



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 04:26 PM GMT

PDB ID : 2X9T  
Title : STRUCTURE OF THE 70S RIBOSOME BOUND TO RELEASE FACTOR 2  
AND A SUBSTRATE ANALOG PROVIDES INSIGHTS INTO CATALYSIS  
OF PEPTIDE RELEASE  
Authors : Jin, H.; Kelley, A.C.; Loakes, D.; Ramakrishnan, V.  
Deposited on : 2010-03-24  
Resolution : 3.10 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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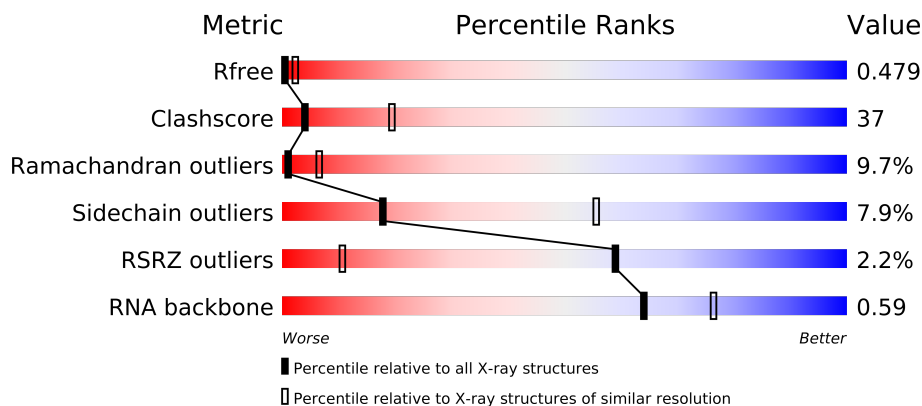
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.10 Å.

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



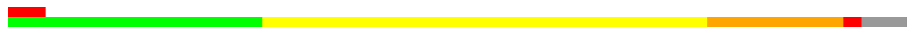
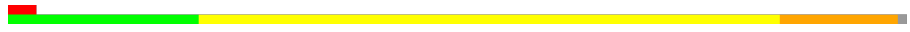


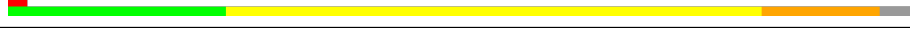
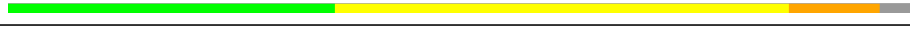
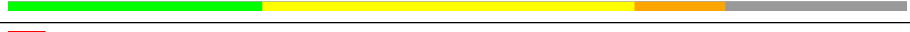



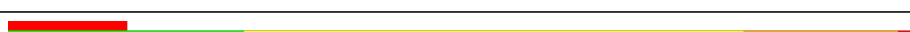
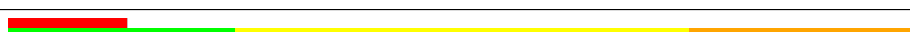
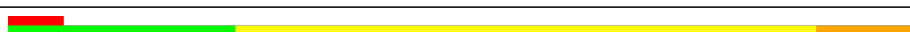
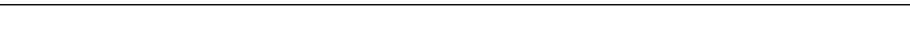
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 66092                       | 1007 (3.18-3.02)                                      |
| Clashscore            | 79885                       | 1078 (3.16-3.04)                                      |
| Ramachandran outliers | 78287                       | 1044 (3.16-3.04)                                      |
| Sidechain outliers    | 78261                       | 1044 (3.16-3.04)                                      |
| RSRZ outliers         | 66119                       | 1008 (3.18-3.02)                                      |
| RNA backbone          | 1838                        | 1047 (3.60-2.60)                                      |

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   | B     | 256    |                  |
| 3   | C     | 239    |                  |
| 4   | D     | 209    |                  |
| 5   | E     | 162    |                  |
| 6   | F     | 101    |                  |
| 7   | G     | 156    |                  |
| 8   | H     | 138    |                  |
| 9   | I     | 128    |                  |
| 10  | J     | 105    |                  |
| 11  | K     | 129    |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 12  | L     | 132    |  |
| 13  | M     | 126    |  |
| 14  | N     | 61     |  |
| 15  | O     | 89     |  |
| 16  | P     | 88     |  |
| 17  | Q     | 105    |  |
| 18  | R     | 88     |  |
| 19  | S     | 93     |  |
| 20  | T     | 106    |  |
| 21  | U     | 27     |  |
| 22  | V     | 77     |  |
| 22  | W     | 77     |  |
| 23  | X     | 8      |  |
| 24  | Y     | 351    |  |

## 2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 58261 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 RRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1   | A     | 1504     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32329 | 14390 | 5992 | 10444 | 1503 |         |         |       |

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | B     | 235      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1901  | 1213 | 342 | 341 | 5 |         |         |       |

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | C     | 207      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1613  | 1016 | 315 | 281 | 1 |         |         |       |

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | D     | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1703  | 1066 | 339 | 291 | 7 |         |         |       |

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | E     | 151      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1147  | 724 | 218 | 201 | 4 |         |         |       |

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | F     | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 843   | 531 | 155 | 154 | 3 |         |         |       |

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | G     | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1257  | 781 | 252 | 218 | 6 |         |         |       |

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | H     | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1116  | 705 | 215 | 193 | 3 |         |         |       |

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9   | I     | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1011  | 639 | 198 | 174 |   |         |         |       |

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | J     | 99       | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 795   | 499 | 157 | 138 | 1 |         |         |       |

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | K     | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 885   | 549 | 168 | 165 | 3 |         |         |       |

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | L     | 125      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 971   | 611 | 196 | 163 | 1 |         |         |       |

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | M     | 125      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 988   | 611 | 206 | 169 | 2 |         |         |       |

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14 TYPE Z.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 14  | N     | 60       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 492   | 312 | 104 | 72 | 4 |         |         |       |

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15  | O     | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 734   | 459 | 147 | 126 | 2 |         |         |       |

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | P     | 84       | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 701   | 443 | 140 | 117 | 1 |         |         |       |

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17  | Q     | 100      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 824   | 528 | 152 | 142 | 2 |         |         |       |

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

| Mol | Chain | Residues | Atoms |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 18  | R     | 70       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 574   | 367 | 112 | 95 |         |         |       |

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | S     | 79       | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 630   | 403 | 115 | 110 | 2 |         |         |       |

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20  | T     | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 763   | 470 | 162 | 129 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 21  | U     | 25       | Total | C   | N  | O  | 0       | 0       | 1     |
|     |       |          | 209   | 128 | 51 | 30 |         |         |       |

- Molecule 22 is a RNA chain called E-SITE TRNA PHE OR P-SITE TRNA PHE (UNMODIFIED BASES).

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 22  | V     | 77       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1630  | 732 | 292 | 531 | 75 |         |         |       |
| 22  | W     | 77       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1630  | 732 | 292 | 531 | 75 |         |         |       |

- Molecule 23 is a RNA chain called MRNA.

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 23  | X     | 8        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 165   | 76 | 29 | 53 | 7 |         |         |       |

- Molecule 24 is a protein called PEPTIDE CHAIN RELEASE FACTOR 2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 24  | Y     | 351      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2801  | 1752 | 506 | 535 | 8 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 25  | Z     | 546      | Total | Mg  | 0       | 0       |
|     |       |          | 546   | 546 |         |         |

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

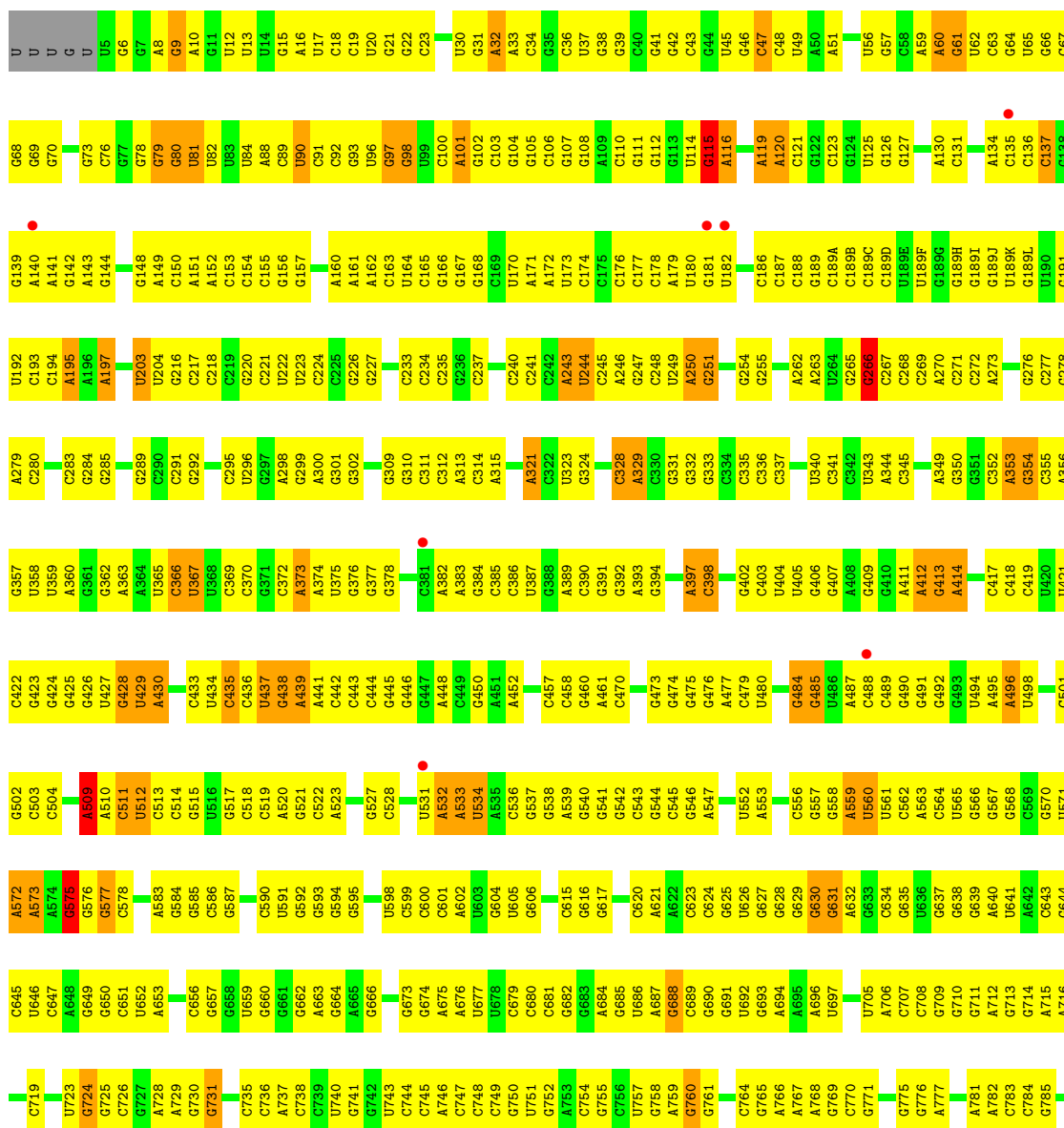
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 26  | Z     | 3        | Total | Zn | 0       | 0       |
|     |       |          | 3     | 3  |         |         |

### 3 Residue-property plots

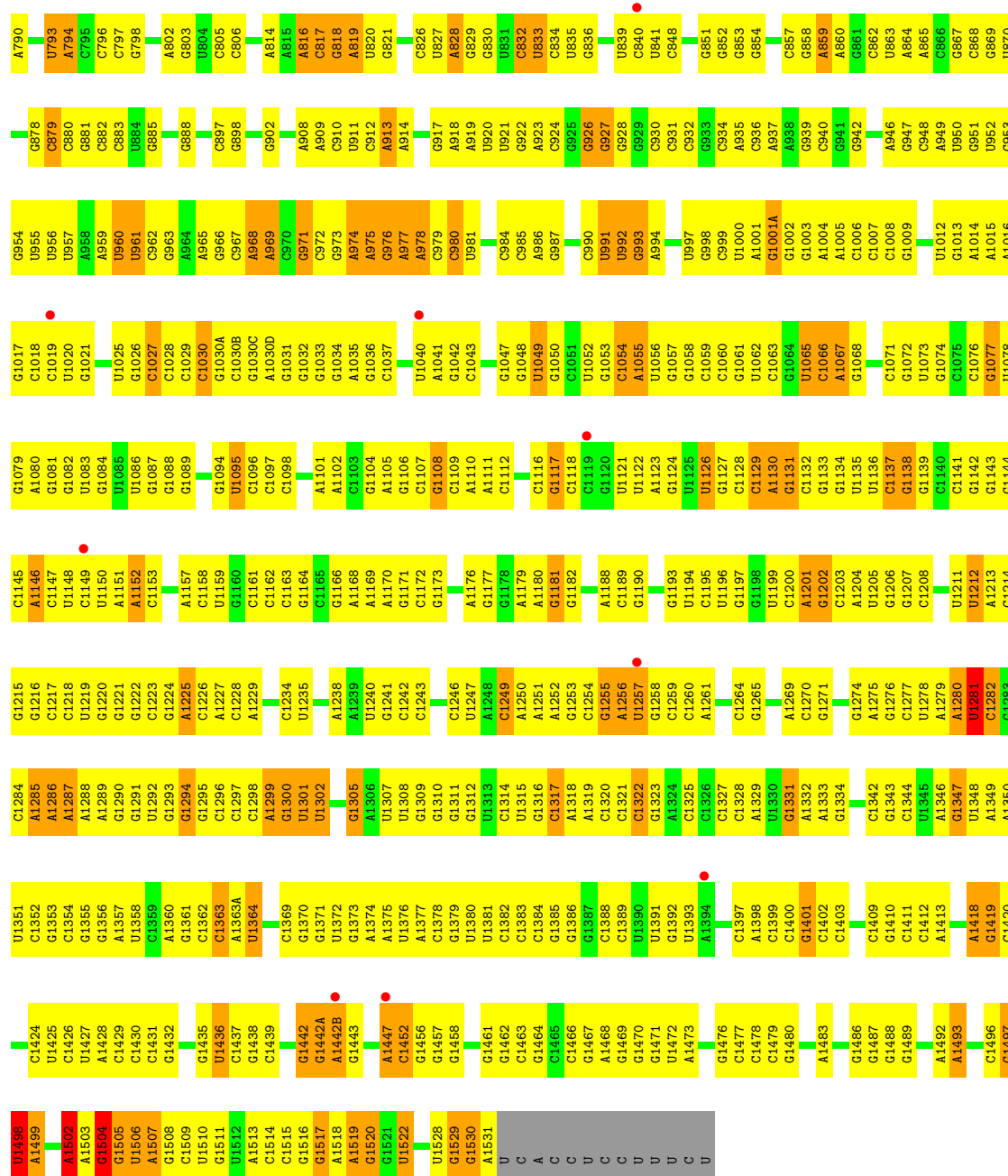
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 rRNA

Chain A: 

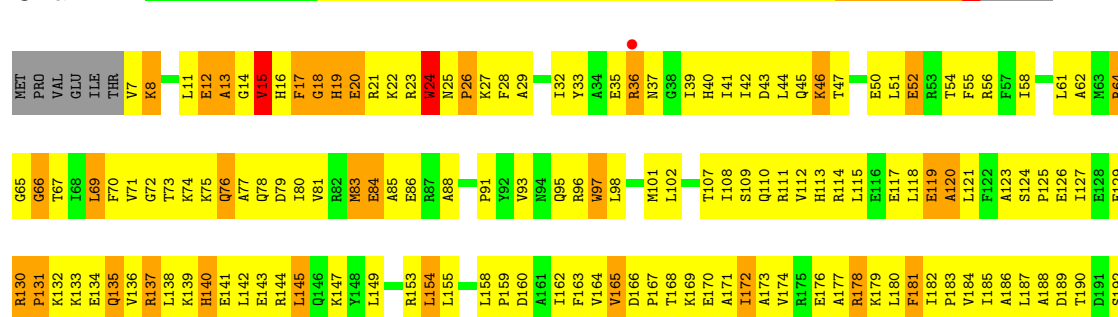






## • Molecule 2: 30S RIBOSOMAL PROTEIN S2

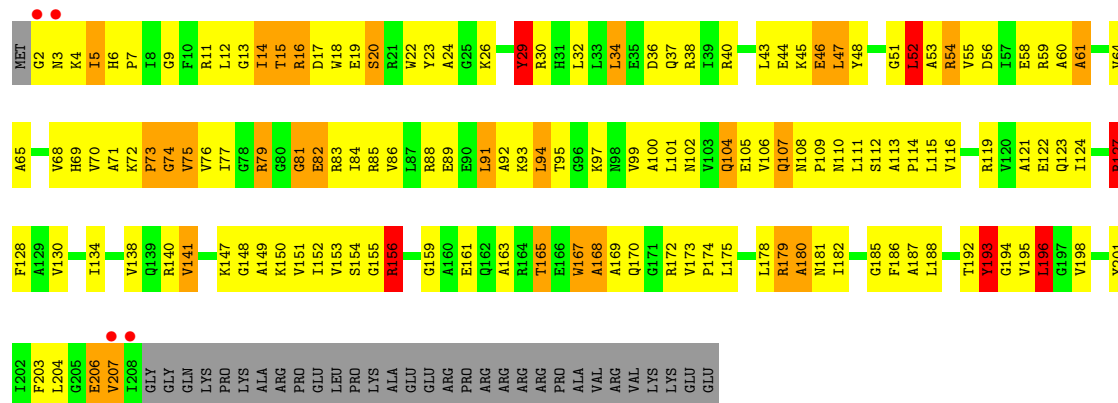
Chain B:





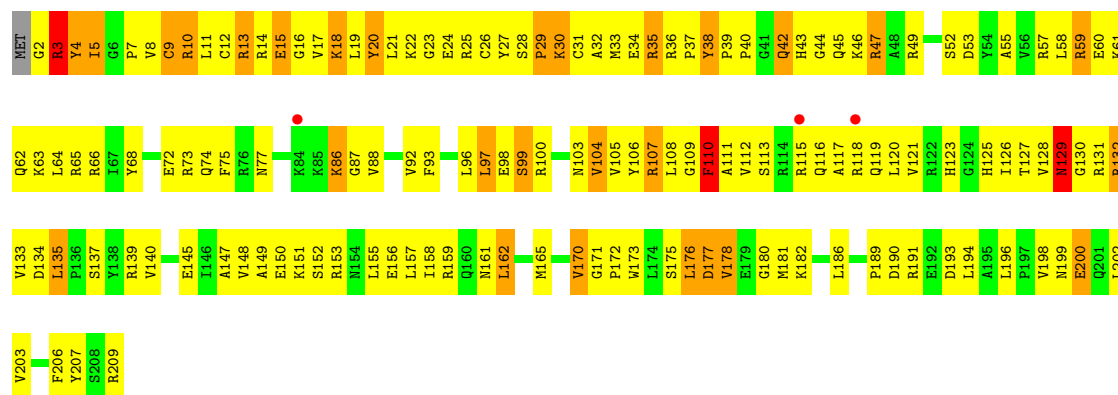
### • Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain C:



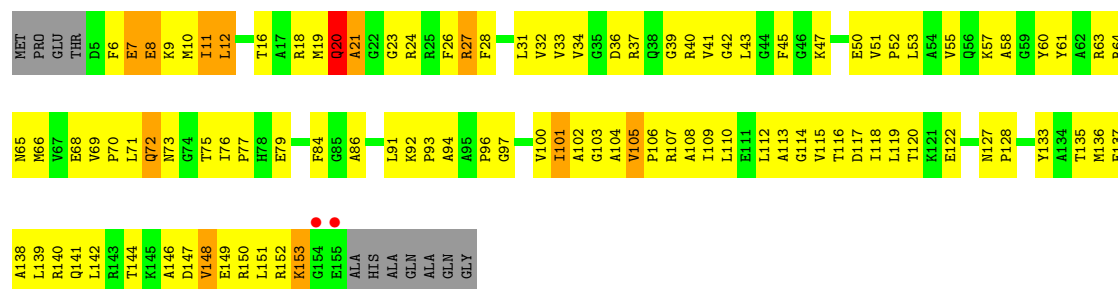
### • Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain D:



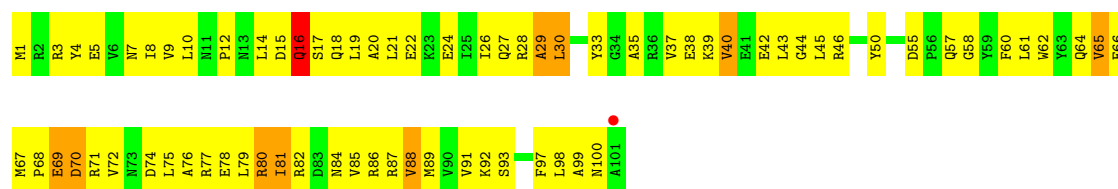
### • Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain E:



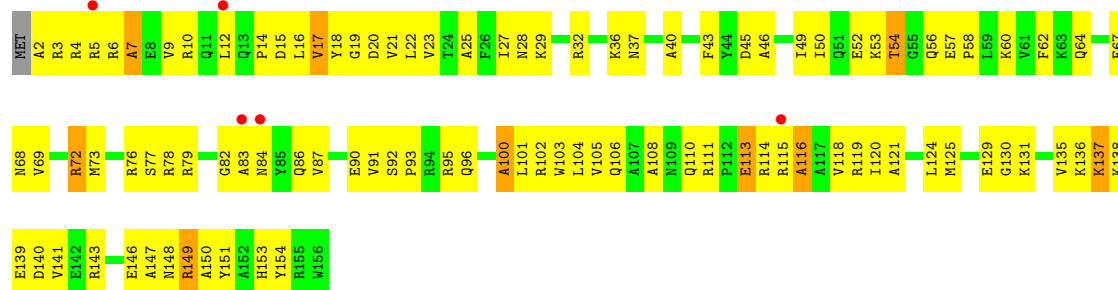
### • Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain F:



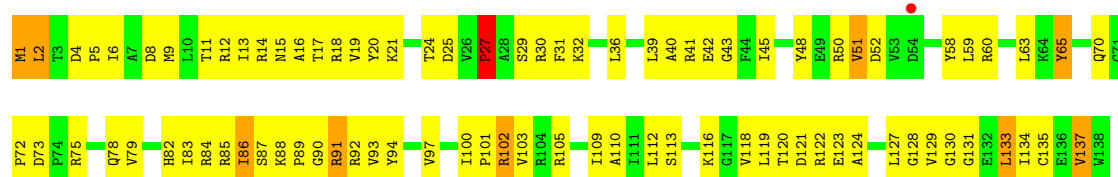
- Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain G:



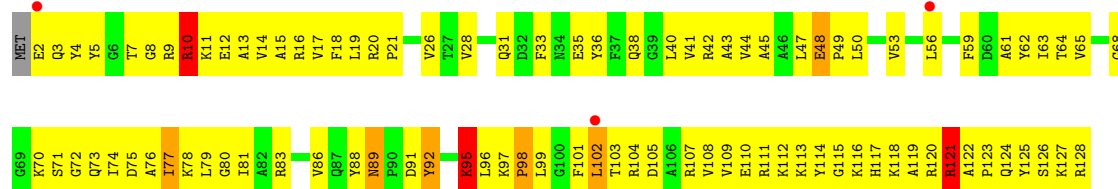
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain H:



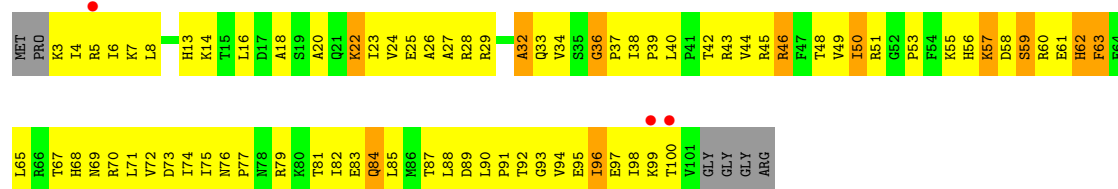
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain I:

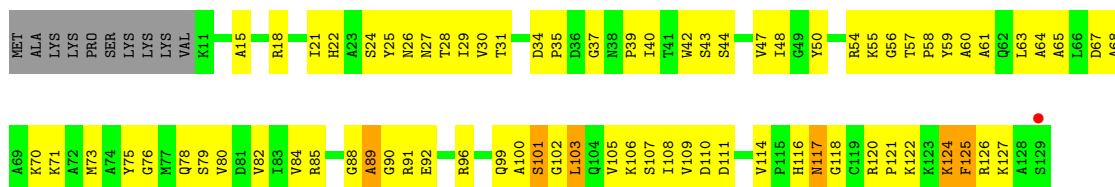


- Molecule 10: 30S RIBOSOMAL PROTEIN S10

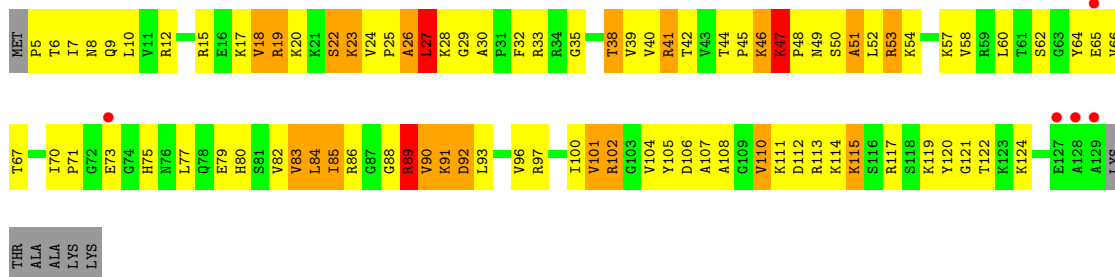
Chain J:



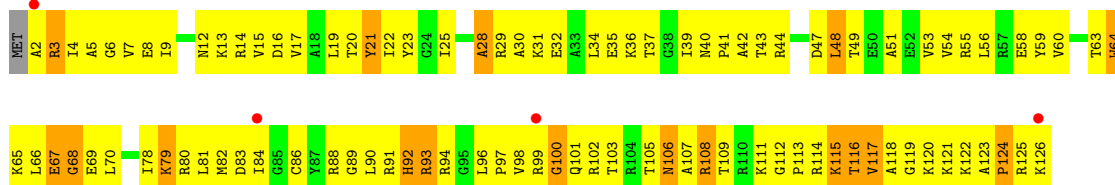
- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain K: 

- Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain L: 

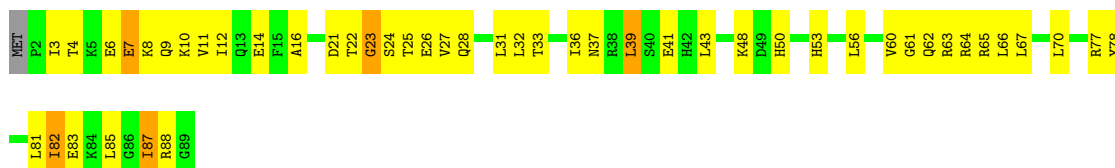
- Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain M: 

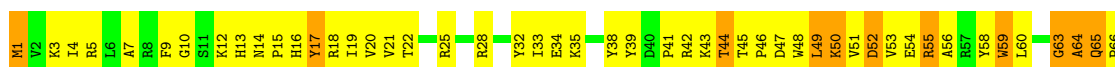
- Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain N: 

- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain O: 

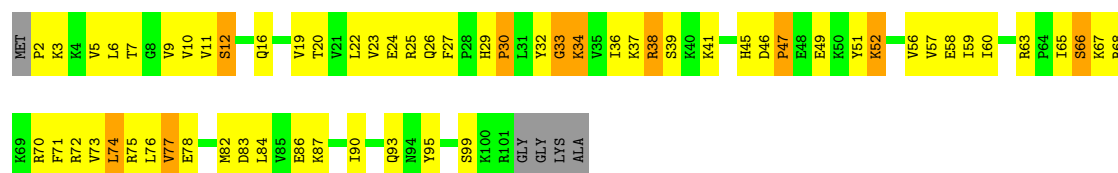
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain P: 



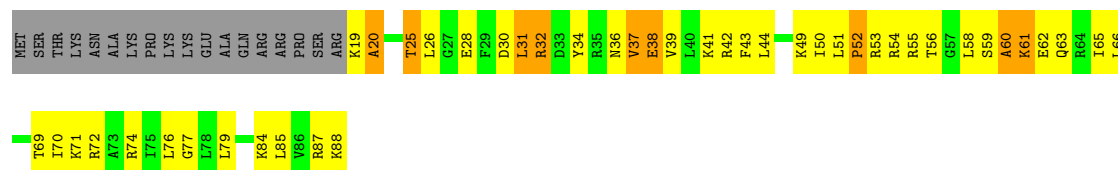
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain Q:



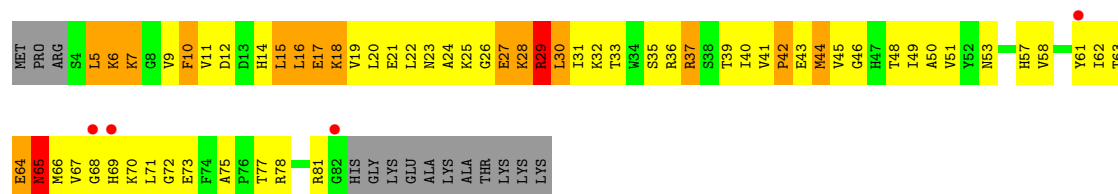
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain R:



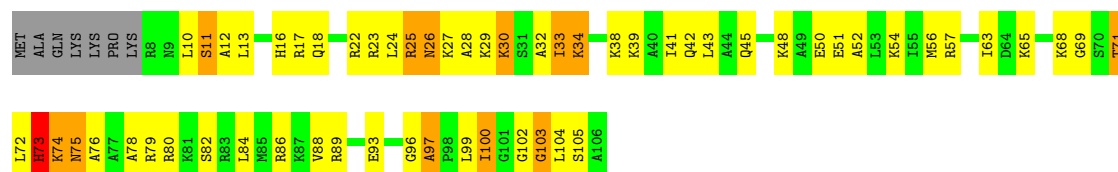
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain S:



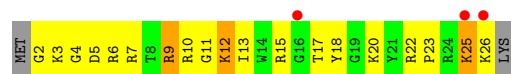
• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain T:



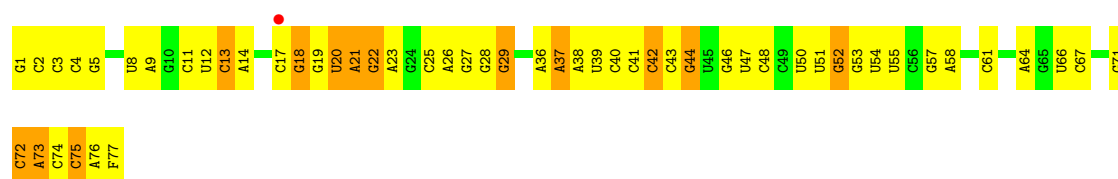
• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain U:



• Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE (UNMODIFIED BASES)

Chain V:



- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE (UNMODIFIED BASES)

Chain W:



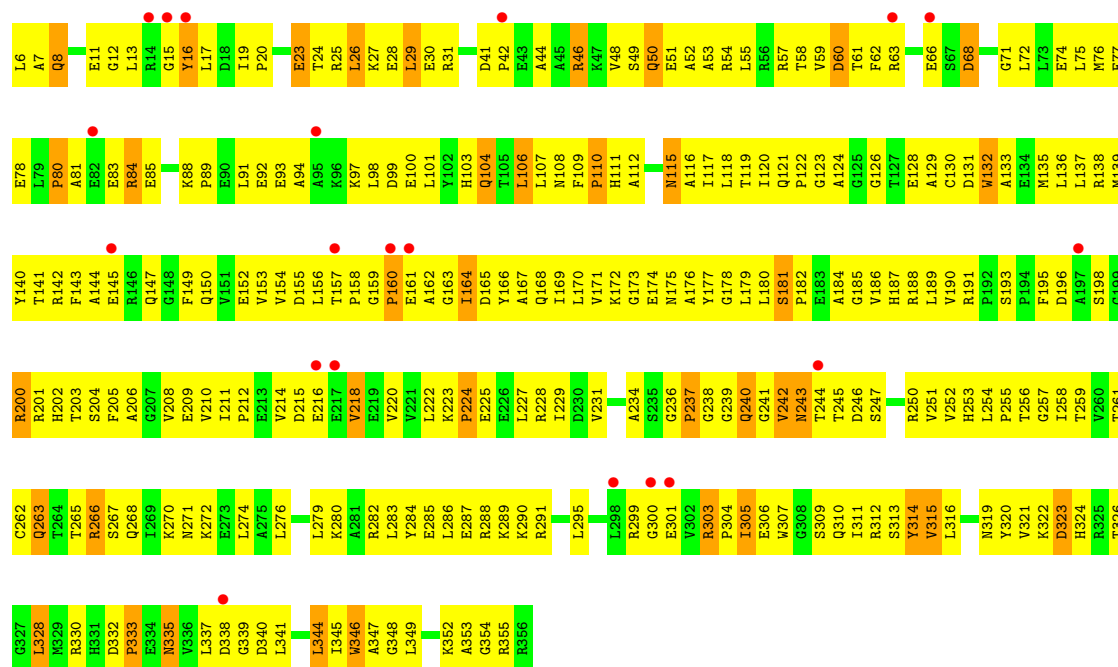
- Molecule 23: MRNA

Chain X:



- Molecule 24: PEPTIDE CHAIN RELEASE FACTOR 2

Chain Y:



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 211.42Å 452.50Å 625.44Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 47.86 – 3.10<br>49.71 – 3.00                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 100.0 (47.86-3.10)<br>99.6 (49.71-3.00)                     | Depositor<br>EDS |
| $R_{merge}$   | 0.16  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.59 (at 3.01Å)   | Xtriage          |
| Refinement program  | CNS 1.2   | Depositor        |
| R, $R_{free}$   | 0.223 , 0.264<br>0.478 , 0.479                              | Depositor<br>DCC |
| $R_{free}$ test set   | 52374 reflections (4.65%)                                   | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 55.0  | Xtriage          |
| Anisotropy  | 0.035   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.29 , 73.4   | EDS              |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| L-test for twinning   | $\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$ | Xtriage          |
| Outliers  | 0 of 1179114 reflections                                    | Xtriage          |
| $F_o, F_c$ correlation  | 0.45  | EDS              |
| Total number of atoms   | 58261   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 105.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% 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: MG, ZN, 8AN, PHA

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     | 0.39         | 0/36190     | 0.69        | 11/56486 (0.0%) |
| 2   | B     | 0.33         | 0/1936      | 0.58        | 0/2611          |
| 3   | C     | 0.32         | 0/1637      | 0.54        | 0/2207          |
| 4   | D     | 0.33         | 0/1733      | 0.62        | 0/2318          |
| 5   | E     | 0.35         | 0/1163      | 0.62        | 0/1566          |
| 6   | F     | 0.34         | 0/856       | 0.64        | 0/1154          |
| 7   | G     | 0.31         | 0/1276      | 0.56        | 0/1709          |
| 8   | H     | 0.32         | 0/1136      | 0.62        | 0/1527          |
| 9   | I     | 0.32         | 0/1027      | 0.58        | 0/1372          |
| 10  | J     | 0.33         | 0/808       | 0.56        | 0/1087          |
| 11  | K     | 0.36         | 0/900       | 0.59        | 0/1213          |
| 12  | L     | 0.36         | 0/987       | 0.67        | 0/1322          |
| 13  | M     | 0.32         | 0/994       | 0.56        | 0/1322          |
| 14  | N     | 0.33         | 0/501       | 0.55        | 0/664           |
| 15  | O     | 0.33         | 0/745       | 0.58        | 0/992           |
| 16  | P     | 0.34         | 0/717       | 0.58        | 0/965           |
| 17  | Q     | 0.35         | 0/837       | 0.61        | 0/1119          |
| 18  | R     | 0.34         | 0/579       | 0.60        | 0/768           |
| 19  | S     | 0.34         | 0/643       | 0.57        | 0/867           |
| 20  | T     | 0.29         | 0/765       | 0.58        | 0/1007          |
| 21  | U     | 0.42         | 0/213       | 0.50        | 0/279           |
| 22  | V     | 0.44         | 0/1784      | 0.69        | 0/2780          |
| 22  | W     | 0.36         | 0/1784      | 0.70        | 0/2780          |
| 23  | X     | 0.45         | 0/184       | 0.76        | 0/284           |
| 24  | Y     | 0.33         | 0/2849      | 0.66        | 0/3848          |
| All | All   | 0.37         | 0/62244     | 0.66        | 11/92247 (0.0%) |

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



| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 1                   | 17                  |
| 22  | V     | 0                   | 1                   |
| 22  | W     | 0                   | 3                   |
| All | All   | 1                   | 21                  |

There are no bond length outliers.

All (11) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 1498 | U    | C2'-C3'-O3' | 8.75  | 128.75      | 109.50   |
| 1   | A     | 1504 | G    | C2'-C3'-O3' | 8.30  | 127.77      | 109.50   |
| 1   | A     | 115  | G    | C2'-C3'-O3' | 7.59  | 126.20      | 109.50   |
| 1   | A     | 575  | G    | C2'-C3'-O3' | 7.24  | 125.42      | 109.50   |
| 1   | A     | 366  | C    | C2'-C3'-O3' | 7.14  | 125.22      | 109.50   |
| 1   | A     | 913  | A    | C2'-C3'-O3' | 7.09  | 125.10      | 109.50   |
| 1   | A     | 266  | G    | C2'-C3'-O3' | 6.47  | 124.06      | 113.70   |
| 1   | A     | 1067 | A    | C2'-C3'-O3' | 6.30  | 123.78      | 113.70   |
| 1   | A     | 1504 | G    | C4'-C3'-O3' | 5.82  | 124.63      | 113.00   |
| 1   | A     | 920  | U    | C5'-C4'-C3' | -5.56 | 107.10      | 116.00   |
| 1   | A     | 509  | A    | C2'-C3'-O3' | 5.05  | 121.78      | 113.70   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 1   | A     | 1504 | G    | C3'  |

All (21) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | A     | 1077 | G    | Sidechain |
| 1   | A     | 1181 | G    | Sidechain |
| 1   | A     | 1281 | U    | Sidechain |
| 1   | A     | 1418 | A    | Sidechain |
| 1   | A     | 1436 | U    | Sidechain |
| 1   | A     | 1502 | A    | Sidechain |
| 1   | A     | 1517 | G    | Sidechain |
| 1   | A     | 1519 | A    | Sidechain |
| 1   | A     | 1522 | U    | Sidechain |
| 1   | A     | 21   | G    | Sidechain |
| 1   | A     | 575  | G    | Sidechain |
| 1   | A     | 587  | G    | Sidechain |
| 1   | A     | 760  | G    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 832 | C    | Sidechain |
| 1   | A     | 879 | C    | Sidechain |
| 1   | A     | 897 | C    | Sidechain |
| 1   | A     | 898 | G    | Sidechain |
| 22  | V     | 29  | G    | Sidechain |
| 22  | W     | 19  | G    | Sidechain |
| 22  | W     | 20  | U    | Sidechain |
| 22  | W     | 70  | G    | 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     | 32329 | 0        | 16316    | 1207    | 0            |
| 2   | B     | 1901  | 0        | 1951     | 259     | 0            |
| 3   | C     | 1613  | 0        | 1677     | 196     | 0            |
| 4   | D     | 1703  | 0        | 1763     | 207     | 0            |
| 5   | E     | 1147  | 0        | 1207     | 125     | 0            |
| 6   | F     | 843   | 0        | 857      | 93      | 0            |
| 7   | G     | 1257  | 0        | 1296     | 121     | 0            |
| 8   | H     | 1116  | 0        | 1177     | 113     | 0            |
| 9   | I     | 1011  | 0        | 1041     | 129     | 0            |
| 10  | J     | 795   | 0        | 840      | 144     | 0            |
| 11  | K     | 885   | 0        | 904      | 77      | 0            |
| 12  | L     | 971   | 0        | 1057     | 124     | 0            |
| 13  | M     | 988   | 0        | 1055     | 150     | 0            |
| 14  | N     | 492   | 0        | 529      | 65      | 0            |
| 15  | O     | 734   | 0        | 771      | 52      | 0            |
| 16  | P     | 701   | 0        | 720      | 87      | 0            |
| 17  | Q     | 824   | 0        | 891      | 63      | 0            |
| 18  | R     | 574   | 0        | 644      | 59      | 0            |
| 19  | S     | 630   | 0        | 651      | 100     | 0            |
| 20  | T     | 763   | 0        | 861      | 78      | 0            |
| 21  | U     | 209   | 0        | 221      | 26      | 0            |
| 22  | V     | 1630  | 0        | 831      | 58      | 0            |
| 22  | W     | 1630  | 0        | 832      | 95      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 23  | X     | 165   | 0        | 87       | 17      | 0            |
| 24  | Y     | 2801  | 0        | 2816     | 393     | 0            |
| 25  | Z     | 546   | 0        | 0        | 0       | 0            |
| 26  | Z     | 3     | 0        | 0        | 0       | 0            |
| All | All   | 58261 | 0        | 40995    | 3675    | 0            |

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 37.

All (3675) close contacts within the same asymmetric unit are listed below.

| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 4:D:128:VAL:HG12  | 4:D:129:ASN:H     | 1.08        | 1.16     |
| 22:V:72:C:H2'     | 22:V:73:A:H5''    | 1.24        | 1.15     |
| 4:D:86:LYS:HE3    | 4:D:87:GLY:H      | 1.00        | 1.12     |
| 24:Y:111:HIS:NE2  | 24:Y:214:VAL:HB   | 1.67        | 1.09     |
| 2:B:172:ILE:H     | 2:B:172:ILE:HD12  | 1.20        | 1.06     |
| 13:M:88:ARG:HA    | 13:M:98:VAL:HG11  | 1.37        | 1.05     |
| 19:S:6:LYS:HG2    | 19:S:7:LYS:HE3    | 1.38        | 1.04     |
| 24:Y:209:GLU:OE2  | 24:Y:303:ARG:CD   | 2.06        | 1.04     |
| 22:W:16:U:H3'     | 22:W:17:C:H5'     | 1.34        | 1.03     |
| 24:Y:238:GLY:HA3  | 24:Y:242:VAL:HB   | 1.38        | 1.03     |
| 5:E:102:ALA:HB1   | 5:E:106:PRO:HG2   | 1.41        | 1.03     |
| 24:Y:287:GLU:HA   | 24:Y:290:LYS:HE3  | 1.42        | 1.02     |
| 1:A:979:C:H3'     | 1:A:980:C:H5''    | 1.38        | 1.01     |
| 1:A:975:A:H4'     | 1:A:976:G:H5''    | 1.43        | 1.00     |
| 2:B:71:VAL:HG13   | 2:B:93:VAL:HB     | 1.42        | 1.00     |
| 10:J:50:ILE:HD13  | 10:J:50:ILE:H     | 1.26        | 0.99     |
| 6:F:30:LEU:H      | 6:F:30:LEU:HD23   | 1.27        | 0.99     |
| 4:D:18:LYS:HB2    | 4:D:33:MET:HG2    | 1.42        | 0.99     |
| 3:C:150:LYS:HB3   | 3:C:201:TYR:HB2   | 1.44        | 0.99     |
| 22:W:39:U:H2'     | 22:W:40:C:H5''    | 1.44        | 0.98     |
| 1:A:1107:C:H2'    | 1:A:1108:G:H5''   | 1.44        | 0.98     |
| 3:C:14:ILE:HG12   | 3:C:15:THR:H      | 1.27        | 0.98     |
| 24:Y:252:VAL:HG13 | 24:Y:259:THR:HG22 | 1.46        | 0.97     |
| 1:A:1256:A:H61    | 1:A:1278:U:H1'    | 1.26        | 0.97     |
| 1:A:1116:C:H2'    | 1:A:1117:G:H5''   | 1.47        | 0.96     |
| 1:A:939:G:H5''    | 7:G:102:ARG:HH12  | 1.30        | 0.96     |
| 4:D:176:LEU:HG    | 4:D:177:ASP:H     | 1.29        | 0.96     |
| 1:A:1128:C:H1'    | 1:A:1146:A:H61    | 1.31        | 0.95     |
| 4:D:86:LYS:HE3    | 4:D:87:GLY:N      | 1.80        | 0.95     |
| 13:M:124:PRO:HD2  | 24:Y:163:GLY:H    | 1.26        | 0.95     |
| 22:W:50:U:H4'     | 22:W:65:G:H22     | 1.30        | 0.95     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 24:Y:61:THR:HG21  | 24:Y:101:LEU:HD13 | 1.45        | 0.95     |
| 2:B:168:THR:HG23  | 2:B:192:SER:OG    | 1.68        | 0.94     |
| 1:A:673:G:H2'     | 1:A:674:G:C8      | 2.02        | 0.94     |
| 2:B:185:ILE:HG22  | 2:B:199:TYR:HB2   | 1.49        | 0.94     |
| 2:B:22:LYS:HA     | 2:B:22:LYS:HE2    | 1.46        | 0.94     |
| 19:S:10:PHE:HZ    | 19:S:70:LYS:HZ3   | 1.10        | 0.93     |
| 6:F:91:VAL:HG11   | 18:R:72:ARG:HH12  | 1.34        | 0.93     |
| 11:K:99:GLN:HG2   | 11:K:105:VAL:HG11 | 1.50        | 0.93     |
| 8:H:87:SER:HB2    | 8:H:93:VAL:HB     | 1.49        | 0.93     |
| 15:O:33:THR:HG21  | 15:O:85:LEU:HD21  | 1.50        | 0.93     |
| 2:B:178:ARG:HB2   | 2:B:178:ARG:HH11  | 1.34        | 0.92     |
| 24:Y:323:ASP:HB3  | 24:Y:326:THR:HG22 | 1.49        | 0.92     |
| 22:V:41:C:H3'     | 22:V:42:C:H5''    | 1.49        | 0.92     |
| 1:A:137:C:H42     | 1:A:226:G:H1      | 1.10        | 0.92     |
| 1:A:266:G:H5''    | 1:A:268:C:H41     | 1.35        | 0.92     |
| 24:Y:182:PRO:HG3  | 24:Y:345:ILE:HG23 | 1.52        | 0.92     |
| 1:A:192:U:H4'     | 20:T:103:GLY:H    | 1.33        | 0.92     |
| 13:M:125:ARG:HG3  | 24:Y:160:PRO:HD2  | 1.50        | 0.91     |
| 3:C:70:VAL:HG12   | 3:C:72:LYS:H      | 1.34        | 0.91     |
| 16:P:22:THR:HA    | 16:P:33:ILE:HG12  | 1.53        | 0.91     |
| 2:B:231:GLU:HB2   | 2:B:232:PRO:HD2   | 1.52        | 0.91     |
| 1:A:15:G:H4'      | 5:E:24:ARG:HH12   | 1.34        | 0.91     |
| 13:M:126:LYS:N    | 24:Y:162:ALA:H    | 1.68        | 0.91     |
| 4:D:74:GLN:HA     | 4:D:77:ASN:HD22   | 1.35        | 0.90     |
| 24:Y:150:GLN:HE21 | 24:Y:172:LYS:NZ   | 1.69        | 0.90     |
| 10:J:3:LYS:HD2    | 10:J:77:PRO:HG3   | 1.54        | 0.90     |
| 9:I:28:VAL:HG22   | 9:I:63:ILE:HB     | 1.52        | 0.90     |
| 19:S:32:LYS:HA    | 19:S:50:ALA:HB3   | 1.51        | 0.89     |
| 13:M:78:ILE:HA    | 13:M:81:LEU:HD12  | 1.54        | 0.89     |
| 22:W:25:C:H2'     | 22:W:26:A:H8      | 1.36        | 0.89     |
| 12:L:18:VAL:HG23  | 12:L:19:ARG:H     | 1.34        | 0.89     |
| 22:V:72:C:C2'     | 22:V:73:A:H5''    | 2.02        | 0.89     |
| 1:A:413:G:H4'     | 1:A:414:A:H5''    | 1.52        | 0.89     |
| 4:D:128:VAL:HG12  | 4:D:129:ASN:N     | 1.87        | 0.89     |
| 1:A:1057:G:H5''   | 3:C:154:SER:HB2   | 1.54        | 0.88     |
| 10:J:43:ARG:HB2   | 10:J:67:THR:HB    | 1.54        | 0.88     |
| 24:Y:239:GLY:H    | 24:Y:242:VAL:HG12 | 1.39        | 0.88     |
| 3:C:6:HIS:HD2     | 3:C:7:PRO:HD2     | 1.36        | 0.88     |
| 5:E:51:VAL:HB     | 5:E:52:PRO:HD3    | 1.56        | 0.88     |
| 1:A:735:C:H2'     | 1:A:736:C:H6      | 1.36        | 0.88     |
| 13:M:3:ARG:HH21   | 13:M:7:VAL:HG22   | 1.37        | 0.88     |
| 13:M:124:PRO:CD   | 24:Y:163:GLY:H    | 1.86        | 0.88     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 1:A:473:G:H4'     | 16:P:81:ARG:HH21   | 1.37        | 0.88     |
| 9:I:65:VAL:HG21   | 9:I:73:GLN:HB3     | 1.54        | 0.88     |
| 22:W:68:C:H2'     | 22:W:69:G:H8       | 1.39        | 0.88     |
| 5:E:7:GLU:HG2     | 5:E:112:LEU:HD22   | 1.55        | 0.87     |
| 5:E:76:ILE:HD11   | 5:E:142:LEU:HD21   | 1.53        | 0.87     |
| 19:S:78:ARG:HH11  | 19:S:81:ARG:HH12   | 1.15        | 0.87     |
| 1:A:424:G:H2'     | 1:A:425:G:H8       | 1.38        | 0.87     |
| 10:J:4:ILE:HD11   | 10:J:77:PRO:HB3    | 1.54        | 0.87     |
| 5:E:41:VAL:HG22   | 5:E:113:ALA:HA     | 1.57        | 0.87     |
| 1:A:942:G:H21     | 9:I:124:GLN:HE22   | 1.23        | 0.86     |
| 7:G:37:ASN:HD21   | 9:I:40:LEU:HA      | 1.38        | 0.86     |
| 20:T:57:ARG:HH22  | 20:T:100:ILE:HG12  | 1.39        | 0.86     |
| 2:B:165:VAL:HG23  | 2:B:166:ASP:H      | 1.39        | 0.86     |
| 24:Y:286:LEU:HA   | 24:Y:289:LYS:HD2   | 1.57        | 0.86     |
| 24:Y:209:GLU:OE2  | 24:Y:303:ARG:HD3   | 1.75        | 0.85     |
| 3:C:32:LEU:HB3    | 3:C:59:ARG:HH22    | 1.39        | 0.85     |
| 24:Y:198:SER:HB2  | 24:Y:200:ARG:HG3   | 1.56        | 0.85     |
| 20:T:57:ARG:NH2   | 20:T:100:ILE:HG12  | 1.92        | 0.85     |
| 12:L:25:PRO:C     | 12:L:27:LEU:H      | 1.78        | 0.85     |
| 6:F:77:ARG:NH1    | 6:F:77:ARG:HB3     | 1.90        | 0.85     |
| 4:D:128:VAL:CG1   | 4:D:129:ASN:H      | 1.88        | 0.85     |
| 7:G:102:ARG:HG2   | 7:G:106:GLN:HE21   | 1.41        | 0.85     |
| 24:Y:326:THR:HG23 | 24:Y:328:LEU:H     | 1.42        | 0.85     |
| 9:I:26:VAL:HG22   | 9:I:61:ALA:HB3     | 1.58        | 0.85     |
| 22:V:51:U:H2'     | 22:V:52:G:C8       | 2.11        | 0.85     |
| 22:W:72:C:H2'     | 22:W:73:A:O4'      | 1.75        | 0.85     |
| 1:A:1028:C:H2'    | 1:A:1029:C:H5'     | 1.57        | 0.85     |
| 2:B:33:TYR:HB2    | 2:B:43:ASP:HB2     | 1.56        | 0.85     |
| 1:A:1030(A):G:H2' | 1:A:1030(B):C:H5'' | 1.56        | 0.84     |
| 18:R:56:THR:HB    | 18:R:58:LEU:HD13   | 1.56        | 0.84     |
| 9:I:50:LEU:HD21   | 9:I:81:ILE:HG22    | 1.57        | 0.84     |
| 22:W:59:U:H2'     | 22:W:60:U:H6       | 1.41        | 0.84     |
| 12:L:6:THR:HG23   | 12:L:9:GLN:HE21    | 1.41        | 0.84     |
| 22:W:76:8AN:H4'   | 22:W:77:PHA:O      | 1.77        | 0.84     |
| 9:I:9:ARG:HG2     | 9:I:14:VAL:HG22    | 1.60        | 0.84     |
| 1:A:1347:G:N2     | 1:A:1373:G:H2'     | 1.93        | 0.83     |
| 10:J:26:ALA:HA    | 10:J:29:ARG:HH12   | 1.41        | 0.83     |
| 22:W:59:U:H2'     | 22:W:60:U:C6       | 2.13        | 0.83     |
| 1:A:939:G:C5'     | 7:G:102:ARG:HH12   | 1.91        | 0.83     |
| 19:S:29:ARG:HD2   | 19:S:30:LEU:H      | 1.42        | 0.83     |
| 2:B:118:LEU:HB3   | 2:B:142:LEU:HD12   | 1.60        | 0.83     |
| 16:P:45:THR:HG22  | 16:P:47:ASP:H      | 1.43        | 0.83     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:728:A:H2'    | 1:A:729:A:C8      | 2.14        | 0.83     |
| 12:L:84:LEU:HD12 | 12:L:104:VAL:HG11 | 1.59        | 0.83     |
| 2:B:233:SER:HB2  | 2:B:234:PRO:HD2   | 1.57        | 0.83     |
| 2:B:80:ILE:H     | 2:B:80:ILE:HD12   | 1.42        | 0.83     |
| 19:S:42:PRO:O    | 19:S:43:GLU:HB3   | 1.77        | 0.83     |
| 9:I:10:ARG:HH21  | 9:I:11:LYS:HB2    | 1.41        | 0.83     |
| 24:Y:283:LEU:HB3 | 24:Y:287:GLU:OE2  | 1.78        | 0.83     |
| 24:Y:287:GLU:O   | 24:Y:290:LYS:HG2  | 1.79        | 0.83     |
| 12:L:6:THR:H     | 12:L:9:GLN:HE21   | 1.23        | 0.82     |
| 2:B:55:PHE:HA    | 2:B:58:ILE:HD12   | 1.60        | 0.82     |
| 24:Y:279:LEU:O   | 24:Y:283:LEU:HG   | 1.78        | 0.82     |
| 12:L:47:LYS:HB3  | 12:L:48:PRO:CD    | 2.09        | 0.82     |
| 1:A:976:G:H5'    | 1:A:1358:U:O2'    | 1.79        | 0.82     |
| 1:A:922:G:H4'    | 5:E:20:GLN:HA     | 1.62        | 0.82     |
| 5:E:101:ILE:HD11 | 5:E:119:LEU:HD23  | 1.60        | 0.82     |
| 4:D:59:ARG:HA    | 4:D:59:ARG:HE     | 1.44        | 0.82     |
| 9:I:4:TYR:HB2    | 9:I:19:LEU:HB2    | 1.61        | 0.82     |
| 2:B:231:GLU:HB2  | 2:B:232:PRO:CD    | 2.10        | 0.82     |
| 3:C:113:ALA:HB3  | 3:C:114:PRO:HD3   | 1.62        | 0.82     |
| 1:A:1502:A:H2    | 1:A:1505:G:H1     | 1.25        | 0.82     |
| 12:L:53:ARG:HH11 | 12:L:53:ARG:HG2   | 1.42        | 0.82     |
| 1:A:939:G:H5''   | 7:G:102:ARG:NH1   | 1.95        | 0.81     |
| 5:E:92:LYS:HB3   | 5:E:119:LEU:HB2   | 1.62        | 0.81     |
| 1:A:1321:C:C5'   | 1:A:1322:C:H5''   | 2.10        | 0.81     |
| 18:R:31:LEU:HD23 | 18:R:31:LEU:H     | 1.45        | 0.81     |
| 1:A:1292:U:H2'   | 1:A:1293:G:C8     | 2.14        | 0.81     |
| 12:L:57:LYS:HG2  | 12:L:67:THR:HG22  | 1.63        | 0.81     |
| 1:A:990:C:H2'    | 1:A:991:U:C6      | 2.16        | 0.81     |
| 8:H:11:THR:HG22  | 8:H:15:ASN:HD21   | 1.46        | 0.81     |
| 8:H:11:THR:HG22  | 8:H:15:ASN:ND2    | 1.96        | 0.81     |
| 9:I:15:ALA:HB2   | 9:I:65:VAL:HG23   | 1.62        | 0.81     |
| 19:S:43:GLU:HG2  | 19:S:44:MET:HE1   | 1.60        | 0.81     |
| 4:D:93:PHE:O     | 4:D:97:LEU:HB2    | 1.81        | 0.81     |
| 10:J:24:VAL:HG21 | 10:J:37:PRO:HG3   | 1.61        | 0.81     |
| 13:M:126:LYS:N   | 24:Y:162:ALA:N    | 2.29        | 0.80     |
| 22:W:63:G:H2'    | 22:W:64:A:H5'     | 1.62        | 0.80     |
| 19:S:16:LEU:HD12 | 19:S:16:LEU:H     | 1.45        | 0.80     |
| 3:C:34:LEU:HD21  | 3:C:38:ARG:HD2    | 1.63        | 0.80     |
| 1:A:223:U:H2'    | 1:A:224:C:H6      | 1.46        | 0.80     |
| 24:Y:209:GLU:CD  | 24:Y:303:ARG:HD3  | 2.00        | 0.80     |
| 1:A:1116:C:C2'   | 1:A:1117:G:H5''   | 2.12        | 0.80     |
| 9:I:17:VAL:HG13  | 9:I:81:ILE:HD13   | 1.63        | 0.80     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:590:C:H2'     | 1:A:591:U:H6      | 1.45        | 0.80     |
| 8:H:89:PRO:HA     | 8:H:92:ARG:HH11   | 1.47        | 0.80     |
| 3:C:16:ARG:NH1    | 3:C:16:ARG:HB2    | 1.96        | 0.80     |
| 1:A:624:C:H2'     | 1:A:625:G:H8      | 1.46        | 0.80     |
| 3:C:101:LEU:HD23  | 3:C:102:ASN:N     | 1.97        | 0.80     |
| 1:A:444:C:H2'     | 1:A:445:G:C8      | 2.17        | 0.80     |
| 6:F:68:PRO:HG2    | 6:F:71:ARG:HG3    | 1.63        | 0.80     |
| 1:A:1137:C:H4'    | 1:A:1138:G:C2     | 2.16        | 0.80     |
| 7:G:84:ASN:ND2    | 22:W:37:A:H61     | 1.79        | 0.79     |
| 4:D:30:LYS:C      | 4:D:32:ALA:H      | 1.86        | 0.79     |
| 24:Y:115:ASN:HA   | 24:Y:176:ALA:HB3  | 1.62        | 0.79     |
| 16:P:28:ARG:HH11  | 16:P:28:ARG:HG2   | 1.46        | 0.79     |
| 3:C:36:ASP:HB3    | 3:C:40:ARG:HH12   | 1.46        | 0.79     |
| 24:Y:288:ARG:HB3  | 24:Y:288:ARG:HH11 | 1.46        | 0.79     |
| 2:B:141:GLU:O     | 2:B:145:LEU:HB2   | 1.82        | 0.79     |
| 7:G:100:ALA:O     | 7:G:104:LEU:HD23  | 1.82        | 0.79     |
| 11:K:85:ARG:HG2   | 11:K:111:ASP:O    | 1.83        | 0.79     |
| 1:A:15:G:H4'      | 5:E:24:ARG:NH1    | 1.97        | 0.79     |
| 3:C:32:LEU:HB3    | 3:C:59:ARG:NH2    | 1.97        | 0.79     |
| 24:Y:49:SER:O     | 24:Y:53:ALA:HB2   | 1.81        | 0.79     |
| 1:A:973:G:H3'     | 1:A:974:A:H5''    | 1.65        | 0.79     |
| 1:A:1278:U:H5''   | 1:A:1279:A:O4'    | 1.83        | 0.79     |
| 4:D:12:CYS:HA     | 4:D:19:LEU:H      | 1.47        | 0.78     |
| 24:Y:131:ASP:HA   | 24:Y:163:GLY:HA2  | 1.64        | 0.78     |
| 1:A:601:C:H2'     | 1:A:602:A:H8      | 1.47        | 0.78     |
| 24:Y:41:ASP:HB3   | 24:Y:44:ALA:HB3   | 1.66        | 0.78     |
| 24:Y:112:ALA:HA   | 24:Y:177:TYR:HD2  | 1.47        | 0.78     |
| 19:S:18:LYS:O     | 19:S:22:LEU:HD23  | 1.82        | 0.78     |
| 1:A:1435:G:H2'    | 1:A:1436:U:C6     | 2.18        | 0.78     |
| 3:C:6:HIS:ND1     | 14:N:49:HIS:HB3   | 1.98        | 0.78     |
| 24:Y:295:LEU:CD1  | 24:Y:299:ARG:HH21 | 1.97        | 0.78     |
| 6:F:19:LEU:HD23   | 6:F:19:LEU:O      | 1.84        | 0.78     |
| 24:Y:150:GLN:HE21 | 24:Y:172:LYS:HZ3  | 1.30        | 0.78     |
| 24:Y:270:LYS:O    | 24:Y:274:LEU:HD13 | 1.82        | 0.78     |
| 22:W:57:G:H2'     | 22:W:58:A:H5'     | 1.64        | 0.78     |
| 1:A:392:G:H2'     | 1:A:393:A:H8      | 1.48        | 0.78     |
| 22:V:26:A:H61     | 22:V:44:G:H1      | 1.29        | 0.78     |
| 1:A:1305:G:H5'    | 21:U:4:GLY:HA3    | 1.63        | 0.78     |
| 4:D:196:LEU:H     | 4:D:196:LEU:HD12  | 1.48        | 0.78     |
| 24:Y:181:SER:H    | 24:Y:182:PRO:HD2  | 1.48        | 0.78     |
| 1:A:1005:A:N6     | 1:A:1025:U:H4'    | 1.99        | 0.78     |
| 4:D:49:ARG:HE     | 4:D:49:ARG:HA     | 1.48        | 0.78     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 3:C:175:LEU:HD21  | 3:C:201:TYR:HE2   | 1.46        | 0.78     |
| 7:G:79:ARG:HH21   | 23:X:14:A:H61     | 1.33        | 0.78     |
| 7:G:15:ASP:HB3    | 7:G:19:GLY:N      | 2.00        | 0.77     |
| 24:Y:288:ARG:NH1  | 24:Y:288:ARG:HB3  | 1.98        | 0.77     |
| 18:R:37:VAL:HG23  | 18:R:38:GLU:H     | 1.49        | 0.77     |
| 1:A:392:G:H2'     | 1:A:393:A:C8      | 2.19        | 0.77     |
| 1:A:255:G:H1'     | 17:Q:16:GLN:NE2   | 1.99        | 0.77     |
| 22:V:21:A:H2'     | 22:V:22:G:H5''    | 1.65        | 0.77     |
| 4:D:176:LEU:HG    | 4:D:178:VAL:H     | 1.48        | 0.77     |
| 1:A:1057:G:H5''   | 3:C:154:SER:CB    | 2.14        | 0.77     |
| 24:Y:214:VAL:HG13 | 24:Y:215:ASP:H    | 1.47        | 0.77     |
| 11:K:29:ILE:HG13  | 11:K:44:SER:HB3   | 1.67        | 0.77     |
| 5:E:100:VAL:HG12  | 5:E:118:ILE:HG22  | 1.65        | 0.77     |
| 2:B:91:PRO:HG3    | 2:B:154:LEU:HB2   | 1.65        | 0.77     |
| 22:V:41:C:C3'     | 22:V:42:C:H5''    | 2.14        | 0.77     |
| 5:E:6:PHE:HB2     | 5:E:34:VAL:HG22   | 1.65        | 0.77     |
| 7:G:15:ASP:HB3    | 7:G:19:GLY:H      | 1.50        | 0.77     |
| 8:H:91:ARG:HG2    | 8:H:91:ARG:HH11   | 1.49        | 0.77     |
| 24:Y:81:ALA:HB1   | 24:Y:84:ARG:HH21  | 1.50        | 0.77     |
| 6:F:100:ASN:O     | 18:R:28:GLU:HG2   | 1.85        | 0.77     |
| 1:A:1355:G:H2'    | 1:A:1356:G:H8     | 1.49        | 0.77     |
| 1:A:878:G:H5'     | 8:H:89:PRO:HG2    | 1.67        | 0.76     |
| 20:T:11:SER:HA    | 20:T:13:LEU:HD12  | 1.67        | 0.76     |
| 1:A:954:G:H21     | 1:A:1227:A:H62    | 1.33        | 0.76     |
| 13:M:124:PRO:N    | 24:Y:162:ALA:HA   | 2.00        | 0.76     |
| 4:D:110:PHE:H     | 4:D:110:PHE:HD1   | 1.32        | 0.76     |
| 1:A:728:A:H2'     | 1:A:729:A:H8      | 1.49        | 0.76     |
| 22:W:28:G:H2'     | 22:W:29:G:C8      | 2.20        | 0.76     |
| 10:J:49:VAL:HG23  | 14:N:41:ARG:HB2   | 1.67        | 0.76     |
| 24:Y:130:CYS:HB3  | 24:Y:164:ILE:H    | 1.49        | 0.76     |
| 9:I:53:VAL:HG12   | 9:I:95:LYS:HE3    | 1.66        | 0.76     |
| 20:T:56:MET:HG3   | 20:T:84:LEU:CD1   | 2.15        | 0.76     |
| 2:B:124:SER:OG    | 2:B:125:PRO:HD2   | 1.85        | 0.76     |
| 24:Y:344:LEU:HD23 | 24:Y:344:LEU:H    | 1.49        | 0.76     |
| 7:G:113:GLU:CG    | 7:G:119:ARG:HG2   | 2.16        | 0.76     |
| 20:T:75:ASN:N     | 20:T:75:ASN:HD22  | 1.80        | 0.76     |
| 16:P:53:VAL:HG12  | 16:P:79:VAL:HG22  | 1.68        | 0.76     |
| 12:L:70:ILE:HG12  | 12:L:100:ILE:HD12 | 1.66        | 0.76     |
| 16:P:13:HIS:O     | 16:P:15:PRO:HD3   | 1.85        | 0.76     |
| 3:C:180:ALA:HB1   | 3:C:203:PHE:HE1   | 1.50        | 0.76     |
| 6:F:77:ARG:HH11   | 6:F:77:ARG:HB3    | 1.48        | 0.76     |
| 1:A:235:C:H5'     | 17:Q:70:ARG:HG2   | 1.66        | 0.76     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 4:D:112:VAL:HG12 | 4:D:116:GLN:OE1  | 1.86        | 0.76     |
| 4:D:176:LEU:CG   | 4:D:177:ASP:H    | 1.99        | 0.76     |
| 19:S:29:ARG:CD   | 19:S:30:LEU:H    | 1.97        | 0.76     |
| 22:W:28:G:H2'    | 22:W:29:G:H8     | 1.51        | 0.76     |
| 22:W:16:U:H3'    | 22:W:17:C:C5'    | 2.13        | 0.75     |
| 13:M:124:PRO:HD2 | 24:Y:163:GLY:N   | 2.01        | 0.75     |
| 12:L:47:LYS:HB3  | 12:L:48:PRO:HD3  | 1.68        | 0.75     |
| 1:A:1513:A:H2'   | 1:A:1514:C:C6    | 2.21        | 0.75     |
| 8:H:36:LEU:HA    | 8:H:39:LEU:HD23  | 1.69        | 0.75     |
| 1:A:67:C:H2'     | 1:A:68:G:C8      | 2.20        | 0.75     |
| 1:A:976:G:N2     | 1:A:1362:C:H2'   | 2.00        | 0.75     |
| 10:J:49:VAL:CG2  | 14:N:41:ARG:HB2  | 2.15        | 0.75     |
| 19:S:48:THR:HG22 | 19:S:61:TYR:HA   | 1.68        | 0.75     |
| 2:B:101:MET:HA   | 2:B:108:ILE:HG13 | 1.68        | 0.75     |
| 1:A:1425:U:H2'   | 1:A:1426:C:H6    | 1.49        | 0.75     |
| 13:M:32:GLU:O    | 13:M:35:GLU:HG2  | 1.85        | 0.75     |
| 1:A:532:A:N6     | 3:C:156:ARG:HH12 | 1.83        | 0.75     |
| 1:A:377:G:H2'    | 1:A:378:G:H8     | 1.51        | 0.75     |
| 5:E:92:LYS:O     | 5:E:118:ILE:HD12 | 1.86        | 0.75     |
| 22:W:19:G:H2'    | 22:W:20:U:C6     | 2.21        | 0.75     |
| 10:J:6:ILE:HG22  | 10:J:98:ILE:HG13 | 1.69        | 0.75     |
| 17:Q:7:THR:HG22  | 17:Q:58:GLU:HG2  | 1.67        | 0.75     |
| 1:A:737:A:H2'    | 1:A:738:C:C6     | 2.22        | 0.75     |
| 2:B:120:ALA:O    | 2:B:121:LEU:HD23 | 1.87        | 0.75     |
| 8:H:101:PRO:HG2  | 8:H:133:LEU:HD11 | 1.69        | 0.75     |
| 22:W:19:G:H2'    | 22:W:20:U:C5     | 2.21        | 0.75     |
| 24:Y:186:VAL:HB  | 24:Y:309:SER:O   | 1.87        | 0.75     |
| 10:J:4:ILE:HD12  | 10:J:4:ILE:H     | 1.51        | 0.75     |
| 24:Y:80:PRO:HB3  | 24:Y:85:GLU:OE1  | 1.87        | 0.75     |
| 1:A:1163:C:H2'   | 1:A:1164:G:H8    | 1.51        | 0.75     |
| 2:B:208:ILE:HA   | 2:B:211:ILE:HD12 | 1.69        | 0.74     |
| 2:B:166:ASP:HB3  | 2:B:169:LYS:HB2  | 1.68        | 0.74     |
| 5:E:150:ARG:HA   | 5:E:153:LYS:HE2  | 1.69        | 0.74     |
| 2:B:170:GLU:O    | 2:B:174:VAL:HG23 | 1.86        | 0.74     |
| 24:Y:25:ARG:HH11 | 24:Y:29:LEU:HD23 | 1.51        | 0.74     |
| 21:U:9:ARG:HA    | 21:U:9:ARG:HH11  | 1.50        | 0.74     |
| 1:A:405:U:H3'    | 1:A:406:G:H5'    | 1.68        | 0.74     |
| 22:W:50:U:H4'    | 22:W:65:G:N2     | 2.03        | 0.74     |
| 1:A:1107:C:C2'   | 1:A:1108:G:H5''  | 2.16        | 0.74     |
| 22:V:1:G:H2'     | 22:V:2:C:H6      | 1.50        | 0.74     |
| 2:B:224:GLN:HA   | 2:B:229:VAL:HG22 | 1.69        | 0.74     |
| 14:N:23:ARG:NH1  | 14:N:30:ALA:HB2  | 2.02        | 0.74     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 12:L:89:ARG:HA   | 12:L:97:ARG:HA    | 1.69        | 0.74     |
| 10:J:38:ILE:HD11 | 10:J:71:LEU:HD23  | 1.68        | 0.74     |
| 22:W:57:G:C2'    | 22:W:58:A:H5'     | 2.18        | 0.74     |
| 24:Y:238:GLY:HA3 | 24:Y:242:VAL:CB   | 2.16        | 0.74     |
| 5:E:50:GLU:HG3   | 5:E:52:PRO:HD2    | 1.69        | 0.74     |
| 3:C:121:ALA:HB2  | 3:C:198:VAL:HG21  | 1.70        | 0.74     |
| 15:O:33:THR:HG21 | 15:O:85:LEU:CD2   | 2.17        | 0.74     |
| 2:B:194:PRO:HG2  | 2:B:195:ASP:OD1   | 1.87        | 0.74     |
| 12:L:25:PRO:O    | 12:L:27:LEU:HD13  | 1.87        | 0.74     |
| 3:C:71:ALA:HB2   | 3:C:106:VAL:HB    | 1.70        | 0.74     |
| 22:W:38:A:H2'    | 22:W:39:U:H5''    | 1.70        | 0.74     |
| 1:A:192:U:H2'    | 1:A:193:C:C6      | 2.22        | 0.74     |
| 1:A:491:G:H2'    | 1:A:492:G:H8      | 1.51        | 0.74     |
| 1:A:963:G:H21    | 10:J:55:LYS:HZ2   | 1.34        | 0.74     |
| 1:A:1027:C:H2'   | 1:A:1028:C:C5     | 2.23        | 0.74     |
| 5:E:31:LEU:HD23  | 5:E:45:PHE:HB2    | 1.68        | 0.74     |
| 2:B:178:ARG:HH22 | 2:B:196:LEU:C     | 1.92        | 0.73     |
| 1:A:1003:G:H2'   | 1:A:1004:A:O4'    | 1.88        | 0.73     |
| 1:A:1030:C:H2'   | 1:A:1030(A):G:H5' | 1.70        | 0.73     |
| 1:A:1321:C:C3'   | 1:A:1322:C:H5''   | 2.18        | 0.73     |
| 9:I:115:GLY:O    | 9:I:116:LYS:HG3   | 1.88        | 0.73     |
| 1:A:1343:G:H2'   | 1:A:1344:C:C6     | 2.22        | 0.73     |
| 3:C:14:ILE:HG12  | 3:C:15:THR:N      | 2.02        | 0.73     |
| 19:S:78:ARG:HB2  | 19:S:81:ARG:HH11  | 1.52        | 0.73     |
| 19:S:11:VAL:HG13 | 19:S:16:LEU:HD11  | 1.69        | 0.73     |
| 10:J:33:GLN:O    | 10:J:75:ILE:HG12  | 1.88        | 0.73     |
| 13:M:19:LEU:HA   | 13:M:22:ILE:HD13  | 1.70        | 0.73     |
| 3:C:206:GLU:HG2  | 3:C:207:VAL:H     | 1.53        | 0.73     |
| 22:V:77:PHA:N    | 22:V:77:PHA:HD2   | 2.02        | 0.73     |
| 19:S:6:LYS:HD2   | 19:S:6:LYS:H      | 1.52        | 0.73     |
| 24:Y:118:LEU:CD2 | 24:Y:210:VAL:HG22 | 2.17        | 0.73     |
| 2:B:187:LEU:HD23 | 2:B:201:ILE:HG22  | 1.70        | 0.73     |
| 1:A:474:G:H2'    | 1:A:475:G:C8      | 2.22        | 0.73     |
| 12:L:70:ILE:HD13 | 12:L:77:LEU:HD12  | 1.71        | 0.73     |
| 7:G:146:GLU:HG2  | 7:G:149:ARG:HH12  | 1.51        | 0.73     |
| 1:A:997:U:H2'    | 1:A:998:G:C8      | 2.23        | 0.73     |
| 13:M:49:THR:HG22 | 13:M:51:ALA:H     | 1.54        | 0.73     |
| 1:A:979:C:C3'    | 1:A:980:C:H5''    | 2.18        | 0.73     |
| 8:H:88:LYS:HB3   | 8:H:89:PRO:HD2    | 1.68        | 0.73     |
| 20:T:39:LYS:O    | 20:T:42:GLN:HB3   | 1.88        | 0.73     |
| 1:A:674:G:H2'    | 1:A:675:A:H8      | 1.51        | 0.73     |
| 8:H:11:THR:HG23  | 8:H:14:ARG:NH1    | 2.03        | 0.73     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:353:A:H5'     | 1:A:353:A:H8      | 1.54        | 0.73     |
| 3:C:127:ARG:HD2   | 3:C:127:ARG:N     | 2.04        | 0.73     |
| 2:B:97:TRP:CH2    | 2:B:173:ALA:HA    | 2.23        | 0.73     |
| 1:A:685:G:O2'     | 1:A:686:U:H5'     | 1.88        | 0.73     |
| 24:Y:312:ARG:HE   | 24:Y:344:LEU:HD12 | 1.54        | 0.73     |
| 1:A:1397:C:H2'    | 24:Y:198:SER:OG   | 1.87        | 0.73     |
| 1:A:1028:C:C2'    | 1:A:1029:C:H5'    | 2.19        | 0.73     |
| 1:A:223:U:H2'     | 1:A:224:C:C6      | 2.24        | 0.73     |
| 8:H:86:ILE:HG12   | 8:H:135:CYS:HA    | 1.70        | 0.73     |
| 13:M:91:ARG:HB2   | 13:M:98:VAL:HG22  | 1.71        | 0.72     |
| 5:E:76:ILE:HG13   | 5:E:142:LEU:HD13  | 1.70        | 0.72     |
| 1:A:1294:G:H2'    | 1:A:1295:G:H8     | 1.52        | 0.72     |
| 10:J:7:LYS:HD3    | 10:J:71:LEU:HD13  | 1.70        | 0.72     |
| 3:C:76:VAL:HG23   | 3:C:77:ILE:HG13   | 1.71        | 0.72     |
| 16:P:19:ILE:H     | 16:P:19:ILE:HD12  | 1.54        | 0.72     |
| 9:I:97:LYS:HB3    | 9:I:98:PRO:HD3    | 1.71        | 0.72     |
| 24:Y:303:ARG:H    | 24:Y:304:PRO:HD3  | 1.55        | 0.72     |
| 13:M:82:MET:HB2   | 13:M:93:ARG:NH1   | 2.03        | 0.72     |
| 5:E:9:LYS:HB2     | 5:E:112:LEU:HD11  | 1.71        | 0.72     |
| 24:Y:26:LEU:HB2   | 24:Y:55:LEU:HD21  | 1.69        | 0.72     |
| 1:A:407:G:O2'     | 4:D:116:GLN:HG3   | 1.89        | 0.72     |
| 1:A:939:G:H5''    | 7:G:102:ARG:HH22  | 1.53        | 0.72     |
| 18:R:88:LYS:HD3   | 18:R:88:LYS:C     | 2.10        | 0.72     |
| 1:A:17:U:H2'      | 1:A:18:C:C6       | 2.23        | 0.72     |
| 7:G:77:SER:HA     | 7:G:86:GLN:HA     | 1.72        | 0.72     |
| 24:Y:118:LEU:HD22 | 24:Y:208:VAL:CG1  | 2.20        | 0.72     |
| 22:W:38:A:H3'     | 22:W:39:U:H5''    | 1.70        | 0.72     |
| 1:A:1321:C:H5'    | 1:A:1322:C:H5''   | 1.70        | 0.72     |
| 24:Y:27:LYS:HA    | 24:Y:30:GLU:HG3   | 1.71        | 0.72     |
| 10:J:48:THR:HA    | 10:J:62:HIS:HB3   | 1.71        | 0.72     |
| 8:H:19:VAL:HG21   | 8:H:21:LYS:HE2    | 1.71        | 0.72     |
| 22:W:20:U:O2      | 22:W:20:U:H2'     | 1.89        | 0.72     |
| 1:A:1143:G:H2'    | 1:A:1144:G:C8     | 2.25        | 0.72     |
| 22:V:21:A:C2'     | 22:V:22:G:H5''    | 2.20        | 0.72     |
| 1:A:91:C:O2       | 1:A:91:C:H2'      | 1.89        | 0.72     |
| 1:A:73:G:H1       | 1:A:96:U:H3       | 1.36        | 0.72     |
| 1:A:434:U:H2'     | 1:A:435:C:C6      | 2.24        | 0.72     |
| 5:E:71:LEU:O      | 5:E:72:GLN:HG3    | 1.90        | 0.72     |
| 2:B:17:PHE:HD1    | 2:B:44:LEU:HD11   | 1.53        | 0.72     |
| 2:B:69:LEU:HD22   | 2:B:91:PRO:HB2    | 1.71        | 0.72     |
| 8:H:6:ILE:HD12    | 8:H:6:ILE:H       | 1.55        | 0.72     |
| 12:L:28:LYS:HE3   | 12:L:33:ARG:HH12  | 1.53        | 0.72     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 2:B:201:ILE:HG21  | 2:B:214:ILE:HG21  | 1.71        | 0.72     |
| 1:A:601:C:H2'     | 1:A:602:A:C8      | 2.25        | 0.72     |
| 8:H:86:ILE:HG21   | 8:H:133:LEU:HD22  | 1.70        | 0.72     |
| 7:G:147:ALA:C     | 7:G:148:ASN:HD22  | 1.92        | 0.72     |
| 13:M:112:GLY:HA2  | 13:M:113:PRO:HD2  | 1.71        | 0.72     |
| 4:D:68:TYR:CD2    | 4:D:97:LEU:HD22   | 2.24        | 0.72     |
| 1:A:1352:C:H2'    | 1:A:1353:G:C8     | 2.24        | 0.72     |
| 2:B:98:LEU:O      | 2:B:101:MET:HG3   | 1.90        | 0.72     |
| 9:I:13:ALA:HB2    | 9:I:68:GLY:HA3    | 1.71        | 0.72     |
| 1:A:865:A:H5'     | 1:A:1078:U:O4     | 1.89        | 0.71     |
| 2:B:130:ARG:NH2   | 2:B:138:LEU:HD11  | 2.05        | 0.71     |
| 5:E:42:GLY:HA3    | 5:E:66:MET:HG2    | 1.72        | 0.71     |
| 24:Y:326:THR:HG21 | 24:Y:328:LEU:HD22 | 1.71        | 0.71     |
| 24:Y:341:LEU:O    | 24:Y:345:ILE:HG13 | 1.90        | 0.71     |
| 1:A:878:G:C5'     | 8:H:89:PRO:HG2    | 2.20        | 0.71     |
| 1:A:36:C:H4'      | 12:L:122:THR:O    | 1.90        | 0.71     |
| 18:R:31:LEU:CD2   | 18:R:31:LEU:H     | 2.03        | 0.71     |
| 24:Y:88:LYS:HB2   | 24:Y:89:PRO:HD3   | 1.71        | 0.71     |
| 9:I:88:TYR:O      | 9:I:89:ASN:HB2    | 1.90        | 0.71     |
| 1:A:750:G:H1'     | 15:O:23:GLY:H     | 1.56        | 0.71     |
| 13:M:90:LEU:C     | 13:M:92:HIS:H     | 1.93        | 0.71     |
| 1:A:1243:C:H42    | 1:A:1294:G:H22    | 1.37        | 0.71     |
| 4:D:126:ILE:HG22  | 4:D:127:THR:N     | 2.05        | 0.71     |
| 17:Q:57:VAL:HG12  | 17:Q:76:LEU:HA    | 1.73        | 0.71     |
| 24:Y:13:LEU:HA    | 24:Y:16:TYR:HB2   | 1.73        | 0.71     |
| 4:D:64:LEU:HB2    | 4:D:198:VAL:HG11  | 1.73        | 0.71     |
| 9:I:7:THR:HB      | 9:I:83:ARG:NH1    | 2.06        | 0.71     |
| 10:J:27:ALA:HB2   | 10:J:85:LEU:HD11  | 1.72        | 0.71     |
| 2:B:67:THR:HG21   | 2:B:155:LEU:HD11  | 1.72        | 0.71     |
| 1:A:1031:G:H2'    | 1:A:1032:G:O4'    | 1.89        | 0.71     |
| 4:D:14:ARG:HD2    | 4:D:59:ARG:NH1    | 2.06        | 0.71     |
| 3:C:20:SER:HB2    | 3:C:40:ARG:HH22   | 1.54        | 0.71     |
| 24:Y:190:VAL:HB   | 24:Y:315:VAL:HB   | 1.70        | 0.71     |
| 1:A:250:A:H4'     | 1:A:251:G:O5'     | 1.91        | 0.71     |
| 15:O:4:THR:OG1    | 15:O:7:GLU:HB2    | 1.90        | 0.71     |
| 4:D:86:LYS:CE     | 4:D:87:GLY:H      | 1.91        | 0.71     |
| 24:Y:209:GLU:OE2  | 24:Y:303:ARG:NE   | 2.23        | 0.71     |
| 10:J:50:ILE:HD11  | 14:N:41:ARG:NH1   | 2.05        | 0.71     |
| 22:W:38:A:C3'     | 22:W:39:U:H5''    | 2.20        | 0.71     |
| 1:A:650:G:O2'     | 1:A:651:C:H5'     | 1.91        | 0.71     |
| 24:Y:285:GLU:HA   | 24:Y:288:ARG:NH1  | 2.06        | 0.70     |
| 22:W:39:U:C2'     | 22:W:40:C:H5''    | 2.19        | 0.70     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 9:I:95:LYS:HD3    | 9:I:96:LEU:N      | 2.05        | 0.70     |
| 4:D:60:GLU:OE2    | 4:D:198:VAL:HA    | 1.90        | 0.70     |
| 1:A:333:G:H4'     | 20:T:16:HIS:CE1   | 2.26        | 0.70     |
| 7:G:64:GLN:HE21   | 7:G:68:ASN:HD21   | 1.38        | 0.70     |
| 1:A:1314:C:OP2    | 19:S:6:LYS:HG3    | 1.91        | 0.70     |
| 1:A:963:G:N2      | 10:J:55:LYS:HZ2   | 1.89        | 0.70     |
| 4:D:31:CYS:C      | 4:D:33:MET:H      | 1.94        | 0.70     |
| 4:D:32:ALA:O      | 4:D:35:ARG:HG3    | 1.90        | 0.70     |
| 9:I:15:ALA:HA     | 9:I:65:VAL:HA     | 1.73        | 0.70     |
| 2:B:54:THR:HG21   | 2:B:201:ILE:HD11  | 1.73        | 0.70     |
| 1:A:1363(A):A:H4' | 1:A:1364:U:H5''   | 1.72        | 0.70     |
| 24:Y:303:ARG:O    | 24:Y:303:ARG:HG2  | 1.91        | 0.70     |
| 4:D:33:MET:C      | 4:D:35:ARG:H      | 1.93        | 0.70     |
| 1:A:1112:C:O2     | 3:C:179:ARG:HG2   | 1.91        | 0.70     |
| 24:Y:68:ASP:OD2   | 24:Y:94:ALA:HB1   | 1.90        | 0.70     |
| 6:F:86:ARG:O      | 6:F:87:ARG:HG2    | 1.91        | 0.70     |
| 10:J:50:ILE:HA    | 10:J:60:ARG:HB2   | 1.74        | 0.70     |
| 1:A:1256:A:N6     | 1:A:1278:U:H1'    | 2.02        | 0.70     |
| 1:A:1242:C:P      | 21:U:10:ARG:HH22  | 2.15        | 0.70     |
| 8:H:40:ALA:C      | 8:H:42:GLU:H      | 1.94        | 0.70     |
| 24:Y:303:ARG:N    | 24:Y:304:PRO:HD3  | 2.06        | 0.70     |
| 1:A:1134:G:H2'    | 1:A:1135:U:H5'    | 1.73        | 0.70     |
| 1:A:1054:C:O2'    | 1:A:1055:A:H5'    | 1.92        | 0.70     |
| 1:A:328:C:H4'     | 1:A:329:A:H5'     | 1.72        | 0.70     |
| 4:D:128:VAL:O     | 4:D:130:GLY:N     | 2.24        | 0.70     |
| 2:B:185:ILE:CG2   | 2:B:199:TYR:HB2   | 2.22        | 0.70     |
| 2:B:178:ARG:HH11  | 2:B:178:ARG:CB    | 2.05        | 0.70     |
| 1:A:1347:G:H22    | 1:A:1373:G:H2'    | 1.53        | 0.70     |
| 18:R:70:ILE:O     | 18:R:74:ARG:HG3   | 1.91        | 0.70     |
| 10:J:4:ILE:HD12   | 10:J:4:ILE:N      | 2.06        | 0.70     |
| 2:B:46:LYS:HE3    | 2:B:46:LYS:HA     | 1.74        | 0.70     |
| 4:D:49:ARG:NE     | 4:D:49:ARG:HA     | 2.06        | 0.70     |
| 17:Q:59:ILE:CG2   | 17:Q:71:PHE:HB3   | 2.21        | 0.70     |
| 14:N:23:ARG:HD2   | 14:N:28:GLY:O     | 1.92        | 0.70     |
| 13:M:84:ILE:HG13  | 19:S:66:MET:SD    | 2.32        | 0.70     |
| 13:M:3:ARG:NH2    | 13:M:7:VAL:HG22   | 2.07        | 0.70     |
| 2:B:114:ARG:O     | 2:B:118:LEU:HG    | 1.91        | 0.70     |
| 4:D:132:ARG:HH11  | 4:D:132:ARG:HG2   | 1.57        | 0.70     |
| 1:A:1348:U:H4'    | 9:I:120:ARG:HD2   | 1.73        | 0.70     |
| 11:K:80:VAL:HG13  | 11:K:103:LEU:HD11 | 1.72        | 0.70     |
| 10:J:8:LEU:HD23   | 10:J:96:ILE:CG2   | 2.22        | 0.70     |
| 1:A:973:G:O4'     | 10:J:55:LYS:HG3   | 1.92        | 0.70     |

