 20  | S     | 647   | 0        | 673      | 82      | 0            |
| 21  | T     | 762   | 0        | 859      | 61      | 0            |
| 22  | V     | 208   | 0        | 221      | 22      | 0            |
| 23  | A     | 94    | 0        | 0        | 0       | 0            |
| 23  | D     | 1     | 0        | 0        | 0       | 0            |
| 23  | H     | 1     | 0        | 0        | 0       | 0            |
| 24  | D     | 1     | 0        | 0        | 0       | 0            |
| 24  | N     | 1     | 0        | 0        | 0       | 0            |
| 25  | A     | 36    | 0        | 36       | 8       | 0            |
| All | All   | 51906 | 0        | 36691    | 3082    | 1            |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 35.

All (3082) close contacts within the same asymmetric unit are listed below.

| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 13:L:28:LYS:HD2  | 13:L:33:ARG:HH22 | 1.08        | 1.12     |
| 1:A:1443:G:H5''  | 1:A:1446:A:H5'   | 1.21        | 1.11     |
| 5:D:36:ARG:H     | 5:D:37:PRO:HD3   | 1.02        | 1.10     |
| 3:B:84:GLU:HB3   | 3:B:219:VAL:HG21 | 1.30        | 1.09     |
| 11:J:45:ARG:HH11 | 11:J:45:ARG:HB3  | 1.01        | 1.09     |
| 13:L:41:ARG:HG2  | 13:L:42:THR:H    | 1.10        | 1.09     |
| 1:A:80:G:H3'     | 1:A:81:U:H5''    | 1.33        | 1.08     |
| 3:B:77:ALA:HB2   | 3:B:211:ILE:HD13 | 1.15        | 1.08     |
| 4:C:25:GLY:HA2   | 4:C:29:TYR:HB2   | 1.32        | 1.07     |
| 12:K:110:ASP:HB2 | 19:R:88:LYS:HD2  | 1.33        | 1.07     |
| 10:I:8:GLY:HA2   | 10:I:79:LEU:HD12 | 1.34        | 1.06     |
| 11:J:51:ARG:HB2  | 11:J:59:SER:HB3  | 1.32        | 1.05     |
| 1:A:761:G:H4'    | 18:Q:103:GLY:H   | 1.21        | 1.04     |
| 20:S:33:THR:HG22 | 20:S:35:SER:H    | 1.15        | 1.04     |
| 9:H:119:LEU:HD12 | 9:H:124:ALA:HA   | 1.36        | 1.04     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 16:O:56:LEU:HA   | 16:O:59:MET:HE2  | 1.37        | 1.03     |
| 18:Q:104:LYS:HZ3 | 18:Q:104:LYS:H   | 1.05        | 1.02     |
| 1:A:1047:G:H5''  | 15:N:4:LYS:HD2   | 1.41        | 1.02     |
| 4:C:91:LEU:HD21  | 4:C:99:VAL:HG13  | 1.41        | 1.01     |
| 11:J:45:ARG:NH1  | 11:J:45:ARG:HB3  | 1.75        | 1.01     |
| 14:M:49:THR:HG22 | 14:M:51:ALA:H    | 1.24        | 1.01     |
| 1:A:1057:G:H5''  | 4:C:154:SER:HB2  | 1.41        | 1.01     |
| 4:C:94:LEU:HD23  | 4:C:95:THR:HG23  | 1.43        | 1.00     |
| 14:M:10:PRO:HB2  | 14:M:18:ALA:HB1  | 1.43        | 0.99     |
| 5:D:187:ARG:HE   | 5:D:188:LEU:H    | 1.02        | 0.99     |
| 13:L:60:LEU:HD11 | 13:L:85:ILE:HD12 | 1.40        | 0.99     |
| 21:T:39:LYS:HD2  | 21:T:55:ILE:HD13 | 1.43        | 0.99     |
| 6:E:51:VAL:HB    | 6:E:52:PRO:HD3   | 1.44        | 0.99     |
| 5:D:187:ARG:HH21 | 5:D:188:LEU:HG   | 1.29        | 0.98     |
| 13:L:33:ARG:HG2  | 13:L:60:LEU:HD12 | 1.46        | 0.98     |
| 1:A:1131:G:H1    | 1:A:1143:G:H21   | 1.03        | 0.97     |
| 1:A:761:G:H4'    | 18:Q:103:GLY:N   | 1.78        | 0.97     |
| 3:B:74:LYS:NZ    | 3:B:206:ASP:HA   | 1.81        | 0.96     |
| 1:A:64:G:H4'     | 1:A:65:U:O5'     | 1.65        | 0.96     |
| 3:B:74:LYS:HZ2   | 3:B:206:ASP:HA   | 1.30        | 0.95     |
| 5:D:36:ARG:N     | 5:D:37:PRO:HD3   | 1.82        | 0.95     |
| 5:D:140:VAL:HG11 | 5:D:146:ILE:HD11 | 1.46        | 0.95     |
| 12:K:54:ARG:HH11 | 12:K:54:ARG:HB3  | 1.31        | 0.94     |
| 1:A:1305:G:HO2'  | 1:A:1306:A:H8    | 0.96        | 0.94     |
| 1:A:1125:U:H3    | 11:J:5:ARG:HH21  | 1.08        | 0.94     |
| 4:C:3:ASN:N      | 4:C:3:ASN:HD22   | 1.65        | 0.93     |
| 3:B:91:PRO:HG3   | 3:B:154:LEU:HB2  | 1.48        | 0.93     |
| 1:A:1137:C:H4'   | 1:A:1138:G:C2    | 2.04        | 0.93     |
| 3:B:67:THR:HA    | 3:B:90:MET:HE1   | 1.50        | 0.93     |
| 7:F:8:ILE:HD11   | 7:F:79:LEU:HD13  | 1.47        | 0.93     |
| 1:A:1305:G:O2'   | 1:A:1306:A:H8    | 1.52        | 0.93     |
| 9:H:19:VAL:HG23  | 9:H:21:LYS:HD3   | 1.51        | 0.92     |
| 13:L:75:HIS:HD2  | 13:L:77:LEU:H    | 1.16        | 0.92     |
| 12:K:40:ILE:HG22 | 12:K:41:THR:HG23 | 1.49        | 0.92     |
| 13:L:24:VAL:HG13 | 13:L:98:TYR:HE2  | 1.34        | 0.91     |
| 1:A:1286:A:C3'   | 1:A:1287:A:H5''  | 2.00        | 0.91     |
| 18:Q:104:LYS:H   | 18:Q:104:LYS:NZ  | 1.69        | 0.90     |
| 1:A:1286:A:C2'   | 1:A:1287:A:H5''  | 2.02        | 0.90     |
| 1:A:1281:U:H5'   | 1:A:1282:C:H5    | 1.34        | 0.90     |
| 8:G:78:ARG:HB2   | 8:G:156:TRP:HZ3  | 1.35        | 0.90     |
| 1:A:243:A:H4'    | 1:A:244:U:H5'    | 1.54        | 0.90     |
| 19:R:36:ASN:ND2  | 19:R:38:GLU:HG2  | 1.87        | 0.90     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:686:U:HO2'   | 1:A:687:A:H8     | 0.90        | 0.90     |
| 1:A:1230:C:H1'   | 14:M:126:LYS:HA  | 1.52        | 0.90     |
| 1:A:7:G:H5'      | 1:A:298:A:O4'    | 1.72        | 0.90     |
| 1:A:351:G:H4'    | 1:A:352:C:OP1    | 1.71        | 0.89     |
| 1:A:1086:U:H3    | 1:A:1099:G:H22   | 0.93        | 0.89     |
| 5:D:25:ARG:NH1   | 5:D:30:LYS:HB3   | 1.88        | 0.89     |
| 3:B:77:ALA:HB2   | 3:B:211:ILE:CD1  | 2.03        | 0.89     |
| 1:A:1116:C:H2'   | 1:A:1117:G:H5''  | 1.52        | 0.89     |
| 4:C:3:ASN:HD22   | 4:C:3:ASN:H      | 1.19        | 0.88     |
| 1:A:1286:A:H2'   | 1:A:1287:A:H5''  | 1.54        | 0.88     |
| 4:C:195:VAL:O    | 4:C:196:LEU:HD23 | 1.74        | 0.87     |
| 1:A:1250:A:H4'   | 10:I:68:GLY:N    | 1.90        | 0.87     |
| 18:Q:97:SER:HB2  | 18:Q:103:GLY:N   | 1.90        | 0.87     |
| 5:D:199:ASN:HD21 | 5:D:201:GLN:HB3  | 1.40        | 0.86     |
| 1:A:1226:C:H4'   | 1:A:1227:A:OP1   | 1.72        | 0.86     |
| 4:C:108:ASN:ND2  | 4:C:111:LEU:HG   | 1.89        | 0.86     |
| 4:C:52:LEU:H     | 4:C:52:LEU:HD23  | 1.39        | 0.86     |
| 19:R:55:ARG:HB3  | 19:R:55:ARG:NH1  | 1.90        | 0.86     |
| 1:A:1152:A:H5''  | 11:J:13:HIS:HD2  | 1.40        | 0.85     |
| 3:B:178:ARG:HG3  | 3:B:178:ARG:HH11 | 1.39        | 0.85     |
| 5:D:187:ARG:HE   | 5:D:188:LEU:N    | 1.72        | 0.85     |
| 8:G:78:ARG:HB2   | 8:G:156:TRP:CZ3  | 2.12        | 0.85     |
| 11:J:62:HIS:HB3  | 15:N:59:ALA:HB3  | 1.57        | 0.85     |
| 1:A:954:G:H21    | 1:A:1227:A:H62   | 1.25        | 0.85     |
| 1:A:974:A:OP1    | 15:N:31:ARG:HG2  | 1.76        | 0.85     |
| 5:D:36:ARG:H     | 5:D:37:PRO:CD    | 1.85        | 0.84     |
| 5:D:23:GLY:HA3   | 5:D:112:VAL:HG12 | 1.57        | 0.84     |
| 6:E:80:ILE:CD1   | 6:E:91:LEU:HB2   | 2.08        | 0.84     |
| 1:A:664:G:H22    | 1:A:741:G:H1     | 1.20        | 0.84     |
| 3:B:124:SER:HB2  | 3:B:125:PRO:HD2  | 1.60        | 0.84     |
| 1:A:438:G:H4'    | 1:A:439:A:OP1    | 1.75        | 0.84     |
| 1:A:371:G:O2'    | 1:A:372:C:H5'    | 1.77        | 0.84     |
| 4:C:131:ARG:HG2  | 4:C:135:LYS:HE3  | 1.59        | 0.84     |
| 1:A:975:A:H5'    | 1:A:975:A:H8     | 1.40        | 0.84     |
| 9:H:1:MET:HG2    | 9:H:2:LEU:H      | 1.43        | 0.84     |
| 11:J:19:SER:HB2  | 11:J:91:PRO:HG3  | 1.58        | 0.84     |
| 5:D:156:GLU:HG2  | 5:D:160:GLN:HE21 | 1.42        | 0.84     |
| 7:F:10:LEU:HD12  | 7:F:59:TYR:HB3   | 1.60        | 0.84     |
| 1:A:1356:G:H2'   | 1:A:1357:A:C8    | 2.13        | 0.83     |
| 13:L:41:ARG:HG2  | 13:L:42:THR:N    | 1.93        | 0.83     |
| 1:A:1286:A:H3'   | 1:A:1287:A:H5''  | 1.57        | 0.83     |
| 3:B:130:ARG:HH22 | 4:C:207:VAL:HG23 | 1.43        | 0.83     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 5:D:150:GLU:CD   | 5:D:150:GLU:H    | 1.82        | 0.83     |
| 4:C:112:SER:HB2  | 4:C:115:LEU:HD12 | 1.59        | 0.83     |
| 12:K:91:ARG:NH1  | 19:R:88:LYS:HE2  | 1.94        | 0.83     |
| 11:J:39:PRO:HA   | 11:J:70:ARG:HH11 | 1.44        | 0.82     |
| 20:S:55:LYS:HG2  | 20:S:56:GLN:HE21 | 1.43        | 0.82     |
| 1:A:1443:G:C5'   | 1:A:1446:A:H5'   | 2.07        | 0.82     |
| 13:L:70:ILE:HD13 | 13:L:77:LEU:HD12 | 1.59        | 0.82     |
| 1:A:1117:G:H4'   | 10:I:104:ARG:NH1 | 1.93        | 0.82     |
| 13:L:28:LYS:HD2  | 13:L:33:ARG:NH2  | 1.91        | 0.82     |
| 1:A:1347:G:N2    | 1:A:1373:G:H2'   | 1.92        | 0.82     |
| 3:B:197:VAL:HB   | 3:B:200:ILE:HG12 | 1.59        | 0.82     |
| 4:C:58:GLU:HB3   | 11:J:92:THR:HG21 | 1.62        | 0.82     |
| 6:E:9:LYS:HD2    | 6:E:112:LEU:HD21 | 1.61        | 0.82     |
| 1:A:1060:C:C5    | 4:C:2:GLY:HA3    | 2.14        | 0.82     |
| 4:C:174:PRO:HB2  | 4:C:177:THR:HG22 | 1.60        | 0.81     |
| 1:A:80:G:H3'     | 1:A:81:U:C5'     | 2.09        | 0.81     |
| 1:A:1137:C:H4'   | 1:A:1138:G:N2    | 1.95        | 0.81     |
| 1:A:1065:U:H4'   | 1:A:1066:C:O5'   | 1.79        | 0.81     |
| 20:S:64:GLU:O    | 20:S:67:VAL:HG23 | 1.80        | 0.81     |
| 1:A:1412:C:H2'   | 1:A:1413:A:H8    | 1.44        | 0.81     |
| 1:A:80:G:C3'     | 1:A:81:U:H5''    | 2.10        | 0.80     |
| 1:A:686:U:O2'    | 1:A:687:A:H8     | 1.64        | 0.80     |
| 6:E:81:GLU:HG2   | 6:E:90:VAL:HG22  | 1.61        | 0.80     |
| 11:J:51:ARG:HG2  | 11:J:51:ARG:HH11 | 1.46        | 0.80     |
| 10:I:9:ARG:HG2   | 10:I:14:VAL:HG22 | 1.64        | 0.80     |
| 8:G:95:ARG:HG2   | 8:G:99:LEU:HD11  | 1.62        | 0.80     |
| 14:M:50:GLU:O    | 14:M:54:VAL:HG23 | 1.81        | 0.80     |
| 3:B:80:ILE:HD11  | 3:B:208:ILE:HG23 | 1.62        | 0.80     |
| 20:S:33:THR:HG22 | 20:S:35:SER:N    | 1.95        | 0.80     |
| 1:A:1493:A:O2'   | 1:A:1494:G:H5'   | 1.82        | 0.80     |
| 1:A:1236:A:H4'   | 1:A:1304:G:H4'   | 1.62        | 0.80     |
| 1:A:1025:U:H2'   | 1:A:1026:G:C8    | 2.16        | 0.80     |
| 1:A:1238:A:H5'   | 1:A:1336:C:H41   | 1.44        | 0.80     |
| 1:A:1190:G:OP1   | 4:C:4:LYS:HA     | 1.80        | 0.80     |
| 5:D:61:LYS:HD2   | 5:D:207:TYR:OH   | 1.81        | 0.80     |
| 1:A:1279:A:H5''  | 1:A:1280:A:OP1   | 1.82        | 0.80     |
| 3:B:132:LYS:HA   | 3:B:135:GLN:HB3  | 1.63        | 0.80     |
| 1:A:839:U:H5'    | 1:A:840:C:C5     | 2.16        | 0.80     |
| 5:D:199:ASN:ND2  | 5:D:201:GLN:HB3  | 1.96        | 0.79     |
| 1:A:953:G:H1'    | 14:M:125:ARG:CB  | 2.12        | 0.79     |
| 1:A:1182:G:H4'   | 1:A:1183:A:O5'   | 1.82        | 0.79     |
| 1:A:1006:C:H2'   | 1:A:1007:C:H6    | 1.46        | 0.79     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:328:C:O2     | 1:A:328:C:H2'     | 1.82        | 0.79     |
| 14:M:11:ARG:HG3  | 14:M:12:ASN:N     | 1.96        | 0.79     |
| 13:L:27:LEU:HG   | 13:L:28:LYS:H     | 1.48        | 0.79     |
| 12:K:57:THR:HG23 | 12:K:60:ALA:H     | 1.48        | 0.79     |
| 4:C:58:GLU:H     | 4:C:65:ALA:HB3    | 1.48        | 0.79     |
| 3:B:22:LYS:HD2   | 3:B:35:GLU:OE1    | 1.83        | 0.79     |
| 13:L:24:VAL:HG13 | 13:L:98:TYR:CE2   | 2.18        | 0.79     |
| 1:A:1132:C:H2'   | 1:A:1133:G:C8     | 2.18        | 0.79     |
| 1:A:1251:A:H2'   | 1:A:1252:A:C8     | 2.17        | 0.79     |
| 1:A:1366:C:H2'   | 1:A:1367:C:H6     | 1.47        | 0.79     |
| 3:B:16:HIS:NE2   | 3:B:214:ILE:HG12  | 1.97        | 0.79     |
| 14:M:52:GLU:HG2  | 14:M:55:ARG:HH21  | 1.48        | 0.79     |
| 6:E:110:LEU:HD13 | 6:E:118:ILE:HD12  | 1.65        | 0.79     |
| 1:A:1502:A:H2    | 1:A:1505:G:H1     | 1.31        | 0.79     |
| 15:N:26:ARG:NH1  | 15:N:47:LEU:HG    | 1.98        | 0.79     |
| 11:J:37:PRO:HA   | 11:J:72:VAL:HG22  | 1.62        | 0.78     |
| 1:A:1475:G:H2'   | 1:A:1476:G:H8     | 1.46        | 0.78     |
| 9:H:138:TRP:OXT  | 9:H:138:TRP:HE3   | 1.65        | 0.78     |
| 1:A:1488:G:H2'   | 1:A:1489:G:C8     | 2.19        | 0.78     |
| 1:A:435:C:H2'    | 1:A:436:C:H6      | 1.49        | 0.78     |
| 4:C:15:THR:O     | 4:C:16:ARG:HB2    | 1.80        | 0.78     |
| 16:O:29:VAL:HG12 | 16:O:85:LEU:CD1   | 2.13        | 0.78     |
| 4:C:52:LEU:HD21  | 4:C:118:GLN:HE22  | 1.46        | 0.78     |
| 21:T:14:LYS:O    | 21:T:18:GLN:HG3   | 1.84        | 0.78     |
| 1:A:620:C:C2     | 5:D:135:LEU:HD13  | 2.17        | 0.78     |
| 1:A:1343:G:H1'   | 10:I:121:ARG:HH12 | 1.49        | 0.78     |
| 1:A:1116:C:C2'   | 1:A:1117:G:H5''   | 2.13        | 0.78     |
| 13:L:41:ARG:CG   | 13:L:42:THR:H     | 1.93        | 0.78     |
| 1:A:975:A:H4'    | 1:A:976:G:H5'     | 1.66        | 0.78     |
| 20:S:17:GLU:HA   | 20:S:20:LEU:HD11  | 1.66        | 0.78     |
| 8:G:79:ARG:HG2   | 8:G:84:ASN:OD1    | 1.81        | 0.78     |
| 16:O:16:ALA:HB1  | 16:O:21:ASP:HB3   | 1.65        | 0.78     |
| 1:A:1487:G:O2'   | 1:A:1488:G:H5'    | 1.83        | 0.78     |
| 3:B:161:ALA:HB1  | 3:B:185:ILE:HD11  | 1.64        | 0.78     |
| 5:D:104:VAL:HG11 | 5:D:146:ILE:HD13  | 1.66        | 0.78     |
| 4:C:108:ASN:HD22 | 4:C:111:LEU:HG    | 1.46        | 0.78     |
| 1:A:393:A:O2'    | 1:A:394:G:H5'     | 1.84        | 0.77     |
| 1:A:1086:U:H3    | 1:A:1099:G:N2     | 1.76        | 0.77     |
| 1:A:538:G:OP2    | 13:L:115:LYS:HG3  | 1.84        | 0.77     |
| 1:A:706:A:H1'    | 12:K:29:ILE:HD11  | 1.65        | 0.77     |
| 6:E:93:PRO:HG2   | 9:H:105:ARG:HE    | 1.48        | 0.77     |
| 1:A:250:A:H4'    | 1:A:251:G:O5'     | 1.82        | 0.77     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 8:G:18:TYR:HB3   | 8:G:59:LEU:HD22   | 1.66        | 0.77     |
| 17:P:58:TYR:O    | 17:P:61:SER:HB3   | 1.85        | 0.77     |
| 10:I:86:VAL:HG13 | 10:I:90:PRO:HA    | 1.65        | 0.77     |
| 1:A:1443:G:H5''  | 1:A:1446:A:C5'    | 2.08        | 0.77     |
| 5:D:70:ILE:HD11  | 5:D:100:ARG:CZ    | 2.15        | 0.77     |
| 3:B:142:LEU:HB3  | 3:B:146:GLN:HE21  | 1.50        | 0.77     |
| 1:A:382:A:H2'    | 1:A:383:A:C8      | 2.19        | 0.77     |
| 13:L:27:LEU:O    | 13:L:29:GLY:N     | 2.18        | 0.76     |
| 7:F:33:TYR:HB2   | 7:F:75:LEU:HD23   | 1.67        | 0.76     |
| 1:A:1256:A:H4'   | 1:A:1257:U:H5'    | 1.67        | 0.76     |
| 1:A:1497:G:H2'   | 1:A:1498:U:H5'    | 1.68        | 0.76     |
| 13:L:33:ARG:CD   | 13:L:62:SER:HB3   | 2.15        | 0.76     |
| 1:A:1495:U:O4    | 25:A:1632:HYG:H2  | 1.86        | 0.76     |
| 9:H:51:VAL:HG21  | 9:H:60:ARG:HG2    | 1.66        | 0.76     |
| 17:P:21:VAL:HG21 | 17:P:59:TRP:CD1   | 2.21        | 0.76     |
| 4:C:177:THR:HG23 | 4:C:180:ALA:HB2   | 1.68        | 0.76     |
| 1:A:939:G:H2'    | 1:A:940:C:C6      | 2.21        | 0.76     |
| 3:B:102:LEU:HD21 | 3:B:162:ILE:CD1   | 2.15        | 0.76     |
| 1:A:141:A:H1'    | 1:A:182:U:O2      | 1.86        | 0.76     |
| 10:I:16:ARG:HB2  | 10:I:64:THR:HB    | 1.68        | 0.76     |
| 21:T:56:MET:HG3  | 21:T:88:VAL:HG21  | 1.68        | 0.76     |
| 18:Q:24:GLU:OE2  | 18:Q:37:LYS:HD3   | 1.85        | 0.76     |
| 12:K:77:MET:O    | 12:K:78:GLN:HG3   | 1.86        | 0.76     |
| 13:L:110:VAL:O   | 13:L:122:THR:HG21 | 1.85        | 0.76     |
| 1:A:1278:U:H5''  | 1:A:1279:A:H5'    | 1.68        | 0.75     |
| 1:A:1004:A:H5''  | 1:A:1025:U:C5     | 2.20        | 0.75     |
| 7:F:100:ASN:HD22 | 19:R:23:LYS:HG2   | 1.51        | 0.75     |
| 1:A:1064:G:H4'   | 1:A:1065:U:H5'    | 1.68        | 0.75     |
| 1:A:1152:A:H5''  | 11:J:13:HIS:CD2   | 2.21        | 0.75     |
| 1:A:1391:U:H2'   | 1:A:1392:G:C8     | 2.21        | 0.75     |
| 10:I:10:ARG:HG2  | 10:I:75:ASP:HB2   | 1.68        | 0.75     |
| 20:S:70:LYS:O    | 20:S:72:GLY:N     | 2.20        | 0.75     |
| 1:A:761:G:C2     | 18:Q:105:ALA:HB3  | 2.21        | 0.75     |
| 1:A:1281:U:H5'   | 1:A:1282:C:C5     | 2.20        | 0.75     |
| 1:A:501:C:H2'    | 1:A:502:G:H8      | 1.52        | 0.75     |
| 4:C:191:THR:HG22 | 4:C:192:THR:N     | 1.99        | 0.75     |
| 13:L:25:PRO:C    | 13:L:27:LEU:H     | 1.86        | 0.75     |
| 1:A:1497:G:C2'   | 1:A:1498:U:H5'    | 2.16        | 0.75     |
| 11:J:61:GLU:OE1  | 15:N:45:ARG:NH1   | 2.19        | 0.75     |
| 4:C:174:PRO:HB2  | 4:C:177:THR:CG2   | 2.17        | 0.75     |
| 3:B:80:ILE:HD13  | 3:B:212:GLN:HB2   | 1.69        | 0.75     |
| 10:I:48:GLU:HA   | 10:I:51:ARG:NH1   | 2.02        | 0.75     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 4:C:38:ARG:HH11  | 4:C:38:ARG:HG3    | 1.52        | 0.75     |
| 5:D:8:VAL:HG21   | 5:D:115:ARG:NH1   | 2.02        | 0.74     |
| 21:T:54:LYS:HG3  | 21:T:100:ILE:HD13 | 1.67        | 0.74     |
| 1:A:1064:G:H4'   | 1:A:1065:U:C5'    | 2.18        | 0.74     |
| 19:R:36:ASN:HD22 | 19:R:38:GLU:HG2   | 1.50        | 0.74     |
| 3:B:122:PHE:HE2  | 3:B:139:LYS:HG2   | 1.51        | 0.74     |
| 18:Q:21:VAL:HG21 | 18:Q:59:ILE:HD11  | 1.70        | 0.74     |
| 1:A:8:A:N6       | 5:D:209:ARG:HB2   | 2.03        | 0.74     |
| 15:N:14:PRO:C    | 15:N:16:PHE:H     | 1.88        | 0.74     |
| 1:A:839:U:O2     | 1:A:839:U:H2'     | 1.87        | 0.74     |
| 14:M:4:ILE:HG22  | 14:M:5:ALA:N      | 2.03        | 0.74     |
| 1:A:434:U:H2'    | 1:A:435:C:C6      | 2.23        | 0.74     |
| 10:I:70:LYS:O    | 10:I:74:ILE:HG13  | 1.88        | 0.74     |
| 14:M:88:ARG:HD2  | 20:S:3:ARG:HH21   | 1.52        | 0.74     |
| 5:D:191:ARG:HD2  | 5:D:191:ARG:O     | 1.87        | 0.74     |
| 12:K:54:ARG:O    | 12:K:57:THR:HG22  | 1.86        | 0.74     |
| 1:A:1278:U:H5''  | 1:A:1279:A:C5'    | 2.18        | 0.74     |
| 8:G:46:ALA:O     | 8:G:50:ILE:HG13   | 1.87        | 0.74     |
| 7:F:101:ALA:HA   | 19:R:28:GLU:HB3   | 1.69        | 0.74     |
| 1:A:129(A):G:O2' | 1:A:190(E):U:H2'  | 1.88        | 0.74     |
| 5:D:35:ARG:O     | 5:D:36:ARG:HB2    | 1.87        | 0.74     |
| 1:A:1498:U:H4'   | 1:A:1519:A:H2     | 1.51        | 0.74     |
| 14:M:14:ARG:HG3  | 14:M:44:ARG:NH1   | 2.03        | 0.74     |
| 1:A:975:A:H5'    | 1:A:975:A:C8      | 2.23        | 0.74     |
| 7:F:26:ILE:HG21  | 7:F:63:TYR:HE2    | 1.53        | 0.74     |
| 4:C:107:GLN:NE2  | 4:C:107:GLN:H     | 1.86        | 0.73     |
| 6:E:93:PRO:CG    | 9:H:105:ARG:HE    | 2.01        | 0.73     |
| 1:A:1250:A:H4'   | 10:I:68:GLY:H     | 1.51        | 0.73     |
| 11:J:53:PRO:HA   | 15:N:41:ARG:HH21  | 1.53        | 0.73     |
| 5:D:114:ARG:HG3  | 5:D:114:ARG:HH11  | 1.51        | 0.73     |
| 13:L:33:ARG:HD3  | 13:L:62:SER:HB3   | 1.70        | 0.73     |
| 1:A:1490:C:H2'   | 1:A:1491:G:H8     | 1.51        | 0.73     |
| 4:C:110:ASN:HD21 | 4:C:140:ARG:HB3   | 1.53        | 0.73     |
| 14:M:59:TYR:O    | 14:M:63:THR:HB    | 1.89        | 0.73     |
| 11:J:30:SER:O    | 11:J:78:ASN:HB2   | 1.89        | 0.73     |
| 8:G:18:TYR:CD2   | 8:G:59:LEU:HB2    | 2.24        | 0.73     |
| 7:F:101:ALA:HB2  | 19:R:28:GLU:HB2   | 1.69        | 0.73     |
| 1:A:173:U:H5'    | 1:A:197:A:O4'     | 1.89        | 0.73     |
| 20:S:22:LEU:HD22 | 20:S:28:LYS:HB2   | 1.69        | 0.73     |
| 18:Q:45:HIS:NE2  | 18:Q:47:PRO:HG3   | 2.02        | 0.73     |
| 1:A:1298:C:C5    | 8:G:114:ARG:HD3   | 2.23        | 0.73     |
| 15:N:27:CYS:SG   | 15:N:29:ARG:HB2   | 2.29        | 0.73     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:1241:G:H2'   | 1:A:1242:C:C6    | 2.23        | 0.73     |
| 5:D:170:VAL:HG12 | 5:D:174:LEU:HB2  | 1.70        | 0.73     |
| 4:C:43:LEU:HD23  | 4:C:43:LEU:N     | 2.04        | 0.73     |
| 5:D:24:GLU:HG2   | 5:D:25:ARG:H     | 1.52        | 0.72     |
| 10:I:78:LYS:HD3  | 10:I:101:PHE:HD2 | 1.55        | 0.72     |
| 4:C:23:TYR:CD2   | 4:C:24:ALA:N     | 2.57        | 0.72     |
| 1:A:405:U:H3'    | 1:A:406:G:H5'    | 1.71        | 0.72     |
| 14:M:78:ILE:HA   | 14:M:81:LEU:HD21 | 1.71        | 0.72     |
| 9:H:9:MET:SD     | 9:H:32:LYS:HG2   | 2.29        | 0.72     |
| 5:D:25:ARG:HH12  | 5:D:30:LYS:HB3   | 1.54        | 0.72     |
| 16:O:45:VAL:HG12 | 16:O:46:HIS:H    | 1.53        | 0.72     |
| 1:A:1040:U:H2'   | 1:A:1041:A:C8    | 2.23        | 0.72     |
| 12:K:84:VAL:HG21 | 19:R:88:LYS:HD3  | 1.71        | 0.72     |
| 5:D:187:ARG:NE   | 5:D:188:LEU:H    | 1.84        | 0.72     |
| 5:D:32:ALA:C     | 5:D:34:GLU:H     | 1.93        | 0.72     |
| 1:A:1226:C:H5''  | 14:M:103:THR:OG1 | 1.89        | 0.72     |
| 12:K:110:ASP:HB2 | 19:R:88:LYS:CD   | 2.14        | 0.72     |
| 10:I:79:LEU:HD13 | 10:I:83:ARG:HD2  | 1.72        | 0.72     |
| 6:E:80:ILE:HD12  | 6:E:91:LEU:HB2   | 1.69        | 0.72     |
| 11:J:22:LYS:HE2  | 11:J:90:LEU:HB2  | 1.72        | 0.72     |
| 1:A:992:U:H4'    | 1:A:993:G:O5'    | 1.89        | 0.72     |
| 1:A:701:C:H5'    | 1:A:703:G:O4'    | 1.90        | 0.72     |
| 3:B:8:LYS:O      | 3:B:9:GLU:HB2    | 1.87        | 0.72     |
| 19:R:74:ARG:HB3  | 19:R:81:PHE:CE1  | 2.25        | 0.72     |
| 3:B:84:GLU:HB3   | 3:B:219:VAL:CG2  | 2.17        | 0.71     |
| 1:A:243:A:C4'    | 1:A:244:U:H5'    | 2.20        | 0.71     |
| 1:A:1355:G:O2'   | 1:A:1356:G:H5'   | 1.90        | 0.71     |
| 14:M:78:ILE:HG22 | 14:M:82:MET:HE3  | 1.72        | 0.71     |
| 1:A:1372:U:OP1   | 10:I:71:SER:HB3  | 1.89        | 0.71     |
| 17:P:28:ARG:HG3  | 17:P:29:ASP:OD2  | 1.90        | 0.71     |
| 5:D:29:PRO:O     | 5:D:30:LYS:HG3   | 1.90        | 0.71     |
| 9:H:1:MET:HG2    | 9:H:2:LEU:N      | 2.05        | 0.71     |
| 1:A:1475:G:H2'   | 1:A:1476:G:C8    | 2.25        | 0.71     |
| 1:A:1189:C:OP1   | 11:J:51:ARG:NH2  | 2.23        | 0.71     |
| 1:A:840:C:H5''   | 1:A:841:U:OP1    | 1.89        | 0.71     |
| 3:B:116:GLU:HG2  | 3:B:153:ARG:NH1  | 2.04        | 0.71     |
| 1:A:953:G:H1'    | 14:M:125:ARG:HB3 | 1.71        | 0.71     |
| 4:C:29:TYR:OH    | 15:N:54:PRO:HG2  | 1.91        | 0.71     |
| 1:A:195:A:H4'    | 21:T:68:LYS:HE2  | 1.71        | 0.71     |
| 4:C:188:LEU:CD1  | 4:C:189:ALA:H    | 2.04        | 0.71     |
| 20:S:15:LEU:HA   | 20:S:18:LYS:HB3  | 1.73        | 0.71     |
| 3:B:42:ILE:HD11  | 3:B:189:ASP:HB2  | 1.72        | 0.71     |

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| Atom-1            | Atom-2           | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:A:382:A:H2'     | 1:A:383:A:H8     | 1.55        | 0.71     |
| 1:A:448:A:OP2     | 1:A:485:G:N2     | 2.24        | 0.71     |
| 11:J:5:ARG:HA     | 11:J:73:ASP:OD1  | 1.91        | 0.71     |
| 4:C:188:LEU:HD13  | 4:C:189:ALA:H    | 1.56        | 0.71     |
| 13:L:83:VAL:HG22  | 13:L:84:LEU:H    | 1.55        | 0.71     |
| 1:A:923:A:OP1     | 6:E:21:ALA:HB2   | 1.90        | 0.71     |
| 4:C:3:ASN:N       | 4:C:3:ASN:ND2    | 2.32        | 0.71     |
| 11:J:39:PRO:O     | 11:J:40:LEU:HB2  | 1.89        | 0.71     |
| 21:T:57:ARG:HH21  | 21:T:100:ILE:CG2 | 2.03        | 0.71     |
| 1:A:791:G:H2'     | 1:A:792:A:H5'    | 1.73        | 0.71     |
| 1:A:135:C:O2      | 17:P:1:MET:HB2   | 1.90        | 0.71     |
| 16:O:39:LEU:HD22  | 16:O:56:LEU:HD13 | 1.71        | 0.70     |
| 1:A:254:G:O2'     | 1:A:255:G:H5'    | 1.91        | 0.70     |
| 11:J:32:ALA:HB2   | 11:J:75:ILE:O    | 1.91        | 0.70     |
| 18:Q:76:LEU:HD23  | 18:Q:77:VAL:N    | 2.06        | 0.70     |
| 1:A:1028:C:H2'    | 1:A:1029:C:C6    | 2.25        | 0.70     |
| 1:A:760:G:O6      | 18:Q:105:ALA:HB2 | 1.91        | 0.70     |
| 12:K:27:ASN:HA    | 12:K:56:GLY:HA2  | 1.73        | 0.70     |
| 1:A:1006:C:H2'    | 1:A:1007:C:C6    | 2.26        | 0.70     |
| 7:F:86:ARG:O      | 7:F:87:ARG:HG2   | 1.92        | 0.70     |
| 16:O:26:GLU:OE1   | 16:O:77:ARG:HD2  | 1.90        | 0.70     |
| 6:E:12:LEU:HD13   | 6:E:31:LEU:HB2   | 1.70        | 0.70     |
| 1:A:1141:C:H2'    | 1:A:1142:G:H8    | 1.57        | 0.70     |
| 19:R:86:VAL:O     | 19:R:87:ARG:HB2  | 1.90        | 0.70     |
| 1:A:1498:U:H4'    | 1:A:1519:A:C2    | 2.26        | 0.70     |
| 3:B:139:LYS:O     | 3:B:143:GLU:HG2  | 1.90        | 0.70     |
| 7:F:21:LEU:O      | 7:F:24:GLU:HB3   | 1.91        | 0.70     |
| 1:A:1148:U:H2'    | 1:A:1149:C:O4'   | 1.91        | 0.70     |
| 4:C:120:VAL:O     | 4:C:124:ILE:HG13 | 1.90        | 0.70     |
| 13:L:47:LYS:CB    | 13:L:48:PRO:HD3  | 2.22        | 0.70     |
| 12:K:77:MET:HE3   | 12:K:80:VAL:HG22 | 1.73        | 0.70     |
| 4:C:107:GLN:H     | 4:C:107:GLN:CD   | 1.95        | 0.70     |
| 4:C:6:HIS:CD2     | 4:C:8:ILE:HB     | 2.27        | 0.70     |
| 20:S:17:GLU:O     | 20:S:21:GLU:HG3  | 1.91        | 0.70     |
| 4:C:64:VAL:HB     | 4:C:99:VAL:CG2   | 2.22        | 0.69     |
| 3:B:76:GLN:HG3    | 3:B:206:ASP:OD1  | 1.92        | 0.69     |
| 4:C:179:ARG:HD3   | 4:C:206:GLU:HG2  | 1.72        | 0.69     |
| 10:I:108:VAL:HG12 | 10:I:109:VAL:N   | 2.07        | 0.69     |
| 12:K:84:VAL:HG11  | 12:K:95:ILE:HD11 | 1.73        | 0.69     |
| 1:A:1426:C:H2'    | 1:A:1427:U:C6    | 2.27        | 0.69     |
| 1:A:1132:C:H2'    | 1:A:1133:G:H8    | 1.54        | 0.69     |
| 1:A:939:G:H5''    | 8:G:102:ARG:NH2  | 2.08        | 0.69     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:677:U:H3     | 1:A:713:G:H22     | 1.41        | 0.69     |
| 1:A:1167:A:H2'   | 1:A:1168:A:C8     | 2.28        | 0.69     |
| 4:C:35:GLU:HG3   | 4:C:95:THR:HG21   | 1.74        | 0.69     |
| 4:C:180:ALA:O    | 4:C:181:ASN:HB3   | 1.91        | 0.69     |
| 1:A:918:A:H2'    | 1:A:919:A:C8      | 2.28        | 0.69     |
| 14:M:3:ARG:HA    | 14:M:8:GLU:O      | 1.92        | 0.69     |
| 11:J:34:VAL:HG22 | 11:J:74:ILE:HG23  | 1.75        | 0.69     |
| 18:Q:53:LEU:HD11 | 18:Q:85:VAL:HG11  | 1.73        | 0.69     |
| 7:F:80:ARG:NH1   | 7:F:88:VAL:HB     | 2.07        | 0.69     |
| 1:A:824:C:H2'    | 1:A:825:G:H8      | 1.58        | 0.69     |
| 14:M:65:LYS:HG3  | 14:M:69:GLU:OE2   | 1.93        | 0.69     |
| 10:I:2:GLU:OE1   | 10:I:3:GLN:HB2    | 1.92        | 0.69     |
| 14:M:49:THR:HG22 | 14:M:51:ALA:N     | 2.04        | 0.69     |
| 19:R:39:VAL:O    | 19:R:42:ARG:HB2   | 1.93        | 0.69     |
| 1:A:1250:A:H4'   | 10:I:68:GLY:CA    | 2.23        | 0.69     |
| 1:A:1113:C:H4'   | 4:C:14:ILE:HD11   | 1.74        | 0.69     |
| 1:A:1415:G:H2'   | 1:A:1416:G:H8     | 1.58        | 0.69     |
| 13:L:83:VAL:HG22 | 13:L:84:LEU:N     | 2.07        | 0.69     |
| 13:L:47:LYS:CB   | 13:L:48:PRO:CD    | 2.71        | 0.69     |
| 16:O:87:ILE:O    | 16:O:88:ARG:HB2   | 1.93        | 0.69     |
| 4:C:130:VAL:HG12 | 4:C:134:ILE:HD11  | 1.73        | 0.69     |
| 8:G:23:VAL:O     | 8:G:27:ILE:HG13   | 1.93        | 0.69     |
| 1:A:401:C:H2'    | 1:A:402:G:H8      | 1.57        | 0.69     |
| 1:A:149:A:H2'    | 1:A:150:C:C6      | 2.26        | 0.69     |
| 1:A:948:C:OP1    | 14:M:109:THR:HG22 | 1.92        | 0.69     |
| 8:G:138:LYS:C    | 8:G:138:LYS:HD3   | 2.13        | 0.69     |
| 8:G:95:ARG:HG2   | 8:G:99:LEU:CD1    | 2.23        | 0.69     |
| 14:M:11:ARG:HG3  | 14:M:12:ASN:H     | 1.54        | 0.69     |
| 17:P:20:VAL:HG23 | 17:P:34:GLU:O     | 1.93        | 0.69     |
| 1:A:946:A:H2'    | 1:A:947:G:C8      | 2.27        | 0.69     |
| 4:C:52:LEU:HD23  | 4:C:52:LEU:N      | 2.07        | 0.69     |
| 6:E:51:VAL:O     | 6:E:55:VAL:HG23   | 1.93        | 0.69     |
| 1:A:99:C:H2'     | 1:A:101:A:C8      | 2.27        | 0.69     |
| 12:K:43:SER:HA   | 12:K:47:VAL:HG21  | 1.74        | 0.68     |
| 5:D:33:MET:HE3   | 5:D:37:PRO:HB3    | 1.74        | 0.68     |
| 10:I:8:GLY:HA2   | 10:I:79:LEU:CD1   | 2.18        | 0.68     |
| 1:A:243:A:H4'    | 1:A:244:U:C5'     | 2.22        | 0.68     |
| 1:A:113:G:H1'    | 1:A:354:G:H5'     | 1.75        | 0.68     |
| 1:A:1412:C:H2'   | 1:A:1413:A:C8     | 2.27        | 0.68     |
| 1:A:1241:G:H2'   | 1:A:1242:C:H6     | 1.58        | 0.68     |
| 1:A:1004:A:H5''  | 1:A:1025:U:C4     | 2.27        | 0.68     |
| 1:A:1343:G:H2'   | 1:A:1344:C:C6     | 2.28        | 0.68     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 10:I:48:GLU:HA   | 10:I:51:ARG:HH11 | 1.57        | 0.68     |
| 18:Q:63:ARG:HG2  | 18:Q:64:PRO:HD2  | 1.75        | 0.68     |
| 19:R:37:VAL:O    | 19:R:41:LYS:HB2  | 1.93        | 0.68     |
| 1:A:476:G:H2'    | 1:A:477:G:H8     | 1.58        | 0.68     |
| 4:C:50:ALA:HB1   | 4:C:70:VAL:HG11  | 1.75        | 0.68     |
| 1:A:1499:A:O2'   | 1:A:1500:A:H5'   | 1.94        | 0.68     |
| 1:A:1163:C:H2'   | 1:A:1164:G:H8    | 1.58        | 0.68     |
| 7:F:38:GLU:O     | 7:F:39:LYS:HB3   | 1.92        | 0.68     |
| 19:R:43:PHE:C    | 19:R:51:LEU:HD12 | 2.14        | 0.68     |
| 1:A:1411:C:H2'   | 1:A:1412:C:C6    | 2.28        | 0.68     |
| 21:T:54:LYS:HG3  | 21:T:100:ILE:CD1 | 2.23        | 0.68     |
| 3:B:143:GLU:O    | 3:B:147:LYS:HG3  | 1.93        | 0.68     |
| 1:A:1256:A:N6    | 1:A:1278:U:H1'   | 2.09        | 0.68     |
| 5:D:24:GLU:HG2   | 5:D:25:ARG:N     | 2.08        | 0.68     |
| 3:B:25:ASN:C     | 3:B:25:ASN:HD22  | 1.96        | 0.68     |
| 13:L:126:LYS:HD2 | 13:L:126:LYS:N   | 2.06        | 0.68     |
| 11:J:51:ARG:CB   | 11:J:59:SER:HB3  | 2.17        | 0.68     |
| 1:A:1281:U:H4'   | 1:A:1282:C:OP2   | 1.93        | 0.68     |
| 11:J:49:VAL:HG11 | 15:N:41:ARG:O    | 1.92        | 0.68     |
| 19:R:45:SER:C    | 19:R:47:THR:H    | 1.96        | 0.68     |
| 1:A:285:G:O2'    | 1:A:286:G:H5'    | 1.93        | 0.68     |
| 20:S:62:ILE:HD12 | 20:S:66:MET:HG3  | 1.76        | 0.68     |
| 1:A:1160:G:O2'   | 1:A:1161:C:H5'   | 1.94        | 0.68     |
| 14:M:40:ASN:HD22 | 14:M:41:PRO:CD   | 2.07        | 0.68     |
| 1:A:1053:G:C3'   | 1:A:1054:C:H5'   | 2.23        | 0.68     |
| 4:C:79:ARG:HG2   | 4:C:82:GLU:HG2   | 1.74        | 0.68     |
| 13:L:45:PRO:HD3  | 13:L:51:ALA:O    | 1.94        | 0.68     |
| 1:A:1257:U:H4'   | 1:A:1258:G:C5'   | 2.24        | 0.67     |
| 19:R:53:ARG:HH21 | 19:R:60:GLY:N    | 1.91        | 0.67     |
| 1:A:1286:A:H2'   | 1:A:1287:A:C5'   | 2.23        | 0.67     |
| 18:Q:59:ILE:HG23 | 18:Q:71:PHE:HB3  | 1.75        | 0.67     |
| 9:H:7:ALA:HA     | 9:H:85:ARG:HG3   | 1.76        | 0.67     |
| 1:A:1124:G:H5'   | 11:J:35:SER:O    | 1.95        | 0.67     |
| 11:J:54:PHE:O    | 11:J:55:LYS:HG2  | 1.94        | 0.67     |
| 17:P:67:THR:HG22 | 17:P:68:ASP:N    | 2.09        | 0.67     |
| 1:A:996:A:H2'    | 1:A:997:U:C6     | 2.30        | 0.67     |
| 1:A:1289:A:H2'   | 1:A:1290:G:H5'   | 1.77        | 0.67     |
| 6:E:80:ILE:H     | 6:E:80:ILE:HD12  | 1.58        | 0.67     |
| 4:C:8:ILE:HG23   | 4:C:16:ARG:HG2   | 1.75        | 0.67     |
| 1:A:1262:C:H2'   | 1:A:1263:C:C6    | 2.29        | 0.67     |
| 22:V:6:ARG:CD    | 22:V:15:ARG:NH1  | 2.57        | 0.67     |
| 1:A:1533:C:H2'   | 1:A:1533:C:O2    | 1.93        | 0.67     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 14:M:36:LYS:HD2  | 14:M:59:TYR:CZ   | 2.30        | 0.67     |
| 1:A:255:G:H1'    | 18:Q:16:GLN:NE2  | 2.09        | 0.67     |
| 6:E:43:LEU:HD11  | 6:E:132:ALA:HB1  | 1.77        | 0.67     |
| 19:R:55:ARG:HB3  | 19:R:55:ARG:HH11 | 1.58        | 0.67     |
| 19:R:87:ARG:HG2  | 19:R:87:ARG:HH11 | 1.60        | 0.67     |
| 6:E:40:ARG:HG2   | 6:E:68:GLU:OE2   | 1.95        | 0.67     |
| 11:J:45:ARG:NH2  | 15:N:36:PHE:CD2  | 2.62        | 0.67     |
| 3:B:15:VAL:HG11  | 3:B:209:ARG:C    | 2.15        | 0.67     |
| 12:K:19:ALA:HB2  | 12:K:80:VAL:HG11 | 1.75        | 0.67     |
| 14:M:40:ASN:HD22 | 14:M:41:PRO:HD2  | 1.60        | 0.67     |
| 16:O:17:ARG:NH1  | 16:O:77:ARG:NH1  | 2.43        | 0.67     |
| 20:S:42:PRO:O    | 20:S:45:VAL:HG23 | 1.94        | 0.67     |
| 1:A:560:U:H5'    | 1:A:566:G:N2     | 2.10        | 0.67     |
| 1:A:975:A:O2'    | 15:N:32:SER:HB2  | 1.94        | 0.67     |
| 18:Q:59:ILE:HG22 | 18:Q:71:PHE:CD1  | 2.29        | 0.67     |
| 1:A:1510:U:H2'   | 1:A:1511:G:C8    | 2.30        | 0.67     |
| 12:K:69:ALA:O    | 12:K:73:MET:HG2  | 1.95        | 0.67     |
| 1:A:1502:A:H2    | 1:A:1505:G:N1    | 1.92        | 0.67     |
| 1:A:130:A:OP2    | 1:A:190(E):U:H2' | 1.95        | 0.67     |
| 4:C:150:LYS:HE2  | 4:C:152:ILE:HD11 | 1.76        | 0.67     |
| 6:E:64:ARG:O     | 6:E:65:ASN:HB3   | 1.95        | 0.67     |
| 9:H:36:LEU:HD12  | 9:H:59:LEU:HD13  | 1.77        | 0.67     |
| 1:A:1305:G:H5'   | 22:V:4:GLY:HA3   | 1.75        | 0.67     |
| 6:E:118:ILE:HG22 | 6:E:119:LEU:N    | 2.10        | 0.67     |
| 13:L:47:LYS:HB2  | 13:L:48:PRO:CD   | 2.25        | 0.67     |
| 1:A:1285:A:H4'   | 1:A:1286:A:O5'   | 1.94        | 0.66     |
| 11:J:39:PRO:HA   | 11:J:70:ARG:NH1  | 2.10        | 0.66     |
| 3:B:102:LEU:HD21 | 3:B:162:ILE:HD11 | 1.75        | 0.66     |
| 22:V:6:ARG:HD3   | 22:V:15:ARG:NH1  | 2.10        | 0.66     |
| 1:A:650:G:O2'    | 1:A:651:C:H5'    | 1.95        | 0.66     |
| 1:A:107:G:C2'    | 1:A:108:G:H5'    | 2.25        | 0.66     |
| 3:B:84:GLU:OE1   | 3:B:216:SER:HA   | 1.95        | 0.66     |
| 1:A:972:C:P      | 11:J:57:LYS:HD3  | 2.35        | 0.66     |
| 11:J:4:ILE:HG22  | 11:J:6:ILE:HG23  | 1.76        | 0.66     |
| 11:J:8:LEU:CD2   | 11:J:96:ILE:HG12 | 2.24        | 0.66     |
| 1:A:1248:A:H1'   | 10:I:70:LYS:NZ   | 2.11        | 0.66     |
| 13:L:6:THR:OG1   | 13:L:9:GLN:HG3   | 1.96        | 0.66     |
| 3:B:124:SER:HB2  | 3:B:125:PRO:CD   | 2.26        | 0.66     |
| 5:D:162:LEU:HD12 | 5:D:181:MET:HE2  | 1.76        | 0.66     |
| 10:I:4:TYR:CE2   | 10:I:88:TYR:HA   | 2.30        | 0.66     |
| 1:A:838:G:H2'    | 1:A:839:U:H5''   | 1.77        | 0.66     |
| 1:A:1425:U:H2'   | 1:A:1426:C:C6    | 2.31        | 0.66     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 16:O:29:VAL:HG11 | 16:O:67:LEU:HD21 | 1.78        | 0.66     |
| 1:A:1202:G:C2'   | 1:A:1203:C:H5'   | 2.26        | 0.66     |
| 3:B:23:ARG:NH1   | 3:B:24:TRP:HA    | 2.11        | 0.66     |
| 1:A:1347:G:O2'   | 1:A:1348:U:OP2   | 2.13        | 0.66     |
| 16:O:26:GLU:HA   | 16:O:81:LEU:HD11 | 1.76        | 0.66     |
| 1:A:1195:C:H3'   | 1:A:1196:U:H5''  | 1.76        | 0.66     |
| 17:P:39:TYR:CD2  | 17:P:73:LEU:HD11 | 2.30        | 0.66     |
| 1:A:723:U:O2     | 1:A:723:U:H2'    | 1.95        | 0.66     |
| 4:C:6:HIS:HD2    | 4:C:8:ILE:HB     | 1.60        | 0.66     |
| 1:A:1037:C:H2'   | 1:A:1038:C:C6    | 2.31        | 0.66     |
| 17:P:34:GLU:OE2  | 17:P:55:ARG:HD3  | 1.95        | 0.66     |
| 22:V:5:ASP:O     | 22:V:11:GLY:HA3  | 1.96        | 0.66     |
| 9:H:31:PHE:O     | 9:H:35:ILE:HG13  | 1.96        | 0.66     |
| 11:J:40:LEU:HD22 | 11:J:41:PRO:HD2  | 1.77        | 0.66     |
| 1:A:1040:U:H2'   | 1:A:1041:A:H8    | 1.60        | 0.66     |
| 16:O:31:LEU:HD12 | 16:O:31:LEU:H    | 1.59        | 0.66     |
| 1:A:390:C:O3'    | 17:P:28:ARG:NH2  | 2.29        | 0.66     |
| 4:C:113:ALA:HB3  | 4:C:114:PRO:HD3  | 1.77        | 0.66     |
| 1:A:1142:G:H2'   | 1:A:1143:G:O4'   | 1.96        | 0.66     |
| 9:H:60:ARG:HG3   | 9:H:60:ARG:HH11  | 1.59        | 0.66     |
| 1:A:1145:C:O2'   | 1:A:1146:A:H8    | 1.79        | 0.66     |
| 1:A:130:A:C8     | 18:Q:63:ARG:HG3  | 2.31        | 0.66     |
| 1:A:1423:G:O2'   | 1:A:1424:C:H5'   | 1.97        | 0.65     |
| 1:A:197:A:H4'    | 1:A:198:G:O5'    | 1.96        | 0.65     |
| 1:A:1202:G:O2'   | 1:A:1203:C:H5'   | 1.96        | 0.65     |
| 13:L:75:HIS:CD2  | 13:L:77:LEU:H    | 2.06        | 0.65     |
| 6:E:115:VAL:HG11 | 6:E:118:ILE:CD1  | 2.25        | 0.65     |
| 20:S:52:TYR:HA   | 20:S:56:GLN:O    | 1.96        | 0.65     |
| 1:A:953:G:O4'    | 14:M:125:ARG:HA  | 1.95        | 0.65     |
| 9:H:103:VAL:CG2  | 9:H:110:ALA:HB2  | 2.27        | 0.65     |
| 1:A:489:C:H2'    | 1:A:490:G:H8     | 1.60        | 0.65     |
| 11:J:8:LEU:HB3   | 11:J:16:LEU:HD22 | 1.78        | 0.65     |
| 13:L:59:ARG:HD3  | 13:L:65:GLU:HG3  | 1.77        | 0.65     |
| 1:A:812:C:HO2'   | 1:A:813:U:P      | 2.20        | 0.65     |
| 5:D:140:VAL:CG1  | 5:D:146:ILE:HD11 | 2.24        | 0.65     |
| 6:E:35:GLY:HA3   | 6:E:112:LEU:HB3  | 1.76        | 0.65     |
| 18:Q:18:THR:OG1  | 18:Q:69:LYS:HE3  | 1.96        | 0.65     |
| 16:O:17:ARG:HH11 | 16:O:17:ARG:HG3  | 1.61        | 0.65     |
| 3:B:23:ARG:HH11  | 3:B:24:TRP:HA    | 1.60        | 0.65     |
| 22:V:6:ARG:HD3   | 22:V:15:ARG:HH12 | 1.60        | 0.65     |
| 4:C:190:ARG:HB3  | 4:C:190:ARG:NH1  | 2.12        | 0.65     |
| 3:B:97:TRP:HZ2   | 3:B:102:LEU:HD13 | 1.61        | 0.65     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:1527:C:O2'    | 1:A:1528:U:H5'    | 1.97        | 0.65     |
| 1:A:1195:C:H2'    | 1:A:1197:G:H5'    | 1.79        | 0.65     |
| 5:D:4:TYR:O       | 5:D:5:ILE:HB      | 1.95        | 0.65     |
| 6:E:79:GLU:CD     | 6:E:79:GLU:H      | 2.00        | 0.65     |
| 1:A:1348:U:H2'    | 1:A:1349:A:H8     | 1.60        | 0.65     |
| 1:A:1428:A:H2'    | 1:A:1429:C:C6     | 2.31        | 0.65     |
| 18:Q:15:MET:HE3   | 18:Q:43:LEU:HD22  | 1.78        | 0.65     |
| 5:D:121:VAL:O     | 5:D:134:ASP:HA    | 1.96        | 0.65     |
| 1:A:1021:G:H2'    | 1:A:1022:G:O4'    | 1.97        | 0.65     |
| 1:A:1225:A:H2'    | 1:A:1225:A:N3     | 2.12        | 0.65     |
| 1:A:353:A:H5'     | 1:A:353:A:H8      | 1.62        | 0.65     |
| 3:B:215:LEU:O     | 3:B:219:VAL:HG23  | 1.97        | 0.65     |
| 5:D:142:PRO:HG2   | 5:D:187:ARG:NH2   | 2.12        | 0.65     |
| 19:R:53:ARG:HH21  | 19:R:60:GLY:H     | 1.45        | 0.65     |
| 10:I:81:ILE:O     | 10:I:85:LEU:HB2   | 1.97        | 0.65     |
| 5:D:16:GLY:O      | 5:D:33:MET:HE2    | 1.97        | 0.64     |
| 1:A:761:G:N3      | 18:Q:105:ALA:HB3  | 2.12        | 0.64     |
| 10:I:78:LYS:HD3   | 10:I:101:PHE:CD2  | 2.32        | 0.64     |
| 1:A:509:A:H5'     | 5:D:54:TYR:HD2    | 1.62        | 0.64     |
| 1:A:1037:C:H2'    | 1:A:1038:C:H6     | 1.62        | 0.64     |
| 17:P:8:ARG:HB2    | 17:P:28:ARG:NH1   | 2.12        | 0.64     |
| 10:I:118:LYS:O    | 10:I:119:ALA:HB3  | 1.95        | 0.64     |
| 14:M:117:VAL:HG12 | 14:M:118:ALA:N    | 2.12        | 0.64     |
| 14:M:102:ARG:HB2  | 14:M:102:ARG:HH11 | 1.62        | 0.64     |
| 5:D:70:ILE:HD11   | 5:D:100:ARG:NE    | 2.12        | 0.64     |
| 13:L:120:TYR:O    | 13:L:122:THR:HG23 | 1.98        | 0.64     |
| 13:L:60:LEU:CD1   | 13:L:85:ILE:HD12  | 2.22        | 0.64     |
| 1:A:1411:C:H2'    | 1:A:1412:C:H6     | 1.61        | 0.64     |
| 21:T:54:LYS:HE3   | 21:T:100:ILE:HD11 | 1.79        | 0.64     |
| 1:A:1323:G:H2'    | 1:A:1324:A:C8     | 2.32        | 0.64     |
| 18:Q:12:SER:HB3   | 18:Q:20:THR:HB    | 1.80        | 0.64     |
| 6:E:51:VAL:HB     | 6:E:52:PRO:CD     | 2.25        | 0.64     |
| 11:J:78:ASN:O     | 11:J:80:LYS:N     | 2.30        | 0.64     |
| 9:H:6:ILE:HD11    | 9:H:31:PHE:CD2    | 2.32        | 0.64     |
| 6:E:15:ARG:O      | 6:E:15:ARG:HD2    | 1.98        | 0.64     |
| 1:A:1251:A:H4'    | 10:I:12:GLU:OE2   | 1.98        | 0.64     |
| 21:T:67:ALA:HA    | 21:T:73:HIS:H     | 1.62        | 0.64     |
| 3:B:184:VAL:N     | 3:B:198:ASP:OD2   | 2.31        | 0.64     |
| 5:D:190:ASP:HB2   | 5:D:193:ASP:OD2   | 1.98        | 0.64     |
| 1:A:939:G:H2'     | 1:A:940:C:H6      | 1.63        | 0.64     |
| 6:E:31:LEU:HD22   | 6:E:43:LEU:HD21   | 1.79        | 0.64     |
| 1:A:1368:G:O2'    | 1:A:1369:C:H5'    | 1.98        | 0.64     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:920:U:H2'    | 1:A:921:U:C6      | 2.33        | 0.64     |
| 1:A:1117:G:H5'   | 1:A:1117:G:H8     | 1.62        | 0.64     |
| 17:P:59:TRP:HB3  | 17:P:64:ALA:HB2   | 1.80        | 0.64     |
| 1:A:735:C:O2'    | 1:A:736:C:H5'     | 1.98        | 0.64     |
| 1:A:1306:A:N6    | 1:A:1331:G:H1'    | 2.13        | 0.64     |
| 6:E:75:THR:HG23  | 6:E:76:ILE:N      | 2.12        | 0.64     |
| 6:E:86:ALA:HB3   | 6:E:125:SER:HB2   | 1.80        | 0.64     |
| 4:C:95:THR:C     | 4:C:97:LYS:H      | 2.02        | 0.63     |
| 14:M:37:THR:O    | 14:M:37:THR:HG22  | 1.98        | 0.63     |
| 4:C:14:ILE:HG22  | 4:C:15:THR:H      | 1.62        | 0.63     |
| 3:B:69:LEU:HD12  | 3:B:155:LEU:HD11  | 1.80        | 0.63     |
| 21:T:89:ARG:HE   | 21:T:104:LEU:HD22 | 1.63        | 0.63     |
| 4:C:26:LYS:HD3   | 4:C:26:LYS:N      | 2.13        | 0.63     |
| 15:N:57:ARG:HG2  | 15:N:58:LYS:H     | 1.63        | 0.63     |
| 5:D:55:ALA:O     | 5:D:59:ARG:HG2    | 1.98        | 0.63     |
| 4:C:155:GLY:O    | 4:C:156:ARG:HB2   | 1.97        | 0.63     |
| 1:A:328:C:H4'    | 1:A:329:A:O5'     | 1.98        | 0.63     |
| 3:B:95:GLN:O     | 3:B:96:ARG:HD2    | 1.98        | 0.63     |
| 1:A:1131:G:H1    | 1:A:1143:G:N2     | 1.86        | 0.63     |
| 1:A:1329:A:P     | 14:M:28:ALA:HB3   | 2.38        | 0.63     |
| 5:D:25:ARG:C     | 5:D:27:TYR:H      | 2.01        | 0.63     |
| 1:A:620:C:N1     | 5:D:135:LEU:HD13  | 2.13        | 0.63     |
| 1:A:254:G:OP1    | 18:Q:67:LYS:O     | 2.14        | 0.63     |
| 1:A:411:A:N9     | 1:A:413:G:H1'     | 2.14        | 0.63     |
| 8:G:71:PRO:HD3   | 8:G:103:TRP:HZ3   | 1.62        | 0.63     |
| 3:B:28:PHE:CZ    | 3:B:189:ASP:HA    | 2.34        | 0.63     |
| 5:D:104:VAL:HG11 | 5:D:146:ILE:CD1   | 2.29        | 0.63     |
| 10:I:100:GLY:O   | 10:I:102:LEU:N    | 2.31        | 0.63     |
| 1:A:190(F):G:H4' | 1:A:190(G):G:OP2  | 1.98        | 0.63     |
| 19:R:47:THR:HG23 | 19:R:83:GLU:H     | 1.64        | 0.63     |
| 1:A:31:G:N1      | 1:A:48:C:H5''     | 2.14        | 0.63     |
| 19:R:25:THR:O    | 19:R:26:LEU:HB2   | 1.98        | 0.63     |
| 4:C:34:LEU:O     | 4:C:34:LEU:HD23   | 1.98        | 0.63     |
| 1:A:657:G:H4'    | 16:O:28:GLN:HG2   | 1.80        | 0.63     |
| 1:A:1484:C:H2'   | 1:A:1485:U:H6     | 1.63        | 0.63     |
| 11:J:35:SER:HB2  | 11:J:72:VAL:O     | 1.98        | 0.63     |
| 6:E:115:VAL:HG11 | 6:E:118:ILE:HD11  | 1.80        | 0.63     |
| 1:A:1250:A:H2'   | 1:A:1251:A:C8     | 2.33        | 0.63     |
| 11:J:90:LEU:H    | 11:J:91:PRO:HD2   | 1.62        | 0.63     |
| 1:A:1520:G:O2'   | 1:A:1521:G:H5'    | 1.99        | 0.63     |
| 7:F:30:LEU:HB3   | 7:F:35:ALA:HB3    | 1.80        | 0.63     |
| 17:P:43:LYS:HG3  | 17:P:48:TRP:CD2   | 2.34        | 0.63     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:149:A:O2'     | 1:A:150:C:H5'     | 1.99        | 0.63     |
| 1:A:267:C:H2'     | 1:A:268:C:C6      | 2.34        | 0.63     |
| 4:C:52:LEU:H      | 4:C:52:LEU:CD2    | 2.11        | 0.63     |
| 1:A:1257:U:H4'    | 1:A:1258:G:H5'    | 1.80        | 0.63     |
| 6:E:80:ILE:HD13   | 6:E:91:LEU:HD12   | 1.80        | 0.63     |
| 1:A:1216:G:H5''   | 15:N:5:ALA:CB     | 2.29        | 0.63     |
| 15:N:59:ALA:O     | 15:N:60:SER:CB    | 2.47        | 0.62     |
| 4:C:84:ILE:O      | 4:C:88:ARG:HB2    | 1.98        | 0.62     |
| 11:J:54:PHE:CD2   | 11:J:55:LYS:HD3   | 2.33        | 0.62     |
| 3:B:75:LYS:HE3    | 3:B:78:GLN:OE1    | 1.98        | 0.62     |
| 1:A:1413:A:O2'    | 1:A:1414:U:H5'    | 1.98        | 0.62     |
| 1:A:1425:U:H2'    | 1:A:1426:C:H6     | 1.63        | 0.62     |
| 3:B:142:LEU:HB3   | 3:B:146:GLN:NE2   | 2.14        | 0.62     |
| 1:A:476:G:H2'     | 1:A:477:G:C8      | 2.34        | 0.62     |
| 13:L:42:THR:CG2   | 13:L:52:LEU:HB3   | 2.29        | 0.62     |
| 20:S:16:LEU:O     | 20:S:19:VAL:HG12  | 1.99        | 0.62     |
| 10:I:111:ARG:HD3  | 10:I:112:LYS:N    | 2.14        | 0.62     |
| 3:B:42:ILE:HD12   | 3:B:203:GLY:HA2   | 1.80        | 0.62     |
| 1:A:1298:C:H2'    | 8:G:114:ARG:HH12  | 1.65        | 0.62     |
| 1:A:175:C:H2'     | 1:A:176:C:H6      | 1.64        | 0.62     |
| 18:Q:79:SER:O     | 18:Q:80:GLY:O     | 2.17        | 0.62     |
| 3:B:178:ARG:O     | 9:H:71:GLY:HA2    | 2.00        | 0.62     |
| 14:M:62:ASN:O     | 14:M:63:THR:HB    | 2.00        | 0.62     |
| 13:L:47:LYS:HB3   | 13:L:48:PRO:HD3   | 1.79        | 0.62     |
| 3:B:27:LYS:HD3    | 3:B:195:ASP:OD2   | 1.99        | 0.62     |
| 1:A:370:C:O2'     | 1:A:371:G:H5'     | 1.98        | 0.62     |
| 1:A:1347:G:H22    | 1:A:1373:G:H2'    | 1.64        | 0.62     |
| 25:A:1632:HYG:O30 | 25:A:1632:HYG:H12 | 1.99        | 0.62     |
| 25:A:1632:HYG:O14 | 25:A:1632:HYG:H1  | 1.98        | 0.62     |
| 20:S:29:ARG:O     | 20:S:30:LEU:HB2   | 2.00        | 0.62     |
| 14:M:45:VAL:O     | 14:M:48:LEU:HB2   | 1.99        | 0.62     |
| 1:A:477:G:H2'     | 1:A:478:A:H8      | 1.65        | 0.62     |
| 1:A:107:G:H2'     | 1:A:108:G:H5'     | 1.81        | 0.62     |
| 6:E:120:THR:HG23  | 6:E:121:LYS:N     | 2.13        | 0.62     |
| 7:F:95:GLU:H      | 7:F:95:GLU:CD     | 2.03        | 0.62     |
| 1:A:664:G:OP1     | 19:R:64:ARG:HD2   | 2.00        | 0.62     |
| 14:M:77:ASN:O     | 14:M:80:ARG:HB3   | 1.98        | 0.62     |
| 4:C:11:ARG:HH11   | 4:C:11:ARG:HG2    | 1.65        | 0.62     |
| 16:O:55:GLY:O     | 16:O:59:MET:HG3   | 1.99        | 0.62     |
| 1:A:1305:G:C5'    | 22:V:4:GLY:HA3    | 2.29        | 0.62     |
| 11:J:38:ILE:HG13  | 11:J:72:VAL:H     | 1.65        | 0.62     |
| 1:A:1366:C:H2'    | 1:A:1367:C:C6     | 2.32        | 0.62     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 5:D:196:LEU:C     | 5:D:198:VAL:H     | 2.02        | 0.62     |
| 1:A:1216:G:H5''   | 15:N:5:ALA:HB2    | 1.82        | 0.62     |
| 1:A:1314:C:H2'    | 1:A:1315:U:C6     | 2.34        | 0.62     |
| 1:A:791:G:H2'     | 1:A:792:A:C5'     | 2.29        | 0.62     |
| 13:L:55:VAL:HG12  | 13:L:56:ALA:N     | 2.14        | 0.62     |
| 1:A:835:U:OP1     | 19:R:64:ARG:NH2   | 2.33        | 0.61     |
| 7:F:69:GLU:N      | 7:F:69:GLU:OE1    | 2.33        | 0.61     |
| 14:M:14:ARG:HB3   | 14:M:16:ASP:OD1   | 2.00        | 0.61     |
| 14:M:117:VAL:HG12 | 14:M:118:ALA:H    | 1.65        | 0.61     |
| 8:G:139:GLU:O     | 8:G:143:ARG:HG3   | 2.00        | 0.61     |
| 13:L:38:THR:HG22  | 13:L:39:VAL:HG23  | 1.81        | 0.61     |
| 19:R:72:ARG:O     | 19:R:75:ILE:HG22  | 2.00        | 0.61     |
| 3:B:18:GLY:CA     | 3:B:41:ILE:HA     | 2.30        | 0.61     |
| 11:J:8:LEU:HB2    | 11:J:70:ARG:HB2   | 1.81        | 0.61     |
| 19:R:38:GLU:OE1   | 19:R:38:GLU:N     | 2.33        | 0.61     |
| 1:A:614:A:H2'     | 1:A:615:C:C6      | 2.34        | 0.61     |
| 4:C:47:LEU:N      | 4:C:47:LEU:HD12   | 2.16        | 0.61     |
| 7:F:36:ARG:HH11   | 7:F:36:ARG:HG2    | 1.64        | 0.61     |
| 6:E:24:ARG:HH11   | 6:E:24:ARG:HG2    | 1.66        | 0.61     |
| 5:D:173:TRP:HB2   | 5:D:187:ARG:O     | 2.00        | 0.61     |
| 1:A:1356:G:H2'    | 1:A:1357:A:H8     | 1.62        | 0.61     |
| 1:A:1346:A:N1     | 1:A:1374:A:H5''   | 2.15        | 0.61     |
| 15:N:11:LYS:O     | 15:N:13:THR:N     | 2.33        | 0.61     |
| 1:A:524:G:H2'     | 1:A:525:C:C6      | 2.35        | 0.61     |
| 1:A:1425:U:O2'    | 1:A:1426:C:H5'    | 2.00        | 0.61     |
| 17:P:22:THR:HA    | 17:P:33:ILE:HG13  | 1.81        | 0.61     |
| 17:P:52:ASP:OD2   | 17:P:55:ARG:HB2   | 2.01        | 0.61     |
| 1:A:1397:C:H4'    | 1:A:1398:A:OP2    | 2.00        | 0.61     |
| 19:R:16:PRO:O     | 19:R:17:SER:HB3   | 2.00        | 0.61     |
| 13:L:17:LYS:HA    | 13:L:17:LYS:HE3   | 1.80        | 0.61     |
| 1:A:1307:U:H5'    | 14:M:109:THR:HG21 | 1.83        | 0.61     |
| 1:A:1352:C:H2'    | 1:A:1353:G:C8     | 2.36        | 0.61     |
| 14:M:11:ARG:CG    | 14:M:12:ASN:N     | 2.62        | 0.61     |
| 1:A:373:A:O2'     | 1:A:374:A:H5'     | 2.00        | 0.61     |
| 3:B:53:ARG:NH1    | 3:B:199:TYR:CD2   | 2.69        | 0.61     |
| 18:Q:74:LEU:C     | 18:Q:74:LEU:HD23  | 2.21        | 0.61     |
| 1:A:1057:G:H5''   | 4:C:154:SER:CB    | 2.23        | 0.61     |
| 1:A:953:G:C1'     | 14:M:125:ARG:HA   | 2.31        | 0.61     |
| 1:A:1112:C:O2     | 4:C:179:ARG:HB3   | 1.99        | 0.61     |
| 1:A:1489:G:H2'    | 1:A:1490:C:C6     | 2.35        | 0.61     |
| 20:S:30:LEU:HD23  | 20:S:48:THR:O     | 2.00        | 0.61     |
| 22:V:6:ARG:CD     | 22:V:15:ARG:HH12  | 2.14        | 0.61     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:1016:A:H2'   | 1:A:1017:G:O4'   | 2.01        | 0.61     |
| 1:A:1218:C:H2'   | 1:A:1219:U:C6    | 2.35        | 0.61     |
| 16:O:38:ARG:O    | 16:O:41:GLU:HB3  | 2.00        | 0.61     |
| 13:L:33:ARG:HD2  | 13:L:62:SER:HB3  | 1.82        | 0.61     |
| 4:C:46:GLU:O     | 4:C:48:TYR:N     | 2.32        | 0.61     |
| 1:A:344:A:H4'    | 1:A:345:C:OP2    | 2.01        | 0.61     |
| 1:A:646:U:H2'    | 1:A:647:C:C6     | 2.36        | 0.61     |
| 8:G:12:LEU:H     | 8:G:12:LEU:HD12  | 1.65        | 0.61     |
| 4:C:47:LEU:CD1   | 4:C:47:LEU:H     | 2.14        | 0.61     |
| 4:C:91:LEU:CD2   | 4:C:99:VAL:HG13  | 2.24        | 0.61     |
| 11:J:62:HIS:HB3  | 15:N:59:ALA:CB   | 2.30        | 0.61     |
| 3:B:23:ARG:O     | 3:B:24:TRP:O     | 2.19        | 0.61     |
| 10:I:65:VAL:HG21 | 10:I:73:GLN:HB3  | 1.81        | 0.61     |
| 1:A:1320:C:N3    | 20:S:36:ARG:HG3  | 2.16        | 0.61     |
| 11:J:49:VAL:HG12 | 15:N:41:ARG:HD2  | 1.82        | 0.61     |
| 14:M:88:ARG:HD2  | 20:S:3:ARG:NH2   | 2.16        | 0.61     |
| 19:R:47:THR:HA   | 19:R:83:GLU:HB2  | 1.81        | 0.61     |
| 1:A:1195:C:H3'   | 1:A:1196:U:C5'   | 2.30        | 0.61     |
| 1:A:35:G:H2'     | 1:A:36:C:C6      | 2.36        | 0.61     |
| 1:A:580:U:H2'    | 1:A:581:G:O4'    | 2.01        | 0.60     |
| 21:T:56:MET:HE3  | 21:T:88:VAL:HG11 | 1.81        | 0.60     |
| 14:M:22:ILE:HD12 | 14:M:25:ILE:HD12 | 1.83        | 0.60     |
| 14:M:52:GLU:HG2  | 14:M:55:ARG:NH2  | 2.15        | 0.60     |
| 3:B:17:PHE:HB3   | 3:B:44:LEU:HD11  | 1.83        | 0.60     |
| 4:C:112:SER:CB   | 4:C:115:LEU:HD12 | 2.31        | 0.60     |
| 1:A:1163:C:H2'   | 1:A:1164:G:C8    | 2.36        | 0.60     |
| 4:C:13:GLY:HA3   | 15:N:57:ARG:CZ   | 2.30        | 0.60     |
| 8:G:85:TYR:HD1   | 8:G:154:TYR:HE1  | 1.48        | 0.60     |
| 1:A:437:U:H5''   | 5:D:155:LEU:HD22 | 1.82        | 0.60     |
| 1:A:1066:C:O2'   | 1:A:1067:A:H5'   | 2.01        | 0.60     |
| 4:C:110:ASN:ND2  | 4:C:140:ARG:HB3  | 2.15        | 0.60     |
| 6:E:12:LEU:CD1   | 6:E:31:LEU:HB2   | 2.31        | 0.60     |
| 1:A:765:G:H1     | 1:A:812:C:H2'    | 1.66        | 0.60     |
| 1:A:232:G:H1'    | 1:A:262:A:N1     | 2.16        | 0.60     |
| 13:L:27:LEU:C    | 13:L:29:GLY:N    | 2.53        | 0.60     |
| 5:D:30:LYS:C     | 5:D:32:ALA:H     | 2.03        | 0.60     |
| 1:A:1223:C:P     | 20:S:78:ARG:HH12 | 2.24        | 0.60     |
| 9:H:138:TRP:OXT  | 9:H:138:TRP:CE3  | 2.51        | 0.60     |
| 5:D:209:ARG:HG2  | 5:D:209:ARG:HH11 | 1.66        | 0.60     |
| 11:J:31:GLY:HA2  | 11:J:78:ASN:HD22 | 1.66        | 0.60     |
| 11:J:82:ILE:O    | 11:J:86:MET:HB2  | 2.01        | 0.60     |
| 1:A:1111:A:H2'   | 1:A:1112:C:C6    | 2.35        | 0.60     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 9:H:51:VAL:HG21  | 9:H:60:ARG:CG    | 2.31        | 0.60     |
| 17:P:21:VAL:HG21 | 17:P:59:TRP:CG   | 2.36        | 0.60     |
| 4:C:191:THR:CG2  | 4:C:192:THR:N    | 2.64        | 0.60     |
| 5:D:3:ARG:HE     | 5:D:71:SER:HB3   | 1.67        | 0.60     |
| 1:A:474:G:H2'    | 1:A:475:G:H8     | 1.66        | 0.60     |
| 1:A:761:G:H5''   | 18:Q:102:GLY:HA3 | 1.82        | 0.60     |
| 1:A:1047:G:C5'   | 15:N:4:LYS:HD2   | 2.27        | 0.60     |
| 4:C:47:LEU:HD12  | 4:C:47:LEU:H     | 1.66        | 0.60     |
| 3:B:18:GLY:HA3   | 3:B:41:ILE:HA    | 1.84        | 0.60     |
| 11:J:38:ILE:HB   | 11:J:71:LEU:HB3  | 1.83        | 0.60     |
| 17:P:20:VAL:HG21 | 17:P:32:TYR:CG   | 2.37        | 0.60     |
| 1:A:1053:G:C4'   | 1:A:1054:C:H5'   | 2.31        | 0.60     |
| 1:A:513:C:H2'    | 1:A:514:C:H6     | 1.66        | 0.60     |
| 9:H:14:ARG:O     | 9:H:18:ARG:HD3   | 2.00        | 0.60     |
| 5:D:176:LEU:HA   | 5:D:183:GLY:HA2  | 1.83        | 0.60     |
| 10:I:49:PRO:HD3  | 10:I:78:LYS:HG2  | 1.83        | 0.60     |
| 14:M:33:ALA:HA   | 14:M:59:TYR:HE2  | 1.66        | 0.60     |
| 13:L:55:VAL:HG12 | 13:L:56:ALA:H    | 1.66        | 0.60     |
| 1:A:10:A:OP2     | 6:E:126:ARG:HG2  | 2.02        | 0.60     |
| 1:A:1409:C:H2'   | 1:A:1410:G:H8    | 1.67        | 0.60     |
| 20:S:33:THR:HG22 | 20:S:34:TRP:N    | 2.17        | 0.60     |
| 11:J:69:ASN:O    | 11:J:70:ARG:HD3  | 2.02        | 0.60     |
| 1:A:1522:U:O2'   | 1:A:1523:G:H5'   | 2.02        | 0.60     |
| 7:F:14:LEU:HA    | 7:F:18:GLN:NE2   | 2.16        | 0.60     |
| 1:A:1168:A:H2'   | 1:A:1169:A:C8    | 2.36        | 0.60     |
| 10:I:24:GLY:HA2  | 10:I:59:PHE:O    | 2.02        | 0.60     |
| 19:R:61:LYS:O    | 19:R:65:ILE:HG13 | 2.01        | 0.60     |
| 1:A:969:A:N6     | 14:M:124:PRO:HB3 | 2.16        | 0.60     |
| 5:D:13:ARG:HA    | 5:D:33:MET:SD    | 2.42        | 0.60     |
| 3:B:206:ASP:CG   | 3:B:207:ALA:H    | 2.04        | 0.60     |
| 5:D:150:GLU:HG3  | 5:D:153:ARG:NH2  | 2.16        | 0.60     |
| 20:S:16:LEU:C    | 20:S:18:LYS:H    | 2.04        | 0.60     |
| 1:A:765:G:N2     | 1:A:812:C:O2'    | 2.34        | 0.60     |
| 1:A:1521:G:H2'   | 1:A:1522:U:C6    | 2.37        | 0.60     |
| 12:K:72:ALA:HB1  | 12:K:77:MET:HG3  | 1.84        | 0.60     |
| 13:L:46:LYS:NZ   | 13:L:47:LYS:HG3  | 2.17        | 0.60     |
| 8:G:71:PRO:HD3   | 8:G:103:TRP:CZ3  | 2.37        | 0.60     |
| 1:A:1229:A:OP2   | 14:M:114:ARG:HD3 | 2.02        | 0.59     |
| 1:A:1223:C:OP1   | 1:A:1224:G:H3'   | 2.02        | 0.59     |
| 14:M:14:ARG:HG3  | 14:M:44:ARG:HH12 | 1.65        | 0.59     |
| 1:A:518:C:O2'    | 13:L:50:SER:HB3  | 2.02        | 0.59     |
| 1:A:16:A:O2'     | 1:A:17:U:H5'     | 2.01        | 0.59     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 14:M:60:VAL:HG12 | 14:M:66:LEU:HD11 | 1.83        | 0.59     |
| 20:S:44:MET:O    | 20:S:47:HIS:HB2  | 2.02        | 0.59     |
| 3:B:178:ARG:NH1  | 3:B:178:ARG:HG3  | 2.08        | 0.59     |
| 11:J:53:PRO:HA   | 15:N:41:ARG:NH2  | 2.17        | 0.59     |
| 1:A:222:U:H2'    | 1:A:223:U:C6     | 2.37        | 0.59     |
| 6:E:12:LEU:C     | 6:E:12:LEU:HD22  | 2.23        | 0.59     |
| 1:A:532:A:H2'    | 1:A:533:A:C5'    | 2.32        | 0.59     |
| 1:A:673:G:H2'    | 1:A:674:G:C8     | 2.37        | 0.59     |
| 4:C:179:ARG:CD   | 4:C:206:GLU:HG2  | 2.32        | 0.59     |
| 3:B:101:MET:N    | 3:B:108:ILE:HD12 | 2.17        | 0.59     |
| 9:H:29:SER:OG    | 9:H:32:LYS:HB2   | 2.03        | 0.59     |
| 21:T:82:SER:O    | 21:T:86:ARG:HB2  | 2.02        | 0.59     |
| 1:A:164:U:H2'    | 1:A:165:C:H6     | 1.67        | 0.59     |
| 11:J:12:ASP:HB3  | 11:J:15:THR:CG2  | 2.32        | 0.59     |
| 7:F:25:ILE:HD12  | 7:F:82:ARG:HD2   | 1.83        | 0.59     |
| 4:C:33:LEU:O     | 4:C:33:LEU:HD23  | 2.01        | 0.59     |
| 4:C:92:ALA:C     | 4:C:94:LEU:H     | 2.05        | 0.59     |
| 6:E:9:LYS:CD     | 6:E:112:LEU:HD21 | 2.31        | 0.59     |
| 16:O:29:VAL:HG12 | 16:O:85:LEU:HD12 | 1.84        | 0.59     |
| 21:T:76:ALA:O    | 21:T:80:ARG:HG2  | 2.02        | 0.59     |
| 1:A:547:A:H4'    | 1:A:548:G:O5'    | 2.02        | 0.59     |
| 16:O:56:LEU:HA   | 16:O:59:MET:CE   | 2.23        | 0.59     |
| 17:P:51:VAL:O    | 17:P:52:ASP:HB3  | 2.00        | 0.59     |
| 1:A:1054:C:OP1   | 1:A:1197:G:OP1   | 2.21        | 0.59     |
| 1:A:22:G:O2'     | 1:A:23:C:H5'     | 2.02        | 0.59     |
| 21:T:59:ALA:O    | 21:T:63:ILE:HG13 | 2.01        | 0.59     |
| 1:A:321:A:O2'    | 1:A:322:C:H5'    | 2.03        | 0.59     |
| 18:Q:67:LYS:O    | 18:Q:68:ARG:HB3  | 2.01        | 0.59     |
| 1:A:731:G:O2'    | 1:A:732:C:H5'    | 2.03        | 0.59     |
| 8:G:116:ALA:HA   | 8:G:119:ARG:CZ   | 2.32        | 0.59     |
| 1:A:1392:G:H21   | 1:A:1502:A:H8    | 1.48        | 0.59     |
| 1:A:1369:C:H2'   | 1:A:1370:G:C8    | 2.38        | 0.59     |
| 16:O:41:GLU:OE2  | 16:O:41:GLU:HA   | 2.02        | 0.59     |
| 5:D:127:THR:HG23 | 5:D:128:VAL:N    | 2.18        | 0.59     |
| 1:A:427:U:OP1    | 5:D:13:ARG:NH2   | 2.35        | 0.59     |
| 18:Q:97:SER:HB2  | 18:Q:102:GLY:C   | 2.23        | 0.59     |
| 4:C:42:LEU:O     | 4:C:46:GLU:HG2   | 2.03        | 0.59     |
| 1:A:1283:G:O2'   | 1:A:1284:C:H5'   | 2.02        | 0.59     |
| 1:A:1226:C:N4    | 14:M:104:ARG:HD2 | 2.17        | 0.59     |
| 1:A:392:G:H2'    | 1:A:393:A:C8     | 2.37        | 0.59     |
| 9:H:83:ILE:O     | 9:H:83:ILE:HG23  | 2.03        | 0.59     |
| 5:D:3:ARG:HH22   | 5:D:74:GLN:CD    | 2.06        | 0.59     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:627:G:O2'    | 1:A:628:G:H5'    | 2.02        | 0.59     |
| 1:A:187:C:O2     | 21:T:105:SER:HB3 | 2.01        | 0.59     |
| 9:H:119:LEU:HD12 | 9:H:124:ALA:CA   | 2.23        | 0.59     |
| 1:A:1305:G:N2    | 1:A:1331:G:O2'   | 2.35        | 0.59     |
| 11:J:40:LEU:HD12 | 11:J:69:ASN:HB3  | 1.85        | 0.59     |
| 1:A:1236:A:H2'   | 1:A:1237:C:C6    | 2.38        | 0.59     |
| 3:B:230:VAL:HG13 | 3:B:231:GLU:OE2  | 2.02        | 0.59     |
| 8:G:38:LEU:O     | 8:G:38:LEU:HD12  | 2.03        | 0.59     |
| 16:O:3:ILE:HD12  | 16:O:3:ILE:N     | 2.18        | 0.59     |
| 1:A:1064:G:C4'   | 1:A:1065:U:H5'   | 2.33        | 0.59     |
| 10:I:125:TYR:CD1 | 10:I:128:ARG:HB2 | 2.38        | 0.59     |
| 5:D:32:ALA:C     | 5:D:34:GLU:N     | 2.54        | 0.59     |
| 1:A:1172:C:H2'   | 1:A:1173:G:H8    | 1.65        | 0.59     |
| 4:C:25:GLY:CA    | 4:C:29:TYR:HB2   | 2.21        | 0.58     |
| 11:J:8:LEU:HD23  | 11:J:96:ILE:HG12 | 1.83        | 0.58     |
| 3:B:124:SER:CB   | 3:B:125:PRO:HD2  | 2.32        | 0.58     |
| 1:A:371:G:C2'    | 1:A:372:C:H5'    | 2.33        | 0.58     |
| 10:I:49:PRO:O    | 10:I:52:ALA:HB3  | 2.02        | 0.58     |
| 1:A:266:G:C8     | 1:A:266:G:H5''   | 2.38        | 0.58     |
| 10:I:4:TYR:CD2   | 10:I:88:TYR:HA   | 2.38        | 0.58     |
| 12:K:48:ILE:HD13 | 12:K:63:LEU:CB   | 2.33        | 0.58     |
| 11:J:49:VAL:O    | 11:J:60:ARG:HA   | 2.04        | 0.58     |
| 3:B:97:TRP:HZ3   | 3:B:176:GLU:OE2  | 1.86        | 0.58     |
| 1:A:17:U:H2'     | 1:A:18:C:C6      | 2.38        | 0.58     |
| 14:M:102:ARG:HB2 | 14:M:102:ARG:NH1 | 2.17        | 0.58     |
| 12:K:95:ILE:O    | 12:K:99:GLN:HG3  | 2.03        | 0.58     |
| 18:Q:97:SER:OG   | 18:Q:98:LEU:N    | 2.35        | 0.58     |
| 4:C:64:VAL:HB    | 4:C:99:VAL:HG21  | 1.85        | 0.58     |
| 5:D:28:SER:O     | 5:D:30:LYS:N     | 2.36        | 0.58     |
| 3:B:124:SER:O    | 3:B:127:ILE:HG13 | 2.03        | 0.58     |
| 5:D:162:LEU:HD12 | 5:D:181:MET:CE   | 2.33        | 0.58     |
| 1:A:1238:A:C8    | 1:A:1303:C:H1'   | 2.39        | 0.58     |
| 17:P:6:LEU:HB3   | 17:P:17:TYR:CD2  | 2.38        | 0.58     |
| 1:A:1278:U:H5    | 11:J:99:LYS:NZ   | 2.01        | 0.58     |
| 11:J:38:ILE:HD12 | 11:J:71:LEU:HD12 | 1.85        | 0.58     |
| 1:A:977:A:H2'    | 1:A:978:A:H5''   | 1.84        | 0.58     |
| 1:A:37:U:O2'     | 1:A:38:G:H5'     | 2.03        | 0.58     |
| 1:A:911:U:H2'    | 1:A:912:C:C6     | 2.39        | 0.58     |
| 1:A:828:A:H2'    | 1:A:829:G:O4'    | 2.03        | 0.58     |
| 1:A:683:G:H2'    | 1:A:684:A:C8     | 2.38        | 0.58     |
| 3:B:114:ARG:NH1  | 3:B:118:LEU:HD21 | 2.17        | 0.58     |
| 11:J:46:ARG:NH1  | 11:J:64:GLU:HG2  | 2.18        | 0.58     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 4:C:155:GLY:O    | 4:C:196:LEU:HD22 | 2.03        | 0.58     |
| 3:B:12:GLU:OE2   | 3:B:213:LEU:HD11 | 2.04        | 0.58     |
| 1:A:1038:C:H2'   | 1:A:1039:C:C6    | 2.39        | 0.58     |
| 1:A:1343:G:H1'   | 10:I:121:ARG:NH1 | 2.18        | 0.58     |
| 7:F:33:TYR:HA    | 7:F:71:ARG:NH2   | 2.17        | 0.58     |
| 1:A:255:G:H2'    | 1:A:256:U:C6     | 2.39        | 0.58     |
| 1:A:1333:A:H2'   | 1:A:1334:G:O4'   | 2.03        | 0.58     |
| 1:A:178:C:O2'    | 1:A:179:A:H5'    | 2.03        | 0.58     |
| 18:Q:26:GLN:O    | 18:Q:27:PHE:HB3  | 2.03        | 0.58     |
| 4:C:177:THR:O    | 4:C:177:THR:HG23 | 2.03        | 0.58     |
| 17:P:19:ILE:HG22 | 17:P:36:ILE:HG13 | 1.86        | 0.58     |
| 10:I:48:GLU:N    | 10:I:49:PRO:HD2  | 2.18        | 0.58     |
| 1:A:761:G:C4'    | 18:Q:103:GLY:H   | 2.08        | 0.58     |
| 8:G:113:GLU:HG2  | 8:G:119:ARG:HG2  | 1.85        | 0.58     |
| 7:F:19:LEU:HD23  | 7:F:19:LEU:C     | 2.24        | 0.58     |
| 3:B:52:GLU:O     | 3:B:56:ARG:HB2   | 2.03        | 0.58     |
| 1:A:403:C:O2'    | 1:A:404:U:H5'    | 2.03        | 0.58     |
| 4:C:108:ASN:C    | 4:C:110:ASN:H    | 2.06        | 0.58     |
| 1:A:1113:C:H1'   | 4:C:178:LEU:HD21 | 1.86        | 0.58     |
| 3:B:16:HIS:NE2   | 3:B:214:ILE:CG1  | 2.67        | 0.58     |
| 1:A:1039:C:O2'   | 1:A:1040:U:H5'   | 2.03        | 0.58     |
| 13:L:27:LEU:C    | 13:L:29:GLY:H    | 2.07        | 0.58     |
| 3:B:88:ALA:C     | 3:B:90:MET:H     | 2.07        | 0.58     |
| 1:A:243:A:C5'    | 1:A:244:U:H5'    | 2.34        | 0.58     |
| 7:F:10:LEU:HD11  | 7:F:59:TYR:HD2   | 1.69        | 0.58     |
| 1:A:1262:C:H2'   | 1:A:1263:C:H6    | 1.68        | 0.58     |
| 4:C:60:ALA:O     | 4:C:61:ALA:HB3   | 2.03        | 0.58     |
| 7:F:94:GLN:HE21  | 19:R:32:ARG:HD3  | 1.68        | 0.58     |
| 1:A:1515:C:O2'   | 1:A:1516:G:H5'   | 2.04        | 0.58     |
| 5:D:8:VAL:O      | 5:D:10:ARG:N     | 2.37        | 0.58     |
| 6:E:105:VAL:HB   | 6:E:106:PRO:HD3  | 1.86        | 0.58     |
| 1:A:1239:A:H62   | 1:A:1299:A:H62   | 1.50        | 0.58     |
| 3:B:179:LYS:HA   | 9:H:72:PRO:HD3   | 1.85        | 0.58     |
| 17:P:20:VAL:HG22 | 17:P:21:VAL:O    | 2.03        | 0.57     |
| 9:H:101:PRO:HG3  | 9:H:133:LEU:HD11 | 1.85        | 0.57     |
| 1:A:1286:A:C8    | 1:A:1287:A:H5''  | 2.39        | 0.57     |
| 3:B:116:GLU:HG2  | 3:B:153:ARG:HH12 | 1.70        | 0.57     |
| 10:I:11:LYS:HG2  | 10:I:11:LYS:O    | 2.03        | 0.57     |
| 1:A:959:A:H3'    | 1:A:960:U:H5''   | 1.84        | 0.57     |
| 1:A:542:G:O2'    | 1:A:543:C:H5'    | 2.04        | 0.57     |
| 1:A:1347:G:O2'   | 1:A:1348:U:P     | 2.62        | 0.57     |
| 1:A:1026:G:H2'   | 1:A:1027:C:H5'   | 1.85        | 0.57     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 3:B:132:LYS:C    | 3:B:134:GLU:H     | 2.07        | 0.57     |
| 16:O:70:LEU:HD12 | 16:O:78:TYR:HB2   | 1.84        | 0.57     |
| 1:A:1310:G:O6    | 20:S:2:PRO:HB3    | 2.04        | 0.57     |
| 1:A:1101:A:H4'   | 1:A:1102:A:O5'    | 2.04        | 0.57     |
| 1:A:105:G:H2'    | 1:A:106:C:C6      | 2.39        | 0.57     |
| 8:G:69:VAL:HG21  | 8:G:104:LEU:HD21  | 1.86        | 0.57     |
| 1:A:5:U:H2'      | 1:A:5:U:O2        | 2.04        | 0.57     |
| 1:A:1153:C:H2'   | 1:A:1154:G:H8     | 1.69        | 0.57     |
| 7:F:4:TYR:OH     | 7:F:69:GLU:HB3    | 2.04        | 0.57     |
| 1:A:129(A):G:O2' | 1:A:130:A:OP2     | 2.23        | 0.57     |
| 13:L:46:LYS:HZ3  | 13:L:47:LYS:HG3   | 1.69        | 0.57     |
| 1:A:203:U:H5''   | 1:A:204:U:OP1     | 2.04        | 0.57     |
| 3:B:97:TRP:CZ2   | 3:B:101:MET:HB2   | 2.39        | 0.57     |
| 1:A:824:C:H2'    | 1:A:825:G:C8      | 2.38        | 0.57     |
| 1:A:376:G:H5''   | 17:P:5:ARG:HD2    | 1.86        | 0.57     |
| 1:A:930:C:O2'    | 1:A:931:C:H5'     | 2.04        | 0.57     |
| 22:V:24:ARG:O    | 22:V:25:LYS:HB2   | 2.05        | 0.57     |
| 4:C:195:VAL:C    | 4:C:196:LEU:HD23  | 2.24        | 0.57     |
| 5:D:142:PRO:HA   | 5:D:185:PHE:O     | 2.04        | 0.57     |
| 6:E:116:THR:HG23 | 6:E:117:ASP:OD2   | 2.03        | 0.57     |
| 5:D:152:SER:O    | 5:D:158:ILE:HD12  | 2.04        | 0.57     |
| 9:H:103:VAL:HG21 | 9:H:110:ALA:HB2   | 1.86        | 0.57     |
| 1:A:993:G:H4'    | 1:A:994:A:OP2     | 2.03        | 0.57     |
| 1:A:881:G:P      | 13:L:12:ARG:HH22  | 2.27        | 0.57     |
| 13:L:86:ARG:HB3  | 13:L:101:VAL:HG23 | 1.87        | 0.57     |
| 4:C:157:ILE:HD11 | 4:C:166:GLU:HB2   | 1.87        | 0.57     |
| 17:P:10:GLY:HA3  | 17:P:15:PRO:HA    | 1.86        | 0.57     |
| 3:B:221:LEU:O    | 3:B:221:LEU:HD13  | 2.05        | 0.57     |
| 3:B:19:HIS:NE2   | 3:B:206:ASP:HB3   | 2.20        | 0.57     |
| 1:A:1229:A:H2'   | 1:A:1230:C:H6     | 1.69        | 0.57     |
| 1:A:1117:G:H4'   | 10:I:104:ARG:HH12 | 1.66        | 0.57     |
| 1:A:736:C:H2'    | 1:A:737:A:C8      | 2.39        | 0.57     |
| 10:I:97:LYS:HG2  | 10:I:102:LEU:HD12 | 1.87        | 0.57     |
| 1:A:164:U:H2'    | 1:A:165:C:C6      | 2.39        | 0.57     |
| 1:A:1286:A:H3'   | 1:A:1287:A:C5'    | 2.32        | 0.57     |
| 20:S:63:THR:O    | 20:S:66:MET:HG2   | 2.05        | 0.57     |
| 3:B:213:LEU:HD23 | 3:B:213:LEU:C     | 2.26        | 0.57     |
| 3:B:132:LYS:HG2  | 3:B:135:GLN:OE1   | 2.05        | 0.57     |
| 1:A:448:A:O2'    | 1:A:449:C:H5'     | 2.05        | 0.57     |
| 14:M:94:ARG:HH12 | 20:S:81:ARG:HD3   | 1.70        | 0.57     |
| 12:K:84:VAL:HG23 | 12:K:110:ASP:HA   | 1.86        | 0.57     |
| 4:C:35:GLU:CG    | 4:C:95:THR:HG21   | 2.35        | 0.57     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 4:C:188:LEU:CD1  | 4:C:195:VAL:HG13 | 2.35        | 0.57     |
| 11:J:49:VAL:HG13 | 15:N:41:ARG:HB2  | 1.85        | 0.57     |
| 1:A:974:A:OP2    | 15:N:41:ARG:NH1  | 2.38        | 0.57     |
| 10:I:43:ALA:O    | 10:I:45:ALA:N    | 2.38        | 0.57     |
| 1:A:826:C:H2'    | 1:A:827:U:H6     | 1.70        | 0.57     |
| 16:O:36:ILE:HD11 | 16:O:60:VAL:HA   | 1.86        | 0.56     |
| 3:B:12:GLU:C     | 3:B:14:GLY:N     | 2.58        | 0.56     |
| 1:A:1182:G:O2'   | 1:A:1183:A:OP2   | 2.23        | 0.56     |
| 6:E:72:GLN:O     | 6:E:75:THR:HG22  | 2.05        | 0.56     |
| 1:A:188:C:H4'    | 21:T:89:ARG:NH1  | 2.19        | 0.56     |
| 7:F:22:GLU:OE2   | 7:F:84:ASN:HB2   | 2.04        | 0.56     |
| 4:C:83:ARG:C     | 4:C:85:ARG:H     | 2.07        | 0.56     |
| 17:P:6:LEU:HB3   | 17:P:17:TYR:HD2  | 1.70        | 0.56     |
| 22:V:6:ARG:HD2   | 22:V:15:ARG:NH1  | 2.19        | 0.56     |
| 1:A:780:A:O2'    | 1:A:781:A:H5''   | 2.04        | 0.56     |
| 22:V:7:ARG:O     | 22:V:7:ARG:HG3   | 2.05        | 0.56     |
| 1:A:1072:G:H2'   | 1:A:1073:U:C6    | 2.39        | 0.56     |
| 3:B:88:ALA:O     | 3:B:90:MET:N     | 2.37        | 0.56     |
| 6:E:41:VAL:HG13  | 6:E:113:ALA:HA   | 1.86        | 0.56     |
| 3:B:122:PHE:O    | 3:B:123:ALA:HB2  | 2.04        | 0.56     |
| 22:V:17:THR:O    | 22:V:22:ARG:HD3  | 2.05        | 0.56     |
| 1:A:1231:G:O3'   | 10:I:126:SER:HB3 | 2.05        | 0.56     |
| 1:A:112:G:H4'    | 1:A:389:A:H5''   | 1.87        | 0.56     |
| 5:D:112:VAL:HG23 | 5:D:161:ASN:HD21 | 1.68        | 0.56     |
| 6:E:80:ILE:CD1   | 6:E:91:LEU:HD12  | 2.35        | 0.56     |
| 1:A:1003(A):G:C2 | 1:A:1004:A:H1'   | 2.41        | 0.56     |
| 1:A:435:C:H2'    | 1:A:436:C:C6     | 2.36        | 0.56     |
| 3:B:101:MET:HA   | 3:B:108:ILE:HD12 | 1.88        | 0.56     |
| 3:B:73:THR:HG23  | 3:B:95:GLN:O     | 2.05        | 0.56     |
| 1:A:393:A:HO2'   | 1:A:394:G:H5'    | 1.68        | 0.56     |
| 1:A:149:A:H2'    | 1:A:150:C:H6     | 1.70        | 0.56     |
| 15:N:21:TYR:HE2  | 15:N:23:ARG:NE   | 2.03        | 0.56     |
| 20:S:41:VAL:HG23 | 20:S:43:GLU:HG2  | 1.86        | 0.56     |
| 17:P:81:ARG:CG   | 17:P:83:GLU:HG2  | 2.34        | 0.56     |
| 1:A:1117:G:H21   | 1:A:1180:A:H1'   | 1.71        | 0.56     |
| 3:B:130:ARG:HH22 | 4:C:207:VAL:CG2  | 2.17        | 0.56     |
| 14:M:81:LEU:HD22 | 14:M:81:LEU:N    | 2.20        | 0.56     |
| 1:A:477:G:H2'    | 1:A:478:A:C8     | 2.39        | 0.56     |
| 8:G:145:ALA:C    | 8:G:147:ALA:H    | 2.08        | 0.56     |
| 1:A:1245:A:H2'   | 1:A:1246:C:C6    | 2.40        | 0.56     |
| 20:S:5:LEU:O     | 20:S:6:LYS:CB    | 2.52        | 0.56     |
| 9:H:120:THR:H    | 9:H:123:GLU:HB2  | 1.71        | 0.56     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 9:H:123:GLU:O    | 9:H:127:LEU:HD23 | 2.05        | 0.56     |
| 4:C:154:SER:OG   | 4:C:155:GLY:N    | 2.39        | 0.56     |
| 1:A:1141:C:H2'   | 1:A:1142:G:C8    | 2.40        | 0.56     |
| 3:B:111:ARG:HB3  | 3:B:149:LEU:HD11 | 1.88        | 0.56     |
| 15:N:59:ALA:O    | 15:N:60:SER:HB2  | 2.04        | 0.56     |
| 4:C:177:THR:CG2  | 4:C:180:ALA:HB2  | 2.36        | 0.56     |
| 1:A:838:G:C2'    | 1:A:839:U:H5''   | 2.34        | 0.56     |
| 13:L:50:SER:O    | 13:L:51:ALA:HB2  | 2.05        | 0.56     |
| 1:A:1263:C:H2'   | 1:A:1264:C:C6    | 2.40        | 0.56     |
| 1:A:765:G:H22    | 1:A:812:C:HO2'   | 1.53        | 0.56     |
| 10:I:93:ARG:HD3  | 10:I:97:LYS:HE3  | 1.88        | 0.56     |
| 4:C:137:ALA:O    | 4:C:141:VAL:HG23 | 2.06        | 0.56     |
| 13:L:25:PRO:C    | 13:L:27:LEU:N    | 2.58        | 0.56     |
| 12:K:48:ILE:HD13 | 12:K:63:LEU:HB3  | 1.86        | 0.56     |
| 20:S:15:LEU:O    | 20:S:19:VAL:N    | 2.38        | 0.56     |
| 20:S:20:LEU:HA   | 20:S:23:ASN:ND2  | 2.20        | 0.56     |
| 18:Q:53:LEU:C    | 18:Q:53:LEU:HD12 | 2.26        | 0.56     |
| 1:A:882:C:O2'    | 1:A:883:C:H5'    | 2.05        | 0.56     |
| 8:G:26:PHE:CE2   | 8:G:30:ILE:HD11  | 2.41        | 0.56     |
| 6:E:150:ARG:HH11 | 6:E:150:ARG:HG3  | 1.71        | 0.56     |
| 9:H:118:VAL:C    | 9:H:119:LEU:HD23 | 2.26        | 0.56     |
| 1:A:112:G:N2     | 1:A:354:G:H5'    | 2.21        | 0.56     |
| 1:A:390:C:H2'    | 1:A:391:G:C8     | 2.41        | 0.56     |
| 5:D:43:HIS:CE1   | 5:D:46:LYS:HZ2   | 2.22        | 0.56     |
| 1:A:151:A:H2'    | 1:A:152:A:O4'    | 2.06        | 0.56     |
| 1:A:818:G:C3'    | 1:A:819:A:H5''   | 2.35        | 0.56     |
| 21:T:43:LEU:HD13 | 21:T:51:GLU:HG3  | 1.88        | 0.56     |
| 13:L:60:LEU:CD2  | 13:L:66:VAL:HG22 | 2.36        | 0.56     |
| 1:A:1257:U:H4'   | 1:A:1258:G:O5'   | 2.06        | 0.56     |
| 19:R:48:GLY:O    | 19:R:74:ARG:NH2  | 2.37        | 0.56     |
| 18:Q:80:GLY:O    | 18:Q:81:ARG:HB3  | 2.06        | 0.56     |
| 1:A:883:C:O2'    | 1:A:884:U:H5'    | 2.06        | 0.56     |
| 8:G:21:VAL:HG23  | 8:G:22:LEU:N     | 2.20        | 0.56     |
| 1:A:193:C:H2'    | 1:A:194:C:C6     | 2.41        | 0.56     |
| 17:P:4:ILE:HG13  | 17:P:64:ALA:HB1  | 1.88        | 0.56     |
| 1:A:353:A:H5'    | 1:A:353:A:C8     | 2.41        | 0.56     |
| 1:A:1268:A:H2'   | 1:A:1269:A:C8    | 2.41        | 0.56     |
| 5:D:107:ARG:HD2  | 5:D:173:TRP:CZ2  | 2.41        | 0.56     |
| 11:J:96:ILE:HG22 | 11:J:97:GLU:H    | 1.69        | 0.56     |
| 19:R:22:VAL:HG23 | 19:R:55:ARG:O    | 2.05        | 0.56     |
| 1:A:407:G:H2'    | 1:A:408:A:H8     | 1.71        | 0.56     |
| 6:E:11:ILE:HB    | 6:E:31:LEU:HB3   | 1.88        | 0.56     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 13:L:126:LYS:N   | 13:L:126:LYS:CD  | 2.69        | 0.56     |
| 1:A:877:C:O2'    | 1:A:878:G:H5'    | 2.05        | 0.56     |
| 1:A:1316:G:N2    | 1:A:1318:A:H3'   | 2.21        | 0.56     |
| 19:R:33:ASP:OD2  | 19:R:36:ASN:HB2  | 2.06        | 0.55     |
| 1:A:1347:G:H3'   | 10:I:108:VAL:O   | 2.06        | 0.55     |
| 3:B:15:VAL:CG2   | 3:B:209:ARG:HG3  | 2.35        | 0.55     |
| 1:A:743:U:H2'    | 1:A:744:C:C6     | 2.42        | 0.55     |
| 16:O:53:HIS:O    | 16:O:56:LEU:HB3  | 2.06        | 0.55     |
| 1:A:1287:A:H2'   | 1:A:1288:A:C8    | 2.41        | 0.55     |
| 1:A:755:G:OP2    | 16:O:65:ARG:HD2  | 2.06        | 0.55     |
| 19:R:86:VAL:O    | 19:R:87:ARG:CB   | 2.53        | 0.55     |
| 1:A:969:A:H61    | 14:M:124:PRO:HB3 | 1.70        | 0.55     |
| 9:H:19:VAL:CG2   | 9:H:21:LYS:HD3   | 2.32        | 0.55     |
| 4:C:130:VAL:O    | 4:C:134:ILE:HG13 | 2.06        | 0.55     |
| 1:A:187:C:C2     | 21:T:105:SER:HB3 | 2.41        | 0.55     |
| 3:B:223:ILE:HG21 | 3:B:230:VAL:CG2  | 2.37        | 0.55     |
| 1:A:358:U:H2'    | 1:A:359:U:C6     | 2.42        | 0.55     |
| 10:I:53:VAL:O    | 10:I:54:ASP:HB2  | 2.06        | 0.55     |
| 18:Q:97:SER:HB2  | 18:Q:103:GLY:CA  | 2.36        | 0.55     |
| 7:F:8:ILE:CD1    | 7:F:79:LEU:HD13  | 2.29        | 0.55     |
| 19:R:53:ARG:HE   | 19:R:59:SER:C    | 2.10        | 0.55     |
| 1:A:1003:G:N2    | 1:A:1039:C:C2    | 2.75        | 0.55     |
| 5:D:19:LEU:HD22  | 5:D:67:ILE:HG12  | 1.88        | 0.55     |
| 1:A:501:C:H2'    | 1:A:502:G:C8     | 2.37        | 0.55     |
| 9:H:7:ALA:HB2    | 9:H:85:ARG:HD2   | 1.88        | 0.55     |
| 1:A:513:C:H2'    | 1:A:514:C:C6     | 2.42        | 0.55     |
| 1:A:357:G:O2'    | 1:A:358:U:H5'    | 2.07        | 0.55     |
| 5:D:111:ALA:HB3  | 5:D:117:ALA:HB2  | 1.88        | 0.55     |
| 15:N:24:CYS:HB3  | 15:N:28:GLY:H    | 1.71        | 0.55     |
| 3:B:188:ALA:O    | 3:B:202:PRO:HA   | 2.06        | 0.55     |
| 11:J:46:ARG:HH11 | 11:J:64:GLU:HB3  | 1.71        | 0.55     |
| 3:B:17:PHE:H     | 3:B:44:LEU:HD21  | 1.71        | 0.55     |
| 1:A:1427:U:H2'   | 1:A:1428:A:C8    | 2.41        | 0.55     |
| 1:A:730:G:N2     | 1:A:765:G:H5''   | 2.22        | 0.55     |
| 1:A:268:C:H2'    | 1:A:269:C:H6     | 1.71        | 0.55     |
| 6:E:102:ALA:HB1  | 6:E:120:THR:HG21 | 1.88        | 0.55     |
| 10:I:65:VAL:CG2  | 10:I:73:GLN:HB3  | 2.35        | 0.55     |
| 1:A:1091:U:O2    | 1:A:1093:A:C8    | 2.60        | 0.55     |
| 5:D:131:ARG:H    | 5:D:131:ARG:HD2  | 1.71        | 0.55     |
| 11:J:51:ARG:H    | 11:J:59:SER:CB   | 2.20        | 0.55     |
| 3:B:15:VAL:HG11  | 3:B:210:SER:N    | 2.21        | 0.55     |
| 1:A:382:A:C2     | 1:A:383:A:C4     | 2.94        | 0.55     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 10:I:10:ARG:HG2  | 10:I:75:ASP:CB    | 2.35        | 0.55     |
| 4:C:191:THR:HG21 | 4:C:193:TYR:CZ    | 2.42        | 0.55     |
| 4:C:38:ARG:NH1   | 4:C:38:ARG:HG3    | 2.22        | 0.55     |
| 16:O:71:GLN:HB2  | 16:O:78:TYR:CD1   | 2.41        | 0.55     |
| 1:A:1130:A:OP2   | 1:A:1130:A:H3'    | 2.07        | 0.55     |
| 1:A:1000:U:H2'   | 1:A:1001:A:C8     | 2.41        | 0.55     |
| 3:B:160:ASP:O    | 3:B:183:PRO:HD2   | 2.06        | 0.55     |
| 8:G:133:GLY:O    | 8:G:137:LYS:HG3   | 2.07        | 0.55     |
| 3:B:77:ALA:CB    | 3:B:211:ILE:HD13  | 2.10        | 0.55     |
| 13:L:70:ILE:CD1  | 13:L:77:LEU:HD12  | 2.36        | 0.55     |
| 1:A:1154:G:O2'   | 1:A:1155:G:H5'    | 2.07        | 0.55     |
| 4:C:76:VAL:HG11  | 4:C:103:VAL:HG21  | 1.89        | 0.55     |
| 20:S:67:VAL:O    | 20:S:69:HIS:N     | 2.40        | 0.55     |
| 14:M:3:ARG:HG2   | 14:M:9:ILE:HG23   | 1.89        | 0.55     |
| 7:F:76:ALA:O     | 7:F:80:ARG:HG3    | 2.06        | 0.55     |
| 1:A:101:A:O2'    | 1:A:102:G:H5'     | 2.06        | 0.55     |
| 11:J:27:ALA:HB2  | 11:J:85:LEU:HD21  | 1.89        | 0.55     |
| 1:A:532:A:H2'    | 1:A:533:A:H5'     | 1.87        | 0.55     |
| 4:C:116:VAL:HG21 | 4:C:202:ILE:HD11  | 1.87        | 0.55     |
| 5:D:25:ARG:C     | 5:D:27:TYR:N      | 2.60        | 0.55     |
| 1:A:954:G:H5''   | 14:M:120:LYS:HD3  | 1.88        | 0.55     |
| 16:O:29:VAL:HG12 | 16:O:85:LEU:HD11  | 1.88        | 0.55     |
| 3:B:101:MET:CA   | 3:B:108:ILE:HD12  | 2.37        | 0.55     |
| 7:F:36:ARG:NH1   | 7:F:36:ARG:HG2    | 2.21        | 0.55     |
| 10:I:97:LYS:CG   | 10:I:102:LEU:HD12 | 2.36        | 0.55     |
| 22:V:7:ARG:HA    | 22:V:12:LYS:HE2   | 1.89        | 0.55     |
| 1:A:546:G:OP1    | 5:D:73:ARG:HB2    | 2.07        | 0.55     |
| 19:R:73:ALA:CB   | 19:R:79:LEU:HD12  | 2.37        | 0.55     |
| 1:A:748:C:H1'    | 1:A:749:C:H5      | 1.72        | 0.55     |
| 1:A:659:U:O2'    | 1:A:660:G:H5'     | 2.07        | 0.55     |
| 5:D:17:VAL:HG12  | 5:D:18:LYS:N      | 2.22        | 0.55     |
| 15:N:59:ALA:HB1  | 15:N:61:TRP:CZ3   | 2.42        | 0.55     |
| 3:B:209:ARG:HE   | 3:B:239:VAL:HG11  | 1.71        | 0.55     |
| 12:K:14:VAL:O    | 12:K:15:ALA:HB3   | 2.06        | 0.55     |
| 4:C:83:ARG:C     | 4:C:85:ARG:N      | 2.59        | 0.55     |
| 16:O:28:GLN:OE1  | 16:O:66:LEU:HD11  | 2.07        | 0.55     |
| 1:A:162:A:H8     | 1:A:162:A:O5'     | 1.90        | 0.55     |
| 6:E:83:GLU:HG3   | 6:E:88:LYS:HG3    | 1.88        | 0.55     |
| 6:E:152:ARG:NH2  | 9:H:107:LEU:O     | 2.39        | 0.55     |
| 20:S:7:LYS:HG3   | 20:S:7:LYS:O      | 2.07        | 0.55     |
| 5:D:36:ARG:N     | 5:D:37:PRO:CD     | 2.58        | 0.55     |
| 3:B:178:ARG:NH1  | 9:H:71:GLY:O      | 2.40        | 0.55     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:972:C:O5'    | 11:J:57:LYS:HD3   | 2.07        | 0.55     |
| 13:L:55:VAL:CG1  | 13:L:67:THR:HG23  | 2.36        | 0.55     |
| 8:G:108:ALA:O    | 8:G:119:ARG:HD2   | 2.06        | 0.55     |
| 1:A:192:U:H1'    | 21:T:103:GLY:HA2  | 1.88        | 0.55     |
| 1:A:1381:U:O2'   | 1:A:1382:C:H5'    | 2.07        | 0.55     |
| 11:J:45:ARG:NH1  | 11:J:45:ARG:CB    | 2.63        | 0.54     |
| 1:A:1060:C:O2'   | 1:A:1061:G:H5'    | 2.07        | 0.54     |
| 19:R:26:LEU:HD11 | 19:R:39:VAL:HG23  | 1.89        | 0.54     |
| 13:L:126:LYS:H   | 13:L:126:LYS:CD   | 2.20        | 0.54     |
| 1:A:972:C:OP1    | 11:J:57:LYS:NZ    | 2.37        | 0.54     |
| 6:E:15:ARG:HD3   | 6:E:26:PHE:CD2    | 2.41        | 0.54     |
| 10:I:93:ARG:NH1  | 10:I:97:LYS:NZ    | 2.54        | 0.54     |
| 1:A:204:U:H4'    | 1:A:216:G:O5'     | 2.05        | 0.54     |
| 20:S:43:GLU:CD   | 20:S:43:GLU:H     | 2.09        | 0.54     |
| 6:E:84:PHE:CE2   | 6:E:133:TYR:HD1   | 2.25        | 0.54     |
| 8:G:53:LYS:O     | 8:G:54:THR:HG23   | 2.07        | 0.54     |
| 15:N:9:LYS:HD3   | 15:N:9:LYS:C      | 2.28        | 0.54     |
| 5:D:16:GLY:O     | 5:D:33:MET:CE     | 2.56        | 0.54     |
| 11:J:96:ILE:HG22 | 11:J:97:GLU:N     | 2.22        | 0.54     |
| 11:J:23:ILE:N    | 11:J:23:ILE:HD12  | 2.22        | 0.54     |
| 16:O:17:ARG:NH1  | 16:O:77:ARG:HH11  | 2.05        | 0.54     |
| 1:A:921:U:O2     | 6:E:19:MET:HB2    | 2.07        | 0.54     |
| 1:A:1454:G:O2'   | 1:A:1455:G:H5'    | 2.06        | 0.54     |
| 5:D:145:GLU:HG3  | 5:D:184:LYS:HE2   | 1.88        | 0.54     |
| 6:E:87:SER:HB3   | 6:E:131:ILE:HD13  | 1.89        | 0.54     |
| 4:C:29:TYR:CZ    | 15:N:54:PRO:HG2   | 2.42        | 0.54     |
| 16:O:60:VAL:O    | 16:O:64:ARG:HG2   | 2.07        | 0.54     |
| 5:D:173:TRP:CD2  | 5:D:189:PRO:HB3   | 2.42        | 0.54     |
| 11:J:36:GLY:O    | 11:J:72:VAL:HA    | 2.07        | 0.54     |
| 20:S:40:ILE:HG21 | 20:S:62:ILE:CD1   | 2.38        | 0.54     |
| 1:A:706:A:C1'    | 12:K:29:ILE:HD11  | 2.37        | 0.54     |
| 1:A:1202:G:H2'   | 1:A:1203:C:H5'    | 1.90        | 0.54     |
| 1:A:911:U:H2'    | 1:A:912:C:H6      | 1.72        | 0.54     |
| 1:A:794:A:H2'    | 1:A:795:C:C6      | 2.42        | 0.54     |
| 1:A:694:A:H5'    | 12:K:53:SER:HB2   | 1.89        | 0.54     |
| 4:C:188:LEU:O    | 4:C:189:ALA:HB2   | 2.07        | 0.54     |
| 4:C:147:LYS:HE2  | 4:C:205:GLY:HA2   | 1.89        | 0.54     |
| 7:F:4:TYR:CZ     | 7:F:72:VAL:HG21   | 2.43        | 0.54     |
| 21:T:50:GLU:HG2  | 21:T:100:ILE:HG13 | 1.89        | 0.54     |
| 1:A:542:G:OP1    | 5:D:10:ARG:NH2    | 2.40        | 0.54     |
| 11:J:81:THR:C    | 11:J:83:GLU:H     | 2.11        | 0.54     |
| 18:Q:15:MET:CE   | 18:Q:43:LEU:HD22  | 2.37        | 0.54     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 16:O:87:ILE:CG2  | 16:O:88:ARG:N    | 2.70        | 0.54     |
| 6:E:101:ILE:O    | 6:E:120:THR:HB   | 2.07        | 0.54     |
| 1:A:965:A:C2     | 14:M:124:PRO:HB2 | 2.42        | 0.54     |
| 1:A:983:A:H5'    | 1:A:984:C:OP2    | 2.06        | 0.54     |
| 16:O:39:LEU:HD22 | 16:O:56:LEU:HB2  | 1.89        | 0.54     |
| 3:B:74:LYS:HZ3   | 3:B:76:GLN:HB2   | 1.71        | 0.54     |
| 4:C:191:THR:HG22 | 4:C:193:TYR:H    | 1.73        | 0.54     |
| 16:O:26:GLU:HA   | 16:O:81:LEU:CD1  | 2.37        | 0.54     |
| 14:M:8:GLU:HG3   | 14:M:22:ILE:HG23 | 1.88        | 0.54     |
| 6:E:15:ARG:O     | 6:E:16:THR:O     | 2.25        | 0.54     |
| 8:G:37:ASN:ND2   | 10:I:41:VAL:HG23 | 2.22        | 0.54     |
| 11:J:44:VAL:HG22 | 11:J:66:ARG:HB3  | 1.88        | 0.54     |
| 8:G:15:ASP:OD1   | 8:G:17:VAL:HB    | 2.07        | 0.54     |
| 1:A:1308:U:H2'   | 1:A:1309:G:C8    | 2.42        | 0.54     |
| 1:A:443:C:O2'    | 1:A:444:C:H5'    | 2.07        | 0.54     |
| 1:A:189:G:H2'    | 1:A:190:C:C6     | 2.43        | 0.54     |
| 15:N:3:ARG:NH2   | 15:N:6:LEU:HG    | 2.22        | 0.54     |
| 4:C:48:TYR:HA    | 4:C:52:LEU:HD22  | 1.90        | 0.54     |
| 14:M:6:GLY:O     | 14:M:7:VAL:HG22  | 2.08        | 0.54     |
| 10:I:111:ARG:NH1 | 10:I:111:ARG:HG3 | 2.22        | 0.54     |
| 19:R:73:ALA:HB3  | 19:R:79:LEU:HD12 | 1.89        | 0.54     |
| 18:Q:34:LYS:HD3  | 18:Q:35:VAL:O    | 2.08        | 0.54     |
| 18:Q:66:SER:O    | 18:Q:70:ARG:NH1  | 2.40        | 0.54     |
| 13:L:75:HIS:HD2  | 13:L:77:LEU:N    | 1.97        | 0.54     |
| 1:A:974:A:H8     | 1:A:974:A:OP1    | 1.91        | 0.54     |
| 1:A:1425:U:H3    | 1:A:1475:G:H1    | 1.54        | 0.54     |
| 9:H:103:VAL:HB   | 9:H:108:GLY:O    | 2.08        | 0.54     |
| 3:B:144:ARG:HG3  | 3:B:145:LEU:H    | 1.72        | 0.54     |
| 11:J:84:GLN:O    | 11:J:88:LEU:HD12 | 2.08        | 0.54     |
| 14:M:81:LEU:HA   | 14:M:84:ILE:HG12 | 1.89        | 0.54     |
| 18:Q:68:ARG:O    | 18:Q:69:LYS:HB2  | 2.06        | 0.54     |
| 11:J:3:LYS:N     | 11:J:75:ILE:HA   | 2.23        | 0.54     |
| 15:N:9:LYS:HD3   | 15:N:9:LYS:O     | 2.07        | 0.54     |
| 17:P:74:LEU:O    | 17:P:79:VAL:HG23 | 2.07        | 0.54     |
| 1:A:865:A:H5'    | 1:A:1078:U:O4    | 2.07        | 0.54     |
| 3:B:74:LYS:HZ1   | 3:B:206:ASP:HA   | 1.68        | 0.54     |
| 15:N:41:ARG:HG3  | 15:N:42:ILE:N    | 2.22        | 0.54     |
| 14:M:16:ASP:HB3  | 14:M:41:PRO:HB3  | 1.88        | 0.54     |
| 1:A:1014:A:H2'   | 1:A:1015:A:C8    | 2.43        | 0.54     |
| 1:A:106:C:O2     | 1:A:379:C:H4'    | 2.07        | 0.54     |
| 9:H:56:LYS:N     | 9:H:56:LYS:HD2   | 2.22        | 0.54     |
| 3:B:92:TYR:CD1   | 3:B:151:GLY:HA3  | 2.43        | 0.54     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 10:I:108:VAL:CG1 | 10:I:109:VAL:N   | 2.70        | 0.54     |
| 6:E:112:LEU:N    | 6:E:112:LEU:HD23 | 2.22        | 0.54     |
| 8:G:83:ALA:HB3   | 8:G:85:TYR:CE2   | 2.42        | 0.54     |
| 16:O:78:TYR:CZ   | 16:O:82:ILE:HD11 | 2.42        | 0.54     |
| 1:A:818:G:C2'    | 1:A:819:A:H5''   | 2.37        | 0.54     |
| 1:A:807:A:H2'    | 1:A:808:C:C6     | 2.42        | 0.54     |
| 18:Q:60:ILE:HD13 | 18:Q:61:GLU:N    | 2.23        | 0.54     |
| 11:J:45:ARG:O    | 11:J:64:GLU:HA   | 2.08        | 0.54     |
| 16:O:39:LEU:HD13 | 16:O:59:MET:CE   | 2.38        | 0.54     |
| 4:C:32:LEU:HD21  | 4:C:59:ARG:HD2   | 1.90        | 0.54     |
| 11:J:16:LEU:HD13 | 11:J:70:ARG:HG2  | 1.88        | 0.54     |
| 1:A:336:C:O2'    | 1:A:337:C:H5'    | 2.07        | 0.54     |
| 3:B:134:GLU:C    | 3:B:136:VAL:H    | 2.11        | 0.54     |
| 9:H:23:SER:OG    | 9:H:60:ARG:HD2   | 2.08        | 0.54     |
| 18:Q:76:LEU:HD23 | 18:Q:76:LEU:C    | 2.28        | 0.54     |
| 9:H:18:ARG:N     | 9:H:18:ARG:HD2   | 2.23        | 0.54     |
| 1:A:187:C:N3     | 21:T:105:SER:HB3 | 2.23        | 0.54     |
| 1:A:1524:C:OP1   | 12:K:120:ARG:NH1 | 2.41        | 0.54     |
| 5:D:187:ARG:NH2  | 5:D:188:LEU:HG   | 2.12        | 0.53     |
| 19:R:55:ARG:HH11 | 19:R:55:ARG:CB   | 2.21        | 0.53     |
| 1:A:1521:G:H2'   | 1:A:1522:U:H6    | 1.73        | 0.53     |
| 1:A:1004:A:H5''  | 1:A:1025:U:O4    | 2.08        | 0.53     |
| 12:K:15:ALA:HA   | 12:K:77:MET:HA   | 1.88        | 0.53     |
| 1:A:148:G:H2'    | 1:A:149:A:C8     | 2.43        | 0.53     |
| 1:A:1417:G:H2'   | 1:A:1482:G:H22   | 1.72        | 0.53     |
| 1:A:613:C:O2'    | 1:A:614:A:H5'    | 2.08        | 0.53     |
| 20:S:5:LEU:O     | 20:S:6:LYS:HB2   | 2.08        | 0.53     |
| 1:A:1232:U:H5''  | 10:I:124:GLN:O   | 2.08        | 0.53     |
| 3:B:228:GLY:O    | 3:B:229:VAL:C    | 2.47        | 0.53     |
| 1:A:1441:G:H4'   | 1:A:1442:G:C5    | 2.44        | 0.53     |
| 13:L:43:VAL:HG12 | 13:L:44:THR:N    | 2.23        | 0.53     |
| 9:H:17:THR:HB    | 9:H:78:GLN:OE1   | 2.08        | 0.53     |
| 5:D:39:PRO:HG2   | 5:D:44:GLY:HA2   | 1.90        | 0.53     |
| 3:B:19:HIS:CE1   | 3:B:206:ASP:HB3  | 2.43        | 0.53     |
| 11:J:24:VAL:HG12 | 11:J:28:ARG:HE   | 1.73        | 0.53     |
| 6:E:89:ILE:HD13  | 6:E:90:VAL:N     | 2.23        | 0.53     |
| 11:J:30:SER:OG   | 11:J:81:THR:HA   | 2.07        | 0.53     |
| 4:C:152:ILE:HB   | 4:C:199:LYS:HB2  | 1.90        | 0.53     |
| 8:G:122:HIS:HA   | 8:G:125:MET:HE3  | 1.89        | 0.53     |
| 21:T:10:LEU:O    | 21:T:12:ALA:N    | 2.40        | 0.53     |
| 5:D:107:ARG:HD2  | 5:D:173:TRP:HZ2  | 1.72        | 0.53     |
| 4:C:191:THR:HG22 | 4:C:192:THR:H    | 1.71        | 0.53     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 3:B:144:ARG:HG3  | 3:B:145:LEU:N     | 2.22        | 0.53     |
| 13:L:48:PRO:HG2  | 13:L:49:ASN:H     | 1.73        | 0.53     |
| 1:A:812:C:O2'    | 1:A:813:U:P       | 2.66        | 0.53     |
| 1:A:1102:A:H2'   | 1:A:1103:C:C6     | 2.43        | 0.53     |
| 4:C:145:GLY:O    | 4:C:146:ALA:O     | 2.26        | 0.53     |
| 1:A:505:G:H2'    | 1:A:506:G:C8      | 2.43        | 0.53     |
| 18:Q:29:HIS:CE1  | 18:Q:31:LEU:H     | 2.27        | 0.53     |
| 11:J:47:PHE:CE2  | 15:N:37:PHE:HE1   | 2.26        | 0.53     |
| 1:A:913:A:H1'    | 1:A:914:A:O4'     | 2.09        | 0.53     |
| 1:A:200:G:H2'    | 1:A:201:C:O4'     | 2.08        | 0.53     |
| 1:A:959:A:C2     | 1:A:1222:G:O4'    | 2.62        | 0.53     |
| 4:C:180:ALA:HB1  | 4:C:203:PHE:CE1   | 2.43        | 0.53     |
| 3:B:162:ILE:O    | 3:B:185:ILE:HD12  | 2.09        | 0.53     |
| 3:B:97:TRP:CZ3   | 3:B:176:GLU:OE2   | 2.61        | 0.53     |
| 6:E:102:ALA:CB   | 6:E:120:THR:HG21  | 2.38        | 0.53     |
| 1:A:556:C:O2'    | 1:A:557:G:H5'     | 2.08        | 0.53     |
| 16:O:39:LEU:CD2  | 16:O:56:LEU:HB2   | 2.38        | 0.53     |
| 1:A:954:G:C5'    | 14:M:120:LYS:HD3  | 2.39        | 0.53     |
| 4:C:106:VAL:HG11 | 4:C:115:LEU:CD1   | 2.38        | 0.53     |
| 16:O:30:ALA:HA   | 16:O:85:LEU:HD21  | 1.90        | 0.53     |
| 17:P:20:VAL:HG23 | 17:P:34:GLU:C     | 2.29        | 0.53     |
| 21:T:57:ARG:HH21 | 21:T:100:ILE:HG23 | 1.72        | 0.53     |
| 3:B:25:ASN:HD22  | 3:B:27:LYS:H      | 1.56        | 0.53     |
| 1:A:490:G:H2'    | 1:A:491:G:H8      | 1.74        | 0.53     |
| 6:E:120:THR:CG2  | 6:E:121:LYS:N     | 2.72        | 0.53     |
| 5:D:127:THR:CG2  | 5:D:128:VAL:N     | 2.71        | 0.53     |
| 1:A:826:C:H2'    | 1:A:827:U:C6      | 2.44        | 0.53     |
| 19:R:27:GLY:O    | 19:R:29:PHE:HD2   | 1.90        | 0.53     |
| 1:A:986:A:H1'    | 20:S:54:GLY:O     | 2.09        | 0.53     |
| 3:B:162:ILE:C    | 3:B:185:ILE:HD12  | 2.29        | 0.53     |
| 3:B:69:LEU:HD22  | 3:B:71:VAL:HG22   | 1.90        | 0.53     |
| 15:N:8:GLU:O     | 15:N:11:LYS:HB2   | 2.09        | 0.53     |
| 14:M:81:LEU:O    | 14:M:89:GLY:HA3   | 2.08        | 0.53     |
| 1:A:614:A:H2'    | 1:A:615:C:H6      | 1.74        | 0.53     |
| 3:B:53:ARG:NH1   | 3:B:199:TYR:HD2   | 2.06        | 0.53     |
| 1:A:260:G:H2'    | 1:A:261:U:C6      | 2.44        | 0.53     |
| 5:D:64:LEU:HG    | 5:D:198:VAL:HG11  | 1.91        | 0.53     |
| 1:A:392:G:H2'    | 1:A:393:A:H8      | 1.72        | 0.53     |
| 9:H:23:SER:O     | 9:H:24:THR:HB     | 2.09        | 0.53     |
| 1:A:229:U:H5''   | 17:P:33:ILE:HD13  | 1.89        | 0.53     |
| 3:B:137:ARG:HB3  | 3:B:137:ARG:NH1   | 2.24        | 0.53     |
| 16:O:81:LEU:O    | 16:O:81:LEU:HD23  | 2.08        | 0.53     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 8:G:12:LEU:N     | 8:G:12:LEU:HD12   | 2.24        | 0.53     |
| 17:P:81:ARG:HB2  | 17:P:81:ARG:NH1   | 2.23        | 0.53     |
| 1:A:818:G:O2'    | 1:A:819:A:H5''    | 2.08        | 0.53     |
| 1:A:797:C:O2'    | 1:A:798:G:H5'     | 2.09        | 0.53     |
| 4:C:35:GLU:CD    | 4:C:95:THR:HG21   | 2.29        | 0.53     |
| 20:S:51:VAL:O    | 20:S:57:HIS:HA    | 2.09        | 0.53     |
| 3:B:187:LEU:HD13 | 3:B:187:LEU:O     | 2.09        | 0.53     |
| 4:C:172:ARG:HH12 | 4:C:174:PRO:HG3   | 1.73        | 0.53     |
| 15:N:14:PRO:HB2  | 15:N:16:PHE:O     | 2.09        | 0.53     |
| 1:A:255:G:H2'    | 1:A:256:U:H6      | 1.72        | 0.53     |
| 18:Q:18:THR:HG23 | 18:Q:69:LYS:HE2   | 1.91        | 0.53     |
| 1:A:476:G:O2'    | 1:A:477:G:H5'     | 2.09        | 0.53     |
| 1:A:268:C:H2'    | 1:A:269:C:C6      | 2.43        | 0.53     |
| 1:A:258:G:O2'    | 1:A:259:G:H5'     | 2.09        | 0.53     |
| 1:A:1070:U:H2'   | 1:A:1071:C:H6     | 1.72        | 0.53     |
| 4:C:37:GLN:NE2   | 15:N:52:GLN:OE1   | 2.39        | 0.53     |
| 13:L:85:ILE:HG23 | 13:L:98:TYR:HB2   | 1.91        | 0.53     |
| 1:A:1288:A:H1'   | 1:A:1352:C:O2'    | 2.08        | 0.53     |
| 15:N:12:ARG:O    | 15:N:14:PRO:N     | 2.42        | 0.53     |
| 13:L:45:PRO:HB2  | 13:L:49:ASN:O     | 2.09        | 0.53     |
| 1:A:650:G:C2'    | 1:A:651:C:H5'     | 2.39        | 0.53     |
| 10:I:105:ASP:OD1 | 10:I:107:ARG:HG3  | 2.09        | 0.53     |
| 1:A:1044:A:H2'   | 1:A:1045:C:C4'    | 2.39        | 0.53     |
| 1:A:948:C:O2'    | 1:A:949:A:H5'     | 2.09        | 0.53     |
| 4:C:10:PHE:CZ    | 4:C:178:LEU:HD13  | 2.44        | 0.53     |
| 1:A:1498:U:O4    | 25:A:1632:HYG:H24 | 2.09        | 0.53     |
| 8:G:70:LYS:HB3   | 8:G:96:GLN:HG2    | 1.91        | 0.53     |
| 14:M:5:ALA:O     | 14:M:6:GLY:C      | 2.48        | 0.53     |
| 1:A:1053:G:H4'   | 1:A:1054:C:H5'    | 1.91        | 0.53     |
| 1:A:403:C:H2'    | 1:A:404:U:H6      | 1.73        | 0.53     |
| 19:R:19:LYS:O    | 19:R:20:ALA:HB3   | 2.09        | 0.53     |
| 1:A:420:U:H2'    | 1:A:422:C:C5      | 2.44        | 0.53     |
| 1:A:287:U:O2'    | 1:A:288:A:H5'     | 2.09        | 0.53     |
| 1:A:853:G:O2'    | 1:A:854:G:H5'     | 2.09        | 0.53     |
| 13:L:97:ARG:HB2  | 13:L:98:TYR:CE1   | 2.44        | 0.52     |
| 11:J:46:ARG:HH11 | 11:J:64:GLU:CB    | 2.22        | 0.52     |
| 11:J:7:LYS:NZ    | 11:J:40:LEU:HD11  | 2.24        | 0.52     |
| 3:B:124:SER:CB   | 3:B:125:PRO:CD    | 2.87        | 0.52     |
| 7:F:44:GLY:HA2   | 7:F:59:TYR:CE1    | 2.44        | 0.52     |
| 1:A:575:G:OP1    | 1:A:575:G:H4'     | 2.08        | 0.52     |
| 3:B:19:HIS:HB2   | 3:B:204:ASN:OD1   | 2.09        | 0.52     |
| 14:M:33:ALA:HB2  | 14:M:64:TRP:CH2   | 2.44        | 0.52     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 14:M:78:ILE:HG22 | 14:M:82:MET:CE   | 2.39        | 0.52     |
| 9:H:9:MET:HB2    | 9:H:32:LYS:HD3   | 1.91        | 0.52     |
| 1:A:1319:A:H5'   | 1:A:1320:C:OP1   | 2.09        | 0.52     |
| 1:A:217:C:O2'    | 1:A:218:C:H5'    | 2.08        | 0.52     |
| 1:A:1438:G:H2'   | 1:A:1439:C:C6    | 2.43        | 0.52     |
| 5:D:190:ASP:O    | 5:D:194:LEU:HD23 | 2.09        | 0.52     |
| 11:J:6:ILE:HD11  | 11:J:72:VAL:CG1  | 2.39        | 0.52     |
| 1:A:393:A:C2'    | 1:A:394:G:H5'    | 2.39        | 0.52     |
| 7:F:100:ASN:ND2  | 19:R:23:LYS:HG2  | 2.22        | 0.52     |
| 1:A:190(E):U:O2' | 18:Q:63:ARG:NH2  | 2.42        | 0.52     |
| 1:A:1370:G:O2'   | 1:A:1371:G:H5'   | 2.10        | 0.52     |
| 8:G:85:TYR:HD1   | 8:G:154:TYR:CE1  | 2.27        | 0.52     |
| 22:V:7:ARG:O     | 22:V:8:THR:HG23  | 2.09        | 0.52     |
| 1:A:1453:G:H2'   | 1:A:1454:G:O4'   | 2.10        | 0.52     |
| 1:A:1126:U:H1'   | 1:A:1280:A:C6    | 2.44        | 0.52     |
| 16:O:27:VAL:O    | 16:O:30:ALA:HB3  | 2.09        | 0.52     |
| 1:A:1248:A:H1'   | 10:I:70:LYS:HZ2  | 1.73        | 0.52     |
| 14:M:84:ILE:HG22 | 20:S:65:ASN:HD22 | 1.74        | 0.52     |
| 7:F:18:GLN:O     | 7:F:21:LEU:HB3   | 2.10        | 0.52     |
| 16:O:87:ILE:O    | 16:O:88:ARG:CB   | 2.57        | 0.52     |
| 1:A:1172:C:O2'   | 1:A:1173:G:H5'   | 2.09        | 0.52     |
| 1:A:757:U:H2'    | 1:A:758:G:O4'    | 2.09        | 0.52     |
| 1:A:1136:U:H5''  | 1:A:1137:C:OP2   | 2.10        | 0.52     |
| 4:C:110:ASN:O    | 4:C:111:LEU:HD23 | 2.10        | 0.52     |
| 11:J:60:ARG:N    | 11:J:60:ARG:HD2  | 2.24        | 0.52     |
| 3:B:126:GLU:O    | 3:B:129:GLU:HB2  | 2.09        | 0.52     |
| 1:A:1414:U:H2'   | 1:A:1415:G:C8    | 2.44        | 0.52     |
| 3:B:15:VAL:HG21  | 3:B:209:ARG:HG3  | 1.90        | 0.52     |
| 8:G:15:ASP:HB3   | 8:G:19:GLY:N     | 2.24        | 0.52     |
| 1:A:103:C:P      | 21:T:17:ARG:HH11 | 2.33        | 0.52     |
| 1:A:663:A:O2'    | 1:A:664:G:H5'    | 2.10        | 0.52     |
| 11:J:62:HIS:CB   | 15:N:59:ALA:HB3  | 2.35        | 0.52     |
| 13:L:119:LYS:O   | 13:L:120:TYR:HB2 | 2.10        | 0.52     |
| 17:P:67:THR:CG2  | 17:P:68:ASP:N    | 2.73        | 0.52     |
| 3:B:72:GLY:HA3   | 3:B:81:VAL:HG21  | 1.91        | 0.52     |
| 1:A:567:G:H2'    | 1:A:568:G:O4'    | 2.10        | 0.52     |
| 6:E:144:THR:HG22 | 6:E:145:LYS:N    | 2.25        | 0.52     |
| 3:B:19:HIS:HD2   | 3:B:205:ASP:OD1  | 1.92        | 0.52     |
| 3:B:71:VAL:O     | 3:B:165:VAL:HG23 | 2.09        | 0.52     |
| 18:Q:17:LYS:HA   | 18:Q:46:ASP:O    | 2.10        | 0.52     |
| 4:C:151:VAL:HG12 | 4:C:152:ILE:N    | 2.24        | 0.52     |
| 21:T:33:ILE:HD13 | 21:T:63:ILE:HG12 | 1.92        | 0.52     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:690:G:H2'    | 1:A:691:G:O4'    | 2.10        | 0.52     |
| 1:A:989:C:O2'    | 1:A:990:C:H5'    | 2.10        | 0.52     |
| 8:G:48:LYS:O     | 8:G:51:GLN:HB2   | 2.10        | 0.52     |
| 1:A:47:C:C6      | 1:A:365:U:H2'    | 2.44        | 0.52     |
| 13:L:85:ILE:HG23 | 13:L:98:TYR:CB   | 2.39        | 0.52     |
| 9:H:121:ASP:HB2  | 9:H:125:ARG:HH21 | 1.74        | 0.52     |
| 3:B:119:GLU:CD   | 3:B:153:ARG:HH22 | 2.13        | 0.52     |
| 10:I:9:ARG:CG    | 10:I:14:VAL:HG22 | 2.37        | 0.52     |
| 4:C:107:GLN:O    | 4:C:108:ASN:CB   | 2.57        | 0.52     |
| 3:B:12:GLU:C     | 3:B:14:GLY:H     | 2.12        | 0.52     |
| 1:A:1460:A:H2'   | 1:A:1461:G:O4'   | 2.10        | 0.52     |
| 1:A:1306:A:H2'   | 1:A:1307:U:O4'   | 2.10        | 0.52     |
| 5:D:70:ILE:HD11  | 5:D:100:ARG:HD2  | 1.92        | 0.52     |
| 1:A:543:C:O2'    | 1:A:544:G:H5'    | 2.09        | 0.52     |
| 15:N:14:PRO:C    | 15:N:16:PHE:N    | 2.59        | 0.52     |
| 4:C:13:GLY:HA3   | 15:N:57:ARG:NH2  | 2.24        | 0.52     |
| 1:A:744:C:H2'    | 1:A:745:C:C6     | 2.45        | 0.52     |
| 3:B:18:GLY:HA2   | 3:B:42:ILE:H     | 1.75        | 0.52     |
| 18:Q:59:ILE:CG2  | 18:Q:71:PHE:CD1  | 2.93        | 0.52     |
| 1:A:1264:C:H2'   | 1:A:1265:G:H8    | 1.75        | 0.52     |
| 14:M:15:VAL:HG23 | 14:M:43:THR:O    | 2.10        | 0.52     |
| 13:L:60:LEU:HD21 | 13:L:66:VAL:HG22 | 1.92        | 0.51     |
| 18:Q:104:LYS:N   | 18:Q:104:LYS:NZ  | 2.50        | 0.51     |
| 12:K:54:ARG:HH11 | 12:K:54:ARG:CB   | 2.15        | 0.51     |
| 1:A:1286:A:H8    | 1:A:1287:A:H5''  | 1.75        | 0.51     |
| 5:D:70:ILE:HD11  | 5:D:100:ARG:CD   | 2.40        | 0.51     |
| 4:C:23:TYR:O     | 4:C:24:ALA:HB2   | 2.09        | 0.51     |
| 4:C:190:ARG:CB   | 4:C:190:ARG:HH11 | 2.22        | 0.51     |
| 8:G:41:ARG:O     | 8:G:42:ILE:C     | 2.47        | 0.51     |
| 7:F:97:PHE:HB2   | 19:R:32:ARG:NH1  | 2.25        | 0.51     |
| 6:E:103:GLY:O    | 6:E:107:ARG:HB3  | 2.09        | 0.51     |
| 19:R:39:VAL:HG13 | 19:R:40:LEU:N    | 2.25        | 0.51     |
| 1:A:1250:A:H5''  | 10:I:68:GLY:N    | 2.25        | 0.51     |
| 1:A:1222:G:P     | 20:S:77:THR:HG21 | 2.49        | 0.51     |
| 1:A:1405:G:O6    | 25:A:1632:HYG:N7 | 2.42        | 0.51     |
| 1:A:1491:G:N2    | 1:A:1492:A:H62   | 2.06        | 0.51     |
| 3:B:10:LEU:HD23  | 3:B:48:MET:HG3   | 1.92        | 0.51     |
| 20:S:22:LEU:HD21 | 20:S:28:LYS:HD2  | 1.92        | 0.51     |
| 14:M:5:ALA:O     | 14:M:7:VAL:N     | 2.43        | 0.51     |
| 1:A:1028:C:H2'   | 1:A:1029:C:H6    | 1.71        | 0.51     |
| 1:A:1368:G:P     | 10:I:112:LYS:O   | 2.68        | 0.51     |
| 1:A:459:G:H3'    | 1:A:460:A:C5'    | 2.39        | 0.51     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 9:H:119:LEU:CD1  | 9:H:124:ALA:HA   | 2.23        | 0.51     |
| 1:A:393:A:OP2    | 17:P:12:LYS:HE2  | 2.11        | 0.51     |
| 21:T:53:LEU:O    | 21:T:57:ARG:HD2  | 2.11        | 0.51     |
| 4:C:26:LYS:CD    | 4:C:26:LYS:N     | 2.73        | 0.51     |
| 9:H:11:THR:HG22  | 9:H:15:ASN:ND2   | 2.26        | 0.51     |
| 15:N:22:THR:O    | 15:N:23:ARG:HB2  | 2.09        | 0.51     |
| 1:A:738:C:OP1    | 7:F:92:LYS:HE3   | 2.10        | 0.51     |
| 1:A:860:A:H2'    | 1:A:861:G:O4'    | 2.11        | 0.51     |
| 10:I:36:TYR:CD2  | 10:I:37:PHE:CE2  | 2.98        | 0.51     |
| 1:A:316:G:H2'    | 1:A:317:G:H8     | 1.75        | 0.51     |
| 1:A:761:G:H1'    | 18:Q:104:LYS:O   | 2.11        | 0.51     |
| 1:A:1127:G:H5''  | 10:I:66:ARG:HH22 | 1.75        | 0.51     |
| 3:B:197:VAL:CB   | 3:B:200:ILE:HG12 | 2.38        | 0.51     |
| 1:A:1038:C:H2'   | 1:A:1039:C:H6    | 1.76        | 0.51     |
| 6:E:47:LYS:HD2   | 6:E:47:LYS:N     | 2.25        | 0.51     |
| 1:A:190(B):C:H2' | 1:A:190(C):C:O4' | 2.10        | 0.51     |
| 13:L:54:LYS:N    | 13:L:54:LYS:HD2  | 2.25        | 0.51     |
| 1:A:1348:U:H2'   | 1:A:1349:A:C8    | 2.45        | 0.51     |
| 3:B:239:VAL:HG12 | 3:B:239:VAL:O    | 2.11        | 0.51     |
| 1:A:1036:G:H2'   | 1:A:1037:C:O4'   | 2.10        | 0.51     |
| 1:A:328:C:O2     | 1:A:328:C:C2'    | 2.56        | 0.51     |
| 3:B:102:LEU:HD21 | 3:B:162:ILE:HD12 | 1.90        | 0.51     |
| 14:M:78:ILE:O    | 14:M:81:LEU:CD2  | 2.58        | 0.51     |
| 18:Q:12:SER:HB3  | 18:Q:20:THR:CB   | 2.41        | 0.51     |
| 1:A:736:C:H2'    | 1:A:737:A:H8     | 1.76        | 0.51     |
| 1:A:737:A:H1'    | 7:F:73:ASN:HD21  | 1.75        | 0.51     |
| 13:L:38:THR:HG22 | 13:L:39:VAL:CG2  | 2.39        | 0.51     |
| 7:F:94:GLN:NE2   | 19:R:32:ARG:HD3  | 2.25        | 0.51     |
| 1:A:308:C:H2'    | 1:A:309:G:H8     | 1.75        | 0.51     |
| 9:H:45:ILE:HG13  | 9:H:47:GLY:N     | 2.26        | 0.51     |
| 14:M:37:THR:HG23 | 14:M:55:ARG:HB3  | 1.93        | 0.51     |
| 1:A:1415:G:H2'   | 1:A:1416:G:C8    | 2.43        | 0.51     |
| 16:O:27:VAL:HG12 | 16:O:31:LEU:CD1  | 2.41        | 0.51     |
| 3:B:137:ARG:HH11 | 3:B:137:ARG:HB3  | 1.76        | 0.51     |
| 18:Q:63:ARG:HG2  | 18:Q:64:PRO:CD   | 2.41        | 0.51     |
| 1:A:407:G:H2'    | 1:A:408:A:C8     | 2.45        | 0.51     |
| 1:A:652:U:O4     | 1:A:752:G:O2'    | 2.23        | 0.51     |
| 4:C:33:LEU:HD11  | 15:N:53:LEU:CD2  | 2.41        | 0.51     |
| 16:O:56:LEU:O    | 16:O:60:VAL:HG23 | 2.11        | 0.51     |
| 4:C:52:LEU:CD2   | 4:C:118:GLN:HE22 | 2.21        | 0.51     |
| 4:C:20:SER:HB3   | 4:C:22:TRP:NE1   | 2.25        | 0.51     |
| 1:A:953:G:H1'    | 14:M:125:ARG:HA  | 1.92        | 0.51     |