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| Atom-1            | Atom-2           | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 17:Q:59:ILE:HG21  | 17:Q:71:PHE:HB3  | 1.72        | 0.70     |
| 1:A:1241:G:H2'    | 1:A:1242:C:C6    | 2.27        | 0.70     |
| 4:D:129:ASN:HD22  | 4:D:129:ASN:N    | 1.89        | 0.70     |
| 6:F:69:GLU:O      | 6:F:72:VAL:HG12  | 1.91        | 0.70     |
| 16:P:20:VAL:HG23  | 16:P:34:GLU:O    | 1.92        | 0.70     |
| 8:H:90:GLY:O      | 12:L:7:ILE:HG21  | 1.92        | 0.70     |
| 24:Y:141:THR:O    | 24:Y:145:GLU:HG3 | 1.92        | 0.70     |
| 24:Y:312:ARG:HD2  | 24:Y:314:TYR:CZ  | 2.27        | 0.69     |
| 2:B:187:LEU:HD22  | 2:B:201:ILE:O    | 1.92        | 0.69     |
| 1:A:503:C:H2'     | 1:A:504:C:H6     | 1.56        | 0.69     |
| 15:O:16:ALA:HB1   | 15:O:21:ASP:HB3  | 1.73        | 0.69     |
| 24:Y:137:LEU:HD23 | 24:Y:137:LEU:O   | 1.91        | 0.69     |
| 1:A:659:U:O2'     | 1:A:660:G:H5'    | 1.92        | 0.69     |
| 5:E:42:GLY:CA     | 5:E:66:MET:HG2   | 2.22        | 0.69     |
| 1:A:438:G:H4'     | 1:A:439:A:OP1    | 1.92        | 0.69     |
| 1:A:1172:C:H2'    | 1:A:1173:G:H8    | 1.58        | 0.69     |
| 24:Y:135:MET:HB3  | 24:Y:138:ARG:NH1 | 2.07        | 0.69     |
| 13:M:2:ALA:N      | 13:M:9:ILE:HG23  | 2.08        | 0.69     |
| 1:A:67:C:H2'      | 1:A:68:G:H8      | 1.58        | 0.69     |
| 1:A:537:G:H2'     | 1:A:538:G:H8     | 1.57        | 0.69     |
| 1:A:1264:C:H2'    | 1:A:1265:G:C8    | 2.27        | 0.69     |
| 1:A:489:C:H2'     | 1:A:490:G:H8     | 1.57        | 0.69     |
| 7:G:140:ASP:HA    | 7:G:143:ARG:NH1  | 2.07        | 0.69     |
| 24:Y:112:ALA:HA   | 24:Y:177:TYR:CD2 | 2.26        | 0.69     |
| 5:E:102:ALA:HB1   | 5:E:106:PRO:CG   | 2.21        | 0.69     |
| 1:A:390:C:H2'     | 1:A:391:G:C8     | 2.28        | 0.69     |
| 1:A:1355:G:H2'    | 1:A:1356:G:C8    | 2.27        | 0.69     |
| 3:C:123:GLN:O     | 3:C:128:PHE:HB2  | 1.92        | 0.69     |
| 1:A:1255:G:H2'    | 1:A:1255:G:N3    | 2.06        | 0.69     |
| 6:F:12:PRO:HG3    | 6:F:57:GLN:O     | 1.92        | 0.69     |
| 2:B:71:VAL:HB     | 2:B:164:VAL:HG22 | 1.73        | 0.69     |
| 1:A:1126:U:H2'    | 1:A:1127:G:O4'   | 1.92        | 0.69     |
| 1:A:736:C:H2'     | 1:A:737:A:C8     | 2.27        | 0.69     |
| 1:A:1321:C:H3'    | 1:A:1322:C:H5''  | 1.75        | 0.69     |
| 10:J:75:ILE:HG13  | 10:J:76:ASN:H    | 1.58        | 0.69     |
| 24:Y:136:LEU:HD11 | 24:Y:187:HIS:HB2 | 1.73        | 0.69     |
| 1:A:243:A:H4'     | 1:A:244:U:O5'    | 1.91        | 0.69     |
| 1:A:1128:C:C5'    | 9:I:16:ARG:HH12  | 2.06        | 0.69     |
| 1:A:194:C:H2'     | 1:A:195:A:H5''   | 1.75        | 0.69     |
| 2:B:162:ILE:O     | 2:B:185:ILE:HG12 | 1.93        | 0.69     |
| 24:Y:138:ARG:HD2  | 24:Y:142:ARG:NH2 | 2.08        | 0.69     |
| 9:I:102:LEU:HD23  | 9:I:103:THR:N    | 2.07        | 0.69     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 8:H:118:VAL:O     | 8:H:119:LEU:HD23  | 1.92        | 0.69     |
| 6:F:82:ARG:HB2    | 6:F:85:VAL:HG23   | 1.75        | 0.69     |
| 13:M:83:ASP:CG    | 13:M:84:ILE:H     | 1.97        | 0.68     |
| 13:M:120:LYS:HD3  | 13:M:121:LYS:N    | 2.07        | 0.68     |
| 16:P:20:VAL:HG21  | 16:P:32:TYR:CD2   | 2.27        | 0.68     |
| 1:A:262:A:H2'     | 1:A:263:A:C8      | 2.29        | 0.68     |
| 13:M:124:PRO:HB2  | 24:Y:163:GLY:C    | 2.14        | 0.68     |
| 22:W:68:C:H2'     | 22:W:69:G:C8      | 2.25        | 0.68     |
| 10:J:8:LEU:HD23   | 10:J:96:ILE:HG22  | 1.74        | 0.68     |
| 24:Y:141:THR:HG22 | 24:Y:145:GLU:OE2  | 1.93        | 0.68     |
| 2:B:219:VAL:O     | 2:B:223:ILE:HG13  | 1.93        | 0.68     |
| 24:Y:223:LYS:C    | 24:Y:225:GLU:H    | 1.97        | 0.68     |
| 14:N:6:LEU:HD22   | 14:N:23:ARG:NH2   | 2.08        | 0.68     |
| 3:C:53:ALA:HB2    | 3:C:115:LEU:HD21  | 1.74        | 0.68     |
| 1:A:979:C:H3'     | 1:A:980:C:C5'     | 2.20        | 0.68     |
| 10:J:34:VAL:HG22  | 10:J:74:ILE:HG22  | 1.74        | 0.68     |
| 4:D:150:GLU:CD    | 4:D:151:LYS:H     | 1.95        | 0.68     |
| 2:B:77:ALA:O      | 2:B:81:VAL:HG23   | 1.94        | 0.68     |
| 24:Y:237:PRO:O    | 24:Y:242:VAL:HG11 | 1.93        | 0.68     |
| 1:A:192:U:H5'     | 20:T:102:GLY:HA2  | 1.75        | 0.68     |
| 19:S:64:GLU:HG3   | 19:S:65:ASN:H     | 1.58        | 0.68     |
| 24:Y:241:GLY:O    | 24:Y:244:THR:N    | 2.27        | 0.68     |
| 6:F:3:ARG:HG3     | 6:F:3:ARG:HH11    | 1.59        | 0.68     |
| 1:A:1152:A:H2'    | 1:A:1153:C:H6     | 1.57        | 0.68     |
| 7:G:82:GLY:HA2    | 23:X:14:A:N6      | 2.08        | 0.68     |
| 1:A:59:A:C5'      | 1:A:60:A:H5''     | 2.24        | 0.68     |
| 1:A:1012:U:H2'    | 1:A:1013:G:C8     | 2.28        | 0.68     |
| 8:H:30:ARG:HB3    | 8:H:30:ARG:NH1    | 2.09        | 0.68     |
| 6:F:16:GLN:CD     | 6:F:16:GLN:H      | 1.97        | 0.68     |
| 19:S:67:VAL:HG23  | 19:S:68:GLY:H     | 1.58        | 0.68     |
| 4:D:129:ASN:H     | 4:D:129:ASN:ND2   | 1.92        | 0.68     |
| 9:I:28:VAL:HA     | 9:I:63:ILE:O      | 1.94        | 0.68     |
| 19:S:50:ALA:HB1   | 19:S:57:HIS:HB3   | 1.75        | 0.68     |
| 1:A:1240:U:OP2    | 7:G:116:ALA:HB2   | 1.94        | 0.68     |
| 9:I:118:LYS:O     | 9:I:119:ALA:HB3   | 1.94        | 0.68     |
| 4:D:150:GLU:CD    | 4:D:151:LYS:N     | 2.48        | 0.68     |
| 17:Q:9:VAL:HG12   | 17:Q:56:VAL:HG22  | 1.75        | 0.68     |
| 1:A:191:G:H1'     | 20:T:105:SER:HB3  | 1.76        | 0.68     |
| 1:A:1158:C:H2'    | 1:A:1158:C:O2     | 1.94        | 0.68     |
| 4:D:35:ARG:O      | 4:D:37:PRO:HD3    | 1.93        | 0.67     |
| 10:J:6:ILE:O      | 10:J:6:ILE:HD12   | 1.94        | 0.67     |
| 7:G:120:ILE:H     | 7:G:120:ILE:HD12  | 1.59        | 0.67     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:1149:C:H2'    | 1:A:1150:U:C6     | 2.30        | 0.67     |
| 21:U:6:ARG:O      | 21:U:12:LYS:HE3   | 1.94        | 0.67     |
| 1:A:930:C:O2'     | 1:A:931:C:H5'     | 1.94        | 0.67     |
| 22:W:19:G:H8      | 22:W:20:U:H5      | 1.41        | 0.67     |
| 7:G:151:TYR:OH    | 11:K:54:ARG:HD3   | 1.94        | 0.67     |
| 24:Y:120:ILE:HB   | 24:Y:167:ALA:HB3  | 1.76        | 0.67     |
| 3:C:34:LEU:O      | 3:C:38:ARG:HG3    | 1.94        | 0.67     |
| 1:A:1379:G:O6     | 7:G:2:ALA:HB3     | 1.94        | 0.67     |
| 1:A:1388:C:H2'    | 1:A:1389:C:C6     | 2.29        | 0.67     |
| 1:A:1356:G:H2'    | 1:A:1357:A:C8     | 2.28        | 0.67     |
| 1:A:1148:U:H2'    | 1:A:1149:C:O4'    | 1.93        | 0.67     |
| 1:A:1152:A:H5''   | 10:J:13:HIS:CD2   | 2.29        | 0.67     |
| 12:L:28:LYS:HD2   | 12:L:30:ALA:HB2   | 1.76        | 0.67     |
| 6:F:67:MET:HB2    | 6:F:68:PRO:HD2    | 1.77        | 0.67     |
| 3:C:153:VAL:HG22  | 3:C:198:VAL:HG12  | 1.77        | 0.67     |
| 2:B:194:PRO:O     | 2:B:196:LEU:N     | 2.28        | 0.67     |
| 12:L:6:THR:HG23   | 12:L:9:GLN:NE2    | 2.09        | 0.67     |
| 11:K:111:ASP:OD2  | 18:R:84:LYS:HE2   | 1.94        | 0.67     |
| 1:A:473:G:H4'     | 16:P:81:ARG:NH2   | 2.09        | 0.67     |
| 3:C:180:ALA:HB1   | 3:C:203:PHE:CE1   | 2.30        | 0.67     |
| 1:A:59:A:H5''     | 1:A:60:A:H5''     | 1.77        | 0.67     |
| 4:D:127:THR:HG23  | 4:D:147:ALA:HB3   | 1.76        | 0.67     |
| 7:G:73:MET:HG2    | 7:G:90:GLU:HA     | 1.76        | 0.67     |
| 19:S:6:LYS:CG     | 19:S:7:LYS:HE3    | 2.22        | 0.67     |
| 3:C:175:LEU:HD21  | 3:C:201:TYR:CE2   | 2.30        | 0.67     |
| 15:O:78:TYR:O     | 15:O:82:ILE:HG22  | 1.94        | 0.67     |
| 7:G:146:GLU:HG2   | 7:G:149:ARG:NH1   | 2.10        | 0.67     |
| 2:B:17:PHE:CD1    | 2:B:44:LEU:HD11   | 2.30        | 0.67     |
| 10:J:56:HIS:O     | 10:J:58:ASP:N     | 2.27        | 0.67     |
| 22:W:38:A:C2'     | 22:W:39:U:H5''    | 2.25        | 0.67     |
| 8:H:97:VAL:HG21   | 8:H:128:GLY:HA2   | 1.77        | 0.67     |
| 20:T:48:LYS:O     | 20:T:52:ALA:HB2   | 1.95        | 0.67     |
| 24:Y:118:LEU:HD11 | 24:Y:180:LEU:HD22 | 1.77        | 0.66     |
| 1:A:473:G:C4'     | 16:P:81:ARG:HH21  | 2.08        | 0.66     |
| 1:A:475:G:H2'     | 1:A:476:G:H8      | 1.60        | 0.66     |
| 1:A:942:G:H21     | 9:I:124:GLN:NE2   | 1.91        | 0.66     |
| 1:A:444:C:H2'     | 1:A:445:G:H8      | 1.57        | 0.66     |
| 7:G:113:GLU:HG2   | 7:G:119:ARG:HG2   | 1.76        | 0.66     |
| 1:A:750:G:N3      | 15:O:23:GLY:HA3   | 2.09        | 0.66     |
| 1:A:735:C:H2'     | 1:A:736:C:C6      | 2.24        | 0.66     |
| 1:A:1261:A:C2     | 1:A:1275:A:H1'    | 2.31        | 0.66     |
| 1:A:1391:U:H2'    | 1:A:1392:G:C8     | 2.31        | 0.66     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 24:Y:239:GLY:H    | 24:Y:242:VAL:CG1  | 2.08        | 0.66     |
| 16:P:45:THR:HG23  | 16:P:46:PRO:HD2   | 1.76        | 0.66     |
| 2:B:211:ILE:O     | 2:B:215:LEU:HD23  | 1.96        | 0.66     |
| 3:C:73:PRO:HG2    | 3:C:74:GLY:H      | 1.61        | 0.66     |
| 20:T:89:ARG:HD2   | 20:T:104:LEU:HD11 | 1.77        | 0.66     |
| 2:B:187:LEU:HA    | 2:B:201:ILE:HB    | 1.78        | 0.66     |
| 24:Y:119:THR:HG23 | 24:Y:166:TYR:CE1  | 2.31        | 0.66     |
| 1:A:192:U:H4'     | 20:T:103:GLY:N    | 2.10        | 0.66     |
| 2:B:223:ILE:HA    | 2:B:226:ARG:HB3   | 1.78        | 0.66     |
| 1:A:8:A:N6        | 4:D:209:ARG:HB2   | 2.10        | 0.66     |
| 1:A:1141:C:H2'    | 1:A:1142:G:C8     | 2.30        | 0.66     |
| 10:J:26:ALA:HB3   | 10:J:85:LEU:HD21  | 1.78        | 0.66     |
| 13:M:16:ASP:OD2   | 13:M:17:VAL:HG23  | 1.96        | 0.66     |
| 1:A:383:A:C2'     | 1:A:384:G:H5'     | 2.25        | 0.66     |
| 13:M:8:GLU:OE1    | 13:M:22:ILE:HG13  | 1.95        | 0.66     |
| 4:D:121:VAL:HA    | 4:D:126:ILE:HD13  | 1.78        | 0.66     |
| 1:A:620:C:H2'     | 1:A:621:A:O4'     | 1.94        | 0.66     |
| 3:C:89:GLU:O      | 3:C:93:LYS:HB2    | 1.96        | 0.66     |
| 2:B:14:GLY:O      | 2:B:15:VAL:HG13   | 1.95        | 0.66     |
| 24:Y:240:GLN:HA   | 24:Y:243:ASN:ND2  | 2.11        | 0.66     |
| 11:K:21:ILE:HD13  | 11:K:82:VAL:HG13  | 1.77        | 0.66     |
| 13:M:78:ILE:HG23  | 13:M:92:HIS:ND1   | 2.11        | 0.66     |
| 3:C:92:ALA:HB2    | 3:C:99:VAL:HG22   | 1.78        | 0.66     |
| 3:C:43:LEU:O      | 3:C:47:LEU:HB3    | 1.94        | 0.66     |
| 1:A:155:C:H2'     | 1:A:156:G:C8      | 2.30        | 0.66     |
| 18:R:36:ASN:HB3   | 18:R:39:VAL:HG21  | 1.77        | 0.66     |
| 2:B:107:THR:HA    | 2:B:110:GLN:HE21  | 1.59        | 0.66     |
| 24:Y:118:LEU:HD23 | 24:Y:210:VAL:HG22 | 1.76        | 0.66     |
| 3:C:59:ARG:HG2    | 3:C:64:VAL:HA     | 1.78        | 0.66     |
| 9:I:17:VAL:CG1    | 9:I:81:ILE:HD13   | 2.26        | 0.66     |
| 19:S:49:ILE:HD12  | 19:S:71:LEU:HD21  | 1.77        | 0.66     |
| 18:R:36:ASN:HB3   | 18:R:39:VAL:CG2   | 2.26        | 0.66     |
| 1:A:1317:C:OP2    | 14:N:17:LYS:HG2   | 1.96        | 0.66     |
| 19:S:6:LYS:HD2    | 19:S:6:LYS:N      | 2.11        | 0.66     |
| 4:D:17:VAL:O      | 4:D:17:VAL:HG12   | 1.96        | 0.66     |
| 24:Y:19:ILE:O     | 24:Y:23:GLU:HB2   | 1.95        | 0.66     |
| 1:A:32:A:H2'      | 1:A:33:A:C8       | 2.32        | 0.65     |
| 23:X:19:U:C2      | 24:Y:126:GLY:HA3  | 2.31        | 0.65     |
| 15:O:48:LYS:HA    | 15:O:48:LYS:HE2   | 1.77        | 0.65     |
| 1:A:1277:C:H2'    | 1:A:1278:U:H5'    | 1.77        | 0.65     |
| 1:A:939:G:H5''    | 7:G:102:ARG:NH2   | 2.11        | 0.65     |
| 13:M:123:ALA:C    | 24:Y:162:ALA:HA   | 2.16        | 0.65     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 12:L:90:VAL:O     | 12:L:92:ASP:N     | 2.29        | 0.65     |
| 24:Y:295:LEU:HD13 | 24:Y:299:ARG:HH21 | 1.59        | 0.65     |
| 13:M:23:TYR:O     | 13:M:66:LEU:HA    | 1.95        | 0.65     |
| 19:S:40:ILE:HG21  | 19:S:62:ILE:HD11  | 1.79        | 0.65     |
| 1:A:1079:G:H2'    | 1:A:1080:A:C8     | 2.32        | 0.65     |
| 20:T:56:MET:HG3   | 20:T:84:LEU:HD12  | 1.78        | 0.65     |
| 24:Y:129:ALA:HA   | 24:Y:204:SER:HB3  | 1.77        | 0.65     |
| 1:A:1205:U:H1'    | 3:C:195:VAL:HG21  | 1.77        | 0.65     |
| 1:A:805:C:H2'     | 1:A:806:C:H6      | 1.62        | 0.65     |
| 1:A:1260:C:OP1    | 1:A:1284:C:H4'    | 1.97        | 0.65     |
| 4:D:43:HIS:O      | 4:D:45:GLN:N      | 2.29        | 0.65     |
| 3:C:52:LEU:H      | 3:C:52:LEU:HD23   | 1.61        | 0.65     |
| 24:Y:81:ALA:HB3   | 24:Y:84:ARG:HE    | 1.62        | 0.65     |
| 12:L:115:LYS:O    | 12:L:117:ARG:HG3  | 1.97        | 0.65     |
| 24:Y:218:VAL:HG23 | 24:Y:284:TYR:OH   | 1.97        | 0.65     |
| 24:Y:150:GLN:NE2  | 24:Y:172:LYS:NZ   | 2.43        | 0.65     |
| 1:A:1152:A:H2'    | 1:A:1153:C:C6     | 2.32        | 0.65     |
| 1:A:736:C:H2'     | 1:A:737:A:H8      | 1.62        | 0.65     |
| 5:E:101:ILE:HD13  | 5:E:101:ILE:N     | 2.11        | 0.65     |
| 5:E:40:ARG:HG2    | 5:E:40:ARG:HH11   | 1.61        | 0.65     |
| 6:F:97:PHE:HB2    | 18:R:32:ARG:NH1   | 2.11        | 0.65     |
| 1:A:1468:A:H2'    | 1:A:1469:G:O4'    | 1.97        | 0.65     |
| 19:S:24:ALA:O     | 19:S:25:LYS:HB2   | 1.95        | 0.65     |
| 7:G:12:LEU:HD13   | 7:G:25:ALA:HB2    | 1.78        | 0.65     |
| 1:A:272:C:H2'     | 1:A:273:A:H8      | 1.62        | 0.65     |
| 2:B:21:ARG:HB3    | 2:B:39:ILE:HG23   | 1.79        | 0.65     |
| 1:A:1016:A:H2'    | 1:A:1017:G:O4'    | 1.97        | 0.65     |
| 1:A:1249:C:H5'    | 1:A:1249:C:H6     | 1.61        | 0.65     |
| 5:E:105:VAL:H     | 5:E:106:PRO:HD2   | 1.62        | 0.65     |
| 1:A:1127:G:H21    | 1:A:1147:C:H41    | 1.45        | 0.65     |
| 20:T:50:GLU:HA    | 20:T:100:ILE:HG22 | 1.77        | 0.65     |
| 1:A:1030(B):C:H2' | 1:A:1030(C):G:H5' | 1.79        | 0.65     |
| 16:P:51:VAL:HG11  | 16:P:74:LEU:CD2   | 2.27        | 0.65     |
| 10:J:33:GLN:H     | 10:J:75:ILE:HD11  | 1.62        | 0.65     |
| 24:Y:256:THR:HG22 | 24:Y:258:ILE:HG13 | 1.79        | 0.65     |
| 1:A:716:A:N3      | 11:K:118:GLY:HA2  | 2.12        | 0.65     |
| 5:E:110:LEU:O     | 5:E:115:VAL:HB    | 1.97        | 0.65     |
| 24:Y:184:ALA:HA   | 24:Y:208:VAL:O    | 1.98        | 0.65     |
| 22:W:63:G:C2'     | 22:W:64:A:H5'     | 2.26        | 0.65     |
| 1:A:137:C:N4      | 1:A:226:G:H1      | 1.91        | 0.65     |
| 12:L:25:PRO:C     | 12:L:27:LEU:N     | 2.50        | 0.65     |
| 2:B:18:GLY:H      | 2:B:42:ILE:HG22   | 1.61        | 0.65     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 9:I:113:LYS:N    | 9:I:113:LYS:HD2   | 2.12        | 0.65     |
| 1:A:143:A:H2     | 1:A:220:G:H1      | 1.44        | 0.65     |
| 1:A:59:A:H1'     | 1:A:354:G:N2      | 2.11        | 0.64     |
| 16:P:18:ARG:HD3  | 16:P:35:LYS:HE3   | 1.79        | 0.64     |
| 3:C:54:ARG:NH1   | 3:C:56:ASP:HB2    | 2.12        | 0.64     |
| 6:F:98:LEU:HG    | 18:R:30:ASP:HB2   | 1.79        | 0.64     |
| 8:H:83:ILE:HD13  | 8:H:137:VAL:HG13  | 1.79        | 0.64     |
| 1:A:834:C:H2'    | 1:A:835:U:C6      | 2.32        | 0.64     |
| 1:A:757:U:H2'    | 1:A:758:G:O4'     | 1.97        | 0.64     |
| 10:J:23:ILE:HG23 | 10:J:85:LEU:HD13  | 1.79        | 0.64     |
| 21:U:2:GLY:O     | 21:U:4:GLY:N      | 2.28        | 0.64     |
| 24:Y:81:ALA:HB1  | 24:Y:84:ARG:NH2   | 2.10        | 0.64     |
| 1:A:491:G:H2'    | 1:A:492:G:C8      | 2.31        | 0.64     |
| 3:C:54:ARG:HH12  | 3:C:56:ASP:HB2    | 1.63        | 0.64     |
| 1:A:1312:G:H1    | 1:A:1325:C:H42    | 1.44        | 0.64     |
| 2:B:136:VAL:O    | 2:B:140:HIS:HB2   | 1.97        | 0.64     |
| 1:A:123:C:OP1    | 1:A:312:C:H5'     | 1.98        | 0.64     |
| 6:F:60:PHE:C     | 6:F:61:LEU:HD12   | 2.17        | 0.64     |
| 13:M:115:LYS:O   | 13:M:117:VAL:N    | 2.30        | 0.64     |
| 15:O:37:ASN:HD22 | 15:O:37:ASN:N     | 1.94        | 0.64     |
| 1:A:973:G:H1'    | 10:J:55:LYS:HE2   | 1.80        | 0.64     |
| 24:Y:115:ASN:HB3 | 24:Y:172:LYS:HA   | 1.78        | 0.64     |
| 1:A:1372:U:H5''  | 9:I:71:SER:HB3    | 1.79        | 0.64     |
| 6:F:14:LEU:HB3   | 6:F:18:GLN:HE21   | 1.63        | 0.64     |
| 1:A:617:G:H4'    | 16:P:44:THR:O     | 1.96        | 0.64     |
| 1:A:186:C:H2'    | 1:A:187:C:H6      | 1.62        | 0.64     |
| 10:J:50:ILE:HD13 | 10:J:50:ILE:N     | 2.07        | 0.64     |
| 3:C:9:GLY:HA2    | 3:C:12:LEU:HG     | 1.79        | 0.64     |
| 11:K:107:SER:C   | 11:K:108:ILE:HD12 | 2.18        | 0.64     |
| 16:P:48:TRP:O    | 16:P:49:LEU:HB2   | 1.98        | 0.64     |
| 5:E:101:ILE:H    | 5:E:101:ILE:HD13  | 1.62        | 0.64     |
| 18:R:66:LEU:HG   | 18:R:70:ILE:HD11  | 1.78        | 0.64     |
| 13:M:67:GLU:CD   | 13:M:68:GLY:H     | 2.00        | 0.64     |
| 1:A:1062:U:H2'   | 1:A:1063:C:C6     | 2.33        | 0.64     |
| 4:D:92:VAL:O     | 4:D:96:LEU:HD13   | 1.97        | 0.64     |
| 4:D:175:SER:HB3  | 4:D:186:LEU:HD11  | 1.77        | 0.64     |
| 24:Y:81:ALA:CB   | 24:Y:84:ARG:HE    | 2.11        | 0.64     |
| 7:G:111:ARG:HB3  | 7:G:113:GLU:OE2   | 1.97        | 0.64     |
| 1:A:539:A:OP2    | 12:L:115:LYS:HE3  | 1.97        | 0.64     |
| 1:A:853:G:H2'    | 1:A:854:G:H8      | 1.63        | 0.64     |
| 1:A:723:U:H5''   | 1:A:724:G:OP2     | 1.98        | 0.64     |
| 13:M:19:LEU:H    | 13:M:19:LEU:HD22  | 1.62        | 0.64     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 19:S:64:GLU:HG3   | 19:S:65:ASN:OD1   | 1.97        | 0.64     |
| 20:T:30:LYS:HE3   | 20:T:30:LYS:O     | 1.97        | 0.64     |
| 2:B:172:ILE:H     | 2:B:172:ILE:CD1   | 1.97        | 0.64     |
| 1:A:961:U:O2'     | 1:A:962:C:H5'     | 1.97        | 0.64     |
| 1:A:1128:C:H5''   | 9:I:16:ARG:HH12   | 1.61        | 0.64     |
| 24:Y:72:LEU:HD13  | 24:Y:91:LEU:HG    | 1.80        | 0.64     |
| 16:P:72:ARG:HH21  | 16:P:73:LEU:HD21  | 1.62        | 0.64     |
| 1:A:537:G:H2'     | 1:A:538:G:C8      | 2.32        | 0.64     |
| 1:A:1095:U:H2'    | 1:A:1096:C:C6     | 2.33        | 0.64     |
| 5:E:93:PRO:HG2    | 8:H:105:ARG:HH21  | 1.62        | 0.64     |
| 4:D:129:ASN:ND2   | 4:D:145:GLU:H     | 1.96        | 0.64     |
| 4:D:28:SER:HB2    | 4:D:30:LYS:HE2    | 1.78        | 0.64     |
| 4:D:28:SER:CB     | 4:D:30:LYS:HE2    | 2.26        | 0.64     |
| 1:A:1116:C:C3'    | 1:A:1117:G:H5''   | 2.27        | 0.64     |
| 1:A:1243:C:N4     | 1:A:1294:G:H22    | 1.96        | 0.64     |
| 1:A:403:C:H2'     | 1:A:404:U:H6      | 1.63        | 0.64     |
| 10:J:75:ILE:HG13  | 10:J:76:ASN:N     | 2.13        | 0.64     |
| 1:A:359:U:H2'     | 1:A:360:A:C8      | 2.33        | 0.64     |
| 3:C:6:HIS:CD2     | 3:C:7:PRO:HD2     | 2.28        | 0.64     |
| 1:A:1510:U:H2'    | 1:A:1511:G:C8     | 2.33        | 0.64     |
| 1:A:984:C:H2'     | 1:A:985:C:C6      | 2.32        | 0.64     |
| 4:D:18:LYS:HB2    | 4:D:33:MET:CG     | 2.23        | 0.64     |
| 11:K:82:VAL:HB    | 11:K:108:ILE:HG13 | 1.80        | 0.64     |
| 5:E:41:VAL:CG2    | 5:E:113:ALA:HA    | 2.28        | 0.64     |
| 12:L:89:ARG:HB2   | 12:L:89:ARG:HH11  | 1.62        | 0.64     |
| 24:Y:138:ARG:HH22 | 24:Y:337:LEU:CD1  | 2.11        | 0.64     |
| 1:A:489:C:H2'     | 1:A:490:G:C8      | 2.33        | 0.64     |
| 19:S:20:LEU:HA    | 19:S:23:ASN:ND2   | 2.13        | 0.64     |
| 5:E:33:VAL:HG11   | 5:E:109:ILE:HA    | 1.80        | 0.64     |
| 20:T:89:ARG:NH2   | 20:T:104:LEU:HD21 | 2.13        | 0.63     |
| 1:A:1288:A:N1     | 1:A:1371:G:H1'    | 2.13        | 0.63     |
| 1:A:1015:A:H2'    | 1:A:1016:A:C8     | 2.34        | 0.63     |
| 24:Y:224:PRO:HA   | 24:Y:227:LEU:HB2  | 1.80        | 0.63     |
| 1:A:1277:C:C2'    | 1:A:1278:U:H5'    | 2.29        | 0.63     |
| 4:D:112:VAL:HG12  | 4:D:116:GLN:CD    | 2.18        | 0.63     |
| 1:A:1325:C:H5'    | 21:U:15:ARG:HE    | 1.63        | 0.63     |
| 1:A:359:U:H2'     | 1:A:360:A:H8      | 1.63        | 0.63     |
| 24:Y:227:LEU:HD11 | 24:Y:276:LEU:CD2  | 2.28        | 0.63     |
| 11:K:27:ASN:OD1   | 11:K:55:LYS:HB3   | 1.98        | 0.63     |
| 11:K:15:ALA:HA    | 11:K:76:GLY:O     | 1.98        | 0.63     |
| 8:H:51:VAL:HG11   | 8:H:60:ARG:HB2    | 1.80        | 0.63     |
| 24:Y:117:ILE:HB   | 24:Y:211:ILE:HG13 | 1.78        | 0.63     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 11:K:21:ILE:HD12 | 11:K:21:ILE:N    | 2.13        | 0.63     |
| 7:G:78:ARG:HG2   | 7:G:79:ARG:H     | 1.62        | 0.63     |
| 5:E:137:GLU:HG3  | 5:E:141:GLN:NE2  | 2.14        | 0.63     |
| 10:J:61:GLU:HG2  | 14:N:58:LYS:HE2  | 1.81        | 0.63     |
| 15:O:27:VAL:O    | 15:O:31:LEU:HD23 | 1.98        | 0.63     |
| 1:A:834:C:H2'    | 1:A:835:U:H6     | 1.62        | 0.63     |
| 1:A:828:A:H2'    | 1:A:829:G:O4'    | 1.98        | 0.63     |
| 1:A:460:G:O6     | 1:A:470:C:H5''   | 1.98        | 0.63     |
| 4:D:14:ARG:HA    | 4:D:39:PRO:HB3   | 1.81        | 0.63     |
| 17:Q:7:THR:CG2   | 17:Q:58:GLU:HG2  | 2.28        | 0.63     |
| 21:U:9:ARG:NH1   | 21:U:9:ARG:HA    | 2.13        | 0.63     |
| 12:L:23:LYS:O    | 12:L:24:VAL:HG23 | 1.98        | 0.63     |
| 1:A:1258:G:H2'   | 1:A:1259:C:C6    | 2.34        | 0.63     |
| 1:A:1259:C:H42   | 1:A:1276:G:H1    | 1.45        | 0.63     |
| 1:A:189(K):U:H2' | 1:A:189(L):G:C8  | 2.33        | 0.63     |
| 24:Y:287:GLU:CA  | 24:Y:290:LYS:HE3 | 2.24        | 0.63     |
| 1:A:1026:G:H3'   | 1:A:1027:C:C5'   | 2.29        | 0.63     |
| 1:A:538:G:OP2    | 12:L:115:LYS:HG3 | 1.98        | 0.63     |
| 1:A:1488:G:O2'   | 1:A:1489:G:H5'   | 1.98        | 0.63     |
| 17:Q:26:GLN:O    | 17:Q:27:PHE:HB3  | 1.98        | 0.63     |
| 19:S:5:LEU:HD13  | 19:S:6:LYS:H     | 1.64        | 0.63     |
| 10:J:50:ILE:HA   | 10:J:60:ARG:CB   | 2.28        | 0.63     |
| 17:Q:27:PHE:CE1  | 17:Q:36:ILE:HD11 | 2.34        | 0.63     |
| 8:H:103:VAL:HG21 | 8:H:110:ALA:HB2  | 1.79        | 0.63     |
| 6:F:75:LEU:O     | 6:F:79:LEU:HG    | 1.99        | 0.63     |
| 3:C:52:LEU:HD23  | 3:C:52:LEU:N     | 2.13        | 0.63     |
| 1:A:1055:A:H2    | 3:C:194:GLY:HA2  | 1.64        | 0.63     |
| 10:J:6:ILE:O     | 10:J:71:LEU:HD12 | 1.99        | 0.63     |
| 10:J:96:ILE:HD13 | 10:J:96:ILE:N    | 2.14        | 0.63     |
| 14:N:26:ARG:HG3  | 14:N:39:LEU:HD22 | 1.79        | 0.63     |
| 2:B:112:VAL:C    | 2:B:114:ARG:H    | 2.01        | 0.63     |
| 1:A:519:C:H2'    | 1:A:520:A:H8     | 1.63        | 0.63     |
| 6:F:88:VAL:O     | 6:F:88:VAL:HG12  | 1.98        | 0.63     |
| 24:Y:97:LYS:C    | 24:Y:99:ASP:H    | 2.00        | 0.63     |
| 1:A:651:C:O2'    | 1:A:652:U:H5'    | 1.99        | 0.62     |
| 16:P:15:PRO:HB2  | 16:P:41:PRO:HG3  | 1.81        | 0.62     |
| 1:A:1425:U:H2'   | 1:A:1426:C:C6    | 2.33        | 0.62     |
| 1:A:1071:C:H2'   | 1:A:1072:G:H8    | 1.64        | 0.62     |
| 13:M:111:LYS:O   | 13:M:113:PRO:HD2 | 1.99        | 0.62     |
| 16:P:20:VAL:HG21 | 16:P:32:TYR:CG   | 2.34        | 0.62     |
| 5:E:137:GLU:HG3  | 5:E:141:GLN:HE21 | 1.64        | 0.62     |
| 9:I:56:LEU:O     | 9:I:56:LEU:HD23  | 1.99        | 0.62     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:1227:A:OP2   | 13:M:111:LYS:HE2  | 1.99        | 0.62     |
| 24:Y:122:PRO:HG3 | 24:Y:164:ILE:O    | 1.99        | 0.62     |
| 19:S:40:ILE:HD13 | 19:S:62:ILE:HD13  | 1.80        | 0.62     |
| 1:A:503:C:H2'    | 1:A:504:C:C6      | 2.35        | 0.62     |
| 3:C:91:LEU:HB3   | 3:C:99:VAL:HG11   | 1.81        | 0.62     |
| 2:B:213:LEU:HD23 | 2:B:213:LEU:O     | 1.99        | 0.62     |
| 1:A:1052:U:H5'   | 24:Y:319:ASN:ND2  | 2.15        | 0.62     |
| 24:Y:117:ILE:O   | 24:Y:210:VAL:HA   | 1.99        | 0.62     |
| 4:D:9:CYS:SG     | 4:D:31:CYS:O      | 2.58        | 0.62     |
| 2:B:32:ILE:HD12  | 2:B:40:HIS:CD2    | 2.35        | 0.62     |
| 1:A:775:G:O2'    | 1:A:776:G:H5'     | 1.99        | 0.62     |
| 13:M:34:LEU:HD13 | 13:M:41:PRO:HG3   | 1.81        | 0.62     |
| 24:Y:180:LEU:O   | 24:Y:210:VAL:HG11 | 2.00        | 0.62     |
| 1:A:1054:C:H3'   | 1:A:1054:C:O2     | 1.99        | 0.62     |
| 24:Y:135:MET:O   | 24:Y:138:ARG:HG2  | 1.98        | 0.62     |
| 1:A:833:U:H2'    | 1:A:834:C:C6      | 2.34        | 0.62     |
| 4:D:88:VAL:O     | 4:D:92:VAL:HG23   | 1.99        | 0.62     |
| 7:G:87:VAL:HG11  | 7:G:154:TYR:O     | 2.00        | 0.62     |
| 1:A:114:U:H2'    | 1:A:115:G:C8      | 2.34        | 0.62     |
| 1:A:1128:C:H1'   | 1:A:1146:A:N6     | 2.10        | 0.62     |
| 3:C:71:ALA:CB    | 3:C:106:VAL:HB    | 2.29        | 0.62     |
| 19:S:18:LYS:O    | 19:S:21:GLU:HG2   | 1.98        | 0.62     |
| 1:A:328:C:H4'    | 1:A:329:A:C5'     | 2.29        | 0.62     |
| 1:A:950:U:H2'    | 1:A:951:G:H8      | 1.64        | 0.62     |
| 1:A:639:G:H2'    | 1:A:640:A:H8      | 1.64        | 0.62     |
| 3:C:11:ARG:HB3   | 3:C:15:THR:HB     | 1.82        | 0.62     |
| 1:A:457:C:H2'    | 1:A:458:C:C6      | 2.35        | 0.62     |
| 19:S:29:ARG:N    | 19:S:29:ARG:HD2   | 2.15        | 0.62     |
| 4:D:18:LYS:HG3   | 4:D:31:CYS:SG     | 2.40        | 0.62     |
| 1:A:191:G:C4     | 20:T:105:SER:HB3  | 2.34        | 0.62     |
| 17:Q:45:HIS:HB2  | 17:Q:65:ILE:HD13  | 1.81        | 0.62     |
| 19:S:40:ILE:HD11 | 19:S:71:LEU:HD23  | 1.80        | 0.62     |
| 6:F:79:LEU:HD12  | 6:F:88:VAL:CG1    | 2.30        | 0.62     |
| 4:D:3:ARG:NH2    | 4:D:118:ARG:HD3   | 2.15        | 0.62     |
| 1:A:1081:G:H5''  | 5:E:18:ARG:HD3    | 1.80        | 0.62     |
| 1:A:556:C:O2'    | 1:A:557:G:H5'     | 1.99        | 0.62     |
| 4:D:129:ASN:N    | 4:D:129:ASN:ND2   | 2.47        | 0.62     |
| 1:A:1319:A:OP2   | 19:S:5:LEU:HD23   | 1.99        | 0.62     |
| 24:Y:241:GLY:O   | 24:Y:242:VAL:C    | 2.38        | 0.62     |
| 11:K:21:ILE:CD1  | 11:K:82:VAL:HG13  | 2.30        | 0.62     |
| 11:K:110:ASP:O   | 18:R:84:LYS:HD2   | 1.99        | 0.62     |
| 3:C:51:GLY:O     | 3:C:53:ALA:N      | 2.33        | 0.62     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:383:A:H2'    | 1:A:384:G:H5'    | 1.81        | 0.62     |
| 4:D:106:TYR:CD1  | 4:D:113:SER:HA   | 2.35        | 0.62     |
| 1:A:457:C:H2'    | 1:A:458:C:H6     | 1.65        | 0.61     |
| 24:Y:55:LEU:HA   | 24:Y:58:THR:OG1  | 2.00        | 0.61     |
| 3:C:173:VAL:O    | 3:C:175:LEU:HD12 | 2.00        | 0.61     |
| 1:A:15:G:H2'     | 1:A:16:A:H8      | 1.65        | 0.61     |
| 13:M:115:LYS:C   | 13:M:117:VAL:H   | 2.03        | 0.61     |
| 1:A:221:C:H2'    | 1:A:222:U:H6     | 1.65        | 0.61     |
| 21:U:25:LYS:HG2  | 21:U:26:LYS:N    | 2.15        | 0.61     |
| 22:V:12:U:H3     | 22:V:23:A:H61    | 1.47        | 0.61     |
| 24:Y:234:ALA:HB2 | 24:Y:247:SER:OG  | 2.00        | 0.61     |
| 2:B:164:VAL:O    | 2:B:186:ALA:HB1  | 2.00        | 0.61     |
| 9:I:40:LEU:O     | 9:I:42:ARG:N     | 2.27        | 0.61     |
| 1:A:393:A:O2'    | 1:A:394:G:H5'    | 2.00        | 0.61     |
| 2:B:44:LEU:N     | 2:B:44:LEU:HD12  | 2.15        | 0.61     |
| 2:B:24:TRP:CZ3   | 2:B:26:PRO:HA    | 2.35        | 0.61     |
| 1:A:148:G:H2'    | 1:A:149:A:H8     | 1.64        | 0.61     |
| 22:W:19:G:H4'    | 22:W:57:G:H22    | 1.64        | 0.61     |
| 22:W:55:U:H2'    | 22:W:56:C:C5     | 2.36        | 0.61     |
| 6:F:3:ARG:HB3    | 6:F:93:SER:HB2   | 1.81        | 0.61     |
| 1:A:1029:C:H4'   | 1:A:1033:G:N2    | 2.16        | 0.61     |
| 1:A:539:A:H2'    | 1:A:540:G:C8     | 2.34        | 0.61     |
| 1:A:155:C:H2'    | 1:A:156:G:H8     | 1.66        | 0.61     |
| 8:H:20:TYR:HA    | 8:H:65:TYR:CE2   | 2.35        | 0.61     |
| 24:Y:241:GLY:C   | 24:Y:243:ASN:N   | 2.51        | 0.61     |
| 14:N:29:ARG:HG2  | 14:N:40:CYS:HB2  | 1.82        | 0.61     |
| 1:A:67:C:O2'     | 1:A:171:A:H1'    | 2.00        | 0.61     |
| 3:C:155:GLY:O    | 3:C:156:ARG:HB2  | 1.99        | 0.61     |
| 2:B:88:ALA:HB2   | 2:B:219:VAL:HG13 | 1.83        | 0.61     |
| 21:U:6:ARG:NE    | 21:U:15:ARG:HH12 | 1.98        | 0.61     |
| 1:A:533:A:H1'    | 1:A:534:U:OP1    | 2.00        | 0.61     |
| 1:A:1486:G:H2'   | 1:A:1487:G:O4'   | 2.00        | 0.61     |
| 13:M:88:ARG:HA   | 13:M:98:VAL:CG1  | 2.22        | 0.61     |
| 5:E:6:PHE:HB2    | 5:E:34:VAL:CG2   | 2.31        | 0.61     |
| 12:L:60:LEU:C    | 12:L:62:SER:H    | 2.03        | 0.61     |
| 1:A:1321:C:H5'   | 1:A:1322:C:C5'   | 2.30        | 0.61     |
| 10:J:37:PRO:HA   | 10:J:72:VAL:HG22 | 1.82        | 0.61     |
| 6:F:8:ILE:HG22   | 6:F:9:VAL:N      | 2.15        | 0.61     |
| 1:A:397:A:N3     | 1:A:397:A:H3'    | 2.15        | 0.61     |
| 7:G:131:LYS:O    | 7:G:131:LYS:HG3  | 2.01        | 0.61     |
| 22:W:61:C:H2'    | 22:W:62:C:C6     | 2.36        | 0.61     |
| 3:C:104:GLN:CD   | 3:C:105:GLU:H    | 2.04        | 0.61     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 12:L:18:VAL:HG23  | 12:L:19:ARG:N     | 2.13        | 0.61     |
| 12:L:25:PRO:O     | 12:L:27:LEU:N     | 2.33        | 0.61     |
| 10:J:26:ALA:CA    | 10:J:29:ARG:HH12  | 2.13        | 0.61     |
| 1:A:538:G:O3'     | 12:L:114:LYS:HD2  | 2.00        | 0.61     |
| 1:A:1442(A):G:C3' | 1:A:1442(B):A:H5' | 2.31        | 0.61     |
| 15:O:8:LYS:O      | 15:O:12:ILE:HG13  | 2.01        | 0.61     |
| 9:I:50:LEU:O      | 9:I:53:VAL:HG22   | 2.01        | 0.61     |
| 1:A:522:C:H42     | 1:A:528:C:H42     | 1.48        | 0.61     |
| 1:A:1220:G:H2'    | 1:A:1221:G:H8     | 1.64        | 0.61     |
| 24:Y:153:VAL:HG13 | 24:Y:153:VAL:O    | 2.01        | 0.61     |
| 4:D:14:ARG:HB2    | 4:D:40:PRO:HD2    | 1.83        | 0.61     |
| 1:A:1294:G:H2'    | 1:A:1295:G:C8     | 2.34        | 0.61     |
| 8:H:11:THR:HG23   | 8:H:14:ARG:HH12   | 1.65        | 0.61     |
| 11:K:58:PRO:HD3   | 11:K:89:ALA:HB1   | 1.83        | 0.61     |
| 1:A:136:C:H4'     | 16:P:1:MET:HE2    | 1.82        | 0.61     |
| 8:H:6:ILE:CD1     | 8:H:6:ILE:H       | 2.14        | 0.61     |
| 1:A:221:C:H2'     | 1:A:222:U:C6      | 2.36        | 0.61     |
| 1:A:100:C:H2'     | 1:A:101:A:C8      | 2.36        | 0.61     |
| 1:A:69:G:H2'      | 1:A:70:G:H8       | 1.66        | 0.61     |
| 5:E:55:VAL:O      | 5:E:58:ALA:HB3    | 2.00        | 0.60     |
| 10:J:38:ILE:HG13  | 10:J:71:LEU:HB3   | 1.83        | 0.60     |
| 1:A:1112:C:C4     | 3:C:178:LEU:HD23  | 2.36        | 0.60     |
| 1:A:1030(D):A:H2' | 1:A:1031:G:H5'    | 1.83        | 0.60     |
| 2:B:132:LYS:HG3   | 2:B:135:GLN:NE2   | 2.15        | 0.60     |
| 4:D:109:GLY:O     | 4:D:111:ALA:N     | 2.34        | 0.60     |
| 24:Y:137:LEU:HD12 | 24:Y:167:ALA:HB1  | 1.82        | 0.60     |
| 5:E:76:ILE:HD11   | 5:E:142:LEU:CD2   | 2.28        | 0.60     |
| 16:P:74:LEU:O     | 16:P:79:VAL:HG23  | 2.01        | 0.60     |
| 10:J:6:ILE:HG22   | 10:J:98:ILE:CG1   | 2.30        | 0.60     |
| 4:D:117:ALA:O     | 4:D:121:VAL:HG23  | 2.00        | 0.60     |
| 1:A:1325:C:H4'    | 21:U:17:THR:HG21  | 1.81        | 0.60     |
| 20:T:79:ARG:HA    | 20:T:82:SER:OG    | 2.01        | 0.60     |
| 20:T:82:SER:O     | 20:T:86:ARG:HB2   | 2.01        | 0.60     |
| 4:D:30:LYS:HB3    | 4:D:35:ARG:CZ     | 2.31        | 0.60     |
| 1:A:137:C:H1'     | 16:P:63:GLY:HA3   | 1.84        | 0.60     |
| 9:I:43:ALA:HA     | 9:I:74:ILE:HG21   | 1.82        | 0.60     |
| 18:R:52:PRO:O     | 18:R:56:THR:HG23  | 2.01        | 0.60     |
| 2:B:18:GLY:HA2    | 2:B:42:ILE:HG22   | 1.83        | 0.60     |
| 8:H:40:ALA:O      | 8:H:42:GLU:N      | 2.35        | 0.60     |
| 1:A:1346:A:N1     | 1:A:1374:A:H5''   | 2.16        | 0.60     |
| 1:A:180:U:H2'     | 1:A:181:G:H5''    | 1.83        | 0.60     |
| 12:L:82:VAL:HG23  | 12:L:106:ASP:OD2  | 2.01        | 0.60     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 22:V:40:C:H2'    | 22:V:41:C:H6      | 1.65        | 0.60     |
| 1:A:923:A:OP1    | 5:E:21:ALA:HB2    | 2.02        | 0.60     |
| 22:V:1:G:H2'     | 22:V:2:C:C6       | 2.35        | 0.60     |
| 1:A:1439:C:H5'   | 20:T:38:LYS:HZ1   | 1.66        | 0.60     |
| 1:A:543:C:H2'    | 1:A:544:G:H8      | 1.66        | 0.60     |
| 4:D:22:LYS:HG3   | 4:D:26:CYS:SG     | 2.41        | 0.60     |
| 10:J:38:ILE:HG12 | 10:J:71:LEU:O     | 2.00        | 0.60     |
| 24:Y:135:MET:HB3 | 24:Y:138:ARG:HH12 | 1.65        | 0.60     |
| 10:J:63:PHE:HA   | 14:N:59:ALA:H     | 1.66        | 0.60     |
| 6:F:7:ASN:HD21   | 18:R:34:TYR:HE1   | 1.49        | 0.60     |
| 1:A:1498:U:C5    | 23:X:17:U:H5'     | 2.36        | 0.60     |
| 24:Y:326:THR:HB  | 24:Y:347:ALA:HB1  | 1.83        | 0.60     |
| 13:M:89:GLY:O    | 13:M:93:ARG:HD2   | 2.02        | 0.60     |
| 9:I:40:LEU:C     | 9:I:42:ARG:H      | 2.05        | 0.60     |
| 24:Y:26:LEU:HB2  | 24:Y:55:LEU:HD11  | 1.83        | 0.60     |
| 1:A:254:G:OP1    | 17:Q:67:LYS:O     | 2.19        | 0.60     |
| 1:A:1053:G:N7    | 1:A:1200:C:H5''   | 2.16        | 0.60     |
| 1:A:1291:G:H4'   | 9:I:38:GLN:O      | 2.01        | 0.60     |
| 2:B:165:VAL:HG23 | 2:B:166:ASP:N     | 2.14        | 0.60     |
| 1:A:413:G:H1'    | 1:A:428:G:N2      | 2.16        | 0.60     |
| 4:D:13:ARG:O     | 4:D:15:GLU:N      | 2.32        | 0.60     |
| 1:A:519:C:H2'    | 1:A:520:A:C8      | 2.36        | 0.60     |
| 22:V:77:PHA:N    | 22:V:77:PHA:CD2   | 2.64        | 0.60     |
| 7:G:148:ASN:C    | 7:G:150:ALA:H     | 2.04        | 0.60     |
| 4:D:127:THR:HA   | 4:D:132:ARG:HA    | 1.82        | 0.60     |
| 1:A:1188:A:H2'   | 1:A:1189:C:O4'    | 2.02        | 0.60     |
| 1:A:1007:C:H2'   | 1:A:1008:C:C6     | 2.36        | 0.60     |
| 24:Y:239:GLY:O   | 24:Y:243:ASN:ND2  | 2.35        | 0.60     |
| 1:A:1201:A:H1'   | 1:A:1202:G:OP2    | 2.02        | 0.60     |
| 4:D:26:CYS:HA    | 4:D:31:CYS:HA     | 1.84        | 0.60     |
| 16:P:49:LEU:HD12 | 16:P:50:LYS:H     | 1.66        | 0.60     |
| 10:J:5:ARG:HA    | 10:J:73:ASP:OD1   | 2.01        | 0.60     |
| 1:A:430:A:OP2    | 4:D:8:VAL:HG22    | 2.01        | 0.60     |
| 17:Q:82:MET:O    | 17:Q:86:GLU:HG2   | 2.01        | 0.60     |
| 1:A:1026:G:H3'   | 1:A:1027:C:H5'    | 1.84        | 0.60     |
| 17:Q:67:LYS:HA   | 17:Q:70:ARG:HH12  | 1.66        | 0.60     |
| 1:A:999:C:O2'    | 1:A:1000:U:H5'    | 2.01        | 0.60     |
| 1:A:684:A:H2'    | 1:A:685:G:C8      | 2.37        | 0.60     |
| 1:A:1269:A:H5'   | 21:U:18:TYR:O     | 2.02        | 0.60     |
| 1:A:69:G:H2'     | 1:A:70:G:C8       | 2.36        | 0.60     |
| 20:T:23:ARG:O    | 20:T:27:LYS:HB2   | 2.01        | 0.60     |
| 24:Y:6:LEU:C     | 24:Y:8:GLN:H      | 2.04        | 0.60     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 22:V:73:A:N3      | 22:V:73:A:H5'     | 2.16        | 0.60     |
| 7:G:78:ARG:HG2    | 7:G:79:ARG:N      | 2.16        | 0.60     |
| 13:M:13:LYS:HA    | 13:M:44:ARG:HH11  | 1.65        | 0.60     |
| 1:A:402:G:O2'     | 1:A:403:C:H5'     | 2.01        | 0.60     |
| 8:H:20:TYR:HE2    | 8:H:75:ARG:HD2    | 1.66        | 0.60     |
| 4:D:173:TRP:CZ3   | 4:D:193:ASP:HB3   | 2.37        | 0.60     |
| 13:M:108:ARG:N    | 13:M:108:ARG:HD2  | 2.17        | 0.59     |
| 13:M:123:ALA:HB1  | 24:Y:162:ALA:HB2  | 1.82        | 0.59     |
| 4:D:13:ARG:NH1    | 4:D:38:TYR:O      | 2.34        | 0.59     |
| 19:S:19:VAL:O     | 19:S:22:LEU:HB2   | 2.02        | 0.59     |
| 3:C:73:PRO:O      | 3:C:76:VAL:HG13   | 2.02        | 0.59     |
| 1:A:433:C:H2'     | 1:A:434:U:C6      | 2.37        | 0.59     |
| 1:A:1438:G:H2'    | 1:A:1439:C:C6     | 2.37        | 0.59     |
| 1:A:373:A:O2'     | 1:A:374:A:H5'     | 2.01        | 0.59     |
| 24:Y:214:VAL:HG13 | 24:Y:215:ASP:N    | 2.17        | 0.59     |
| 24:Y:196:ASP:OD1  | 24:Y:200:ARG:HB2  | 2.02        | 0.59     |
| 1:A:590:C:H2'     | 1:A:591:U:C6      | 2.33        | 0.59     |
| 1:A:1137:C:H4'    | 1:A:1138:G:N2     | 2.17        | 0.59     |
| 17:Q:76:LEU:HD12  | 17:Q:77:VAL:H     | 1.66        | 0.59     |
| 2:B:8:LYS:HD3     | 2:B:217:ARG:NH1   | 2.17        | 0.59     |
| 24:Y:128:GLU:HG2  | 24:Y:204:SER:OG   | 2.03        | 0.59     |
| 1:A:1442(A):G:H3' | 1:A:1442(B):A:H5' | 1.84        | 0.59     |
| 7:G:36:LYS:HB2    | 7:G:36:LYS:NZ     | 2.17        | 0.59     |
| 1:A:194:C:C2'     | 1:A:195:A:H5''    | 2.31        | 0.59     |
| 3:C:70:VAL:O      | 3:C:105:GLU:HA    | 2.02        | 0.59     |
| 16:P:43:LYS:HA    | 16:P:48:TRP:HB3   | 1.84        | 0.59     |
| 3:C:75:VAL:O      | 3:C:83:ARG:HG2    | 2.02        | 0.59     |
| 10:J:16:LEU:HD23  | 10:J:94:VAL:CG1   | 2.31        | 0.59     |
| 7:G:129:GLU:OE2   | 7:G:131:LYS:HE2   | 2.02        | 0.59     |
| 1:A:1285:A:H1'    | 1:A:1286:A:OP2    | 2.01        | 0.59     |
| 1:A:16:A:O2'      | 1:A:17:U:H5'      | 2.02        | 0.59     |
| 3:C:36:ASP:HB3    | 3:C:40:ARG:NH1    | 2.15        | 0.59     |
| 22:V:20:U:H5'     | 22:V:21:A:OP2     | 2.03        | 0.59     |
| 1:A:377:G:OP1     | 16:P:3:LYS:HD2    | 2.01        | 0.59     |
| 4:D:126:ILE:N     | 4:D:126:ILE:HD12  | 2.17        | 0.59     |
| 4:D:121:VAL:O     | 4:D:134:ASP:HA    | 2.02        | 0.59     |
| 19:S:63:THR:HG22  | 19:S:66:MET:SD    | 2.42        | 0.59     |
| 19:S:66:MET:HA    | 19:S:69:HIS:HD2   | 1.68        | 0.59     |
| 1:A:1161:C:H2'    | 1:A:1162:C:C6     | 2.37        | 0.59     |
| 10:J:87:THR:C     | 10:J:89:ASP:H     | 2.06        | 0.59     |
| 2:B:20:GLU:HB2    | 2:B:190:THR:OG1   | 2.01        | 0.59     |
| 24:Y:180:LEU:O    | 24:Y:210:VAL:HG21 | 2.02        | 0.59     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:1132:C:O2'    | 1:A:1133:G:H5'    | 2.02        | 0.59     |
| 2:B:18:GLY:H      | 2:B:42:ILE:CG2    | 2.15        | 0.59     |
| 16:P:28:ARG:NH1   | 16:P:28:ARG:HG2   | 2.17        | 0.59     |
| 23:X:19:U:O2      | 24:Y:126:GLY:HA3  | 2.02        | 0.59     |
| 14:N:12:ARG:NH1   | 14:N:14:PRO:HD3   | 2.18        | 0.59     |
| 22:W:31:A:H2'     | 22:W:32:U:H5'     | 1.85        | 0.59     |
| 12:L:6:THR:H      | 12:L:9:GLN:NE2    | 1.99        | 0.59     |
| 1:A:522:C:N4      | 1:A:528:C:H42     | 2.01        | 0.59     |
| 1:A:97:G:O2'      | 1:A:98:G:H5''     | 2.01        | 0.59     |
| 8:H:6:ILE:HD12    | 8:H:6:ILE:N       | 2.17        | 0.59     |
| 10:J:16:LEU:HD13  | 10:J:70:ARG:HD2   | 1.83        | 0.59     |
| 18:R:25:THR:HG22  | 18:R:42:ARG:NH1   | 2.18        | 0.59     |
| 1:A:954:G:H21     | 1:A:1227:A:N6     | 1.98        | 0.59     |
| 13:M:108:ARG:CZ   | 13:M:114:ARG:HG2  | 2.32        | 0.59     |
| 1:A:1318:A:H1'    | 19:S:37:ARG:HH21  | 1.65        | 0.59     |
| 24:Y:99:ASP:O     | 24:Y:103:HIS:HB2  | 2.03        | 0.59     |
| 1:A:950:U:H2'     | 1:A:951:G:C8      | 2.38        | 0.59     |
| 4:D:128:VAL:HG12  | 4:D:129:ASN:ND2   | 2.18        | 0.59     |
| 1:A:975:A:H8      | 1:A:975:A:H5'     | 1.68        | 0.59     |
| 12:L:47:LYS:HD2   | 12:L:47:LYS:C     | 2.23        | 0.59     |
| 1:A:1305:G:OP1    | 21:U:2:GLY:HA3    | 2.02        | 0.59     |
| 10:J:48:THR:HA    | 10:J:62:HIS:CB    | 2.33        | 0.59     |
| 4:D:100:ARG:CZ    | 4:D:137:SER:HA    | 2.33        | 0.59     |
| 19:S:53:ASN:O     | 19:S:77:THR:HG22  | 2.01        | 0.59     |
| 12:L:102:ARG:HD2  | 12:L:108:ALA:O    | 2.03        | 0.59     |
| 1:A:477:A:O2'     | 1:A:479:C:H5'     | 2.03        | 0.59     |
| 24:Y:252:VAL:HG22 | 24:Y:259:THR:HB   | 1.84        | 0.59     |
| 1:A:191:G:H1'     | 20:T:105:SER:CB   | 2.33        | 0.59     |
| 13:M:9:ILE:N      | 13:M:9:ILE:HD12   | 2.17        | 0.59     |
| 1:A:1030:C:C2'    | 1:A:1030(A):G:H5' | 2.32        | 0.59     |
| 3:C:77:ILE:O      | 3:C:83:ARG:HB3    | 2.03        | 0.59     |
| 5:E:10:MET:HA     | 5:E:32:VAL:HG22   | 1.84        | 0.59     |
| 18:R:19:LYS:O     | 18:R:20:ALA:HB2   | 2.02        | 0.59     |
| 1:A:349:A:O2'     | 1:A:350:G:H5'     | 2.03        | 0.59     |
| 1:A:1270:C:O2'    | 1:A:1271:G:H5'    | 2.02        | 0.59     |
| 10:J:90:LEU:N     | 10:J:91:PRO:HD3   | 2.18        | 0.59     |
| 17:Q:52:LYS:HD2   | 17:Q:52:LYS:H     | 1.67        | 0.59     |
| 13:M:125:ARG:HD2  | 24:Y:165:ASP:CB   | 2.33        | 0.59     |
| 5:E:6:PHE:HD1     | 5:E:63:ARG:NH1    | 2.00        | 0.59     |
| 24:Y:13:LEU:O     | 24:Y:17:LEU:HG    | 2.03        | 0.59     |
| 7:G:79:ARG:NH2    | 23:X:14:A:H61     | 1.99        | 0.59     |
| 2:B:69:LEU:HD23   | 2:B:159:PRO:HG2   | 1.85        | 0.59     |

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| Atom-1            | Atom-2           | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:A:156:G:O2'     | 1:A:157:G:H5'    | 2.02        | 0.59     |
| 14:N:12:ARG:NH1   | 14:N:12:ARG:HB2  | 2.17        | 0.59     |
| 1:A:336:C:H2'     | 1:A:337:C:H6     | 1.67        | 0.59     |
| 17:Q:74:LEU:HD12  | 17:Q:75:ARG:HG2  | 1.84        | 0.59     |
| 1:A:1281:U:H4'    | 1:A:1282:C:OP2   | 2.03        | 0.59     |
| 6:F:33:TYR:HE2    | 6:F:74:ASP:HB2   | 1.68        | 0.59     |
| 7:G:60:LYS:HD2    | 7:G:60:LYS:N     | 2.18        | 0.59     |
| 1:A:737:A:H2'     | 1:A:738:C:H6     | 1.67        | 0.58     |
| 3:C:53:ALA:HB2    | 3:C:115:LEU:CD2  | 2.32        | 0.58     |
| 17:Q:9:VAL:HG11   | 17:Q:84:LEU:HD12 | 1.84        | 0.58     |
| 1:A:1496:C:H2'    | 1:A:1497:G:O4'   | 2.01        | 0.58     |
| 1:A:137:C:H1'     | 16:P:63:GLY:CA   | 2.34        | 0.58     |
| 22:V:50:U:H2'     | 22:V:51:U:O4'    | 2.02        | 0.58     |
| 2:B:96:ARG:N      | 2:B:96:ARG:HD2   | 2.18        | 0.58     |
| 1:A:1439:C:H5'    | 20:T:38:LYS:NZ   | 2.17        | 0.58     |
| 22:V:55:U:N3      | 22:V:57:G:H5''   | 2.18        | 0.58     |
| 18:R:53:ARG:C     | 18:R:55:ARG:H    | 2.05        | 0.58     |
| 13:M:126:LYS:N    | 24:Y:161:GLU:N   | 2.50        | 0.58     |
| 1:A:1152:A:H5''   | 10:J:13:HIS:HD2  | 1.67        | 0.58     |
| 1:A:1030:C:H5     | 1:A:1033:G:N1    | 2.01        | 0.58     |
| 18:R:38:GLU:HA    | 18:R:41:LYS:HB3  | 1.84        | 0.58     |
| 11:K:22:HIS:HB3   | 11:K:29:ILE:CG2  | 2.33        | 0.58     |
| 7:G:118:VAL:HG23  | 7:G:119:ARG:H    | 1.67        | 0.58     |
| 1:A:1169:A:H2'    | 1:A:1170:A:C8    | 2.38        | 0.58     |
| 1:A:107:G:C2'     | 1:A:108:G:H5'    | 2.33        | 0.58     |
| 2:B:172:ILE:HD12  | 2:B:172:ILE:N    | 2.05        | 0.58     |
| 24:Y:120:ILE:HG23 | 24:Y:133:ALA:HB1 | 1.84        | 0.58     |
| 21:U:2:GLY:C      | 21:U:4:GLY:H     | 2.05        | 0.58     |
| 24:Y:76:MET:CE    | 24:Y:88:LYS:HE2  | 2.33        | 0.58     |
| 1:A:1053:G:C3'    | 1:A:1054:C:H5'   | 2.34        | 0.58     |
| 6:F:45:LEU:C      | 6:F:45:LEU:HD23  | 2.24        | 0.58     |
| 3:C:53:ALA:O      | 3:C:54:ARG:HB2   | 2.04        | 0.58     |
| 24:Y:272:LYS:O    | 24:Y:276:LEU:HG  | 2.04        | 0.58     |
| 1:A:1218:C:H2'    | 1:A:1219:U:C6    | 2.38        | 0.58     |
| 2:B:117:GLU:HG2   | 2:B:117:GLU:O    | 2.03        | 0.58     |
| 7:G:22:LEU:HD23   | 7:G:22:LEU:O     | 2.03        | 0.58     |
| 13:M:82:MET:HB2   | 13:M:93:ARG:CZ   | 2.32        | 0.58     |
| 13:M:3:ARG:HG2    | 13:M:9:ILE:HD11  | 1.85        | 0.58     |
| 22:V:50:U:H3      | 22:V:64:A:H61    | 1.50        | 0.58     |
| 2:B:142:LEU:HD23  | 2:B:142:LEU:O    | 2.03        | 0.58     |
| 1:A:1320:C:H2'    | 1:A:1321:C:O4'   | 2.03        | 0.58     |
| 24:Y:52:ALA:O     | 24:Y:55:LEU:HB2  | 2.03        | 0.58     |

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| Atom-1            | Atom-2           | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 9:I:31:GLN:NE2    | 9:I:36:TYR:HA    | 2.18        | 0.58     |
| 1:A:1281:U:H5'    | 1:A:1282:C:C5    | 2.38        | 0.58     |
| 22:V:9:A:H8       | 22:V:11:C:N4     | 2.02        | 0.58     |
| 24:Y:189:LEU:O    | 24:Y:203:THR:HA  | 2.03        | 0.58     |
| 1:A:1134:G:C2'    | 1:A:1135:U:H5'   | 2.34        | 0.58     |
| 22:V:20:U:C5      | 22:V:21:A:H1'    | 2.39        | 0.58     |
| 2:B:236:TYR:HA    | 2:B:239:VAL:CG2  | 2.34        | 0.58     |
| 1:A:994:A:N1      | 1:A:1047:G:H4'   | 2.18        | 0.58     |
| 22:W:16:U:N3      | 22:W:18:G:H2'    | 2.18        | 0.58     |
| 24:Y:61:THR:HG21  | 24:Y:101:LEU:CD1 | 2.29        | 0.58     |
| 19:S:29:ARG:HD2   | 19:S:30:LEU:N    | 2.15        | 0.58     |
| 2:B:18:GLY:N      | 2:B:42:ILE:HG22  | 2.19        | 0.58     |
| 6:F:68:PRO:CG     | 6:F:71:ARG:HG3   | 2.31        | 0.58     |
| 2:B:16:HIS:HB3    | 2:B:210:SER:CB   | 2.33        | 0.58     |
| 1:A:358:U:H2'     | 1:A:359:U:C6     | 2.39        | 0.58     |
| 10:J:44:VAL:HG12  | 10:J:46:ARG:HD2  | 1.85        | 0.58     |
| 1:A:1234:C:O2'    | 1:A:1235:U:H5'   | 2.03        | 0.58     |
| 1:A:882:C:O2'     | 1:A:883:C:H5'    | 2.04        | 0.58     |
| 24:Y:236:GLY:O    | 24:Y:237:PRO:O   | 2.21        | 0.58     |
| 15:O:82:ILE:C     | 15:O:82:ILE:HD13 | 2.24        | 0.58     |
| 12:L:38:THR:OG1   | 12:L:39:VAL:HG23 | 2.04        | 0.58     |
| 12:L:24:VAL:HG22  | 12:L:97:ARG:HB3  | 1.86        | 0.58     |
| 2:B:218:ALA:O     | 2:B:222:ILE:HG12 | 2.03        | 0.58     |
| 3:C:187:ALA:C     | 3:C:188:LEU:HD22 | 2.24        | 0.58     |
| 3:C:16:ARG:HH11   | 3:C:16:ARG:HB2   | 1.66        | 0.58     |
| 24:Y:57:ARG:HA    | 24:Y:60:ASP:OD1  | 2.03        | 0.58     |
| 24:Y:312:ARG:HE   | 24:Y:344:LEU:CD1 | 2.16        | 0.58     |
| 19:S:46:GLY:H     | 19:S:62:ILE:HG23 | 1.67        | 0.58     |
| 19:S:46:GLY:N     | 19:S:62:ILE:HG23 | 2.19        | 0.58     |
| 3:C:116:VAL:O     | 3:C:119:ARG:HB3  | 2.04        | 0.58     |
| 17:Q:3:LYS:HD2    | 17:Q:60:ILE:HD11 | 1.86        | 0.58     |
| 8:H:12:ARG:HH12   | 8:H:27:PRO:CD    | 2.17        | 0.58     |
| 2:B:36:ARG:O      | 2:B:37:ASN:HB3   | 2.04        | 0.58     |
| 1:A:673:G:H2'     | 1:A:674:G:H8     | 1.61        | 0.58     |
| 1:A:625:G:H2'     | 1:A:626:U:C6     | 2.39        | 0.58     |
| 2:B:17:PHE:HD2    | 2:B:17:PHE:H     | 1.52        | 0.58     |
| 1:A:1383:C:H2'    | 1:A:1384:C:H6    | 1.69        | 0.58     |
| 11:K:92:GLU:HG3   | 11:K:96:ARG:HD2  | 1.84        | 0.58     |
| 2:B:162:ILE:HD11  | 2:B:184:VAL:HG22 | 1.86        | 0.57     |
| 4:D:9:CYS:HB3     | 4:D:32:ALA:HB2   | 1.86        | 0.57     |
| 24:Y:150:GLN:HE21 | 24:Y:172:LYS:HZ1 | 1.48        | 0.57     |
| 16:P:43:LYS:C     | 16:P:45:THR:H    | 2.07        | 0.57     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 22:V:26:A:N6      | 22:V:44:G:H1      | 2.00        | 0.57     |
| 1:A:376:G:O2'     | 1:A:377:G:H5'     | 2.03        | 0.57     |
| 2:B:7:VAL:C       | 2:B:217:ARG:HH22  | 2.07        | 0.57     |
| 1:A:637:G:H2'     | 1:A:638:G:H8      | 1.69        | 0.57     |
| 4:D:8:VAL:HG11    | 4:D:115:ARG:NH1   | 2.19        | 0.57     |
| 7:G:37:ASN:ND2    | 9:I:40:LEU:HA     | 2.14        | 0.57     |
| 2:B:119:GLU:C     | 2:B:121:LEU:H     | 2.07        | 0.57     |
| 1:A:692:U:H5      | 11:K:26:ASN:HD22  | 1.53        | 0.57     |
| 7:G:87:VAL:HG21   | 7:G:154:TYR:HB3   | 1.86        | 0.57     |
| 1:A:237:C:H4'     | 17:Q:25:ARG:HH12  | 1.69        | 0.57     |
| 1:A:1059:C:O2     | 10:J:53:PRO:HG3   | 2.04        | 0.57     |
| 22:W:70:G:H2'     | 22:W:71:G:H8      | 1.69        | 0.57     |
| 1:A:1381:U:H5     | 1:A:1382:C:C4     | 2.21        | 0.57     |
| 8:H:5:PRO:O       | 8:H:8:ASP:HB3     | 2.04        | 0.57     |
| 1:A:1212:U:H2'    | 24:Y:78:GLU:OE2   | 2.03        | 0.57     |
| 13:M:65:LYS:CE    | 13:M:69:GLU:HG3   | 2.34        | 0.57     |
| 1:A:107:G:H2'     | 1:A:108:G:H5'     | 1.86        | 0.57     |
| 1:A:1327:C:H2'    | 1:A:1328:C:C6     | 2.39        | 0.57     |
| 1:A:1203:C:H2'    | 1:A:1204:A:C8     | 2.40        | 0.57     |
| 13:M:91:ARG:CB    | 13:M:98:VAL:HG22  | 2.34        | 0.57     |
| 24:Y:229:ILE:HG23 | 24:Y:251:VAL:HG12 | 1.85        | 0.57     |
| 4:D:28:SER:O      | 4:D:30:LYS:N      | 2.37        | 0.57     |
| 1:A:939:G:H5''    | 7:G:102:ARG:CZ    | 2.33        | 0.57     |
| 24:Y:326:THR:CB   | 24:Y:347:ALA:HB1  | 2.35        | 0.57     |
| 1:A:475:G:H2'     | 1:A:476:G:C8      | 2.38        | 0.57     |
| 1:A:1288:A:O2'    | 1:A:1289:A:H5'    | 2.04        | 0.57     |
| 1:A:1499:A:H1'    | 1:A:1520:G:C5'    | 2.35        | 0.57     |
| 24:Y:241:GLY:O    | 24:Y:243:ASN:N    | 2.38        | 0.57     |
| 2:B:80:ILE:CD1    | 2:B:80:ILE:H      | 2.16        | 0.57     |
| 5:E:12:LEU:C      | 5:E:12:LEU:HD22   | 2.25        | 0.57     |
| 1:A:66:G:H4'      | 1:A:173:U:C5      | 2.39        | 0.57     |
| 1:A:165:C:H2'     | 1:A:166:G:H8      | 1.69        | 0.57     |
| 3:C:134:ILE:HG23  | 3:C:151:VAL:HB    | 1.87        | 0.57     |
| 14:N:25:VAL:HG23  | 14:N:38:GLY:O     | 2.03        | 0.57     |
| 2:B:72:GLY:HA2    | 2:B:165:VAL:HG22  | 1.87        | 0.57     |
| 24:Y:116:ALA:HA   | 24:Y:212:PRO:HA   | 1.85        | 0.57     |
| 1:A:594:G:H1      | 1:A:645:C:H42     | 1.51        | 0.57     |
| 1:A:624:C:H4'     | 16:P:10:GLY:HA2   | 1.85        | 0.57     |
| 17:Q:51:TYR:CD2   | 17:Q:57:VAL:HG11  | 2.40        | 0.57     |
| 8:H:40:ALA:C      | 8:H:42:GLU:N      | 2.58        | 0.57     |
| 1:A:1296:C:H5'    | 1:A:1297:C:OP2    | 2.05        | 0.57     |
| 12:L:27:LEU:HB2   | 12:L:33:ARG:HD2   | 1.85        | 0.57     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 16:P:45:THR:HG22 | 16:P:47:ASP:N     | 2.18        | 0.57     |
| 12:L:53:ARG:HG2  | 12:L:53:ARG:NH1   | 2.18        | 0.57     |
| 20:T:75:ASN:ND2  | 20:T:75:ASN:N     | 2.53        | 0.57     |
| 2:B:121:LEU:O    | 2:B:127:ILE:HD11  | 2.04        | 0.57     |
| 5:E:36:ASP:OD2   | 5:E:40:ARG:HB2    | 2.05        | 0.57     |
| 1:A:888:G:H4'    | 1:A:1488:G:O2'    | 2.04        | 0.57     |
| 1:A:148:G:H2'    | 1:A:149:A:C8      | 2.40        | 0.57     |
| 1:A:397:A:H5'    | 1:A:398:C:OP1     | 2.05        | 0.57     |
| 1:A:512:U:H2'    | 1:A:513:C:C6      | 2.40        | 0.57     |
| 1:A:663:A:O2'    | 1:A:664:G:H5'     | 2.04        | 0.57     |
| 24:Y:112:ALA:HB1 | 24:Y:178:GLY:CA   | 2.35        | 0.57     |
| 24:Y:184:ALA:HB2 | 24:Y:210:VAL:HG23 | 1.87        | 0.57     |
| 3:C:186:PHE:CZ   | 3:C:188:LEU:HD11  | 2.39        | 0.57     |
| 24:Y:181:SER:N   | 24:Y:182:PRO:HD2  | 2.19        | 0.57     |
| 24:Y:182:PRO:CG  | 24:Y:345:ILE:HG23 | 2.31        | 0.57     |
| 9:I:17:VAL:HG21  | 9:I:81:ILE:N      | 2.20        | 0.57     |
| 1:A:1305:G:H22   | 1:A:1331:G:H1'    | 1.69        | 0.57     |
| 24:Y:76:MET:HG3  | 24:Y:88:LYS:HE2   | 1.87        | 0.57     |
| 1:A:1264:C:H2'   | 1:A:1265:G:H8     | 1.66        | 0.57     |
| 7:G:120:ILE:N    | 7:G:120:ILE:HD12  | 2.19        | 0.57     |
| 8:H:120:THR:OG1  | 8:H:123:GLU:HG3   | 2.05        | 0.57     |
| 1:A:63:C:H42     | 1:A:104:G:H1      | 1.52        | 0.57     |
| 4:D:65:ARG:HD2   | 4:D:72:GLU:HA     | 1.85        | 0.57     |
| 15:O:39:LEU:HD12 | 15:O:56:LEU:HB2   | 1.86        | 0.57     |
| 4:D:18:LYS:HE2   | 4:D:31:CYS:HB2    | 1.85        | 0.57     |
| 1:A:1005:A:H2'   | 1:A:1006:C:H5'    | 1.87        | 0.57     |
| 1:A:552:U:O2'    | 1:A:553:A:H5'     | 2.05        | 0.57     |
| 24:Y:77:GLU:HB2  | 24:Y:84:ARG:HG2   | 1.86        | 0.57     |
| 1:A:532:A:H61    | 3:C:156:ARG:HH12  | 1.50        | 0.57     |
| 2:B:140:HIS:O    | 2:B:144:ARG:HG2   | 2.05        | 0.57     |
| 8:H:51:VAL:CG1   | 8:H:60:ARG:HB2    | 2.34        | 0.57     |
| 4:D:100:ARG:NH1  | 4:D:137:SER:HA    | 2.19        | 0.57     |
| 1:A:707:C:O2'    | 1:A:708:C:H5'     | 2.05        | 0.57     |
| 1:A:1194:U:H2'   | 1:A:1195:C:C6     | 2.39        | 0.57     |
| 13:M:118:ALA:HB1 | 13:M:119:GLY:N    | 2.20        | 0.57     |
| 24:Y:29:LEU:HG   | 24:Y:51:GLU:HB2   | 1.85        | 0.57     |
| 9:I:111:ARG:HG2  | 9:I:112:LYS:N     | 2.19        | 0.57     |
| 13:M:49:THR:O    | 13:M:53:VAL:HG23  | 2.05        | 0.57     |
| 3:C:119:ARG:HH11 | 3:C:119:ARG:HG3   | 1.70        | 0.57     |
| 13:M:69:GLU:HA   | 13:M:70:LEU:N     | 2.20        | 0.57     |
| 1:A:1097:C:O2'   | 1:A:1098:C:H5'    | 2.05        | 0.57     |
| 1:A:1058:G:H2'   | 1:A:1059:C:C6     | 2.39        | 0.57     |