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| Atom-1            | Atom-2           | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:A:1153:C:P      | 11:J:13:HIS:HE2  | 2.33        | 0.51     |
| 1:A:1222:G:OP1    | 20:S:77:THR:HG21 | 2.11        | 0.51     |
| 9:H:104:ARG:HG2   | 9:H:104:ARG:HH11 | 1.76        | 0.51     |
| 20:S:45:VAL:HG12  | 20:S:46:GLY:N    | 2.26        | 0.51     |
| 1:A:881:G:OP2     | 13:L:12:ARG:NH2  | 2.44        | 0.51     |
| 6:E:13:ILE:HG22   | 6:E:30:ALA:HA    | 1.92        | 0.51     |
| 1:A:1057:G:O2'    | 1:A:1058:G:H5'   | 2.11        | 0.51     |
| 4:C:107:GLN:O     | 4:C:108:ASN:HB3  | 2.10        | 0.51     |
| 1:A:848:C:H2'     | 1:A:849:C:C6     | 2.46        | 0.51     |
| 9:H:60:ARG:NH1    | 9:H:60:ARG:HG3   | 2.25        | 0.51     |
| 14:M:33:ALA:HA    | 14:M:59:TYR:CE2  | 2.45        | 0.51     |
| 14:M:78:ILE:HA    | 14:M:81:LEU:CD2  | 2.40        | 0.51     |
| 13:L:83:VAL:CG2   | 13:L:84:LEU:H    | 2.21        | 0.51     |
| 4:C:157:ILE:CD1   | 4:C:166:GLU:HB2  | 2.40        | 0.51     |
| 1:A:279:A:H5''    | 1:A:280:C:H3'    | 1.93        | 0.51     |
| 1:A:399:G:H2'     | 1:A:400:C:C6     | 2.45        | 0.51     |
| 1:A:1153:C:H2'    | 1:A:1154:G:C8    | 2.46        | 0.51     |
| 4:C:106:VAL:HG11  | 4:C:115:LEU:HD11 | 1.93        | 0.51     |
| 1:A:1003(A):G:H2' | 1:A:1004:A:H4'   | 1.93        | 0.51     |
| 5:D:3:ARG:HH22    | 5:D:74:GLN:CG    | 2.23        | 0.51     |
| 1:A:332:G:O2'     | 1:A:333:G:H5'    | 2.10        | 0.51     |
| 1:A:1207:G:O2'    | 1:A:1208:C:H5'   | 2.11        | 0.51     |
| 1:A:424:G:O2'     | 1:A:425:G:H5'    | 2.11        | 0.51     |
| 6:E:92:LYS:O      | 6:E:118:ILE:HG23 | 2.11        | 0.51     |
| 1:A:112:G:H21     | 1:A:354:G:H5'    | 1.76        | 0.51     |
| 4:C:14:ILE:O      | 4:C:16:ARG:N     | 2.43        | 0.51     |
| 5:D:153:ARG:HG2   | 5:D:181:MET:SD   | 2.50        | 0.51     |
| 8:G:72:ARG:HG2    | 8:G:142:GLU:OE1  | 2.11        | 0.51     |
| 15:N:26:ARG:HH12  | 15:N:47:LEU:HG   | 1.72        | 0.51     |
| 7:F:75:LEU:HD13   | 7:F:75:LEU:O     | 2.09        | 0.51     |
| 21:T:50:GLU:HG3   | 21:T:99:LEU:HD12 | 1.93        | 0.51     |
| 1:A:501:C:OP1     | 13:L:117:ARG:NH2 | 2.43        | 0.51     |
| 7:F:14:LEU:HA     | 7:F:18:GLN:HE21  | 1.74        | 0.51     |
| 5:D:4:TYR:CG      | 5:D:5:ILE:N      | 2.79        | 0.51     |
| 10:I:111:ARG:HD3  | 10:I:112:LYS:H   | 1.74        | 0.51     |
| 1:A:411:A:C4      | 1:A:413:G:H1'    | 2.46        | 0.51     |
| 8:G:85:TYR:O      | 8:G:87:VAL:HG23  | 2.11        | 0.51     |
| 1:A:459:G:H3'     | 1:A:460:A:H5''   | 1.93        | 0.51     |
| 6:E:144:THR:HB    | 6:E:147:ASP:OD2  | 2.11        | 0.51     |
| 1:A:1504:G:OP1    | 1:A:1507:A:H4'   | 2.11        | 0.51     |
| 11:J:20:ALA:O     | 11:J:24:VAL:HG23 | 2.10        | 0.50     |
| 16:O:31:LEU:N     | 16:O:31:LEU:HD12 | 2.25        | 0.50     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 4:C:11:ARG:HG2   | 4:C:11:ARG:NH1    | 2.27        | 0.50     |
| 8:G:143:ARG:O    | 8:G:145:ALA:O     | 2.29        | 0.50     |
| 1:A:731:G:H5'    | 1:A:766:A:H4'     | 1.93        | 0.50     |
| 11:J:45:ARG:HH11 | 11:J:45:ARG:CB    | 1.95        | 0.50     |
| 19:R:42:ARG:NH1  | 19:R:42:ARG:HG3   | 2.25        | 0.50     |
| 5:D:165:MET:HE2  | 5:D:176:LEU:HD13  | 1.93        | 0.50     |
| 1:A:1238:A:N7    | 1:A:1303:C:H1'    | 2.26        | 0.50     |
| 1:A:142:G:O2'    | 1:A:196:A:N1      | 2.32        | 0.50     |
| 11:J:12:ASP:HB3  | 11:J:15:THR:HG22  | 1.93        | 0.50     |
| 15:N:24:CYS:HB3  | 15:N:28:GLY:N     | 2.26        | 0.50     |
| 3:B:17:PHE:CD1   | 3:B:17:PHE:C      | 2.85        | 0.50     |
| 3:B:17:PHE:HD1   | 3:B:17:PHE:C      | 2.15        | 0.50     |
| 11:J:6:ILE:HG22  | 11:J:98:ILE:HG12  | 1.93        | 0.50     |
| 19:R:42:ARG:HH11 | 19:R:42:ARG:HG3   | 1.77        | 0.50     |
| 13:L:119:LYS:O   | 13:L:120:TYR:CB   | 2.60        | 0.50     |
| 4:C:34:LEU:HG    | 15:N:25:VAL:HG21  | 1.93        | 0.50     |
| 1:A:437:U:O2'    | 5:D:123:HIS:CD2   | 2.64        | 0.50     |
| 1:A:861:G:O2'    | 1:A:862:C:H5'     | 2.11        | 0.50     |
| 5:D:6:GLY:O      | 5:D:7:PRO:C       | 2.47        | 0.50     |
| 1:A:1477:C:H2'   | 1:A:1478:C:H6     | 1.76        | 0.50     |
| 4:C:188:LEU:HD11 | 4:C:195:VAL:HG13  | 1.92        | 0.50     |
| 1:A:1149:C:H2'   | 1:A:1150:U:C6     | 2.47        | 0.50     |
| 1:A:337:C:H2'    | 1:A:338:A:H8      | 1.76        | 0.50     |
| 1:A:1346:A:O2'   | 1:A:1347:G:OP2    | 2.27        | 0.50     |
| 1:A:509:A:N3     | 1:A:543:C:O2'     | 2.36        | 0.50     |
| 13:L:84:LEU:HD22 | 13:L:104:VAL:HG11 | 1.94        | 0.50     |
| 1:A:551:U:H2'    | 1:A:552:U:C6      | 2.47        | 0.50     |
| 1:A:707:C:OP1    | 12:K:85:ARG:NH1   | 2.45        | 0.50     |
| 1:A:1176:A:H2'   | 1:A:1177:G:C8     | 2.46        | 0.50     |
| 10:I:58:ARG:HD2  | 10:I:58:ARG:O     | 2.11        | 0.50     |
| 1:A:961:U:O2'    | 1:A:962:C:H5'     | 2.11        | 0.50     |
| 12:K:99:GLN:HG2  | 12:K:105:VAL:HG21 | 1.93        | 0.50     |
| 11:J:56:HIS:O    | 11:J:58:ASP:N     | 2.44        | 0.50     |
| 3:B:98:LEU:O     | 3:B:101:MET:HG3   | 2.11        | 0.50     |
| 18:Q:81:ARG:O    | 18:Q:81:ARG:HG3   | 2.12        | 0.50     |
| 18:Q:27:PHE:CE1  | 18:Q:36:ILE:HD11  | 2.47        | 0.50     |
| 1:A:1326:C:OP1   | 22:V:12:LYS:NZ    | 2.44        | 0.50     |
| 1:A:933:G:OP2    | 8:G:3:ARG:HB3     | 2.11        | 0.50     |
| 13:L:26:ALA:O    | 13:L:27:LEU:O     | 2.30        | 0.50     |
| 1:A:281:G:O2'    | 1:A:282:A:OP2     | 2.24        | 0.50     |
| 3:B:16:HIS:CD2   | 3:B:210:SER:HG    | 2.30        | 0.50     |
| 1:A:918:A:H2'    | 1:A:919:A:H8      | 1.75        | 0.50     |