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| Atom-1            | Atom-2           | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 4:D:53:ASP:O      | 4:D:57:ARG:HD3   | 2.05        | 0.57     |
| 22:W:64:A:H2'     | 22:W:65:G:C8     | 2.39        | 0.56     |
| 3:C:150:LYS:HE2   | 3:C:152:ILE:HD11 | 1.87        | 0.56     |
| 1:A:1001(A):G:H2' | 1:A:1002:G:O4'   | 2.05        | 0.56     |
| 1:A:93:G:O2'      | 1:A:96:U:H5'     | 2.05        | 0.56     |
| 1:A:936:C:H2'     | 1:A:937:A:C8     | 2.40        | 0.56     |
| 7:G:12:LEU:CD1    | 7:G:25:ALA:HB2   | 2.35        | 0.56     |
| 1:A:186:C:H2'     | 1:A:187:C:C6     | 2.39        | 0.56     |
| 1:A:1220:G:H2'    | 1:A:1221:G:C8    | 2.40        | 0.56     |
| 24:Y:6:LEU:O      | 24:Y:8:GLN:N     | 2.38        | 0.56     |
| 4:D:58:LEU:HD23   | 4:D:62:GLN:HG2   | 1.86        | 0.56     |
| 1:A:189(A):C:H2'  | 1:A:189(B):C:C6  | 2.40        | 0.56     |
| 1:A:189(C):C:O2'  | 1:A:189(D):C:H5' | 2.04        | 0.56     |
| 1:A:46:G:O2'      | 1:A:365:U:H1'    | 2.05        | 0.56     |
| 22:V:18:G:H21     | 22:V:58:A:H5'    | 1.70        | 0.56     |
| 24:Y:98:LEU:O     | 24:Y:98:LEU:HD23 | 2.05        | 0.56     |
| 17:Q:12:SER:HB3   | 17:Q:20:THR:HB   | 1.85        | 0.56     |
| 4:D:129:ASN:HD21  | 4:D:145:GLU:N    | 2.03        | 0.56     |
| 19:S:22:LEU:HA    | 19:S:27:GLU:CD   | 2.26        | 0.56     |
| 8:H:30:ARG:CB     | 8:H:30:ARG:HH11  | 2.17        | 0.56     |
| 1:A:542:G:P       | 4:D:10:ARG:HH22  | 2.27        | 0.56     |
| 1:A:1411:C:O2'    | 1:A:1412:C:H5'   | 2.05        | 0.56     |
| 24:Y:106:LEU:HD23 | 24:Y:106:LEU:C   | 2.24        | 0.56     |
| 1:A:1228:C:H2'    | 1:A:1229:A:H8    | 1.70        | 0.56     |
| 22:W:49:C:H3'     | 22:W:50:U:H6     | 1.69        | 0.56     |
| 1:A:1144:G:H21    | 1:A:1146:A:H62   | 1.53        | 0.56     |
| 24:Y:61:THR:C     | 24:Y:63:ARG:H    | 2.09        | 0.56     |
| 13:M:90:LEU:HD13  | 13:M:94:ARG:NH2  | 2.20        | 0.56     |
| 1:A:1033:G:H2'    | 1:A:1034:G:H5'   | 1.86        | 0.56     |
| 1:A:1399:C:C2     | 1:A:1502:A:N6    | 2.73        | 0.56     |
| 10:J:24:VAL:HG22  | 10:J:72:VAL:HG11 | 1.87        | 0.56     |
| 7:G:17:VAL:HG12   | 7:G:18:TYR:CD1   | 2.40        | 0.56     |
| 11:K:29:ILE:CG1   | 11:K:44:SER:HB3  | 2.34        | 0.56     |
| 13:M:30:ALA:C     | 13:M:32:GLU:H    | 2.09        | 0.56     |
| 1:A:1452:C:H5'    | 1:A:1456:G:C5    | 2.40        | 0.56     |
| 1:A:539:A:H2'     | 1:A:540:G:H8     | 1.70        | 0.56     |
| 1:A:243:A:H4'     | 1:A:244:U:C5'    | 2.35        | 0.56     |
| 3:C:112:SER:HB3   | 3:C:115:LEU:HD12 | 1.88        | 0.56     |
| 6:F:17:SER:O      | 6:F:21:LEU:HD23  | 2.05        | 0.56     |
| 3:C:46:GLU:O      | 3:C:47:LEU:HB2   | 2.05        | 0.56     |
| 1:A:356:A:H2'     | 1:A:357:G:H8     | 1.68        | 0.56     |
| 1:A:477:A:H2'     | 1:A:479:C:H6     | 1.70        | 0.56     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:545:C:O2'     | 1:A:546:G:H5'     | 2.04        | 0.56     |
| 24:Y:330:ARG:HG2  | 24:Y:332:ASP:OD1  | 2.05        | 0.56     |
| 4:D:133:VAL:HG12  | 4:D:135:LEU:H     | 1.70        | 0.56     |
| 1:A:688:G:H2'     | 1:A:689:C:H6      | 1.69        | 0.56     |
| 1:A:1333:A:H2'    | 1:A:1334:G:O4'    | 2.05        | 0.56     |
| 13:M:58:GLU:C     | 13:M:60:VAL:H     | 2.07        | 0.56     |
| 1:A:192:U:C4'     | 20:T:103:GLY:H    | 2.11        | 0.56     |
| 19:S:22:LEU:HA    | 19:S:27:GLU:OE2   | 2.05        | 0.56     |
| 22:V:25:C:H2'     | 22:V:26:A:C8      | 2.40        | 0.56     |
| 24:Y:81:ALA:HB3   | 24:Y:84:ARG:HB2   | 1.87        | 0.56     |
| 1:A:1457:G:H2'    | 1:A:1458:G:H8     | 1.70        | 0.56     |
| 21:U:6:ARG:HE     | 21:U:15:ARG:HH12  | 1.54        | 0.56     |
| 22:W:50:U:C4'     | 22:W:65:G:H22     | 2.10        | 0.56     |
| 7:G:102:ARG:HG2   | 7:G:106:GLN:NE2   | 2.17        | 0.56     |
| 13:M:125:ARG:HA   | 24:Y:159:GLY:HA3  | 1.87        | 0.56     |
| 1:A:865:A:H5'     | 1:A:1078:U:C4     | 2.40        | 0.56     |
| 9:I:4:TYR:CB      | 9:I:19:LEU:HB2    | 2.35        | 0.56     |
| 1:A:521:G:H4'     | 12:L:73:GLU:HG2   | 1.86        | 0.56     |
| 8:H:14:ARG:O      | 8:H:18:ARG:HD3    | 2.04        | 0.56     |
| 1:A:390:C:O3'     | 16:P:28:ARG:NH2   | 2.39        | 0.56     |
| 17:Q:45:HIS:O     | 17:Q:73:VAL:HG23  | 2.05        | 0.56     |
| 19:S:33:THR:HG23  | 19:S:51:VAL:HA    | 1.88        | 0.56     |
| 1:A:562:C:H4'     | 1:A:563:A:O5'     | 2.06        | 0.56     |
| 24:Y:279:LEU:HD23 | 24:Y:283:LEU:HD11 | 1.88        | 0.56     |
| 4:D:32:ALA:C      | 4:D:35:ARG:HG3    | 2.25        | 0.56     |
| 1:A:1004:A:H62    | 1:A:1034:G:H8     | 1.53        | 0.56     |
| 12:L:90:VAL:HG12  | 12:L:90:VAL:O     | 2.06        | 0.56     |
| 11:K:67:ASP:OD1   | 11:K:71:LYS:HE3   | 2.06        | 0.56     |
| 1:A:369:C:O2'     | 1:A:370:C:H5'     | 2.06        | 0.56     |
| 14:N:24:CYS:HB2   | 14:N:29:ARG:HB3   | 1.87        | 0.56     |
| 15:O:82:ILE:HG12  | 15:O:87:ILE:HG13  | 1.88        | 0.56     |
| 4:D:74:GLN:HA     | 4:D:77:ASN:ND2    | 2.15        | 0.56     |
| 1:A:424:G:H2'     | 1:A:425:G:C8      | 2.30        | 0.56     |
| 4:D:49:ARG:HE     | 4:D:49:ARG:CA     | 2.17        | 0.56     |
| 22:W:29:G:H2'     | 22:W:30:G:H8      | 1.70        | 0.56     |
| 8:H:51:VAL:HG11   | 8:H:60:ARG:HD3    | 1.86        | 0.56     |
| 15:O:56:LEU:O     | 15:O:60:VAL:HG23  | 2.06        | 0.56     |
| 4:D:23:GLY:O      | 4:D:27:TYR:HD1    | 1.88        | 0.56     |
| 1:A:946:A:H2'     | 1:A:947:G:C8      | 2.40        | 0.56     |
| 24:Y:344:LEU:CD2  | 24:Y:344:LEU:H    | 2.17        | 0.56     |
| 10:J:3:LYS:O      | 10:J:100:THR:HG23 | 2.05        | 0.56     |
| 1:A:1033:G:C2'    | 1:A:1034:G:H5'    | 2.36        | 0.56     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 10:J:29:ARG:HH11 | 10:J:29:ARG:HG2  | 1.69        | 0.56     |
| 2:B:47:THR:HG22  | 2:B:51:LEU:HD11  | 1.88        | 0.56     |
| 5:E:144:THR:O    | 5:E:148:VAL:HG23 | 2.06        | 0.56     |
| 8:H:120:THR:HG23 | 8:H:123:GLU:OE1  | 2.06        | 0.56     |
| 1:A:1073:U:H2'   | 1:A:1074:G:C8    | 2.41        | 0.56     |
| 1:A:6:G:H4'      | 1:A:298:A:H4'    | 1.88        | 0.56     |
| 18:R:87:ARG:HB3  | 18:R:87:ARG:NH1  | 2.20        | 0.56     |
| 13:M:125:ARG:HD3 | 24:Y:130:CYS:SG  | 2.46        | 0.56     |
| 24:Y:50:GLN:O    | 24:Y:53:ALA:HB3  | 2.05        | 0.56     |
| 1:A:254:G:O2'    | 1:A:255:G:H5'    | 2.06        | 0.56     |
| 10:J:38:ILE:HG13 | 10:J:38:ILE:O    | 2.06        | 0.56     |
| 8:H:84:ARG:O     | 8:H:135:CYS:HB2  | 2.06        | 0.56     |
| 1:A:512:U:H2'    | 1:A:513:C:H6     | 1.69        | 0.56     |
| 1:A:708:C:H2'    | 1:A:709:G:H8     | 1.71        | 0.56     |
| 1:A:134:A:H61    | 16:P:25:ARG:NH1  | 2.04        | 0.56     |
| 16:P:75:ARG:HH11 | 16:P:75:ARG:HG3  | 1.71        | 0.56     |
| 13:M:123:ALA:HB1 | 24:Y:161:GLU:O   | 2.05        | 0.56     |
| 24:Y:26:LEU:HD12 | 24:Y:26:LEU:C    | 2.27        | 0.56     |
| 2:B:126:GLU:HA   | 2:B:129:GLU:HG2  | 1.87        | 0.56     |
| 12:L:24:VAL:HG12 | 12:L:24:VAL:O    | 2.04        | 0.56     |
| 1:A:96:U:O2'     | 1:A:97:G:H8      | 1.89        | 0.56     |
| 1:A:37:U:O2'     | 1:A:38:G:H5'     | 2.06        | 0.56     |
| 2:B:86:GLU:C     | 2:B:88:ALA:H     | 2.08        | 0.56     |
| 1:A:180:U:H2'    | 1:A:181:G:C5'    | 2.35        | 0.56     |
| 13:M:86:CYS:HB2  | 19:S:73:GLU:HG2  | 1.89        | 0.55     |
| 22:W:38:A:H2'    | 22:W:39:U:C5'    | 2.35        | 0.55     |
| 1:A:523:A:N6     | 12:L:53:ARG:HH12 | 2.04        | 0.55     |
| 10:J:20:ALA:O    | 10:J:24:VAL:HG23 | 2.05        | 0.55     |
| 1:A:1343:G:H1'   | 9:I:121:ARG:HH12 | 1.72        | 0.55     |
| 8:H:19:VAL:CG2   | 8:H:21:LYS:HE2   | 2.36        | 0.55     |
| 4:D:126:ILE:HG22 | 4:D:127:THR:H    | 1.70        | 0.55     |
| 2:B:36:ARG:HG2   | 2:B:36:ARG:HH11  | 1.71        | 0.55     |
| 15:O:36:ILE:HG23 | 15:O:56:LEU:HD11 | 1.87        | 0.55     |
| 10:J:81:THR:C    | 10:J:83:GLU:H    | 2.09        | 0.55     |
| 10:J:49:VAL:O    | 10:J:60:ARG:HB2  | 2.06        | 0.55     |
| 24:Y:172:LYS:O   | 24:Y:176:ALA:HB2 | 2.06        | 0.55     |
| 5:E:50:GLU:HB3   | 5:E:53:LEU:HD12  | 1.88        | 0.55     |
| 9:I:3:GLN:OE1    | 9:I:20:ARG:NH2   | 2.39        | 0.55     |
| 2:B:145:LEU:CD1  | 2:B:149:LEU:HD12 | 2.36        | 0.55     |
| 6:F:1:MET:HB3    | 6:F:66:GLU:HG2   | 1.87        | 0.55     |
| 24:Y:46:ARG:O    | 24:Y:46:ARG:NE   | 2.40        | 0.55     |
| 4:D:119:GLN:HG2  | 4:D:123:HIS:CD2  | 2.41        | 0.55     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:998:G:O2'     | 1:A:999:C:H5'     | 2.06        | 0.55     |
| 2:B:16:HIS:HB3    | 2:B:210:SER:HA    | 1.87        | 0.55     |
| 1:A:1060:C:C5     | 3:C:2:GLY:HA3     | 2.40        | 0.55     |
| 22:W:16:U:C6      | 22:W:18:G:H5''    | 2.41        | 0.55     |
| 2:B:22:LYS:CA     | 2:B:22:LYS:HE2    | 2.26        | 0.55     |
| 15:O:82:ILE:HG23  | 15:O:83:GLU:H     | 1.70        | 0.55     |
| 1:A:16:A:N1       | 1:A:919:A:H2      | 2.05        | 0.55     |
| 12:L:45:PRO:HG3   | 12:L:53:ARG:HD3   | 1.88        | 0.55     |
| 1:A:445:G:H2'     | 1:A:446:G:H8      | 1.71        | 0.55     |
| 11:K:111:ASP:HA   | 18:R:84:LYS:HD2   | 1.88        | 0.55     |
| 5:E:11:ILE:HG22   | 5:E:12:LEU:N      | 2.21        | 0.55     |
| 5:E:12:LEU:CD1    | 5:E:31:LEU:HB3    | 2.36        | 0.55     |
| 1:A:501:C:H2'     | 1:A:502:G:C8      | 2.41        | 0.55     |
| 1:A:692:U:OP1     | 11:K:124:LYS:HE2  | 2.06        | 0.55     |
| 2:B:19:HIS:O      | 2:B:20:GLU:O      | 2.24        | 0.55     |
| 10:J:44:VAL:CG1   | 10:J:46:ARG:HD2   | 2.36        | 0.55     |
| 13:M:99:ARG:HB2   | 13:M:101:GLN:NE2  | 2.22        | 0.55     |
| 24:Y:144:ALA:HB1  | 24:Y:149:PHE:HB2  | 1.89        | 0.55     |
| 1:A:628:G:H2'     | 1:A:629:G:C8      | 2.41        | 0.55     |
| 24:Y:205:PHE:HE2  | 24:Y:310:GLN:NE2  | 2.05        | 0.55     |
| 24:Y:251:VAL:HG23 | 24:Y:279:LEU:HD12 | 1.87        | 0.55     |
| 20:T:57:ARG:NH1   | 20:T:102:GLY:HA3  | 2.21        | 0.55     |
| 9:I:19:LEU:O      | 9:I:20:ARG:HG3    | 2.05        | 0.55     |
| 2:B:18:GLY:CA     | 2:B:42:ILE:HG22   | 2.36        | 0.55     |
| 1:A:926:G:N2      | 1:A:1505:G:H2'    | 2.22        | 0.55     |
| 1:A:255:G:H1'     | 17:Q:16:GLN:HE21  | 1.71        | 0.55     |
| 3:C:156:ARG:HD3   | 3:C:194:GLY:HA3   | 1.88        | 0.55     |
| 4:D:199:ASN:HD22  | 4:D:202:LEU:HG    | 1.71        | 0.55     |
| 24:Y:227:LEU:HD11 | 24:Y:276:LEU:HD22 | 1.86        | 0.55     |
| 16:P:17:TYR:CD1   | 16:P:17:TYR:N     | 2.74        | 0.55     |
| 22:V:66:U:H2'     | 22:V:67:C:O4'     | 2.07        | 0.55     |
| 24:Y:306:GLU:HG3  | 24:Y:307:TRP:H    | 1.69        | 0.55     |
| 22:W:55:U:O2'     | 22:W:56:C:H5      | 1.90        | 0.55     |
| 10:J:58:ASP:O     | 10:J:59:SER:C     | 2.45        | 0.55     |
| 1:A:1128:C:H4'    | 9:I:16:ARG:HH12   | 1.71        | 0.55     |
| 1:A:15:G:H2'      | 1:A:16:A:C8       | 2.41        | 0.55     |
| 1:A:626:U:H5''    | 16:P:38:TYR:CD2   | 2.42        | 0.55     |
| 12:L:75:HIS:HD2   | 12:L:77:LEU:HB2   | 1.72        | 0.55     |
| 4:D:126:ILE:CG2   | 4:D:127:THR:N     | 2.69        | 0.55     |
| 2:B:11:LEU:C      | 2:B:213:LEU:HD11  | 2.27        | 0.55     |
| 1:A:637:G:H2'     | 1:A:638:G:C8      | 2.42        | 0.55     |
| 22:W:70:G:H4'     | 22:W:71:G:OP1     | 2.06        | 0.55     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:165:C:H2'     | 1:A:166:G:C8      | 2.42        | 0.55     |
| 13:M:54:VAL:O     | 13:M:58:GLU:HG2   | 2.07        | 0.55     |
| 22:W:6:G:N2       | 22:W:7:A:H62      | 2.05        | 0.55     |
| 1:A:1040:U:H2'    | 1:A:1041:A:C8     | 2.42        | 0.55     |
| 3:C:52:LEU:CD2    | 3:C:52:LEU:H      | 2.18        | 0.55     |
| 1:A:1042:G:O2'    | 1:A:1043:C:H5'    | 2.07        | 0.55     |
| 1:A:783:C:O2'     | 1:A:784:C:H5'     | 2.07        | 0.55     |
| 1:A:1463:C:O2'    | 1:A:1464:G:H5'    | 2.07        | 0.55     |
| 1:A:1229:A:OP2    | 13:M:114:ARG:HD3  | 2.06        | 0.55     |
| 24:Y:323:ASP:CB   | 24:Y:326:THR:HG22 | 2.32        | 0.55     |
| 5:E:146:ALA:O     | 5:E:149:GLU:HG2   | 2.06        | 0.55     |
| 12:L:117:ARG:NH2  | 12:L:124:LYS:HB2  | 2.22        | 0.55     |
| 19:S:39:THR:HG22  | 19:S:40:ILE:N     | 2.22        | 0.55     |
| 2:B:135:GLN:O     | 2:B:139:LYS:HG2   | 2.06        | 0.55     |
| 24:Y:321:VAL:HG23 | 24:Y:333:PRO:HA   | 1.88        | 0.55     |
| 1:A:710:G:O2'     | 1:A:711:G:H5'     | 2.06        | 0.55     |
| 2:B:102:LEU:HD12  | 2:B:102:LEU:N     | 2.21        | 0.55     |
| 3:C:20:SER:HB2    | 3:C:40:ARG:NH2    | 2.22        | 0.55     |
| 8:H:91:ARG:CG     | 8:H:91:ARG:HH11   | 2.19        | 0.55     |
| 2:B:76:GLN:O      | 2:B:208:ILE:HG23  | 2.07        | 0.55     |
| 15:O:37:ASN:N     | 15:O:37:ASN:ND2   | 2.55        | 0.55     |
| 3:C:148:GLY:HA3   | 3:C:172:ARG:O     | 2.07        | 0.55     |
| 1:A:1224:G:H4'    | 13:M:102:ARG:NH1  | 2.22        | 0.55     |
| 2:B:162:ILE:HD13  | 2:B:177:ALA:CB    | 2.36        | 0.55     |
| 13:M:112:GLY:HA2  | 13:M:113:PRO:CD   | 2.36        | 0.55     |
| 4:D:55:ALA:O      | 4:D:59:ARG:HG2    | 2.07        | 0.55     |
| 19:S:22:LEU:HD13  | 19:S:27:GLU:HB2   | 1.89        | 0.55     |
| 5:E:147:ASP:O     | 5:E:151:LEU:HG    | 2.07        | 0.55     |
| 1:A:76:C:H42      | 1:A:93:G:H1       | 1.54        | 0.55     |
| 9:I:79:LEU:HD11   | 9:I:83:ARG:HH21   | 1.72        | 0.55     |
| 1:A:1073:U:H2'    | 1:A:1074:G:H8     | 1.71        | 0.55     |
| 1:A:1169:A:H2'    | 1:A:1170:A:H8     | 1.72        | 0.55     |
| 2:B:204:ASN:ND2   | 2:B:206:ASP:H     | 2.05        | 0.55     |
| 1:A:1519:A:C3'    | 1:A:1520:G:H5'    | 2.36        | 0.55     |
| 1:A:867:G:O2'     | 1:A:868:C:H5'     | 2.06        | 0.55     |
| 2:B:97:TRP:HZ2    | 2:B:102:LEU:HD13  | 1.71        | 0.55     |
| 1:A:1226:C:H4'    | 1:A:1227:A:OP1    | 2.07        | 0.55     |
| 1:A:1424:C:O2'    | 1:A:1425:U:H5'    | 2.07        | 0.55     |
| 13:M:14:ARG:HA    | 13:M:43:THR:O     | 2.06        | 0.55     |
| 13:M:83:ASP:OD2   | 13:M:84:ILE:N     | 2.37        | 0.55     |
| 2:B:136:VAL:HG13  | 2:B:140:HIS:ND1   | 2.21        | 0.55     |
| 3:C:60:ALA:O      | 3:C:61:ALA:HB2    | 2.05        | 0.55     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 24:Y:185:GLY:HA3  | 24:Y:311:ILE:CG2  | 2.37        | 0.55     |
| 1:A:1190:G:OP1    | 3:C:5:ILE:HG23    | 2.07        | 0.55     |
| 10:J:57:LYS:O     | 10:J:57:LYS:HG3   | 2.06        | 0.54     |
| 15:O:67:LEU:HD11  | 15:O:87:ILE:HD12  | 1.89        | 0.54     |
| 1:A:644:G:H5'     | 8:H:92:ARG:NH2    | 2.22        | 0.54     |
| 6:F:97:PHE:HB2    | 18:R:32:ARG:HH11  | 1.72        | 0.54     |
| 12:L:119:LYS:HB2  | 12:L:120:TYR:HD1  | 1.72        | 0.54     |
| 1:A:744:C:H2'     | 1:A:745:C:C6      | 2.42        | 0.54     |
| 1:A:484:G:H4'     | 1:A:485:G:O5'     | 2.08        | 0.54     |
| 2:B:93:VAL:HG21   | 2:B:97:TRP:CD1    | 2.41        | 0.54     |
| 1:A:135:C:H2'     | 1:A:136:C:H5'     | 1.89        | 0.54     |
| 1:A:1053:G:C6     | 1:A:1199:U:H2'    | 2.42        | 0.54     |
| 16:P:64:ALA:O     | 16:P:65:GLN:C     | 2.46        | 0.54     |
| 1:A:537:G:H5''    | 12:L:113:ARG:NH1  | 2.21        | 0.54     |
| 1:A:638:G:O2'     | 1:A:639:G:H5'     | 2.08        | 0.54     |
| 10:J:90:LEU:N     | 10:J:91:PRO:CD    | 2.70        | 0.54     |
| 24:Y:106:LEU:C    | 24:Y:108:ASN:H    | 2.11        | 0.54     |
| 3:C:167:TRP:O     | 3:C:168:ALA:HB3   | 2.07        | 0.54     |
| 8:H:29:SER:HB3    | 8:H:32:LYS:CG     | 2.37        | 0.54     |
| 2:B:52:GLU:O      | 2:B:56:ARG:HG2    | 2.07        | 0.54     |
| 24:Y:118:LEU:HD21 | 24:Y:210:VAL:HG22 | 1.88        | 0.54     |
| 4:D:25:ARG:NH1    | 4:D:30:LYS:HB2    | 2.23        | 0.54     |
| 19:S:28:LYS:NZ    | 19:S:29:ARG:NH2   | 2.55        | 0.54     |
| 2:B:114:ARG:O     | 2:B:114:ARG:HD3   | 2.07        | 0.54     |
| 5:E:72:GLN:O      | 5:E:75:THR:HG22   | 2.08        | 0.54     |
| 7:G:148:ASN:N     | 7:G:148:ASN:HD22  | 2.02        | 0.54     |
| 1:A:328:C:HO2'    | 1:A:329:A:P       | 2.29        | 0.54     |
| 2:B:15:VAL:HG23   | 2:B:16:HIS:CE1    | 2.42        | 0.54     |
| 1:A:314:C:O2'     | 1:A:315:A:H5'     | 2.06        | 0.54     |
| 22:W:70:G:H2'     | 22:W:71:G:C8      | 2.42        | 0.54     |
| 1:A:1427:U:H2'    | 1:A:1428:A:H8     | 1.72        | 0.54     |
| 24:Y:107:LEU:HD23 | 24:Y:107:LEU:O    | 2.07        | 0.54     |
| 2:B:167:PRO:HG3   | 2:B:188:ALA:CB    | 2.37        | 0.54     |
| 24:Y:152:GLU:O    | 24:Y:169:ILE:HG23 | 2.07        | 0.54     |
| 15:O:82:ILE:HG23  | 15:O:83:GLU:N     | 2.22        | 0.54     |
| 22:W:76:8AN:C4'   | 22:W:77:PHA:O     | 2.54        | 0.54     |
| 1:A:922:G:H2'     | 1:A:923:A:C8      | 2.42        | 0.54     |
| 2:B:44:LEU:H      | 2:B:44:LEU:HD12   | 1.72        | 0.54     |
| 2:B:164:VAL:HG12  | 2:B:165:VAL:N     | 2.23        | 0.54     |
| 13:M:96:LEU:HB3   | 13:M:97:PRO:HD2   | 1.88        | 0.54     |
| 24:Y:283:LEU:O    | 24:Y:287:GLU:HB2  | 2.07        | 0.54     |
| 3:C:7:PRO:O       | 3:C:11:ARG:HG2    | 2.08        | 0.54     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 13:M:126:LYS:N   | 24:Y:161:GLU:H   | 2.06        | 0.54     |
| 1:A:625:G:H2'    | 1:A:626:U:H6     | 1.70        | 0.54     |
| 24:Y:41:ASP:CB   | 24:Y:44:ALA:HB3  | 2.35        | 0.54     |
| 12:L:89:ARG:CB   | 12:L:89:ARG:HH11 | 2.20        | 0.54     |
| 3:C:73:PRO:C     | 3:C:76:VAL:HG22  | 2.28        | 0.54     |
| 3:C:83:ARG:O     | 3:C:86:VAL:HG22  | 2.08        | 0.54     |
| 7:G:73:MET:HA    | 7:G:91:VAL:HG23  | 1.90        | 0.54     |
| 24:Y:124:ALA:O   | 24:Y:129:ALA:HB2 | 2.08        | 0.54     |
| 1:A:272:C:H2'    | 1:A:273:A:C8     | 2.43        | 0.54     |
| 1:A:1082:G:O2'   | 1:A:1083:U:H5'   | 2.07        | 0.54     |
| 3:C:130:VAL:O    | 3:C:134:ILE:HG13 | 2.07        | 0.54     |
| 7:G:45:ASP:O     | 7:G:49:ILE:HG12  | 2.08        | 0.54     |
| 1:A:102:G:H2'    | 1:A:103:C:C6     | 2.43        | 0.54     |
| 13:M:112:GLY:O   | 13:M:113:PRO:HG2 | 2.07        | 0.54     |
| 1:A:980:C:H3'    | 1:A:981:U:C6     | 2.43        | 0.54     |
| 3:C:71:ALA:CA    | 3:C:106:VAL:HB   | 2.37        | 0.54     |
| 9:I:43:ALA:C     | 9:I:45:ALA:H     | 2.11        | 0.54     |
| 9:I:26:VAL:HG13  | 9:I:61:ALA:O     | 2.07        | 0.54     |
| 1:A:1026:G:N3    | 1:A:1026:G:H2'   | 2.21        | 0.54     |
| 1:A:1027:C:H2'   | 1:A:1028:C:C6    | 2.42        | 0.54     |
| 18:R:31:LEU:N    | 18:R:31:LEU:HD23 | 2.17        | 0.54     |
| 24:Y:50:GLN:HE21 | 24:Y:50:GLN:C    | 2.11        | 0.54     |
| 15:O:7:GLU:O     | 15:O:10:LYS:HB3  | 2.08        | 0.54     |
| 11:K:24:SER:O    | 11:K:26:ASN:N    | 2.41        | 0.54     |
| 2:B:204:ASN:C    | 2:B:204:ASN:HD22 | 2.11        | 0.54     |
| 4:D:129:ASN:HD21 | 4:D:145:GLU:H    | 1.55        | 0.54     |
| 10:J:57:LYS:HE3  | 10:J:60:ARG:HH22 | 1.72        | 0.54     |
| 1:A:1128:C:C1'   | 1:A:1146:A:H61   | 2.13        | 0.54     |
| 3:C:58:GLU:HB2   | 3:C:65:ALA:HB3   | 1.89        | 0.54     |
| 8:H:11:THR:HA    | 8:H:14:ARG:NH1   | 2.22        | 0.54     |
| 7:G:118:VAL:HG23 | 7:G:119:ARG:N    | 2.23        | 0.54     |
| 16:P:19:ILE:HD11 | 16:P:39:TYR:HB2  | 1.88        | 0.54     |
| 17:Q:76:LEU:HD12 | 17:Q:77:VAL:N    | 2.21        | 0.54     |
| 19:S:36:ARG:HB2  | 19:S:72:GLY:CA   | 2.38        | 0.54     |
| 1:A:203:U:H4'    | 1:A:216:G:C4     | 2.43        | 0.54     |
| 1:A:41:G:H2'     | 1:A:42:G:H8      | 1.73        | 0.54     |
| 22:W:12:U:H3     | 22:W:23:A:H61    | 1.55        | 0.54     |
| 15:O:6:GLU:OE1   | 15:O:6:GLU:N     | 2.40        | 0.54     |
| 22:W:19:G:H8     | 22:W:20:U:C5     | 2.23        | 0.54     |
| 4:D:33:MET:C     | 4:D:35:ARG:N     | 2.61        | 0.54     |
| 1:A:921:U:O2     | 5:E:19:MET:HB2   | 2.08        | 0.54     |
| 1:A:878:G:H5'    | 8:H:89:PRO:CG    | 2.35        | 0.54     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 5:E:147:ASP:HA    | 5:E:150:ARG:NH1   | 2.22        | 0.54     |
| 1:A:692:U:O2      | 1:A:694:A:C8      | 2.61        | 0.54     |
| 22:V:53:G:H2'     | 22:V:54:U:H6      | 1.72        | 0.54     |
| 12:L:119:LYS:O    | 12:L:120:TYR:HB2  | 2.07        | 0.54     |
| 1:A:233:C:O2'     | 1:A:234:C:H5'     | 2.07        | 0.54     |
| 1:A:977:A:H2'     | 1:A:978:A:H5'     | 1.89        | 0.54     |
| 24:Y:313:SER:OG   | 24:Y:324:HIS:HE1  | 1.91        | 0.54     |
| 1:A:1256:A:H5'    | 1:A:1257:U:OP1    | 2.08        | 0.54     |
| 13:M:125:ARG:CA   | 24:Y:159:GLY:HA3  | 2.38        | 0.54     |
| 7:G:69:VAL:CG1    | 7:G:100:ALA:HA    | 2.38        | 0.54     |
| 24:Y:25:ARG:O     | 24:Y:29:LEU:HB2   | 2.07        | 0.54     |
| 1:A:265:G:O3'     | 17:Q:66:SER:HA    | 2.08        | 0.54     |
| 2:B:222:ILE:O     | 2:B:226:ARG:HB2   | 2.08        | 0.54     |
| 1:A:1203:C:H2'    | 1:A:1204:A:H8     | 1.73        | 0.54     |
| 1:A:627:G:O2'     | 1:A:628:G:H5'     | 2.07        | 0.54     |
| 1:A:473:G:H2'     | 1:A:474:G:C8      | 2.43        | 0.54     |
| 5:E:27:ARG:HG2    | 5:E:28:PHE:N      | 2.22        | 0.54     |
| 6:F:84:ASN:O      | 6:F:86:ARG:HG3    | 2.08        | 0.54     |
| 24:Y:136:LEU:HD11 | 24:Y:187:HIS:CB   | 2.38        | 0.54     |
| 24:Y:223:LYS:C    | 24:Y:225:GLU:N    | 2.61        | 0.54     |
| 19:S:36:ARG:HB2   | 19:S:72:GLY:HA2   | 1.90        | 0.54     |
| 24:Y:224:PRO:HA   | 24:Y:227:LEU:HD12 | 1.90        | 0.54     |
| 8:H:109:ILE:HG12  | 8:H:110:ALA:N     | 2.22        | 0.54     |
| 2:B:36:ARG:HD2    | 2:B:36:ARG:N      | 2.22        | 0.54     |
| 1:A:605:U:H2'     | 1:A:606:G:O4'     | 2.07        | 0.54     |
| 1:A:1086:U:H2'    | 1:A:1087:G:H8     | 1.74        | 0.54     |
| 1:A:975:A:C4'     | 1:A:976:G:H5''    | 2.27        | 0.53     |
| 19:S:22:LEU:HD13  | 19:S:27:GLU:CB    | 2.38        | 0.53     |
| 1:A:591:U:H2'     | 1:A:592:G:C8      | 2.43        | 0.53     |
| 17:Q:66:SER:O     | 17:Q:70:ARG:NH1   | 2.41        | 0.53     |
| 8:H:82:HIS:CE1    | 8:H:84:ARG:HB2    | 2.43        | 0.53     |
| 5:E:47:LYS:HD3    | 5:E:47:LYS:N      | 2.23        | 0.53     |
| 16:P:19:ILE:N     | 16:P:19:ILE:HD12  | 2.22        | 0.53     |
| 7:G:64:GLN:NE2    | 7:G:68:ASN:HD21   | 2.05        | 0.53     |
| 24:Y:138:ARG:NH2  | 24:Y:337:LEU:HB3  | 2.23        | 0.53     |
| 2:B:219:VAL:O     | 2:B:222:ILE:HB    | 2.07        | 0.53     |
| 6:F:16:GLN:O      | 6:F:20:ALA:HB2    | 2.08        | 0.53     |
| 12:L:110:VAL:CG2  | 12:L:120:TYR:HB3  | 2.37        | 0.53     |
| 1:A:323:U:H2'     | 1:A:324:G:O4'     | 2.08        | 0.53     |
| 1:A:879:C:O2'     | 1:A:880:C:H5'     | 2.08        | 0.53     |
| 1:A:309:G:O2'     | 1:A:310:G:H5'     | 2.08        | 0.53     |
| 22:V:74:C:OP2     | 24:Y:266:ARG:NH1  | 2.41        | 0.53     |