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| Atom-1            | Atom-2           | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 21:T:94:ALA:O     | 21:T:95:ALA:HB3  | 2.10        | 0.50     |
| 9:H:91:ARG:CG     | 13:L:7:ILE:HG13  | 2.41        | 0.50     |
| 1:A:624:C:H2'     | 1:A:625:G:H8     | 1.76        | 0.50     |
| 3:B:19:HIS:CD2    | 3:B:205:ASP:OD1  | 2.64        | 0.50     |
| 21:T:102:GLY:O    | 21:T:104:LEU:N   | 2.39        | 0.50     |
| 18:Q:59:ILE:CG2   | 18:Q:71:PHE:HB3  | 2.42        | 0.50     |
| 14:M:29:ARG:HB3   | 14:M:64:TRP:CH2  | 2.47        | 0.50     |
| 14:M:78:ILE:O     | 14:M:81:LEU:HD22 | 2.12        | 0.50     |
| 1:A:505:G:H2'     | 1:A:506:G:H8     | 1.77        | 0.50     |
| 5:D:151:LYS:HD2   | 5:D:151:LYS:H    | 1.77        | 0.50     |
| 21:T:39:LYS:CD    | 21:T:55:ILE:HD13 | 2.31        | 0.50     |
| 1:A:1250:A:H5'    | 10:I:68:GLY:O    | 2.12        | 0.50     |
| 1:A:1113:C:H6     | 1:A:1113:C:O5'   | 1.95        | 0.50     |
| 3:B:187:LEU:HD23  | 3:B:201:ILE:HG22 | 1.92        | 0.50     |
| 1:A:1392:G:H2'    | 1:A:1393:U:H6    | 1.77        | 0.50     |
| 3:B:103:THR:HB    | 3:B:176:GLU:CD   | 2.32        | 0.50     |
| 1:A:276:G:C2'     | 1:A:277:C:H5'    | 2.42        | 0.50     |
| 19:R:52:PRO:HB2   | 19:R:54:ARG:HD3  | 1.93        | 0.50     |
| 1:A:965:A:H2      | 14:M:124:PRO:HB2 | 1.77        | 0.50     |
| 6:E:148:VAL:O     | 6:E:152:ARG:HG3  | 2.12        | 0.50     |
| 1:A:190:C:H2'     | 1:A:190(A):C:C6  | 2.47        | 0.50     |
| 1:A:91:C:O2'      | 1:A:92:C:H5'     | 2.11        | 0.50     |
| 1:A:522:C:H41     | 13:L:53:ARG:HH22 | 1.60        | 0.50     |
| 4:C:87:LEU:C      | 4:C:89:GLU:N     | 2.65        | 0.50     |
| 1:A:190(J):U:H2'  | 1:A:190(K):G:C8  | 2.47        | 0.50     |
| 1:A:1306:A:C2     | 1:A:1307:U:H1'   | 2.47        | 0.50     |
| 11:J:24:VAL:CG1   | 11:J:28:ARG:HE   | 2.25        | 0.50     |
| 1:A:298:A:H2'     | 1:A:299:G:O4'    | 2.12        | 0.50     |
| 1:A:1116:C:H2'    | 1:A:1117:G:C5'   | 2.34        | 0.50     |
| 1:A:1002:G:H2'    | 1:A:1003:G:O4'   | 2.12        | 0.50     |
| 1:A:270:A:H2'     | 1:A:271:C:C6     | 2.47        | 0.50     |
| 8:G:135:VAL:O     | 8:G:139:GLU:HG3  | 2.12        | 0.50     |
| 1:A:628:G:O2'     | 1:A:629:G:H5'    | 2.11        | 0.50     |
| 22:V:24:ARG:O     | 22:V:25:LYS:CB   | 2.60        | 0.50     |
| 12:K:85:ARG:HG3   | 12:K:85:ARG:HH11 | 1.77        | 0.50     |
| 1:A:1030(C):G:H2' | 1:A:1030(D):A:C8 | 2.47        | 0.50     |
| 4:C:167:TRP:O     | 4:C:168:ALA:HB3  | 2.12        | 0.50     |
| 9:H:20:TYR:CE1    | 9:H:76:PRO:HD2   | 2.47        | 0.50     |
| 1:A:1330:U:H2'    | 1:A:1331:G:H5'   | 1.94        | 0.49     |
| 12:K:13:GLN:HA    | 12:K:75:TYR:O    | 2.11        | 0.49     |
| 1:A:1277:C:H2'    | 1:A:1278:U:H5'   | 1.94        | 0.49     |
| 1:A:1251:A:H4'    | 10:I:12:GLU:CD   | 2.32        | 0.49     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 19:R:58:LEU:HD22 | 19:R:62:GLU:HB3  | 1.93        | 0.49     |
| 3:B:137:ARG:O    | 3:B:140:HIS:HB2  | 2.12        | 0.49     |
| 7:F:36:ARG:HH12  | 7:F:38:GLU:HG2   | 1.77        | 0.49     |
| 10:I:93:ARG:NH1  | 10:I:97:LYS:HZ2  | 2.09        | 0.49     |
| 1:A:521:G:OP1    | 13:L:73:GLU:O    | 2.29        | 0.49     |
| 1:A:666:G:H5'    | 1:A:726:C:H1'    | 1.92        | 0.49     |
| 3:B:181:PHE:CD2  | 9:H:70:GLN:HB3   | 2.47        | 0.49     |
| 4:C:22:TRP:CZ3   | 4:C:32:LEU:HD22  | 2.46        | 0.49     |
| 1:A:1139:G:O2'   | 1:A:1140:C:P     | 2.70        | 0.49     |
| 1:A:5:U:HO2'     | 1:A:6:G:P        | 2.35        | 0.49     |
| 3:B:130:ARG:NH2  | 4:C:207:VAL:HG23 | 2.22        | 0.49     |
| 1:A:1042:G:O2'   | 1:A:1043:C:H5'   | 2.12        | 0.49     |
| 5:D:63:LYS:O     | 5:D:64:LEU:C     | 2.51        | 0.49     |
| 9:H:104:ARG:NH2  | 9:H:138:TRP:CH2  | 2.80        | 0.49     |
| 4:C:191:THR:CG2  | 4:C:192:THR:H    | 2.24        | 0.49     |
| 19:R:51:LEU:HB2  | 19:R:56:THR:HG22 | 1.94        | 0.49     |
| 1:A:109:A:H2'    | 1:A:326:G:N2     | 2.27        | 0.49     |
| 1:A:1420:C:H2'   | 1:A:1421:G:H8    | 1.76        | 0.49     |
| 3:B:57:PHE:O     | 3:B:60:ASP:HB3   | 2.12        | 0.49     |
| 3:B:17:PHE:HD1   | 3:B:18:GLY:N     | 2.10        | 0.49     |
| 11:J:34:VAL:CG2  | 11:J:74:ILE:HG23 | 2.43        | 0.49     |
| 1:A:1498:U:C4'   | 1:A:1519:A:H2    | 2.24        | 0.49     |
| 12:K:19:ALA:HB2  | 12:K:80:VAL:CG1  | 2.43        | 0.49     |
| 3:B:23:ARG:NH1   | 3:B:24:TRP:CA    | 2.75        | 0.49     |
| 20:S:45:VAL:C    | 20:S:47:HIS:H    | 2.15        | 0.49     |
| 1:A:818:G:H3'    | 1:A:819:A:C5'    | 2.42        | 0.49     |
| 1:A:444:C:O2'    | 1:A:445:G:H5'    | 2.12        | 0.49     |
| 1:A:625:G:H4'    | 17:P:16:HIS:CD2  | 2.48        | 0.49     |
| 3:B:164:VAL:HG12 | 3:B:186:ALA:CB   | 2.42        | 0.49     |
| 11:J:51:ARG:NH1  | 11:J:51:ARG:HG2  | 2.21        | 0.49     |
| 1:A:1061:G:C2'   | 1:A:1062:U:H5'   | 2.43        | 0.49     |
| 7:F:75:LEU:HD13  | 7:F:75:LEU:C     | 2.33        | 0.49     |
| 21:T:53:LEU:HD13 | 21:T:101:GLY:N   | 2.27        | 0.49     |
| 1:A:448:A:H62    | 1:A:486:U:H3     | 1.59        | 0.49     |
| 1:A:443:C:H2'    | 1:A:444:C:H6     | 1.78        | 0.49     |
| 1:A:1442:G:H2'   | 1:A:1442:G:N3    | 2.26        | 0.49     |
| 13:L:53:ARG:CB   | 13:L:93:LEU:HD11 | 2.43        | 0.49     |
| 8:G:110:GLN:OE1  | 8:G:110:GLN:HA   | 2.11        | 0.49     |
| 1:A:6:G:C4       | 6:E:119:LEU:HD11 | 2.47        | 0.49     |
| 11:J:54:PHE:CE2  | 11:J:55:LYS:HD3  | 2.48        | 0.49     |
| 4:C:131:ARG:O    | 4:C:135:LYS:HG3  | 2.12        | 0.49     |
| 3:B:16:HIS:CE1   | 3:B:214:ILE:HG12 | 2.47        | 0.49     |

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| Atom-1            | Atom-2           | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:A:141:A:H1'     | 1:A:182:U:C2     | 2.47        | 0.49     |
| 15:N:12:ARG:O     | 15:N:13:THR:C    | 2.51        | 0.49     |
| 10:I:111:ARG:HH11 | 10:I:111:ARG:HG3 | 1.77        | 0.49     |
| 1:A:77:G:O2'      | 1:A:78:G:H5'     | 2.13        | 0.49     |
| 10:I:89:ASN:ND2   | 10:I:91:ASP:HB2  | 2.28        | 0.49     |
| 11:J:51:ARG:N     | 11:J:59:SER:CB   | 2.76        | 0.49     |
| 4:C:88:ARG:O      | 4:C:91:LEU:HD22  | 2.11        | 0.49     |
| 3:B:109:SER:O     | 3:B:112:VAL:N    | 2.42        | 0.49     |
| 1:A:1256:A:H5'    | 1:A:1258:G:O4'   | 2.13        | 0.49     |
| 11:J:71:LEU:O     | 11:J:72:VAL:HB   | 2.13        | 0.49     |
| 1:A:687:A:H4'     | 1:A:688:G:O5'    | 2.11        | 0.49     |
| 1:A:1085:U:O3'    | 1:A:1086:U:H6    | 1.96        | 0.49     |
| 20:S:62:ILE:CD1   | 20:S:66:MET:HG3  | 2.42        | 0.49     |
| 1:A:1413:A:H2     | 1:A:1487:G:H22   | 1.58        | 0.49     |
| 3:B:103:THR:HB    | 3:B:176:GLU:OE1  | 2.12        | 0.49     |
| 10:I:46:ALA:HA    | 10:I:78:LYS:HB2  | 1.95        | 0.49     |
| 3:B:144:ARG:O     | 3:B:147:LYS:N    | 2.44        | 0.49     |
| 1:A:447:G:H2'     | 1:A:485:G:N2     | 2.27        | 0.49     |
| 10:I:65:VAL:HG13  | 10:I:65:VAL:O    | 2.12        | 0.49     |
| 1:A:537:G:OP1     | 13:L:113:ARG:NH2 | 2.46        | 0.49     |
| 3:B:26:PRO:O      | 3:B:29:ALA:HB2   | 2.13        | 0.49     |
| 19:R:46:GLU:CD    | 19:R:46:GLU:H    | 2.16        | 0.49     |
| 1:A:123:C:OP1     | 1:A:312:C:H5'    | 2.12        | 0.49     |
| 4:C:20:SER:HB3    | 4:C:22:TRP:HE1   | 1.78        | 0.49     |
| 4:C:95:THR:O      | 4:C:97:LYS:N     | 2.44        | 0.49     |
| 5:D:158:ILE:HG22  | 5:D:181:MET:HE2  | 1.95        | 0.49     |
| 6:E:112:LEU:C     | 6:E:114:GLY:N    | 2.65        | 0.49     |
| 1:A:1023:G:H2'    | 1:A:1023:G:N3    | 2.26        | 0.49     |
| 1:A:1399:C:C2     | 1:A:1502:A:N6    | 2.80        | 0.49     |
| 1:A:485:G:C2'     | 1:A:486:U:OP2    | 2.61        | 0.49     |
| 1:A:1053:G:O2'    | 1:A:1199:U:H5    | 1.96        | 0.49     |
| 9:H:11:THR:HA     | 9:H:14:ARG:NH1   | 2.28        | 0.49     |
| 16:O:70:LEU:HD12  | 16:O:78:TYR:CB   | 2.43        | 0.49     |
| 1:A:929:G:O2'     | 1:A:930:C:H5'    | 2.12        | 0.49     |
| 4:C:87:LEU:O      | 4:C:89:GLU:N     | 2.46        | 0.49     |
| 1:A:1470:G:O2'    | 1:A:1471:G:H5'   | 2.13        | 0.49     |
| 1:A:1118:C:H1'    | 1:A:1179:A:C4    | 2.48        | 0.49     |
| 15:N:44:LEU:O     | 15:N:44:LEU:HD12 | 2.12        | 0.49     |
| 1:A:1226:C:H5''   | 14:M:103:THR:HG1 | 1.75        | 0.49     |
| 8:G:72:ARG:HA     | 8:G:96:GLN:NE2   | 2.27        | 0.49     |
| 3:B:209:ARG:HH11  | 3:B:209:ARG:HG2  | 1.78        | 0.49     |
| 11:J:80:LYS:O     | 11:J:84:GLN:HG3  | 2.12        | 0.49     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:390:C:H2'    | 1:A:391:G:H8      | 1.77        | 0.49     |
| 10:I:118:LYS:O   | 10:I:119:ALA:CB   | 2.61        | 0.49     |
| 1:A:1417:G:O2'   | 1:A:1483:A:N6     | 2.45        | 0.49     |
| 1:A:646:U:H2'    | 1:A:647:C:H6      | 1.78        | 0.49     |
| 5:D:38:TYR:HB2   | 5:D:39:PRO:HD2    | 1.95        | 0.49     |
| 5:D:92:VAL:O     | 5:D:96:LEU:HD13   | 2.12        | 0.49     |
| 21:T:42:GLN:CA   | 21:T:42:GLN:HE21  | 2.24        | 0.49     |
| 20:S:51:VAL:HG12 | 20:S:52:TYR:N     | 2.28        | 0.49     |
| 15:N:29:ARG:HH11 | 15:N:29:ARG:HG2   | 1.77        | 0.49     |
| 5:D:3:ARG:NE     | 5:D:71:SER:H      | 2.11        | 0.49     |
| 21:T:79:ARG:O    | 21:T:80:ARG:C     | 2.51        | 0.49     |
| 7:F:19:LEU:HD23  | 7:F:20:ALA:N      | 2.28        | 0.49     |
| 1:A:552:U:H4'    | 13:L:86:ARG:O     | 2.12        | 0.49     |
| 1:A:1128:C:O2'   | 1:A:1130:A:C8     | 2.65        | 0.49     |
| 3:B:182:ILE:O    | 3:B:183:PRO:C     | 2.50        | 0.49     |
| 1:A:913:A:O2'    | 1:A:914:A:OP2     | 2.28        | 0.49     |
| 14:M:31:LYS:O    | 14:M:35:GLU:HB2   | 2.12        | 0.49     |
| 14:M:97:PRO:HB2  | 14:M:101:GLN:OE1  | 2.12        | 0.49     |
| 1:A:246:A:N6     | 1:A:281:G:H1'     | 2.27        | 0.49     |
| 5:D:24:GLU:O     | 5:D:25:ARG:HB3    | 2.13        | 0.49     |
| 4:C:179:ARG:C    | 4:C:179:ARG:HD2   | 2.33        | 0.49     |
| 4:C:172:ARG:HB3  | 4:C:172:ARG:HH11  | 1.78        | 0.49     |
| 1:A:1487:G:H2'   | 1:A:1488:G:H8     | 1.77        | 0.49     |
| 1:A:1238:A:H2    | 1:A:1241:G:N3     | 2.10        | 0.49     |
| 14:M:84:ILE:O    | 14:M:86:CYS:N     | 2.46        | 0.49     |
| 1:A:1216:G:H2'   | 1:A:1217:C:H6     | 1.78        | 0.49     |
| 7:F:94:GLN:HB2   | 19:R:32:ARG:HD3   | 1.95        | 0.49     |
| 1:A:420:U:O2'    | 1:A:421:U:H5''    | 2.13        | 0.49     |
| 4:C:52:LEU:HG    | 4:C:52:LEU:O      | 2.13        | 0.48     |
| 4:C:42:LEU:HD12  | 4:C:94:LEU:CD1    | 2.43        | 0.48     |
| 3:B:119:GLU:CD   | 3:B:153:ARG:NH2   | 2.66        | 0.48     |
| 11:J:4:ILE:HG23  | 11:J:98:ILE:HG21  | 1.95        | 0.48     |
| 19:R:36:ASN:HB3  | 19:R:39:VAL:HG12  | 1.94        | 0.48     |
| 1:A:5:U:O2       | 1:A:5:U:C2'       | 2.61        | 0.48     |
| 4:C:123:GLN:HE22 | 4:C:140:ARG:HH22  | 1.61        | 0.48     |
| 1:A:1346:A:C4    | 8:G:10:ARG:NH2    | 2.81        | 0.48     |
| 4:C:58:GLU:HB2   | 4:C:65:ALA:HB2    | 1.95        | 0.48     |
| 5:D:68:TYR:CE2   | 5:D:97:LEU:HB3    | 2.48        | 0.48     |
| 5:D:68:TYR:CD2   | 5:D:97:LEU:HB3    | 2.48        | 0.48     |
| 16:O:27:VAL:HG12 | 16:O:31:LEU:HD11  | 1.94        | 0.48     |
| 1:A:1075:C:H5'   | 3:B:103:THR:HG21  | 1.95        | 0.48     |
| 21:T:53:LEU:HD21 | 21:T:104:LEU:HD12 | 1.95        | 0.48     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:B:59:GLU:O     | 3:B:62:ALA:HB3   | 2.12        | 0.48     |
| 20:S:80:TYR:CD2  | 20:S:81:ARG:N    | 2.80        | 0.48     |
| 8:G:15:ASP:O     | 8:G:19:GLY:HA2   | 2.12        | 0.48     |
| 6:E:107:ARG:HG2  | 6:E:108:ALA:N    | 2.27        | 0.48     |
| 20:S:74:PHE:N    | 20:S:74:PHE:CD1  | 2.80        | 0.48     |
| 5:D:98:GLU:HA    | 5:D:103:ASN:ND2  | 2.28        | 0.48     |
| 5:D:24:GLU:CG    | 5:D:25:ARG:H     | 2.25        | 0.48     |
| 1:A:959:A:H2     | 1:A:1221:G:N3    | 2.11        | 0.48     |
| 3:B:239:VAL:HB   | 3:B:240:GLN:NE2  | 2.28        | 0.48     |
| 1:A:1238:A:C2    | 1:A:1241:G:N3    | 2.81        | 0.48     |
| 14:M:36:LYS:HD2  | 14:M:59:TYR:OH   | 2.13        | 0.48     |
| 1:A:1202:G:H2'   | 1:A:1203:C:C5'   | 2.42        | 0.48     |
| 1:A:256:U:H5'    | 18:Q:17:LYS:HZ1  | 1.78        | 0.48     |
| 6:E:43:LEU:CD2   | 6:E:44:GLY:N     | 2.76        | 0.48     |
| 1:A:1095:U:H2'   | 1:A:1096:C:C6    | 2.48        | 0.48     |
| 1:A:1514:C:H2'   | 1:A:1515:C:C6    | 2.47        | 0.48     |
| 1:A:783:C:O2'    | 1:A:784:C:H5'    | 2.13        | 0.48     |
| 1:A:248:C:O2'    | 1:A:249:U:H5'    | 2.13        | 0.48     |
| 7:F:53:ALA:C     | 7:F:55:ASP:H     | 2.16        | 0.48     |
| 4:C:18:TRP:HE3   | 4:C:18:TRP:H     | 1.59        | 0.48     |
| 1:A:425:G:O2'    | 1:A:426:G:H5'    | 2.13        | 0.48     |
| 3:B:125:PRO:HG2  | 3:B:126:GLU:H    | 1.78        | 0.48     |
| 4:C:43:LEU:N     | 4:C:43:LEU:CD2   | 2.73        | 0.48     |
| 1:A:622:A:C8     | 1:A:623:C:C5     | 3.01        | 0.48     |
| 1:A:1197:G:C2'   | 1:A:1198:G:H5'   | 2.44        | 0.48     |
| 1:A:108:G:N2     | 1:A:109:A:N1     | 2.61        | 0.48     |
| 1:A:162:A:H2'    | 1:A:163:C:O4'    | 2.13        | 0.48     |
| 1:A:1172:C:H2'   | 1:A:1173:G:C8    | 2.47        | 0.48     |
| 1:A:75:G:O2'     | 1:A:76:C:H5'     | 2.14        | 0.48     |
| 3:B:82:ARG:O     | 3:B:86:GLU:HG3   | 2.13        | 0.48     |
| 1:A:832:C:O2'    | 1:A:833:U:H5'    | 2.13        | 0.48     |
| 1:A:1472:U:O2'   | 1:A:1473:A:H5'   | 2.12        | 0.48     |
| 1:A:1296:C:H4'   | 1:A:1302:U:C5    | 2.48        | 0.48     |
| 1:A:1231:G:H4'   | 10:I:126:SER:CB  | 2.44        | 0.48     |
| 3:B:130:ARG:HB3  | 3:B:131:PRO:HD2  | 1.96        | 0.48     |
| 1:A:1492:A:H2'   | 1:A:1493:A:C8    | 2.48        | 0.48     |
| 18:Q:59:ILE:HG22 | 18:Q:71:PHE:HD1  | 1.76        | 0.48     |
| 13:L:47:LYS:HB2  | 13:L:48:PRO:HD3  | 1.92        | 0.48     |
| 14:M:60:VAL:CG1  | 14:M:66:LEU:HD11 | 2.44        | 0.48     |
| 17:P:39:TYR:O    | 17:P:41:PRO:HD3  | 2.13        | 0.48     |
| 1:A:1020:U:H2'   | 1:A:1021:G:H8    | 1.78        | 0.48     |
| 10:I:93:ARG:CD   | 10:I:97:LYS:HE3  | 2.44        | 0.48     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 6:E:102:ALA:HB2   | 6:E:120:THR:HB    | 1.96        | 0.48     |
| 4:C:7:PRO:HG2     | 4:C:184:TYR:HB2   | 1.96        | 0.48     |
| 21:T:45:GLN:CB    | 21:T:91:LEU:HD22  | 2.42        | 0.48     |
| 14:M:110:ARG:HG2  | 14:M:110:ARG:HH11 | 1.78        | 0.48     |
| 9:H:126:LYS:C     | 9:H:128:GLY:H     | 2.17        | 0.48     |
| 1:A:639:G:O2'     | 1:A:640:A:H5'     | 2.12        | 0.48     |
| 13:L:98:TYR:CD1   | 13:L:98:TYR:N     | 2.81        | 0.48     |
| 11:J:46:ARG:HH11  | 11:J:64:GLU:HG2   | 1.78        | 0.48     |
| 11:J:51:ARG:CG    | 11:J:51:ARG:HH11  | 2.20        | 0.48     |
| 3:B:17:PHE:CD1    | 3:B:18:GLY:N      | 2.81        | 0.48     |
| 3:B:33:TYR:O      | 3:B:34:ALA:HB2    | 2.13        | 0.48     |
| 1:A:1230:C:O2'    | 1:A:1231:G:H5'    | 2.14        | 0.48     |
| 1:A:1402:C:O2     | 1:A:1500:A:N1     | 2.47        | 0.48     |
| 1:A:1248:A:H1'    | 10:I:70:LYS:HZ1   | 1.78        | 0.48     |
| 14:M:40:ASN:HD22  | 14:M:41:PRO:N     | 2.11        | 0.48     |
| 11:J:32:ALA:HB2   | 11:J:76:ASN:HD22  | 1.79        | 0.48     |
| 3:B:230:VAL:CG1   | 3:B:231:GLU:N     | 2.77        | 0.48     |
| 1:A:1269:A:C2     | 1:A:1313:U:O4'    | 2.67        | 0.48     |
| 14:M:15:VAL:C     | 14:M:17:VAL:H     | 2.16        | 0.48     |
| 6:E:57:LYS:HG2    | 6:E:61:TYR:CE2    | 2.48        | 0.48     |
| 1:A:553:A:H2'     | 1:A:554:C:C6      | 2.48        | 0.48     |
| 4:C:5:ILE:HD12    | 4:C:5:ILE:O       | 2.14        | 0.48     |
| 1:A:1531:A:O5'    | 1:A:1531:A:H8     | 1.96        | 0.48     |
| 1:A:1532:U:H6     | 1:A:1532:U:O5'    | 1.97        | 0.48     |
| 3:B:115:LEU:O     | 3:B:119:GLU:HG3   | 2.13        | 0.48     |
| 1:A:1488:G:H2'    | 1:A:1489:G:H8     | 1.73        | 0.48     |
| 1:A:267:C:H2'     | 1:A:268:C:H6      | 1.78        | 0.48     |
| 1:A:875:C:H1'     | 9:H:15:ASN:OD1    | 2.14        | 0.48     |
| 1:A:218:C:H2'     | 1:A:219:C:C6      | 2.49        | 0.48     |
| 1:A:33:A:H2'      | 1:A:34:C:C6       | 2.48        | 0.48     |
| 14:M:110:ARG:HH11 | 14:M:110:ARG:CG   | 2.27        | 0.48     |
| 13:L:40:VAL:O     | 13:L:40:VAL:HG12  | 2.13        | 0.48     |
| 9:H:38:ILE:N      | 9:H:38:ILE:HD12   | 2.27        | 0.48     |
| 3:B:84:GLU:CB     | 3:B:219:VAL:HG21  | 2.22        | 0.48     |
| 18:Q:104:LYS:O    | 18:Q:105:ALA:HB2  | 2.14        | 0.48     |
| 12:K:26:ASN:O     | 12:K:27:ASN:HB2   | 2.14        | 0.48     |
| 1:A:1305:G:H2'    | 1:A:1331:G:N2     | 2.28        | 0.48     |
| 1:A:244:U:O4      | 1:A:906:G:H1'     | 2.13        | 0.48     |
| 14:M:121:LYS:O    | 14:M:123:ALA:N    | 2.47        | 0.48     |
| 4:C:70:VAL:HG12   | 4:C:72:LYS:H      | 1.78        | 0.48     |
| 5:D:65:ARG:HA     | 5:D:75:PHE:CE1    | 2.48        | 0.48     |
| 7:F:67:MET:HE1    | 7:F:72:VAL:HA     | 1.95        | 0.48     |

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| Atom-1            | Atom-2           | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:A:197:A:N1      | 1:A:220:G:O2'    | 2.45        | 0.48     |
| 3:B:8:LYS:O       | 3:B:9:GLU:CB     | 2.60        | 0.48     |
| 1:A:737:A:H1'     | 7:F:73:ASN:ND2   | 2.29        | 0.48     |
| 8:G:145:ALA:C     | 8:G:147:ALA:N    | 2.66        | 0.48     |
| 6:E:150:ARG:HG3   | 6:E:150:ARG:NH1  | 2.29        | 0.48     |
| 1:A:458:C:H2'     | 1:A:459:G:O4'    | 2.14        | 0.48     |
| 6:E:144:THR:HG22  | 6:E:146:ALA:H    | 1.79        | 0.48     |
| 4:C:77:ILE:HG22   | 4:C:81:GLY:HA2   | 1.95        | 0.48     |
| 11:J:48:THR:OG1   | 11:J:62:HIS:CD2  | 2.66        | 0.48     |
| 4:C:204:LEU:O     | 4:C:205:GLY:C    | 2.51        | 0.48     |
| 10:I:108:VAL:HG12 | 10:I:109:VAL:H   | 1.78        | 0.48     |
| 5:D:64:LEU:HD13   | 5:D:75:PHE:HZ    | 1.79        | 0.48     |
| 9:H:108:GLY:HA3   | 9:H:138:TRP:HB3  | 1.96        | 0.48     |
| 21:T:72:LEU:HD23  | 21:T:72:LEU:HA   | 1.72        | 0.48     |
| 15:N:23:ARG:HD3   | 15:N:30:ALA:HB2  | 1.96        | 0.48     |
| 1:A:1420:C:H2'    | 1:A:1421:G:C8    | 2.49        | 0.48     |
| 1:A:635:G:O2'     | 1:A:636:U:H5'    | 2.13        | 0.48     |
| 1:A:41:G:H2'      | 1:A:42:G:H8      | 1.78        | 0.48     |
| 14:M:79:LYS:O     | 14:M:83:ASP:OD2  | 2.32        | 0.48     |
| 5:D:33:MET:HE3    | 5:D:37:PRO:CB    | 2.40        | 0.48     |
| 11:J:51:ARG:N     | 11:J:59:SER:HB3  | 2.29        | 0.48     |
| 1:A:760:G:O6      | 18:Q:105:ALA:CB  | 2.59        | 0.48     |
| 4:C:32:LEU:HD23   | 4:C:32:LEU:O     | 2.14        | 0.48     |
| 4:C:95:THR:C      | 4:C:97:LYS:N     | 2.67        | 0.48     |
| 1:A:1256:A:H61    | 1:A:1278:U:H1'   | 1.75        | 0.48     |
| 11:J:19:SER:O     | 11:J:23:ILE:HD13 | 2.14        | 0.48     |
| 1:A:959:A:H2'     | 1:A:960:U:O4'    | 2.14        | 0.48     |
| 1:A:1426:C:H2'    | 1:A:1427:U:H6    | 1.78        | 0.48     |
| 1:A:1096:C:O2'    | 1:A:1097:C:H5'   | 2.14        | 0.48     |
| 1:A:736:C:OP2     | 19:R:68:LYS:HE2  | 2.14        | 0.48     |
| 13:L:67:THR:HG22  | 13:L:96:VAL:HG13 | 1.96        | 0.48     |
| 20:S:5:LEU:O      | 20:S:6:LYS:HG3   | 2.14        | 0.48     |
| 1:A:1380:U:O2'    | 1:A:1381:U:OP2   | 2.31        | 0.48     |
| 1:A:913:A:O2'     | 1:A:914:A:P      | 2.72        | 0.48     |
| 1:A:862:C:O2'     | 1:A:863:U:H5'    | 2.14        | 0.48     |
| 1:A:308:C:H2'     | 1:A:309:G:C8     | 2.48        | 0.48     |
| 1:A:523:A:H61     | 13:L:92:ASP:HB2  | 1.78        | 0.48     |
| 14:M:96:LEU:O     | 14:M:110:ARG:NH1 | 2.47        | 0.48     |
| 1:A:934:C:C4      | 1:A:1345:U:C5    | 3.02        | 0.48     |
| 1:A:39:G:O2'      | 1:A:40:C:H5'     | 2.13        | 0.48     |
| 6:E:137:GLU:O     | 6:E:141:GLN:HG3  | 2.13        | 0.48     |
| 6:E:143:ARG:NH1   | 9:H:77:GLU:OE2   | 2.46        | 0.48     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:1306:A:O2'   | 14:M:109:THR:HG21 | 2.13        | 0.48     |
| 1:A:1152:A:H2'   | 1:A:1153:C:C6     | 2.49        | 0.48     |
| 5:D:162:LEU:HD23 | 5:D:165:MET:HG3   | 1.96        | 0.48     |
| 1:A:1005:A:H2'   | 1:A:1006:C:H5'    | 1.94        | 0.48     |
| 1:A:1392:G:H2'   | 1:A:1393:U:C6     | 2.49        | 0.48     |
| 21:T:50:GLU:O    | 21:T:100:ILE:HD12 | 2.14        | 0.48     |
| 1:A:197:A:H1'    | 1:A:198:G:O4'     | 2.14        | 0.48     |
| 7:F:11:ASN:O     | 7:F:14:LEU:HG     | 2.13        | 0.48     |
| 19:R:46:GLU:CD   | 19:R:46:GLU:N     | 2.67        | 0.48     |
| 8:G:124:LEU:O    | 8:G:127:ALA:HB3   | 2.14        | 0.48     |
| 4:C:33:LEU:HD23  | 4:C:33:LEU:C      | 2.33        | 0.47     |
| 12:K:56:GLY:O    | 12:K:57:THR:O     | 2.32        | 0.47     |
| 3:B:92:TYR:CE1   | 3:B:151:GLY:HA3   | 2.48        | 0.47     |
| 1:A:1277:C:C2'   | 1:A:1278:U:H5'    | 2.43        | 0.47     |
| 1:A:953:G:H1'    | 14:M:125:ARG:CA   | 2.44        | 0.47     |
| 4:C:108:ASN:OD1  | 4:C:110:ASN:HB2   | 2.14        | 0.47     |
| 3:B:208:ILE:O    | 3:B:210:SER:N     | 2.47        | 0.47     |
| 16:O:87:ILE:HG22 | 16:O:88:ARG:N     | 2.29        | 0.47     |
| 13:L:58:VAL:O    | 13:L:65:GLU:HA    | 2.14        | 0.47     |
| 4:C:60:ALA:O     | 4:C:61:ALA:CB     | 2.61        | 0.47     |
| 1:A:1064:G:H4'   | 1:A:1065:U:H5''   | 1.92        | 0.47     |
| 1:A:1065:U:H5''  | 1:A:1066:C:H5'    | 1.97        | 0.47     |
| 17:P:55:ARG:O    | 17:P:56:ALA:C     | 2.51        | 0.47     |
| 1:A:1298:C:C4    | 8:G:114:ARG:HD3   | 2.49        | 0.47     |
| 1:A:255:G:H1'    | 18:Q:16:GLN:HE22  | 1.79        | 0.47     |
| 1:A:1056:U:O2    | 1:A:1056:U:H2'    | 2.13        | 0.47     |
| 1:A:920:U:H2'    | 1:A:921:U:H6      | 1.78        | 0.47     |
| 1:A:498:U:O2'    | 1:A:499:A:H5'     | 2.14        | 0.47     |
| 1:A:1516:G:H2'   | 1:A:1518:A:OP2    | 2.14        | 0.47     |
| 5:D:88:VAL:O     | 5:D:92:VAL:HG23   | 2.14        | 0.47     |
| 6:E:115:VAL:HG11 | 6:E:118:ILE:HG13  | 1.97        | 0.47     |
| 20:S:63:THR:HG22 | 20:S:64:GLU:N     | 2.30        | 0.47     |
| 1:A:994:A:H8     | 1:A:994:A:OP1     | 1.97        | 0.47     |
| 1:A:518:C:H5''   | 1:A:519:C:C6      | 2.49        | 0.47     |
| 4:C:190:ARG:NH1  | 4:C:190:ARG:CB    | 2.78        | 0.47     |
| 1:A:216:G:H2'    | 1:A:217:C:C6      | 2.49        | 0.47     |
| 1:A:409:G:H2'    | 1:A:410:G:O4'     | 2.13        | 0.47     |
| 10:I:5:TYR:O     | 10:I:84:ALA:HA    | 2.14        | 0.47     |
| 4:C:42:LEU:HD12  | 4:C:94:LEU:HD12   | 1.97        | 0.47     |
| 4:C:188:LEU:HD13 | 4:C:189:ALA:N     | 2.27        | 0.47     |
| 1:A:1286:A:C8    | 1:A:1287:A:C5'    | 2.96        | 0.47     |
| 5:D:53:ASP:O     | 5:D:57:ARG:HD3    | 2.14        | 0.47     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 8:G:114:ARG:HG2  | 8:G:114:ARG:HH11 | 1.79        | 0.47     |
| 1:A:792:A:H4'    | 1:A:793:U:H5''   | 1.97        | 0.47     |
| 1:A:1513:A:H2'   | 1:A:1514:C:C6    | 2.49        | 0.47     |
| 7:F:91:VAL:HG12  | 7:F:92:LYS:O     | 2.14        | 0.47     |
| 14:M:32:GLU:O    | 14:M:35:GLU:HB3  | 2.15        | 0.47     |
| 1:A:582:U:C2     | 1:A:760:G:C6     | 3.02        | 0.47     |
| 4:C:46:GLU:C     | 4:C:48:TYR:H     | 2.16        | 0.47     |
| 1:A:1250:A:H5''  | 10:I:67:GLY:C    | 2.35        | 0.47     |
| 1:A:438:G:C4'    | 1:A:439:A:OP1    | 2.55        | 0.47     |
| 5:D:67:ILE:HG22  | 5:D:68:TYR:CD1   | 2.49        | 0.47     |
| 20:S:20:LEU:C    | 20:S:22:LEU:N    | 2.68        | 0.47     |
| 14:M:34:LEU:CD1  | 14:M:41:PRO:HA   | 2.45        | 0.47     |
| 1:A:276:G:O2'    | 1:A:277:C:H5'    | 2.14        | 0.47     |
| 4:C:79:ARG:CG    | 4:C:82:GLU:HG2   | 2.42        | 0.47     |
| 1:A:31:G:C2      | 1:A:48:C:H5''    | 2.50        | 0.47     |
| 7:F:95:GLU:N     | 7:F:95:GLU:CD    | 2.68        | 0.47     |
| 1:A:160:A:H1'    | 1:A:344:A:N7     | 2.28        | 0.47     |
| 10:I:69:GLY:O    | 10:I:73:GLN:HG3  | 2.14        | 0.47     |
| 1:A:356:A:O2'    | 1:A:357:G:H5'    | 2.15        | 0.47     |
| 1:A:802:A:H2'    | 1:A:803:G:O4'    | 2.15        | 0.47     |
| 1:A:60:A:H4'     | 1:A:61:G:O5'     | 2.14        | 0.47     |
| 17:P:26:ARG:HE   | 17:P:31:LYS:HB3  | 1.78        | 0.47     |
| 4:C:47:LEU:N     | 4:C:47:LEU:CD1   | 2.76        | 0.47     |
| 4:C:110:ASN:HB3  | 4:C:144:SER:OG   | 2.13        | 0.47     |
| 1:A:1367:C:H5'   | 11:J:60:ARG:NH1  | 2.29        | 0.47     |
| 4:C:205:GLY:O    | 4:C:206:GLU:HB2  | 2.13        | 0.47     |
| 5:D:160:GLN:O    | 5:D:163:GLU:HB3  | 2.14        | 0.47     |
| 9:H:103:VAL:HG23 | 9:H:110:ALA:HB2  | 1.96        | 0.47     |
| 10:I:120:ARG:O   | 10:I:122:ALA:N   | 2.47        | 0.47     |
| 9:H:51:VAL:HG12  | 9:H:52:ASP:N     | 2.29        | 0.47     |
| 21:T:56:MET:HE1  | 21:T:104:LEU:HG  | 1.97        | 0.47     |
| 3:B:195:ASP:O    | 9:H:74:PRO:HG3   | 2.14        | 0.47     |
| 1:A:488:C:O2'    | 1:A:489:C:H5'    | 2.15        | 0.47     |
| 1:A:730:G:H21    | 1:A:765:G:H5''   | 1.78        | 0.47     |
| 6:E:24:ARG:NH1   | 6:E:24:ARG:HG2   | 2.27        | 0.47     |
| 1:A:743:U:H2'    | 1:A:744:C:H6     | 1.78        | 0.47     |
| 1:A:103:C:OP1    | 21:T:17:ARG:HD2  | 2.14        | 0.47     |
| 4:C:77:ILE:CG2   | 4:C:81:GLY:HA2   | 2.45        | 0.47     |
| 1:A:1327:C:O2'   | 1:A:1328:C:H5'   | 2.14        | 0.47     |
| 1:A:67:C:H4'     | 1:A:172:A:O4'    | 2.14        | 0.47     |
| 1:A:836:G:C6     | 1:A:851:G:C6     | 3.02        | 0.47     |
| 13:L:33:ARG:HH11 | 13:L:62:SER:HB3  | 1.80        | 0.47     |

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| Atom-1          | Atom-2           | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 4:C:28:GLN:O    | 4:C:31:HIS:N     | 2.40        | 0.47     |
| 4:C:156:ARG:NH2 | 4:C:161:GLU:HA   | 2.29        | 0.47     |
| 3:B:206:ASP:CG  | 3:B:207:ALA:N    | 2.68        | 0.47     |
| 1:A:1279:A:O2'  | 1:A:1282:C:N4    | 2.48        | 0.47     |
| 1:A:6:G:H4'     | 1:A:298:A:H4'    | 1.95        | 0.47     |
| 5:D:30:LYS:O    | 5:D:32:ALA:N     | 2.48        | 0.47     |
| 1:A:1366:C:HO2' | 11:J:60:ARG:HH22 | 1.61        | 0.47     |
| 11:J:49:VAL:CG1 | 15:N:41:ARG:HB2  | 2.44        | 0.47     |
| 1:A:974:A:P     | 15:N:31:ARG:HG2  | 2.55        | 0.47     |
| 4:C:71:ALA:HA   | 4:C:106:VAL:HB   | 1.96        | 0.47     |
| 1:A:1238:A:H5'  | 1:A:1336:C:N4    | 2.21        | 0.47     |
| 1:A:1303:C:H2'  | 1:A:1304:G:H5'   | 1.97        | 0.47     |
| 5:D:196:LEU:C   | 5:D:198:VAL:N    | 2.68        | 0.47     |
| 5:D:78:LEU:CD1  | 5:D:97:LEU:HD23  | 2.44        | 0.47     |
| 8:G:18:TYR:HD2  | 8:G:59:LEU:HD22  | 1.80        | 0.47     |
| 8:G:59:LEU:O    | 8:G:63:LYS:HG3   | 2.15        | 0.47     |
| 1:A:1298:C:H2'  | 8:G:114:ARG:NH1  | 2.29        | 0.47     |
| 6:E:31:LEU:HD22 | 6:E:43:LEU:CD2   | 2.44        | 0.47     |
| 3:B:23:ARG:HH12 | 3:B:191:ASP:HA   | 1.79        | 0.47     |
| 1:A:781:A:H2    | 1:A:1514:C:C4'   | 2.28        | 0.47     |
| 1:A:854:G:C6    | 1:A:855:G:N7     | 2.82        | 0.47     |
| 1:A:1213:A:N1   | 1:A:1215:G:H1'   | 2.29        | 0.47     |
| 14:M:46:LYS:HE2 | 14:M:47:ASP:OD1  | 2.14        | 0.47     |
| 6:E:33:VAL:HG11 | 6:E:109:ILE:HA   | 1.97        | 0.47     |
| 7:F:43:LEU:N    | 7:F:43:LEU:HD22  | 2.29        | 0.47     |
| 16:O:10:LYS:HD2 | 16:O:10:LYS:O    | 2.14        | 0.47     |
| 3:B:119:GLU:OE1 | 3:B:153:ARG:NH2  | 2.37        | 0.47     |
| 3:B:151:GLY:C   | 3:B:153:ARG:H    | 2.17        | 0.47     |
| 4:C:70:VAL:HG21 | 4:C:76:VAL:HG21  | 1.96        | 0.47     |
| 1:A:1523:G:OP1  | 12:K:123:LYS:HD2 | 2.15        | 0.47     |
| 12:K:46:GLY:O   | 12:K:47:VAL:C    | 2.52        | 0.47     |
| 9:H:84:ARG:HD2  | 9:H:85:ARG:O     | 2.14        | 0.47     |
| 1:A:649:G:O2'   | 1:A:650:G:H5'    | 2.14        | 0.47     |
| 7:F:12:PRO:HG3  | 7:F:55:ASP:OD1   | 2.15        | 0.47     |
| 7:F:62:TRP:CD1  | 19:R:35:ARG:NH1  | 2.83        | 0.47     |
| 13:L:89:ARG:HG2 | 13:L:97:ARG:HA   | 1.95        | 0.47     |
| 1:A:1060:C:C4   | 4:C:2:GLY:HA3    | 2.50        | 0.47     |
| 1:A:1138:G:H2'  | 1:A:1140:C:H5'   | 1.97        | 0.47     |
| 1:A:953:G:N7    | 14:M:104:ARG:NH2 | 2.62        | 0.47     |
| 19:R:53:ARG:C   | 19:R:55:ARG:H    | 2.18        | 0.47     |
| 19:R:45:SER:C   | 19:R:47:THR:N    | 2.66        | 0.47     |
| 1:A:1440:C:H2'  | 1:A:1441:G:H5'   | 1.97        | 0.47     |

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| Atom-1            | Atom-2           | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:A:42:G:H2'      | 1:A:43:C:C6      | 2.50        | 0.47     |
| 1:A:138:G:O2'     | 1:A:139:G:H5'    | 2.15        | 0.47     |
| 17:P:9:PHE:CE2    | 17:P:18:ARG:HD2  | 2.50        | 0.47     |
| 13:L:71:PRO:O     | 13:L:102:ARG:HD2 | 2.15        | 0.47     |
| 1:A:115:G:H1'     | 1:A:116:A:N7     | 2.29        | 0.47     |
| 1:A:760:G:H2'     | 1:A:761:G:H5'    | 1.97        | 0.47     |
| 1:A:337:C:H2'     | 1:A:338:A:C8     | 2.50        | 0.47     |
| 15:N:60:SER:H     | 15:N:61:TRP:HE3  | 1.63        | 0.47     |
| 4:C:8:ILE:C       | 4:C:10:PHE:N     | 2.69        | 0.47     |
| 3:B:95:GLN:OE1    | 3:B:95:GLN:HA    | 2.14        | 0.47     |
| 6:E:76:ILE:O      | 6:E:93:PRO:HB3   | 2.15        | 0.47     |
| 6:E:31:LEU:HD23   | 6:E:31:LEU:HA    | 1.66        | 0.47     |
| 1:A:148:G:H2'     | 1:A:149:A:H8     | 1.79        | 0.47     |
| 18:Q:27:PHE:CZ    | 18:Q:36:ILE:HD11 | 2.50        | 0.47     |
| 1:A:1187:G:OP1    | 10:I:113:LYS:HE2 | 2.15        | 0.47     |
| 4:C:121:ALA:O     | 4:C:125:GLU:HG3  | 2.15        | 0.47     |
| 1:A:1253:G:H2'    | 1:A:1254:C:C6    | 2.50        | 0.46     |
| 12:K:109:VAL:HG13 | 19:R:85:LEU:O    | 2.15        | 0.46     |
| 1:A:1058:G:O2'    | 1:A:1059:C:H5'   | 2.15        | 0.46     |
| 5:D:109:GLY:HA3   | 5:D:165:MET:SD   | 2.55        | 0.46     |
| 1:A:1347:G:HO2'   | 1:A:1373:G:H1    | 1.62        | 0.46     |
| 4:C:182:ILE:HG12  | 4:C:203:PHE:HD1  | 1.80        | 0.46     |
| 1:A:264:U:O2'     | 18:Q:64:PRO:HB2  | 2.14        | 0.46     |
| 1:A:266:G:O3'     | 18:Q:67:LYS:HB2  | 2.14        | 0.46     |
| 14:M:9:ILE:N      | 14:M:9:ILE:HD12  | 2.30        | 0.46     |
| 1:A:1480:G:O2'    | 1:A:1481:U:H5'   | 2.16        | 0.46     |
| 1:A:965:A:H4'     | 1:A:966:G:O5'    | 2.15        | 0.46     |
| 3:B:59:GLU:HG2    | 3:B:221:LEU:HD11 | 1.96        | 0.46     |
| 1:A:189:G:H2'     | 1:A:190:C:H6     | 1.80        | 0.46     |
| 1:A:426:G:O2'     | 1:A:427:U:H5'    | 2.15        | 0.46     |
| 1:A:1123:A:H4'    | 11:J:37:PRO:HD2  | 1.96        | 0.46     |
| 1:A:243:A:H5''    | 1:A:244:U:H5'    | 1.97        | 0.46     |
| 6:E:79:GLU:N      | 6:E:79:GLU:OE1   | 2.47        | 0.46     |
| 20:S:20:LEU:C     | 20:S:22:LEU:H    | 2.17        | 0.46     |
| 5:D:58:LEU:HD23   | 5:D:206:PHE:CE1  | 2.50        | 0.46     |
| 1:A:373:A:H1'     | 1:A:481:G:H1'    | 1.96        | 0.46     |
| 1:A:812:C:O2'     | 1:A:813:U:OP2    | 2.23        | 0.46     |
| 1:A:1020:U:H2'    | 1:A:1021:G:C8    | 2.50        | 0.46     |
| 1:A:163:C:O2'     | 1:A:164:U:H5'    | 2.16        | 0.46     |
| 1:A:781:A:H2'     | 1:A:782:A:H5'    | 1.96        | 0.46     |
| 1:A:93:G:O2'      | 1:A:95:U:H5'     | 2.15        | 0.46     |
| 9:H:75:ARG:HA     | 9:H:76:PRO:HD3   | 1.67        | 0.46     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 21:T:45:GLN:HB2  | 21:T:91:LEU:HD22 | 1.97        | 0.46     |
| 1:A:814:A:N7     | 1:A:816:A:C4     | 2.83        | 0.46     |
| 1:A:774:G:O2'    | 1:A:775:G:H5'    | 2.16        | 0.46     |
| 1:A:590:C:O2'    | 1:A:591:U:H5'    | 2.15        | 0.46     |
| 15:N:45:ARG:HH11 | 15:N:45:ARG:HG3  | 1.80        | 0.46     |
| 1:A:1138:G:N3    | 1:A:1138:G:H3'   | 2.31        | 0.46     |
| 1:A:338:A:H2     | 1:A:351:G:H22    | 1.62        | 0.46     |
| 19:R:59:SER:OG   | 19:R:62:GLU:HG3  | 2.15        | 0.46     |
| 3:B:236:TYR:HA   | 3:B:239:VAL:HG23 | 1.96        | 0.46     |
| 3:B:103:THR:HA   | 3:B:180:LEU:HD11 | 1.97        | 0.46     |
| 3:B:97:TRP:CH2   | 3:B:176:GLU:CD   | 2.89        | 0.46     |
| 6:E:76:ILE:HG23  | 6:E:142:LEU:HD22 | 1.97        | 0.46     |
| 19:R:87:ARG:HG2  | 19:R:87:ARG:NH1  | 2.29        | 0.46     |
| 1:A:977:A:C2'    | 1:A:978:A:H5''   | 2.45        | 0.46     |
| 8:G:24:THR:HG22  | 8:G:28:ASN:HD21  | 1.80        | 0.46     |
| 9:H:114:THR:C    | 9:H:116:LYS:H    | 2.19        | 0.46     |
| 1:A:1049:U:H1'   | 1:A:1201:A:N7    | 2.30        | 0.46     |
| 12:K:54:ARG:NH1  | 12:K:54:ARG:HB3  | 2.14        | 0.46     |
| 1:A:1068:G:N2    | 1:A:1191:A:N3    | 2.61        | 0.46     |
| 1:A:954:G:H2'    | 1:A:955:U:C6     | 2.50        | 0.46     |
| 1:A:1005:A:C2'   | 1:A:1006:C:H5'   | 2.46        | 0.46     |
| 1:A:269:C:H2'    | 1:A:270:A:C8     | 2.49        | 0.46     |
| 6:E:102:ALA:HA   | 6:E:120:THR:CG2  | 2.45        | 0.46     |
| 18:Q:74:LEU:C    | 18:Q:74:LEU:CD2  | 2.83        | 0.46     |
| 9:H:28:ALA:HB3   | 9:H:57:PRO:HB2   | 1.96        | 0.46     |
| 10:I:113:LYS:HD2 | 10:I:113:LYS:H   | 1.79        | 0.46     |
| 1:A:750:G:H1'    | 16:O:22:THR:OG1  | 2.15        | 0.46     |
| 1:A:938:A:H8     | 1:A:938:A:O5'    | 1.98        | 0.46     |
| 13:L:28:LYS:HG3  | 13:L:33:ARG:HH12 | 1.79        | 0.46     |
| 1:A:761:G:H2'    | 1:A:762:C:C6     | 2.51        | 0.46     |
| 1:A:1256:A:H4'   | 1:A:1257:U:C5'   | 2.40        | 0.46     |
| 4:C:108:ASN:C    | 4:C:110:ASN:N    | 2.69        | 0.46     |
| 11:J:54:PHE:HD2  | 11:J:55:LYS:HD3  | 1.77        | 0.46     |
| 1:A:960:U:H1'    | 1:A:1223:C:H5'   | 1.98        | 0.46     |
| 10:I:44:VAL:HG12 | 10:I:44:VAL:O    | 2.16        | 0.46     |
| 1:A:791:G:C2'    | 1:A:792:A:C5'    | 2.94        | 0.46     |
| 4:C:83:ARG:HA    | 4:C:86:VAL:HG23  | 1.98        | 0.46     |
| 1:A:722:A:H4'    | 1:A:723:U:C5     | 2.50        | 0.46     |
| 10:I:111:ARG:O   | 10:I:119:ALA:HB2 | 2.16        | 0.46     |
| 1:A:397:A:H5'    | 1:A:398:C:P      | 2.56        | 0.46     |
| 1:A:865:A:H2'    | 1:A:866:C:C6     | 2.51        | 0.46     |
| 1:A:89:C:O2'     | 1:A:90:U:H5'     | 2.15        | 0.46     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 21:T:42:GLN:O    | 21:T:45:GLN:HB3   | 2.16        | 0.46     |
| 1:A:247:G:OP2    | 18:Q:100:LYS:HG3  | 2.16        | 0.46     |
| 18:Q:10:VAL:HG13 | 18:Q:19:VAL:HB    | 1.98        | 0.46     |
| 7:F:40:VAL:CG2   | 7:F:41:GLU:N      | 2.79        | 0.46     |
| 1:A:452:A:H2'    | 1:A:453:A:H8      | 1.81        | 0.46     |
| 8:G:141:VAL:O    | 8:G:144:MET:HB2   | 2.16        | 0.46     |
| 13:L:27:LEU:HG   | 13:L:28:LYS:N     | 2.24        | 0.46     |
| 1:A:1063:C:H2'   | 1:A:1064:G:C8     | 2.50        | 0.46     |
| 14:M:26:GLY:O    | 14:M:28:ALA:N     | 2.49        | 0.46     |
| 4:C:50:ALA:HB2   | 4:C:75:VAL:HB     | 1.96        | 0.46     |
| 4:C:173:VAL:N    | 4:C:174:PRO:CD    | 2.78        | 0.46     |
| 1:A:1003(A):G:N1 | 1:A:1004:A:H1'    | 2.30        | 0.46     |
| 21:T:56:MET:HG2  | 21:T:84:LEU:HD11  | 1.98        | 0.46     |
| 1:A:135:C:C2     | 17:P:1:MET:HB2    | 2.50        | 0.46     |
| 1:A:16:A:N1      | 1:A:919:A:H2      | 2.12        | 0.46     |
| 1:A:619:U:N3     | 5:D:134:ASP:OD1   | 2.48        | 0.46     |
| 1:A:980:C:H2'    | 1:A:981:U:O4'     | 2.16        | 0.46     |
| 4:C:141:VAL:O    | 4:C:146:ALA:HB3   | 2.16        | 0.46     |
| 5:D:130:GLY:O    | 5:D:131:ARG:C     | 2.53        | 0.46     |
| 15:N:50:LYS:HD3  | 15:N:52:GLN:NE2   | 2.31        | 0.46     |
| 1:A:154:C:H2'    | 1:A:155:C:H6      | 1.81        | 0.46     |
| 1:A:51:A:H4'     | 1:A:52:G:C5'      | 2.46        | 0.46     |
| 1:A:995:C:H2'    | 1:A:995:C:O2      | 2.14        | 0.46     |
| 5:D:98:GLU:HG2   | 5:D:189:PRO:HG3   | 1.98        | 0.46     |
| 1:A:1494:G:OP2   | 25:A:1632:HYG:O11 | 2.30        | 0.46     |
| 3:B:208:ILE:HG22 | 3:B:209:ARG:N     | 2.31        | 0.46     |
| 5:D:196:LEU:O    | 5:D:198:VAL:N     | 2.42        | 0.46     |
| 7:F:30:LEU:HA    | 7:F:75:LEU:HD21   | 1.96        | 0.46     |
| 18:Q:15:MET:HB2  | 18:Q:18:THR:HB    | 1.98        | 0.46     |
| 1:A:98:U:O2'     | 1:A:99:C:H5'      | 2.15        | 0.46     |
| 1:A:815:A:H4'    | 1:A:817:C:C4      | 2.51        | 0.46     |
| 18:Q:81:ARG:NH2  | 18:Q:83:ASP:OD2   | 2.47        | 0.46     |
| 1:A:1244:C:O2'   | 1:A:1245:A:H5'    | 2.16        | 0.46     |
| 1:A:1525:G:P     | 12:K:120:ARG:HH22 | 2.39        | 0.46     |
| 1:A:1070:U:O2'   | 1:A:1071:C:H5'    | 2.16        | 0.46     |
| 3:B:224:GLN:O    | 3:B:226:ARG:N     | 2.48        | 0.46     |
| 3:B:83:MET:HE3   | 3:B:235:SER:N     | 2.30        | 0.46     |
| 1:A:1127:G:N2    | 1:A:1144:G:N2     | 2.64        | 0.46     |
| 1:A:1085:U:O3'   | 1:A:1086:U:C6     | 2.69        | 0.46     |
| 14:M:120:LYS:HE2 | 14:M:123:ALA:HB2  | 1.98        | 0.46     |
| 19:R:53:ARG:HE   | 19:R:60:GLY:N     | 2.13        | 0.46     |
| 3:B:197:VAL:HB   | 3:B:200:ILE:CG1   | 2.39        | 0.46     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 4:C:174:PRO:O    | 4:C:177:THR:HG22  | 2.16        | 0.46     |
| 1:A:839:U:C2'    | 1:A:839:U:O2      | 2.60        | 0.46     |
| 6:E:76:ILE:HG23  | 6:E:77:PRO:HD2    | 1.97        | 0.46     |
| 13:L:46:LYS:O    | 13:L:47:LYS:C     | 2.54        | 0.46     |
| 17:P:17:TYR:CE1  | 17:P:41:PRO:HG2   | 2.51        | 0.46     |
| 1:A:463:A:H2'    | 1:A:474:G:O4'     | 2.15        | 0.46     |
| 1:A:106:C:O2'    | 1:A:379:C:H5''    | 2.16        | 0.46     |
| 13:L:86:ARG:HG3  | 13:L:86:ARG:HH11  | 1.80        | 0.46     |
| 20:S:5:LEU:O     | 20:S:6:LYS:CG     | 2.64        | 0.46     |
| 1:A:193:C:H2'    | 1:A:194:C:H6      | 1.80        | 0.46     |
| 1:A:192:U:O2'    | 1:A:193:C:H5'     | 2.16        | 0.46     |
| 1:A:259:G:O2'    | 1:A:260:G:H5'     | 2.15        | 0.46     |
| 21:T:38:LYS:O    | 21:T:42:GLN:HB2   | 2.15        | 0.46     |
| 1:A:583:A:H2'    | 1:A:584:G:O4'     | 2.16        | 0.46     |
| 5:D:103:ASN:O    | 5:D:106:TYR:HB3   | 2.16        | 0.46     |
| 1:A:1285:A:H8    | 1:A:1285:A:OP1    | 1.99        | 0.46     |
| 6:E:115:VAL:HG11 | 6:E:118:ILE:CG1   | 2.46        | 0.46     |
| 4:C:139:GLN:O    | 4:C:143:GLU:N     | 2.37        | 0.46     |
| 3:B:97:TRP:HH2   | 3:B:176:GLU:CD    | 2.20        | 0.46     |
| 1:A:1056:U:H5'   | 4:C:163:ALA:CB    | 2.46        | 0.46     |
| 1:A:1145:C:O2'   | 1:A:1146:A:C8     | 2.64        | 0.46     |
| 21:T:67:ALA:HB2  | 21:T:77:ALA:HB2   | 1.97        | 0.46     |
| 5:D:17:VAL:CG1   | 5:D:18:LYS:N      | 2.79        | 0.46     |
| 3:B:105:PHE:HB2  | 3:B:158:LEU:HD21  | 1.97        | 0.46     |
| 1:A:581:G:HO2'   | 18:Q:105:ALA:C    | 2.18        | 0.46     |
| 4:C:64:VAL:HB    | 4:C:99:VAL:HB     | 1.98        | 0.46     |
| 15:N:59:ALA:HB1  | 15:N:61:TRP:HZ3   | 1.79        | 0.46     |
| 4:C:139:GLN:O    | 4:C:140:ARG:C     | 2.54        | 0.46     |
| 1:A:960:U:O2'    | 1:A:1223:C:H4'    | 2.16        | 0.46     |
| 10:I:108:VAL:CG1 | 10:I:109:VAL:H    | 2.29        | 0.46     |
| 6:E:112:LEU:C    | 6:E:114:GLY:H     | 2.18        | 0.46     |
| 1:A:1004:A:C8    | 1:A:1037:C:O2     | 2.69        | 0.46     |
| 1:A:1183:A:C2'   | 1:A:1184:G:OP1    | 2.64        | 0.46     |
| 1:A:1343:G:C1'   | 10:I:121:ARG:HH12 | 2.25        | 0.46     |
| 5:D:114:ARG:NH1  | 5:D:114:ARG:HG3   | 2.26        | 0.46     |
| 1:A:253:U:H2'    | 1:A:254:G:H8      | 1.79        | 0.46     |
| 13:L:6:THR:HG1   | 13:L:9:GLN:HG3    | 1.79        | 0.46     |
| 1:A:21:G:H2'     | 1:A:22:G:C8       | 2.50        | 0.46     |
| 14:M:94:ARG:HH12 | 20:S:81:ARG:CD    | 2.29        | 0.46     |
| 1:A:1044:A:H2'   | 1:A:1045:C:C5'    | 2.46        | 0.46     |
| 1:A:1118:C:H2'   | 1:A:1119:C:H6     | 1.80        | 0.46     |
| 1:A:1150:U:H6    | 1:A:1150:U:O5'    | 2.00        | 0.45     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 11:J:40:LEU:HB3  | 11:J:69:ASN:HB2  | 1.98        | 0.45     |
| 19:R:39:VAL:CG1  | 19:R:40:LEU:N    | 2.78        | 0.45     |
| 1:A:1220:G:H1'   | 20:S:52:TYR:HD2  | 1.82        | 0.45     |
| 6:E:9:LYS:HG3    | 6:E:112:LEU:HD11 | 1.97        | 0.45     |
| 6:E:93:PRO:HG3   | 9:H:105:ARG:HE   | 1.79        | 0.45     |
| 1:A:406:G:H2'    | 1:A:407:G:H8     | 1.82        | 0.45     |
| 1:A:101:A:H2'    | 1:A:102:G:H8     | 1.81        | 0.45     |
| 1:A:421:U:H5'    | 1:A:422:C:H5     | 1.80        | 0.45     |
| 1:A:248:C:C2'    | 1:A:249:U:H5'    | 2.46        | 0.45     |
| 1:A:767:A:H2'    | 1:A:768:A:C8     | 2.51        | 0.45     |
| 4:C:35:GLU:CG    | 4:C:59:ARG:HH22  | 2.29        | 0.45     |
| 4:C:156:ARG:HH21 | 4:C:161:GLU:HA   | 1.82        | 0.45     |
| 1:A:1286:A:C3'   | 1:A:1287:A:C5'   | 2.85        | 0.45     |
| 1:A:1256:A:H2    | 1:A:1258:G:C2    | 2.33        | 0.45     |
| 8:G:156:TRP:OXT  | 8:G:156:TRP:HD1  | 2.00        | 0.45     |
| 1:A:281:G:HO2'   | 1:A:282:A:P      | 2.39        | 0.45     |
| 4:C:172:ARG:HB3  | 4:C:172:ARG:NH1  | 2.32        | 0.45     |
| 5:D:68:TYR:OH    | 5:D:196:LEU:HD11 | 2.16        | 0.45     |
| 10:I:120:ARG:O   | 10:I:121:ARG:C   | 2.54        | 0.45     |
| 10:I:42:ARG:O    | 10:I:43:ALA:C    | 2.54        | 0.45     |
| 7:F:101:ALA:CA   | 19:R:28:GLU:HB3  | 2.42        | 0.45     |
| 22:V:15:ARG:O    | 22:V:17:THR:HG23 | 2.17        | 0.45     |
| 6:E:65:ASN:CG    | 6:E:65:ASN:O     | 2.55        | 0.45     |
| 21:T:73:HIS:C    | 21:T:74:LYS:HG2  | 2.37        | 0.45     |
| 6:E:102:ALA:HA   | 6:E:120:THR:HG22 | 1.98        | 0.45     |
| 1:A:437:U:C5'    | 5:D:155:LEU:HD22 | 2.45        | 0.45     |
| 1:A:1514:C:H2'   | 1:A:1515:C:H6    | 1.80        | 0.45     |
| 14:M:94:ARG:NH1  | 20:S:81:ARG:HD3  | 2.30        | 0.45     |
| 5:D:145:GLU:CG   | 5:D:184:LYS:HE2  | 2.47        | 0.45     |
| 7:F:43:LEU:N     | 7:F:43:LEU:CD2   | 2.79        | 0.45     |
| 20:S:61:TYR:HD2  | 20:S:61:TYR:C    | 2.19        | 0.45     |
| 11:J:21:GLN:O    | 11:J:25:GLU:HG3  | 2.16        | 0.45     |
| 4:C:91:LEU:HD23  | 4:C:92:ALA:N     | 2.31        | 0.45     |
| 1:A:1286:A:H8    | 1:A:1287:A:C5'   | 2.29        | 0.45     |
| 11:J:8:LEU:HD21  | 11:J:96:ILE:HG12 | 1.97        | 0.45     |
| 8:G:78:ARG:HD2   | 8:G:156:TRP:CE3  | 2.50        | 0.45     |
| 1:A:1366:C:C2    | 1:A:1367:C:C5    | 3.04        | 0.45     |
| 3:B:134:GLU:C    | 3:B:136:VAL:N    | 2.69        | 0.45     |
| 16:O:45:VAL:HB   | 16:O:46:HIS:ND1  | 2.31        | 0.45     |
| 4:C:7:PRO:O      | 4:C:11:ARG:HD2   | 2.15        | 0.45     |
| 16:O:71:GLN:HG3  | 16:O:78:TYR:CE2  | 2.52        | 0.45     |
| 13:L:32:PHE:CE1  | 13:L:86:ARG:HB2  | 2.52        | 0.45     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:1313:U:OP2   | 20:S:6:LYS:HA    | 2.16        | 0.45     |
| 1:A:1308:U:H2'   | 1:A:1309:G:H8    | 1.81        | 0.45     |
| 6:E:28:PHE:O     | 6:E:47:LYS:HA    | 2.16        | 0.45     |
| 3:B:224:GLN:C    | 3:B:226:ARG:H    | 2.20        | 0.45     |
| 1:A:429:U:H4'    | 1:A:430:A:O5'    | 2.16        | 0.45     |
| 10:I:7:THR:HG22  | 10:I:8:GLY:N     | 2.31        | 0.45     |
| 1:A:1149:C:OP1   | 10:I:9:ARG:HD3   | 2.15        | 0.45     |
| 1:A:1229:A:H2'   | 1:A:1230:C:C6    | 2.50        | 0.45     |
| 6:E:115:VAL:HG12 | 6:E:116:THR:N    | 2.31        | 0.45     |
| 1:A:334:C:H2'    | 1:A:335:C:C6     | 2.52        | 0.45     |
| 5:D:24:GLU:CG    | 5:D:25:ARG:N     | 2.78        | 0.45     |
| 5:D:162:LEU:HD13 | 5:D:181:MET:HG2  | 1.98        | 0.45     |
| 3:B:208:ILE:C    | 3:B:210:SER:N    | 2.70        | 0.45     |
| 7:F:35:ALA:HA    | 7:F:67:MET:HB3   | 1.97        | 0.45     |
| 1:A:993:G:HO2'   | 1:A:994:A:P      | 2.40        | 0.45     |
| 10:I:97:LYS:O    | 10:I:100:GLY:N   | 2.39        | 0.45     |
| 1:A:682:G:O2'    | 1:A:683:G:H5'    | 2.16        | 0.45     |
| 20:S:61:TYR:CD2  | 20:S:61:TYR:C    | 2.89        | 0.45     |
| 7:F:45:LEU:HA    | 7:F:58:GLY:O     | 2.16        | 0.45     |
| 13:L:87:GLY:H    | 13:L:98:TYR:HB3  | 1.81        | 0.45     |
| 13:L:42:THR:HG22 | 13:L:52:LEU:HB3  | 1.96        | 0.45     |
| 1:A:1063:C:H3'   | 1:A:1064:G:H2'   | 1.99        | 0.45     |
| 5:D:165:MET:HE2  | 5:D:176:LEU:CD1  | 2.46        | 0.45     |
| 1:A:1486:G:H2'   | 1:A:1487:G:C8    | 2.52        | 0.45     |
| 10:I:44:VAL:HG13 | 10:I:51:ARG:NH2  | 2.31        | 0.45     |
| 1:A:1021:G:C2    | 1:A:1022:G:H1'   | 2.52        | 0.45     |
| 10:I:118:LYS:NZ  | 10:I:118:LYS:CB  | 2.80        | 0.45     |
| 5:D:3:ARG:NH2    | 5:D:74:GLN:HG3   | 2.31        | 0.45     |
| 17:P:81:ARG:HB2  | 17:P:81:ARG:HH11 | 1.82        | 0.45     |
| 1:A:818:G:C3'    | 1:A:819:A:C5'    | 2.94        | 0.45     |
| 1:A:96:G:O2'     | 1:A:97:G:H5'     | 2.17        | 0.45     |
| 1:A:1051:C:O2'   | 1:A:1052:U:H5'   | 2.16        | 0.45     |
| 5:D:205:GLU:O    | 5:D:208:SER:HB2  | 2.16        | 0.45     |
| 1:A:291:C:O2'    | 1:A:292:G:H5'    | 2.17        | 0.45     |
| 3:B:112:VAL:O    | 3:B:116:GLU:HG3  | 2.16        | 0.45     |
| 3:B:117:GLU:O    | 3:B:120:ALA:HB3  | 2.16        | 0.45     |
| 1:A:975:A:C5'    | 1:A:975:A:C8     | 2.97        | 0.45     |
| 1:A:1392:G:N2    | 1:A:1502:A:H8    | 2.14        | 0.45     |
| 1:A:538:G:H2'    | 1:A:539:A:C8     | 2.52        | 0.45     |
| 19:R:47:THR:HA   | 19:R:83:GLU:CB   | 2.47        | 0.45     |
| 1:A:375:U:C2     | 1:A:376:G:C8     | 3.05        | 0.45     |
| 10:I:19:LEU:CD1  | 10:I:85:LEU:HD12 | 2.47        | 0.45     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 16:O:70:LEU:HD12 | 16:O:78:TYR:CA    | 2.47        | 0.45     |
| 8:G:26:PHE:O     | 8:G:30:ILE:HG13   | 2.16        | 0.45     |
| 1:A:1070:U:H2'   | 1:A:1071:C:C6     | 2.51        | 0.45     |
| 3:B:100:GLY:O    | 3:B:104:ASN:N     | 2.48        | 0.45     |
| 1:A:1435:G:H2'   | 1:A:1436:U:C6     | 2.51        | 0.45     |
| 7:F:48:LEU:HD13  | 7:F:52:ILE:HD12   | 1.99        | 0.45     |
| 17:P:47:ASP:OD2  | 17:P:47:ASP:C     | 2.54        | 0.45     |
| 5:D:60:GLU:HA    | 5:D:60:GLU:OE1    | 2.17        | 0.45     |
| 13:L:27:LEU:O    | 13:L:28:LYS:C     | 2.55        | 0.45     |
| 12:K:49:GLY:O    | 12:K:50:TYR:C     | 2.54        | 0.45     |
| 1:A:113:G:C1'    | 1:A:354:G:H5'     | 2.45        | 0.45     |
| 3:B:132:LYS:HE2  | 3:B:135:GLN:OE1   | 2.17        | 0.45     |
| 1:A:1181:G:O2'   | 1:A:1182:G:O4'    | 2.34        | 0.45     |
| 3:B:103:THR:N    | 3:B:176:GLU:OE1   | 2.44        | 0.45     |
| 5:D:170:VAL:O    | 5:D:171:GLY:C     | 2.55        | 0.45     |
| 4:C:152:ILE:N    | 4:C:199:LYS:O     | 2.50        | 0.45     |
| 1:A:1533:C:C2'   | 1:A:1533:C:O2     | 2.64        | 0.45     |
| 10:I:97:LYS:HE2  | 10:I:102:LEU:HD12 | 1.98        | 0.45     |
| 11:J:12:ASP:OD1  | 11:J:14:LYS:N     | 2.49        | 0.45     |
| 1:A:1300:G:O2'   | 1:A:1301:U:H6     | 2.00        | 0.45     |
| 12:K:38:ASN:HA   | 12:K:39:PRO:HD2   | 1.78        | 0.45     |
| 18:Q:9:VAL:HG21  | 18:Q:84:LEU:HD13  | 1.97        | 0.45     |
| 1:A:45:U:H2'     | 1:A:46:G:C8       | 2.52        | 0.45     |
| 9:H:112:LEU:HD23 | 9:H:112:LEU:H     | 1.82        | 0.45     |
| 4:C:12:LEU:HA    | 4:C:12:LEU:HD23   | 1.63        | 0.45     |
| 16:O:40:SER:O    | 16:O:44:LYS:HG2   | 2.17        | 0.45     |
| 5:D:189:PRO:HB2  | 5:D:194:LEU:HD21  | 1.98        | 0.45     |
| 12:K:48:ILE:O    | 12:K:49:GLY:C     | 2.55        | 0.45     |
| 1:A:953:G:H2'    | 1:A:954:G:O4'     | 2.16        | 0.45     |
| 1:A:1221:G:O3'   | 20:S:77:THR:HG21  | 2.15        | 0.45     |
| 3:B:187:LEU:HA   | 3:B:201:ILE:O     | 2.17        | 0.45     |
| 1:A:1003(A):G:C6 | 1:A:1004:A:H1'    | 2.52        | 0.45     |
| 1:A:838:G:N2     | 1:A:849:C:C2      | 2.85        | 0.45     |
| 20:S:13:ASP:HA   | 20:S:16:LEU:HB3   | 1.98        | 0.45     |
| 7:F:67:MET:CE    | 7:F:72:VAL:HA     | 2.46        | 0.45     |
| 8:G:46:ALA:HB1   | 8:G:121:ALA:HB2   | 1.99        | 0.45     |
| 1:A:129(A):G:N3  | 1:A:190(E):U:H5'  | 2.31        | 0.45     |
| 11:J:30:SER:HB3  | 11:J:80:LYS:CG    | 2.47        | 0.45     |
| 1:A:792:A:H4'    | 1:A:793:U:C5'     | 2.47        | 0.45     |
| 1:A:147:G:O2'    | 1:A:148:G:H5'     | 2.17        | 0.45     |
| 3:B:25:ASN:ND2   | 3:B:27:LYS:H      | 2.14        | 0.45     |
| 10:I:4:TYR:CZ    | 10:I:88:TYR:HD1   | 2.35        | 0.45     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 13:L:59:ARG:NH1  | 13:L:65:GLU:HG2  | 2.32        | 0.45     |
| 1:A:231:G:O2'    | 1:A:232:G:H5'    | 2.17        | 0.45     |
| 17:P:81:ARG:CB   | 17:P:81:ARG:HH11 | 2.30        | 0.45     |
| 1:A:1440:C:C2'   | 1:A:1441:G:H5'   | 2.47        | 0.45     |
| 5:D:151:LYS:N    | 5:D:151:LYS:HD2  | 2.32        | 0.45     |
| 4:C:87:LEU:C     | 4:C:89:GLU:H     | 2.20        | 0.45     |
| 1:A:640:A:O2'    | 1:A:641:U:H5'    | 2.17        | 0.45     |
| 1:A:893:C:H2'    | 1:A:894:G:C8     | 2.51        | 0.45     |
| 4:C:129:ALA:HB3  | 4:C:132:ARG:HD2  | 1.99        | 0.45     |
| 1:A:300:A:H2'    | 1:A:301:G:O4'    | 2.17        | 0.45     |
| 1:A:1069:C:O2'   | 1:A:1192:C:H1'   | 2.17        | 0.45     |
| 5:D:33:MET:HE3   | 5:D:37:PRO:CA    | 2.47        | 0.45     |
| 11:J:51:ARG:H    | 11:J:59:SER:HB3  | 1.80        | 0.45     |
| 1:A:1305:G:H5''  | 22:V:4:GLY:C     | 2.37        | 0.45     |
| 11:J:34:VAL:HG12 | 11:J:36:GLY:N    | 2.31        | 0.45     |
| 1:A:986:A:C2     | 1:A:1220:G:C2    | 3.05        | 0.45     |
| 16:O:27:VAL:O    | 16:O:30:ALA:N    | 2.50        | 0.45     |
| 10:I:46:ALA:O    | 10:I:49:PRO:HD2  | 2.17        | 0.45     |
| 1:A:130:A:N7     | 18:Q:63:ARG:HG3  | 2.32        | 0.45     |
| 16:O:45:VAL:O    | 16:O:46:HIS:C    | 2.54        | 0.45     |
| 1:A:560:U:H4'    | 1:A:561:U:H5''   | 1.97        | 0.45     |
| 1:A:1509:C:C2'   | 1:A:1510:U:H5'   | 2.46        | 0.45     |
| 1:A:1217:C:O2'   | 1:A:1218:C:H5'   | 2.17        | 0.45     |
| 3:B:75:LYS:HD3   | 3:B:75:LYS:O     | 2.17        | 0.45     |
| 1:A:1409:C:H2'   | 1:A:1410:G:C8    | 2.50        | 0.45     |
| 15:N:21:TYR:O    | 15:N:21:TYR:CD2  | 2.70        | 0.45     |
| 9:H:91:ARG:HG2   | 13:L:7:ILE:HG13  | 1.98        | 0.45     |
| 1:A:822:C:O2'    | 1:A:823:G:H5'    | 2.17        | 0.45     |
| 1:A:385:C:H2'    | 1:A:386:C:C6     | 2.52        | 0.45     |
| 3:B:167:PRO:O    | 3:B:171:ALA:N    | 2.50        | 0.45     |
| 10:I:79:LEU:CD1  | 10:I:83:ARG:HD2  | 2.45        | 0.45     |
| 4:C:91:LEU:C     | 4:C:91:LEU:HD23  | 2.38        | 0.45     |
| 1:A:243:A:N6     | 1:A:281:G:O2'    | 2.50        | 0.45     |
| 5:D:199:ASN:HD21 | 5:D:201:GLN:CB   | 2.19        | 0.45     |
| 4:C:180:ALA:O    | 4:C:181:ASN:CB   | 2.62        | 0.45     |
| 4:C:43:LEU:HD23  | 4:C:43:LEU:H     | 1.79        | 0.45     |
| 11:J:94:VAL:HG12 | 11:J:95:GLU:N    | 2.32        | 0.45     |
| 1:A:1129:C:O2'   | 1:A:1130:A:OP2   | 2.27        | 0.45     |
| 21:T:10:LEU:O    | 21:T:13:LEU:HD12 | 2.17        | 0.45     |
| 1:A:1176:A:H2'   | 1:A:1177:G:O4'   | 2.16        | 0.45     |
| 13:L:53:ARG:HD2  | 13:L:53:ARG:N    | 2.32        | 0.45     |
| 1:A:61:G:O2'     | 1:A:62:U:H5'     | 2.17        | 0.45     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:456:C:H2'    | 1:A:457:C:C6     | 2.52        | 0.45     |
| 1:A:967:C:H2'    | 1:A:968:A:C8     | 2.52        | 0.45     |
| 13:L:24:VAL:HG12 | 13:L:24:VAL:O    | 2.17        | 0.44     |
| 1:A:1305:G:N2    | 1:A:1331:G:HO2'  | 2.15        | 0.44     |
| 11:J:34:VAL:HG12 | 11:J:36:GLY:H    | 1.82        | 0.44     |
| 11:J:38:ILE:O    | 11:J:70:ARG:HA   | 2.17        | 0.44     |
| 1:A:281:G:O2'    | 1:A:282:A:P      | 2.74        | 0.44     |
| 1:A:1115:C:H1'   | 15:N:61:TRP:O    | 2.17        | 0.44     |
| 3:B:101:MET:HG2  | 3:B:108:ILE:HD13 | 1.97        | 0.44     |
| 3:B:108:ILE:CG2  | 3:B:108:ILE:O    | 2.65        | 0.44     |
| 1:A:939:G:H5''   | 8:G:102:ARG:HH22 | 1.78        | 0.44     |
| 21:T:53:LEU:HD21 | 21:T:104:LEU:CD1 | 2.46        | 0.44     |
| 14:M:48:LEU:HD23 | 14:M:48:LEU:HA   | 1.85        | 0.44     |
| 1:A:446:G:O2'    | 1:A:447:G:H5'    | 2.17        | 0.44     |
| 1:A:922:G:N3     | 1:A:1398:A:H2    | 2.15        | 0.44     |
| 1:A:16:A:C2'     | 1:A:17:U:H5'     | 2.47        | 0.44     |
| 19:R:43:PHE:HD1  | 19:R:66:LEU:HD11 | 1.81        | 0.44     |
| 1:A:1055:A:C6    | 1:A:1056:U:C6    | 3.04        | 0.44     |
| 4:C:82:GLU:O     | 4:C:85:ARG:HB3   | 2.17        | 0.44     |
| 1:A:437:U:H5''   | 5:D:155:LEU:CD2  | 2.44        | 0.44     |
| 1:A:836:G:C6     | 1:A:851:G:C5     | 3.05        | 0.44     |
| 1:A:900:A:H2'    | 1:A:901:A:C8     | 2.52        | 0.44     |
| 1:A:412:A:N1     | 5:D:35:ARG:HB3   | 2.32        | 0.44     |
| 1:A:1059:C:O2'   | 1:A:1060:C:H5'   | 2.17        | 0.44     |
| 6:E:118:ILE:CG2  | 6:E:119:LEU:N    | 2.79        | 0.44     |
| 5:D:25:ARG:HA    | 5:D:28:SER:OG    | 2.17        | 0.44     |
| 4:C:70:VAL:C     | 4:C:106:VAL:HG23 | 2.37        | 0.44     |
| 1:A:491:G:H2'    | 1:A:492:G:H8     | 1.82        | 0.44     |
| 1:A:19:C:OP1     | 6:E:125:SER:OG   | 2.24        | 0.44     |
| 1:A:1216:G:H2'   | 1:A:1217:C:C6    | 2.52        | 0.44     |
| 8:G:20:ASP:OD1   | 8:G:21:VAL:N     | 2.50        | 0.44     |
| 1:A:1129:C:O2'   | 1:A:1130:A:P     | 2.75        | 0.44     |
| 1:A:1477:C:H2'   | 1:A:1478:C:C6    | 2.51        | 0.44     |
| 9:H:112:LEU:N    | 9:H:112:LEU:HD23 | 2.33        | 0.44     |
| 15:N:18:VAL:C    | 15:N:20:ALA:H    | 2.20        | 0.44     |
| 3:B:156:LYS:O    | 3:B:156:LYS:HD3  | 2.17        | 0.44     |
| 12:K:110:ASP:HB3 | 19:R:85:LEU:HB3  | 2.00        | 0.44     |
| 9:H:120:THR:O    | 9:H:121:ASP:C    | 2.55        | 0.44     |
| 3:B:109:SER:C    | 3:B:111:ARG:H    | 2.20        | 0.44     |
| 19:R:55:ARG:HB3  | 19:R:55:ARG:CZ   | 2.46        | 0.44     |
| 5:D:150:GLU:HG3  | 5:D:153:ARG:HH21 | 1.83        | 0.44     |
| 5:D:162:LEU:HA   | 5:D:162:LEU:HD23 | 1.66        | 0.44     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:538:G:O2'    | 1:A:539:A:H5'    | 2.17        | 0.44     |
| 10:I:43:ALA:C    | 10:I:45:ALA:H    | 2.20        | 0.44     |
| 14:M:80:ARG:C    | 14:M:82:MET:N    | 2.70        | 0.44     |
| 1:A:1096:C:H2'   | 1:A:1097:C:H6    | 1.82        | 0.44     |
| 1:A:1161:C:H2'   | 1:A:1162:C:H6    | 1.83        | 0.44     |
| 1:A:1162:C:H2'   | 1:A:1163:C:C6    | 2.52        | 0.44     |
| 1:A:1129:C:OP1   | 10:I:62:TYR:CE2  | 2.71        | 0.44     |
| 9:H:39:LEU:HD11  | 9:H:137:VAL:HG21 | 2.00        | 0.44     |
| 12:K:30:VAL:HG21 | 12:K:65:ALA:HA   | 1.98        | 0.44     |
| 11:J:65:LEU:C    | 11:J:65:LEU:HD23 | 2.38        | 0.44     |
| 4:C:30:ARG:HG2   | 4:C:30:ARG:HH11  | 1.83        | 0.44     |
| 1:A:1231:G:H4'   | 10:I:126:SER:HB3 | 1.98        | 0.44     |
| 1:A:337:C:O2'    | 1:A:338:A:H5'    | 2.18        | 0.44     |
| 3:B:178:ARG:NH1  | 3:B:178:ARG:CG   | 2.76        | 0.44     |
| 3:B:80:ILE:CD1   | 3:B:212:GLN:HB2  | 2.43        | 0.44     |
| 3:B:10:LEU:CD2   | 3:B:48:MET:HG3   | 2.48        | 0.44     |
| 3:B:132:LYS:O    | 3:B:136:VAL:HG23 | 2.17        | 0.44     |
| 12:K:17:GLY:O    | 12:K:80:VAL:HA   | 2.17        | 0.44     |
| 3:B:140:HIS:O    | 3:B:143:GLU:HB2  | 2.18        | 0.44     |
| 14:M:80:ARG:C    | 14:M:82:MET:H    | 2.18        | 0.44     |
| 3:B:231:GLU:OE1  | 3:B:232:PRO:O    | 2.35        | 0.44     |
| 7:F:94:GLN:CB    | 19:R:32:ARG:HD3  | 2.46        | 0.44     |
| 3:B:58:ILE:O     | 3:B:59:GLU:C     | 2.56        | 0.44     |
| 1:A:818:G:H3'    | 1:A:819:A:H5''   | 2.00        | 0.44     |
| 1:A:452:A:H2'    | 1:A:453:A:C8     | 2.53        | 0.44     |
| 13:L:18:VAL:CG1  | 13:L:19:ARG:N    | 2.80        | 0.44     |
| 20:S:50:ALA:HA   | 20:S:58:VAL:O    | 2.18        | 0.44     |
| 1:A:294:U:H2'    | 1:A:295:C:H6     | 1.83        | 0.44     |
| 12:K:12:ARG:O    | 12:K:13:GLN:HB2  | 2.18        | 0.44     |
| 1:A:1127:G:H1'   | 1:A:1148:U:H3    | 1.81        | 0.44     |
| 1:A:1221:G:H1'   | 20:S:54:GLY:HA3  | 2.00        | 0.44     |
| 3:B:10:LEU:HG    | 3:B:48:MET:HE1   | 1.99        | 0.44     |
| 20:S:28:LYS:HG2  | 20:S:29:ARG:N    | 2.32        | 0.44     |
| 20:S:30:LEU:O    | 20:S:31:ILE:HD13 | 2.18        | 0.44     |
| 3:B:97:TRP:CZ2   | 3:B:102:LEU:HD13 | 2.48        | 0.44     |
| 9:H:24:THR:HG22  | 9:H:61:VAL:O     | 2.18        | 0.44     |
| 3:B:122:PHE:CE2  | 3:B:139:LYS:HG2  | 2.41        | 0.44     |
| 1:A:252:U:H2'    | 1:A:253:U:C6     | 2.53        | 0.44     |
| 14:M:24:GLY:HA3  | 14:M:66:LEU:HD22 | 1.99        | 0.44     |
| 17:P:71:ARG:HD3  | 17:P:75:ARG:HH21 | 1.83        | 0.44     |
| 1:A:396:G:O2'    | 1:A:398:C:OP1    | 2.27        | 0.44     |
| 8:G:38:LEU:O     | 8:G:42:ILE:HG13  | 2.17        | 0.44     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:179:A:H2'    | 1:A:180:U:C6      | 2.52        | 0.44     |
| 1:A:1461:G:O2'   | 1:A:1462:G:H5'    | 2.17        | 0.44     |
| 5:D:151:LYS:CD   | 5:D:151:LYS:H     | 2.31        | 0.44     |
| 1:A:313:A:H2'    | 1:A:314:C:C6      | 2.53        | 0.44     |
| 1:A:424:G:H2'    | 1:A:425:G:H8      | 1.83        | 0.44     |
| 15:N:3:ARG:CZ    | 15:N:6:LEU:HG     | 2.48        | 0.44     |
| 15:N:3:ARG:O     | 15:N:4:LYS:C      | 2.53        | 0.44     |
| 1:A:1190:G:C2'   | 1:A:1191:A:OP2    | 2.65        | 0.44     |
| 11:J:69:ASN:O    | 11:J:70:ARG:CD    | 2.66        | 0.44     |
| 1:A:113:G:H1'    | 1:A:354:G:C5'     | 2.45        | 0.44     |
| 1:A:952:U:O2'    | 1:A:953:G:H5'     | 2.17        | 0.44     |
| 3:B:125:PRO:C    | 3:B:127:ILE:H     | 2.20        | 0.44     |
| 25:A:1632:HYG:C1 | 25:A:1632:HYG:O14 | 2.65        | 0.44     |
| 8:G:138:LYS:HE2  | 8:G:142:GLU:OE1   | 2.17        | 0.44     |
| 8:G:95:ARG:O     | 8:G:96:GLN:C      | 2.56        | 0.44     |
| 3:B:132:LYS:C    | 3:B:134:GLU:N     | 2.70        | 0.44     |
| 1:A:1427:U:H2'   | 1:A:1428:A:H8     | 1.81        | 0.44     |
| 11:J:30:SER:HB3  | 11:J:80:LYS:HG3   | 1.99        | 0.44     |
| 14:M:73:GLU:O    | 14:M:74:VAL:C     | 2.56        | 0.44     |
| 14:M:74:VAL:O    | 14:M:77:ASN:HB2   | 2.18        | 0.44     |
| 1:A:518:C:H4'    | 1:A:519:C:O5'     | 2.18        | 0.44     |
| 19:R:52:PRO:HB2  | 19:R:54:ARG:CD    | 2.47        | 0.44     |
| 3:B:24:TRP:CG    | 3:B:25:ASN:N      | 2.85        | 0.44     |
| 4:C:79:ARG:HG3   | 4:C:79:ARG:O      | 2.16        | 0.44     |
| 12:K:69:ALA:O    | 12:K:73:MET:N     | 2.50        | 0.44     |
| 10:I:58:ARG:CG   | 10:I:58:ARG:HH11  | 2.31        | 0.44     |
| 1:A:636:U:C5'    | 18:Q:2:PRO:HG2    | 2.47        | 0.44     |
| 1:A:166:G:O2'    | 1:A:167:G:H5'     | 2.18        | 0.44     |
| 1:A:942:G:C2     | 1:A:943:U:C6      | 3.05        | 0.44     |
| 1:A:224:C:H2'    | 1:A:225:C:H6      | 1.83        | 0.44     |
| 1:A:1115:C:O2'   | 1:A:1116:C:H5'    | 2.17        | 0.44     |
| 7:F:44:GLY:O     | 7:F:59:TYR:HA     | 2.17        | 0.44     |
| 3:B:8:LYS:HD3    | 3:B:9:GLU:N       | 2.32        | 0.44     |
| 6:E:43:LEU:HD23  | 6:E:44:GLY:H      | 1.82        | 0.44     |
| 1:A:375:U:H4'    | 17:P:17:TYR:CE2   | 2.51        | 0.44     |
| 1:A:411:A:C8     | 1:A:413:G:H1'     | 2.53        | 0.44     |
| 16:O:71:GLN:HB2  | 16:O:78:TYR:CE1   | 2.52        | 0.44     |
| 17:P:82:GLN:O    | 17:P:83:GLU:C     | 2.56        | 0.44     |
| 3:B:181:PHE:HD2  | 9:H:70:GLN:HB3    | 1.81        | 0.44     |
| 1:A:52:G:H2'     | 1:A:53:A:H8       | 1.82        | 0.44     |
| 3:B:87:ARG:NH2   | 3:B:220:ASP:OD1   | 2.39        | 0.44     |
| 1:A:1272:G:H2'   | 1:A:1273:G:H8     | 1.82        | 0.44     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 12:K:48:ILE:HD13  | 12:K:63:LEU:HB2   | 1.99        | 0.44     |
| 1:A:1352:C:H2'    | 1:A:1353:G:O4'    | 2.17        | 0.44     |
| 3:B:109:SER:C     | 3:B:111:ARG:N     | 2.70        | 0.44     |
| 19:R:52:PRO:O     | 19:R:56:THR:HG23  | 2.18        | 0.44     |
| 19:R:47:THR:C     | 19:R:49:LYS:H     | 2.21        | 0.44     |
| 1:A:781:A:H2      | 1:A:1514:C:H4'    | 1.82        | 0.44     |
| 1:A:458:C:O2'     | 1:A:459:G:H5'     | 2.18        | 0.44     |
| 1:A:409:G:O2'     | 1:A:410:G:H5'     | 2.18        | 0.44     |
| 3:B:167:PRO:HG2   | 3:B:192:SER:OG    | 2.18        | 0.44     |
| 4:C:30:ARG:HG2    | 4:C:30:ARG:NH1    | 2.32        | 0.44     |
| 12:K:82:VAL:HG23  | 12:K:105:VAL:HG13 | 2.00        | 0.44     |
| 9:H:119:LEU:HD23  | 9:H:119:LEU:N     | 2.33        | 0.44     |
| 14:M:37:THR:CG2   | 14:M:37:THR:O     | 2.65        | 0.44     |
| 14:M:26:GLY:C     | 14:M:28:ALA:N     | 2.71        | 0.44     |
| 1:A:1347:G:C2'    | 1:A:1348:U:OP2    | 2.65        | 0.44     |
| 5:D:68:TYR:N      | 5:D:68:TYR:CD1    | 2.85        | 0.44     |
| 1:A:250:A:C2      | 1:A:274:A:C6      | 3.06        | 0.44     |
| 8:G:18:TYR:N      | 8:G:18:TYR:CD1    | 2.85        | 0.44     |
| 10:I:49:PRO:CD    | 10:I:78:LYS:HG2   | 2.48        | 0.44     |
| 3:B:23:ARG:HH11   | 3:B:24:TRP:CA     | 2.30        | 0.44     |
| 9:H:4:ASP:HB3     | 9:H:7:ALA:HB3     | 2.00        | 0.44     |
| 1:A:1417:G:N2     | 1:A:1484:C:N4     | 2.66        | 0.44     |
| 18:Q:80:GLY:O     | 18:Q:81:ARG:CB    | 2.66        | 0.44     |
| 3:B:53:ARG:HH11   | 3:B:53:ARG:HG2    | 1.83        | 0.44     |
| 1:A:160:A:H1'     | 1:A:344:A:C5      | 2.52        | 0.44     |
| 1:A:186:C:H2'     | 1:A:187:C:H6      | 1.83        | 0.44     |
| 1:A:1490:C:O2'    | 1:A:1491:G:H5'    | 2.18        | 0.43     |
| 25:A:1632:HYG:H30 | 25:A:1632:HYG:H12 | 1.81        | 0.43     |
| 1:A:1202:G:O4'    | 15:N:29:ARG:HD3   | 2.18        | 0.43     |
| 1:A:253:U:H2'     | 1:A:254:G:C8      | 2.53        | 0.43     |
| 6:E:11:ILE:HG23   | 6:E:105:VAL:HG22  | 2.00        | 0.43     |
| 1:A:489:C:H2'     | 1:A:490:G:C8      | 2.46        | 0.43     |
| 1:A:1249:C:O2'    | 10:I:73:GLN:NE2   | 2.51        | 0.43     |
| 1:A:864:A:H2'     | 1:A:865:A:C8      | 2.53        | 0.43     |
| 1:A:1394:A:C5     | 1:A:1501:C:H4'    | 2.53        | 0.43     |
| 1:A:1272:G:O2'    | 1:A:1273:G:H5'    | 2.18        | 0.43     |
| 1:A:718:G:H5'     | 1:A:719:C:OP2     | 2.18        | 0.43     |
| 3:B:84:GLU:HG3    | 3:B:215:LEU:HB3   | 2.00        | 0.43     |
| 1:A:1353:G:OP2    | 22:V:3:LYS:HE2    | 2.18        | 0.43     |
| 5:D:162:LEU:CD1   | 5:D:181:MET:HG2   | 2.48        | 0.43     |
| 1:A:1223:C:P      | 20:S:78:ARG:NH1   | 2.90        | 0.43     |
| 1:A:1519:A:H2'    | 1:A:1520:G:H5'    | 2.00        | 0.43     |