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| Atom-1            | Atom-2           | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 8:H:58:TYR:O      | 8:H:59:LEU:HD23  | 2.07        | 0.53     |
| 24:Y:111:HIS:CE1  | 24:Y:214:VAL:HB  | 2.42        | 0.53     |
| 1:A:1227:A:H2'    | 1:A:1228:C:O5'   | 2.08        | 0.53     |
| 12:L:58:VAL:O     | 12:L:60:LEU:HD22 | 2.08        | 0.53     |
| 1:A:1005:A:C2'    | 1:A:1006:C:H5'   | 2.38        | 0.53     |
| 5:E:19:MET:O      | 5:E:20:GLN:HB2   | 2.08        | 0.53     |
| 11:K:22:HIS:HB3   | 11:K:29:ILE:HG22 | 1.90        | 0.53     |
| 24:Y:76:MET:HE2   | 24:Y:88:LYS:HE2  | 1.90        | 0.53     |
| 20:T:84:LEU:O     | 20:T:88:VAL:HG23 | 2.08        | 0.53     |
| 1:A:1007:C:H2'    | 1:A:1008:C:C5    | 2.43        | 0.53     |
| 2:B:204:ASN:HD22  | 2:B:206:ASP:H    | 1.55        | 0.53     |
| 5:E:68:GLU:O      | 5:E:70:PRO:HD3   | 2.08        | 0.53     |
| 1:A:81:U:H2'      | 1:A:82:U:C6      | 2.43        | 0.53     |
| 2:B:163:PHE:HA    | 2:B:185:ILE:O    | 2.08        | 0.53     |
| 2:B:167:PRO:HG2   | 2:B:192:SER:OG   | 2.09        | 0.53     |
| 2:B:75:LYS:HD3    | 2:B:78:GLN:NE2   | 2.24        | 0.53     |
| 1:A:939:G:H2'     | 1:A:940:C:C6     | 2.44        | 0.53     |
| 1:A:458:C:N4      | 1:A:474:G:H1     | 2.07        | 0.53     |
| 12:L:27:LEU:C     | 12:L:29:GLY:H    | 2.11        | 0.53     |
| 1:A:1104:G:H4'    | 2:B:111:ARG:NH1  | 2.23        | 0.53     |
| 24:Y:52:ALA:HA    | 24:Y:55:LEU:HD13 | 1.89        | 0.53     |
| 5:E:12:LEU:HD13   | 5:E:31:LEU:HB3   | 1.90        | 0.53     |
| 1:A:1015:A:H2'    | 1:A:1016:A:H8    | 1.73        | 0.53     |
| 1:A:1097:C:H2'    | 1:A:1098:C:H6    | 1.73        | 0.53     |
| 18:R:53:ARG:NH1   | 18:R:60:ALA:HA   | 2.24        | 0.53     |
| 1:A:300:A:H2'     | 1:A:301:G:O4'    | 2.07        | 0.53     |
| 15:O:70:LEU:HD11  | 15:O:77:ARG:HG3  | 1.90        | 0.53     |
| 22:W:56:C:N3      | 22:W:57:G:N7     | 2.56        | 0.53     |
| 4:D:18:LYS:HE2    | 4:D:31:CYS:CB    | 2.38        | 0.53     |
| 1:A:674:G:H2'     | 1:A:675:A:C8     | 2.39        | 0.53     |
| 1:A:192:U:H2'     | 1:A:193:C:H6     | 1.71        | 0.53     |
| 20:T:104:LEU:HD23 | 20:T:105:SER:N   | 2.23        | 0.53     |
| 12:L:58:VAL:O     | 12:L:65:GLU:HA   | 2.08        | 0.53     |
| 22:V:51:U:H2'     | 22:V:52:G:H8     | 1.69        | 0.53     |
| 1:A:390:C:H2'     | 1:A:391:G:H8     | 1.71        | 0.53     |
| 24:Y:17:LEU:O     | 24:Y:20:PRO:HD2  | 2.08        | 0.53     |
| 1:A:170:U:O2'     | 1:A:171:A:H5'    | 2.08        | 0.53     |
| 3:C:179:ARG:HH21  | 3:C:207:VAL:HG22 | 1.72        | 0.53     |
| 1:A:639:G:O2'     | 1:A:640:A:H5'    | 2.08        | 0.53     |
| 1:A:1381:U:H5     | 1:A:1382:C:C5    | 2.27        | 0.53     |
| 1:A:646:U:H2'     | 1:A:647:C:C6     | 2.43        | 0.53     |
| 1:A:599:C:H4'     | 8:H:130:GLY:HA3  | 1.90        | 0.53     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:1478:C:O2'   | 1:A:1479:C:H5'    | 2.08        | 0.53     |
| 24:Y:209:GLU:OE2 | 24:Y:303:ARG:HD2  | 2.04        | 0.53     |
| 4:D:31:CYS:C     | 4:D:33:MET:N      | 2.62        | 0.53     |
| 24:Y:120:ILE:CG2 | 24:Y:133:ALA:HB1  | 2.39        | 0.53     |
| 15:O:63:ARG:NH1  | 15:O:87:ILE:HG21  | 2.23        | 0.53     |
| 1:A:865:A:C2     | 1:A:918:A:H4'     | 2.44        | 0.53     |
| 12:L:104:VAL:O   | 12:L:107:ALA:HB3  | 2.09        | 0.53     |
| 4:D:47:ARG:NE    | 4:D:49:ARG:HH22   | 2.05        | 0.53     |
| 1:A:383:A:H2'    | 1:A:384:G:O4'     | 2.08        | 0.53     |
| 5:E:93:PRO:HG2   | 8:H:105:ARG:NH2   | 2.23        | 0.53     |
| 1:A:1060:C:C4    | 3:C:2:GLY:HA3     | 2.43        | 0.53     |
| 1:A:1086:U:H2'   | 1:A:1087:G:O4'    | 2.09        | 0.53     |
| 3:C:107:GLN:H    | 3:C:107:GLN:NE2   | 2.06        | 0.53     |
| 24:Y:154:VAL:O   | 24:Y:154:VAL:HG12 | 2.09        | 0.53     |
| 8:H:45:ILE:O     | 8:H:45:ILE:HG13   | 2.07        | 0.53     |
| 1:A:918:A:H2'    | 1:A:919:A:C8      | 2.43        | 0.53     |
| 16:P:3:LYS:O     | 16:P:21:VAL:HA    | 2.08        | 0.53     |
| 10:J:16:LEU:HD23 | 10:J:94:VAL:HG13  | 1.90        | 0.53     |
| 4:D:152:SER:HA   | 4:D:155:LEU:CD1   | 2.38        | 0.53     |
| 7:G:29:LYS:HB2   | 7:G:105:VAL:HG21  | 1.89        | 0.53     |
| 1:A:487:A:H2'    | 1:A:488:C:O4'     | 2.08        | 0.53     |
| 1:A:1223:C:P     | 19:S:78:ARG:HH21  | 2.31        | 0.53     |
| 9:I:45:ALA:HA    | 9:I:48:GLU:OE1    | 2.08        | 0.53     |
| 1:A:1034:G:H2'   | 1:A:1035:A:C5     | 2.43        | 0.53     |
| 9:I:4:TYR:HA     | 9:I:88:TYR:CE1    | 2.44        | 0.53     |
| 9:I:18:PHE:HD1   | 9:I:62:TYR:CD2    | 2.26        | 0.53     |
| 12:L:47:LYS:HE2  | 12:L:48:PRO:HD3   | 1.89        | 0.53     |
| 12:L:50:SER:O    | 12:L:51:ALA:HB2   | 2.09        | 0.53     |
| 14:N:7:ILE:O     | 14:N:11:LYS:HG2   | 2.08        | 0.53     |
| 10:J:33:GLN:N    | 10:J:75:ILE:HD11  | 2.24        | 0.53     |
| 1:A:1118:C:H5'   | 9:I:104:ARG:HD2   | 1.90        | 0.53     |
| 1:A:1316:G:O2'   | 14:N:18:VAL:HG11  | 2.08        | 0.53     |
| 24:Y:268:GLN:O   | 24:Y:272:LYS:HG3  | 2.09        | 0.53     |
| 1:A:829:G:O2'    | 1:A:830:G:H5'     | 2.08        | 0.53     |
| 1:A:1008:C:H42   | 1:A:1021:G:H1     | 1.55        | 0.53     |
| 8:H:122:ARG:CZ   | 8:H:122:ARG:HB2   | 2.37        | 0.53     |
| 24:Y:139:MET:HE3 | 24:Y:341:LEU:HD21 | 1.91        | 0.53     |
| 1:A:474:G:H2'    | 1:A:475:G:H8      | 1.70        | 0.53     |
| 9:I:5:TYR:HD2    | 9:I:18:PHE:CE2    | 2.26        | 0.53     |
| 19:S:9:VAL:O     | 19:S:11:VAL:N     | 2.41        | 0.53     |
| 10:J:98:ILE:O    | 10:J:99:LYS:HD3   | 2.08        | 0.53     |
| 13:M:19:LEU:HD22 | 13:M:19:LEU:N     | 2.24        | 0.53     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 3:C:92:ALA:HA     | 3:C:95:THR:HB     | 1.90        | 0.53     |
| 6:F:79:LEU:HD12   | 6:F:88:VAL:HG13   | 1.91        | 0.53     |
| 2:B:19:HIS:CG     | 2:B:20:GLU:H      | 2.26        | 0.53     |
| 1:A:545:C:H5''    | 4:D:72:GLU:HG2    | 1.91        | 0.53     |
| 12:L:110:VAL:HG21 | 12:L:120:TYR:HB3  | 1.91        | 0.53     |
| 24:Y:156:LEU:HD23 | 24:Y:157:THR:N    | 2.24        | 0.53     |
| 1:A:84:U:O2'      | 1:A:88:A:H5'      | 2.09        | 0.53     |
| 23:X:15:A:C4      | 23:X:15:A:H5''    | 2.44        | 0.53     |
| 2:B:185:ILE:HG22  | 2:B:199:TYR:CB    | 2.32        | 0.53     |
| 3:C:186:PHE:CZ    | 3:C:188:LEU:HD21  | 2.44        | 0.53     |
| 2:B:80:ILE:N      | 2:B:80:ILE:HD12   | 2.20        | 0.53     |
| 1:A:116:A:H8      | 1:A:116:A:O5'     | 1.91        | 0.53     |
| 1:A:237:C:H4'     | 17:Q:25:ARG:NH1   | 2.24        | 0.53     |
| 1:A:163:C:O2'     | 1:A:164:U:H5'     | 2.09        | 0.53     |
| 1:A:751:U:C2'     | 1:A:752:G:H5'     | 2.39        | 0.53     |
| 2:B:93:VAL:HG11   | 2:B:97:TRP:HD1    | 1.73        | 0.53     |
| 24:Y:116:ALA:HB1  | 24:Y:210:VAL:HG12 | 1.91        | 0.53     |
| 13:M:79:LYS:O     | 13:M:82:MET:HB3   | 2.08        | 0.53     |
| 2:B:142:LEU:HA    | 2:B:145:LEU:HB2   | 1.91        | 0.53     |
| 2:B:29:ALA:HA     | 2:B:32:ILE:HG22   | 1.91        | 0.53     |
| 4:D:15:GLU:OE1    | 4:D:15:GLU:HA     | 2.08        | 0.53     |
| 24:Y:29:LEU:HG    | 24:Y:51:GLU:CB    | 2.39        | 0.53     |
| 1:A:1211:U:H5'    | 1:A:1212:U:OP1    | 2.09        | 0.53     |
| 24:Y:81:ALA:HB3   | 24:Y:84:ARG:NE    | 2.24        | 0.53     |
| 16:P:51:VAL:HG11  | 16:P:74:LEU:HD23  | 1.91        | 0.53     |
| 1:A:353:A:H5'     | 1:A:353:A:C8      | 2.41        | 0.53     |
| 7:G:136:LYS:O     | 7:G:140:ASP:HB2   | 2.09        | 0.53     |
| 1:A:1158:C:C2'    | 1:A:1158:C:O2     | 2.57        | 0.53     |
| 20:T:18:GLN:O     | 20:T:22:ARG:HG3   | 2.09        | 0.53     |
| 1:A:862:C:O2'     | 1:A:863:U:H5'     | 2.08        | 0.53     |
| 13:M:105:THR:O    | 13:M:106:ASN:C    | 2.47        | 0.53     |
| 6:F:39:LYS:O      | 6:F:40:VAL:HB     | 2.10        | 0.52     |
| 4:D:31:CYS:O      | 4:D:32:ALA:HB3    | 2.09        | 0.52     |
| 1:A:1144:G:H21    | 1:A:1146:A:N6     | 2.06        | 0.52     |
| 24:Y:348:GLY:O    | 24:Y:352:LYS:HB2  | 2.09        | 0.52     |
| 13:M:90:LEU:C     | 13:M:92:HIS:N     | 2.60        | 0.52     |
| 9:I:48:GLU:N      | 9:I:49:PRO:HD2    | 2.24        | 0.52     |
| 1:A:1123:A:H4'    | 10:J:36:GLY:HA3   | 1.89        | 0.52     |
| 1:A:437:U:H2'     | 1:A:438:G:O4'     | 2.09        | 0.52     |
| 24:Y:142:ARG:HB2  | 24:Y:338:ASP:O    | 2.08        | 0.52     |
| 1:A:47:C:H5''     | 1:A:365:U:C6      | 2.44        | 0.52     |
| 1:A:1478:C:H2'    | 1:A:1479:C:H6     | 1.73        | 0.52     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 5:E:135:THR:O    | 5:E:138:ALA:N     | 2.42        | 0.52     |
| 3:C:34:LEU:CD2   | 3:C:38:ARG:HD2    | 2.37        | 0.52     |
| 9:I:112:LYS:HA   | 9:I:119:ALA:HB2   | 1.90        | 0.52     |
| 20:T:26:ASN:N    | 20:T:26:ASN:HD22  | 2.06        | 0.52     |
| 1:A:797:C:OP1    | 11:K:124:LYS:HE3  | 2.09        | 0.52     |
| 1:A:543:C:C2     | 1:A:544:G:C8      | 2.97        | 0.52     |
| 19:S:51:VAL:O    | 19:S:58:VAL:HG22  | 2.09        | 0.52     |
| 11:K:61:ALA:CB   | 11:K:90:GLY:HA3   | 2.39        | 0.52     |
| 24:Y:239:GLY:O   | 24:Y:243:ASN:CG   | 2.48        | 0.52     |
| 12:L:65:GLU:HG2  | 12:L:65:GLU:O     | 2.09        | 0.52     |
| 1:A:1004:A:H5'   | 1:A:1005:A:OP1    | 2.08        | 0.52     |
| 1:A:523:A:H61    | 12:L:53:ARG:HH12  | 1.56        | 0.52     |
| 12:L:53:ARG:NH1  | 12:L:92:ASP:OD2   | 2.42        | 0.52     |
| 24:Y:25:ARG:NH1  | 24:Y:29:LEU:HD23  | 2.22        | 0.52     |
| 1:A:407:G:H1'    | 4:D:119:GLN:OE1   | 2.10        | 0.52     |
| 1:A:1055:A:C2    | 3:C:194:GLY:HA2   | 2.44        | 0.52     |
| 7:G:148:ASN:C    | 7:G:150:ALA:N     | 2.62        | 0.52     |
| 1:A:1172:C:H2'   | 1:A:1173:G:C8     | 2.40        | 0.52     |
| 1:A:715:A:O2'    | 1:A:716:A:H5'     | 2.10        | 0.52     |
| 1:A:1096:C:O2'   | 1:A:1097:C:H5'    | 2.09        | 0.52     |
| 4:D:61:LYS:HG3   | 4:D:203:VAL:HG13  | 1.91        | 0.52     |
| 9:I:53:VAL:HB    | 9:I:92:TYR:CE2    | 2.45        | 0.52     |
| 1:A:243:A:O2'    | 1:A:244:U:OP2     | 2.27        | 0.52     |
| 19:S:20:LEU:HA   | 19:S:23:ASN:HD22  | 1.72        | 0.52     |
| 1:A:1052:U:H5'   | 24:Y:319:ASN:HD22 | 1.75        | 0.52     |
| 1:A:541:G:H2'    | 1:A:542:G:H8      | 1.73        | 0.52     |
| 1:A:1060:C:H2'   | 1:A:1061:G:H8     | 1.75        | 0.52     |
| 1:A:1529:G:H4'   | 1:A:1530:G:OP2    | 2.10        | 0.52     |
| 8:H:13:ILE:O     | 8:H:17:THR:HG23   | 2.10        | 0.52     |
| 1:A:280:C:O2     | 17:Q:38:ARG:HG3   | 2.09        | 0.52     |
| 7:G:76:ARG:HG2   | 7:G:76:ARG:HH11   | 1.75        | 0.52     |
| 1:A:192:U:C4'    | 20:T:103:GLY:N    | 2.71        | 0.52     |
| 2:B:121:LEU:HD21 | 2:B:126:GLU:OE2   | 2.10        | 0.52     |
| 1:A:1242:C:H5''  | 21:U:10:ARG:HH12  | 1.74        | 0.52     |
| 15:O:16:ALA:HA   | 15:O:27:VAL:CG2   | 2.40        | 0.52     |
| 1:A:383:A:H2'    | 1:A:384:G:C5'     | 2.39        | 0.52     |
| 1:A:104:G:H4'    | 1:A:174:C:O4'     | 2.09        | 0.52     |
| 1:A:179:A:H2'    | 1:A:180:U:H6      | 1.74        | 0.52     |
| 1:A:711:G:O2'    | 1:A:712:A:H5'     | 2.10        | 0.52     |
| 24:Y:263:GLN:HA  | 24:Y:271:ASN:ND2  | 2.25        | 0.52     |
| 18:R:43:PHE:O    | 18:R:51:LEU:HD12  | 2.09        | 0.52     |
| 5:E:105:VAL:HB   | 5:E:106:PRO:HD3   | 1.92        | 0.52     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 5:E:8:GLU:N       | 5:E:34:VAL:HG23   | 2.24        | 0.52     |
| 9:I:42:ARG:NH1    | 9:I:71:SER:OG     | 2.42        | 0.52     |
| 1:A:1029:C:H4'    | 1:A:1033:G:H22    | 1.74        | 0.52     |
| 7:G:16:LEU:O      | 7:G:17:VAL:HG23   | 2.10        | 0.52     |
| 13:M:21:TYR:C     | 13:M:22:ILE:HD12  | 2.30        | 0.52     |
| 16:P:19:ILE:H     | 16:P:19:ILE:CD1   | 2.23        | 0.52     |
| 12:L:7:ILE:CG2    | 12:L:8:ASN:N      | 2.72        | 0.52     |
| 24:Y:138:ARG:HH22 | 24:Y:337:LEU:HD13 | 1.73        | 0.52     |
| 15:O:48:LYS:CA    | 15:O:48:LYS:HE2   | 2.40        | 0.52     |
| 1:A:104:G:O2'     | 1:A:105:G:H5'     | 2.09        | 0.52     |
| 1:A:1438:G:H2'    | 1:A:1439:C:H6     | 1.74        | 0.52     |
| 3:C:5:ILE:O       | 3:C:5:ILE:HD13    | 2.09        | 0.52     |
| 24:Y:263:GLN:O    | 24:Y:263:GLN:HG2  | 2.10        | 0.52     |
| 1:A:558:G:H2'     | 1:A:559:A:H2      | 1.74        | 0.52     |
| 20:T:51:GLU:HA    | 20:T:54:LYS:NZ    | 2.24        | 0.52     |
| 3:C:37:GLN:NE2    | 14:N:52:GLN:OE1   | 2.42        | 0.52     |
| 1:A:1206:G:H4'    | 3:C:192:THR:O     | 2.10        | 0.52     |
| 1:A:1447:A:N3     | 1:A:1447:A:H2'    | 2.23        | 0.52     |
| 13:M:88:ARG:CA    | 13:M:98:VAL:HG11  | 2.23        | 0.52     |
| 9:I:65:VAL:HG21   | 9:I:73:GLN:CB     | 2.33        | 0.52     |
| 7:G:69:VAL:HG12   | 7:G:100:ALA:HA    | 1.91        | 0.52     |
| 24:Y:26:LEU:CB    | 24:Y:55:LEU:HD11  | 2.40        | 0.52     |
| 17:Q:59:ILE:HG23  | 17:Q:72:ARG:O     | 2.09        | 0.52     |
| 12:L:24:VAL:CG2   | 12:L:97:ARG:HB3   | 2.39        | 0.52     |
| 2:B:130:ARG:HB3   | 2:B:134:GLU:HG3   | 1.91        | 0.52     |
| 7:G:140:ASP:HA    | 7:G:143:ARG:HH11  | 1.73        | 0.52     |
| 2:B:223:ILE:HG12  | 2:B:226:ARG:CZ    | 2.40        | 0.52     |
| 22:V:53:G:H2'     | 22:V:54:U:C6      | 2.45        | 0.52     |
| 1:A:615:C:H2'     | 1:A:616:G:O4'     | 2.10        | 0.52     |
| 4:D:161:ASN:O     | 4:D:162:LEU:HG    | 2.09        | 0.52     |
| 7:G:6:ARG:HG2     | 7:G:6:ARG:O       | 2.09        | 0.52     |
| 2:B:185:ILE:HA    | 2:B:199:TYR:O     | 2.10        | 0.52     |
| 4:D:20:TYR:CD1    | 4:D:20:TYR:N      | 2.78        | 0.52     |
| 24:Y:257:GLY:O    | 24:Y:259:THR:HG23 | 2.10        | 0.52     |
| 1:A:1351:U:O2'    | 1:A:1352:C:H5'    | 2.09        | 0.52     |
| 1:A:1369:C:H2'    | 1:A:1370:G:C8     | 2.45        | 0.52     |
| 8:H:20:TYR:HD1    | 8:H:65:TYR:CD2    | 2.26        | 0.52     |
| 1:A:1019:C:O2'    | 1:A:1020:U:H5'    | 2.09        | 0.52     |
| 17:Q:90:ILE:HG23  | 17:Q:93:GLN:NE2   | 2.25        | 0.52     |
| 24:Y:238:GLY:CA   | 24:Y:242:VAL:HB   | 2.26        | 0.52     |
| 9:I:77:ILE:O      | 9:I:77:ILE:HG22   | 2.09        | 0.52     |
| 22:W:25:C:H2'     | 22:W:26:A:C8      | 2.29        | 0.52     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 23:X:20:A:N6     | 24:Y:195:PHE:HB2  | 2.25        | 0.52     |
| 2:B:200:ILE:HG22 | 2:B:201:ILE:N     | 2.24        | 0.52     |
| 2:B:42:ILE:HD11  | 2:B:202:PRO:HB2   | 1.92        | 0.52     |
| 16:P:9:PHE:HB2   | 16:P:16:HIS:O     | 2.10        | 0.52     |
| 4:D:132:ARG:NH1  | 4:D:132:ARG:HG2   | 2.23        | 0.52     |
| 4:D:149:ALA:HB3  | 4:D:152:SER:OG    | 2.10        | 0.52     |
| 8:H:65:TYR:CD1   | 8:H:65:TYR:N      | 2.78        | 0.52     |
| 2:B:238:LEU:HG   | 2:B:239:VAL:N     | 2.25        | 0.52     |
| 9:I:122:ALA:HB1  | 9:I:123:PRO:HD2   | 1.92        | 0.52     |
| 6:F:89:MET:SD    | 18:R:76:LEU:HD21  | 2.50        | 0.52     |
| 9:I:64:THR:O     | 9:I:64:THR:HG22   | 2.08        | 0.52     |
| 24:Y:152:GLU:OE1 | 24:Y:170:LEU:HD23 | 2.09        | 0.52     |
| 24:Y:309:SER:O   | 24:Y:310:GLN:HG3  | 2.10        | 0.52     |
| 22:W:59:U:N1     | 22:W:60:U:H5      | 2.08        | 0.52     |
| 24:Y:242:VAL:CG1 | 24:Y:243:ASN:N    | 2.72        | 0.52     |
| 3:C:186:PHE:CE2  | 3:C:188:LEU:HD21  | 2.44        | 0.52     |
| 1:A:1143:G:H2'   | 1:A:1144:G:H8     | 1.73        | 0.52     |
| 1:A:16:A:N1      | 1:A:919:A:C2      | 2.78        | 0.52     |
| 1:A:1151:A:HO2'  | 1:A:1152:A:H8     | 1.58        | 0.52     |
| 12:L:42:THR:OG1  | 12:L:52:LEU:HB3   | 2.10        | 0.52     |
| 1:A:624:C:H2'    | 1:A:625:G:C8      | 2.37        | 0.52     |
| 4:D:119:GLN:O    | 4:D:123:HIS:CD2   | 2.63        | 0.52     |
| 1:A:1315:U:H2'   | 1:A:1316:G:O4'    | 2.10        | 0.52     |
| 10:J:63:PHE:HD1  | 14:N:58:LYS:HG2   | 1.74        | 0.52     |
| 13:M:116:THR:O   | 13:M:116:THR:HG22 | 2.10        | 0.52     |
| 1:A:1088:G:H2'   | 1:A:1089:G:H8     | 1.74        | 0.52     |
| 1:A:9:G:H2'      | 1:A:10:A:H8       | 1.75        | 0.52     |
| 1:A:119:A:O2'    | 1:A:120:A:OP2     | 2.21        | 0.52     |
| 2:B:70:PHE:HA    | 2:B:163:PHE:O     | 2.10        | 0.51     |
| 22:W:16:U:C2     | 22:W:18:G:H3'     | 2.44        | 0.51     |
| 22:W:52:G:N1     | 22:W:62:C:N4      | 2.58        | 0.51     |
| 10:J:49:VAL:HG22 | 10:J:50:ILE:N     | 2.25        | 0.51     |
| 3:C:16:ARG:HG3   | 3:C:17:ASP:O      | 2.10        | 0.51     |
| 1:A:1279:A:N3    | 1:A:1279:A:H2'    | 2.25        | 0.51     |
| 1:A:1029:C:H2'   | 1:A:1030(A):G:C5  | 2.45        | 0.51     |
| 2:B:67:THR:HG21  | 2:B:155:LEU:CD1   | 2.38        | 0.51     |
| 1:A:90:U:OP2     | 1:A:91:C:H5'      | 2.10        | 0.51     |
| 1:A:385:C:O2'    | 1:A:386:C:H5'     | 2.10        | 0.51     |
| 3:C:47:LEU:HD11  | 3:C:68:VAL:HG11   | 1.91        | 0.51     |
| 8:H:103:VAL:CG2  | 8:H:110:ALA:HB2   | 2.39        | 0.51     |
| 2:B:25:ASN:O     | 2:B:27:LYS:N      | 2.43        | 0.51     |
| 1:A:42:G:H2'     | 1:A:43:C:C6       | 2.46        | 0.51     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:820:U:H4'    | 1:A:821:G:OP2    | 2.10        | 0.51     |
| 2:B:158:LEU:HD22 | 2:B:182:ILE:HD11 | 1.92        | 0.51     |
| 1:A:1298:C:N4    | 7:G:114:ARG:HB3  | 2.25        | 0.51     |
| 24:Y:346:TRP:N   | 24:Y:346:TRP:HE3 | 2.08        | 0.51     |
| 1:A:1372:U:OP1   | 9:I:72:GLY:N     | 2.43        | 0.51     |
| 24:Y:23:GLU:OE1  | 24:Y:26:LEU:HD23 | 2.10        | 0.51     |
| 1:A:1302:U:C5    | 13:M:17:VAL:HG21 | 2.46        | 0.51     |
| 1:A:1053:G:N7    | 1:A:1199:U:H3'   | 2.25        | 0.51     |
| 19:S:62:ILE:HD12 | 19:S:66:MET:CE   | 2.41        | 0.51     |
| 3:C:119:ARG:HH21 | 3:C:140:ARG:HE   | 1.59        | 0.51     |
| 24:Y:119:THR:CG2 | 24:Y:166:TYR:HE1 | 2.23        | 0.51     |
| 17:Q:11:VAL:O    | 17:Q:12:SER:HB2  | 2.10        | 0.51     |
| 1:A:1409:C:H2'   | 1:A:1410:G:H8    | 1.74        | 0.51     |
| 1:A:102:G:H2'    | 1:A:103:C:H6     | 1.75        | 0.51     |
| 1:A:1307:U:H2'   | 1:A:1308:U:C6    | 2.46        | 0.51     |
| 1:A:814:A:N7     | 1:A:816:A:C4     | 2.78        | 0.51     |
| 19:S:6:LYS:O     | 19:S:7:LYS:HD3   | 2.11        | 0.51     |
| 12:L:26:ALA:C    | 12:L:27:LEU:HD22 | 2.31        | 0.51     |
| 1:A:1002:G:H2'   | 1:A:1003:G:H5'   | 1.93        | 0.51     |
| 5:E:101:ILE:CD1  | 5:E:119:LEU:HD23 | 2.35        | 0.51     |
| 1:A:1505:G:H5''  | 1:A:1506:U:H5''  | 1.92        | 0.51     |
| 17:Q:59:ILE:HD12 | 17:Q:73:VAL:HA   | 1.91        | 0.51     |
| 1:A:1287:A:C2    | 1:A:1353:G:H1'   | 2.45        | 0.51     |
| 4:D:126:ILE:CG2  | 4:D:127:THR:H    | 2.23        | 0.51     |
| 10:J:8:LEU:HB3   | 10:J:16:LEU:HD21 | 1.93        | 0.51     |
| 2:B:223:ILE:HG12 | 2:B:226:ARG:NH2  | 2.26        | 0.51     |
| 1:A:793:U:H5'    | 1:A:794:A:O5'    | 2.09        | 0.51     |
| 11:K:126:ARG:CZ  | 11:K:126:ARG:HB3 | 2.40        | 0.51     |
| 20:T:24:LEU:HD13 | 20:T:24:LEU:C    | 2.30        | 0.51     |
| 2:B:167:PRO:HG3  | 2:B:188:ALA:HB2  | 1.91        | 0.51     |
| 1:A:963:G:H21    | 10:J:55:LYS:CD   | 2.23        | 0.51     |
| 4:D:33:MET:O     | 4:D:35:ARG:N     | 2.41        | 0.51     |
| 1:A:997:U:H2'    | 1:A:998:G:H8     | 1.76        | 0.51     |
| 8:H:51:VAL:HG11  | 8:H:60:ARG:CD    | 2.41        | 0.51     |
| 4:D:61:LYS:NZ    | 4:D:62:GLN:HE21  | 2.07        | 0.51     |
| 10:J:92:THR:HG23 | 10:J:93:GLY:N    | 2.25        | 0.51     |
| 1:A:130:A:C8     | 17:Q:63:ARG:HG3  | 2.44        | 0.51     |
| 22:W:16:U:C3'    | 22:W:17:C:H5'    | 2.25        | 0.51     |
| 1:A:1318:A:H4'   | 19:S:10:PHE:HB2  | 1.92        | 0.51     |
| 22:V:40:C:H2'    | 22:V:41:C:C6     | 2.45        | 0.51     |
| 7:G:69:VAL:HG21  | 7:G:104:LEU:HD21 | 1.93        | 0.51     |
| 1:A:60:A:H8      | 1:A:60:A:P       | 2.34        | 0.51     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:559:A:H4'     | 1:A:560:U:H5''    | 1.92        | 0.51     |
| 1:A:1127:G:O2'    | 1:A:1128:C:H5'    | 2.11        | 0.51     |
| 1:A:1372:U:H2'    | 1:A:1373:G:O4'    | 2.10        | 0.51     |
| 22:V:50:U:O2'     | 22:V:51:U:H5'     | 2.11        | 0.51     |
| 5:E:20:GLN:O      | 5:E:23:GLY:O      | 2.29        | 0.51     |
| 11:K:111:ASP:HA   | 18:R:84:LYS:CD    | 2.41        | 0.51     |
| 13:M:14:ARG:NH2   | 13:M:16:ASP:OD1   | 2.44        | 0.51     |
| 2:B:139:LYS:O     | 2:B:143:GLU:HG3   | 2.10        | 0.51     |
| 1:A:1081:G:O2'    | 1:A:1082:G:H5'    | 2.10        | 0.51     |
| 6:F:8:ILE:CG2     | 6:F:9:VAL:N       | 2.73        | 0.51     |
| 1:A:826:C:H2'     | 1:A:827:U:C6      | 2.45        | 0.51     |
| 22:W:6:G:H21      | 22:W:7:A:H62      | 1.58        | 0.51     |
| 11:K:79:SER:OG    | 11:K:106:LYS:HE3  | 2.11        | 0.51     |
| 15:O:3:ILE:HG13   | 15:O:3:ILE:O      | 2.10        | 0.51     |
| 5:E:91:LEU:HD22   | 5:E:91:LEU:N      | 2.25        | 0.51     |
| 5:E:140:ARG:HG2   | 5:E:140:ARG:O     | 2.11        | 0.51     |
| 10:J:13:HIS:CE1   | 10:J:14:LYS:HG3   | 2.45        | 0.51     |
| 1:A:735:C:O2'     | 1:A:736:C:H5'     | 2.11        | 0.51     |
| 1:A:423:G:C2'     | 1:A:424:G:H5'     | 2.41        | 0.51     |
| 19:S:31:ILE:HG23  | 19:S:31:ILE:O     | 2.11        | 0.51     |
| 1:A:1399:C:H4'    | 1:A:1400:C:O5'    | 2.11        | 0.51     |
| 1:A:1502:A:H2     | 1:A:1505:G:N1     | 2.02        | 0.51     |
| 1:A:1205:U:C1'    | 3:C:195:VAL:HG21  | 2.41        | 0.51     |
| 24:Y:227:LEU:HD11 | 24:Y:276:LEU:HD21 | 1.91        | 0.51     |
| 14:N:9:LYS:HG3    | 14:N:12:ARG:NH2   | 2.26        | 0.51     |
| 1:A:1499:A:H1'    | 1:A:1520:G:H5''   | 1.91        | 0.51     |
| 4:D:52:SER:O      | 4:D:53:ASP:C      | 2.49        | 0.51     |
| 1:A:151:A:H2'     | 1:A:152:A:H5'     | 1.93        | 0.51     |
| 9:I:65:VAL:HB     | 9:I:77:ILE:HD11   | 1.93        | 0.51     |
| 16:P:49:LEU:O     | 16:P:50:LYS:HB2   | 2.11        | 0.51     |
| 3:C:34:LEU:HD23   | 3:C:34:LEU:C      | 2.31        | 0.51     |
| 1:A:1305:G:C2     | 1:A:1331:G:N3     | 2.79        | 0.51     |
| 17:Q:65:ILE:O     | 17:Q:66:SER:HB3   | 2.10        | 0.51     |
| 5:E:31:LEU:HD21   | 5:E:43:LEU:HD11   | 1.91        | 0.51     |
| 11:K:78:GLN:O     | 11:K:103:LEU:HD13 | 2.11        | 0.51     |
| 13:M:65:LYS:O     | 13:M:66:LEU:N     | 2.43        | 0.51     |
| 24:Y:149:PHE:HZ   | 24:Y:179:LEU:HD22 | 1.76        | 0.51     |
| 1:A:1427:U:H2'    | 1:A:1428:A:C8     | 2.46        | 0.51     |
| 11:K:79:SER:HB2   | 11:K:106:LYS:HE3  | 1.93        | 0.51     |
| 1:A:425:G:O2'     | 1:A:426:G:H5'     | 2.11        | 0.51     |
| 24:Y:72:LEU:HB2   | 24:Y:91:LEU:HG    | 1.93        | 0.51     |
| 13:M:65:LYS:HB2   | 13:M:69:GLU:O     | 2.09        | 0.51     |

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| Atom-1            | Atom-2           | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 16:P:7:ALA:O      | 16:P:17:TYR:HA   | 2.11        | 0.51     |
| 1:A:1329:A:P      | 13:M:28:ALA:HB3  | 2.51        | 0.51     |
| 1:A:514:C:O2'     | 1:A:515:G:H5'    | 2.11        | 0.51     |
| 1:A:681:C:O2'     | 1:A:682:G:H5'    | 2.11        | 0.51     |
| 2:B:61:LEU:HA     | 2:B:64:ARG:HD2   | 1.92        | 0.51     |
| 1:A:976:G:P       | 14:N:32:SER:H    | 2.35        | 0.51     |
| 13:M:125:ARG:HA   | 24:Y:159:GLY:CA  | 2.41        | 0.51     |
| 3:C:70:VAL:HG12   | 3:C:71:ALA:N     | 2.26        | 0.51     |
| 1:A:1151:A:H5''   | 10:J:42:THR:H    | 1.76        | 0.51     |
| 18:R:50:ILE:HD12  | 18:R:70:ILE:HG21 | 1.92        | 0.51     |
| 1:A:1250:A:H2     | 1:A:1370:G:H1'   | 1.76        | 0.51     |
| 24:Y:315:VAL:HG11 | 24:Y:320:TYR:CZ  | 2.46        | 0.51     |
| 1:A:1149:C:H2'    | 1:A:1150:U:H6    | 1.75        | 0.51     |
| 1:A:1072:G:H2'    | 1:A:1073:U:C6    | 2.46        | 0.51     |
| 1:A:105:G:H2'     | 1:A:106:C:C6     | 2.46        | 0.51     |
| 16:P:17:TYR:HD1   | 16:P:17:TYR:H    | 1.59        | 0.51     |
| 1:A:479:C:H2'     | 1:A:480:U:C6     | 2.46        | 0.51     |
| 4:D:61:LYS:HD2    | 4:D:207:TYR:OH   | 2.11        | 0.51     |
| 2:B:182:ILE:HG22  | 2:B:183:PRO:O    | 2.11        | 0.51     |
| 9:I:126:SER:O     | 9:I:127:LYS:HB3  | 2.11        | 0.51     |
| 1:A:56:U:H2'      | 1:A:57:G:C8      | 2.46        | 0.51     |
| 2:B:97:TRP:CZ2    | 2:B:173:ALA:HA   | 2.45        | 0.50     |
| 22:W:19:G:C8      | 22:W:20:U:H5     | 2.25        | 0.50     |
| 15:O:81:LEU:HD11  | 15:O:85:LEU:HD12 | 1.92        | 0.50     |
| 10:J:4:ILE:HD13   | 10:J:74:ILE:CD1  | 2.41        | 0.50     |
| 13:M:89:GLY:O     | 13:M:92:HIS:HB2  | 2.12        | 0.50     |
| 1:A:423:G:H2'     | 1:A:424:G:H5'    | 1.93        | 0.50     |
| 16:P:67:THR:HB    | 16:P:70:ALA:HB3  | 1.92        | 0.50     |
| 7:G:148:ASN:O     | 7:G:150:ALA:N    | 2.44        | 0.50     |
| 7:G:135:VAL:HG12  | 7:G:139:GLU:OE2  | 2.10        | 0.50     |
| 1:A:311:C:HO2'    | 1:A:312:C:H5'    | 1.75        | 0.50     |
| 2:B:236:TYR:HA    | 2:B:239:VAL:HG21 | 1.93        | 0.50     |
| 7:G:101:LEU:O     | 7:G:105:VAL:HG23 | 2.12        | 0.50     |
| 11:K:31:THR:OG1   | 11:K:42:TRP:HB3  | 2.12        | 0.50     |
| 1:A:972:C:O2'     | 10:J:55:LYS:HG2  | 2.11        | 0.50     |
| 4:D:19:LEU:HD12   | 4:D:19:LEU:N     | 2.26        | 0.50     |
| 1:A:475:G:O2'     | 1:A:476:G:H5'    | 2.12        | 0.50     |
| 5:E:76:ILE:CG1    | 5:E:77:PRO:HD2   | 2.41        | 0.50     |
| 1:A:1036:G:H3'    | 1:A:1037:C:C6    | 2.46        | 0.50     |
| 9:I:18:PHE:HD1    | 9:I:62:TYR:HD2   | 1.58        | 0.50     |
| 1:A:1352:C:H2'    | 1:A:1353:G:H8    | 1.74        | 0.50     |
| 1:A:376:G:OP2     | 16:P:67:THR:HG21 | 2.11        | 0.50     |

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| Atom-1            | Atom-2           | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 10:J:8:LEU:O      | 10:J:16:LEU:HD21 | 2.10        | 0.50     |
| 19:S:58:VAL:HG21  | 19:S:75:ALA:HB2  | 1.93        | 0.50     |
| 6:F:42:GLU:HG2    | 6:F:42:GLU:O     | 2.11        | 0.50     |
| 17:Q:24:GLU:HG2   | 17:Q:39:SER:HB3  | 1.93        | 0.50     |
| 1:A:962:C:H2'     | 1:A:963:G:H8     | 1.75        | 0.50     |
| 22:W:68:C:O2'     | 22:W:69:G:H5'    | 2.10        | 0.50     |
| 3:C:82:GLU:O      | 3:C:86:VAL:HG13  | 2.12        | 0.50     |
| 1:A:382:A:H2'     | 1:A:383:A:C8     | 2.46        | 0.50     |
| 1:A:375:U:H4'     | 16:P:17:TYR:CE2  | 2.47        | 0.50     |
| 2:B:209:ARG:HH11  | 2:B:239:VAL:CG1  | 2.24        | 0.50     |
| 1:A:300:A:H1'     | 1:A:565:U:O2     | 2.11        | 0.50     |
| 11:K:79:SER:CB    | 11:K:106:LYS:HE3 | 2.41        | 0.50     |
| 24:Y:109:PHE:HB3  | 24:Y:110:PRO:HD2 | 1.91        | 0.50     |
| 1:A:1476:G:H2'    | 1:A:1477:C:H6    | 1.75        | 0.50     |
| 1:A:1207:G:O2'    | 1:A:1208:C:H5'   | 2.12        | 0.50     |
| 10:J:29:ARG:HG2   | 10:J:29:ARG:NH1  | 2.26        | 0.50     |
| 4:D:14:ARG:HD2    | 4:D:59:ARG:HH12  | 1.76        | 0.50     |
| 12:L:45:PRO:HD3   | 12:L:51:ALA:O    | 2.11        | 0.50     |
| 24:Y:50:GLN:C     | 24:Y:50:GLN:NE2  | 2.65        | 0.50     |
| 1:A:1251:A:H2'    | 1:A:1252:A:C8    | 2.46        | 0.50     |
| 10:J:39:PRO:HB3   | 10:J:70:ARG:NH1  | 2.26        | 0.50     |
| 24:Y:187:HIS:N    | 24:Y:206:ALA:O   | 2.40        | 0.50     |
| 2:B:16:HIS:HB3    | 2:B:210:SER:CA   | 2.42        | 0.50     |
| 14:N:59:ALA:O     | 14:N:60:SER:HB2  | 2.12        | 0.50     |
| 1:A:1246:C:H2'    | 1:A:1247:U:H6    | 1.76        | 0.50     |
| 1:A:340:U:H2'     | 1:A:341:C:C6     | 2.47        | 0.50     |
| 24:Y:59:VAL:HG12  | 24:Y:59:VAL:O    | 2.11        | 0.50     |
| 22:V:72:C:C3'     | 22:V:73:A:H5''   | 2.42        | 0.50     |
| 3:C:188:LEU:HD22  | 3:C:188:LEU:N    | 2.26        | 0.50     |
| 3:C:16:ARG:CB     | 3:C:16:ARG:HH11  | 2.25        | 0.50     |
| 5:E:7:GLU:O       | 5:E:8:GLU:HB3    | 2.11        | 0.50     |
| 9:I:112:LYS:HD3   | 9:I:112:LYS:O    | 2.10        | 0.50     |
| 4:D:126:ILE:H     | 4:D:126:ILE:HD12 | 1.77        | 0.50     |
| 1:A:1030(D):A:C2' | 1:A:1031:G:H5'   | 2.41        | 0.50     |
| 20:T:43:LEU:HB3   | 20:T:48:LYS:HB2  | 1.94        | 0.50     |
| 1:A:1316:G:H2'    | 1:A:1317:C:H5''  | 1.92        | 0.50     |
| 24:Y:74:GLU:C     | 24:Y:75:LEU:HD22 | 2.32        | 0.50     |
| 1:A:679:C:O2'     | 1:A:680:C:H5'    | 2.12        | 0.50     |
| 24:Y:303:ARG:N    | 24:Y:304:PRO:CD  | 2.75        | 0.50     |
| 6:F:39:LYS:HG2    | 6:F:40:VAL:H     | 1.76        | 0.50     |
| 13:M:120:LYS:HD3  | 13:M:121:LYS:O   | 2.11        | 0.50     |
| 13:M:94:ARG:CZ    | 19:S:81:ARG:HG3  | 2.41        | 0.50     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 14:N:23:ARG:HH11  | 14:N:30:ALA:HB2   | 1.76        | 0.50     |
| 3:C:140:ARG:HH11  | 3:C:140:ARG:HG3   | 1.75        | 0.50     |
| 1:A:1316:G:H5'    | 14:N:17:LYS:HE3   | 1.93        | 0.50     |
| 18:R:32:ARG:HA    | 18:R:69:THR:HG21  | 1.93        | 0.50     |
| 1:A:358:U:H2'     | 1:A:359:U:H6      | 1.76        | 0.50     |
| 1:A:986:A:H2'     | 1:A:987:G:C8      | 2.47        | 0.50     |
| 11:K:34:ASP:HB3   | 11:K:40:ILE:HD11  | 1.94        | 0.50     |
| 17:Q:10:VAL:HG13  | 17:Q:19:VAL:HB    | 1.92        | 0.50     |
| 3:C:30:ARG:HB2    | 14:N:36:PHE:O     | 2.11        | 0.50     |
| 1:A:963:G:H21     | 10:J:55:LYS:HD2   | 1.76        | 0.50     |
| 4:D:26:CYS:O      | 4:D:31:CYS:HB2    | 2.11        | 0.50     |
| 10:J:100:THR:HG22 | 10:J:100:THR:O    | 2.11        | 0.50     |
| 12:L:91:LYS:HD3   | 12:L:91:LYS:C     | 2.32        | 0.50     |
| 18:R:31:LEU:HD12  | 18:R:66:LEU:HB2   | 1.94        | 0.50     |
| 1:A:389:A:H2'     | 1:A:390:C:H5'     | 1.93        | 0.50     |
| 8:H:30:ARG:CB     | 8:H:30:ARG:NH1    | 2.74        | 0.50     |
| 2:B:95:GLN:HE21   | 2:B:147:LYS:CG    | 2.25        | 0.50     |
| 20:T:73:HIS:O     | 20:T:74:LYS:C     | 2.50        | 0.50     |
| 4:D:42:GLN:O      | 4:D:42:GLN:HG2    | 2.12        | 0.50     |
| 24:Y:48:VAL:HG12  | 24:Y:48:VAL:O     | 2.12        | 0.50     |
| 10:J:50:ILE:H     | 10:J:50:ILE:CD1   | 2.07        | 0.50     |
| 6:F:62:TRP:CH2    | 6:F:64:GLN:HB2    | 2.47        | 0.50     |
| 13:M:125:ARG:HA   | 24:Y:159:GLY:C    | 2.32        | 0.50     |
| 20:T:57:ARG:HH12  | 20:T:100:ILE:HG13 | 1.77        | 0.50     |
| 1:A:418:C:H2'     | 1:A:419:C:H6      | 1.74        | 0.50     |
| 3:C:113:ALA:HB3   | 3:C:114:PRO:CD    | 2.39        | 0.50     |
| 1:A:719:C:N4      | 18:R:71:LYS:HE2   | 2.27        | 0.50     |
| 1:A:377:G:H2'     | 1:A:378:G:C8      | 2.39        | 0.50     |
| 9:I:83:ARG:HA     | 9:I:86:VAL:HG12   | 1.93        | 0.50     |
| 7:G:120:ILE:HG22  | 7:G:124:LEU:HD12  | 1.94        | 0.50     |
| 24:Y:153:VAL:O    | 24:Y:153:VAL:CG1  | 2.60        | 0.50     |
| 1:A:1086:U:O2'    | 1:A:1087:G:H5'    | 2.12        | 0.50     |
| 2:B:97:TRP:CZ2    | 2:B:102:LEU:HD13  | 2.47        | 0.50     |
| 10:J:49:VAL:HG21  | 14:N:41:ARG:HB2   | 1.93        | 0.50     |
| 1:A:1133:G:H22    | 1:A:1143:G:H1'    | 1.77        | 0.50     |
| 9:I:65:VAL:CG2    | 9:I:73:GLN:HB3    | 2.35        | 0.50     |
| 9:I:4:TYR:HE1     | 9:I:21:PRO:HD3    | 1.76        | 0.50     |
| 9:I:17:VAL:HG21   | 9:I:80:GLY:C      | 2.32        | 0.50     |
| 4:D:15:GLU:HG3    | 4:D:63:LYS:HE2    | 1.94        | 0.50     |
| 1:A:911:U:H2'     | 1:A:912:C:C6      | 2.47        | 0.50     |
| 6:F:45:LEU:HD11   | 6:F:57:GLN:OE1    | 2.11        | 0.50     |
| 11:K:125:PHE:N    | 11:K:125:PHE:HD1  | 2.09        | 0.50     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 8:H:110:ALA:O    | 8:H:112:LEU:HD22  | 2.12        | 0.50     |
| 2:B:212:GLN:HG3  | 2:B:235:SER:HB2   | 1.94        | 0.50     |
| 15:O:70:LEU:HD12 | 15:O:70:LEU:O     | 2.12        | 0.50     |
| 24:Y:262:CYS:O   | 24:Y:263:GLN:HB2  | 2.11        | 0.50     |
| 2:B:180:LEU:C    | 2:B:182:ILE:H     | 2.15        | 0.50     |
| 1:A:245:C:O2     | 1:A:283:C:N3      | 2.44        | 0.50     |
| 1:A:859:A:H2'    | 1:A:860:A:O4'     | 2.11        | 0.50     |
| 2:B:97:TRP:HZ3   | 2:B:172:ILE:HG22  | 1.76        | 0.49     |
| 22:W:19:G:H4'    | 22:W:59:U:O4      | 2.12        | 0.49     |
| 6:F:4:TYR:HA     | 6:F:91:VAL:O      | 2.12        | 0.49     |
| 1:A:942:G:N2     | 9:I:124:GLN:NE2   | 2.60        | 0.49     |
| 22:V:51:U:O5'    | 22:V:51:U:H6      | 1.94        | 0.49     |
| 10:J:6:ILE:CG2   | 10:J:98:ILE:HG23  | 2.42        | 0.49     |
| 9:I:118:LYS:O    | 9:I:119:ALA:CB    | 2.60        | 0.49     |
| 5:E:152:ARG:HD3  | 8:H:42:GLU:O      | 2.11        | 0.49     |
| 17:Q:9:VAL:CG1   | 17:Q:56:VAL:HG22  | 2.42        | 0.49     |
| 5:E:36:ASP:O     | 5:E:37:ARG:HB2    | 2.12        | 0.49     |
| 8:H:12:ARG:NH1   | 8:H:27:PRO:HD2    | 2.27        | 0.49     |
| 24:Y:253:HIS:CD2 | 24:Y:255:PRO:HG2  | 2.47        | 0.49     |
| 24:Y:282:ARG:HB3 | 24:Y:282:ARG:HH21 | 1.77        | 0.49     |
| 5:E:105:VAL:HB   | 5:E:106:PRO:CD    | 2.42        | 0.49     |
| 24:Y:120:ILE:O   | 24:Y:120:ILE:HG22 | 2.11        | 0.49     |
| 1:A:191:G:C1'    | 20:T:105:SER:HB3  | 2.41        | 0.49     |
| 1:A:738:C:H5''   | 6:F:69:GLU:HB2    | 1.95        | 0.49     |
| 9:I:4:TYR:HA     | 9:I:88:TYR:CZ     | 2.47        | 0.49     |
| 5:E:73:ASN:N     | 5:E:73:ASN:HD22   | 2.10        | 0.49     |
| 24:Y:132:TRP:CE3 | 24:Y:135:MET:HB2  | 2.46        | 0.49     |
| 3:C:91:LEU:C     | 3:C:93:LYS:H      | 2.16        | 0.49     |
| 22:V:12:U:H2'    | 22:V:13:C:H5''    | 1.94        | 0.49     |
| 1:A:573:A:N3     | 1:A:883:C:O2'     | 2.43        | 0.49     |
| 1:A:712:A:O2'    | 1:A:713:G:H5'     | 2.12        | 0.49     |
| 1:A:881:G:OP2    | 12:L:12:ARG:NH2   | 2.45        | 0.49     |
| 11:K:126:ARG:HB3 | 11:K:126:ARG:NH1  | 2.27        | 0.49     |
| 3:C:147:LYS:HD2  | 3:C:204:LEU:O     | 2.11        | 0.49     |
| 1:A:1226:C:OP1   | 13:M:91:ARG:NH1   | 2.45        | 0.49     |
| 4:D:9:CYS:HB3    | 4:D:32:ALA:CB     | 2.42        | 0.49     |
| 3:C:150:LYS:HG3  | 3:C:169:ALA:HB2   | 1.94        | 0.49     |
| 13:M:123:ALA:CB  | 24:Y:162:ALA:HB2  | 2.42        | 0.49     |
| 1:A:509:A:H5''   | 4:D:55:ALA:HB2    | 1.93        | 0.49     |
| 24:Y:85:GLU:HA   | 24:Y:88:LYS:HG2   | 1.94        | 0.49     |
| 1:A:61:G:H2'     | 1:A:62:U:O4'      | 2.13        | 0.49     |
| 1:A:696:A:O2'    | 1:A:697:U:H5'     | 2.12        | 0.49     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 10:J:40:LEU:N    | 10:J:69:ASN:O    | 2.45        | 0.49     |
| 24:Y:228:ARG:HD2 | 24:Y:228:ARG:O   | 2.12        | 0.49     |
| 14:N:31:ARG:HG3  | 14:N:31:ARG:HH11 | 1.77        | 0.49     |
| 1:A:1107:C:C3'   | 1:A:1108:G:H5''  | 2.42        | 0.49     |
| 13:M:120:LYS:HE2 | 13:M:122:LYS:HZ2 | 1.77        | 0.49     |
| 5:E:76:ILE:HG13  | 5:E:142:LEU:CD1  | 2.40        | 0.49     |
| 1:A:1026:G:C3'   | 1:A:1027:C:H5'   | 2.42        | 0.49     |
| 2:B:54:THR:HG21  | 2:B:201:ILE:CD1  | 2.42        | 0.49     |
| 1:A:926:G:H21    | 1:A:1505:G:H2'   | 1.77        | 0.49     |
| 12:L:41:ARG:HD3  | 12:L:42:THR:C    | 2.33        | 0.49     |
| 1:A:433:C:H2'    | 1:A:434:U:H6     | 1.77        | 0.49     |
| 24:Y:223:LYS:O   | 24:Y:225:GLU:N   | 2.45        | 0.49     |
| 1:A:1014:A:H2'   | 1:A:1015:A:C8    | 2.47        | 0.49     |
| 24:Y:276:LEU:O   | 24:Y:280:LYS:HG3 | 2.12        | 0.49     |
| 1:A:542:G:OP1    | 4:D:10:ARG:NH2   | 2.46        | 0.49     |
| 1:A:1166:G:H2'   | 1:A:1169:A:OP2   | 2.12        | 0.49     |
| 1:A:22:G:O2'     | 1:A:23:C:H5'     | 2.12        | 0.49     |
| 24:Y:306:GLU:HG3 | 24:Y:307:TRP:N   | 2.27        | 0.49     |
| 6:F:26:ILE:O     | 6:F:29:ALA:HB3   | 2.12        | 0.49     |
| 24:Y:72:LEU:HD22 | 24:Y:91:LEU:HG   | 1.94        | 0.49     |
| 16:P:51:VAL:O    | 16:P:53:VAL:N    | 2.45        | 0.49     |
| 16:P:67:THR:HB   | 16:P:70:ALA:CB   | 2.42        | 0.49     |
| 17:Q:7:THR:HG22  | 17:Q:58:GLU:CG   | 2.40        | 0.49     |
| 12:L:22:SER:O    | 12:L:24:VAL:N    | 2.46        | 0.49     |
| 13:M:19:LEU:CA   | 13:M:22:ILE:HD13 | 2.41        | 0.49     |
| 1:A:1379:G:O2'   | 1:A:1380:U:H5'   | 2.13        | 0.49     |
| 24:Y:119:THR:CG2 | 24:Y:166:TYR:CE1 | 2.95        | 0.49     |
| 3:C:95:THR:HG22  | 3:C:97:LYS:H     | 1.78        | 0.49     |
| 1:A:189(J):G:O2' | 1:A:189(K):U:H5' | 2.13        | 0.49     |
| 1:A:176:C:O2'    | 1:A:177:C:H5'    | 2.12        | 0.49     |
| 1:A:546:G:OP1    | 4:D:73:ARG:HB2   | 2.11        | 0.49     |
| 24:Y:149:PHE:CD1 | 24:Y:173:GLY:HA3 | 2.48        | 0.49     |
| 1:A:1040:U:H2'   | 1:A:1041:A:H8    | 1.77        | 0.49     |
| 2:B:180:LEU:O    | 2:B:182:ILE:N    | 2.45        | 0.49     |
| 1:A:857:C:H2'    | 1:A:858:G:O4'    | 2.12        | 0.49     |
| 3:C:79:ARG:HG3   | 3:C:79:ARG:HH11  | 1.77        | 0.49     |
| 22:V:76:8AN:H4'  | 22:V:76:8AN:O1P  | 2.12        | 0.49     |
| 1:A:1126:U:O2'   | 1:A:1127:G:H5'   | 2.12        | 0.49     |
| 12:L:18:VAL:O    | 12:L:19:ARG:HB3  | 2.12        | 0.49     |
| 24:Y:27:LYS:HE3  | 24:Y:31:ARG:NH2  | 2.28        | 0.49     |
| 16:P:13:HIS:C    | 16:P:15:PRO:HD3  | 2.33        | 0.49     |
| 9:I:104:ARG:O    | 9:I:104:ARG:HG2  | 2.13        | 0.49     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:1096:C:H2'    | 1:A:1097:C:C6     | 2.48        | 0.49     |
| 4:D:57:ARG:NH2    | 5:E:107:ARG:HD3   | 2.27        | 0.49     |
| 23:X:15:A:N3      | 23:X:15:A:H5''    | 2.26        | 0.49     |
| 1:A:1127:G:N2     | 1:A:1147:C:H41    | 2.07        | 0.49     |
| 20:T:89:ARG:HB2   | 20:T:104:LEU:HD11 | 1.94        | 0.49     |
| 22:V:50:U:H3      | 22:V:64:A:N6      | 2.10        | 0.49     |
| 18:R:50:ILE:CD1   | 18:R:70:ILE:HG21  | 2.43        | 0.49     |
| 7:G:79:ARG:HG3    | 7:G:83:ALA:O      | 2.13        | 0.49     |
| 9:I:112:LYS:HD3   | 9:I:112:LYS:C     | 2.33        | 0.49     |
| 1:A:1112:C:H1'    | 3:C:179:ARG:CD    | 2.42        | 0.49     |
| 13:M:65:LYS:NZ    | 13:M:70:LEU:HD23  | 2.27        | 0.49     |
| 11:K:124:LYS:HZ3  | 11:K:125:PHE:HE1  | 1.60        | 0.49     |
| 4:D:173:TRP:CE3   | 4:D:193:ASP:HB3   | 2.48        | 0.49     |
| 1:A:599:C:H4'     | 8:H:130:GLY:CA    | 2.43        | 0.49     |
| 1:A:139:G:H2'     | 1:A:140:A:H8      | 1.78        | 0.49     |
| 1:A:583:A:H2'     | 1:A:584:G:O4'     | 2.13        | 0.49     |
| 24:Y:137:LEU:HD23 | 24:Y:137:LEU:C    | 2.32        | 0.49     |
| 1:A:656:C:H2'     | 1:A:657:G:H8      | 1.78        | 0.49     |
| 1:A:865:A:H2      | 1:A:918:A:H4'     | 1.78        | 0.49     |
| 9:I:20:ARG:HG3    | 9:I:20:ARG:HH11   | 1.77        | 0.49     |
| 1:A:1288:A:H2'    | 1:A:1289:A:H8     | 1.78        | 0.49     |
| 2:B:187:LEU:CD1   | 2:B:205:ASP:HA    | 2.43        | 0.49     |
| 8:H:91:ARG:NH1    | 8:H:91:ARG:HG2    | 2.24        | 0.49     |
| 13:M:43:THR:O     | 13:M:44:ARG:HD3   | 2.13        | 0.49     |
| 19:S:40:ILE:HG21  | 19:S:62:ILE:CD1   | 2.43        | 0.49     |
| 1:A:438:G:H2'     | 1:A:494:U:O4      | 2.12        | 0.49     |
| 18:R:30:ASP:OD1   | 18:R:32:ARG:HB2   | 2.12        | 0.49     |
| 1:A:832:C:O2'     | 1:A:833:U:H6      | 1.95        | 0.49     |
| 1:A:115:G:H1'     | 1:A:116:A:N7      | 2.27        | 0.49     |
| 1:A:302:G:N3      | 1:A:556:C:H4'     | 2.28        | 0.49     |
| 19:S:58:VAL:HG23  | 19:S:58:VAL:O     | 2.12        | 0.49     |
| 1:A:760:G:H2'     | 1:A:761:G:H5'     | 1.95        | 0.49     |
| 2:B:28:PHE:HD1    | 2:B:28:PHE:O      | 1.95        | 0.49     |
| 19:S:73:GLU:O     | 19:S:73:GLU:HG2   | 2.12        | 0.49     |
| 24:Y:186:VAL:HG13 | 24:Y:305:ILE:HD13 | 1.94        | 0.49     |
| 24:Y:242:VAL:O    | 24:Y:243:ASN:C    | 2.51        | 0.49     |
| 22:W:31:A:C2'     | 22:W:32:U:H5'     | 2.43        | 0.49     |
| 1:A:1116:C:H2'    | 1:A:1117:G:C5'    | 2.30        | 0.49     |
| 3:C:179:ARG:O     | 3:C:206:GLU:HG3   | 2.13        | 0.49     |
| 1:A:438:G:C4'     | 1:A:439:A:OP1     | 2.60        | 0.49     |
| 1:A:984:C:H2'     | 1:A:985:C:H6      | 1.75        | 0.49     |
| 6:F:76:ALA:HB1    | 6:F:80:ARG:NH2    | 2.28        | 0.49     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:977:A:C2'     | 1:A:978:A:H5'     | 2.43        | 0.49     |
| 4:D:189:PRO:HB2   | 4:D:194:LEU:HD21  | 1.94        | 0.49     |
| 24:Y:118:LEU:HA   | 24:Y:209:GLU:O    | 2.12        | 0.49     |
| 24:Y:242:VAL:HA   | 24:Y:245:THR:CG2  | 2.43        | 0.49     |
| 3:C:14:ILE:CG1    | 3:C:15:THR:H      | 2.05        | 0.49     |
| 1:A:675:A:H1'     | 11:K:116:HIS:CD2  | 2.48        | 0.49     |
| 2:B:178:ARG:HH11  | 2:B:178:ARG:CG    | 2.26        | 0.49     |
| 1:A:926:G:C6      | 1:A:1505:G:C5     | 3.01        | 0.49     |
| 19:S:15:LEU:O     | 19:S:19:VAL:HG23  | 2.13        | 0.49     |
| 2:B:208:ILE:HA    | 2:B:211:ILE:CD1   | 2.42        | 0.49     |
| 20:T:42:GLN:HA    | 20:T:42:GLN:HE21  | 1.76        | 0.49     |
| 2:B:21:ARG:CZ     | 2:B:39:ILE:HG12   | 2.43        | 0.49     |
| 1:A:143:A:N1      | 1:A:220:G:O6      | 2.46        | 0.49     |
| 4:D:8:VAL:HB      | 4:D:21:LEU:HD12   | 1.94        | 0.49     |
| 1:A:1410:G:H2'    | 1:A:1411:C:C6     | 2.48        | 0.49     |
| 16:P:55:ARG:HA    | 16:P:55:ARG:HE    | 1.77        | 0.49     |
| 1:A:1121:U:H2'    | 1:A:1122:U:C6     | 2.48        | 0.49     |
| 1:A:1065:U:O2'    | 1:A:1066:C:P      | 2.71        | 0.49     |
| 1:A:634:C:H2'     | 1:A:635:G:H8      | 1.77        | 0.49     |
| 9:I:95:LYS:HD3    | 9:I:95:LYS:C      | 2.33        | 0.48     |
| 1:A:1104:G:H2'    | 1:A:1105:A:H8     | 1.77        | 0.48     |
| 24:Y:27:LYS:C     | 24:Y:29:LEU:H     | 2.16        | 0.48     |
| 2:B:65:GLY:O      | 2:B:67:THR:N      | 2.46        | 0.48     |
| 3:C:77:ILE:HA     | 3:C:84:ILE:HB     | 1.95        | 0.48     |
| 20:T:26:ASN:O     | 20:T:30:LYS:HB2   | 2.13        | 0.48     |
| 1:A:677:U:H3      | 1:A:713:G:H22     | 1.59        | 0.48     |
| 22:W:46:G:OP1     | 22:W:46:G:H3'     | 2.13        | 0.48     |
| 24:Y:118:LEU:HD22 | 24:Y:208:VAL:HG12 | 1.95        | 0.48     |
| 6:F:92:LYS:NZ     | 6:F:92:LYS:CB     | 2.76        | 0.48     |
| 11:K:105:VAL:HB   | 11:K:108:ILE:HD11 | 1.95        | 0.48     |
| 13:M:90:LEU:O     | 13:M:92:HIS:N     | 2.46        | 0.48     |
| 19:S:29:ARG:CD    | 19:S:30:LEU:N     | 2.73        | 0.48     |
| 1:A:521:G:O2'     | 1:A:522:C:H5'     | 2.12        | 0.48     |
| 1:A:724:G:O2'     | 1:A:725:G:H5'     | 2.13        | 0.48     |
| 20:T:29:LYS:O     | 20:T:33:ILE:HG13  | 2.12        | 0.48     |
| 14:N:9:LYS:HG3    | 14:N:12:ARG:HH22  | 1.78        | 0.48     |
| 1:A:279:A:OP2     | 17:Q:95:TYR:OH    | 2.31        | 0.48     |
| 2:B:93:VAL:HG11   | 2:B:97:TRP:CD1    | 2.47        | 0.48     |
| 4:D:12:CYS:SG     | 4:D:19:LEU:O      | 2.72        | 0.48     |
| 1:A:328:C:O2'     | 1:A:329:A:P       | 2.71        | 0.48     |
| 4:D:2:GLY:O       | 4:D:3:ARG:O       | 2.31        | 0.48     |
| 1:A:298:A:H2'     | 1:A:299:G:O4'     | 2.13        | 0.48     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:1307:U:H2'   | 1:A:1308:U:H6    | 1.78        | 0.48     |
| 1:A:411:A:H2'    | 1:A:412:A:H4'    | 1.94        | 0.48     |
| 24:Y:112:ALA:O   | 24:Y:177:TYR:HB3 | 2.13        | 0.48     |
| 24:Y:123:GLY:HA3 | 24:Y:305:ILE:CG2 | 2.43        | 0.48     |
| 22:W:52:G:N3     | 22:W:63:G:O6     | 2.45        | 0.48     |
| 10:J:3:LYS:HZ3   | 10:J:77:PRO:HD2  | 1.79        | 0.48     |
| 12:L:33:ARG:HA   | 12:L:33:ARG:HE   | 1.78        | 0.48     |
| 3:C:44:GLU:HA    | 3:C:52:LEU:HD11  | 1.95        | 0.48     |
| 16:P:20:VAL:HG22 | 16:P:21:VAL:N    | 2.29        | 0.48     |
| 10:J:16:LEU:HD13 | 10:J:16:LEU:O    | 2.13        | 0.48     |
| 1:A:1469:G:O2'   | 1:A:1470:G:H5'   | 2.13        | 0.48     |
| 1:A:797:C:O2'    | 1:A:798:G:H5'    | 2.13        | 0.48     |
| 11:K:125:PHE:CD1 | 11:K:125:PHE:N   | 2.79        | 0.48     |
| 1:A:189(I):G:O2' | 1:A:189(J):G:H5' | 2.13        | 0.48     |
| 1:A:1060:C:H5''  | 10:J:51:ARG:HB3  | 1.94        | 0.48     |
| 11:K:43:SER:HB3  | 11:K:68:ALA:HB2  | 1.95        | 0.48     |
| 1:A:818:G:H3'    | 1:A:819:A:C5'    | 2.43        | 0.48     |
| 2:B:71:VAL:O     | 2:B:164:VAL:HG13 | 2.12        | 0.48     |
| 13:M:112:GLY:HA2 | 13:M:113:PRO:CG  | 2.43        | 0.48     |
| 22:W:39:U:H3'    | 22:W:40:C:C5'    | 2.44        | 0.48     |
| 1:A:1057:G:H5''  | 3:C:154:SER:OG   | 2.12        | 0.48     |
| 1:A:1104:G:O2'   | 1:A:1105:A:H5'   | 2.14        | 0.48     |
| 18:R:74:ARG:HA   | 18:R:79:LEU:O    | 2.13        | 0.48     |
| 24:Y:30:GLU:OE2  | 24:Y:31:ARG:HB2  | 2.13        | 0.48     |
| 5:E:150:ARG:HA   | 5:E:153:LYS:CE   | 2.42        | 0.48     |
| 1:A:501:C:H2'    | 1:A:502:G:H8     | 1.78        | 0.48     |
| 10:J:61:GLU:CG   | 14:N:58:LYS:HE2  | 2.43        | 0.48     |
| 6:F:7:ASN:O      | 6:F:8:ILE:HG13   | 2.14        | 0.48     |
| 15:O:61:GLY:O    | 15:O:64:ARG:HB3  | 2.13        | 0.48     |
| 4:D:129:ASN:ND2  | 4:D:145:GLU:N    | 2.59        | 0.48     |
| 2:B:78:GLN:O     | 2:B:81:VAL:HB    | 2.14        | 0.48     |
| 1:A:954:G:H2'    | 1:A:955:U:C6     | 2.49        | 0.48     |
| 22:W:19:G:N2     | 22:W:56:C:H42    | 2.11        | 0.48     |
| 10:J:50:ILE:CD1  | 14:N:41:ARG:HD3  | 2.44        | 0.48     |
| 14:N:29:ARG:HG2  | 14:N:40:CYS:CB   | 2.42        | 0.48     |
| 3:C:71:ALA:CB    | 3:C:109:PRO:HB3  | 2.44        | 0.48     |
| 9:I:43:ALA:O     | 9:I:45:ALA:N     | 2.43        | 0.48     |
| 1:A:1028:C:H2'   | 1:A:1029:C:C5'   | 2.36        | 0.48     |
| 1:A:511:C:H1'    | 4:D:43:HIS:HE2   | 1.78        | 0.48     |
| 1:A:223:U:O5'    | 1:A:223:U:H6     | 1.97        | 0.48     |
| 24:Y:72:LEU:HG   | 24:Y:76:MET:HE1  | 1.95        | 0.48     |
| 5:E:11:ILE:HD12  | 5:E:31:LEU:CD1   | 2.44        | 0.48     |

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| Atom-1            | Atom-2           | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:A:437:U:H2'     | 1:A:438:G:C8     | 2.48        | 0.48     |
| 7:G:139:GLU:O     | 7:G:143:ARG:HG3  | 2.13        | 0.48     |
| 6:F:97:PHE:N      | 18:R:30:ASP:OD1  | 2.47        | 0.48     |
| 1:A:724:G:H2'     | 1:A:725:G:H8     | 1.77        | 0.48     |
| 2:B:20:GLU:CG     | 2:B:189:ASP:OD2  | 2.62        | 0.48     |
| 14:N:12:ARG:CB    | 14:N:12:ARG:HH11 | 2.27        | 0.48     |
| 3:C:138:VAL:HG13  | 3:C:149:ALA:CB   | 2.43        | 0.48     |
| 1:A:299:G:H2'     | 1:A:300:A:C8     | 2.48        | 0.48     |
| 1:A:784:C:H2'     | 1:A:785:G:H8     | 1.77        | 0.48     |
| 20:T:63:ILE:HG23  | 20:T:72:LEU:HD13 | 1.95        | 0.48     |
| 1:A:167:G:O2'     | 1:A:168:G:H5'    | 2.13        | 0.48     |
| 14:N:48:ALA:HB2   | 14:N:53:LEU:HD12 | 1.95        | 0.48     |
| 1:A:1202:G:H1'    | 14:N:29:ARG:HD3  | 1.95        | 0.48     |
| 6:F:35:ALA:HB1    | 6:F:65:VAL:HG21  | 1.96        | 0.48     |
| 3:C:11:ARG:HH11   | 3:C:11:ARG:HG2   | 1.78        | 0.48     |
| 20:T:50:GLU:HA    | 20:T:100:ILE:CG2 | 2.42        | 0.48     |
| 5:E:7:GLU:O       | 5:E:8:GLU:CB     | 2.62        | 0.48     |
| 1:A:427:U:OP1     | 4:D:40:PRO:HA    | 2.14        | 0.48     |
| 4:D:59:ARG:HE     | 4:D:59:ARG:CA    | 2.18        | 0.48     |
| 24:Y:54:ARG:O     | 24:Y:58:THR:HG23 | 2.14        | 0.48     |
| 24:Y:83:GLU:HB3   | 24:Y:84:ARG:NH1  | 2.29        | 0.48     |
| 1:A:376:G:H2'     | 1:A:377:G:H8     | 1.78        | 0.48     |
| 3:C:76:VAL:HG23   | 3:C:77:ILE:N     | 2.29        | 0.48     |
| 1:A:539:A:P       | 12:L:114:LYS:HD2 | 2.53        | 0.48     |
| 1:A:1071:C:H2'    | 1:A:1072:G:C8    | 2.46        | 0.48     |
| 1:A:1072:G:H2'    | 1:A:1073:U:H6    | 1.79        | 0.48     |
| 19:S:53:ASN:HD22  | 19:S:58:VAL:CG1  | 2.26        | 0.48     |
| 1:A:1499:A:H1'    | 1:A:1520:G:H5'   | 1.96        | 0.48     |
| 1:A:164:U:O2'     | 1:A:165:C:H5'    | 2.12        | 0.48     |
| 1:A:630:G:H2'     | 1:A:630:G:N3     | 2.29        | 0.48     |
| 1:A:751:U:H2'     | 1:A:752:G:H5'    | 1.94        | 0.48     |
| 1:A:818:G:C3'     | 1:A:819:A:H5''   | 2.44        | 0.48     |
| 18:R:59:SER:OG    | 18:R:62:GLU:HG2  | 2.12        | 0.48     |
| 1:A:1418:A:C2     | 1:A:1483:A:C2    | 3.02        | 0.48     |
| 9:I:4:TYR:O       | 9:I:18:PHE:HA    | 2.14        | 0.48     |
| 1:A:519:C:OP1     | 24:Y:188:ARG:NH1 | 2.47        | 0.48     |
| 24:Y:295:LEU:HD13 | 24:Y:295:LEU:O   | 2.13        | 0.48     |
| 1:A:564:C:H5'     | 17:Q:32:TYR:CE2  | 2.48        | 0.48     |
| 13:M:67:GLU:CG    | 13:M:68:GLY:N    | 2.77        | 0.48     |
| 11:K:24:SER:O     | 11:K:27:ASN:N    | 2.44        | 0.48     |
| 4:D:3:ARG:O       | 4:D:3:ARG:HD3    | 2.13        | 0.48     |
| 1:A:881:G:P       | 12:L:12:ARG:HH22 | 2.37        | 0.48     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:1128:C:C4'   | 9:I:16:ARG:HH12   | 2.26        | 0.48     |
| 13:M:124:PRO:N   | 24:Y:163:GLY:H    | 2.12        | 0.48     |
| 15:O:25:THR:O    | 15:O:28:GLN:N     | 2.47        | 0.48     |
| 12:L:60:LEU:HD23 | 12:L:64:TYR:HB2   | 1.96        | 0.48     |
| 18:R:56:THR:CB   | 18:R:58:LEU:HD13  | 2.37        | 0.48     |
| 10:J:27:ALA:HB2  | 10:J:85:LEU:CD1   | 2.40        | 0.48     |
| 1:A:649:G:H2'    | 1:A:650:G:H8      | 1.78        | 0.48     |
| 24:Y:17:LEU:C    | 24:Y:20:PRO:HD2   | 2.34        | 0.48     |
| 24:Y:85:GLU:O    | 24:Y:89:PRO:HD3   | 2.13        | 0.48     |
| 4:D:119:GLN:HG2  | 4:D:123:HIS:HD2   | 1.78        | 0.48     |
| 1:A:171:A:H2'    | 1:A:172:A:C8      | 2.48        | 0.48     |
| 4:D:120:LEU:HB3  | 4:D:126:ILE:HD11  | 1.95        | 0.48     |
| 1:A:1261:A:N1    | 1:A:1275:A:H1'    | 2.29        | 0.48     |
| 1:A:154:C:O2'    | 1:A:155:C:H5'     | 2.14        | 0.48     |
| 1:A:357:G:OP1    | 1:A:367:U:H5''    | 2.13        | 0.48     |
| 4:D:8:VAL:HG11   | 4:D:115:ARG:CZ    | 2.43        | 0.48     |
| 14:N:12:ARG:NH1  | 14:N:12:ARG:CB    | 2.76        | 0.48     |
| 13:M:56:LEU:HD13 | 13:M:60:VAL:HG21  | 1.94        | 0.48     |
| 24:Y:185:GLY:HA3 | 24:Y:311:ILE:HG21 | 1.96        | 0.48     |
| 2:B:73:THR:HG22  | 2:B:95:GLN:O      | 2.13        | 0.48     |
| 1:A:295:C:H2'    | 1:A:296:U:C6      | 2.48        | 0.48     |
| 1:A:64:G:H4'     | 1:A:65:U:H5''     | 1.96        | 0.48     |
| 24:Y:130:CYS:C   | 24:Y:163:GLY:HA3  | 2.34        | 0.48     |
| 3:C:22:TRP:CH2   | 3:C:32:LEU:HB2    | 2.48        | 0.48     |
| 7:G:15:ASP:CB    | 7:G:20:ASP:H      | 2.27        | 0.48     |
| 8:H:39:LEU:H     | 8:H:39:LEU:HD22   | 1.78        | 0.48     |
| 1:A:539:A:OP1    | 12:L:114:LYS:HD2  | 2.14        | 0.48     |
| 10:J:16:LEU:HA   | 10:J:94:VAL:HG21  | 1.96        | 0.48     |
| 4:D:152:SER:HA   | 4:D:155:LEU:HD12  | 1.96        | 0.48     |
| 7:G:25:ALA:HA    | 7:G:28:ASN:HD22   | 1.79        | 0.48     |
| 6:F:33:TYR:CE2   | 6:F:74:ASP:HB2    | 2.49        | 0.48     |
| 1:A:818:G:O2'    | 1:A:819:A:H5''    | 2.14        | 0.48     |
| 1:A:965:A:C2     | 1:A:969:A:C2      | 3.02        | 0.48     |
| 1:A:967:C:H2'    | 1:A:968:A:C8      | 2.49        | 0.48     |
| 2:B:137:ARG:HG2  | 2:B:137:ARG:HH11  | 1.78        | 0.48     |
| 1:A:125:U:H2'    | 1:A:126:G:C8      | 2.48        | 0.48     |
| 6:F:27:GLN:HE21  | 6:F:27:GLN:HA     | 1.79        | 0.48     |
| 24:Y:231:VAL:HB  | 24:Y:246:ASP:HB3  | 1.96        | 0.48     |
| 4:D:12:CYS:HB3   | 4:D:18:LYS:HA     | 1.94        | 0.47     |
| 3:C:186:PHE:HD1  | 3:C:198:VAL:O     | 1.97        | 0.47     |
| 24:Y:60:ASP:CG   | 24:Y:61:THR:N     | 2.67        | 0.47     |
| 5:E:69:VAL:HG21  | 5:E:113:ALA:HB1   | 1.94        | 0.47     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:B:233:SER:HB2  | 2:B:234:PRO:CD   | 2.38        | 0.47     |
| 22:V:1:G:O2'     | 22:V:2:C:H5'     | 2.14        | 0.47     |
| 13:M:48:LEU:HG   | 13:M:53:VAL:HG22 | 1.95        | 0.47     |
| 20:T:26:ASN:N    | 20:T:26:ASN:ND2  | 2.61        | 0.47     |
| 4:D:190:ASP:HB3  | 4:D:193:ASP:OD2  | 2.13        | 0.47     |
| 2:B:212:GLN:NE2  | 2:B:216:SER:HB2  | 2.28        | 0.47     |
| 16:P:55:ARG:O    | 16:P:58:TYR:HB3  | 2.14        | 0.47     |
| 1:A:1508:G:H2'   | 1:A:1509:C:C6    | 2.48        | 0.47     |
| 9:I:75:ASP:HA    | 9:I:78:LYS:NZ    | 2.28        | 0.47     |
| 1:A:248:C:O2'    | 1:A:249:U:H5'    | 2.13        | 0.47     |
| 22:W:55:U:O2     | 22:W:55:U:O4'    | 2.32        | 0.47     |
| 1:A:1371:G:OP2   | 9:I:11:LYS:HD2   | 2.13        | 0.47     |
| 13:M:16:ASP:O    | 13:M:30:ALA:HB1  | 2.14        | 0.47     |
| 16:P:4:ILE:CD1   | 16:P:64:ALA:HB1  | 2.44        | 0.47     |
| 1:A:76:C:N4      | 1:A:93:G:H1      | 2.12        | 0.47     |
| 1:A:186:C:O2'    | 1:A:187:C:H5'    | 2.14        | 0.47     |
| 4:D:3:ARG:O      | 4:D:5:ILE:HG13   | 2.14        | 0.47     |
| 8:H:12:ARG:HH12  | 8:H:27:PRO:HD3   | 1.78        | 0.47     |
| 8:H:29:SER:HB3   | 8:H:32:LYS:HG3   | 1.96        | 0.47     |
| 22:V:3:C:H2'     | 22:V:4:C:C6      | 2.48        | 0.47     |
| 5:E:57:LYS:HB3   | 5:E:61:TYR:CE2   | 2.49        | 0.47     |
| 1:A:643:C:H5'    | 8:H:31:PHE:CD1   | 2.48        | 0.47     |
| 7:G:23:VAL:HG12  | 7:G:23:VAL:O     | 2.14        | 0.47     |
| 1:A:959:A:H2'    | 1:A:960:U:H4'    | 1.95        | 0.47     |
| 4:D:20:TYR:H     | 4:D:20:TYR:HD1   | 1.61        | 0.47     |
| 1:A:413:G:H4'    | 1:A:414:A:C5'    | 2.36        | 0.47     |
| 1:A:1357:A:H61   | 1:A:1363(A):A:H2 | 1.60        | 0.47     |
| 12:L:22:SER:C    | 12:L:24:VAL:H    | 2.18        | 0.47     |
| 9:I:118:LYS:NZ   | 9:I:118:LYS:HB3  | 2.29        | 0.47     |
| 13:M:19:LEU:H    | 13:M:19:LEU:CD2  | 2.27        | 0.47     |
| 3:C:119:ARG:HH21 | 3:C:140:ARG:NE   | 2.12        | 0.47     |
| 1:A:189(K):U:H2' | 1:A:189(L):G:H8  | 1.76        | 0.47     |
| 1:A:336:C:O2'    | 1:A:337:C:H5'    | 2.13        | 0.47     |
| 1:A:1383:C:H2'   | 1:A:1384:C:C6    | 2.48        | 0.47     |
| 3:C:138:VAL:HG13 | 3:C:149:ALA:HB3  | 1.95        | 0.47     |
| 1:A:746:A:O2'    | 1:A:747:C:H5'    | 2.15        | 0.47     |
| 2:B:79:ASP:HB2   | 2:B:80:ILE:HD12  | 1.96        | 0.47     |
| 1:A:1288:A:H2'   | 1:A:1289:A:C8    | 2.49        | 0.47     |
| 6:F:68:PRO:HG2   | 6:F:71:ARG:CG    | 2.39        | 0.47     |
| 22:W:27:G:H2'    | 22:W:28:G:C8     | 2.49        | 0.47     |
| 11:K:59:TYR:CE1  | 11:K:63:LEU:HD21 | 2.49        | 0.47     |
| 21:U:12:LYS:CB   | 21:U:22:ARG:HD2  | 2.44        | 0.47     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:986:A:H2'    | 1:A:987:G:H8     | 1.80        | 0.47     |
| 10:J:63:PHE:HB3  | 14:N:58:LYS:HA   | 1.96        | 0.47     |
| 4:D:4:TYR:O      | 4:D:5:ILE:HB     | 2.14        | 0.47     |
| 24:Y:149:PHE:HD1 | 24:Y:173:GLY:HA3 | 1.78        | 0.47     |
| 1:A:9:G:H5''     | 5:E:122:GLU:OE2  | 2.14        | 0.47     |
| 3:C:29:TYR:HE1   | 10:J:65:LEU:HD21 | 1.79        | 0.47     |
| 12:L:111:LYS:HG2 | 12:L:112:ASP:N   | 2.29        | 0.47     |
| 2:B:23:ARG:O     | 2:B:23:ARG:HG3   | 2.14        | 0.47     |
| 1:A:458:C:H2'    | 1:A:460:G:H8     | 1.79        | 0.47     |
| 2:B:118:LEU:HD13 | 2:B:142:LEU:HB2  | 1.96        | 0.47     |
| 19:S:43:GLU:CG   | 19:S:44:MET:HE1  | 2.39        | 0.47     |
| 1:A:421:U:C4     | 3:C:127:ARG:NH1  | 2.82        | 0.47     |
| 4:D:121:VAL:CA   | 4:D:126:ILE:HD13 | 2.45        | 0.47     |
| 1:A:313:A:H2'    | 1:A:314:C:C6     | 2.49        | 0.47     |
| 1:A:1019:C:C2'   | 1:A:1020:U:H5'   | 2.44        | 0.47     |
| 24:Y:109:PHE:CE2 | 24:Y:353:ALA:HB2 | 2.49        | 0.47     |
| 7:G:54:THR:HG23  | 7:G:54:THR:O     | 2.14        | 0.47     |
| 11:K:91:ARG:HD2  | 11:K:91:ARG:C    | 2.34        | 0.47     |
| 1:A:973:G:C3'    | 1:A:974:A:H5''   | 2.41        | 0.47     |
| 6:F:64:GLN:O     | 6:F:65:VAL:HB    | 2.14        | 0.47     |
| 13:M:120:LYS:HE2 | 13:M:122:LYS:NZ  | 2.29        | 0.47     |
| 1:A:473:G:H2'    | 1:A:474:G:H8     | 1.80        | 0.47     |
| 19:S:29:ARG:O    | 19:S:31:ILE:HG22 | 2.15        | 0.47     |
| 2:B:51:LEU:O     | 2:B:55:PHE:HD2   | 1.98        | 0.47     |
| 1:A:922:G:N3     | 1:A:1398:A:H2    | 2.12        | 0.47     |
| 3:C:44:GLU:HA    | 3:C:52:LEU:CD1   | 2.44        | 0.47     |
| 1:A:600:C:O2'    | 1:A:601:C:H5'    | 2.14        | 0.47     |
| 1:A:235:C:C5'    | 17:Q:70:ARG:HG2  | 2.41        | 0.47     |
| 2:B:220:ASP:C    | 2:B:222:ILE:H    | 2.18        | 0.47     |
| 18:R:63:GLN:OE1  | 18:R:63:GLN:HA   | 2.14        | 0.47     |
| 22:W:54:U:H3'    | 22:W:55:U:O2     | 2.15        | 0.47     |
| 6:F:5:GLU:HG2    | 6:F:62:TRP:HZ2   | 1.79        | 0.47     |
| 4:D:176:LEU:HG   | 4:D:177:ASP:N    | 2.13        | 0.47     |
| 24:Y:322:LYS:HD2 | 24:Y:328:LEU:O   | 2.15        | 0.47     |
| 10:J:3:LYS:NZ    | 10:J:77:PRO:HD2  | 2.29        | 0.47     |
| 1:A:218:C:H5'    | 1:A:470:C:N4     | 2.30        | 0.47     |
| 3:C:22:TRP:CZ2   | 14:N:54:PRO:HG2  | 2.50        | 0.47     |
| 1:A:1005:A:C3'   | 1:A:1006:C:H5'   | 2.45        | 0.47     |
| 2:B:115:LEU:HD13 | 2:B:145:LEU:HB3  | 1.95        | 0.47     |
| 2:B:187:LEU:HD11 | 2:B:205:ASP:HA   | 1.96        | 0.47     |
| 12:L:53:ARG:HG2  | 12:L:93:LEU:HD11 | 1.95        | 0.47     |
| 12:L:91:LYS:O    | 12:L:92:ASP:HB2  | 2.14        | 0.47     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 24:Y:26:LEU:O    | 24:Y:30:GLU:CG    | 2.63        | 0.47     |
| 4:D:110:PHE:N    | 4:D:110:PHE:CD1   | 2.78        | 0.47     |
| 1:A:1300:G:O2'   | 1:A:1301:U:P      | 2.73        | 0.47     |
| 16:P:4:ILE:HB    | 16:P:66:PRO:HB3   | 1.97        | 0.47     |
| 1:A:1343:G:H1'   | 9:I:121:ARG:NH1   | 2.29        | 0.47     |
| 17:Q:77:VAL:HG12 | 17:Q:78:GLU:N     | 2.30        | 0.47     |
| 24:Y:138:ARG:HD2 | 24:Y:142:ARG:HH22 | 1.80        | 0.47     |
| 1:A:1493:A:H1'   | 24:Y:124:ALA:HA   | 1.96        | 0.47     |
| 1:A:1493:A:O3'   | 24:Y:126:GLY:HA2  | 2.14        | 0.47     |
| 24:Y:97:LYS:C    | 24:Y:99:ASP:N     | 2.68        | 0.47     |
| 18:R:25:THR:O    | 18:R:25:THR:HG22  | 2.15        | 0.47     |
| 1:A:164:U:H2'    | 1:A:165:C:H6      | 1.80        | 0.47     |
| 20:T:73:HIS:O    | 20:T:76:ALA:HB3   | 2.15        | 0.47     |
| 2:B:28:PHE:CD1   | 2:B:28:PHE:O      | 2.68        | 0.47     |
| 1:A:1403:C:O5'   | 1:A:1403:C:H6     | 1.97        | 0.47     |
| 9:I:70:LYS:O     | 9:I:74:ILE:HG13   | 2.15        | 0.47     |
| 4:D:14:ARG:HA    | 4:D:39:PRO:CB     | 2.45        | 0.47     |
| 22:W:27:G:H1     | 22:W:43:C:N4      | 2.12        | 0.47     |
| 16:P:21:VAL:HG12 | 16:P:34:GLU:O     | 2.14        | 0.47     |
| 12:L:88:GLY:O    | 12:L:89:ARG:O     | 2.33        | 0.47     |
| 8:H:109:ILE:HD11 | 8:H:120:THR:CG2   | 2.43        | 0.47     |
| 1:A:1170:A:H2'   | 1:A:1171:G:H5'    | 1.97        | 0.47     |
| 1:A:1193:G:O2'   | 1:A:1194:U:H5'    | 2.15        | 0.47     |
| 24:Y:174:GLU:OE2 | 24:Y:175:ASN:ND2  | 2.47        | 0.47     |
| 11:K:18:ARG:HH21 | 11:K:37:GLY:N     | 2.13        | 0.47     |
| 1:A:19:C:H2'     | 1:A:20:U:C6       | 2.50        | 0.47     |
| 22:W:9:A:O2'     | 22:W:10:G:N7      | 2.47        | 0.47     |
| 1:A:939:G:H2'    | 1:A:940:C:H6      | 1.78        | 0.47     |
| 5:E:39:GLY:HA2   | 5:E:69:VAL:HB     | 1.97        | 0.47     |
| 12:L:84:LEU:HB3  | 12:L:101:VAL:HB   | 1.97        | 0.47     |
| 7:G:82:GLY:HA2   | 23:X:14:A:H61     | 1.80        | 0.47     |
| 6:F:99:ALA:O     | 6:F:100:ASN:HB2   | 2.15        | 0.47     |
| 1:A:1300:G:H1'   | 1:A:1301:U:H5     | 1.79        | 0.47     |
| 1:A:178:C:H2'    | 1:A:179:A:H8      | 1.79        | 0.47     |
| 1:A:709:G:O2'    | 1:A:710:G:H5'     | 2.15        | 0.47     |
| 17:Q:46:ASP:OD1  | 17:Q:49:GLU:HA    | 2.15        | 0.47     |
| 1:A:517:G:H2'    | 1:A:531:U:C5      | 2.50        | 0.47     |
| 1:A:908:A:H2'    | 1:A:909:A:H8      | 1.80        | 0.47     |
| 22:W:48:C:C5     | 22:W:59:U:H1'     | 2.50        | 0.47     |
| 22:W:63:G:H2'    | 22:W:64:A:C5'     | 2.41        | 0.47     |
| 1:A:963:G:N2     | 10:J:55:LYS:CD    | 2.78        | 0.47     |
| 6:F:29:ALA:HB3   | 6:F:30:LEU:HD23   | 1.97        | 0.47     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 13:M:125:ARG:CB   | 24:Y:159:GLY:HA3  | 2.45        | 0.47     |
| 13:M:125:ARG:CG   | 24:Y:160:PRO:HD2  | 2.34        | 0.47     |
| 12:L:35:GLY:HA3   | 12:L:58:VAL:CG1   | 2.45        | 0.47     |
| 9:I:10:ARG:HH11   | 9:I:105:ASP:N     | 2.13        | 0.47     |
| 18:R:37:VAL:HG23  | 18:R:38:GLU:N     | 2.26        | 0.47     |
| 16:P:39:TYR:CD1   | 16:P:73:LEU:HD13  | 2.49        | 0.47     |
| 1:A:91:C:O2       | 1:A:91:C:C2'      | 2.60        | 0.47     |
| 3:C:119:ARG:HG3   | 3:C:119:ARG:NH1   | 2.29        | 0.47     |
| 2:B:217:ARG:HG3   | 2:B:217:ARG:HH11  | 1.80        | 0.47     |
| 1:A:985:C:H42     | 1:A:1220:G:H1     | 1.62        | 0.47     |
| 1:A:1221:G:O2'    | 1:A:1222:G:H5'    | 2.14        | 0.47     |
| 18:R:25:THR:HG22  | 18:R:42:ARG:HH12  | 1.79        | 0.47     |
| 4:D:65:ARG:HG3    | 4:D:75:PHE:CD1    | 2.50        | 0.47     |
| 1:A:562:C:H1'     | 12:L:15:ARG:HD2   | 1.95        | 0.47     |
| 1:A:643:C:H5'     | 8:H:31:PHE:CE1    | 2.50        | 0.47     |
| 1:A:19:C:H5''     | 5:E:86:ALA:CB     | 2.44        | 0.47     |
| 22:V:37:A:H3'     | 22:V:38:A:H8      | 1.79        | 0.47     |
| 18:R:44:LEU:N     | 18:R:44:LEU:HD12  | 2.30        | 0.47     |
| 1:A:1472:U:O2'    | 1:A:1473:A:H5'    | 2.15        | 0.47     |
| 24:Y:279:LEU:HD23 | 24:Y:283:LEU:CD1  | 2.44        | 0.46     |
| 1:A:1318:A:H1'    | 19:S:37:ARG:NH2   | 2.30        | 0.46     |
| 13:M:14:ARG:HD2   | 13:M:42:ALA:HA    | 1.97        | 0.46     |
| 3:C:156:ARG:NH2   | 3:C:161:GLU:HA    | 2.30        | 0.46     |
| 10:J:6:ILE:HG22   | 10:J:98:ILE:HG23  | 1.96        | 0.46     |
| 1:A:911:U:OP2     | 12:L:97:ARG:NH2   | 2.48        | 0.46     |
| 1:A:1118:C:H1'    | 1:A:1179:A:C4     | 2.50        | 0.46     |
| 13:M:65:LYS:HD2   | 13:M:69:GLU:HG3   | 1.96        | 0.46     |
| 6:F:78:GLU:O      | 6:F:81:ILE:HG13   | 2.15        | 0.46     |
| 1:A:45:U:H2'      | 1:A:46:G:C8       | 2.50        | 0.46     |
| 1:A:604:G:O2'     | 1:A:605:U:H5'     | 2.15        | 0.46     |
| 5:E:135:THR:O     | 5:E:138:ALA:HB3   | 2.15        | 0.46     |
| 24:Y:15:GLY:O     | 24:Y:62:PHE:HE1   | 1.98        | 0.46     |
| 8:H:102:ARG:N     | 8:H:102:ARG:HD3   | 2.30        | 0.46     |
| 20:T:25:ARG:HH11  | 20:T:25:ARG:HG3   | 1.79        | 0.46     |
| 24:Y:116:ALA:HB2  | 24:Y:177:TYR:CD1  | 2.50        | 0.46     |
| 10:J:58:ASP:O     | 10:J:60:ARG:N     | 2.48        | 0.46     |
| 6:F:5:GLU:HG2     | 6:F:62:TRP:CZ2    | 2.50        | 0.46     |
| 24:Y:60:ASP:O     | 24:Y:63:ARG:HB2   | 2.15        | 0.46     |
| 24:Y:139:MET:CE   | 24:Y:341:LEU:HD21 | 2.44        | 0.46     |
| 17:Q:59:ILE:HG22  | 17:Q:71:PHE:HD1   | 1.80        | 0.46     |
| 1:A:1456:G:O3'    | 20:T:39:LYS:NZ    | 2.49        | 0.46     |
| 1:A:59:A:H5'      | 1:A:60:A:H5''     | 1.95        | 0.46     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 4:D:60:GLU:HG2   | 4:D:202:LEU:HD12 | 1.96        | 0.46     |
| 24:Y:155:ASP:HB3 | 24:Y:168:GLN:HB3 | 1.96        | 0.46     |
| 1:A:714:G:H2'    | 1:A:715:A:C8     | 2.50        | 0.46     |
| 3:C:167:TRP:CG   | 3:C:168:ALA:N    | 2.82        | 0.46     |
| 20:T:72:LEU:HD21 | 20:T:80:ARG:HE   | 1.80        | 0.46     |
| 24:Y:24:THR:O    | 24:Y:28:GLU:HG3  | 2.16        | 0.46     |
| 2:B:162:ILE:HG13 | 2:B:162:ILE:O    | 2.15        | 0.46     |
| 6:F:39:LYS:H     | 6:F:64:GLN:HB3   | 1.80        | 0.46     |
| 11:K:54:ARG:NH1  | 22:W:39:U:O2'    | 2.48        | 0.46     |
| 10:J:4:ILE:HB    | 10:J:74:ILE:HD11 | 1.97        | 0.46     |
| 12:L:18:VAL:O    | 12:L:19:ARG:CB   | 2.63        | 0.46     |
| 12:L:93:LEU:O    | 12:L:96:VAL:HG23 | 2.16        | 0.46     |
| 4:D:196:LEU:N    | 4:D:196:LEU:HD12 | 2.23        | 0.46     |
| 1:A:564:C:O2'    | 8:H:91:ARG:NH2   | 2.48        | 0.46     |
| 22:W:29:G:H2'    | 22:W:30:G:C8     | 2.49        | 0.46     |
| 1:A:450:G:H4'    | 16:P:41:PRO:O    | 2.16        | 0.46     |
| 1:A:1242:C:H5''  | 21:U:10:ARG:NH1  | 2.30        | 0.46     |
| 6:F:17:SER:O     | 6:F:20:ALA:HB3   | 2.15        | 0.46     |
| 1:A:33:A:H2'     | 1:A:34:C:C6      | 2.51        | 0.46     |
| 1:A:1309:G:C6    | 1:A:1329:A:C2    | 3.04        | 0.46     |
| 1:A:568:G:O6     | 12:L:5:PRO:HD3   | 2.15        | 0.46     |
| 1:A:1225:A:N3    | 1:A:1225:A:H2'   | 2.30        | 0.46     |
| 13:M:97:PRO:O    | 13:M:98:VAL:HA   | 2.16        | 0.46     |
| 1:A:963:G:H21    | 10:J:55:LYS:NZ   | 2.09        | 0.46     |
| 22:W:39:U:C3'    | 22:W:40:C:C5'    | 2.93        | 0.46     |
| 1:A:1131:G:H2'   | 1:A:1132:C:C6    | 2.51        | 0.46     |
| 13:M:81:LEU:O    | 13:M:89:GLY:HA3  | 2.15        | 0.46     |
| 24:Y:286:LEU:HA  | 24:Y:289:LYS:HB2 | 1.97        | 0.46     |
| 2:B:187:LEU:HD23 | 2:B:201:ILE:CG2  | 2.41        | 0.46     |
| 1:A:1503:A:HO2'  | 1:A:1504:G:P     | 2.37        | 0.46     |
| 1:A:1504:G:OP1   | 1:A:1507:A:H4'   | 2.14        | 0.46     |
| 2:B:8:LYS:O      | 2:B:12:GLU:HG3   | 2.14        | 0.46     |
| 1:A:1437:C:O2'   | 1:A:1438:G:H5'   | 2.14        | 0.46     |
| 1:A:335:C:H2'    | 1:A:336:C:C6     | 2.50        | 0.46     |
| 2:B:204:ASN:ND2  | 2:B:207:ALA:H    | 2.14        | 0.46     |
| 1:A:664:G:H22    | 1:A:741:G:H1     | 1.61        | 0.46     |
| 8:H:121:ASP:CG   | 8:H:122:ARG:H    | 2.18        | 0.46     |
| 8:H:17:THR:HG22  | 8:H:63:LEU:HG    | 1.97        | 0.46     |
| 24:Y:75:LEU:HD22 | 24:Y:75:LEU:N    | 2.30        | 0.46     |
| 24:Y:15:GLY:O    | 24:Y:62:PHE:CE1  | 2.69        | 0.46     |
| 16:P:56:ALA:O    | 16:P:60:LEU:HG   | 2.15        | 0.46     |
| 1:A:1461:G:O2'   | 1:A:1462:G:H5'   | 2.16        | 0.46     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:769:G:O2'     | 1:A:770:C:H5'     | 2.15        | 0.46     |
| 1:A:495:A:H4'     | 1:A:496:A:OP1     | 2.14        | 0.46     |
| 1:A:1227:A:C2'    | 1:A:1228:C:O5'    | 2.64        | 0.46     |
| 22:W:59:U:H2'     | 22:W:60:U:C5      | 2.49        | 0.46     |
| 24:Y:252:VAL:HG13 | 24:Y:259:THR:CG2  | 2.32        | 0.46     |
| 6:F:69:GLU:HG2    | 6:F:70:ASP:N      | 2.31        | 0.46     |
| 23:X:20:A:C2      | 24:Y:202:HIS:HB3  | 2.50        | 0.46     |
| 9:I:4:TYR:CG      | 9:I:19:LEU:HB2    | 2.51        | 0.46     |
| 1:A:729:A:H2'     | 1:A:730:G:H8      | 1.80        | 0.46     |
| 12:L:53:ARG:CG    | 12:L:53:ARG:NH1   | 2.77        | 0.46     |
| 1:A:586:C:H1'     | 1:A:878:G:O2'     | 2.15        | 0.46     |
| 8:H:91:ARG:NH1    | 8:H:91:ARG:CG     | 2.79        | 0.46     |
| 3:C:179:ARG:O     | 3:C:179:ARG:HG3   | 2.15        | 0.46     |
| 7:G:120:ILE:H     | 7:G:120:ILE:CD1   | 2.26        | 0.46     |
| 10:J:61:GLU:OE2   | 14:N:45:ARG:HD2   | 2.15        | 0.46     |
| 2:B:236:TYR:HA    | 2:B:239:VAL:HG23  | 1.97        | 0.46     |
| 4:D:61:LYS:NZ     | 4:D:72:GLU:OE2    | 2.48        | 0.46     |
| 17:Q:24:GLU:OE1   | 17:Q:37:LYS:HD3   | 2.15        | 0.46     |
| 24:Y:209:GLU:CG   | 24:Y:303:ARG:HD3  | 2.46        | 0.46     |
| 13:M:125:ARG:HD2  | 24:Y:165:ASP:HB2  | 1.98        | 0.46     |
| 11:K:108:ILE:N    | 11:K:108:ILE:HD12 | 2.30        | 0.46     |
| 15:O:83:GLU:C     | 15:O:85:LEU:H     | 2.19        | 0.46     |
| 1:A:417:C:O2'     | 1:A:418:C:H5'     | 2.16        | 0.46     |
| 4:D:13:ARG:NH2    | 4:D:36:ARG:HD3    | 2.30        | 0.46     |
| 24:Y:23:GLU:HG3   | 24:Y:26:LEU:HD21  | 1.97        | 0.46     |
| 24:Y:76:MET:HG3   | 24:Y:88:LYS:CE    | 2.45        | 0.46     |
| 10:J:16:LEU:O     | 10:J:16:LEU:HD22  | 2.16        | 0.46     |
| 3:C:112:SER:O     | 3:C:116:VAL:HG23  | 2.14        | 0.46     |
| 4:D:151:LYS:O     | 4:D:155:LEU:HG    | 2.16        | 0.46     |
| 1:A:936:C:H2'     | 1:A:937:A:H8      | 1.79        | 0.46     |
| 2:B:14:GLY:C      | 2:B:15:VAL:HG22   | 2.35        | 0.46     |
| 2:B:7:VAL:CA      | 2:B:217:ARG:HH22  | 2.28        | 0.46     |
| 13:M:67:GLU:CG    | 13:M:68:GLY:H     | 2.29        | 0.46     |
| 8:H:51:VAL:HG23   | 8:H:52:ASP:N      | 2.30        | 0.46     |
| 15:O:39:LEU:CD1   | 15:O:56:LEU:HB2   | 2.45        | 0.46     |
| 22:V:74:C:H2'     | 22:V:75:C:H5'     | 1.97        | 0.46     |
| 1:A:9:G:H5''      | 5:E:122:GLU:CD    | 2.36        | 0.46     |
| 1:A:759:A:H2'     | 1:A:760:G:H5'     | 1.98        | 0.46     |
| 18:R:44:LEU:HA    | 18:R:49:LYS:O     | 2.15        | 0.46     |
| 7:G:50:ILE:C      | 7:G:52:GLU:H      | 2.18        | 0.46     |
| 4:D:16:GLY:HA2    | 4:D:33:MET:HE1    | 1.98        | 0.46     |
| 15:O:85:LEU:O     | 15:O:85:LEU:HD23  | 2.15        | 0.46     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:136:C:H2'    | 1:A:137:C:C6      | 2.51        | 0.46     |
| 24:Y:23:GLU:HA   | 24:Y:26:LEU:HG    | 1.98        | 0.46     |
| 2:B:67:THR:HG21  | 2:B:155:LEU:CG    | 2.46        | 0.46     |
| 7:G:113:GLU:CB   | 7:G:119:ARG:HG2   | 2.46        | 0.46     |
| 1:A:403:C:H2'    | 1:A:404:U:C6      | 2.48        | 0.46     |
| 7:G:103:TRP:CH2  | 7:G:141:VAL:HG21  | 2.51        | 0.46     |
| 1:A:766:A:H2'    | 1:A:767:A:O4'     | 2.16        | 0.46     |
| 5:E:26:PHE:CD1   | 5:E:26:PHE:N      | 2.83        | 0.46     |
| 13:M:91:ARG:HH22 | 13:M:103:THR:HG21 | 1.80        | 0.46     |
| 10:J:24:VAL:O    | 10:J:28:ARG:HG3   | 2.15        | 0.46     |
| 1:A:1305:G:N2    | 1:A:1331:G:N3     | 2.63        | 0.46     |
| 16:P:53:VAL:CG1  | 16:P:79:VAL:HG22  | 2.43        | 0.46     |
| 2:B:224:GLN:HA   | 2:B:229:VAL:CG2   | 2.44        | 0.46     |
| 1:A:1251:A:H4'   | 9:I:12:GLU:OE2    | 2.16        | 0.46     |
| 9:I:83:ARG:O     | 9:I:86:VAL:HG12   | 2.14        | 0.46     |
| 13:M:83:ASP:CG   | 13:M:84:ILE:N     | 2.66        | 0.46     |
| 19:S:40:ILE:HD13 | 19:S:62:ILE:CD1   | 2.46        | 0.46     |
| 1:A:502:G:C2     | 1:A:503:C:O2      | 2.69        | 0.46     |
| 1:A:1157:A:H4'   | 1:A:1158:C:O5'    | 2.16        | 0.46     |
| 1:A:1392:G:O2'   | 1:A:1393:U:H5'    | 2.16        | 0.46     |
| 8:H:112:LEU:HG   | 8:H:112:LEU:O     | 2.16        | 0.46     |
| 1:A:688:G:H2'    | 1:A:689:C:C6      | 2.49        | 0.46     |
| 1:A:1479:C:O2'   | 1:A:1480:G:H5'    | 2.16        | 0.46     |
| 1:A:908:A:H2'    | 1:A:909:A:C8      | 2.51        | 0.46     |
| 1:A:770:C:O2'    | 1:A:771:G:H5'     | 2.15        | 0.46     |
| 1:A:731:G:OP1    | 1:A:766:A:H1'     | 2.16        | 0.46     |
| 11:K:48:ILE:HD11 | 11:K:64:ALA:HA    | 1.96        | 0.46     |
| 5:E:96:PRO:HA    | 5:E:117:ASP:CG    | 2.36        | 0.46     |
| 2:B:168:THR:O    | 2:B:169:LYS:C     | 2.53        | 0.46     |
| 1:A:959:A:H2'    | 1:A:960:U:C4'     | 2.46        | 0.46     |
| 3:C:153:VAL:O    | 3:C:165:THR:HA    | 2.16        | 0.46     |
| 3:C:71:ALA:HA    | 3:C:106:VAL:HB    | 1.97        | 0.46     |
| 5:E:51:VAL:HB    | 5:E:52:PRO:CD     | 2.35        | 0.46     |
| 1:A:1029:C:H2'   | 1:A:1030(A):G:C6  | 2.51        | 0.46     |
| 5:E:100:VAL:HG23 | 5:E:100:VAL:O     | 2.14        | 0.46     |
| 12:L:38:THR:HG23 | 12:L:57:LYS:O     | 2.16        | 0.46     |
| 1:A:1305:G:N2    | 1:A:1331:G:O2'    | 2.49        | 0.46     |
| 1:A:1301:U:H3'   | 1:A:1302:U:H5''   | 1.98        | 0.46     |
| 16:P:20:VAL:HG21 | 16:P:32:TYR:CB    | 2.46        | 0.46     |
| 16:P:21:VAL:HG11 | 16:P:59:TRP:NE1   | 2.30        | 0.46     |
| 13:M:19:LEU:HB3  | 13:M:25:ILE:HG21  | 1.98        | 0.46     |
| 2:B:44:LEU:H     | 2:B:44:LEU:CD1    | 2.29        | 0.46     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:1260:C:H4'    | 1:A:1284:C:H5'    | 1.98        | 0.46     |
| 1:A:598:U:O2'     | 1:A:599:C:H5'     | 2.16        | 0.46     |
| 17:Q:22:LEU:HD12  | 17:Q:23:VAL:N     | 2.30        | 0.46     |
| 5:E:57:LYS:HA     | 5:E:60:TYR:HB3    | 1.98        | 0.46     |
| 1:A:781:A:C3'     | 1:A:782:A:H5'     | 2.46        | 0.46     |
| 3:C:110:ASN:O     | 3:C:141:VAL:HG22  | 2.16        | 0.46     |
| 11:K:114:VAL:HG13 | 11:K:114:VAL:O    | 2.16        | 0.46     |
| 13:M:108:ARG:H    | 13:M:108:ARG:HD2  | 1.81        | 0.46     |
| 24:Y:285:GLU:HA   | 24:Y:288:ARG:HH12 | 1.78        | 0.46     |
| 4:D:29:PRO:O      | 4:D:30:LYS:HB3    | 2.15        | 0.46     |
| 4:D:30:LYS:C      | 4:D:32:ALA:N      | 2.56        | 0.46     |
| 1:A:1127:G:H1     | 1:A:1145:C:N4     | 2.14        | 0.46     |
| 6:F:92:LYS:NZ     | 6:F:92:LYS:HB2    | 2.31        | 0.46     |
| 15:O:78:TYR:OH    | 15:O:88:ARG:HG3   | 2.16        | 0.46     |
| 22:V:28:G:O2'     | 22:V:29:G:H5'     | 2.16        | 0.46     |
| 20:T:89:ARG:CD    | 20:T:104:LEU:HD11 | 2.43        | 0.46     |
| 3:C:40:ARG:O      | 3:C:44:GLU:HB2    | 2.16        | 0.46     |
| 17:Q:45:HIS:CB    | 17:Q:65:ILE:HD13  | 2.46        | 0.46     |
| 1:A:853:G:H2'     | 1:A:854:G:C8      | 2.48        | 0.46     |
| 6:F:79:LEU:HD12   | 6:F:88:VAL:HG11   | 1.97        | 0.46     |
| 1:A:1218:C:P      | 14:N:9:LYS:NZ     | 2.88        | 0.46     |
| 15:O:53:HIS:O     | 15:O:56:LEU:HB3   | 2.16        | 0.46     |
| 14:N:34:TYR:CD1   | 14:N:34:TYR:N     | 2.84        | 0.46     |
| 1:A:1513:A:H2'    | 1:A:1514:C:H6     | 1.80        | 0.45     |
| 1:A:1053:G:O6     | 1:A:1199:U:H2'    | 2.15        | 0.45     |
| 1:A:1123:A:O2'    | 10:J:38:ILE:HG22  | 2.15        | 0.45     |
| 10:J:32:ALA:HB3   | 10:J:75:ILE:HG13  | 1.97        | 0.45     |
| 1:A:1493:A:H4'    | 24:Y:126:GLY:CA   | 2.46        | 0.45     |
| 10:J:63:PHE:HZ    | 14:N:45:ARG:HG3   | 1.81        | 0.45     |
| 1:A:1218:C:P      | 14:N:9:LYS:HZ3    | 2.39        | 0.45     |
| 24:Y:346:TRP:N    | 24:Y:346:TRP:CE3  | 2.84        | 0.45     |
| 1:A:139:G:H2'     | 1:A:140:A:C8      | 2.50        | 0.45     |
| 22:V:4:C:O2'      | 22:V:5:G:H5'      | 2.16        | 0.45     |
| 5:E:57:LYS:HE2    | 5:E:61:TYR:HE2    | 1.82        | 0.45     |
| 1:A:442:C:H2'     | 1:A:443:C:C6      | 2.50        | 0.45     |
| 1:A:1176:A:H2'    | 1:A:1177:G:C8     | 2.51        | 0.45     |
| 2:B:77:ALA:CB     | 2:B:165:VAL:HG11  | 2.45        | 0.45     |
| 2:B:93:VAL:HG21   | 2:B:97:TRP:HD1    | 1.80        | 0.45     |
| 1:A:1228:C:H5''   | 13:M:108:ARG:HH22 | 1.80        | 0.45     |
| 24:Y:283:LEU:O    | 24:Y:287:GLU:CB   | 2.64        | 0.45     |
| 13:M:120:LYS:C    | 13:M:121:LYS:HD2  | 2.37        | 0.45     |
| 19:S:41:VAL:HG12  | 19:S:42:PRO:HD2   | 1.99        | 0.45     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 2:B:200:ILE:HG22  | 2:B:202:PRO:HD3   | 1.97        | 0.45     |
| 2:B:55:PHE:HA     | 2:B:58:ILE:CD1    | 2.38        | 0.45     |
| 12:L:46:LYS:HG2   | 12:L:47:LYS:N     | 2.32        | 0.45     |
| 10:J:28:ARG:HH11  | 10:J:28:ARG:HG2   | 1.82        | 0.45     |
| 1:A:644:G:O2'     | 1:A:645:C:H5'     | 2.15        | 0.45     |
| 1:A:389:A:C2'     | 1:A:390:C:H5'     | 2.46        | 0.45     |
| 24:Y:77:GLU:CG    | 24:Y:84:ARG:HG2   | 2.46        | 0.45     |
| 1:A:1353:G:O2'    | 1:A:1354:C:H5'    | 2.16        | 0.45     |
| 1:A:402:G:C2'     | 1:A:403:C:H5'     | 2.45        | 0.45     |
| 14:N:21:TYR:OH    | 14:N:23:ARG:NH2   | 2.49        | 0.45     |
| 3:C:94:LEU:HD12   | 3:C:94:LEU:C      | 2.36        | 0.45     |
| 8:H:48:TYR:HA     | 8:H:60:ARG:O      | 2.17        | 0.45     |
| 5:E:18:ARG:HG3    | 5:E:18:ARG:HH11   | 1.80        | 0.45     |
| 2:B:19:HIS:CG     | 2:B:20:GLU:N      | 2.84        | 0.45     |
| 2:B:95:GLN:HE21   | 2:B:147:LYS:HG2   | 1.81        | 0.45     |
| 24:Y:282:ARG:CB   | 24:Y:282:ARG:HH21 | 2.28        | 0.45     |
| 1:A:584:G:H2'     | 1:A:585:G:C8      | 2.51        | 0.45     |
| 1:A:1471:G:O2'    | 1:A:1472:U:H5'    | 2.16        | 0.45     |
| 1:A:1228:C:H2'    | 1:A:1229:A:C8     | 2.50        | 0.45     |
| 1:A:218:C:H5'     | 1:A:470:C:H41     | 1.80        | 0.45     |
| 1:A:1001(A):G:O2' | 1:A:1002:G:H5'    | 2.16        | 0.45     |
| 12:L:47:LYS:C     | 12:L:49:ASN:H     | 2.20        | 0.45     |
| 1:A:520:A:OP1     | 12:L:52:LEU:HB2   | 2.16        | 0.45     |
| 19:S:18:LYS:C     | 19:S:22:LEU:HD23  | 2.37        | 0.45     |
| 1:A:112:G:H4'     | 1:A:389:A:H5''    | 1.98        | 0.45     |
| 1:A:1054:C:C3'    | 1:A:1054:C:O2     | 2.65        | 0.45     |
| 1:A:377:G:O2'     | 1:A:378:G:H5'     | 2.17        | 0.45     |
| 5:E:72:GLN:O      | 5:E:73:ASN:HB2    | 2.16        | 0.45     |
| 12:L:117:ARG:HB3  | 12:L:122:THR:HB   | 1.97        | 0.45     |
| 7:G:68:ASN:O      | 7:G:138:LYS:HD2   | 2.16        | 0.45     |
| 4:D:10:ARG:HG2    | 4:D:10:ARG:O      | 2.16        | 0.45     |
| 4:D:98:GLU:O      | 4:D:100:ARG:N     | 2.49        | 0.45     |
| 7:G:23:VAL:O      | 7:G:27:ILE:HG13   | 2.15        | 0.45     |
| 1:A:161:A:H2'     | 1:A:162:A:C8      | 2.51        | 0.45     |
| 9:I:59:PHE:N      | 9:I:59:PHE:CD1    | 2.84        | 0.45     |
| 1:A:1106:G:H2'    | 1:A:1107:C:C6     | 2.52        | 0.45     |
| 13:M:125:ARG:HB2  | 24:Y:159:GLY:HA3  | 1.98        | 0.45     |
| 24:Y:131:ASP:CA   | 24:Y:163:GLY:HA2  | 2.40        | 0.45     |
| 5:E:20:GLN:O      | 5:E:21:ALA:O      | 2.34        | 0.45     |
| 6:F:15:ASP:HB2    | 6:F:16:GLN:NE2    | 2.32        | 0.45     |
| 7:G:120:ILE:HG22  | 7:G:124:LEU:CD1   | 2.46        | 0.45     |
| 3:C:92:ALA:C      | 3:C:94:LEU:H      | 2.19        | 0.45     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:373:A:H2'    | 1:A:374:A:H8      | 1.81        | 0.45     |
| 18:R:25:THR:O    | 18:R:26:LEU:HG    | 2.16        | 0.45     |
| 12:L:102:ARG:CG  | 12:L:102:ARG:HH11 | 2.27        | 0.45     |
| 1:A:41:G:H2'     | 1:A:42:G:C8       | 2.50        | 0.45     |
| 1:A:80:G:H3'     | 1:A:81:U:H5'      | 1.98        | 0.45     |
| 1:A:1298:C:H4'   | 1:A:1299:A:N9     | 2.31        | 0.45     |
| 11:K:70:LYS:O    | 11:K:73:MET:HG2   | 2.15        | 0.45     |
| 1:A:110:C:H2'    | 1:A:111:G:O4'     | 2.17        | 0.45     |
| 9:I:2:GLU:HG2    | 9:I:2:GLU:O       | 2.16        | 0.45     |
| 24:Y:215:ASP:C   | 24:Y:216:GLU:HG3  | 2.35        | 0.45     |
| 22:W:17:C:H2'    | 22:W:17:C:O2      | 2.15        | 0.45     |
| 4:D:12:CYS:O     | 4:D:33:MET:HE2    | 2.16        | 0.45     |
| 1:A:735:C:C2     | 1:A:736:C:C5      | 3.05        | 0.45     |
| 1:A:1034:G:H2'   | 1:A:1035:A:C6     | 2.52        | 0.45     |
| 1:A:592:G:H2'    | 1:A:593:G:H8      | 1.80        | 0.45     |
| 16:P:28:ARG:CG   | 16:P:28:ARG:HH11  | 2.22        | 0.45     |
| 12:L:70:ILE:CD1  | 12:L:77:LEU:HD12  | 2.43        | 0.45     |
| 3:C:156:ARG:NH2  | 3:C:159:GLY:O     | 2.49        | 0.45     |
| 1:A:1020:U:H2'   | 1:A:1021:G:H8     | 1.80        | 0.45     |
| 14:N:14:PRO:O    | 14:N:15:LYS:C     | 2.55        | 0.45     |
| 2:B:204:ASN:HD21 | 2:B:207:ALA:H     | 1.63        | 0.45     |
| 1:A:1329:A:OP1   | 13:M:28:ALA:HB3   | 2.15        | 0.45     |
| 1:A:233:C:H2'    | 1:A:234:C:H6      | 1.82        | 0.45     |
| 1:A:1207:G:H2'   | 1:A:1208:C:H6     | 1.81        | 0.45     |
| 20:T:69:GLY:O    | 20:T:73:HIS:CD2   | 2.69        | 0.45     |
| 24:Y:282:ARG:NH2 | 24:Y:282:ARG:CB   | 2.80        | 0.45     |
| 1:A:932:C:H5''   | 7:G:3:ARG:HD2     | 1.98        | 0.45     |
| 4:D:180:GLY:O    | 4:D:182:LYS:HD2   | 2.16        | 0.45     |
| 2:B:102:LEU:CD1  | 2:B:102:LEU:N     | 2.80        | 0.45     |
| 10:J:50:ILE:HD11 | 14:N:41:ARG:CZ    | 2.46        | 0.45     |
| 22:W:31:A:H1'    | 22:W:40:C:O2      | 2.16        | 0.45     |
| 20:T:57:ARG:NH1  | 20:T:100:ILE:HG13 | 2.31        | 0.45     |
| 1:A:1347:G:H5''  | 9:I:107:ARG:HB3   | 1.98        | 0.45     |
| 2:B:187:LEU:HD13 | 2:B:187:LEU:O     | 2.16        | 0.45     |
| 22:V:25:C:H2'    | 22:V:26:A:H8      | 1.80        | 0.45     |
| 1:A:189(F):U:C4  | 17:Q:72:ARG:CZ    | 2.99        | 0.45     |
| 9:I:113:LYS:H    | 9:I:113:LYS:HD2   | 1.79        | 0.45     |
| 9:I:118:LYS:NZ   | 9:I:118:LYS:CB    | 2.79        | 0.45     |
| 23:X:21:A:N6     | 24:Y:190:VAL:HG13 | 2.32        | 0.45     |
| 6:F:16:GLN:NE2   | 6:F:16:GLN:H      | 2.14        | 0.45     |
| 1:A:1437:C:H2'   | 1:A:1438:G:H8     | 1.81        | 0.45     |
| 1:A:1084:G:H5'   | 1:A:1102:A:OP2    | 2.16        | 0.45     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:754:C:H3'     | 1:A:754:C:O2      | 2.16        | 0.45     |
| 22:W:20:U:O2      | 22:W:20:U:C2'     | 2.62        | 0.45     |
| 22:W:55:U:O4      | 22:W:57:G:H5''    | 2.17        | 0.45     |
| 1:A:972:C:OP2     | 10:J:57:LYS:HE2   | 2.16        | 0.45     |
| 1:A:1133:G:N2     | 1:A:1143:G:H1'    | 2.31        | 0.45     |
| 20:T:57:ARG:CZ    | 20:T:100:ILE:HG12 | 2.44        | 0.45     |
| 1:A:1342:C:H1'    | 9:I:124:GLN:HE21  | 1.81        | 0.45     |
| 18:R:66:LEU:CG    | 18:R:70:ILE:HD11  | 2.45        | 0.45     |
| 19:S:9:VAL:HG12   | 19:S:9:VAL:O      | 2.16        | 0.45     |
| 10:J:98:ILE:N     | 10:J:98:ILE:HD12  | 2.32        | 0.45     |
| 1:A:1349:A:P      | 9:I:118:LYS:NZ    | 2.90        | 0.45     |
| 4:D:148:VAL:HG12  | 4:D:152:SER:HB2   | 1.99        | 0.45     |
| 6:F:97:PHE:CE2    | 18:R:65:ILE:HD12  | 2.52        | 0.45     |
| 4:D:206:PHE:HD2   | 4:D:207:TYR:CE2   | 2.35        | 0.45     |
| 15:O:64:ARG:HG3   | 15:O:64:ARG:HH11  | 1.80        | 0.45     |
| 2:B:179:LYS:HA    | 8:H:72:PRO:HG3    | 1.97        | 0.45     |
| 7:G:121:ALA:O     | 7:G:125:MET:HG3   | 2.16        | 0.45     |
| 24:Y:178:GLY:O    | 24:Y:349:LEU:HD21 | 2.17        | 0.45     |
| 24:Y:242:VAL:HG13 | 24:Y:243:ASN:N    | 2.30        | 0.45     |
| 14:N:41:ARG:HE    | 14:N:42:ILE:HD11  | 1.82        | 0.45     |
| 24:Y:61:THR:C     | 24:Y:63:ARG:N     | 2.69        | 0.45     |
| 12:L:17:LYS:HD3   | 12:L:18:VAL:HG22  | 1.99        | 0.45     |
| 3:C:64:VAL:O      | 3:C:100:ALA:HB3   | 2.16        | 0.45     |
| 2:B:83:MET:O      | 2:B:85:ALA:N      | 2.50        | 0.45     |
| 11:K:22:HIS:HB3   | 11:K:29:ILE:HG23  | 1.99        | 0.45     |
| 5:E:147:ASP:HA    | 5:E:150:ARG:CZ    | 2.46        | 0.45     |
| 1:A:536:C:H2'     | 1:A:537:G:C8      | 2.52        | 0.45     |
| 3:C:47:LEU:HD21   | 3:C:68:VAL:HG11   | 1.98        | 0.45     |
| 2:B:207:ALA:C     | 2:B:209:ARG:N     | 2.70        | 0.45     |
| 1:A:932:C:H5'     | 7:G:4:ARG:CG      | 2.47        | 0.45     |
| 4:D:176:LEU:HG    | 4:D:178:VAL:N     | 2.24        | 0.45     |
| 16:P:50:LYS:HD3   | 16:P:50:LYS:C     | 2.37        | 0.45     |
| 1:A:393:A:C2      | 1:A:394:G:C8      | 3.05        | 0.45     |
| 4:D:196:LEU:H     | 4:D:196:LEU:CD1   | 2.23        | 0.45     |
| 16:P:71:ARG:O     | 16:P:74:LEU:HB2   | 2.16        | 0.45     |
| 7:G:148:ASN:N     | 7:G:148:ASN:ND2   | 2.65        | 0.45     |
| 1:A:321:A:N6      | 1:A:328:C:O2'     | 2.42        | 0.45     |
| 1:A:833:U:H2'     | 1:A:834:C:H6      | 1.77        | 0.45     |
| 8:H:48:TYR:CD1    | 8:H:48:TYR:C      | 2.89        | 0.45     |
| 1:A:1385:G:O2'    | 1:A:1386:G:H5'    | 2.17        | 0.45     |
| 1:A:957:U:H2'     | 1:A:959:A:OP2     | 2.17        | 0.45     |
| 4:D:29:PRO:O      | 4:D:30:LYS:CB     | 2.64        | 0.45     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 9:I:14:VAL:HG12   | 9:I:15:ALA:N      | 2.32        | 0.45     |
| 9:I:88:TYR:O      | 9:I:89:ASN:CB     | 2.64        | 0.45     |
| 22:V:20:U:H5      | 22:V:21:A:HO2'    | 1.62        | 0.45     |
| 24:Y:85:GLU:HA    | 24:Y:88:LYS:CG    | 2.46        | 0.45     |
| 11:K:88:GLY:O     | 11:K:90:GLY:N     | 2.50        | 0.45     |
| 8:H:24:THR:HG22   | 8:H:63:LEU:HD21   | 1.99        | 0.45     |
| 1:A:161:A:O2'     | 1:A:162:A:H5'     | 2.17        | 0.45     |
| 1:A:1290:G:H2'    | 1:A:1290:G:N3     | 2.31        | 0.45     |
| 1:A:1202:G:N1     | 14:N:42:ILE:HG21  | 2.32        | 0.44     |
| 3:C:16:ARG:HB2    | 3:C:16:ARG:CZ     | 2.46        | 0.44     |
| 24:Y:250:ARG:HG2  | 24:Y:250:ARG:O    | 2.17        | 0.44     |
| 11:K:21:ILE:CD1   | 11:K:21:ILE:N     | 2.80        | 0.44     |
| 1:A:1372:U:OP1    | 9:I:71:SER:HB3    | 2.17        | 0.44     |
| 2:B:142:LEU:HA    | 2:B:145:LEU:CB    | 2.47        | 0.44     |
| 2:B:187:LEU:HA    | 2:B:201:ILE:O     | 2.17        | 0.44     |
| 4:D:13:ARG:CB     | 4:D:13:ARG:HH11   | 2.31        | 0.44     |
| 12:L:38:THR:O     | 12:L:79:GLU:HG2   | 2.17        | 0.44     |
| 11:K:84:VAL:CG2   | 11:K:110:ASP:HA   | 2.47        | 0.44     |
| 24:Y:295:LEU:HD13 | 24:Y:299:ARG:NH2  | 2.29        | 0.44     |
| 24:Y:85:GLU:O     | 24:Y:88:LYS:HB2   | 2.16        | 0.44     |
| 8:H:39:LEU:N      | 8:H:39:LEU:HD22   | 2.32        | 0.44     |
| 1:A:376:G:H2'     | 1:A:377:G:C8      | 2.52        | 0.44     |
| 17:Q:7:THR:HG22   | 17:Q:58:GLU:HA    | 1.99        | 0.44     |
| 9:I:112:LYS:HE3   | 9:I:116:LYS:O     | 2.16        | 0.44     |
| 1:A:1194:U:H2'    | 1:A:1195:C:H6     | 1.81        | 0.44     |
| 24:Y:175:ASN:O    | 24:Y:179:LEU:HD13 | 2.17        | 0.44     |
| 1:A:598:U:H4'     | 8:H:94:TYR:CG     | 2.52        | 0.44     |
| 1:A:781:A:H4'     | 1:A:1522:U:O2'    | 2.17        | 0.44     |
| 1:A:284:G:O2'     | 1:A:285:G:H5'     | 2.17        | 0.44     |
| 4:D:99:SER:HB3    | 4:D:140:VAL:O     | 2.17        | 0.44     |
| 1:A:1310:G:O2'    | 1:A:1311:G:H5'    | 2.17        | 0.44     |
| 2:B:174:VAL:HG13  | 2:B:184:VAL:HG11  | 1.99        | 0.44     |
| 1:A:1202:G:C2     | 14:N:42:ILE:HG21  | 2.52        | 0.44     |
| 16:P:81:ARG:HG2   | 16:P:83:GLU:OE2   | 2.17        | 0.44     |
| 3:C:58:GLU:HB2    | 3:C:65:ALA:CB     | 2.47        | 0.44     |
| 4:D:68:TYR:CD1    | 4:D:68:TYR:N      | 2.85        | 0.44     |
| 3:C:52:LEU:CD2    | 3:C:52:LEU:N      | 2.79        | 0.44     |
| 1:A:1458:G:H5'    | 20:T:32:ALA:HB2   | 1.98        | 0.44     |
| 13:M:80:ARG:HH22  | 19:S:69:HIS:CE1   | 2.35        | 0.44     |
| 24:Y:138:ARG:HH12 | 24:Y:337:LEU:HD13 | 1.82        | 0.44     |
| 1:A:1281:U:H5'    | 1:A:1282:C:H5     | 1.83        | 0.44     |
| 4:D:61:LYS:HA     | 4:D:203:VAL:HG22  | 1.99        | 0.44     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:740:U:H4'     | 15:O:39:LEU:HD23  | 1.99        | 0.44     |
| 17:Q:22:LEU:HD11  | 17:Q:39:SER:HB2   | 1.97        | 0.44     |
| 7:G:23:VAL:HG13   | 7:G:43:PHE:CE2    | 2.52        | 0.44     |
| 1:A:932:C:H5'     | 7:G:4:ARG:HG3     | 1.99        | 0.44     |
| 13:M:29:ARG:HD3   | 13:M:64:TRP:CD2   | 2.52        | 0.44     |
| 14:N:13:THR:HG22  | 14:N:13:THR:O     | 2.18        | 0.44     |
| 2:B:74:LYS:HD2    | 2:B:169:LYS:HG3   | 2.00        | 0.44     |
| 1:A:1049:U:H1'    | 1:A:1201:A:N7     | 2.32        | 0.44     |
| 24:Y:312:ARG:HD2  | 24:Y:314:TYR:OH   | 2.16        | 0.44     |
| 20:T:102:GLY:O    | 20:T:104:LEU:N    | 2.51        | 0.44     |
| 9:I:71:SER:HA     | 9:I:74:ILE:HD12   | 1.99        | 0.44     |
| 16:P:42:ARG:C     | 16:P:43:LYS:HD2   | 2.37        | 0.44     |
| 18:R:66:LEU:O     | 18:R:70:ILE:HG13  | 2.18        | 0.44     |
| 1:A:993:G:N3      | 1:A:993:G:H2'     | 2.32        | 0.44     |
| 13:M:20:THR:C     | 13:M:22:ILE:H     | 2.21        | 0.44     |
| 1:A:60:A:H4'      | 1:A:61:G:O5'      | 2.18        | 0.44     |
| 7:G:150:ALA:HA    | 11:K:59:TYR:HB3   | 1.99        | 0.44     |
| 15:O:23:GLY:O     | 15:O:24:SER:HB3   | 2.16        | 0.44     |
| 6:F:43:LEU:HD23   | 6:F:46:ARG:HH11   | 1.81        | 0.44     |
| 1:A:1378:C:C5     | 1:A:1379:G:C4     | 3.06        | 0.44     |
| 1:A:617:G:H1      | 1:A:623:C:H42     | 1.65        | 0.44     |
| 6:F:80:ARG:HG3    | 6:F:88:VAL:HG23   | 1.99        | 0.44     |
| 7:G:36:LYS:HZ3    | 7:G:36:LYS:HB2    | 1.81        | 0.44     |
| 2:B:36:ARG:O      | 2:B:37:ASN:CB     | 2.64        | 0.44     |
| 22:V:53:G:O2'     | 22:V:54:U:H5'     | 2.17        | 0.44     |
| 24:Y:185:GLY:HA3  | 24:Y:311:ILE:HG23 | 2.00        | 0.44     |
| 1:A:690:G:C6      | 1:A:691:G:C6      | 3.05        | 0.44     |
| 20:T:10:LEU:O     | 20:T:12:ALA:N     | 2.40        | 0.44     |
| 1:A:948:C:O2'     | 1:A:949:A:H5'     | 2.17        | 0.44     |
| 8:H:127:LEU:O     | 8:H:129:VAL:HG13  | 2.18        | 0.44     |
| 24:Y:143:PHE:CD2  | 24:Y:180:LEU:HD21 | 2.52        | 0.44     |
| 1:A:962:C:H2'     | 1:A:963:G:C8      | 2.52        | 0.44     |
| 1:A:1133:G:C1'    | 1:A:1142:G:H22    | 2.31        | 0.44     |
| 11:K:108:ILE:HG22 | 18:R:88:LYS:HB3   | 1.99        | 0.44     |
| 22:V:41:C:H2'     | 22:V:41:C:O2      | 2.18        | 0.44     |
| 9:I:47:LEU:C      | 9:I:49:PRO:HD2    | 2.38        | 0.44     |
| 12:L:33:ARG:HG2   | 12:L:60:LEU:HD12  | 1.99        | 0.44     |
| 1:A:1026:G:H2'    | 1:A:1027:C:H5'    | 2.00        | 0.44     |
| 1:A:651:C:H2'     | 1:A:652:U:C6      | 2.52        | 0.44     |
| 1:A:878:G:H5''    | 8:H:89:PRO:HG2    | 1.96        | 0.44     |
| 3:C:155:GLY:HA3   | 3:C:163:ALA:HB1   | 1.98        | 0.44     |
| 13:M:22:ILE:N     | 13:M:22:ILE:HD12  | 2.32        | 0.44     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:1452:C:H4'   | 1:A:1456:G:N3    | 2.32        | 0.44     |
| 1:A:1374:A:H2'   | 1:A:1375:A:H8    | 1.82        | 0.44     |
| 13:M:66:LEU:O    | 13:M:70:LEU:HB2  | 2.18        | 0.44     |
| 8:H:112:LEU:HD23 | 8:H:112:LEU:N    | 2.31        | 0.44     |
| 4:D:106:TYR:HD1  | 4:D:113:SER:HA   | 1.81        | 0.44     |
| 1:A:1437:C:H2'   | 1:A:1438:G:C8    | 2.53        | 0.44     |
| 8:H:25:ASP:HA    | 8:H:59:LEU:O     | 2.17        | 0.44     |
| 1:A:1508:G:H2'   | 1:A:1509:C:O4'   | 2.18        | 0.44     |
| 1:A:12:U:H2'     | 1:A:13:U:H5''    | 1.99        | 0.44     |
| 7:G:5:ARG:C      | 7:G:7:ALA:H      | 2.19        | 0.44     |
| 22:W:38:A:H2'    | 22:W:39:U:C4'    | 2.47        | 0.44     |
| 20:T:50:GLU:HB2  | 20:T:99:LEU:HD12 | 1.99        | 0.44     |
| 12:L:26:ALA:O    | 12:L:27:LEU:O    | 2.35        | 0.44     |
| 1:A:1502:A:H5''  | 1:A:1504:G:C8    | 2.52        | 0.44     |
| 1:A:625:G:H4'    | 16:P:16:HIS:CD2  | 2.52        | 0.44     |
| 22:V:21:A:C3'    | 22:V:22:G:H5''   | 2.48        | 0.44     |
| 1:A:1287:A:H2    | 1:A:1353:G:N3    | 2.16        | 0.44     |
| 9:I:12:GLU:O     | 9:I:68:GLY:N     | 2.51        | 0.44     |
| 9:I:79:LEU:CD1   | 9:I:83:ARG:HH21  | 2.30        | 0.44     |
| 6:F:22:GLU:C     | 6:F:24:GLU:N     | 2.70        | 0.44     |
| 1:A:383:A:O2'    | 1:A:384:G:H5'    | 2.17        | 0.44     |
| 13:M:66:LEU:N    | 13:M:70:LEU:HD12 | 2.32        | 0.44     |
| 13:M:66:LEU:O    | 13:M:70:LEU:N    | 2.51        | 0.44     |
| 1:A:312:C:O2'    | 1:A:313:A:H5'    | 2.18        | 0.44     |
| 1:A:1062:U:H2'   | 1:A:1063:C:C5    | 2.53        | 0.44     |
| 12:L:82:VAL:HG12 | 12:L:83:VAL:H    | 1.82        | 0.44     |
| 3:C:138:VAL:HG12 | 3:C:170:GLN:HE21 | 1.82        | 0.44     |
| 24:Y:332:ASP:HB2 | 24:Y:335:ASN:HB3 | 1.99        | 0.44     |
| 1:A:629:G:H2'    | 1:A:630:G:C8     | 2.53        | 0.44     |
| 1:A:577:G:O2'    | 1:A:578:C:H5'    | 2.18        | 0.44     |
| 7:G:137:LYS:HE2  | 7:G:141:VAL:HG23 | 2.00        | 0.44     |
| 1:A:127:G:HO2'   | 17:Q:2:PRO:N     | 2.16        | 0.44     |
| 3:C:13:GLY:HA2   | 14:N:57:ARG:NE   | 2.33        | 0.44     |
| 22:W:67:C:H3'    | 22:W:67:C:H6     | 1.82        | 0.44     |
| 22:W:18:G:N2     | 22:W:55:U:H6     | 2.15        | 0.44     |
| 22:W:55:U:C2'    | 22:W:56:C:C5     | 3.01        | 0.44     |
| 24:Y:283:LEU:O   | 24:Y:287:GLU:HG3 | 2.18        | 0.44     |
| 19:S:37:ARG:HG3  | 19:S:37:ARG:H    | 1.57        | 0.44     |
| 24:Y:341:LEU:HA  | 24:Y:344:LEU:CD2 | 2.47        | 0.44     |
| 9:I:15:ALA:HB2   | 9:I:65:VAL:CG2   | 2.40        | 0.44     |
| 5:E:51:VAL:O     | 5:E:55:VAL:HG23  | 2.18        | 0.44     |
| 19:S:15:LEU:HD23 | 19:S:35:SER:OG   | 2.17        | 0.44     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 19:S:16:LEU:O    | 19:S:17:GLU:C    | 2.56        | 0.44     |
| 1:A:1305:G:H22   | 1:A:1331:G:C1'   | 2.30        | 0.44     |
| 17:Q:59:ILE:CD1  | 17:Q:73:VAL:HA   | 2.47        | 0.44     |
| 16:P:12:LYS:O    | 16:P:13:HIS:HB2  | 2.18        | 0.44     |
| 12:L:7:ILE:O     | 12:L:10:LEU:HB2  | 2.18        | 0.44     |
| 24:Y:155:ASP:OD1 | 24:Y:166:TYR:HE2 | 2.00        | 0.44     |
| 1:A:1317:C:P     | 14:N:17:LYS:HE2  | 2.58        | 0.44     |
| 1:A:832:C:O2'    | 1:A:833:U:P      | 2.75        | 0.44     |
| 1:A:173:U:H5''   | 1:A:197:A:O4'    | 2.17        | 0.44     |
| 13:M:116:THR:O   | 13:M:118:ALA:N   | 2.50        | 0.44     |
| 8:H:122:ARG:NH1  | 8:H:122:ARG:CB   | 2.81        | 0.44     |
| 4:D:159:ARG:O    | 4:D:162:LEU:HB2  | 2.17        | 0.44     |
| 6:F:28:ARG:HG3   | 6:F:28:ARG:HH11  | 1.82        | 0.44     |
| 7:G:32:ARG:HH11  | 7:G:32:ARG:HG2   | 1.83        | 0.44     |
| 2:B:165:VAL:CG2  | 2:B:166:ASP:H    | 2.15        | 0.44     |
| 22:W:19:G:OP1    | 22:W:60:U:C4     | 2.71        | 0.44     |
| 1:A:963:G:N2     | 10:J:55:LYS:NZ   | 2.63        | 0.44     |
| 24:Y:115:ASN:CB  | 24:Y:172:LYS:HA  | 2.46        | 0.44     |
| 19:S:48:THR:CG2  | 19:S:61:TYR:HD1  | 2.31        | 0.44     |
| 12:L:48:PRO:C    | 12:L:49:ASN:HD22 | 2.19        | 0.44     |
| 24:Y:19:ILE:N    | 24:Y:20:PRO:HD2  | 2.32        | 0.44     |
| 13:M:32:GLU:O    | 13:M:36:LYS:HG2  | 2.18        | 0.44     |
| 5:E:150:ARG:HG3  | 5:E:153:LYS:HE3  | 2.00        | 0.44     |
| 4:D:120:LEU:HD23 | 4:D:125:HIS:HD2  | 1.83        | 0.44     |
| 1:A:1374:A:C4    | 1:A:1375:A:C8    | 3.05        | 0.44     |
| 4:D:100:ARG:HH12 | 4:D:137:SER:CB   | 2.30        | 0.44     |
| 5:E:107:ARG:O    | 5:E:108:ALA:C    | 2.55        | 0.44     |
| 1:A:160:A:H1'    | 1:A:344:A:N7     | 2.33        | 0.44     |
| 4:D:107:ARG:HG2  | 4:D:107:ARG:HH11 | 1.82        | 0.44     |
| 12:L:85:ILE:HD12 | 12:L:85:ILE:HA   | 1.83        | 0.44     |
| 24:Y:304:PRO:HD2 | 24:Y:309:SER:OG  | 2.18        | 0.44     |
| 22:W:49:C:C2'    | 22:W:50:U:H5'    | 2.47        | 0.44     |
| 6:F:3:ARG:HD3    | 6:F:64:GLN:NE2   | 2.32        | 0.44     |
| 1:A:409:G:H5'    | 4:D:25:ARG:HB2   | 2.00        | 0.44     |
| 3:C:152:ILE:O    | 3:C:198:VAL:HA   | 2.17        | 0.44     |
| 24:Y:164:ILE:CD1 | 24:Y:167:ALA:HB2 | 2.47        | 0.44     |
| 3:C:196:LEU:H    | 3:C:196:LEU:CD2  | 2.31        | 0.44     |
| 1:A:1456:G:H2'   | 1:A:1457:G:O4'   | 2.17        | 0.44     |
| 21:U:10:ARG:HA   | 21:U:13:ILE:HB   | 1.99        | 0.44     |
| 1:A:542:G:H2'    | 1:A:543:C:H6     | 1.83        | 0.44     |
| 1:A:1020:U:H2'   | 1:A:1021:G:C8    | 2.53        | 0.44     |
| 1:A:429:U:H1'    | 1:A:430:A:H5''   | 1.99        | 0.44     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:81:U:H2'     | 1:A:82:U:C5       | 2.53        | 0.44     |
| 1:A:84:U:C2'     | 1:A:88:A:H5'      | 2.48        | 0.44     |
| 6:F:37:VAL:HG12  | 6:F:38:GLU:N      | 2.31        | 0.44     |
| 4:D:28:SER:HB2   | 4:D:30:LYS:CE     | 2.48        | 0.44     |
| 4:D:28:SER:HB3   | 4:D:30:LYS:HE2    | 1.97        | 0.44     |
| 22:W:39:U:C3'    | 22:W:40:C:H5''    | 2.47        | 0.44     |
| 5:E:7:GLU:HB3    | 5:E:112:LEU:HD13  | 1.99        | 0.44     |
| 10:J:26:ALA:HA   | 10:J:29:ARG:NH1   | 2.22        | 0.44     |
| 17:Q:5:VAL:HA    | 17:Q:59:ILE:O     | 2.18        | 0.44     |
| 17:Q:45:HIS:HB2  | 17:Q:65:ILE:CD1   | 2.45        | 0.44     |
| 3:C:156:ARG:HD3  | 3:C:194:GLY:CA    | 2.48        | 0.44     |
| 1:A:404:U:H2'    | 1:A:405:U:C6      | 2.53        | 0.44     |
| 8:H:16:ALA:O     | 8:H:19:VAL:HG22   | 2.18        | 0.44     |
| 19:S:62:ILE:HA   | 19:S:66:MET:HE1   | 2.00        | 0.44     |
| 1:A:1179:A:O3'   | 9:I:103:THR:HG23  | 2.16        | 0.44     |
| 1:A:1274:G:H2'   | 1:A:1275:A:C8     | 2.53        | 0.44     |
| 3:C:99:VAL:O     | 3:C:99:VAL:HG23   | 2.18        | 0.44     |
| 1:A:1079:G:C6    | 1:A:1080:A:N6     | 2.86        | 0.44     |
| 1:A:985:C:H2'    | 1:A:986:A:C8      | 2.53        | 0.44     |
| 24:Y:224:PRO:CA  | 24:Y:227:LEU:HB2  | 2.47        | 0.44     |
| 1:A:1439:C:OP1   | 20:T:38:LYS:HD2   | 2.17        | 0.44     |
| 1:A:1280:A:H5'   | 10:J:40:LEU:HD22  | 1.99        | 0.44     |
| 3:C:29:TYR:HD2   | 3:C:29:TYR:O      | 2.01        | 0.44     |
| 11:K:57:THR:HG23 | 11:K:60:ALA:CB    | 2.48        | 0.44     |
| 3:C:14:ILE:HG23  | 3:C:15:THR:N      | 2.33        | 0.43     |
| 24:Y:250:ARG:HG2 | 24:Y:252:VAL:HG23 | 2.00        | 0.43     |
| 24:Y:139:MET:HE2 | 24:Y:341:LEU:HD11 | 2.00        | 0.43     |
| 12:L:60:LEU:C    | 12:L:62:SER:N     | 2.70        | 0.43     |
| 2:B:46:LYS:HE3   | 2:B:46:LYS:CA     | 2.47        | 0.43     |
| 2:B:32:ILE:HA    | 2:B:42:ILE:HA     | 2.00        | 0.43     |
| 1:A:594:G:C2'    | 1:A:595:G:H5'     | 2.48        | 0.43     |
| 7:G:113:GLU:HB2  | 7:G:119:ARG:CG    | 2.48        | 0.43     |
| 3:C:156:ARG:HD3  | 3:C:194:GLY:H     | 1.83        | 0.43     |
| 1:A:1158:C:H42   | 1:A:1181:G:H1     | 1.65        | 0.43     |
| 1:A:123:C:OP1    | 1:A:311:C:O2'     | 2.34        | 0.43     |
| 1:A:533:A:O2'    | 1:A:534:U:H5''    | 2.18        | 0.43     |
| 8:H:17:THR:HB    | 8:H:78:GLN:OE1    | 2.18        | 0.43     |
| 1:A:125:U:H2'    | 1:A:126:G:H8      | 1.83        | 0.43     |
| 1:A:19:C:H2'     | 1:A:20:U:H6       | 1.83        | 0.43     |
| 24:Y:100:GLU:O   | 24:Y:104:GLN:HB2  | 2.18        | 0.43     |
| 1:A:291:C:O2'    | 1:A:292:G:H5'     | 2.18        | 0.43     |
| 13:M:125:ARG:CZ  | 24:Y:165:ASP:OD2  | 2.66        | 0.43     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 10:J:42:THR:HG22 | 10:J:43:ARG:N    | 2.33        | 0.43     |
| 5:E:100:VAL:CG1  | 5:E:118:ILE:HG22 | 2.42        | 0.43     |
| 7:G:15:ASP:HB3   | 7:G:20:ASP:H     | 1.83        | 0.43     |
| 1:A:1514:C:H2'   | 1:A:1515:C:H6    | 1.83        | 0.43     |
| 1:A:1493:A:H4'   | 24:Y:126:GLY:HA2 | 2.00        | 0.43     |
| 20:T:33:ILE:HG22 | 20:T:34:LYS:N    | 2.33        | 0.43     |
| 1:A:630:G:H2'    | 1:A:631:G:H5''   | 2.00        | 0.43     |
| 1:A:1476:G:H2'   | 1:A:1477:C:C6    | 2.52        | 0.43     |
| 22:V:3:C:C2      | 22:V:71:G:N2     | 2.86        | 0.43     |
| 1:A:19:C:H5''    | 5:E:86:ALA:HB3   | 1.99        | 0.43     |
| 1:A:1360:A:H2'   | 1:A:1361:G:O4'   | 2.17        | 0.43     |
| 9:I:33:PHE:C     | 9:I:35:GLU:H     | 2.20        | 0.43     |
| 1:A:656:C:H2'    | 1:A:657:G:C8     | 2.53        | 0.43     |
| 2:B:178:ARG:HA   | 2:B:178:ARG:HD3  | 1.91        | 0.43     |
| 22:V:39:U:O2'    | 22:V:40:C:H5'    | 2.18        | 0.43     |
| 12:L:28:LYS:HG2  | 12:L:28:LYS:O    | 2.17        | 0.43     |
| 1:A:1293:G:O2'   | 1:A:1294:G:C8    | 2.69        | 0.43     |
| 1:A:376:G:HO2'   | 1:A:377:G:H5'    | 1.83        | 0.43     |
| 10:J:38:ILE:CG1  | 10:J:71:LEU:HB3  | 2.47        | 0.43     |
| 1:A:36:C:O2'     | 1:A:37:U:H5'     | 2.17        | 0.43     |
| 10:J:8:LEU:C     | 10:J:16:LEU:HD21 | 2.39        | 0.43     |
| 1:A:1179:A:O2'   | 1:A:1180:A:H5'   | 2.18        | 0.43     |
| 1:A:1275:A:H2'   | 1:A:1276:G:H8    | 1.83        | 0.43     |
| 1:A:1431:C:H2'   | 1:A:1432:G:O4'   | 2.17        | 0.43     |
| 1:A:796:C:O2'    | 1:A:797:C:H5'    | 2.19        | 0.43     |
| 1:A:1168:A:H2'   | 1:A:1169:A:C8    | 2.53        | 0.43     |
| 22:W:70:G:O2'    | 22:W:71:G:O5'    | 2.36        | 0.43     |
| 8:H:29:SER:HB3   | 8:H:32:LYS:HB2   | 2.00        | 0.43     |
| 1:A:1298:C:C4    | 7:G:114:ARG:HD2  | 2.53        | 0.43     |
| 11:K:34:ASP:HB2  | 11:K:35:PRO:CD   | 2.48        | 0.43     |
| 14:N:53:LEU:HD23 | 14:N:53:LEU:HA   | 1.88        | 0.43     |
| 3:C:23:TYR:CG    | 3:C:24:ALA:N     | 2.86        | 0.43     |
| 13:M:88:ARG:HH11 | 13:M:88:ARG:HG2  | 1.83        | 0.43     |
| 24:Y:304:PRO:C   | 24:Y:306:GLU:H   | 2.21        | 0.43     |
| 1:A:976:G:OP1    | 14:N:32:SER:N    | 2.50        | 0.43     |
| 4:D:176:LEU:CG   | 4:D:177:ASP:N    | 2.72        | 0.43     |
| 15:O:81:LEU:CD1  | 15:O:85:LEU:HD12 | 2.48        | 0.43     |
| 19:S:78:ARG:HD2  | 19:S:81:ARG:NH1  | 2.34        | 0.43     |
| 9:I:4:TYR:HB2    | 9:I:19:LEU:CB    | 2.40        | 0.43     |
| 1:A:592:G:O2'    | 1:A:593:G:H5'    | 2.18        | 0.43     |
| 10:J:38:ILE:HD11 | 10:J:71:LEU:CD2  | 2.43        | 0.43     |
| 1:A:1452:C:O4'   | 1:A:1456:G:C2    | 2.72        | 0.43     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 7:G:86:GLN:HG3   | 7:G:86:GLN:O      | 2.17        | 0.43     |
| 2:B:84:GLU:HB3   | 2:B:219:VAL:HG21  | 1.99        | 0.43     |
| 1:A:1018:C:H2'   | 1:A:1019:C:O4'    | 2.19        | 0.43     |
| 1:A:1463:C:C2'   | 1:A:1464:G:H5'    | 2.49        | 0.43     |
| 1:A:836:G:C6     | 1:A:851:G:C6      | 3.06        | 0.43     |
| 1:A:880:C:H2'    | 1:A:881:G:H8      | 1.84        | 0.43     |
| 6:F:42:GLU:C     | 6:F:44:GLY:H      | 2.22        | 0.43     |
| 21:U:5:ASP:O     | 21:U:11:GLY:HA3   | 2.18        | 0.43     |
| 1:A:960:U:O2     | 1:A:960:U:H2'     | 2.18        | 0.43     |
| 13:M:94:ARG:NH1  | 19:S:81:ARG:HG3   | 2.34        | 0.43     |
| 5:E:76:ILE:HG13  | 5:E:77:PRO:HD2    | 1.99        | 0.43     |
| 9:I:40:LEU:C     | 9:I:42:ARG:N      | 2.72        | 0.43     |
| 1:A:532:A:H61    | 3:C:156:ARG:NH1   | 2.14        | 0.43     |
| 1:A:536:C:H2'    | 1:A:537:G:H8      | 1.84        | 0.43     |
| 23:X:21:A:N1     | 24:Y:201:ARG:HD3  | 2.34        | 0.43     |
| 7:G:92:SER:O     | 7:G:93:PRO:C      | 2.57        | 0.43     |
| 9:I:108:VAL:O    | 9:I:110:GLU:N     | 2.52        | 0.43     |
| 16:P:52:ASP:OD2  | 16:P:54:GLU:HB2   | 2.18        | 0.43     |
| 1:A:1228:C:C5'   | 13:M:108:ARG:HH22 | 2.30        | 0.43     |
| 24:Y:117:ILE:CG1 | 24:Y:170:LEU:HD13 | 2.48        | 0.43     |
| 22:W:49:C:O2     | 22:W:49:C:H2'     | 2.18        | 0.43     |
| 14:N:41:ARG:HH11 | 14:N:41:ARG:HG2   | 1.84        | 0.43     |
| 24:Y:326:THR:CG2 | 24:Y:328:LEU:HD22 | 2.46        | 0.43     |
| 20:T:89:ARG:HB2  | 20:T:104:LEU:CD1  | 2.49        | 0.43     |
| 19:S:48:THR:HG22 | 19:S:61:TYR:HD1   | 1.83        | 0.43     |
| 1:A:552:U:H4'    | 12:L:86:ARG:HG2   | 2.00        | 0.43     |
| 19:S:41:VAL:CG1  | 19:S:42:PRO:HD2   | 2.47        | 0.43     |
| 1:A:1356:G:H2'   | 1:A:1357:A:H8     | 1.80        | 0.43     |
| 5:E:146:ALA:O    | 5:E:147:ASP:C     | 2.57        | 0.43     |
| 20:T:42:GLN:HA   | 20:T:42:GLN:NE2   | 2.33        | 0.43     |
| 3:C:83:ARG:C     | 3:C:85:ARG:H      | 2.22        | 0.43     |
| 1:A:503:C:C6     | 1:A:504:C:H5      | 2.36        | 0.43     |
| 24:Y:140:TYR:OH  | 24:Y:187:HIS:NE2  | 2.46        | 0.43     |
| 1:A:142:G:H2'    | 1:A:143:A:C8      | 2.54        | 0.43     |
| 24:Y:234:ALA:HB2 | 24:Y:247:SER:HG   | 1.82        | 0.43     |
| 1:A:1429:C:H2'   | 1:A:1430:C:C6     | 2.54        | 0.43     |
| 1:A:245:C:O2'    | 1:A:246:A:H5'     | 2.18        | 0.43     |
| 2:B:133:LYS:O    | 2:B:137:ARG:HB2   | 2.19        | 0.43     |
| 4:D:191:ARG:NE   | 4:D:200:GLU:OE1   | 2.50        | 0.43     |
| 1:A:276:G:C5     | 1:A:277:C:C5      | 3.06        | 0.43     |
| 12:L:54:LYS:N    | 12:L:54:LYS:HD2   | 2.34        | 0.43     |
| 2:B:77:ALA:O     | 2:B:78:GLN:C      | 2.56        | 0.43     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 22:W:36:A:H2'     | 22:W:37:A:O4'     | 2.18        | 0.43     |
| 1:A:1250:A:C2     | 1:A:1370:G:H1'    | 2.54        | 0.43     |
| 13:M:13:LYS:HA    | 13:M:44:ARG:NH1   | 2.33        | 0.43     |
| 14:N:4:LYS:HD3    | 14:N:7:ILE:HD11   | 2.01        | 0.43     |
| 1:A:1374:A:C5     | 1:A:1375:A:N7     | 2.86        | 0.43     |
| 1:A:32:A:H2'      | 1:A:33:A:H8       | 1.81        | 0.43     |
| 1:A:715:A:H2'     | 1:A:716:A:C8      | 2.54        | 0.43     |
| 1:A:186:C:H5'     | 20:T:78:ALA:HB1   | 2.00        | 0.43     |
| 1:A:9:G:H2'       | 1:A:10:A:C8       | 2.53        | 0.43     |
| 7:G:50:ILE:C      | 7:G:52:GLU:N      | 2.72        | 0.43     |
| 1:A:666:G:H5'     | 1:A:726:C:H1'     | 1.99        | 0.43     |
| 4:D:153:ARG:HG2   | 4:D:181:MET:SD    | 2.59        | 0.43     |
| 12:L:32:PHE:HB3   | 12:L:84:LEU:HD22  | 2.00        | 0.43     |
| 2:B:187:LEU:CD2   | 2:B:201:ILE:O     | 2.64        | 0.43     |
| 24:Y:267:SER:OG   | 24:Y:270:LYS:HG3  | 2.19        | 0.43     |
| 7:G:116:ALA:H     | 7:G:118:VAL:HG22  | 1.84        | 0.43     |
| 5:E:144:THR:C     | 5:E:146:ALA:N     | 2.72        | 0.43     |
| 5:E:73:ASN:N      | 5:E:73:ASN:ND2    | 2.66        | 0.43     |
| 24:Y:218:VAL:HG13 | 24:Y:218:VAL:O    | 2.19        | 0.43     |
| 13:M:115:LYS:C    | 13:M:117:VAL:N    | 2.69        | 0.43     |
| 1:A:1220:G:O3'    | 19:S:36:ARG:HD3   | 2.19        | 0.43     |
| 1:A:693:G:H2'     | 1:A:694:A:O4'     | 2.18        | 0.43     |
| 22:V:12:U:C3'     | 22:V:13:C:H5''    | 2.49        | 0.43     |
| 11:K:56:GLY:O     | 11:K:89:ALA:HB3   | 2.19        | 0.43     |
| 22:V:36:A:C2      | 23:X:17:U:C2      | 3.06        | 0.43     |
| 1:A:827:U:H2'     | 1:A:870:U:O4      | 2.18        | 0.43     |
| 11:K:122:LYS:O    | 11:K:126:ARG:HG3  | 2.19        | 0.43     |
| 1:A:240:C:H2'     | 1:A:241:C:C6      | 2.54        | 0.43     |
| 5:E:84:PHE:CE2    | 5:E:133:TYR:HD1   | 2.37        | 0.43     |
| 5:E:64:ARG:HH11   | 5:E:64:ARG:HG3    | 1.84        | 0.43     |
| 2:B:71:VAL:O      | 2:B:164:VAL:HA    | 2.18        | 0.43     |
| 14:N:24:CYS:SG    | 14:N:40:CYS:N     | 2.85        | 0.43     |
| 3:C:121:ALA:HB2   | 3:C:198:VAL:CG2   | 2.45        | 0.43     |
| 4:D:165:MET:HB3   | 4:D:178:VAL:HG22  | 2.01        | 0.43     |
| 1:A:1144:G:N2     | 1:A:1146:A:H62    | 2.15        | 0.43     |
| 24:Y:326:THR:OG1  | 24:Y:328:LEU:HD13 | 2.19        | 0.43     |
| 24:Y:150:GLN:HB3  | 24:Y:172:LYS:HD3  | 2.01        | 0.43     |
| 4:D:38:TYR:CD2    | 4:D:45:GLN:HB3    | 2.53        | 0.43     |
| 1:A:520:A:OP2     | 12:L:51:ALA:HB1   | 2.18        | 0.43     |
| 18:R:71:LYS:HA    | 18:R:74:ARG:CD    | 2.48        | 0.43     |
| 1:A:389:A:H2'     | 1:A:390:C:C5'     | 2.48        | 0.43     |
| 7:G:100:ALA:C     | 7:G:104:LEU:HD23  | 2.38        | 0.43     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 7:G:15:ASP:OD1   | 7:G:18:TYR:HB2    | 2.19        | 0.43     |
| 24:Y:78:GLU:O    | 24:Y:80:PRO:HD3   | 2.18        | 0.43     |
| 24:Y:85:GLU:O    | 24:Y:85:GLU:HG2   | 2.18        | 0.43     |
| 7:G:113:GLU:HB2  | 7:G:119:ARG:HG2   | 2.00        | 0.43     |
| 3:C:83:ARG:C     | 3:C:85:ARG:N      | 2.72        | 0.43     |
| 1:A:1269:A:H2    | 1:A:1312:G:N3     | 2.17        | 0.43     |
| 12:L:82:VAL:O    | 12:L:83:VAL:HG23  | 2.19        | 0.43     |
| 8:H:12:ARG:NH1   | 8:H:27:PRO:CD     | 2.80        | 0.43     |
| 1:A:1402:C:H2'   | 1:A:1403:C:O4'    | 2.19        | 0.43     |
| 1:A:278:G:OP2    | 17:Q:41:LYS:HE2   | 2.18        | 0.43     |
| 24:Y:283:LEU:C   | 24:Y:285:GLU:H    | 2.21        | 0.43     |
| 10:J:49:VAL:HG23 | 14:N:41:ARG:HD3   | 2.00        | 0.43     |
| 6:F:3:ARG:NH1    | 6:F:38:GLU:OE1    | 2.51        | 0.43     |
| 22:V:29:G:H1     | 22:V:41:C:H42     | 1.66        | 0.43     |
| 24:Y:341:LEU:HA  | 24:Y:344:LEU:HD21 | 2.01        | 0.43     |
| 1:A:192:U:H4'    | 20:T:57:ARG:HD2   | 2.01        | 0.43     |
| 10:J:3:LYS:N     | 10:J:74:ILE:O     | 2.51        | 0.43     |
| 1:A:1152:A:OP1   | 10:J:68:HIS:CD2   | 2.71        | 0.43     |
| 2:B:43:ASP:O     | 2:B:46:LYS:HB2    | 2.19        | 0.43     |
| 1:A:522:C:O2'    | 1:A:523:A:H5'     | 2.18        | 0.43     |
| 24:Y:72:LEU:HD13 | 24:Y:91:LEU:CG    | 2.48        | 0.43     |
| 2:B:96:ARG:O     | 2:B:98:LEU:N      | 2.52        | 0.43     |
| 16:P:3:LYS:C     | 16:P:4:ILE:HD12   | 2.39        | 0.43     |
| 14:N:4:LYS:C     | 14:N:6:LEU:H      | 2.22        | 0.43     |
| 3:C:82:GLU:H     | 3:C:82:GLU:CD     | 2.21        | 0.43     |
| 3:C:91:LEU:C     | 3:C:93:LYS:N      | 2.71        | 0.43     |
| 1:A:9:G:O2'      | 1:A:10:A:H5'      | 2.19        | 0.43     |
| 22:W:21:A:N6     | 22:W:46:G:C4      | 2.87        | 0.43     |
| 7:G:53:LYS:O     | 7:G:54:THR:HB     | 2.19        | 0.43     |
| 8:H:72:PRO:O     | 8:H:73:ASP:HB3    | 2.19        | 0.43     |
| 1:A:572:A:N3     | 1:A:917:G:H1'     | 2.34        | 0.43     |
| 24:Y:112:ALA:HA  | 24:Y:177:TYR:HB3  | 2.01        | 0.42     |
| 24:Y:304:PRO:O   | 24:Y:305:ILE:HB   | 2.19        | 0.42     |
| 4:D:18:LYS:HG3   | 4:D:31:CYS:HB3    | 2.00        | 0.42     |
| 11:K:116:HIS:O   | 11:K:117:ASN:HB2  | 2.17        | 0.42     |
| 1:A:657:G:H4'    | 15:O:28:GLN:HG2   | 2.01        | 0.42     |
| 12:L:27:LEU:O    | 12:L:28:LYS:HB3   | 2.19        | 0.42     |
| 9:I:17:VAL:HG22  | 9:I:81:ILE:CD1    | 2.49        | 0.42     |
| 1:A:1400:C:O5'   | 1:A:1400:C:H6     | 2.01        | 0.42     |
| 1:A:1320:C:C4    | 1:A:1321:C:C4     | 3.07        | 0.42     |
| 24:Y:27:LYS:HE3  | 24:Y:31:ARG:CZ    | 2.49        | 0.42     |
| 21:U:2:GLY:C     | 21:U:4:GLY:N      | 2.71        | 0.42     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 8:H:134:ILE:O    | 8:H:135:CYS:HB3  | 2.18        | 0.42     |
| 7:G:72:ARG:O     | 7:G:91:VAL:HG23  | 2.18        | 0.42     |
| 1:A:355:C:C4     | 1:A:356:A:N7     | 2.87        | 0.42     |
| 18:R:53:ARG:C    | 18:R:55:ARG:N    | 2.72        | 0.42     |
| 4:D:73:ARG:NH1   | 4:D:73:ARG:HG2   | 2.34        | 0.42     |
| 3:C:69:HIS:N     | 3:C:69:HIS:CD2   | 2.85        | 0.42     |
| 2:B:193:ASP:O    | 2:B:193:ASP:OD2  | 2.37        | 0.42     |
| 6:F:30:LEU:H     | 6:F:30:LEU:CD2   | 2.04        | 0.42     |
| 6:F:3:ARG:NH1    | 6:F:3:ARG:HG3    | 2.30        | 0.42     |
| 6:F:5:GLU:HB3    | 6:F:62:TRP:HE1   | 1.84        | 0.42     |
| 3:C:71:ALA:HA    | 3:C:106:VAL:H    | 1.83        | 0.42     |
| 5:E:41:VAL:HG21  | 5:E:113:ALA:CB   | 2.49        | 0.42     |
| 3:C:58:GLU:O     | 3:C:59:ARG:CG    | 2.67        | 0.42     |
| 2:B:43:ASP:OD2   | 2:B:46:LYS:HD2   | 2.19        | 0.42     |
| 10:J:23:ILE:HG23 | 10:J:85:LEU:HD22 | 2.00        | 0.42     |
| 20:T:13:LEU:O    | 20:T:17:ARG:HG3  | 2.18        | 0.42     |
| 3:C:206:GLU:O    | 3:C:207:VAL:C    | 2.57        | 0.42     |
| 1:A:1249:C:H4'   | 9:I:36:TYR:OH    | 2.18        | 0.42     |
| 1:A:186:C:H4'    | 20:T:82:SER:HB3  | 2.00        | 0.42     |
| 1:A:692:U:C5     | 11:K:26:ASN:ND2  | 2.87        | 0.42     |
| 14:N:39:LEU:CD1  | 14:N:47:LEU:HD12 | 2.49        | 0.42     |
| 13:M:100:GLY:C   | 13:M:101:GLN:HG3 | 2.40        | 0.42     |
| 1:A:560:U:H5'    | 1:A:566:G:N2     | 2.34        | 0.42     |
| 10:J:88:LEU:O    | 10:J:88:LEU:HG   | 2.20        | 0.42     |
| 8:H:1:MET:O      | 8:H:2:LEU:O      | 2.36        | 0.42     |
| 7:G:67:GLU:HA    | 7:G:67:GLU:OE2   | 2.18        | 0.42     |
| 22:W:49:C:H2'    | 22:W:50:U:H5'    | 2.00        | 0.42     |
| 1:A:424:G:O2'    | 1:A:425:G:H5'    | 2.20        | 0.42     |
| 19:S:21:GLU:HG3  | 19:S:22:LEU:HD22 | 2.02        | 0.42     |
| 11:K:44:SER:H    | 11:K:47:VAL:CG2  | 2.32        | 0.42     |
| 12:L:22:SER:C    | 12:L:24:VAL:N    | 2.72        | 0.42     |
| 9:I:118:LYS:HZ2  | 9:I:118:LYS:CB   | 2.32        | 0.42     |
| 1:A:321:A:H62    | 1:A:328:C:HO2'   | 1.64        | 0.42     |
| 10:J:8:LEU:HD23  | 10:J:96:ILE:HG21 | 2.00        | 0.42     |
| 19:S:64:GLU:O    | 19:S:65:ASN:C    | 2.58        | 0.42     |
| 1:A:805:C:O2'    | 1:A:806:C:H5'    | 2.19        | 0.42     |
| 5:E:40:ARG:HG2   | 5:E:40:ARG:NH1   | 2.31        | 0.42     |
| 19:S:12:ASP:HB3  | 19:S:14:HIS:CE1  | 2.54        | 0.42     |
| 4:D:88:VAL:HG13  | 5:E:97:GLY:CA    | 2.49        | 0.42     |
| 4:D:175:SER:CB   | 4:D:186:LEU:HD11 | 2.44        | 0.42     |
| 4:D:3:ARG:O      | 4:D:4:TYR:C      | 2.58        | 0.42     |
| 1:A:197:A:C6     | 1:A:221:C:H5'    | 2.54        | 0.42     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:148:G:H1      | 1:A:174:C:H42     | 1.66        | 0.42     |
| 13:M:58:GLU:O     | 13:M:60:VAL:N     | 2.52        | 0.42     |
| 1:A:745:C:H1'     | 1:A:836:G:O2'     | 2.19        | 0.42     |
| 1:A:188:C:H2'     | 1:A:189:G:H8      | 1.85        | 0.42     |
| 4:D:104:VAL:O     | 4:D:104:VAL:HG12  | 2.19        | 0.42     |
| 24:Y:345:ILE:O    | 24:Y:348:GLY:N    | 2.52        | 0.42     |
| 9:I:8:GLY:O       | 9:I:14:VAL:HG13   | 2.19        | 0.42     |
| 2:B:47:THR:O      | 2:B:50:GLU:HB2    | 2.20        | 0.42     |
| 4:D:46:LYS:O      | 4:D:47:ARG:C      | 2.58        | 0.42     |
| 16:P:12:LYS:C     | 16:P:14:ASN:H     | 2.22        | 0.42     |
| 1:A:1055:A:H2     | 3:C:194:GLY:CA    | 2.32        | 0.42     |
| 5:E:139:LEU:C     | 5:E:141:GLN:H     | 2.21        | 0.42     |
| 2:B:213:LEU:HD23  | 2:B:213:LEU:C     | 2.40        | 0.42     |
| 1:A:676:A:O2'     | 1:A:677:U:H5'     | 2.20        | 0.42     |
| 13:M:58:GLU:C     | 13:M:60:VAL:N     | 2.72        | 0.42     |
| 1:A:22:G:H4'      | 1:A:885:G:C8      | 2.54        | 0.42     |
| 1:A:343:U:O2'     | 1:A:344:A:H2'     | 2.19        | 0.42     |
| 4:D:171:GLY:HA2   | 4:D:172:PRO:HD3   | 1.84        | 0.42     |
| 24:Y:137:LEU:HD12 | 24:Y:167:ALA:CB   | 2.49        | 0.42     |
| 13:M:81:LEU:HB3   | 13:M:89:GLY:HA2   | 2.01        | 0.42     |
| 19:S:22:LEU:CD1   | 19:S:27:GLU:HB2   | 2.49        | 0.42     |
| 24:Y:72:LEU:HG    | 24:Y:76:MET:CE    | 2.49        | 0.42     |
| 24:Y:81:ALA:CB    | 24:Y:84:ARG:NE    | 2.78        | 0.42     |
| 3:C:182:ILE:HG12  | 3:C:203:PHE:HD1   | 1.84        | 0.42     |
| 1:A:1457:G:H2'    | 1:A:1458:G:C8     | 2.53        | 0.42     |
| 1:A:353:A:H2'     | 1:A:354:G:OP2     | 2.20        | 0.42     |
| 13:M:68:GLY:O     | 13:M:69:GLU:HB2   | 2.19        | 0.42     |
| 4:D:73:ARG:HG2    | 4:D:73:ARG:HH11   | 1.83        | 0.42     |
| 8:H:122:ARG:NH1   | 8:H:122:ARG:HB2   | 2.35        | 0.42     |
| 10:J:84:GLN:O     | 10:J:88:LEU:N     | 2.47        | 0.42     |
| 7:G:14:PRO:HG3    | 7:G:21:VAL:CG1    | 2.50        | 0.42     |
| 6:F:50:TYR:CE1    | 18:R:77:GLY:HA2   | 2.54        | 0.42     |
| 10:J:95:GLU:HA    | 10:J:95:GLU:OE2   | 2.19        | 0.42     |
| 2:B:164:VAL:HG11  | 2:B:170:GLU:HB2   | 2.01        | 0.42     |
| 2:B:97:TRP:HH2    | 2:B:176:GLU:HB2   | 1.84        | 0.42     |
| 22:W:51:U:H2'     | 22:W:52:G:O4'     | 2.19        | 0.42     |
| 24:Y:242:VAL:O    | 24:Y:245:THR:HG22 | 2.19        | 0.42     |
| 24:Y:245:THR:O    | 24:Y:245:THR:HG23 | 2.19        | 0.42     |
| 4:D:25:ARG:HH22   | 4:D:35:ARG:HH12   | 1.68        | 0.42     |
| 4:D:25:ARG:NH1    | 4:D:30:LYS:O      | 2.52        | 0.42     |
| 3:C:173:VAL:N     | 3:C:174:PRO:HD3   | 2.34        | 0.42     |
| 7:G:151:TYR:N     | 7:G:151:TYR:CD1   | 2.87        | 0.42     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 2:B:178:ARG:CG    | 2:B:178:ARG:NH1   | 2.82        | 0.42     |
| 1:A:1056:U:O2'    | 1:A:1057:G:H5'    | 2.20        | 0.42     |
| 24:Y:196:ASP:OD1  | 24:Y:202:HIS:NE2  | 2.50        | 0.42     |
| 12:L:27:LEU:HD12  | 12:L:64:TYR:CE1   | 2.54        | 0.42     |
| 1:A:1005:A:H62    | 1:A:1025:U:H4'    | 1.82        | 0.42     |
| 2:B:111:ARG:HH21  | 2:B:114:ARG:HG2   | 1.84        | 0.42     |
| 3:C:88:ARG:HG2    | 3:C:101:LEU:HB3   | 2.00        | 0.42     |
| 7:G:113:GLU:O     | 7:G:119:ARG:HD3   | 2.19        | 0.42     |
| 2:B:76:GLN:H      | 2:B:76:GLN:HG3    | 1.57        | 0.42     |
| 11:K:59:TYR:O     | 11:K:63:LEU:HG    | 2.20        | 0.42     |
| 10:J:96:ILE:CD1   | 10:J:96:ILE:N     | 2.83        | 0.42     |
| 11:K:124:LYS:HB3  | 11:K:125:PHE:HD1  | 1.85        | 0.42     |
| 1:A:556:C:C2'     | 1:A:557:G:H5'     | 2.50        | 0.42     |
| 21:U:25:LYS:CG    | 21:U:26:LYS:N     | 2.82        | 0.42     |
| 1:A:818:G:C2'     | 1:A:819:A:H5''    | 2.50        | 0.42     |
| 9:I:78:LYS:NZ     | 9:I:78:LYS:CB     | 2.83        | 0.42     |
| 5:E:94:ALA:O      | 5:E:117:ASP:HB3   | 2.20        | 0.42     |
| 1:A:1419:G:O2'    | 1:A:1420:C:H5'    | 2.20        | 0.42     |
| 1:A:1466:C:C2'    | 1:A:1467:G:H5'    | 2.48        | 0.42     |
| 24:Y:222:LEU:N    | 24:Y:222:LEU:HD22 | 2.34        | 0.42     |
| 1:A:976:G:H22     | 1:A:1362:C:H2'    | 1.80        | 0.42     |
| 4:D:18:LYS:HG3    | 4:D:31:CYS:CB     | 2.50        | 0.42     |
| 24:Y:181:SER:N    | 24:Y:182:PRO:CD   | 2.83        | 0.42     |
| 20:T:100:ILE:O    | 20:T:100:ILE:HG13 | 2.20        | 0.42     |
| 10:J:4:ILE:HD11   | 10:J:77:PRO:CB    | 2.39        | 0.42     |
| 3:C:113:ALA:HB1   | 3:C:185:GLY:N     | 2.35        | 0.42     |
| 1:A:521:G:O5'     | 12:L:73:GLU:HG2   | 2.20        | 0.42     |
| 3:C:155:GLY:O     | 3:C:196:LEU:HD13  | 2.19        | 0.42     |
| 1:A:1317:C:OP1    | 14:N:17:LYS:HE2   | 2.18        | 0.42     |
| 2:B:136:VAL:HA    | 2:B:139:LYS:HB2   | 2.02        | 0.42     |
| 4:D:98:GLU:OE2    | 4:D:103:ASN:ND2   | 2.52        | 0.42     |
| 1:A:1203:C:O2'    | 1:A:1204:A:H5'    | 2.19        | 0.42     |
| 1:A:867:G:H2'     | 1:A:868:C:H6      | 1.83        | 0.42     |
| 1:A:216:G:C2      | 1:A:217:C:N3      | 2.88        | 0.42     |
| 11:K:40:ILE:HG23  | 11:K:75:TYR:CD2   | 2.55        | 0.42     |
| 4:D:42:GLN:O      | 4:D:42:GLN:CG     | 2.68        | 0.42     |
| 15:O:62:GLN:O     | 15:O:66:LEU:HD13  | 2.19        | 0.42     |
| 10:J:49:VAL:CG2   | 10:J:50:ILE:N     | 2.82        | 0.42     |
| 7:G:108:ALA:C     | 7:G:110:GLN:H     | 2.22        | 0.42     |
| 24:Y:326:THR:HG23 | 24:Y:328:LEU:HD13 | 2.02        | 0.42     |
| 1:A:458:C:H2'     | 1:A:460:G:O4'     | 2.20        | 0.42     |
| 1:A:424:G:N3      | 1:A:425:G:C8      | 2.88        | 0.42     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:445:G:H2'    | 1:A:446:G:C8      | 2.54        | 0.42     |
| 1:A:1354:C:H2'   | 1:A:1355:G:H8     | 1.85        | 0.42     |
| 13:M:16:ASP:OD2  | 13:M:17:VAL:N     | 2.53        | 0.42     |
| 1:A:684:A:H2'    | 1:A:685:G:H8      | 1.84        | 0.42     |
| 24:Y:138:ARG:CZ  | 24:Y:337:LEU:HB3  | 2.50        | 0.42     |
| 1:A:382:A:C2     | 1:A:383:A:C4      | 3.07        | 0.42     |
| 6:F:10:LEU:HD13  | 6:F:61:LEU:CD1    | 2.50        | 0.42     |
| 1:A:950:U:H4'    | 1:A:971:G:C2      | 2.54        | 0.42     |
| 1:A:177:C:OP1    | 20:T:65:LYS:HD3   | 2.20        | 0.42     |
| 14:N:12:ARG:HB2  | 14:N:12:ARG:CZ    | 2.50        | 0.42     |
| 1:A:790:A:H2     | 1:A:1497:G:OP1    | 2.02        | 0.42     |
| 7:G:22:LEU:HD23  | 7:G:22:LEU:C      | 2.40        | 0.42     |
| 2:B:95:GLN:HA    | 2:B:95:GLN:OE1    | 2.20        | 0.42     |
| 20:T:73:HIS:O    | 20:T:74:LYS:O     | 2.37        | 0.42     |
| 1:A:19:C:H4'     | 1:A:864:A:O4'     | 2.19        | 0.42     |
| 1:A:948:C:P      | 13:M:109:THR:HG1  | 2.42        | 0.42     |
| 17:Q:29:HIS:HA   | 17:Q:30:PRO:HD2   | 1.82        | 0.42     |
| 1:A:802:A:H3'    | 1:A:803:G:H8      | 1.85        | 0.42     |
| 1:A:141:A:H1'    | 1:A:182:U:C2      | 2.55        | 0.42     |
| 24:Y:300:GLY:O   | 24:Y:301:GLU:HG3  | 2.20        | 0.42     |
| 8:H:4:ASP:CG     | 8:H:85:ARG:HH21   | 2.22        | 0.42     |
| 24:Y:123:GLY:HA3 | 24:Y:305:ILE:HG23 | 2.02        | 0.42     |
| 7:G:95:ARG:O     | 7:G:96:GLN:C      | 2.58        | 0.42     |
| 1:A:1134:G:H2'   | 1:A:1135:U:C5'    | 2.46        | 0.42     |
| 24:Y:312:ARG:HD2 | 24:Y:314:TYR:CE1  | 2.55        | 0.42     |
| 19:S:44:MET:HE3  | 19:S:44:MET:HA    | 2.01        | 0.42     |
| 3:C:155:GLY:O    | 3:C:156:ARG:CB    | 2.66        | 0.42     |
| 2:B:44:LEU:CD1   | 2:B:44:LEU:N      | 2.81        | 0.42     |
| 2:B:12:GLU:O     | 2:B:14:GLY:N      | 2.53        | 0.42     |
| 20:T:30:LYS:O    | 20:T:33:ILE:HB    | 2.20        | 0.42     |
| 1:A:826:C:H5''   | 8:H:12:ARG:HH21   | 1.84        | 0.42     |
| 2:B:37:ASN:OD1   | 2:B:37:ASN:O      | 2.37        | 0.42     |
| 4:D:206:PHE:CD2  | 4:D:207:TYR:CE2   | 3.08        | 0.42     |
| 1:A:1528:U:O3'   | 1:A:1529:G:H3'    | 2.19        | 0.42     |
| 1:A:119:A:H4'    | 1:A:120:A:O5'     | 2.19        | 0.42     |
| 10:J:45:ARG:HB3  | 10:J:65:LEU:HB3   | 2.01        | 0.42     |
| 1:A:1215:G:O2'   | 1:A:1216:G:H5'    | 2.20        | 0.42     |
| 1:A:49:U:O2      | 1:A:362:G:H1'     | 2.20        | 0.42     |
| 2:B:168:THR:O    | 2:B:171:ALA:N     | 2.52        | 0.42     |
| 22:W:55:U:C4     | 22:W:57:G:H5''    | 2.55        | 0.42     |
| 4:D:17:VAL:O     | 4:D:18:LYS:O      | 2.37        | 0.42     |
| 1:A:1134:G:N1    | 1:A:1142:G:C6     | 2.88        | 0.42     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:191:G:N9     | 20:T:105:SER:HB3  | 2.34        | 0.42     |
| 24:Y:150:GLN:NE2 | 24:Y:172:LYS:HZ1  | 2.13        | 0.42     |
| 5:E:8:GLU:CA     | 5:E:34:VAL:HG23   | 2.50        | 0.42     |
| 9:I:89:ASN:O     | 9:I:92:TYR:HB2    | 2.19        | 0.42     |
| 2:B:50:GLU:OE1   | 2:B:200:ILE:HB    | 2.20        | 0.42     |
| 12:L:91:LYS:HA   | 12:L:91:LYS:HE2   | 2.00        | 0.42     |
| 1:A:376:G:H5''   | 16:P:5:ARG:HB2    | 2.01        | 0.42     |
| 8:H:86:ILE:CG2   | 8:H:133:LEU:HD22  | 2.44        | 0.42     |
| 20:T:41:ILE:HG13 | 20:T:42:GLN:N     | 2.34        | 0.42     |
| 21:U:12:LYS:HD2  | 21:U:12:LYS:N     | 2.35        | 0.42     |
| 1:A:833:U:H3     | 1:A:853:G:H1      | 1.67        | 0.42     |
| 14:N:12:ARG:HH12 | 14:N:14:PRO:HD3   | 1.85        | 0.42     |
| 24:Y:106:LEU:C   | 24:Y:108:ASN:N    | 2.72        | 0.42     |
| 1:A:868:C:H2'    | 1:A:869:G:O4'     | 2.19        | 0.42     |
| 13:M:5:ALA:O     | 13:M:6:GLY:C      | 2.58        | 0.42     |
| 2:B:66:GLY:HA2   | 2:B:160:ASP:OD2   | 2.19        | 0.42     |
| 7:G:9:VAL:O      | 7:G:10:ARG:C      | 2.58        | 0.42     |
| 8:H:43:GLY:O     | 8:H:79:VAL:HG11   | 2.20        | 0.42     |
| 13:M:125:ARG:HG3 | 24:Y:160:PRO:CD   | 2.35        | 0.41     |
| 10:J:4:ILE:HD13  | 10:J:74:ILE:HG13  | 2.01        | 0.41     |
| 1:A:1004:A:H3'   | 1:A:1036:G:O6     | 2.20        | 0.41     |
| 1:A:1250:A:H61   | 1:A:1354:C:H1'    | 1.84        | 0.41     |
| 16:P:59:TRP:CE3  | 16:P:59:TRP:HA    | 2.55        | 0.41     |
| 1:A:1111:A:O2'   | 1:A:1112:C:H5'    | 2.20        | 0.41     |
| 1:A:1255:G:C2'   | 1:A:1255:G:N3     | 2.82        | 0.41     |
| 6:F:55:ASP:C     | 6:F:57:GLN:H      | 2.24        | 0.41     |
| 21:U:12:LYS:HB3  | 21:U:22:ARG:HD2   | 2.00        | 0.41     |
| 2:B:15:VAL:C     | 2:B:16:HIS:CG     | 2.93        | 0.41     |
| 7:G:153:HIS:O    | 7:G:154:TYR:HD2   | 2.03        | 0.41     |
| 1:A:336:C:H2'    | 1:A:337:C:C6      | 2.53        | 0.41     |
| 1:A:629:G:H2'    | 1:A:630:G:O4'     | 2.20        | 0.41     |
| 23:X:15:A:N3     | 23:X:15:A:H2'     | 2.34        | 0.41     |
| 5:E:135:THR:O    | 5:E:136:MET:C     | 2.58        | 0.41     |
| 24:Y:254:LEU:N   | 24:Y:255:PRO:HD2  | 2.35        | 0.41     |
| 1:A:767:A:H2'    | 1:A:768:A:O4'     | 2.19        | 0.41     |
| 10:J:79:ARG:HA   | 10:J:82:ILE:HG12  | 2.02        | 0.41     |
| 11:K:100:ALA:O   | 11:K:101:SER:HB3  | 2.20        | 0.41     |
| 24:Y:242:VAL:HA  | 24:Y:245:THR:HG22 | 2.02        | 0.41     |
| 1:A:973:G:C1'    | 10:J:55:LYS:HE2   | 2.48        | 0.41     |
| 3:C:186:PHE:HZ   | 3:C:188:LEU:HD11  | 1.82        | 0.41     |
| 15:O:82:ILE:HD13 | 15:O:83:GLU:N     | 2.35        | 0.41     |
| 20:T:89:ARG:CZ   | 20:T:104:LEU:HD21 | 2.50        | 0.41     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 9:I:9:ARG:HG2     | 9:I:14:VAL:CG2    | 2.41        | 0.41     |
| 2:B:115:LEU:O     | 2:B:118:LEU:HB2   | 2.20        | 0.41     |
| 10:J:28:ARG:NH1   | 10:J:28:ARG:HG2   | 2.34        | 0.41     |
| 7:G:150:ALA:HB2   | 11:K:50:TYR:OH    | 2.20        | 0.41     |
| 1:A:659:U:OP1     | 15:O:9:GLN:NE2    | 2.53        | 0.41     |
| 3:C:47:LEU:HD21   | 3:C:68:VAL:CG1    | 2.50        | 0.41     |
| 1:A:271:C:O2'     | 1:A:272:C:H5'     | 2.20        | 0.41     |
| 24:Y:224:PRO:C    | 24:Y:227:LEU:HB2  | 2.40        | 0.41     |
| 7:G:129:GLU:O     | 7:G:129:GLU:HG2   | 2.20        | 0.41     |
| 3:C:138:VAL:CG2   | 3:C:151:VAL:HG23  | 2.51        | 0.41     |
| 4:D:61:LYS:HD3    | 4:D:206:PHE:CE2   | 2.55        | 0.41     |
| 22:V:18:G:H21     | 22:V:58:A:C5'     | 2.32        | 0.41     |
| 1:A:151:A:C2'     | 1:A:152:A:H5'     | 2.49        | 0.41     |
| 1:A:1216:G:O2'    | 1:A:1217:C:H5'    | 2.19        | 0.41     |
| 17:Q:33:GLY:O     | 17:Q:34:LYS:C     | 2.59        | 0.41     |
| 20:T:96:GLY:O     | 20:T:97:ALA:C     | 2.59        | 0.41     |
| 1:A:1516:G:H2'    | 1:A:1518:A:OP2    | 2.19        | 0.41     |
| 2:B:162:ILE:HD11  | 2:B:184:VAL:HG13  | 2.02        | 0.41     |
| 24:Y:117:ILE:HG12 | 24:Y:170:LEU:HD13 | 2.02        | 0.41     |
| 5:E:102:ALA:HB2   | 5:E:120:THR:OG1   | 2.20        | 0.41     |
| 1:A:939:G:O3'     | 7:G:102:ARG:NH1   | 2.54        | 0.41     |
| 3:C:58:GLU:H      | 3:C:65:ALA:HB3    | 1.84        | 0.41     |
| 1:A:363:A:N7      | 12:L:30:ALA:HB1   | 2.35        | 0.41     |
| 12:L:35:GLY:HA3   | 12:L:58:VAL:HG11  | 2.01        | 0.41     |
| 9:I:81:ILE:O      | 9:I:81:ILE:HG22   | 2.21        | 0.41     |
| 19:S:31:ILE:HG22  | 19:S:48:THR:O     | 2.20        | 0.41     |
| 3:C:48:TYR:HA     | 3:C:52:LEU:CD2    | 2.50        | 0.41     |
| 17:Q:59:ILE:HG22  | 17:Q:71:PHE:CD1   | 2.55        | 0.41     |
| 1:A:376:G:O3'     | 16:P:5:ARG:HD2    | 2.20        | 0.41     |
| 9:I:104:ARG:HG3   | 9:I:104:ARG:HH11  | 1.85        | 0.41     |
| 1:A:153:C:O2'     | 1:A:154:C:H5'     | 2.20        | 0.41     |
| 13:M:65:LYS:HG3   | 13:M:65:LYS:O     | 2.19        | 0.41     |
| 1:A:142:G:H2'     | 1:A:143:A:H8      | 1.85        | 0.41     |
| 19:S:33:THR:CG2   | 19:S:51:VAL:HA    | 2.49        | 0.41     |
| 1:A:134:A:H61     | 16:P:25:ARG:HH12  | 1.67        | 0.41     |
| 1:A:448:A:P       | 1:A:485:G:H22     | 2.43        | 0.41     |
| 1:A:978:A:OP2     | 1:A:1363:C:N4     | 2.46        | 0.41     |
| 1:A:559:A:H4'     | 1:A:560:U:C5'     | 2.50        | 0.41     |
| 5:E:64:ARG:HB2    | 5:E:64:ARG:CZ     | 2.51        | 0.41     |
| 1:A:705:U:C5      | 1:A:706:A:C5      | 3.09        | 0.41     |
| 9:I:99:LEU:HB3    | 9:I:101:PHE:CE1   | 2.55        | 0.41     |
| 6:F:30:LEU:HD12   | 6:F:37:VAL:CG2    | 2.50        | 0.41     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 4:D:20:TYR:HA     | 4:D:26:CYS:SG     | 2.60        | 0.41     |
| 1:A:1128:C:O2'    | 1:A:1130:A:C8     | 2.72        | 0.41     |
| 1:A:1131:G:C6     | 1:A:1132:C:N4     | 2.88        | 0.41     |
| 15:O:25:THR:O     | 15:O:26:GLU:C     | 2.58        | 0.41     |
| 20:T:57:ARG:NH1   | 20:T:100:ILE:CG1  | 2.83        | 0.41     |
| 10:J:25:GLU:C     | 10:J:27:ALA:H     | 2.24        | 0.41     |
| 7:G:15:ASP:OD2    | 7:G:16:LEU:N      | 2.51        | 0.41     |
| 4:D:119:GLN:CG    | 4:D:123:HIS:CD2   | 3.04        | 0.41     |
| 1:A:376:G:P       | 16:P:67:THR:HG21  | 2.60        | 0.41     |
| 20:T:26:ASN:HB2   | 20:T:71:THR:HG23  | 2.03        | 0.41     |
| 15:O:43:LEU:HD11  | 15:O:53:HIS:HA    | 2.03        | 0.41     |
| 1:A:1076:C:C2'    | 1:A:1077:G:H5'    | 2.50        | 0.41     |
| 13:M:37:THR:O     | 13:M:39:ILE:HG13  | 2.21        | 0.41     |
| 16:P:82:GLN:OE1   | 16:P:82:GLN:N     | 2.45        | 0.41     |
| 4:D:128:VAL:CG1   | 4:D:129:ASN:ND2   | 2.82        | 0.41     |
| 24:Y:118:LEU:HD22 | 24:Y:208:VAL:HG13 | 2.01        | 0.41     |
| 22:W:48:C:H3'     | 22:W:50:U:C5      | 2.56        | 0.41     |
| 22:V:76:8AN:H3'   | 24:Y:240:GLN:H    | 1.85        | 0.41     |
| 9:I:15:ALA:CA     | 9:I:65:VAL:HA     | 2.48        | 0.41     |
| 2:B:112:VAL:C     | 2:B:114:ARG:N     | 2.71        | 0.41     |
| 2:B:47:THR:HG22   | 2:B:51:LEU:CD1    | 2.50        | 0.41     |
| 1:A:1053:G:H3'    | 1:A:1054:C:H5'    | 2.01        | 0.41     |
| 17:Q:6:LEU:O      | 17:Q:58:GLU:HA    | 2.21        | 0.41     |
| 1:A:59:A:H3'      | 1:A:331:G:H22     | 1.85        | 0.41     |
| 16:P:18:ARG:O     | 16:P:19:ILE:C     | 2.59        | 0.41     |
| 6:F:97:PHE:CB     | 18:R:32:ARG:HH11  | 2.34        | 0.41     |
| 5:E:110:LEU:CD2   | 5:E:139:LEU:HD21  | 2.51        | 0.41     |
| 1:A:1170:A:C2'    | 1:A:1171:G:H5'    | 2.50        | 0.41     |
| 1:A:1327:C:H5''   | 21:U:20:LYS:HB3   | 2.02        | 0.41     |
| 1:A:662:G:H2'     | 1:A:663:A:C8      | 2.56        | 0.41     |
| 5:E:127:ASN:O     | 5:E:128:PRO:C     | 2.59        | 0.41     |
| 1:A:1109:C:H2'    | 1:A:1110:A:O4'    | 2.21        | 0.41     |
| 1:A:764:C:O2'     | 1:A:765:G:H5'     | 2.21        | 0.41     |
| 1:A:939:G:P       | 7:G:95:ARG:HH22   | 2.44        | 0.41     |
| 1:A:1129:C:H41    | 1:A:1135:U:H3     | 1.68        | 0.41     |
| 13:M:122:LYS:O    | 13:M:123:ALA:HB2  | 2.20        | 0.41     |
| 1:A:226:G:H2'     | 1:A:227:G:H8      | 1.85        | 0.41     |
| 1:A:192:U:H1'     | 20:T:103:GLY:HA2  | 2.02        | 0.41     |
| 5:E:41:VAL:HG21   | 5:E:69:VAL:HG21   | 2.01        | 0.41     |
| 1:A:926:G:C6      | 1:A:1505:G:C6     | 3.09        | 0.41     |
| 12:L:53:ARG:CB    | 12:L:93:LEU:HD11  | 2.50        | 0.41     |
| 5:E:45:PHE:CE2    | 5:E:47:LYS:HD2    | 2.56        | 0.41     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 16:P:18:ARG:HD3   | 16:P:35:LYS:CE    | 2.47        | 0.41     |
| 1:A:1252:A:H2'    | 1:A:1253:G:O4'    | 2.21        | 0.41     |
| 6:F:20:ALA:O      | 6:F:24:GLU:HB2    | 2.20        | 0.41     |
| 1:A:937:A:H1'     | 1:A:1379:G:N2     | 2.36        | 0.41     |
| 13:M:67:GLU:O     | 13:M:69:GLU:N     | 2.54        | 0.41     |
| 18:R:61:LYS:HG2   | 18:R:65:ILE:HD11  | 2.02        | 0.41     |
| 2:B:35:GLU:HA     | 2:B:39:ILE:O      | 2.21        | 0.41     |
| 1:A:1015:A:O5'    | 1:A:1015:A:H8     | 2.03        | 0.41     |
| 1:A:640:A:O2'     | 1:A:641:U:H5'     | 2.20        | 0.41     |
| 22:V:36:A:C2      | 23:X:17:U:O2      | 2.74        | 0.41     |
| 19:S:58:VAL:HG21  | 19:S:75:ALA:CB    | 2.51        | 0.41     |
| 6:F:33:TYR:OH     | 6:F:78:GLU:HB2    | 2.21        | 0.41     |
| 1:A:1328:C:H2'    | 1:A:1329:A:H8     | 1.86        | 0.41     |
| 10:J:18:ALA:O     | 10:J:22:LYS:HB2   | 2.21        | 0.41     |
| 4:D:11:LEU:HD13   | 4:D:66:ARG:HD3    | 2.02        | 0.41     |
| 1:A:956:U:O2'     | 1:A:957:U:H5'     | 2.20        | 0.41     |
| 24:Y:112:ALA:HB1  | 24:Y:178:GLY:HA2  | 2.03        | 0.41     |
| 1:A:963:G:N2      | 10:J:55:LYS:HD2   | 2.35        | 0.41     |
| 3:C:14:ILE:O      | 3:C:16:ARG:N      | 2.53        | 0.41     |
| 6:F:91:VAL:HG12   | 6:F:92:LYS:N      | 2.35        | 0.41     |
| 16:P:45:THR:HG23  | 16:P:46:PRO:CD    | 2.49        | 0.41     |
| 12:L:86:ARG:HB2   | 12:L:101:VAL:CG2  | 2.50        | 0.41     |
| 1:A:921:U:O2'     | 5:E:19:MET:O      | 2.38        | 0.41     |
| 16:P:15:PRO:HB2   | 16:P:41:PRO:CG    | 2.50        | 0.41     |
| 2:B:130:ARG:HA    | 2:B:131:PRO:HD2   | 1.80        | 0.41     |
| 1:A:1254:C:H2'    | 1:A:1255:G:H8     | 1.84        | 0.41     |
| 6:F:21:LEU:O      | 6:F:24:GLU:HB3    | 2.20        | 0.41     |
| 1:A:386:C:O2'     | 1:A:387:U:H5'     | 2.21        | 0.41     |
| 1:A:179:A:H2'     | 1:A:180:U:C6      | 2.54        | 0.41     |
| 11:K:88:GLY:C     | 11:K:90:GLY:H     | 2.23        | 0.41     |
| 8:H:9:MET:O       | 8:H:13:ILE:HG12   | 2.19        | 0.41     |
| 1:A:577:G:C8      | 1:A:816:A:C6      | 3.08        | 0.41     |
| 2:B:95:GLN:NE2    | 2:B:147:LYS:HE2   | 2.35        | 0.41     |
| 11:K:109:VAL:HG13 | 18:R:85:LEU:O     | 2.20        | 0.41     |
| 24:Y:220:VAL:O    | 24:Y:220:VAL:HG12 | 2.19        | 0.41     |
| 3:C:19:GLU:O      | 3:C:19:GLU:HG2    | 2.21        | 0.41     |
| 13:M:124:PRO:HB2  | 24:Y:163:GLY:O    | 2.20        | 0.41     |
| 15:O:63:ARG:HH12  | 15:O:87:ILE:HG21  | 1.86        | 0.41     |
| 24:Y:323:ASP:HB3  | 24:Y:326:THR:CG2  | 2.35        | 0.41     |
| 1:A:194:C:O2'     | 20:T:68:LYS:HD3   | 2.21        | 0.41     |
| 1:A:15:G:C4'      | 5:E:24:ARG:HH22   | 2.34        | 0.41     |
| 19:S:78:ARG:NH1   | 19:S:81:ARG:HH12  | 1.98        | 0.41     |