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| Atom-1            | Atom-2           | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 8:G:18:TYR:CD2    | 8:G:59:LEU:HD22  | 2.52        | 0.43     |
| 1:A:182:U:O4      | 1:A:223:U:H1'    | 2.18        | 0.43     |
| 1:A:1157:A:H4'    | 1:A:1158:C:O5'   | 2.18        | 0.43     |
| 1:A:1054:C:O2'    | 1:A:1055:A:H5''  | 2.18        | 0.43     |
| 11:J:12:ASP:O     | 11:J:15:THR:HG22 | 2.18        | 0.43     |
| 1:A:521:G:O2'     | 1:A:522:C:H5'    | 2.18        | 0.43     |
| 4:C:5:ILE:HD12    | 4:C:5:ILE:C      | 2.38        | 0.43     |
| 1:A:1376:U:H2'    | 1:A:1377:A:C8    | 2.53        | 0.43     |
| 4:C:99:VAL:CG2    | 4:C:100:ALA:N    | 2.81        | 0.43     |
| 8:G:151:TYR:N     | 8:G:151:TYR:CD1  | 2.85        | 0.43     |
| 3:B:88:ALA:C      | 3:B:90:MET:N     | 2.71        | 0.43     |
| 1:A:352:C:H4'     | 1:A:354:G:OP1    | 2.18        | 0.43     |
| 11:J:90:LEU:N     | 11:J:91:PRO:HD2  | 2.29        | 0.43     |
| 21:T:54:LYS:HA    | 21:T:57:ARG:HD3  | 2.00        | 0.43     |
| 1:A:264:U:H4'     | 18:Q:63:ARG:HD3  | 1.99        | 0.43     |
| 1:A:992:U:O2'     | 1:A:993:G:OP2    | 2.31        | 0.43     |
| 7:F:36:ARG:NH1    | 7:F:38:GLU:HG2   | 2.34        | 0.43     |
| 1:A:921:U:O2'     | 6:E:19:MET:O     | 2.28        | 0.43     |
| 11:J:12:ASP:HB3   | 11:J:15:THR:HB   | 2.00        | 0.43     |
| 1:A:586:C:O2'     | 1:A:878:G:H4'    | 2.18        | 0.43     |
| 1:A:1301:U:O2'    | 1:A:1302:U:P     | 2.77        | 0.43     |
| 13:L:34:ARG:HB3   | 13:L:105:TYR:HE1 | 1.83        | 0.43     |
| 1:A:169:C:O2'     | 1:A:170:U:H5'    | 2.18        | 0.43     |
| 4:C:92:ALA:C      | 4:C:94:LEU:N     | 2.70        | 0.43     |
| 3:B:17:PHE:N      | 3:B:44:LEU:HD21  | 2.33        | 0.43     |
| 1:A:1117:G:N2     | 1:A:1180:A:H1'   | 2.33        | 0.43     |
| 1:A:1111:A:H2'    | 1:A:1112:C:H6    | 1.82        | 0.43     |
| 9:H:1:MET:CG      | 9:H:2:LEU:N      | 2.77        | 0.43     |
| 20:S:51:VAL:HG12  | 20:S:52:TYR:H    | 1.82        | 0.43     |
| 1:A:1003(A):G:H2' | 1:A:1004:A:C4'   | 2.47        | 0.43     |
| 1:A:926:G:H3'     | 1:A:1505:G:H21   | 1.83        | 0.43     |
| 1:A:1426:C:O2'    | 1:A:1427:U:H5'   | 2.19        | 0.43     |
| 17:P:38:TYR:O     | 17:P:49:LEU:HD12 | 2.19        | 0.43     |
| 1:A:186:C:H2'     | 1:A:187:C:C6     | 2.53        | 0.43     |
| 6:E:5:ASP:CG      | 6:E:6:PHE:H      | 2.22        | 0.43     |
| 8:G:129:GLU:CB    | 8:G:131:LYS:HE2  | 2.49        | 0.43     |
| 10:I:23:ASN:ND2   | 10:I:23:ASN:C    | 2.72        | 0.43     |
| 15:N:53:LEU:HA    | 15:N:54:PRO:HD2  | 1.85        | 0.43     |
| 4:C:46:GLU:HB2    | 4:C:47:LEU:HD12  | 2.01        | 0.43     |
| 3:B:85:ALA:O      | 3:B:90:MET:O     | 2.37        | 0.43     |
| 3:B:129:GLU:O     | 3:B:130:ARG:HB2  | 2.19        | 0.43     |
| 4:C:8:ILE:C       | 4:C:10:PHE:H     | 2.22        | 0.43     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 4:C:147:LYS:HE2  | 4:C:205:GLY:CA    | 2.48        | 0.43     |
| 1:A:327:A:HO2'   | 1:A:328:C:H6      | 1.65        | 0.43     |
| 17:P:36:ILE:O    | 17:P:51:VAL:O     | 2.36        | 0.43     |
| 5:D:209:ARG:HG2  | 5:D:209:ARG:NH1   | 2.32        | 0.43     |
| 20:S:3:ARG:O     | 20:S:4:SER:HB3    | 2.18        | 0.43     |
| 14:M:40:ASN:HD22 | 14:M:40:ASN:C     | 2.22        | 0.43     |
| 1:A:1298:C:N4    | 8:G:114:ARG:HB3   | 2.33        | 0.43     |
| 1:A:1509:C:O2'   | 1:A:1510:U:H5'    | 2.18        | 0.43     |
| 14:M:117:VAL:CG1 | 14:M:118:ALA:N    | 2.81        | 0.43     |
| 10:I:97:LYS:CE   | 10:I:102:LEU:HD12 | 2.49        | 0.43     |
| 1:A:1417:G:N2    | 1:A:1484:C:H42    | 2.17        | 0.43     |
| 8:G:152:ALA:C    | 8:G:154:TYR:H     | 2.22        | 0.43     |
| 11:J:15:THR:HG23 | 11:J:94:VAL:HG22  | 2.01        | 0.43     |
| 5:D:189:PRO:HB2  | 5:D:194:LEU:CD2   | 2.48        | 0.43     |
| 1:A:1329:A:O2'   | 1:A:1330:U:H5'    | 2.19        | 0.43     |
| 19:R:39:VAL:HG13 | 19:R:40:LEU:HD23  | 2.00        | 0.43     |
| 11:J:53:PRO:O    | 11:J:54:PHE:O     | 2.37        | 0.43     |
| 1:A:755:G:H1'    | 9:H:1:MET:CE      | 2.48        | 0.43     |
| 3:B:16:HIS:CD2   | 3:B:210:SER:OG    | 2.71        | 0.43     |
| 20:S:16:LEU:C    | 20:S:18:LYS:N     | 2.68        | 0.43     |
| 5:D:174:LEU:C    | 5:D:186:LEU:HD12  | 2.39        | 0.43     |
| 5:D:174:LEU:O    | 5:D:186:LEU:HD12  | 2.18        | 0.43     |
| 1:A:1014:A:C2    | 1:A:1219:U:H1'    | 2.53        | 0.43     |
| 11:J:85:LEU:O    | 11:J:87:THR:N     | 2.52        | 0.43     |
| 1:A:1243:C:H2'   | 1:A:1244:C:C6     | 2.54        | 0.43     |
| 9:H:39:LEU:HD13  | 9:H:39:LEU:HA     | 1.87        | 0.43     |
| 3:B:217:ARG:HA   | 3:B:220:ASP:OD2   | 2.19        | 0.43     |
| 8:G:80:VAL:O     | 8:G:82:GLY:N      | 2.51        | 0.43     |
| 10:I:55:ALA:O    | 10:I:57:GLY:N     | 2.51        | 0.43     |
| 1:A:741:G:H5''   | 16:O:39:LEU:HD12  | 2.00        | 0.43     |
| 4:C:114:PRO:O    | 4:C:118:GLN:HG3   | 2.18        | 0.43     |
| 4:C:188:LEU:HD22 | 4:C:188:LEU:HA    | 1.84        | 0.43     |
| 20:S:40:ILE:HB   | 20:S:67:VAL:O     | 2.19        | 0.43     |
| 1:A:250:A:H2     | 1:A:274:A:C6      | 2.36        | 0.43     |
| 18:Q:24:GLU:CD   | 18:Q:37:LYS:HD3   | 2.38        | 0.43     |
| 13:L:83:VAL:CG2  | 13:L:84:LEU:N     | 2.74        | 0.43     |
| 6:E:43:LEU:HD22  | 6:E:44:GLY:N      | 2.34        | 0.43     |
| 1:A:518:C:O2'    | 1:A:519:C:OP2     | 2.30        | 0.43     |
| 1:A:230:G:H2'    | 1:A:231:G:O4'     | 2.19        | 0.43     |
| 6:E:124:GLY:O    | 6:E:126:ARG:N     | 2.52        | 0.43     |
| 1:A:1118:C:H2'   | 1:A:1119:C:C6     | 2.54        | 0.43     |
| 1:A:570:G:H1'    | 1:A:820:U:C4      | 2.53        | 0.43     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:718:G:H4'    | 12:K:117:ASN:HD21 | 1.84        | 0.43     |
| 1:A:156:G:O2'    | 1:A:157:G:H5'     | 2.19        | 0.43     |
| 21:T:61:SER:O    | 21:T:65:LYS:HG3   | 2.18        | 0.43     |
| 13:L:60:LEU:HD21 | 13:L:85:ILE:CD1   | 2.48        | 0.43     |
| 1:A:1064:G:C2    | 1:A:1066:C:N4     | 2.87        | 0.43     |
| 8:G:151:TYR:OH   | 12:K:54:ARG:NE    | 2.52        | 0.43     |
| 1:A:1127:G:H21   | 1:A:1147:C:N4     | 2.17        | 0.43     |
| 1:A:976:G:C8     | 1:A:1358:U:C2     | 3.07        | 0.43     |
| 5:D:156:GLU:HG2  | 5:D:160:GLN:NE2   | 2.21        | 0.43     |
| 5:D:163:GLU:OE2  | 5:D:166:LYS:HE3   | 2.19        | 0.43     |
| 1:A:1402:C:H2'   | 1:A:1403:C:O4'    | 2.18        | 0.43     |
| 3:B:208:ILE:O    | 3:B:209:ARG:C     | 2.57        | 0.43     |
| 1:A:1424:C:O2'   | 1:A:1425:U:H5'    | 2.19        | 0.43     |
| 9:H:60:ARG:CG    | 9:H:60:ARG:NH1    | 2.80        | 0.43     |
| 1:A:502:G:OP1    | 13:L:118:SER:CB   | 2.67        | 0.43     |
| 1:A:542:G:H2'    | 1:A:543:C:H6      | 1.83        | 0.43     |
| 1:A:448:A:O2'    | 1:A:449:C:C5'     | 2.66        | 0.43     |
| 1:A:1009:G:C6    | 1:A:1021:G:C6     | 3.07        | 0.43     |
| 1:A:386:C:C2'    | 1:A:387:U:H5'     | 2.49        | 0.43     |
| 1:A:1034:G:O2'   | 1:A:1035:A:H5'    | 2.19        | 0.43     |
| 3:B:34:ALA:O     | 3:B:41:ILE:N      | 2.51        | 0.43     |
| 11:J:6:ILE:HG13  | 11:J:71:LEU:O     | 2.19        | 0.43     |
| 11:J:55:LYS:O    | 11:J:56:HIS:HB2   | 2.18        | 0.43     |
| 3:B:120:ALA:O    | 3:B:124:SER:HB3   | 2.19        | 0.43     |
| 5:D:61:LYS:HA    | 5:D:203:VAL:HG22  | 2.00        | 0.43     |
| 20:S:20:LEU:HB3  | 20:S:23:ASN:HD22  | 1.84        | 0.43     |
| 1:A:129(A):G:C2  | 1:A:190(E):U:H5'  | 2.54        | 0.43     |
| 5:D:114:ARG:CG   | 5:D:114:ARG:NH1   | 2.82        | 0.43     |
| 1:A:446:G:C2'    | 1:A:447:G:H5'     | 2.49        | 0.43     |
| 21:T:72:LEU:O    | 21:T:73:HIS:O     | 2.36        | 0.43     |
| 1:A:31:G:H1      | 1:A:48:C:H5''     | 1.83        | 0.43     |
| 4:C:7:PRO:CG     | 4:C:184:TYR:HB2   | 2.49        | 0.43     |
| 1:A:421:U:H5'    | 1:A:422:C:C5      | 2.54        | 0.43     |
| 10:I:58:ARG:HD2  | 10:I:58:ARG:C     | 2.39        | 0.43     |
| 10:I:5:TYR:CG    | 10:I:6:GLY:N      | 2.87        | 0.43     |
| 13:L:102:ARG:HB3 | 13:L:102:ARG:HE   | 1.69        | 0.43     |
| 3:B:218:ALA:O    | 3:B:222:ILE:HG13  | 2.18        | 0.43     |
| 12:K:84:VAL:CG2  | 19:R:88:LYS:HD3   | 2.44        | 0.43     |
| 10:I:7:THR:O     | 10:I:15:ALA:O     | 2.37        | 0.43     |
| 11:J:51:ARG:H    | 11:J:59:SER:HB2   | 1.83        | 0.43     |
| 1:A:761:G:H2'    | 1:A:762:C:H6      | 1.83        | 0.43     |
| 14:M:37:THR:CG2  | 14:M:39:ILE:HD11  | 2.49        | 0.43     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:1060:C:OP1   | 15:N:45:ARG:NH2  | 2.49        | 0.43     |
| 11:J:39:PRO:O    | 11:J:69:ASN:O    | 2.37        | 0.43     |
| 1:A:688:G:N3     | 1:A:704:A:C2     | 2.87        | 0.43     |
| 14:M:123:ALA:O   | 14:M:125:ARG:N   | 2.51        | 0.43     |
| 1:A:1221:G:H4'   | 20:S:53:ASN:O    | 2.18        | 0.43     |
| 1:A:434:U:H2'    | 1:A:435:C:H6     | 1.78        | 0.43     |
| 1:A:620:C:H2'    | 1:A:621:A:O4'    | 2.18        | 0.43     |
| 10:I:44:VAL:CG1  | 10:I:51:ARG:NH2  | 2.82        | 0.43     |
| 11:J:30:SER:HB2  | 11:J:80:LYS:HB3  | 2.00        | 0.43     |
| 11:J:3:LYS:HG3   | 11:J:75:ILE:HG23 | 2.01        | 0.43     |
| 1:A:1097:C:H2'   | 1:A:1098:C:C6    | 2.52        | 0.43     |
| 10:I:36:TYR:HD2  | 10:I:37:PHE:CE2  | 2.37        | 0.43     |
| 1:A:92:C:O2'     | 1:A:93:G:H5'     | 2.19        | 0.43     |
| 1:A:452:A:O2'    | 1:A:453:A:O4'    | 2.24        | 0.43     |
| 1:A:386:C:O2'    | 1:A:387:U:H5'    | 2.18        | 0.43     |
| 17:P:65:GLN:HA   | 17:P:66:PRO:HD2  | 1.85        | 0.43     |
| 7:F:78:GLU:O     | 7:F:81:ILE:HG13  | 2.18        | 0.43     |
| 21:T:92:LEU:HD23 | 21:T:92:LEU:HA   | 1.88        | 0.43     |
| 1:A:1280:A:O4'   | 11:J:41:PRO:HG3  | 2.19        | 0.42     |
| 1:A:54:C:H2'     | 1:A:352:C:H41    | 1.84        | 0.42     |
| 3:B:46:LYS:C     | 3:B:48:MET:N     | 2.72        | 0.42     |
| 1:A:849:C:O2'    | 1:A:850:U:H5'    | 2.19        | 0.42     |
| 16:O:8:LYS:HE3   | 16:O:31:LEU:HD23 | 2.01        | 0.42     |
| 17:P:19:ILE:N    | 17:P:37:GLY:O    | 2.52        | 0.42     |
| 17:P:21:VAL:HG12 | 17:P:22:THR:N    | 2.33        | 0.42     |
| 21:T:57:ARG:CG   | 21:T:57:ARG:HH11 | 2.32        | 0.42     |
| 14:M:13:LYS:O    | 14:M:14:ARG:C    | 2.57        | 0.42     |
| 1:A:1262:C:O2'   | 1:A:1263:C:H5'   | 2.19        | 0.42     |
| 8:G:69:VAL:O     | 8:G:69:VAL:HG12  | 2.19        | 0.42     |
| 10:I:89:ASN:C    | 10:I:91:ASP:H    | 2.21        | 0.42     |
| 8:G:75:VAL:CG1   | 8:G:86:GLN:HB3   | 2.49        | 0.42     |
| 10:I:23:ASN:HD22 | 10:I:23:ASN:C    | 2.22        | 0.42     |
| 1:A:720:C:H2'    | 1:A:721:G:C8     | 2.54        | 0.42     |
| 4:C:188:LEU:HD13 | 4:C:195:VAL:HG13 | 2.01        | 0.42     |
| 1:A:1250:A:C4'   | 10:I:68:GLY:H    | 2.28        | 0.42     |
| 1:A:370:C:H2'    | 1:A:371:G:H8     | 1.83        | 0.42     |
| 20:S:67:VAL:HG12 | 20:S:68:GLY:N    | 2.33        | 0.42     |
| 1:A:923:A:O4'    | 1:A:1398:A:C2    | 2.72        | 0.42     |
| 1:A:815:A:N6     | 1:A:1509:C:H1'   | 2.34        | 0.42     |
| 1:A:1368:G:OP2   | 10:I:112:LYS:HD2 | 2.19        | 0.42     |
| 6:E:15:ARG:CD    | 6:E:26:PHE:CD2   | 3.01        | 0.42     |
| 4:C:7:PRO:HG2    | 4:C:184:TYR:CB   | 2.49        | 0.42     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 8:G:145:ALA:O    | 8:G:147:ALA:N    | 2.52        | 0.42     |
| 13:L:32:PHE:HE1  | 13:L:86:ARG:HB2  | 1.84        | 0.42     |
| 20:S:10:PHE:O    | 20:S:39:THR:HB   | 2.19        | 0.42     |
| 1:A:1360:A:H2'   | 1:A:1361:G:O4'   | 2.18        | 0.42     |
| 11:J:51:ARG:N    | 11:J:59:SER:HB2  | 2.34        | 0.42     |
| 3:B:19:HIS:NE2   | 3:B:206:ASP:CB   | 2.82        | 0.42     |
| 4:C:3:ASN:C      | 4:C:4:LYS:HG2    | 2.40        | 0.42     |
| 1:A:1279:A:O2'   | 1:A:1281:U:OP2   | 2.37        | 0.42     |
| 5:D:163:GLU:C    | 5:D:165:MET:N    | 2.71        | 0.42     |
| 1:A:1222:G:O2'   | 1:A:1223:C:H5'   | 2.19        | 0.42     |
| 7:F:80:ARG:HH11  | 7:F:80:ARG:HG2   | 1.84        | 0.42     |
| 4:C:151:VAL:C    | 4:C:152:ILE:HG13 | 2.40        | 0.42     |
| 17:P:17:TYR:HE1  | 17:P:41:PRO:HG2  | 1.83        | 0.42     |
| 1:A:656:C:O2'    | 16:O:28:GLN:OE1  | 2.30        | 0.42     |
| 1:A:265:G:H2'    | 1:A:267:C:H5     | 1.85        | 0.42     |
| 1:A:748:C:H1'    | 1:A:749:C:C5     | 2.53        | 0.42     |
| 1:A:738:C:P      | 7:F:92:LYS:HE3   | 2.59        | 0.42     |
| 20:S:71:LEU:O    | 20:S:74:PHE:N    | 2.39        | 0.42     |
| 4:C:175:LEU:HD11 | 4:C:201:TYR:CE2  | 2.54        | 0.42     |
| 7:F:23:LYS:HE2   | 7:F:23:LYS:HB3   | 1.86        | 0.42     |
| 18:Q:65:ILE:O    | 18:Q:65:ILE:HG22 | 2.19        | 0.42     |
| 21:T:58:LYS:O    | 21:T:62:LEU:HG   | 2.19        | 0.42     |
| 11:J:46:ARG:HD3  | 11:J:64:GLU:HB3  | 2.01        | 0.42     |
| 1:A:1061:G:H2'   | 1:A:1062:U:H5'   | 2.00        | 0.42     |
| 22:V:2:GLY:O     | 22:V:4:GLY:N     | 2.53        | 0.42     |
| 3:B:90:MET:HA    | 3:B:91:PRO:HD3   | 1.85        | 0.42     |
| 3:B:70:PHE:O     | 3:B:92:TYR:HA    | 2.19        | 0.42     |
| 1:A:496:A:H4'    | 1:A:497:A:OP1    | 2.19        | 0.42     |
| 5:D:152:SER:O    | 5:D:154:ASN:N    | 2.53        | 0.42     |
| 3:B:208:ILE:HG21 | 3:B:239:VAL:HA   | 2.01        | 0.42     |
| 1:A:925:G:C2     | 1:A:927:G:C8     | 3.07        | 0.42     |
| 7:F:33:TYR:CB    | 7:F:75:LEU:HD23  | 2.45        | 0.42     |
| 17:P:52:ASP:OD2  | 17:P:55:ARG:HG3  | 2.19        | 0.42     |
| 10:I:99:LEU:HB3  | 10:I:101:PHE:CE1 | 2.54        | 0.42     |
| 15:N:27:CYS:SG   | 15:N:29:ARG:CB   | 3.04        | 0.42     |
| 19:R:87:ARG:HH11 | 19:R:87:ARG:CG   | 2.28        | 0.42     |
| 4:C:86:VAL:O     | 4:C:90:GLU:HB2   | 2.20        | 0.42     |
| 17:P:71:ARG:HG3  | 17:P:80:PHE:CZ   | 2.54        | 0.42     |
| 1:A:20:U:O2'     | 1:A:21:G:H5'     | 2.19        | 0.42     |
| 1:A:1501:C:OP2   | 1:A:1504:G:H2'   | 2.19        | 0.42     |
| 3:B:164:VAL:HG12 | 3:B:186:ALA:HB1  | 2.01        | 0.42     |
| 1:A:41:G:H2'     | 1:A:42:G:C8      | 2.54        | 0.42     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 8:G:75:VAL:HG11  | 8:G:86:GLN:HB3   | 2.01        | 0.42     |
| 1:A:1033:G:H2'   | 1:A:1034:G:C8    | 2.54        | 0.42     |
| 1:A:1010:G:H2'   | 1:A:1011:G:H8    | 1.84        | 0.42     |
| 13:L:89:ARG:O    | 13:L:99:HIS:HE1  | 2.02        | 0.42     |
| 12:K:40:ILE:HG23 | 12:K:75:TYR:CE2  | 2.55        | 0.42     |
| 1:A:1256:A:H5'   | 1:A:1258:G:C1'   | 2.49        | 0.42     |
| 1:A:439:A:C4     | 1:A:497:A:C2     | 3.08        | 0.42     |
| 1:A:1391:U:H2'   | 1:A:1392:G:H8    | 1.79        | 0.42     |
| 1:A:220:G:O2'    | 1:A:221:C:H5'    | 2.19        | 0.42     |
| 17:P:42:ARG:O    | 17:P:43:LYS:C    | 2.58        | 0.42     |
| 17:P:48:TRP:O    | 17:P:49:LEU:HB2  | 2.20        | 0.42     |
| 1:A:401:C:O2'    | 1:A:402:G:H5'    | 2.19        | 0.42     |
| 1:A:376:G:OP2    | 17:P:67:THR:HG21 | 2.20        | 0.42     |
| 1:A:397:A:N3     | 1:A:397:A:H3'    | 2.34        | 0.42     |
| 1:A:1240:U:P     | 8:G:116:ALA:HB2  | 2.59        | 0.42     |
| 1:A:42:G:H2'     | 1:A:43:C:H6      | 1.85        | 0.42     |
| 7:F:78:GLU:HA    | 7:F:81:ILE:CD1   | 2.49        | 0.42     |
| 4:C:84:ILE:O     | 4:C:84:ILE:HG12  | 2.19        | 0.42     |
| 14:M:49:THR:HB   | 14:M:52:GLU:HG3  | 2.00        | 0.42     |
| 14:M:10:PRO:HB3  | 14:M:18:ALA:O    | 2.19        | 0.42     |
| 10:I:127:LYS:HD2 | 10:I:127:LYS:N   | 2.35        | 0.42     |
| 1:A:1113:C:H4'   | 4:C:14:ILE:CD1   | 2.46        | 0.42     |
| 1:A:1113:C:O2'   | 1:A:1114:C:H5'   | 2.19        | 0.42     |
| 4:C:178:LEU:O    | 4:C:179:ARG:CB   | 2.66        | 0.42     |
| 5:D:150:GLU:O    | 5:D:152:SER:N    | 2.53        | 0.42     |
| 20:S:40:ILE:HG21 | 20:S:62:ILE:HD13 | 2.02        | 0.42     |
| 5:D:61:LYS:NZ    | 5:D:62:GLN:NE2   | 2.67        | 0.42     |
| 20:S:22:LEU:CD2  | 20:S:28:LYS:HD2  | 2.49        | 0.42     |
| 20:S:31:ILE:HG22 | 20:S:32:LYS:N    | 2.35        | 0.42     |
| 3:B:25:ASN:ND2   | 3:B:25:ASN:C     | 2.67        | 0.42     |
| 1:A:344:A:H5''   | 1:A:345:C:H5     | 1.85        | 0.42     |
| 1:A:644:G:C5     | 1:A:645:C:C5     | 3.08        | 0.42     |
| 1:A:782:A:C6     | 1:A:801:U:C2     | 3.08        | 0.42     |
| 11:J:8:LEU:CD1   | 11:J:20:ALA:HB2  | 2.49        | 0.42     |
| 8:G:77:SER:O     | 8:G:78:ARG:HB2   | 2.19        | 0.42     |
| 5:D:30:LYS:C     | 5:D:32:ALA:N     | 2.70        | 0.42     |
| 1:A:1403:C:H1'   | 1:A:1500:A:N1    | 2.35        | 0.42     |
| 1:A:323:U:H2'    | 1:A:324:G:O4'    | 2.20        | 0.42     |
| 1:A:449:C:O2     | 17:P:42:ARG:HD2  | 2.20        | 0.42     |
| 4:C:134:ILE:HG23 | 4:C:151:VAL:HB   | 2.01        | 0.42     |
| 1:A:411:A:C2     | 1:A:431:A:N6     | 2.88        | 0.42     |
| 10:I:93:ARG:O    | 10:I:95:LYS:N    | 2.53        | 0.42     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:731:G:OP1    | 1:A:766:A:H1'    | 2.20        | 0.42     |
| 8:G:116:ALA:HA   | 8:G:119:ARG:NH2  | 2.35        | 0.42     |
| 9:H:45:ILE:HG13  | 9:H:47:GLY:H     | 1.85        | 0.42     |
| 1:A:1206:G:C6    | 1:A:1207:G:C5    | 3.08        | 0.42     |
| 1:A:90:U:H2'     | 1:A:91:C:C6      | 2.55        | 0.42     |
| 1:A:1031:G:H2'   | 1:A:1032:G:H8    | 1.85        | 0.42     |
| 7:F:27:GLN:NE2   | 7:F:27:GLN:HA    | 2.34        | 0.42     |
| 13:L:60:LEU:HD23 | 13:L:66:VAL:HG22 | 2.00        | 0.42     |
| 1:A:429:U:OP2    | 5:D:36:ARG:NH1   | 2.52        | 0.42     |
| 4:C:64:VAL:HB    | 4:C:99:VAL:CB    | 2.49        | 0.42     |
| 1:A:1131:G:H2'   | 1:A:1132:C:C6    | 2.54        | 0.42     |
| 12:K:50:TYR:HD1  | 12:K:60:ALA:HB2  | 1.85        | 0.42     |
| 3:B:107:THR:C    | 3:B:109:SER:N    | 2.73        | 0.42     |
| 3:B:68:ILE:H     | 3:B:90:MET:CE    | 2.32        | 0.42     |
| 3:B:85:ALA:CB    | 3:B:92:TYR:HB3   | 2.50        | 0.42     |
| 11:J:34:VAL:HG22 | 11:J:74:ILE:CG2  | 2.48        | 0.42     |
| 1:A:1231:G:OP1   | 10:I:127:LYS:NZ  | 2.53        | 0.42     |
| 10:I:114:TYR:CD1 | 11:J:60:ARG:HB2  | 2.55        | 0.42     |
| 1:A:1041:A:H2'   | 1:A:1042:G:C8    | 2.55        | 0.42     |
| 1:A:1342:C:O2'   | 1:A:1343:G:H5'   | 2.20        | 0.42     |
| 10:I:48:GLU:N    | 10:I:49:PRO:CD   | 2.81        | 0.42     |
| 5:D:57:ARG:HB3   | 5:D:206:PHE:HB2  | 2.00        | 0.42     |
| 14:M:13:LYS:O    | 14:M:45:VAL:HG23 | 2.20        | 0.42     |
| 9:H:7:ALA:HB2    | 9:H:85:ARG:CD    | 2.50        | 0.42     |
| 5:D:126:ILE:HG22 | 5:D:127:THR:N    | 2.35        | 0.42     |
| 4:C:116:VAL:O    | 4:C:119:ARG:HB3  | 2.20        | 0.42     |
| 1:A:460:A:N7     | 1:A:462:G:C6     | 2.88        | 0.42     |
| 1:A:862:C:O4'    | 1:A:874:G:H4'    | 2.20        | 0.42     |
| 1:A:851:G:H2'    | 1:A:852:G:H8     | 1.85        | 0.42     |
| 1:A:275:G:H5'    | 18:Q:14:LYS:HD3  | 2.02        | 0.42     |
| 10:I:26:VAL:HG12 | 10:I:28:VAL:HG23 | 2.01        | 0.42     |
| 4:C:19:GLU:HG2   | 4:C:54:ARG:HE    | 1.85        | 0.42     |
| 5:D:33:MET:HE3   | 5:D:37:PRO:HA    | 2.02        | 0.42     |
| 3:B:189:ASP:OD1  | 3:B:205:ASP:HB3  | 2.20        | 0.42     |
| 1:A:1231:G:H5''  | 10:I:126:SER:CB  | 2.49        | 0.42     |
| 6:E:80:ILE:N     | 6:E:80:ILE:HD12  | 2.29        | 0.42     |
| 1:A:975:A:C4'    | 1:A:976:G:H5'    | 2.42        | 0.42     |
| 5:D:78:LEU:HA    | 5:D:78:LEU:HD23  | 1.73        | 0.42     |
| 1:A:1006:C:O2'   | 1:A:1007:C:H5'   | 2.20        | 0.42     |
| 1:A:321:A:H2'    | 1:A:322:C:C6     | 2.55        | 0.42     |
| 3:B:97:TRP:HH2   | 3:B:176:GLU:OE1  | 2.03        | 0.42     |
| 5:D:170:VAL:CG1  | 5:D:174:LEU:HB2  | 2.45        | 0.42     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 14:M:73:GLU:O    | 14:M:76:ALA:N    | 2.52        | 0.42     |
| 1:A:277:C:H5''   | 18:Q:68:ARG:NH2  | 2.35        | 0.42     |
| 1:A:1508:G:O2'   | 1:A:1509:C:H5'   | 2.18        | 0.42     |
| 1:A:1015:A:H2'   | 1:A:1016:A:C8    | 2.55        | 0.42     |
| 17:P:10:GLY:HA3  | 17:P:14:ASN:O    | 2.19        | 0.42     |
| 20:S:7:LYS:CG    | 20:S:7:LYS:O     | 2.68        | 0.42     |
| 11:J:47:PHE:N    | 11:J:63:PHE:O    | 2.48        | 0.42     |
| 4:C:126:ARG:O    | 4:C:127:ARG:HB2  | 2.20        | 0.42     |
| 10:I:82:ALA:O    | 10:I:96:LEU:HD21 | 2.19        | 0.42     |
| 1:A:858:G:O2'    | 1:A:859:A:H5'    | 2.20        | 0.42     |
| 21:T:93:GLU:OE2  | 21:T:93:GLU:HA   | 2.19        | 0.42     |
| 10:I:127:LYS:C   | 10:I:128:ARG:O   | 2.58        | 0.42     |
| 11:J:22:LYS:NZ   | 11:J:91:PRO:HD3  | 2.34        | 0.42     |
| 4:C:191:THR:HG21 | 4:C:193:TYR:CE1  | 2.55        | 0.42     |
| 1:A:992:U:O2'    | 1:A:993:G:P      | 2.78        | 0.42     |
| 13:L:50:SER:O    | 13:L:51:ALA:CB   | 2.68        | 0.42     |
| 1:A:965:A:C2     | 1:A:969:A:C2     | 3.08        | 0.42     |
| 1:A:930:C:C2'    | 1:A:931:C:H5'    | 2.50        | 0.42     |
| 1:A:557:G:C6     | 1:A:558:G:C6     | 3.08        | 0.42     |
| 6:E:144:THR:N    | 6:E:147:ASP:OD2  | 2.48        | 0.42     |
| 6:E:7:GLU:O      | 6:E:34:VAL:HA    | 2.20        | 0.42     |
| 1:A:724:G:O2'    | 1:A:725:G:H5'    | 2.20        | 0.42     |
| 14:M:23:TYR:HB3  | 14:M:67:GLU:HA   | 2.02        | 0.42     |
| 6:E:110:LEU:O    | 6:E:113:ALA:HB3  | 2.20        | 0.41     |
| 14:M:80:ARG:O    | 14:M:82:MET:N    | 2.53        | 0.41     |
| 1:A:431:A:O2'    | 1:A:432:A:H5'    | 2.20        | 0.41     |
| 1:A:1239:A:H62   | 1:A:1299:A:N6    | 2.18        | 0.41     |
| 13:L:73:GLU:OE2  | 13:L:73:GLU:HA   | 2.19        | 0.41     |
| 1:A:833:U:H2'    | 1:A:834:C:C6     | 2.55        | 0.41     |
| 21:T:62:LEU:N    | 21:T:62:LEU:HD23 | 2.35        | 0.41     |
| 1:A:50:A:N6      | 1:A:361:G:H4'    | 2.35        | 0.41     |
| 20:S:33:THR:HG22 | 20:S:34:TRP:H    | 1.84        | 0.41     |
| 20:S:33:THR:CG2  | 20:S:34:TRP:N    | 2.81        | 0.41     |
| 4:C:47:LEU:CD2   | 4:C:68:VAL:HG11  | 2.51        | 0.41     |
| 3:B:127:ILE:HB   | 3:B:128:GLU:OE1  | 2.19        | 0.41     |
| 3:B:69:LEU:HB3   | 3:B:162:ILE:HG12 | 2.02        | 0.41     |
| 1:A:182:U:H6     | 1:A:182:U:H5'    | 1.85        | 0.41     |
| 5:D:54:TYR:O     | 5:D:55:ALA:C     | 2.59        | 0.41     |
| 1:A:401:C:H2'    | 1:A:402:G:C8     | 2.46        | 0.41     |
| 1:A:285:G:C2'    | 1:A:286:G:H5'    | 2.50        | 0.41     |
| 1:A:397:A:C6     | 1:A:548:G:N7     | 2.88        | 0.41     |
| 8:G:14:PRO:HB2   | 8:G:19:GLY:O     | 2.19        | 0.41     |