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| Atom-1            | Atom-2           | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 2:B:45:GLN:HE21   | 2:B:46:LYS:NZ    | 2.18        | 0.41     |
| 12:L:84:LEU:HG    | 12:L:105:TYR:CE1 | 2.56        | 0.41     |
| 1:A:992:U:O2'     | 1:A:993:G:P      | 2.79        | 0.41     |
| 24:Y:50:GLN:HE21  | 24:Y:51:GLU:N    | 2.19        | 0.41     |
| 17:Q:45:HIS:CD2   | 17:Q:47:PRO:HD3  | 2.56        | 0.41     |
| 22:V:14:A:N6      | 22:V:21:A:H2     | 2.19        | 0.41     |
| 24:Y:76:MET:O     | 24:Y:77:GLU:HG2  | 2.21        | 0.41     |
| 1:A:1357:A:N6     | 1:A:1363(A):A:H2 | 2.18        | 0.41     |
| 22:W:27:G:H1      | 22:W:43:C:H42    | 1.68        | 0.41     |
| 3:C:75:VAL:O      | 3:C:75:VAL:HG12  | 2.20        | 0.41     |
| 1:A:243:A:H4'     | 1:A:244:U:H5''   | 2.03        | 0.41     |
| 1:A:1316:G:O3'    | 14:N:18:VAL:HG13 | 2.21        | 0.41     |
| 1:A:817:C:H1'     | 1:A:819:A:H5'    | 2.03        | 0.41     |
| 7:G:54:THR:OG1    | 7:G:56:GLN:HG2   | 2.21        | 0.41     |
| 2:B:97:TRP:HH2    | 2:B:176:GLU:CG   | 2.34        | 0.41     |
| 19:S:6:LYS:N      | 19:S:6:LYS:CD    | 2.81        | 0.41     |
| 6:F:26:ILE:O      | 6:F:30:LEU:CD2   | 2.69        | 0.41     |
| 6:F:26:ILE:O      | 6:F:30:LEU:HD23  | 2.20        | 0.41     |
| 3:C:11:ARG:O      | 3:C:12:LEU:C     | 2.59        | 0.41     |
| 3:C:14:ILE:CG1    | 3:C:15:THR:N     | 2.72        | 0.41     |
| 6:F:91:VAL:HG11   | 18:R:72:ARG:NH1  | 2.17        | 0.41     |
| 15:O:26:GLU:HA    | 15:O:81:LEU:HD22 | 2.02        | 0.41     |
| 1:A:1036:G:H5''   | 1:A:1037:C:C5    | 2.56        | 0.41     |
| 9:I:5:TYR:HA      | 9:I:17:VAL:O     | 2.21        | 0.41     |
| 9:I:19:LEU:C      | 9:I:20:ARG:HG3   | 2.41        | 0.41     |
| 2:B:111:ARG:HH11  | 2:B:111:ARG:HG2  | 1.86        | 0.41     |
| 12:L:84:LEU:HD12  | 12:L:104:VAL:CG1 | 2.41        | 0.41     |
| 2:B:83:MET:HB3    | 2:B:234:PRO:HG2  | 2.03        | 0.41     |
| 2:B:80:ILE:O      | 2:B:80:ILE:HG22  | 2.20        | 0.41     |
| 6:F:1:MET:HA      | 6:F:67:MET:O     | 2.21        | 0.41     |
| 24:Y:12:GLY:O     | 24:Y:16:TYR:N    | 2.54        | 0.41     |
| 4:D:47:ARG:NE     | 4:D:49:ARG:NH2   | 2.68        | 0.41     |
| 11:K:22:HIS:O     | 11:K:28:THR:HA   | 2.21        | 0.41     |
| 2:B:91:PRO:CG     | 2:B:155:LEU:HD23 | 2.51        | 0.41     |
| 1:A:1300:G:HO2'   | 1:A:1301:U:P     | 2.43        | 0.41     |
| 9:I:113:LYS:H     | 9:I:119:ALA:HA   | 1.85        | 0.41     |
| 1:A:1350:A:P      | 9:I:121:ARG:HG3  | 2.61        | 0.41     |
| 13:M:48:LEU:HG    | 13:M:53:VAL:CG2  | 2.51        | 0.41     |
| 1:A:59:A:H2'      | 1:A:59:A:N3      | 2.36        | 0.41     |
| 24:Y:138:ARG:NH2  | 24:Y:337:LEU:CB  | 2.84        | 0.41     |
| 8:H:119:LEU:HB2   | 8:H:124:ALA:HB2  | 2.02        | 0.41     |
| 24:Y:119:THR:HG22 | 24:Y:121:GLN:HG3 | 2.01        | 0.41     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:1432:G:O2'   | 1:A:1468:A:N6    | 2.52        | 0.41     |
| 1:A:1014:A:H4'   | 19:S:14:HIS:CD2  | 2.56        | 0.41     |
| 1:A:356:A:H2'    | 1:A:357:G:C8     | 2.53        | 0.41     |
| 1:A:1442:G:C6    | 1:A:1442(B):A:H2 | 2.39        | 0.41     |
| 2:B:235:SER:OG   | 2:B:236:TYR:HD1  | 2.04        | 0.41     |
| 1:A:1058:G:C5    | 1:A:1059:C:C4    | 3.09        | 0.41     |
| 15:O:50:HIS:O    | 15:O:53:HIS:HB3  | 2.21        | 0.41     |
| 24:Y:11:GLU:HB3  | 24:Y:98:LEU:HD21 | 2.02        | 0.41     |
| 1:A:563:A:C6     | 1:A:567:G:C2     | 3.08        | 0.41     |
| 11:K:126:ARG:O   | 11:K:127:LYS:C   | 2.58        | 0.41     |
| 9:I:76:ALA:C     | 9:I:78:LYS:H     | 2.24        | 0.41     |
| 3:C:29:TYR:CE1   | 10:J:65:LEU:HD21 | 2.55        | 0.41     |
| 11:K:37:GLY:O    | 11:K:39:PRO:HD3  | 2.21        | 0.41     |
| 3:C:111:LEU:HD23 | 3:C:141:VAL:HG13 | 2.03        | 0.41     |
| 16:P:76:GLN:HG2  | 16:P:76:GLN:O    | 2.21        | 0.41     |
| 1:A:1376:U:H2'   | 1:A:1377:A:C8    | 2.56        | 0.41     |
| 1:A:927:G:O2'    | 1:A:928:G:H5'    | 2.21        | 0.41     |
| 5:E:116:THR:HG22 | 5:E:116:THR:O    | 2.21        | 0.41     |
| 22:W:38:A:H3'    | 22:W:39:U:C5'    | 2.47        | 0.41     |
| 11:K:21:ILE:HA   | 11:K:30:VAL:HG12 | 2.02        | 0.41     |
| 9:I:63:ILE:HD13  | 9:I:77:ILE:CG2   | 2.51        | 0.41     |
| 1:A:924:C:O2'    | 1:A:1502:A:N6    | 2.54        | 0.41     |
| 1:A:1505:G:H4'   | 1:A:1506:U:H5'   | 2.03        | 0.41     |
| 1:A:926:G:C2     | 1:A:1505:G:C8    | 3.09        | 0.41     |
| 12:L:42:THR:HG23 | 12:L:42:THR:O    | 2.21        | 0.41     |
| 12:L:44:THR:HA   | 12:L:45:PRO:HD3  | 1.78        | 0.41     |
| 8:H:11:THR:CG2   | 8:H:14:ARG:HH12  | 2.33        | 0.41     |
| 8:H:88:LYS:HB3   | 8:H:89:PRO:CD    | 2.45        | 0.41     |
| 3:C:88:ARG:HG2   | 3:C:101:LEU:CB   | 2.51        | 0.41     |
| 3:C:156:ARG:CD   | 3:C:194:GLY:HA3  | 2.51        | 0.41     |
| 10:J:6:ILE:HA    | 10:J:97:GLU:O    | 2.21        | 0.41     |
| 10:J:32:ALA:HB1  | 10:J:75:ILE:HD11 | 2.02        | 0.41     |
| 15:O:11:VAL:O    | 15:O:14:GLU:HB3  | 2.21        | 0.41     |
| 6:F:45:LEU:HD23  | 6:F:46:ARG:N     | 2.36        | 0.41     |
| 2:B:223:ILE:HG13 | 2:B:223:ILE:H    | 1.76        | 0.41     |
| 2:B:13:ALA:O     | 2:B:14:GLY:C     | 2.59        | 0.41     |
| 13:M:40:ASN:HA   | 13:M:41:PRO:HD3  | 1.88        | 0.41     |
| 2:B:24:TRP:CG    | 2:B:25:ASN:N     | 2.88        | 0.41     |
| 6:F:78:GLU:HA    | 6:F:78:GLU:OE2   | 2.21        | 0.41     |
| 8:H:12:ARG:HH12  | 8:H:27:PRO:HD2   | 1.81        | 0.41     |
| 1:A:743:U:O2'    | 1:A:744:C:H5'    | 2.22        | 0.41     |
| 1:A:1206:G:O2'   | 3:C:193:TYR:HA   | 2.21        | 0.41     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:B:95:GLN:NE2   | 2:B:147:LYS:CE   | 2.84        | 0.41     |
| 24:Y:282:ARG:HB2 | 24:Y:282:ARG:NH2 | 2.36        | 0.41     |
| 4:D:194:LEU:HD22 | 4:D:194:LEU:N    | 2.36        | 0.41     |
| 1:A:1109:C:O2'   | 1:A:1110:A:H5'   | 2.20        | 0.41     |
| 2:B:97:TRP:CH2   | 2:B:176:GLU:OE2  | 2.74        | 0.40     |
| 1:A:193:C:H2'    | 1:A:194:C:C6     | 2.56        | 0.40     |
| 5:E:63:ARG:C     | 5:E:65:ASN:H     | 2.24        | 0.40     |
| 1:A:418:C:N4     | 1:A:426:G:N1     | 2.69        | 0.40     |
| 2:B:109:SER:C    | 2:B:111:ARG:H    | 2.25        | 0.40     |
| 1:A:509:A:O5'    | 1:A:509:A:H8     | 2.04        | 0.40     |
| 4:D:13:ARG:O     | 4:D:14:ARG:HB3   | 2.21        | 0.40     |
| 1:A:991:U:O2     | 1:A:993:G:C8     | 2.74        | 0.40     |
| 16:P:9:PHE:HB3   | 16:P:10:GLY:H    | 1.73        | 0.40     |
| 24:Y:26:LEU:HB2  | 24:Y:55:LEU:CD2  | 2.45        | 0.40     |
| 5:E:27:ARG:HD3   | 5:E:47:LYS:HB3   | 2.04        | 0.40     |
| 1:A:1000:U:H2'   | 1:A:1001:A:C8    | 2.56        | 0.40     |
| 1:A:1346:A:H5''  | 9:I:120:ARG:HH12 | 1.86        | 0.40     |
| 8:H:83:ILE:CD1   | 8:H:137:VAL:HG22 | 2.51        | 0.40     |
| 15:O:32:LEU:O    | 15:O:36:ILE:HG13 | 2.20        | 0.40     |
| 4:D:99:SER:HB2   | 4:D:139:ARG:HG3  | 2.03        | 0.40     |
| 8:H:1:MET:HE2    | 8:H:1:MET:N      | 2.36        | 0.40     |
| 1:A:141:A:H1'    | 1:A:182:U:O2     | 2.20        | 0.40     |
| 1:A:910:C:H6     | 1:A:910:C:O5'    | 2.04        | 0.40     |
| 2:B:71:VAL:HG13  | 2:B:93:VAL:CB    | 2.31        | 0.40     |
| 13:M:88:ARG:HD3  | 19:S:73:GLU:OE1  | 2.22        | 0.40     |
| 10:J:56:HIS:C    | 10:J:58:ASP:H    | 2.25        | 0.40     |
| 3:C:175:LEU:N    | 3:C:175:LEU:HD12 | 2.37        | 0.40     |
| 7:G:106:GLN:O    | 7:G:110:GLN:HG3  | 2.21        | 0.40     |
| 11:K:30:VAL:HG21 | 11:K:65:ALA:HA   | 2.03        | 0.40     |
| 23:X:20:A:N6     | 24:Y:193:SER:OG  | 2.53        | 0.40     |
| 19:S:41:VAL:O    | 19:S:44:MET:SD   | 2.79        | 0.40     |
| 16:P:67:THR:HG22 | 16:P:68:ASP:N    | 2.37        | 0.40     |
| 1:A:353:A:C2'    | 1:A:354:G:OP2    | 2.70        | 0.40     |
| 3:C:76:VAL:O     | 3:C:84:ILE:HB    | 2.21        | 0.40     |
| 2:B:86:GLU:C     | 2:B:88:ALA:N     | 2.74        | 0.40     |
| 21:U:22:ARG:N    | 21:U:23:PRO:HD3  | 2.36        | 0.40     |
| 1:A:384:G:O2'    | 1:A:385:C:H5'    | 2.22        | 0.40     |
| 5:E:37:ARG:HA    | 5:E:114:GLY:CA   | 2.51        | 0.40     |
| 6:F:58:GLY:O     | 6:F:60:PHE:CD1   | 2.75        | 0.40     |
| 1:A:1332:A:H2'   | 1:A:1333:A:H8    | 1.87        | 0.40     |
| 1:A:630:G:H3'    | 1:A:631:G:H5'    | 2.03        | 0.40     |
| 1:A:1478:C:H2'   | 1:A:1479:C:C6    | 2.55        | 0.40     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 7:G:43:PHE:O     | 7:G:46:ALA:HB3   | 2.20        | 0.40     |
| 4:D:170:VAL:CG1  | 4:D:171:GLY:N    | 2.84        | 0.40     |
| 1:A:1109:C:C2'   | 1:A:1110:A:H5'   | 2.51        | 0.40     |
| 3:C:122:GLU:C    | 3:C:124:ILE:N    | 2.74        | 0.40     |
| 22:V:27:G:H1     | 22:V:43:C:H42    | 1.69        | 0.40     |
| 2:B:41:ILE:HD12  | 2:B:41:ILE:N     | 2.36        | 0.40     |
| 3:C:175:LEU:HD12 | 3:C:175:LEU:H    | 1.86        | 0.40     |
| 20:T:57:ARG:HH12 | 20:T:100:ILE:CG1 | 2.34        | 0.40     |
| 10:J:13:HIS:NE2  | 10:J:14:LYS:HG3  | 2.37        | 0.40     |
| 9:I:47:LEU:N     | 9:I:47:LEU:HD12  | 2.37        | 0.40     |
| 12:L:27:LEU:C    | 12:L:29:GLY:N    | 2.75        | 0.40     |
| 1:A:1399:C:C2    | 1:A:1401:G:C5    | 3.09        | 0.40     |
| 1:A:1354:C:H2'   | 1:A:1355:G:C8    | 2.56        | 0.40     |
| 3:C:74:GLY:O     | 3:C:76:VAL:N     | 2.54        | 0.40     |
| 12:L:7:ILE:HG23  | 12:L:8:ASN:N     | 2.36        | 0.40     |
| 2:B:7:VAL:HA     | 2:B:217:ARG:HH22 | 1.85        | 0.40     |
| 18:R:36:ASN:O    | 18:R:39:VAL:HB   | 2.20        | 0.40     |
| 24:Y:319:ASN:HA  | 24:Y:333:PRO:HG3 | 2.02        | 0.40     |
| 1:A:148:G:O2'    | 1:A:149:A:H5'    | 2.21        | 0.40     |
| 22:V:55:U:C2     | 22:V:57:G:H5''   | 2.55        | 0.40     |
| 1:A:851:G:H2'    | 1:A:852:G:H8     | 1.86        | 0.40     |
| 2:B:56:ARG:HG2   | 2:B:56:ARG:HH11  | 1.85        | 0.40     |
| 1:A:818:G:C3'    | 1:A:819:A:C5'    | 2.99        | 0.40     |
| 8:H:116:LYS:HE2  | 8:H:127:LEU:HD12 | 2.03        | 0.40     |
| 18:R:85:LEU:HD12 | 18:R:85:LEU:N    | 2.35        | 0.40     |
| 1:A:269:C:H2'    | 1:A:270:A:C8     | 2.56        | 0.40     |
| 2:B:181:PHE:CD1  | 8:H:70:GLN:HB3   | 2.55        | 0.40     |
| 1:A:955:U:H2'    | 1:A:956:U:O4'    | 2.20        | 0.40     |
| 22:W:18:G:N2     | 22:W:55:U:H1'    | 2.36        | 0.40     |
| 19:S:28:LYS:HZ1  | 19:S:29:ARG:NH2  | 2.19        | 0.40     |
| 1:A:1104:G:C4    | 1:A:1105:A:C8    | 3.09        | 0.40     |
| 9:I:10:ARG:HD2   | 9:I:105:ASP:N    | 2.36        | 0.40     |
| 1:A:1293:G:O2'   | 1:A:1294:G:P     | 2.79        | 0.40     |
| 19:S:11:VAL:O    | 19:S:11:VAL:HG13 | 2.22        | 0.40     |
| 19:S:16:LEU:O    | 19:S:18:LYS:N    | 2.54        | 0.40     |
| 24:Y:46:ARG:NH1  | 24:Y:50:GLN:HB2  | 2.36        | 0.40     |
| 3:C:156:ARG:HD3  | 3:C:194:GLY:N    | 2.36        | 0.40     |
| 1:A:1456:G:N3    | 1:A:1456:G:H3'   | 2.37        | 0.40     |
| 1:A:439:A:H2'    | 1:A:441:A:O5'    | 2.22        | 0.40     |
| 6:F:14:LEU:HB3   | 6:F:18:GLN:HB2   | 2.03        | 0.40     |
| 1:A:357:G:C2     | 1:A:358:U:C5     | 3.10        | 0.40     |
| 1:A:177:C:O2'    | 1:A:178:C:H5'    | 2.21        | 0.40     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:180:U:C2'     | 1:A:181:G:H5''    | 2.51        | 0.40     |
| 1:A:374:A:C6      | 1:A:375:U:C4      | 3.09        | 0.40     |
| 10:J:87:THR:C     | 10:J:89:ASP:N     | 2.74        | 0.40     |
| 2:B:19:HIS:CD2    | 2:B:20:GLU:OE1    | 2.74        | 0.40     |
| 1:A:826:C:C5'     | 8:H:12:ARG:HH21   | 2.35        | 0.40     |
| 1:A:1428:A:H2'    | 1:A:1429:C:C6     | 2.55        | 0.40     |
| 8:H:100:ILE:HG21  | 8:H:121:ASP:HA    | 2.03        | 0.40     |
| 17:Q:90:ILE:HA    | 17:Q:93:GLN:HB3   | 2.03        | 0.40     |
| 5:E:140:ARG:CG    | 5:E:140:ARG:O     | 2.68        | 0.40     |
| 1:A:760:G:H2'     | 1:A:761:G:C5'     | 2.51        | 0.40     |
| 21:U:5:ASP:C      | 21:U:7:ARG:H      | 2.25        | 0.40     |
| 1:A:78:G:H2'      | 1:A:79:G:O4'      | 2.22        | 0.40     |
| 1:A:952:U:O2'     | 1:A:953:G:H5'     | 2.22        | 0.40     |
| 11:K:120:ARG:HA   | 11:K:121:PRO:HD3  | 1.81        | 0.40     |
| 17:Q:83:ASP:O     | 17:Q:87:LYS:HG2   | 2.21        | 0.40     |
| 8:H:113:SER:O     | 8:H:131:GLY:HA3   | 2.21        | 0.40     |
| 1:A:570:G:H2'     | 1:A:571:U:C6      | 2.56        | 0.40     |
| 24:Y:169:ILE:HG22 | 24:Y:171:VAL:HG23 | 2.04        | 0.40     |
| 5:E:103:GLY:C     | 5:E:105:VAL:H     | 2.24        | 0.40     |
| 2:B:200:ILE:CG2   | 2:B:201:ILE:N     | 2.84        | 0.40     |
| 16:P:4:ILE:N      | 16:P:4:ILE:HD12   | 2.37        | 0.40     |
| 3:C:81:GLY:O      | 3:C:85:ARG:HB2    | 2.21        | 0.40     |
| 15:O:10:LYS:O     | 15:O:14:GLU:HB2   | 2.22        | 0.40     |
| 1:A:189(C):C:C2'  | 1:A:189(D):C:H5'  | 2.51        | 0.40     |
| 1:A:1409:C:H2'    | 1:A:1410:G:C8     | 2.55        | 0.40     |
| 1:A:1412:C:H2'    | 1:A:1413:A:C8     | 2.56        | 0.40     |
| 1:A:563:A:C2      | 1:A:567:G:C6      | 3.10        | 0.40     |
| 8:H:63:LEU:N      | 8:H:63:LEU:HD22   | 2.37        | 0.40     |
| 24:Y:263:GLN:HA   | 24:Y:271:ASN:HD22 | 1.86        | 0.40     |
| 7:G:27:ILE:HG21   | 7:G:40:ALA:HB2    | 2.04        | 0.40     |
| 13:M:37:THR:HA    | 13:M:55:ARG:NH2   | 2.37        | 0.40     |
| 1:A:1048:G:OP2    | 14:N:3:ARG:NH2    | 2.55        | 0.40     |