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| Atom-1          | Atom-2           | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 1:A:312:C:H2'   | 1:A:313:A:C8     | 2.55        | 0.41     |
| 17:P:26:ARG:HG2 | 17:P:26:ARG:HH11 | 1.85        | 0.41     |
| 1:A:637:G:O2'   | 1:A:638:G:H5'    | 2.20        | 0.41     |
| 1:A:124:G:C6    | 1:A:125:U:C4     | 3.08        | 0.41     |
| 1:A:57:G:H2'    | 1:A:58:C:O4'     | 2.19        | 0.41     |
| 1:A:1351:U:O2'  | 1:A:1352:C:H5'   | 2.19        | 0.41     |
| 3:B:109:SER:O   | 3:B:111:ARG:N    | 2.53        | 0.41     |
| 3:B:115:LEU:HG  | 3:B:153:ARG:NH2  | 2.36        | 0.41     |
| 3:B:130:ARG:NH2 | 4:C:207:VAL:CG2  | 2.81        | 0.41     |
| 9:H:1:MET:CG    | 9:H:2:LEU:H      | 2.21        | 0.41     |
| 5:D:61:LYS:NZ   | 5:D:72:GLU:OE2   | 2.53        | 0.41     |
| 5:D:65:ARG:HB2  | 5:D:75:PHE:CE1   | 2.55        | 0.41     |
| 9:H:24:THR:HG23 | 9:H:61:VAL:HB    | 2.02        | 0.41     |
| 1:A:1169:A:H2'  | 1:A:1171:G:O4'   | 2.20        | 0.41     |
| 10:I:19:LEU:C   | 10:I:20:ARG:HG3  | 2.40        | 0.41     |
| 10:I:19:LEU:HB3 | 10:I:59:PHE:CE2  | 2.54        | 0.41     |
| 3:B:53:ARG:HG2  | 3:B:53:ARG:NH1   | 2.35        | 0.41     |
| 1:A:626:U:O2'   | 1:A:627:G:H5'    | 2.19        | 0.41     |
| 1:A:1103:C:H2'  | 1:A:1104:G:O4'   | 2.21        | 0.41     |
| 5:D:43:HIS:O    | 5:D:45:GLN:N     | 2.53        | 0.41     |
| 21:T:94:ALA:O   | 21:T:95:ALA:CB   | 2.68        | 0.41     |
| 5:D:96:LEU:CD1  | 5:D:96:LEU:N     | 2.82        | 0.41     |
| 1:A:767:A:H2'   | 1:A:768:A:H8     | 1.85        | 0.41     |
| 1:A:820:U:H4'   | 1:A:821:G:OP2    | 2.20        | 0.41     |
| 1:A:224:C:H2'   | 1:A:225:C:C6     | 2.54        | 0.41     |
| 1:A:416:G:C5    | 1:A:417:C:C4     | 3.09        | 0.41     |
| 9:H:48:TYR:CD1  | 9:H:48:TYR:C     | 2.93        | 0.41     |
| 13:L:28:LYS:O   | 13:L:29:GLY:C    | 2.57        | 0.41     |
| 9:H:119:LEU:HB3 | 9:H:123:GLU:HB3  | 2.02        | 0.41     |
| 5:D:65:ARG:HE   | 5:D:72:GLU:N     | 2.17        | 0.41     |
| 1:A:926:G:H5'   | 1:A:927:G:O5'    | 2.20        | 0.41     |
| 7:F:101:ALA:HB2 | 19:R:28:GLU:CB   | 2.46        | 0.41     |
| 5:D:114:ARG:CG  | 5:D:114:ARG:HH11 | 2.23        | 0.41     |
| 1:A:448:A:C4    | 1:A:487:A:C2     | 3.08        | 0.41     |
| 1:A:255:G:O6    | 1:A:266:G:O6     | 2.38        | 0.41     |
| 8:G:23:VAL:HG13 | 8:G:43:PHE:CE2   | 2.56        | 0.41     |
| 1:A:1198:G:O2'  | 1:A:1199:U:H5'   | 2.21        | 0.41     |
| 1:A:309:G:O2'   | 1:A:310:G:H5'    | 2.19        | 0.41     |
| 18:Q:51:TYR:CD1 | 18:Q:73:VAL:HG11 | 2.56        | 0.41     |
| 1:A:1468:A:H2'  | 1:A:1469:G:O4'   | 2.20        | 0.41     |
| 9:H:25:ASP:OD1  | 9:H:25:ASP:N     | 2.54        | 0.41     |
| 1:A:281:G:O2'   | 1:A:282:A:C8     | 2.73        | 0.41     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 6:E:92:LYS:HB3   | 6:E:119:LEU:HB2  | 2.01        | 0.41     |
| 14:M:120:LYS:HE2 | 14:M:123:ALA:CB  | 2.50        | 0.41     |
| 19:R:59:SER:O    | 19:R:60:GLY:C    | 2.59        | 0.41     |
| 1:A:1221:G:O2'   | 1:A:1222:G:H5'   | 2.20        | 0.41     |
| 3:B:16:HIS:HE1   | 3:B:213:LEU:HB3  | 1.85        | 0.41     |
| 3:B:180:LEU:HD23 | 3:B:180:LEU:HA   | 1.78        | 0.41     |
| 1:A:393:A:C2     | 1:A:394:G:C8     | 3.08        | 0.41     |
| 1:A:393:A:OP2    | 17:P:12:LYS:CE   | 2.67        | 0.41     |
| 5:D:58:LEU:HD13  | 5:D:58:LEU:C     | 2.41        | 0.41     |
| 4:C:24:ALA:O     | 4:C:26:LYS:HE2   | 2.20        | 0.41     |
| 14:M:22:ILE:HD12 | 14:M:25:ILE:CD1  | 2.49        | 0.41     |
| 1:A:622:A:C8     | 1:A:623:C:C6     | 3.09        | 0.41     |
| 11:J:85:LEU:O    | 11:J:86:MET:C    | 2.58        | 0.41     |
| 22:V:8:THR:O     | 22:V:9:ARG:C     | 2.58        | 0.41     |
| 1:A:607:A:O2'    | 1:A:608:A:H5'    | 2.21        | 0.41     |
| 9:H:73:ASP:OD2   | 9:H:75:ARG:HB2   | 2.21        | 0.41     |
| 1:A:451:A:C2     | 1:A:480:U:C4     | 3.08        | 0.41     |
| 8:G:75:VAL:HG21  | 8:G:144:MET:HB3  | 2.02        | 0.41     |
| 8:G:136:LYS:O    | 8:G:140:ASP:OD1  | 2.38        | 0.41     |
| 12:K:100:ALA:O   | 12:K:102:GLY:N   | 2.53        | 0.41     |
| 1:A:325:A:OP2    | 21:T:70:SER:HB3  | 2.21        | 0.41     |
| 5:D:159:ARG:O    | 5:D:163:GLU:N    | 2.54        | 0.41     |
| 20:S:78:ARG:H    | 20:S:78:ARG:HG2  | 1.57        | 0.41     |
| 16:O:33:THR:OG1  | 16:O:85:LEU:HD13 | 2.21        | 0.41     |
| 3:B:155:LEU:HA   | 3:B:155:LEU:HD23 | 1.90        | 0.41     |
| 9:H:24:THR:HG23  | 9:H:24:THR:O     | 2.21        | 0.41     |
| 9:H:61:VAL:O     | 9:H:63:LEU:HD13  | 2.20        | 0.41     |
| 5:D:52:SER:O     | 5:D:53:ASP:C     | 2.59        | 0.41     |
| 1:A:401:C:H1'    | 1:A:622:A:H1'    | 2.01        | 0.41     |
| 3:B:23:ARG:HD3   | 3:B:23:ARG:C     | 2.41        | 0.41     |
| 1:A:560:U:O2'    | 1:A:561:U:OP2    | 2.28        | 0.41     |
| 5:D:3:ARG:HD3    | 5:D:3:ARG:HA     | 1.80        | 0.41     |
| 17:P:81:ARG:HD3  | 17:P:83:GLU:HG2  | 2.03        | 0.41     |
| 1:A:458:C:C5     | 1:A:459:G:N7     | 2.89        | 0.41     |
| 12:K:85:ARG:HG3  | 12:K:85:ARG:NH1  | 2.34        | 0.41     |
| 6:E:143:ARG:HA   | 6:E:143:ARG:HD3  | 1.78        | 0.41     |
| 1:A:1050:G:O2'   | 1:A:1051:C:H5'   | 2.20        | 0.41     |
| 1:A:899:C:H2'    | 1:A:900:A:C8     | 2.55        | 0.41     |
| 1:A:603:U:O2'    | 1:A:604:G:H5'    | 2.20        | 0.41     |
| 1:A:1079:G:O3'   | 6:E:14:ARG:NH2   | 2.53        | 0.41     |
| 12:K:84:VAL:CG1  | 12:K:95:ILE:HD11 | 2.46        | 0.41     |
| 12:K:99:GLN:HA   | 12:K:105:VAL:CG2 | 2.51        | 0.41     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:685:G:C2     | 1:A:686:U:C4      | 3.08        | 0.41     |
| 10:I:126:SER:OG  | 10:I:127:LYS:N    | 2.52        | 0.41     |
| 1:A:963:G:HO2'   | 11:J:54:PHE:HZ    | 1.67        | 0.41     |
| 10:I:106:ALA:O   | 10:I:108:VAL:HG23 | 2.20        | 0.41     |
| 4:C:148:GLY:HA3  | 4:C:172:ARG:O     | 2.21        | 0.41     |
| 16:O:33:THR:HG23 | 16:O:63:ARG:HH12  | 1.86        | 0.41     |
| 8:G:18:TYR:HD1   | 8:G:18:TYR:H      | 1.67        | 0.41     |
| 4:C:191:THR:HB   | 4:C:194:GLY:H     | 1.86        | 0.41     |
| 10:I:43:ALA:C    | 10:I:45:ALA:N     | 2.74        | 0.41     |
| 16:O:77:ARG:O    | 16:O:80:ALA:HB3   | 2.20        | 0.41     |
| 18:Q:53:LEU:HD12 | 18:Q:54:GLY:N     | 2.36        | 0.41     |
| 9:H:6:ILE:O      | 9:H:10:LEU:HG     | 2.21        | 0.41     |
| 1:A:1145:C:O2'   | 1:A:1146:A:O5'    | 2.34        | 0.41     |
| 8:G:152:ALA:C    | 8:G:154:TYR:N     | 2.74        | 0.41     |
| 1:A:463:A:O2'    | 1:A:474:G:H5'     | 2.21        | 0.41     |
| 6:E:144:THR:CG2  | 6:E:145:LYS:N     | 2.84        | 0.41     |
| 20:S:10:PHE:CD2  | 20:S:11:VAL:N     | 2.88        | 0.41     |
| 12:K:33:THR:OG1  | 12:K:34:ASP:N     | 2.53        | 0.41     |
| 1:A:184:G:H2'    | 1:A:185:A:H8      | 1.86        | 0.41     |
| 9:H:5:PRO:O      | 9:H:8:ASP:HB3     | 2.21        | 0.41     |
| 15:N:36:PHE:O    | 15:N:36:PHE:CD1   | 2.74        | 0.41     |
| 1:A:982:U:H5''   | 15:N:6:LEU:CD1    | 2.51        | 0.41     |
| 6:E:79:GLU:HA    | 6:E:91:LEU:O      | 2.21        | 0.41     |
| 4:C:179:ARG:O    | 4:C:179:ARG:HD2   | 2.20        | 0.41     |
| 1:A:370:C:C2'    | 1:A:371:G:H5'     | 2.50        | 0.41     |
| 1:A:324:G:N2     | 1:A:327:A:H8      | 2.19        | 0.41     |
| 1:A:141:A:O2'    | 1:A:142:G:H5'     | 2.21        | 0.41     |
| 21:T:56:MET:HG2  | 21:T:84:LEU:CD1   | 2.50        | 0.41     |
| 1:A:502:G:H2'    | 1:A:503:C:H6      | 1.86        | 0.41     |
| 14:M:40:ASN:ND2  | 14:M:40:ASN:C     | 2.74        | 0.41     |
| 9:H:9:MET:HG3    | 9:H:26:VAL:HG21   | 2.02        | 0.41     |
| 8:G:71:PRO:HG3   | 8:G:103:TRP:CH2   | 2.56        | 0.41     |
| 8:G:51:GLN:HA    | 8:G:51:GLN:OE1    | 2.20        | 0.41     |
| 6:E:45:PHE:CE2   | 6:E:47:LYS:HE3    | 2.56        | 0.41     |
| 1:A:522:C:H2'    | 1:A:523:A:O4'     | 2.20        | 0.41     |
| 3:B:60:ASP:O     | 3:B:64:ARG:HB2    | 2.21        | 0.41     |
| 1:A:452:A:O2'    | 17:P:72:ARG:HD2   | 2.20        | 0.41     |
| 1:A:1254:C:OP1   | 11:J:45:ARG:HD2   | 2.20        | 0.41     |
| 4:C:28:GLN:O     | 4:C:29:TYR:C      | 2.58        | 0.41     |
| 1:A:1126:U:H2'   | 1:A:1127:G:C8     | 2.56        | 0.41     |
| 1:A:1257:U:O2'   | 1:A:1258:G:OP2    | 2.28        | 0.41     |
| 11:J:4:ILE:HA    | 11:J:100:THR:HA   | 2.01        | 0.41     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:5:U:O2'      | 1:A:6:G:P         | 2.79        | 0.41     |
| 1:A:1117:G:H4'   | 10:I:104:ARG:HH11 | 1.81        | 0.41     |
| 1:A:1227:A:H2'   | 1:A:1228:C:O5'    | 2.21        | 0.41     |
| 11:J:23:ILE:O    | 11:J:23:ILE:HG22  | 2.21        | 0.41     |
| 11:J:22:LYS:HE2  | 11:J:90:LEU:HD12  | 2.02        | 0.41     |
| 5:D:150:GLU:N    | 5:D:150:GLU:CD    | 2.61        | 0.41     |
| 15:N:26:ARG:HH11 | 15:N:47:LEU:HG    | 1.80        | 0.41     |
| 20:S:13:ASP:O    | 20:S:17:GLU:HG2   | 2.21        | 0.41     |
| 1:A:273:A:N6     | 1:A:274:A:C6      | 2.89        | 0.41     |
| 9:H:51:VAL:CG1   | 9:H:52:ASP:N      | 2.84        | 0.41     |
| 10:I:42:ARG:O    | 10:I:44:VAL:N     | 2.53        | 0.41     |
| 10:I:48:GLU:CA   | 10:I:51:ARG:NH1   | 2.79        | 0.41     |
| 10:I:99:LEU:CB   | 10:I:101:PHE:CE1  | 3.03        | 0.41     |
| 5:D:52:SER:C     | 5:D:54:TYR:N      | 2.73        | 0.41     |
| 3:B:122:PHE:O    | 3:B:123:ALA:CB    | 2.67        | 0.41     |
| 14:M:22:ILE:HG21 | 14:M:66:LEU:HD13  | 2.02        | 0.41     |
| 1:A:1196:U:HO2'  | 1:A:1197:G:P      | 2.43        | 0.41     |
| 10:I:93:ARG:HH11 | 10:I:97:LYS:HZ2   | 1.69        | 0.41     |
| 1:A:645:C:O2'    | 1:A:646:U:H5'     | 2.21        | 0.41     |
| 1:A:1442:G:C2'   | 1:A:1442:G:N3     | 2.84        | 0.41     |
| 14:M:15:VAL:C    | 14:M:17:VAL:N     | 2.75        | 0.41     |
| 1:A:652:U:H2'    | 1:A:752:G:N1      | 2.36        | 0.41     |
| 1:A:961:U:C2'    | 1:A:962:C:H5'     | 2.51        | 0.41     |
| 9:H:126:LYS:C    | 9:H:128:GLY:N     | 2.74        | 0.41     |
| 1:A:62:U:H2'     | 1:A:63:C:C6       | 2.56        | 0.41     |
| 1:A:821:G:H2'    | 1:A:822:C:C6      | 2.55        | 0.41     |
| 1:A:718:G:H1'    | 12:K:116:HIS:HA   | 2.03        | 0.41     |
| 1:A:1080:A:C8    | 1:A:1081:G:H1'    | 2.56        | 0.41     |
| 1:A:904:C:H2'    | 1:A:905:U:O4'     | 2.21        | 0.41     |
| 9:H:136:GLU:HG2  | 9:H:136:GLU:O     | 2.19        | 0.41     |
| 1:A:132:C:H2'    | 1:A:133:U:O4'     | 2.21        | 0.41     |
| 16:O:39:LEU:HD13 | 16:O:59:MET:HE2   | 2.03        | 0.41     |
| 3:B:20:GLU:O     | 3:B:39:ILE:HG23   | 2.21        | 0.41     |
| 3:B:33:TYR:HB3   | 3:B:41:ILE:O      | 2.21        | 0.41     |
| 1:A:954:G:H2'    | 1:A:955:U:H6      | 1.85        | 0.41     |
| 4:C:8:ILE:O      | 4:C:10:PHE:N      | 2.54        | 0.41     |
| 1:A:1499:A:H1'   | 1:A:1520:G:H5'    | 2.03        | 0.41     |
| 1:A:1006:C:N3    | 1:A:1023:G:O6     | 2.53        | 0.41     |
| 9:H:60:ARG:HA    | 9:H:60:ARG:HD3    | 1.93        | 0.41     |
| 12:K:15:ALA:CA   | 12:K:77:MET:HA    | 2.50        | 0.41     |
| 5:D:8:VAL:HG11   | 5:D:21:LEU:HB3    | 2.03        | 0.41     |
| 1:A:1317:C:C6    | 15:N:16:PHE:CD2   | 3.09        | 0.41     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 11:J:84:GLN:O    | 11:J:88:LEU:HB2  | 2.21        | 0.41     |
| 1:A:994:A:C8     | 1:A:994:A:OP1    | 2.74        | 0.41     |
| 1:A:922:G:H2'    | 1:A:923:A:C8     | 2.56        | 0.41     |
| 14:M:20:THR:C    | 14:M:22:ILE:H    | 2.24        | 0.41     |
| 8:G:41:ARG:O     | 8:G:44:TYR:N     | 2.54        | 0.41     |
| 9:H:86:ILE:HD12  | 9:H:133:LEU:CD2  | 2.51        | 0.41     |
| 1:A:33:A:N3      | 13:L:32:PHE:HE2  | 2.18        | 0.41     |
| 1:A:586:C:O3'    | 9:H:89:PRO:HB2   | 2.20        | 0.41     |
| 1:A:1337:G:H5''  | 1:A:1338:G:OP1   | 2.21        | 0.41     |
| 1:A:1450:U:H2'   | 1:A:1452:C:C5    | 2.56        | 0.41     |
| 1:A:1062:U:H2'   | 1:A:1063:C:C6    | 2.56        | 0.40     |
| 1:A:1305:G:OP1   | 22:V:2:GLY:N     | 2.53        | 0.40     |
| 22:V:2:GLY:O     | 22:V:3:LYS:C     | 2.59        | 0.40     |
| 1:A:1256:A:O2'   | 1:A:1257:U:P     | 2.79        | 0.40     |
| 1:A:7:G:H5''     | 1:A:298:A:H5'    | 2.03        | 0.40     |
| 11:J:13:HIS:O    | 11:J:17:ASP:OD2  | 2.39        | 0.40     |
| 3:B:126:GLU:HG2  | 3:B:129:GLU:OE1  | 2.20        | 0.40     |
| 4:C:206:GLU:O    | 4:C:207:VAL:O    | 2.39        | 0.40     |
| 10:I:86:VAL:CG1  | 10:I:90:PRO:HA   | 2.44        | 0.40     |
| 13:L:110:VAL:O   | 13:L:122:THR:CG2 | 2.63        | 0.40     |
| 1:A:8:A:C6       | 5:D:209:ARG:HB2  | 2.55        | 0.40     |
| 14:M:44:ARG:HA   | 14:M:44:ARG:HD2  | 1.88        | 0.40     |
| 19:R:87:ARG:CG   | 19:R:87:ARG:NH1  | 2.83        | 0.40     |
| 1:A:1158:C:C5    | 1:A:1160:G:C8    | 3.10        | 0.40     |
| 19:R:51:LEU:HA   | 19:R:52:PRO:HD3  | 1.91        | 0.40     |
| 11:J:82:ILE:O    | 11:J:82:ILE:HG22 | 2.20        | 0.40     |
| 1:A:474:G:OP2    | 17:P:75:ARG:NH1  | 2.53        | 0.40     |
| 1:A:23:C:H2'     | 1:A:24:U:H6      | 1.86        | 0.40     |
| 8:G:104:LEU:HD23 | 8:G:134:ALA:CB   | 2.50        | 0.40     |
| 6:E:127:ASN:O    | 6:E:131:ILE:HG12 | 2.20        | 0.40     |
| 1:A:893:C:H2'    | 1:A:894:G:H8     | 1.86        | 0.40     |
| 1:A:1033:G:H2'   | 1:A:1034:G:H8    | 1.86        | 0.40     |
| 1:A:423:G:C2'    | 1:A:424:G:H5'    | 2.52        | 0.40     |
| 4:C:155:GLY:O    | 4:C:156:ARG:CB   | 2.68        | 0.40     |
| 5:D:187:ARG:HH21 | 5:D:188:LEU:CG   | 2.15        | 0.40     |
| 21:T:36:LEU:HA   | 21:T:39:LYS:HB2  | 2.03        | 0.40     |
| 1:A:1288:A:H2'   | 1:A:1289:A:C8    | 2.56        | 0.40     |
| 8:G:156:TRP:OXT  | 8:G:156:TRP:CD1  | 2.75        | 0.40     |
| 6:E:115:VAL:CG1  | 6:E:116:THR:N    | 2.85        | 0.40     |
| 1:A:1152:A:H2'   | 1:A:1153:C:H6    | 1.86        | 0.40     |
| 1:A:1346:A:C5    | 8:G:10:ARG:NH2   | 2.89        | 0.40     |
| 3:B:200:ILE:HG22 | 3:B:201:ILE:N    | 2.36        | 0.40     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 3:B:236:TYR:HA   | 3:B:239:VAL:CG2   | 2.51        | 0.40     |
| 1:A:322:C:O2'    | 1:A:323:U:H5'     | 2.20        | 0.40     |
| 3:B:96:ARG:O     | 3:B:98:LEU:HD23   | 2.21        | 0.40     |
| 10:I:78:LYS:CD   | 10:I:101:PHE:HD2  | 2.29        | 0.40     |
| 14:M:6:GLY:O     | 14:M:7:VAL:CG2    | 2.69        | 0.40     |
| 1:A:791:G:C2'    | 1:A:792:A:H5'     | 2.48        | 0.40     |
| 1:A:1097:C:O2'   | 1:A:1168:A:N3     | 2.46        | 0.40     |
| 10:I:118:LYS:HB2 | 10:I:118:LYS:HZ2  | 1.86        | 0.40     |
| 19:R:16:PRO:O    | 19:R:17:SER:CB    | 2.68        | 0.40     |
| 1:A:1291:G:H5''  | 8:G:41:ARG:NH2    | 2.37        | 0.40     |
| 14:M:110:ARG:CG  | 14:M:110:ARG:NH1  | 2.84        | 0.40     |
| 10:I:113:LYS:N   | 10:I:113:LYS:HD2  | 2.36        | 0.40     |
| 1:A:340:U:H2'    | 1:A:341:C:C6      | 2.56        | 0.40     |
| 3:B:20:GLU:OE2   | 3:B:205:ASP:OD1   | 2.39        | 0.40     |
| 3:B:18:GLY:HA2   | 3:B:41:ILE:HA     | 2.03        | 0.40     |
| 3:B:107:THR:C    | 3:B:109:SER:H     | 2.25        | 0.40     |
| 11:J:34:VAL:C    | 11:J:36:GLY:H     | 2.24        | 0.40     |
| 11:J:38:ILE:CG2  | 11:J:39:PRO:HD2   | 2.52        | 0.40     |
| 6:E:99:GLY:O     | 6:E:117:ASP:HA    | 2.21        | 0.40     |
| 6:E:115:VAL:CG1  | 6:E:118:ILE:HG13  | 2.51        | 0.40     |
| 1:A:1152:A:O2'   | 1:A:1153:C:H5'    | 2.21        | 0.40     |
| 11:J:23:ILE:CD1  | 11:J:23:ILE:H     | 2.33        | 0.40     |
| 1:A:1404:C:H2'   | 1:A:1405:G:C8     | 2.56        | 0.40     |
| 21:T:18:GLN:O    | 21:T:19:SER:C     | 2.58        | 0.40     |
| 1:A:182:U:OP2    | 1:A:183:G:C8      | 2.74        | 0.40     |
| 13:L:83:VAL:CG2  | 13:L:100:ILE:HG23 | 2.51        | 0.40     |
| 9:H:84:ARG:HB3   | 9:H:84:ARG:HE     | 1.51        | 0.40     |
| 1:A:344:A:O2'    | 1:A:345:C:OP1     | 2.34        | 0.40     |
| 1:A:474:G:H2'    | 1:A:475:G:C8      | 2.50        | 0.40     |
| 8:G:21:VAL:CG2   | 8:G:22:LEU:N      | 2.84        | 0.40     |
| 1:A:309:G:H1'    | 1:A:608:A:C2      | 2.57        | 0.40     |
| 10:I:89:ASN:OD1  | 10:I:91:ASP:HB2   | 2.21        | 0.40     |
| 1:A:536:C:H2'    | 1:A:537:G:C8      | 2.56        | 0.40     |
| 21:T:42:GLN:CA   | 21:T:42:GLN:NE2   | 2.84        | 0.40     |
| 3:B:192:SER:OG   | 3:B:193:ASP:N     | 2.54        | 0.40     |
| 1:A:294:U:H2'    | 1:A:295:C:C6      | 2.56        | 0.40     |
| 1:A:1451:A:H4'   | 1:A:1452:C:OP2    | 2.22        | 0.40     |
| 1:A:679:C:H2'    | 1:A:680:C:C6      | 2.56        | 0.40     |
| 1:A:671:G:H2'    | 1:A:672:U:O4'     | 2.22        | 0.40     |
| 5:D:108:LEU:HA   | 5:D:108:LEU:HD23  | 1.89        | 0.40     |
| 11:J:51:ARG:NH1  | 11:J:51:ARG:CG    | 2.80        | 0.40     |
| 1:A:760:G:H2'    | 1:A:761:G:C5'     | 2.51        | 0.40     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:1068:G:H8    | 1:A:1068:G:OP2   | 2.05        | 0.40     |
| 3:B:85:ALA:HB1   | 3:B:92:TYR:HB3   | 2.04        | 0.40     |
| 1:A:1139:G:O2'   | 1:A:1140:C:OP2   | 2.36        | 0.40     |
| 1:A:335:C:H2'    | 1:A:336:C:H6     | 1.86        | 0.40     |
| 3:B:10:LEU:C     | 3:B:12:GLU:H     | 2.24        | 0.40     |
| 1:A:539:A:H2'    | 1:A:540:G:C8     | 2.57        | 0.40     |
| 8:G:18:TYR:HD2   | 8:G:59:LEU:HB2   | 1.77        | 0.40     |
| 5:D:70:ILE:HD11  | 5:D:100:ARG:NH1  | 2.36        | 0.40     |
| 15:N:8:GLU:HB2   | 15:N:11:LYS:HD2  | 2.04        | 0.40     |
| 7:F:22:GLU:O     | 7:F:26:ILE:HG13  | 2.22        | 0.40     |
| 1:A:528:C:H41    | 13:L:49:ASN:CG   | 2.24        | 0.40     |
| 13:L:47:LYS:HB2  | 13:L:48:PRO:HD2  | 2.02        | 0.40     |
| 9:H:10:LEU:HD22  | 9:H:83:ILE:HD11  | 2.03        | 0.40     |
| 1:A:1481:U:H2'   | 1:A:1482:G:C8    | 2.56        | 0.40     |
| 1:A:981:U:H5'    | 15:N:21:TYR:CE1  | 2.55        | 0.40     |
| 9:H:56:LYS:CB    | 9:H:57:PRO:HD2   | 2.51        | 0.40     |
| 9:H:91:ARG:HG3   | 13:L:7:ILE:HG13  | 2.03        | 0.40     |
| 3:B:30:ARG:HG3   | 3:B:31:TYR:CD2   | 2.56        | 0.40     |
| 8:G:62:PHE:O     | 8:G:65:ALA:HB3   | 2.20        | 0.40     |
| 4:C:36:ASP:HA    | 4:C:39:ILE:HD12  | 2.03        | 0.40     |
| 1:A:119:A:H4'    | 1:A:120:A:O5'    | 2.21        | 0.40     |
| 1:A:455:C:H6     | 1:A:455:C:O5'    | 2.04        | 0.40     |
| 3:B:204:ASN:HD22 | 3:B:207:ALA:CB   | 2.35        | 0.40     |
| 1:A:1127:G:H1'   | 1:A:1148:U:N3    | 2.37        | 0.40     |
| 1:A:1282:C:O2'   | 1:A:1283:G:H5'   | 2.21        | 0.40     |
| 11:J:34:VAL:HA   | 11:J:74:ILE:HG23 | 2.03        | 0.40     |
| 19:R:36:ASN:O    | 19:R:39:VAL:HG12 | 2.21        | 0.40     |
| 4:C:108:ASN:HD22 | 4:C:111:LEU:CG   | 2.27        | 0.40     |
| 5:D:78:LEU:HD13  | 5:D:97:LEU:HD23  | 2.02        | 0.40     |
| 1:A:1423:G:HO2'  | 1:A:1424:C:H5'   | 1.85        | 0.40     |
| 16:O:31:LEU:CD1  | 16:O:31:LEU:H    | 2.31        | 0.40     |
| 3:B:8:LYS:CD     | 3:B:9:GLU:N      | 2.84        | 0.40     |
| 16:O:17:ARG:HH11 | 16:O:17:ARG:CG   | 2.30        | 0.40     |
| 1:A:1178:G:P     | 10:I:97:LYS:NZ   | 2.95        | 0.40     |
| 1:A:179:A:H2'    | 1:A:180:U:H6     | 1.86        | 0.40     |
| 1:A:928:G:O2'    | 1:A:929:G:H5'    | 2.20        | 0.40     |
| 1:A:420:U:C2'    | 1:A:421:U:H5''   | 2.51        | 0.40     |
| 1:A:61:G:C2'     | 1:A:62:U:H5'     | 2.52        | 0.40     |
| 19:R:34:TYR:CD1  | 19:R:35:ARG:HG3  | 2.56        | 0.40     |
| 1:A:1436:U:O2'   | 1:A:1437:C:H5'   | 2.22        | 0.40     |
| 1:A:570:G:N2     | 1:A:571:U:C2     | 2.90        | 0.40     |
| 4:C:126:ARG:C    | 4:C:127:ARG:HG3  | 2.42        | 0.40     |

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| Atom-1           | Atom-2          | Distance(Å) | Clash(Å) |
|------------------|-----------------|-------------|----------|
| 12:K:21:ILE:HD13 | 12:K:94:ALA:HB3 | 2.03        | 0.40     |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1          | Atom-2                 | Distance(Å) | Clash(Å) |
|-----------------|------------------------|-------------|----------|
| 3:B:157:ARG:NH1 | 3:B:157:ARG:NH1[7_555] | 1.94        | 0.26     |

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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 |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 3   | B     | 232/256 (91%) | 172 (74%) | 34 (15%) | 26 (11%) | 1           | 5  |
| 4   | C     | 204/239 (85%) | 132 (65%) | 44 (22%) | 28 (14%) | 0           | 2  |
| 5   | D     | 206/209 (99%) | 153 (74%) | 37 (18%) | 16 (8%)  | 1           | 14 |
| 6   | E     | 148/162 (91%) | 130 (88%) | 15 (10%) | 3 (2%)   | 11          | 58 |
| 7   | F     | 99/101 (98%)  | 83 (84%)  | 13 (13%) | 3 (3%)   | 7           | 46 |
| 8   | G     | 153/156 (98%) | 119 (78%) | 23 (15%) | 11 (7%)  | 2           | 16 |
| 9   | H     | 136/138 (99%) | 118 (87%) | 15 (11%) | 3 (2%)   | 10          | 55 |
| 10  | I     | 125/128 (98%) | 86 (69%)  | 26 (21%) | 13 (10%) | 1           | 7  |
| 11  | J     | 96/105 (91%)  | 59 (62%)  | 19 (20%) | 18 (19%) | 0           | 1  |
| 12  | K     | 117/129 (91%) | 84 (72%)  | 23 (20%) | 10 (8%)  | 1           | 11 |
| 13  | L     | 122/135 (90%) | 90 (74%)  | 22 (18%) | 10 (8%)  | 1           | 13 |
| 14  | M     | 123/126 (98%) | 87 (71%)  | 20 (16%) | 16 (13%) | 0           | 3  |
| 15  | N     | 58/61 (95%)   | 40 (69%)  | 9 (16%)  | 9 (16%)  | 0           | 1  |
| 16  | O     | 86/89 (97%)   | 66 (77%)  | 18 (21%) | 2 (2%)   | 10          | 54 |
| 17  | P     | 86/88 (98%)   | 67 (78%)  | 14 (16%) | 5 (6%)   | 3           | 23 |
| 18  | Q     | 102/105 (97%) | 83 (81%)  | 13 (13%) | 6 (6%)   | 2           | 23 |
| 19  | R     | 71/88 (81%)   | 51 (72%)  | 15 (21%) | 5 (7%)   | 2           | 17 |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 20  | S     | 78/93 (84%)     | 56 (72%)   | 12 (15%)  | 10 (13%) | 0           | 3  |
| 21  | T     | 97/106 (92%)    | 66 (68%)   | 19 (20%)  | 12 (12%) | 1           | 4  |
| 22  | V     | 22/26 (85%)     | 17 (77%)   | 4 (18%)   | 1 (4%)   | 4           | 32 |
| All | All   | 2361/2540 (93%) | 1759 (74%) | 395 (17%) | 207 (9%) | 1           | 11 |

All (207) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | B     | 8   | LYS  |
| 3   | B     | 16  | HIS  |
| 3   | B     | 17  | PHE  |
| 3   | B     | 21  | ARG  |
| 3   | B     | 24  | TRP  |
| 3   | B     | 123 | ALA  |
| 4   | C     | 4   | LYS  |
| 4   | C     | 15  | THR  |
| 4   | C     | 16  | ARG  |
| 4   | C     | 24  | ALA  |
| 4   | C     | 29  | TYR  |
| 4   | C     | 47  | LEU  |
| 4   | C     | 108 | ASN  |
| 4   | C     | 146 | ALA  |
| 4   | C     | 154 | SER  |
| 4   | C     | 179 | ARG  |
| 4   | C     | 189 | ALA  |
| 4   | C     | 206 | GLU  |
| 5   | D     | 29  | PRO  |
| 5   | D     | 36  | ARG  |
| 6   | E     | 16  | THR  |
| 9   | H     | 24  | THR  |
| 9   | H     | 83  | ILE  |
| 9   | H     | 91  | ARG  |
| 10  | I     | 7   | THR  |
| 10  | I     | 43  | ALA  |
| 10  | I     | 44  | VAL  |
| 10  | I     | 101 | PHE  |
| 11  | J     | 30  | SER  |
| 11  | J     | 32  | ALA  |
| 11  | J     | 54  | PHE  |
| 11  | J     | 57  | LYS  |
| 11  | J     | 79  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | J     | 86  | MET  |
| 12  | K     | 57  | THR  |
| 12  | K     | 101 | SER  |
| 13  | L     | 27  | LEU  |
| 13  | L     | 28  | LYS  |
| 13  | L     | 47  | LYS  |
| 14  | M     | 63  | THR  |
| 14  | M     | 67  | GLU  |
| 14  | M     | 107 | ALA  |
| 14  | M     | 122 | LYS  |
| 14  | M     | 124 | PRO  |
| 15  | N     | 22  | THR  |
| 15  | N     | 29  | ARG  |
| 15  | N     | 59  | ALA  |
| 15  | N     | 60  | SER  |
| 16  | O     | 88  | ARG  |
| 17  | P     | 83  | GLU  |
| 18  | Q     | 69  | LYS  |
| 18  | Q     | 80  | GLY  |
| 18  | Q     | 81  | ARG  |
| 18  | Q     | 98  | LEU  |
| 18  | Q     | 104 | LYS  |
| 19  | R     | 87  | ARG  |
| 20  | S     | 6   | LYS  |
| 20  | S     | 9   | VAL  |
| 20  | S     | 71  | LEU  |
| 21  | T     | 11  | SER  |
| 21  | T     | 73  | HIS  |
| 21  | T     | 99  | LEU  |
| 3   | B     | 9   | GLU  |
| 3   | B     | 18  | GLY  |
| 3   | B     | 20  | GLU  |
| 3   | B     | 23  | ARG  |
| 3   | B     | 126 | GLU  |
| 3   | B     | 127 | ILE  |
| 3   | B     | 190 | THR  |
| 3   | B     | 204 | ASN  |
| 3   | B     | 225 | ALA  |
| 4   | C     | 61  | ALA  |
| 5   | D     | 4   | TYR  |
| 5   | D     | 31  | CYS  |
| 5   | D     | 44  | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | D     | 63  | LYS  |
| 5   | D     | 153 | ARG  |
| 5   | D     | 175 | SER  |
| 6   | E     | 11  | ILE  |
| 6   | E     | 125 | SER  |
| 7   | F     | 16  | GLN  |
| 7   | F     | 39  | LYS  |
| 8   | G     | 7   | ALA  |
| 8   | G     | 53  | LYS  |
| 8   | G     | 155 | ARG  |
| 10  | I     | 23  | ASN  |
| 10  | I     | 41  | VAL  |
| 10  | I     | 94  | ALA  |
| 11  | J     | 33  | GLN  |
| 11  | J     | 34  | VAL  |
| 11  | J     | 59  | SER  |
| 11  | J     | 60  | ARG  |
| 11  | J     | 72  | VAL  |
| 12  | K     | 49  | GLY  |
| 12  | K     | 50  | TYR  |
| 12  | K     | 78  | GLN  |
| 12  | K     | 89  | ALA  |
| 13  | L     | 48  | PRO  |
| 13  | L     | 51  | ALA  |
| 13  | L     | 121 | GLY  |
| 14  | M     | 6   | GLY  |
| 14  | M     | 42  | ALA  |
| 14  | M     | 85  | GLY  |
| 14  | M     | 123 | ALA  |
| 15  | N     | 17  | LYS  |
| 17  | P     | 10  | GLY  |
| 17  | P     | 49  | LEU  |
| 19  | R     | 26  | LEU  |
| 20  | S     | 67  | VAL  |
| 20  | S     | 68  | GLY  |
| 20  | S     | 69  | HIS  |
| 21  | T     | 9   | ASN  |
| 21  | T     | 49  | ALA  |
| 21  | T     | 50  | GLU  |
| 21  | T     | 94  | ALA  |
| 21  | T     | 102 | GLY  |
| 3   | B     | 124 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | B     | 232 | PRO  |
| 4   | C     | 26  | LYS  |
| 4   | C     | 88  | ARG  |
| 4   | C     | 167 | TRP  |
| 4   | C     | 168 | ALA  |
| 5   | D     | 10  | ARG  |
| 5   | D     | 151 | LYS  |
| 5   | D     | 179 | GLU  |
| 8   | G     | 77  | SER  |
| 10  | I     | 31  | GLN  |
| 10  | I     | 54  | ASP  |
| 10  | I     | 56  | LEU  |
| 10  | I     | 58  | ARG  |
| 10  | I     | 121 | ARG  |
| 11  | J     | 39  | PRO  |
| 11  | J     | 90  | LEU  |
| 12  | K     | 15  | ALA  |
| 13  | L     | 117 | ARG  |
| 14  | M     | 27  | LYS  |
| 14  | M     | 38  | GLY  |
| 14  | M     | 80  | ARG  |
| 15  | N     | 12  | ARG  |
| 15  | N     | 13  | THR  |
| 15  | N     | 36  | PHE  |
| 19  | R     | 54  | ARG  |
| 21  | T     | 95  | ALA  |
| 21  | T     | 98  | PRO  |
| 22  | V     | 9   | ARG  |
| 3   | B     | 15  | VAL  |
| 3   | B     | 224 | GLN  |
| 4   | C     | 181 | ASN  |
| 4   | C     | 188 | LEU  |
| 5   | D     | 30  | LYS  |
| 5   | D     | 64  | LEU  |
| 8   | G     | 41  | ARG  |
| 8   | G     | 42  | ILE  |
| 8   | G     | 78  | ARG  |
| 8   | G     | 81  | GLY  |
| 11  | J     | 73  | ASP  |
| 11  | J     | 85  | LEU  |
| 12  | K     | 12  | ARG  |
| 12  | K     | 27  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | K     | 102 | GLY  |
| 13  | L     | 41  | ARG  |
| 13  | L     | 126 | LYS  |
| 14  | M     | 73  | GLU  |
| 14  | M     | 74  | VAL  |
| 14  | M     | 86  | CYS  |
| 14  | M     | 121 | LYS  |
| 15  | N     | 19  | ARG  |
| 18  | Q     | 33  | GLY  |
| 21  | T     | 42  | GLN  |
| 3   | B     | 60  | ASP  |
| 3   | B     | 83  | MET  |
| 3   | B     | 95  | GLN  |
| 3   | B     | 125 | PRO  |
| 4   | C     | 127 | ARG  |
| 4   | C     | 156 | ARG  |
| 5   | D     | 5   | ILE  |
| 5   | D     | 32  | ALA  |
| 7   | F     | 32  | ASN  |
| 10  | I     | 88  | TYR  |
| 16  | O     | 84  | LYS  |
| 19  | R     | 20  | ALA  |
| 19  | R     | 62  | GLU  |
| 20  | S     | 65  | ASN  |
| 21  | T     | 74  | LYS  |
| 3   | B     | 209 | ARG  |
| 4   | C     | 96  | GLY  |
| 4   | C     | 157 | ILE  |
| 8   | G     | 83  | ALA  |
| 13  | L     | 116 | SER  |
| 20  | S     | 17  | GLU  |
| 4   | C     | 66  | VAL  |
| 5   | D     | 171 | GLY  |
| 11  | J     | 40  | LEU  |
| 3   | B     | 89  | GLY  |
| 3   | B     | 229 | VAL  |
| 4   | C     | 77  | ILE  |
| 8   | G     | 112 | PRO  |
| 11  | J     | 91  | PRO  |
| 20  | S     | 11  | VAL  |
| 4   | C     | 14  | ILE  |
| 8   | G     | 17  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | S     | 8   | GLY  |
| 4   | C     | 57  | ILE  |
| 11  | J     | 82  | ILE  |
| 17  | P     | 41  | PRO  |
| 17  | P     | 87  | GLY  |
| 4   | C     | 7   | PRO  |

### 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 |     |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 3   | B     | 202/220 (92%)  | 177 (88%) | 25 (12%) | 7           | 31  |
| 4   | C     | 160/188 (85%)  | 140 (88%) | 20 (12%) | 7           | 31  |
| 5   | D     | 180/181 (99%)  | 164 (91%) | 16 (9%)  | 14          | 51  |
| 6   | E     | 115/123 (94%)  | 101 (88%) | 14 (12%) | 7           | 32  |
| 7   | F     | 90/90 (100%)   | 86 (96%)  | 4 (4%)   | 39          | 81  |
| 8   | G     | 126/127 (99%)  | 122 (97%) | 4 (3%)   | 51          | 88  |
| 9   | H     | 119/119 (100%) | 105 (88%) | 14 (12%) | 8           | 34  |
| 10  | I     | 98/99 (99%)    | 89 (91%)  | 9 (9%)   | 13          | 48  |
| 11  | J     | 87/92 (95%)    | 77 (88%)  | 10 (12%) | 8           | 35  |
| 12  | K     | 90/99 (91%)    | 85 (94%)  | 5 (6%)   | 30          | 75  |
| 13  | L     | 104/111 (94%)  | 97 (93%)  | 7 (7%)   | 23          | 67  |
| 14  | M     | 100/101 (99%)  | 84 (84%)  | 16 (16%) | 3           | 18  |
| 15  | N     | 49/50 (98%)    | 45 (92%)  | 4 (8%)   | 17          | 57  |
| 16  | O     | 79/80 (99%)    | 75 (95%)  | 4 (5%)   | 33          | 77  |
| 17  | P     | 74/74 (100%)   | 72 (97%)  | 2 (3%)   | 57          | 90  |
| 18  | Q     | 96/97 (99%)    | 90 (94%)  | 6 (6%)   | 25          | 70  |
| 19  | R     | 64/77 (83%)    | 59 (92%)  | 5 (8%)   | 18          | 60  |
| 20  | S     | 71/80 (89%)    | 64 (90%)  | 7 (10%)  | 11          | 44  |
| 21  | T     | 76/82 (93%)    | 69 (91%)  | 7 (9%)   | 13          | 48  |
| 22  | V     | 19/21 (90%)    | 19 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| All | All   | 1999/2111 (95%) | 1820 (91%) | 179 (9%) | 14          | 50 |

All (179) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | B     | 8   | LYS  |
| 3   | B     | 9   | GLU  |
| 3   | B     | 12  | GLU  |
| 3   | B     | 17  | PHE  |
| 3   | B     | 21  | ARG  |
| 3   | B     | 23  | ARG  |
| 3   | B     | 24  | TRP  |
| 3   | B     | 25  | ASN  |
| 3   | B     | 64  | ARG  |
| 3   | B     | 96  | ARG  |
| 3   | B     | 114 | ARG  |
| 3   | B     | 139 | LYS  |
| 3   | B     | 144 | ARG  |
| 3   | B     | 157 | ARG  |
| 3   | B     | 162 | ILE  |
| 3   | B     | 163 | PHE  |
| 3   | B     | 164 | VAL  |
| 3   | B     | 178 | ARG  |
| 3   | B     | 185 | ILE  |
| 3   | B     | 187 | LEU  |
| 3   | B     | 197 | VAL  |
| 3   | B     | 226 | ARG  |
| 3   | B     | 231 | GLU  |
| 3   | B     | 232 | PRO  |
| 3   | B     | 236 | TYR  |
| 4   | C     | 3   | ASN  |
| 4   | C     | 21  | ARG  |
| 4   | C     | 37  | GLN  |
| 4   | C     | 43  | LEU  |
| 4   | C     | 56  | ASP  |
| 4   | C     | 75  | VAL  |
| 4   | C     | 82  | GLU  |
| 4   | C     | 90  | GLU  |
| 4   | C     | 91  | LEU  |
| 4   | C     | 99  | VAL  |
| 4   | C     | 102 | ASN  |
| 4   | C     | 107 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | C     | 139 | GLN  |
| 4   | C     | 156 | ARG  |
| 4   | C     | 162 | GLN  |
| 4   | C     | 166 | GLU  |
| 4   | C     | 167 | TRP  |
| 4   | C     | 179 | ARG  |
| 4   | C     | 188 | LEU  |
| 4   | C     | 207 | VAL  |
| 5   | D     | 9   | CYS  |
| 5   | D     | 10  | ARG  |
| 5   | D     | 12  | CYS  |
| 5   | D     | 15  | GLU  |
| 5   | D     | 29  | PRO  |
| 5   | D     | 34  | GLU  |
| 5   | D     | 59  | ARG  |
| 5   | D     | 64  | LEU  |
| 5   | D     | 68  | TYR  |
| 5   | D     | 78  | LEU  |
| 5   | D     | 122 | ARG  |
| 5   | D     | 127 | THR  |
| 5   | D     | 157 | LEU  |
| 5   | D     | 176 | LEU  |
| 5   | D     | 194 | LEU  |
| 5   | D     | 199 | ASN  |
| 6   | E     | 12  | LEU  |
| 6   | E     | 31  | LEU  |
| 6   | E     | 43  | LEU  |
| 6   | E     | 52  | PRO  |
| 6   | E     | 56  | GLN  |
| 6   | E     | 63  | ARG  |
| 6   | E     | 68  | GLU  |
| 6   | E     | 73  | ASN  |
| 6   | E     | 79  | GLU  |
| 6   | E     | 80  | ILE  |
| 6   | E     | 89  | ILE  |
| 6   | E     | 120 | THR  |
| 6   | E     | 147 | ASP  |
| 6   | E     | 150 | ARG  |
| 7   | F     | 10  | LEU  |
| 7   | F     | 40  | VAL  |
| 7   | F     | 69  | GLU  |
| 7   | F     | 86  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | G     | 8   | GLU  |
| 8   | G     | 12  | LEU  |
| 8   | G     | 96  | GLN  |
| 8   | G     | 149 | ARG  |
| 9   | H     | 2   | LEU  |
| 9   | H     | 21  | LYS  |
| 9   | H     | 26  | VAL  |
| 9   | H     | 52  | ASP  |
| 9   | H     | 79  | VAL  |
| 9   | H     | 81  | HIS  |
| 9   | H     | 84  | ARG  |
| 9   | H     | 85  | ARG  |
| 9   | H     | 91  | ARG  |
| 9   | H     | 92  | ARG  |
| 9   | H     | 104 | ARG  |
| 9   | H     | 105 | ARG  |
| 9   | H     | 112 | LEU  |
| 9   | H     | 119 | LEU  |
| 10  | I     | 2   | GLU  |
| 10  | I     | 10  | ARG  |
| 10  | I     | 23  | ASN  |
| 10  | I     | 38  | GLN  |
| 10  | I     | 56  | LEU  |
| 10  | I     | 58  | ARG  |
| 10  | I     | 91  | ASP  |
| 10  | I     | 111 | ARG  |
| 10  | I     | 121 | ARG  |
| 11  | J     | 9   | ARG  |
| 11  | J     | 45  | ARG  |
| 11  | J     | 49  | VAL  |
| 11  | J     | 51  | ARG  |
| 11  | J     | 55  | LYS  |
| 11  | J     | 60  | ARG  |
| 11  | J     | 64  | GLU  |
| 11  | J     | 71  | LEU  |
| 11  | J     | 74  | ILE  |
| 11  | J     | 95  | GLU  |
| 12  | K     | 29  | ILE  |
| 12  | K     | 54  | ARG  |
| 12  | K     | 84  | VAL  |
| 12  | K     | 116 | HIS  |
| 12  | K     | 124 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | L     | 7   | ILE  |
| 13  | L     | 17  | LYS  |
| 13  | L     | 33  | ARG  |
| 13  | L     | 53  | ARG  |
| 13  | L     | 98  | TYR  |
| 13  | L     | 113 | ARG  |
| 13  | L     | 126 | LYS  |
| 14  | M     | 9   | ILE  |
| 14  | M     | 32  | GLU  |
| 14  | M     | 40  | ASN  |
| 14  | M     | 44  | ARG  |
| 14  | M     | 48  | LEU  |
| 14  | M     | 56  | LEU  |
| 14  | M     | 63  | THR  |
| 14  | M     | 70  | LEU  |
| 14  | M     | 77  | ASN  |
| 14  | M     | 81  | LEU  |
| 14  | M     | 102 | ARG  |
| 14  | M     | 105 | THR  |
| 14  | M     | 106 | ASN  |
| 14  | M     | 110 | ARG  |
| 14  | M     | 124 | PRO  |
| 14  | M     | 125 | ARG  |
| 15  | N     | 17  | LYS  |
| 15  | N     | 31  | ARG  |
| 15  | N     | 33  | VAL  |
| 15  | N     | 41  | ARG  |
| 16  | O     | 6   | GLU  |
| 16  | O     | 64  | ARG  |
| 16  | O     | 71  | GLN  |
| 16  | O     | 83  | GLU  |
| 17  | P     | 32  | TYR  |
| 17  | P     | 76  | GLN  |
| 18  | Q     | 34  | LYS  |
| 18  | Q     | 38  | ARG  |
| 18  | Q     | 53  | LEU  |
| 18  | Q     | 60  | ILE  |
| 18  | Q     | 70  | ARG  |
| 18  | Q     | 98  | LEU  |
| 19  | R     | 28  | GLU  |
| 19  | R     | 36  | ASN  |
| 19  | R     | 38  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19  | R     | 53  | ARG  |
| 19  | R     | 54  | ARG  |
| 20  | S     | 12  | ASP  |
| 20  | S     | 15  | LEU  |
| 20  | S     | 20  | LEU  |
| 20  | S     | 36  | ARG  |
| 20  | S     | 61  | TYR  |
| 20  | S     | 62  | ILE  |
| 20  | S     | 78  | ARG  |
| 21  | T     | 10  | LEU  |
| 21  | T     | 42  | GLN  |
| 21  | T     | 57  | ARG  |
| 21  | T     | 62  | LEU  |
| 21  | T     | 64  | ASP  |
| 21  | T     | 73  | HIS  |
| 21  | T     | 84  | LEU  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | B     | 25  | ASN  |
| 3   | B     | 113 | HIS  |
| 3   | B     | 140 | HIS  |
| 3   | B     | 146 | GLN  |
| 3   | B     | 204 | ASN  |
| 3   | B     | 240 | GLN  |
| 4   | C     | 3   | ASN  |
| 4   | C     | 6   | HIS  |
| 4   | C     | 31  | HIS  |
| 4   | C     | 69  | HIS  |
| 4   | C     | 98  | ASN  |
| 4   | C     | 104 | GLN  |
| 4   | C     | 107 | GLN  |
| 4   | C     | 108 | ASN  |
| 4   | C     | 110 | ASN  |
| 4   | C     | 118 | GLN  |
| 4   | C     | 123 | GLN  |
| 4   | C     | 139 | GLN  |
| 4   | C     | 176 | HIS  |
| 4   | C     | 181 | ASN  |
| 5   | D     | 62  | GLN  |
| 5   | D     | 77  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | D     | 123 | HIS  |
| 5   | D     | 160 | GLN  |
| 5   | D     | 199 | ASN  |
| 6   | E     | 73  | ASN  |
| 7   | F     | 16  | GLN  |
| 7   | F     | 18  | GLN  |
| 7   | F     | 27  | GLN  |
| 7   | F     | 32  | ASN  |
| 7   | F     | 57  | GLN  |
| 7   | F     | 94  | GLN  |
| 7   | F     | 100 | ASN  |
| 8   | G     | 37  | ASN  |
| 8   | G     | 86  | GLN  |
| 8   | G     | 106 | GLN  |
| 10  | I     | 23  | ASN  |
| 10  | I     | 73  | GLN  |
| 10  | I     | 117 | HIS  |
| 11  | J     | 56  | HIS  |
| 11  | J     | 62  | HIS  |
| 11  | J     | 76  | ASN  |
| 11  | J     | 78  | ASN  |
| 11  | J     | 84  | GLN  |
| 12  | K     | 117 | ASN  |
| 13  | L     | 75  | HIS  |
| 14  | M     | 12  | ASN  |
| 14  | M     | 40  | ASN  |
| 14  | M     | 62  | ASN  |
| 16  | O     | 13  | GLN  |
| 16  | O     | 37  | ASN  |
| 17  | P     | 16  | HIS  |
| 18  | Q     | 16  | GLN  |
| 18  | Q     | 26  | GLN  |
| 19  | R     | 36  | ASN  |
| 20  | S     | 23  | ASN  |
| 20  | S     | 53  | ASN  |
| 20  | S     | 56  | GLN  |
| 21  | T     | 42  | GLN  |
| 21  | T     | 90  | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | A     | 1507/1522 (99%) | 215 (14%)         | 88 (5%)         |
| 2   | X     | 5/6 (83%)       | 0                 | 0               |
| All | All   | 1512/1528 (98%) | 215 (14%)         | 88 (5%)         |

All (215) RNA backbone outliers are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 6      | G    |
| 1   | A     | 7      | G    |
| 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     | 48     | C    |
| 1   | A     | 49     | U    |
| 1   | A     | 51     | A    |
| 1   | A     | 52     | G    |
| 1   | A     | 61     | G    |
| 1   | A     | 62     | U    |
| 1   | A     | 65     | U    |
| 1   | A     | 81     | U    |
| 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     | 182    | U    |
| 1   | A     | 190(D) | U    |
| 1   | A     | 190(E) | U    |
| 1   | A     | 195    | A    |
| 1   | A     | 197    | A    |
| 1   | A     | 198    | G    |
| 1   | A     | 201    | C    |
| 1   | A     | 202    | U    |
| 1   | A     | 203    | U    |
| 1   | A     | 204    | U    |
| 1   | A     | 216    | G    |
| 1   | A     | 244    | U    |
| 1   | A     | 247    | G    |
| 1   | A     | 251    | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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     | 330 | C    |
| 1   | A     | 332 | G    |
| 1   | A     | 344 | A    |
| 1   | A     | 345 | C    |
| 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     | 412 | A    |
| 1   | A     | 413 | G    |
| 1   | A     | 421 | U    |
| 1   | A     | 429 | U    |
| 1   | A     | 430 | A    |
| 1   | A     | 439 | A    |
| 1   | A     | 460 | A    |
| 1   | A     | 461 | C    |
| 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     | 532 | A    |
| 1   | A     | 533 | A    |
| 1   | A     | 534 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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     | 653 | A    |
| 1   | A     | 665 | A    |
| 1   | A     | 687 | A    |
| 1   | A     | 688 | G    |
| 1   | A     | 702 | A    |
| 1   | A     | 703 | G    |
| 1   | A     | 718 | G    |
| 1   | A     | 721 | G    |
| 1   | A     | 723 | U    |
| 1   | A     | 731 | G    |
| 1   | A     | 749 | C    |
| 1   | A     | 755 | G    |
| 1   | A     | 777 | A    |
| 1   | A     | 781 | A    |
| 1   | A     | 792 | A    |
| 1   | A     | 793 | U    |
| 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     | 858 | G    |
| 1   | A     | 902 | G    |
| 1   | A     | 914 | A    |
| 1   | A     | 926 | G    |
| 1   | A     | 927 | G    |
| 1   | A     | 934 | C    |
| 1   | A     | 935 | A    |
| 1   | A     | 945 | G    |
| 1   | A     | 960 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 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     | 1004 | A    |
| 1   | A     | 1005 | A    |
| 1   | A     | 1023 | G    |
| 1   | A     | 1026 | G    |
| 1   | A     | 1045 | C    |
| 1   | A     | 1050 | G    |
| 1   | A     | 1053 | G    |
| 1   | A     | 1054 | C    |
| 1   | A     | 1065 | U    |
| 1   | A     | 1066 | C    |
| 1   | A     | 1068 | G    |
| 1   | A     | 1085 | U    |
| 1   | A     | 1086 | U    |
| 1   | A     | 1094 | G    |
| 1   | A     | 1095 | U    |
| 1   | A     | 1101 | A    |
| 1   | A     | 1102 | A    |
| 1   | A     | 1117 | G    |
| 1   | A     | 1124 | G    |
| 1   | A     | 1125 | U    |
| 1   | A     | 1128 | C    |
| 1   | A     | 1129 | C    |
| 1   | A     | 1130 | A    |
| 1   | A     | 1131 | G    |
| 1   | A     | 1137 | C    |
| 1   | A     | 1138 | G    |
| 1   | A     | 1139 | G    |
| 1   | A     | 1140 | C    |
| 1   | A     | 1145 | C    |
| 1   | A     | 1152 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1159 | U    |
| 1   | A     | 1160 | G    |
| 1   | A     | 1183 | A    |
| 1   | A     | 1184 | G    |
| 1   | A     | 1191 | A    |
| 1   | A     | 1196 | U    |
| 1   | A     | 1197 | G    |
| 1   | A     | 1201 | A    |
| 1   | A     | 1202 | G    |
| 1   | A     | 1212 | U    |
| 1   | A     | 1213 | A    |
| 1   | A     | 1215 | G    |
| 1   | A     | 1225 | A    |
| 1   | A     | 1226 | C    |
| 1   | A     | 1227 | A    |
| 1   | A     | 1257 | U    |
| 1   | A     | 1258 | G    |
| 1   | A     | 1279 | A    |
| 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    |
| 1   | A     | 1301 | U    |
| 1   | A     | 1302 | U    |
| 1   | A     | 1305 | G    |
| 1   | A     | 1320 | C    |
| 1   | A     | 1338 | G    |
| 1   | A     | 1347 | G    |
| 1   | A     | 1348 | U    |
| 1   | A     | 1353 | G    |
| 1   | A     | 1364 | U    |
| 1   | A     | 1381 | U    |
| 1   | A     | 1394 | A    |
| 1   | A     | 1398 | A    |
| 1   | A     | 1442 | G    |
| 1   | A     | 1443 | G    |
| 1   | A     | 1446 | A    |
| 1   | A     | 1452 | C    |
| 1   | A     | 1492 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1497 | 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    |

All (88) RNA pucker outliers are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 5      | U    |
| 1   | A     | 7      | G    |
| 1   | A     | 30     | U    |
| 1   | A     | 48     | C    |
| 1   | A     | 51     | A    |
| 1   | A     | 60     | A    |
| 1   | A     | 64     | G    |
| 1   | A     | 115    | G    |
| 1   | A     | 119    | A    |
| 1   | A     | 129(A) | G    |
| 1   | A     | 181    | G    |
| 1   | A     | 197    | A    |
| 1   | A     | 202    | U    |
| 1   | A     | 204    | U    |
| 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     | 329    | A    |
| 1   | A     | 344    | A    |
| 1   | A     | 351    | G    |
| 1   | A     | 353    | A    |
| 1   | A     | 366    | C    |
| 1   | A     | 372    | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 428  | G    |
| 1   | A     | 429  | U    |
| 1   | A     | 438  | G    |
| 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     | 748  | 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     | 976  | G    |
| 1   | A     | 992  | U    |
| 1   | A     | 993  | G    |
| 1   | A     | 1049 | U    |
| 1   | A     | 1065 | U    |
| 1   | A     | 1067 | A    |
| 1   | A     | 1085 | U    |
| 1   | A     | 1101 | A    |
| 1   | A     | 1117 | G    |
| 1   | A     | 1129 | C    |
| 1   | A     | 1139 | G    |
| 1   | A     | 1182 | G    |
| 1   | A     | 1183 | A    |
| 1   | A     | 1190 | G    |
| 1   | A     | 1196 | U    |
| 1   | A     | 1201 | A    |
| 1   | A     | 1212 | U    |
| 1   | A     | 1214 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1224 | G    |
| 1   | A     | 1225 | A    |
| 1   | A     | 1226 | C    |
| 1   | A     | 1256 | A    |
| 1   | A     | 1257 | U    |
| 1   | A     | 1281 | U    |
| 1   | A     | 1285 | A    |
| 1   | A     | 1300 | G    |
| 1   | A     | 1301 | U    |
| 1   | A     | 1319 | A    |
| 1   | A     | 1346 | A    |
| 1   | A     | 1347 | G    |
| 1   | A     | 1380 | U    |
| 1   | A     | 1397 | C    |
| 1   | A     | 1451 | A    |
| 1   | A     | 1498 | U    |
| 1   | A     | 1502 | A    |
| 1   | A     | 1504 | G    |
| 1   | A     | 1528 | U    |

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 99 ligands modelled in this entry, 98 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 |
| 25  | HYG  | A     | 1632 | -    | 39,39,39     | 2.81 | 21 (53%) | 60,60,60    | 2.33 | 16 (26%) |

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   |
|-----|------|-------|------|------|-----------|------------|---------|
| 25  | HYG  | A     | 1632 | -    | 1/1/16/17 | 0/14/87/87 | 0/2/4/4 |

All (21) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 25  | A     | 1632 | HYG  | C3-C2   | 7.12  | 1.57        | 1.52     |
| 25  | A     | 1632 | HYG  | C27-C33 | 5.98  | 1.61        | 1.52     |
| 25  | A     | 1632 | HYG  | O28-C23 | 5.74  | 1.49        | 1.40     |
| 25  | A     | 1632 | HYG  | O22-C23 | 4.70  | 1.49        | 1.41     |
| 25  | A     | 1632 | HYG  | C23-C24 | 4.24  | 1.66        | 1.51     |
| 25  | A     | 1632 | HYG  | O28-C27 | 3.97  | 1.51        | 1.44     |
| 25  | A     | 1632 | HYG  | C4-N9   | 3.48  | 1.55        | 1.47     |
| 25  | A     | 1632 | HYG  | C26-C27 | 3.31  | 1.61        | 1.52     |
| 25  | A     | 1632 | HYG  | O29-C23 | 3.09  | 1.47        | 1.41     |
| 25  | A     | 1632 | HYG  | O30-C24 | 3.05  | 1.49        | 1.42     |
| 25  | A     | 1632 | HYG  | C1-C6   | 3.04  | 1.61        | 1.52     |
| 25  | A     | 1632 | HYG  | C26-C25 | 2.94  | 1.60        | 1.52     |
| 25  | A     | 1632 | HYG  | C3-C4   | 2.81  | 1.58        | 1.53     |
| 25  | A     | 1632 | HYG  | O29-C12 | -2.80 | 1.38        | 1.43     |
| 25  | A     | 1632 | HYG  | C25-C24 | 2.42  | 1.57        | 1.53     |
| 25  | A     | 1632 | HYG  | C34-C33 | 2.27  | 1.55        | 1.51     |
| 25  | A     | 1632 | HYG  | C10-N9  | 2.19  | 1.53        | 1.46     |
| 25  | A     | 1632 | HYG  | C16-C15 | 2.14  | 1.57        | 1.53     |
| 25  | A     | 1632 | HYG  | O14-C13 | 2.09  | 1.47        | 1.41     |
| 25  | A     | 1632 | HYG  | O18-C13 | 2.09  | 1.47        | 1.41     |
| 25  | A     | 1632 | HYG  | C19-C15 | 2.08  | 1.59        | 1.52     |

All (16) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 25  | A     | 1632 | HYG  | C23-O28-C27 | 7.34 | 118.57      | 111.82   |
| 25  | A     | 1632 | HYG  | C10-N9-C4   | 6.31 | 117.34      | 113.82   |
| 25  | A     | 1632 | HYG  | O28-C27-C33 | 6.03 | 114.83      | 106.93   |
| 25  | A     | 1632 | HYG  | O21-C16-C15 | 5.02 | 122.53      | 109.28   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25  | A     | 1632 | HYG  | O28-C27-C26 | 5.00  | 115.97      | 108.69   |
| 25  | A     | 1632 | HYG  | O21-C16-C17 | 4.71  | 120.85      | 109.85   |
| 25  | A     | 1632 | HYG  | C23-O29-C12 | -4.22 | 97.67       | 106.50   |
| 25  | A     | 1632 | HYG  | C26-C25-C24 | -3.36 | 106.48      | 111.31   |
| 25  | A     | 1632 | HYG  | O22-C23-C24 | -3.30 | 105.02      | 111.47   |
| 25  | A     | 1632 | HYG  | C16-C17-C12 | -3.06 | 105.53      | 113.54   |
| 25  | A     | 1632 | HYG  | C17-C16-C15 | 2.88  | 116.17      | 109.64   |
| 25  | A     | 1632 | HYG  | O18-C6-C1   | 2.72  | 114.15      | 107.16   |
| 25  | A     | 1632 | HYG  | C23-O22-C17 | -2.39 | 101.50      | 106.50   |
| 25  | A     | 1632 | HYG  | O29-C12-C13 | 2.23  | 117.20      | 110.93   |
| 25  | A     | 1632 | HYG  | O22-C17-C16 | 2.22  | 116.83      | 111.24   |
| 25  | A     | 1632 | HYG  | C25-C26-C27 | 2.18  | 114.36      | 109.61   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 25  | A     | 1632 | HYG  | C16  |

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%) | 0.12   | 48 (3%)  | 45  | 11  | 53, 82, 169, 199      | 0     |
| 2   | X     | 6/6 (100%)      | 1.53   | 3 (50%)  | 0   | 0   | 78, 84, 140, 155      | 0     |
| 3   | B     | 234/256 (91%)   | 0.04   | 1 (0%)   | 90  | 57  | 51, 102, 165, 199     | 0     |
| 4   | C     | 206/239 (86%)   | -0.09  | 2 (0%)   | 79  | 33  | 59, 103, 158, 177     | 0     |
| 5   | D     | 208/209 (99%)   | 0.04   | 1 (0%)   | 88  | 51  | 55, 85, 131, 175      | 0     |
| 6   | E     | 150/162 (92%)   | -0.23  | 0        | 100 | 100 | 50, 73, 114, 192      | 0     |
| 7   | F     | 101/101 (100%)  | -0.13  | 0        | 100 | 100 | 66, 109, 144, 174     | 0     |
| 8   | G     | 155/156 (99%)   | -0.09  | 1 (0%)   | 86  | 46  | 58, 100, 150, 177     | 0     |
| 9   | H     | 138/138 (100%)  | -0.19  | 1 (0%)   | 84  | 42  | 41, 70, 106, 153      | 0     |
| 10  | I     | 127/128 (99%)   | 0.08   | 2 (1%)   | 68  | 22  | 62, 109, 150, 175     | 0     |
| 11  | J     | 98/105 (93%)    | 0.64   | 12 (12%) | 5   | 2   | 59, 128, 184, 199     | 0     |
| 12  | K     | 119/129 (92%)   | 0.12   | 3 (2%)   | 54  | 14  | 57, 85, 140, 191      | 0     |
| 13  | L     | 124/135 (91%)   | -0.00  | 0        | 100 | 100 | 44, 83, 128, 182      | 0     |
| 14  | M     | 125/126 (99%)   | 0.52   | 9 (7%)   | 15  | 4   | 61, 99, 158, 193      | 0     |
| 15  | N     | 60/61 (98%)     | 0.17   | 0        | 100 | 100 | 64, 96, 150, 162      | 0     |
| 16  | O     | 88/89 (98%)     | 0.07   | 4 (4%)   | 32  | 7   | 52, 83, 136, 185      | 0     |
| 17  | P     | 88/88 (100%)    | 0.16   | 2 (2%)   | 57  | 15  | 53, 77, 158, 199      | 0     |
| 18  | Q     | 104/105 (99%)   | 0.33   | 7 (6%)   | 17  | 4   | 55, 77, 140, 199      | 0     |
| 19  | R     | 73/88 (82%)     | 0.02   | 1 (1%)   | 72  | 25  | 56, 87, 148, 191      | 0     |
| 20  | S     | 80/93 (86%)     | 0.24   | 4 (5%)   | 28  | 6   | 84, 119, 170, 198     | 0     |
| 21  | T     | 99/106 (93%)    | 0.30   | 4 (4%)   | 36  | 8   | 59, 86, 135, 199      | 0     |
| 22  | V     | 24/26 (92%)     | 0.29   | 0        | 100 | 100 | 60, 91, 127, 143      | 0     |
| All | All   | 3913/4068 (96%) | 0.10   | 105 (2%) | 50  | 13  | 41, 88, 161, 199      | 0     |

All (105) RSRZ outliers are listed below:

| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 14  | M     | 124     | PRO  | 11.6 |
| 1   | A     | 1036    | G    | 8.2  |
| 14  | M     | 123     | ALA  | 7.6  |
| 1   | A     | 1037    | C    | 6.7  |
| 1   | A     | 1005    | A    | 6.7  |
| 1   | A     | 1027    | C    | 6.7  |
| 11  | J     | 33      | GLN  | 6.2  |
| 1   | A     | 1026    | G    | 6.2  |
| 18  | Q     | 105     | ALA  | 6.0  |
| 14  | M     | 125     | ARG  | 5.4  |
| 12  | K     | 129     | SER  | 5.3  |
| 1   | A     | 1001    | A    | 5.2  |
| 21  | T     | 51      | GLU  | 5.2  |
| 14  | M     | 120     | LYS  | 5.1  |
| 1   | A     | 1023    | G    | 4.9  |
| 1   | A     | 1006    | C    | 4.8  |
| 1   | A     | 81      | U    | 4.8  |
| 14  | M     | 121     | LYS  | 4.7  |
| 18  | Q     | 103     | GLY  | 4.6  |
| 1   | A     | 1022    | G    | 4.5  |
| 1   | A     | 1002    | G    | 4.3  |
| 1   | A     | 1274    | G    | 4.3  |
| 1   | A     | 989     | C    | 4.1  |
| 1   | A     | 1275    | A    | 4.1  |
| 18  | Q     | 78      | GLU  | 4.0  |
| 11  | J     | 70      | ARG  | 3.9  |
| 18  | Q     | 104     | LYS  | 3.9  |
| 17  | P     | 87      | GLY  | 3.8  |
| 1   | A     | 1030(B) | C    | 3.8  |
| 1   | A     | 1024    | G    | 3.7  |
| 1   | A     | 990     | C    | 3.7  |
| 1   | A     | 1035    | A    | 3.7  |
| 1   | A     | 1025    | U    | 3.6  |
| 1   | A     | 991     | U    | 3.6  |
| 21  | T     | 48      | LYS  | 3.5  |
| 21  | T     | 103     | GLY  | 3.4  |
| 14  | M     | 126     | LYS  | 3.3  |
| 1   | A     | 1124    | G    | 3.3  |
| 1   | A     | 1029    | C    | 3.1  |
| 1   | A     | 1273    | G    | 3.1  |
| 1   | A     | 841     | U    | 3.1  |
| 3   | B     | 238     | LEU  | 3.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 11  | J     | 89   | ASP  | 3.1  |
| 1   | A     | 848  | C    | 3.0  |
| 1   | A     | 1261 | A    | 3.0  |
| 1   | A     | 1129 | C    | 2.9  |
| 20  | S     | 81   | ARG  | 2.9  |
| 11  | J     | 85   | LEU  | 2.9  |
| 11  | J     | 31   | GLY  | 2.9  |
| 1   | A     | 1004 | A    | 2.9  |
| 1   | A     | 1123 | A    | 2.9  |
| 1   | A     | 1262 | C    | 2.9  |
| 1   | A     | 1488 | G    | 2.9  |
| 18  | Q     | 80   | GLY  | 2.9  |
| 11  | J     | 10   | GLY  | 2.8  |
| 20  | S     | 79   | THR  | 2.8  |
| 14  | M     | 39   | ILE  | 2.7  |
| 16  | O     | 2    | PRO  | 2.7  |
| 11  | J     | 34   | VAL  | 2.7  |
| 1   | A     | 1028 | C    | 2.7  |
| 1   | A     | 341  | C    | 2.7  |
| 1   | A     | 1489 | G    | 2.7  |
| 21  | T     | 43   | LEU  | 2.7  |
| 4   | C     | 105  | GLU  | 2.6  |
| 1   | A     | 1021 | G    | 2.6  |
| 20  | S     | 77   | THR  | 2.6  |
| 1   | A     | 1139 | G    | 2.5  |
| 1   | A     | 1018 | C    | 2.5  |
| 9   | H     | 1    | MET  | 2.5  |
| 1   | A     | 432  | A    | 2.5  |
| 1   | A     | 1144 | G    | 2.5  |
| 18  | Q     | 55   | ASP  | 2.5  |
| 5   | D     | 33   | MET  | 2.5  |
| 2   | X     | 4    | U    | 2.5  |
| 1   | A     | 1260 | C    | 2.4  |
| 2   | X     | 1    | C    | 2.4  |
| 11  | J     | 28   | ARG  | 2.4  |
| 1   | A     | 1003 | G    | 2.4  |
| 1   | A     | 478  | A    | 2.4  |
| 1   | A     | 183  | G    | 2.4  |
| 19  | R     | 18   | ARG  | 2.4  |
| 14  | M     | 36   | LYS  | 2.4  |
| 20  | S     | 3    | ARG  | 2.4  |
| 11  | J     | 39   | PRO  | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 14  | M     | 37   | THR  | 2.4  |
| 1   | A     | 988  | G    | 2.4  |
| 1   | A     | 1276 | G    | 2.4  |
| 16  | O     | 88   | ARG  | 2.3  |
| 10  | I     | 97   | LYS  | 2.3  |
| 11  | J     | 75   | ILE  | 2.3  |
| 1   | A     | 958  | A    | 2.3  |
| 12  | K     | 128  | ALA  | 2.2  |
| 18  | Q     | 79   | SER  | 2.2  |
| 12  | K     | 89   | ALA  | 2.1  |
| 4   | C     | 53   | ALA  | 2.1  |
| 11  | J     | 32   | ALA  | 2.1  |
| 1   | A     | 1038 | C    | 2.1  |
| 16  | O     | 7    | GLU  | 2.1  |
| 10  | I     | 102  | LEU  | 2.1  |
| 1   | A     | 1490 | C    | 2.1  |
| 8   | G     | 62   | PHE  | 2.0  |
| 17  | P     | 88   | ALA  | 2.0  |
| 11  | J     | 16   | LEU  | 2.0  |
| 16  | O     | 3    | ILE  | 2.0  |
| 2   | X     | 2    | U    | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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 | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 23  | MG   | A     | 1557 | 1/1   | 0.65 | -    | 58,58,58,58                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 23  | MG   | A     | 1616 | 1/1   | 0.40 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1581 | 1/1   | 0.49 | -    | 58,58,58,58                 | 1     |
| 23  | MG   | A     | 1573 | 1/1   | 0.73 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1605 | 1/1   | 0.42 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 212  | 1/1   | 0.38 | -    | 58,58,58,58                 | 1     |
| 23  | MG   | A     | 1572 | 1/1   | 0.52 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1603 | 1/1   | 0.32 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1567 | 1/1   | 0.59 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1555 | 1/1   | 0.37 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1602 | 1/1   | 0.74 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 86   | 1/1   | 0.78 | -    | 58,58,58,58                 | 0     |
| 25  | HYG  | A     | 1632 | 36/36 | 0.14 | -    | 41,41,41,41                 | 0     |
| 23  | MG   | A     | 1578 | 1/1   | 0.30 | -    | 58,58,58,58                 | 0     |
| 24  | ZN   | N     | 190  | 1/1   | 0.17 | -    | 66,66,66,66                 | 1     |
| 23  | MG   | A     | 1585 | 1/1   | 0.25 | -    | 58,58,58,58                 | 1     |
| 23  | MG   | H     | 213  | 1/1   | 1.28 | -    | 58,58,58,58                 | 1     |
| 23  | MG   | A     | 1622 | 1/1   | 0.23 | -    | 58,58,58,58                 | 1     |
| 23  | MG   | A     | 211  | 1/1   | 0.67 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1561 | 1/1   | 0.58 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1614 | 1/1   | 0.71 | -    | 58,58,58,58                 | 1     |
| 23  | MG   | A     | 1595 | 1/1   | 0.28 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1582 | 1/1   | 0.25 | -    | 58,58,58,58                 | 1     |
| 24  | ZN   | D     | 300  | 1/1   | 0.31 | -    | 66,66,66,66                 | 0     |
| 23  | MG   | A     | 1551 | 1/1   | 0.70 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1576 | 1/1   | 0.95 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1597 | 1/1   | 0.22 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1624 | 1/1   | 0.32 | -    | 58,58,58,58                 | 1     |
| 23  | MG   | A     | 1620 | 1/1   | 0.37 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1590 | 1/1   | 0.45 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1570 | 1/1   | 0.42 | -    | 58,58,58,58                 | 1     |
| 23  | MG   | A     | 1621 | 1/1   | 0.13 | -    | 58,58,58,58                 | 1     |
| 23  | MG   | A     | 1558 | 1/1   | 0.40 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1626 | 1/1   | 0.26 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1547 | 1/1   | 0.62 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | D     | 215  | 1/1   | 0.23 | -    | 58,58,58,58                 | 1     |
| 23  | MG   | A     | 1629 | 1/1   | 0.32 | -    | 58,58,58,58                 | 1     |
| 23  | MG   | A     | 1571 | 1/1   | 0.68 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1628 | 1/1   | 0.16 | -    | 58,58,58,58                 | 1     |
| 23  | MG   | A     | 1630 | 1/1   | 0.32 | -    | 58,58,58,58                 | 1     |
| 23  | MG   | A     | 1589 | 1/1   | 0.35 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 210  | 1/1   | 0.23 | -    | 58,58,58,58                 | 1     |
| 23  | MG   | A     | 1588 | 1/1   | 0.12 | -    | 58,58,58,58                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 23  | MG   | A     | 87   | 1/1   | 0.48 | -    | 58,58,58,58                 | 1     |
| 23  | MG   | A     | 1548 | 1/1   | 0.32 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1580 | 1/1   | 0.30 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1569 | 1/1   | 0.41 | -    | 58,58,58,58                 | 1     |
| 23  | MG   | A     | 1625 | 1/1   | 0.20 | -    | 58,58,58,58                 | 1     |
| 23  | MG   | A     | 1604 | 1/1   | 0.25 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 214  | 1/1   | 0.75 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1575 | 1/1   | 0.29 | -    | 58,58,58,58                 | 1     |
| 23  | MG   | A     | 1562 | 1/1   | 0.56 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1609 | 1/1   | 0.40 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1600 | 1/1   | 0.51 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1598 | 1/1   | 0.07 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1564 | 1/1   | 0.12 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1607 | 1/1   | 0.68 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1613 | 1/1   | 0.43 | -    | 58,58,58,58                 | 1     |
| 23  | MG   | A     | 1566 | 1/1   | 0.44 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1559 | 1/1   | 0.39 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1627 | 1/1   | 0.46 | -    | 58,58,58,58                 | 1     |
| 23  | MG   | A     | 1619 | 1/1   | 0.23 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1560 | 1/1   | 0.22 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1594 | 1/1   | 0.21 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1612 | 1/1   | 0.35 | -    | 58,58,58,58                 | 1     |
| 23  | MG   | A     | 1617 | 1/1   | 0.46 | -    | 58,58,58,58                 | 1     |
| 23  | MG   | A     | 1549 | 1/1   | 0.84 | -    | 58,58,58,58                 | 1     |
| 23  | MG   | A     | 1550 | 1/1   | 1.34 | -    | 58,58,58,58                 | 1     |
| 23  | MG   | A     | 71   | 1/1   | 0.45 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1610 | 1/1   | 0.33 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1591 | 1/1   | 0.35 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1596 | 1/1   | 0.64 | -    | 58,58,58,58                 | 1     |
| 23  | MG   | A     | 1615 | 1/1   | 1.62 | -    | 58,58,58,58                 | 1     |
| 23  | MG   | A     | 1623 | 1/1   | 1.17 | -    | 58,58,58,58                 | 1     |
| 23  | MG   | A     | 1556 | 1/1   | 1.04 | -    | 58,58,58,58                 | 1     |
| 23  | MG   | A     | 1599 | 1/1   | 0.36 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1552 | 1/1   | 0.15 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1568 | 1/1   | 0.64 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1553 | 1/1   | 0.48 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1554 | 1/1   | 0.58 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1606 | 1/1   | 0.38 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1631 | 1/1   | 0.36 | -    | 58,58,58,58                 | 1     |
| 23  | MG   | A     | 1618 | 1/1   | 0.39 | -    | 58,58,58,58                 | 1     |
| 23  | MG   | A     | 1587 | 1/1   | 0.50 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1592 | 1/1   | 0.17 | -    | 58,58,58,58                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 23  | MG   | A     | 1601 | 1/1   | 0.12 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1546 | 1/1   | 0.39 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1565 | 1/1   | 0.71 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1545 | 1/1   | 0.12 | -    | 58,58,58,58                 | 1     |
| 23  | MG   | A     | 1563 | 1/1   | 0.17 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1586 | 1/1   | 0.56 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1583 | 1/1   | 0.14 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1611 | 1/1   | 0.13 | -    | 58,58,58,58                 | 1     |
| 23  | MG   | A     | 1608 | 1/1   | 0.39 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1593 | 1/1   | 0.27 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1579 | 1/1   | 0.31 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1577 | 1/1   | 0.32 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1584 | 1/1   | 0.44 | -    | 58,58,58,58                 | 0     |
| 23  | MG   | A     | 1574 | 1/1   | 0.41 | -    | 58,58,58,58                 | 0     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.