There are no symmetry-related clashes.

## 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 |    |
|-----|-------|-----------------|------------|-----------|-----------|-------------|----|
| 2   | B     | 233/256 (91%)   | 128 (55%)  | 70 (30%)  | 35 (15%)  | 0           | 1  |
| 3   | C     | 205/239 (86%)   | 129 (63%)  | 42 (20%)  | 34 (17%)  | 0           | 0  |
| 4   | D     | 206/209 (99%)   | 139 (68%)  | 44 (21%)  | 23 (11%)  | 1           | 5  |
| 5   | E     | 149/162 (92%)   | 114 (76%)  | 24 (16%)  | 11 (7%)   | 2           | 11 |
| 6   | F     | 99/101 (98%)    | 73 (74%)   | 18 (18%)  | 8 (8%)    | 1           | 10 |
| 7   | G     | 153/156 (98%)   | 117 (76%)  | 27 (18%)  | 9 (6%)    | 2           | 17 |
| 8   | H     | 136/138 (99%)   | 104 (76%)  | 24 (18%)  | 8 (6%)    | 2           | 17 |
| 9   | I     | 121/128 (94%)   | 86 (71%)   | 24 (20%)  | 11 (9%)   | 1           | 8  |
| 10  | J     | 97/105 (92%)    | 71 (73%)   | 21 (22%)  | 5 (5%)    | 3           | 21 |
| 11  | K     | 117/129 (91%)   | 87 (74%)   | 26 (22%)  | 4 (3%)    | 6           | 32 |
| 12  | L     | 123/132 (93%)   | 84 (68%)   | 21 (17%)  | 18 (15%)  | 0           | 2  |
| 13  | M     | 113/126 (90%)   | 70 (62%)   | 26 (23%)  | 17 (15%)  | 0           | 1  |
| 14  | N     | 58/61 (95%)     | 40 (69%)   | 12 (21%)  | 6 (10%)   | 1           | 6  |
| 15  | O     | 86/89 (97%)     | 66 (77%)   | 18 (21%)  | 2 (2%)    | 10          | 45 |
| 16  | P     | 82/88 (93%)     | 58 (71%)   | 16 (20%)  | 8 (10%)   | 1           | 6  |
| 17  | Q     | 98/105 (93%)    | 76 (78%)   | 12 (12%)  | 10 (10%)  | 1           | 6  |
| 18  | R     | 68/88 (77%)     | 45 (66%)   | 15 (22%)  | 8 (12%)   | 1           | 4  |
| 19  | S     | 77/93 (83%)     | 44 (57%)   | 22 (29%)  | 11 (14%)  | 0           | 2  |
| 20  | T     | 97/106 (92%)    | 63 (65%)   | 24 (25%)  | 10 (10%)  | 1           | 6  |
| 21  | U     | 23/27 (85%)     | 16 (70%)   | 5 (22%)   | 2 (9%)    | 1           | 9  |
| 24  | Y     | 349/351 (99%)   | 272 (78%)  | 55 (16%)  | 22 (6%)   | 2           | 16 |
| All | All   | 2690/2889 (93%) | 1882 (70%) | 546 (20%) | 262 (10%) | 1           | 6  |

All (262) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 12  | GLU  |
| 2   | B     | 15  | VAL  |
| 2   | B     | 19  | HIS  |
| 2   | B     | 20  | GLU  |
| 2   | B     | 24  | TRP  |
| 2   | B     | 64  | ARG  |
| 2   | B     | 97  | TRP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 123 | ALA  |
| 2   | B     | 135 | GLN  |
| 2   | B     | 194 | PRO  |
| 2   | B     | 195 | ASP  |
| 3   | C     | 15  | THR  |
| 3   | C     | 18  | TRP  |
| 3   | C     | 47  | LEU  |
| 3   | C     | 52  | LEU  |
| 3   | C     | 79  | ARG  |
| 3   | C     | 165 | THR  |
| 3   | C     | 167 | TRP  |
| 3   | C     | 207 | VAL  |
| 4   | D     | 3   | ARG  |
| 4   | D     | 4   | TYR  |
| 4   | D     | 5   | ILE  |
| 4   | D     | 30  | LYS  |
| 4   | D     | 44  | GLY  |
| 4   | D     | 110 | PHE  |
| 4   | D     | 129 | ASN  |
| 4   | D     | 177 | ASP  |
| 5   | E     | 11  | ILE  |
| 5   | E     | 21  | ALA  |
| 5   | E     | 153 | LYS  |
| 6   | F     | 40  | VAL  |
| 7   | G     | 115 | ARG  |
| 8   | H     | 2   | LEU  |
| 9   | I     | 41  | VAL  |
| 9   | I     | 44  | VAL  |
| 9   | I     | 89  | ASN  |
| 9   | I     | 109 | VAL  |
| 10  | J     | 57  | LYS  |
| 10  | J     | 59  | SER  |
| 11  | K     | 25  | TYR  |
| 12  | L     | 18  | VAL  |
| 12  | L     | 27  | LEU  |
| 12  | L     | 46  | LYS  |
| 12  | L     | 89  | ARG  |
| 12  | L     | 91  | LYS  |
| 12  | L     | 92  | ASP  |
| 12  | L     | 115 | LYS  |
| 13  | M     | 4   | ILE  |
| 13  | M     | 107 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | M     | 116 | THR  |
| 13  | M     | 117 | VAL  |
| 16  | P     | 52  | ASP  |
| 18  | R     | 20  | ALA  |
| 18  | R     | 37  | VAL  |
| 19  | S     | 10  | PHE  |
| 19  | S     | 28  | LYS  |
| 20  | T     | 11  | SER  |
| 20  | T     | 74  | LYS  |
| 21  | U     | 3   | LYS  |
| 24  | Y     | 110 | PRO  |
| 24  | Y     | 218 | VAL  |
| 24  | Y     | 237 | PRO  |
| 24  | Y     | 263 | GLN  |
| 24  | Y     | 305 | ILE  |
| 2   | B     | 26  | PRO  |
| 2   | B     | 66  | GLY  |
| 2   | B     | 83  | MET  |
| 2   | B     | 84  | GLU  |
| 2   | B     | 120 | ALA  |
| 2   | B     | 154 | LEU  |
| 2   | B     | 165 | VAL  |
| 2   | B     | 181 | PHE  |
| 2   | B     | 204 | ASN  |
| 2   | B     | 230 | VAL  |
| 3   | C     | 4   | LYS  |
| 3   | C     | 45  | LYS  |
| 3   | C     | 61  | ALA  |
| 3   | C     | 73  | PRO  |
| 3   | C     | 74  | GLY  |
| 3   | C     | 156 | ARG  |
| 4   | D     | 18  | LYS  |
| 4   | D     | 24  | GLU  |
| 4   | D     | 99  | SER  |
| 4   | D     | 156 | GLU  |
| 4   | D     | 176 | LEU  |
| 4   | D     | 178 | VAL  |
| 6   | F     | 29  | ALA  |
| 6   | F     | 80  | ARG  |
| 7   | G     | 7   | ALA  |
| 7   | G     | 17  | VAL  |
| 7   | G     | 54  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | H     | 41  | ARG  |
| 8   | H     | 91  | ARG  |
| 9   | I     | 95  | LYS  |
| 9   | I     | 98  | PRO  |
| 10  | J     | 36  | GLY  |
| 11  | K     | 89  | ALA  |
| 11  | K     | 101 | SER  |
| 12  | L     | 19  | ARG  |
| 12  | L     | 22  | SER  |
| 12  | L     | 26  | ALA  |
| 12  | L     | 47  | LYS  |
| 12  | L     | 66  | VAL  |
| 12  | L     | 121 | GLY  |
| 13  | M     | 3   | ARG  |
| 13  | M     | 12  | ASN  |
| 13  | M     | 15  | VAL  |
| 13  | M     | 59  | TYR  |
| 13  | M     | 63  | THR  |
| 13  | M     | 68  | GLY  |
| 13  | M     | 100 | GLY  |
| 13  | M     | 124 | PRO  |
| 14  | N     | 15  | LYS  |
| 14  | N     | 36  | PHE  |
| 14  | N     | 60  | SER  |
| 16  | P     | 50  | LYS  |
| 16  | P     | 63  | GLY  |
| 17  | Q     | 34  | LYS  |
| 17  | Q     | 68  | ARG  |
| 17  | Q     | 74  | LEU  |
| 19  | S     | 29  | ARG  |
| 19  | S     | 30  | LEU  |
| 19  | S     | 64  | GLU  |
| 20  | T     | 25  | ARG  |
| 20  | T     | 103 | GLY  |
| 21  | U     | 25  | LYS  |
| 24  | Y     | 7   | ALA  |
| 24  | Y     | 80  | PRO  |
| 24  | Y     | 106 | LEU  |
| 24  | Y     | 160 | PRO  |
| 24  | Y     | 164 | ILE  |
| 2   | B     | 18  | GLY  |
| 2   | B     | 52  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 62  | ALA  |
| 2   | B     | 113 | HIS  |
| 2   | B     | 153 | ARG  |
| 2   | B     | 232 | PRO  |
| 3   | C     | 29  | TYR  |
| 3   | C     | 46  | GLU  |
| 3   | C     | 81  | GLY  |
| 3   | C     | 91  | LEU  |
| 3   | C     | 94  | LEU  |
| 3   | C     | 181 | ASN  |
| 3   | C     | 206 | GLU  |
| 4   | D     | 157 | LEU  |
| 5   | E     | 7   | GLU  |
| 5   | E     | 20  | GLN  |
| 5   | E     | 27  | ARG  |
| 6   | F     | 65  | VAL  |
| 6   | F     | 70  | ASP  |
| 7   | G     | 58  | PRO  |
| 7   | G     | 116 | ALA  |
| 8   | H     | 27  | PRO  |
| 8   | H     | 50  | ARG  |
| 8   | H     | 86  | ILE  |
| 9   | I     | 102 | LEU  |
| 10  | J     | 32  | ALA  |
| 12  | L     | 23  | LYS  |
| 13  | M     | 106 | ASN  |
| 16  | P     | 49  | LEU  |
| 17  | Q     | 12  | SER  |
| 17  | Q     | 66  | SER  |
| 17  | Q     | 99  | SER  |
| 18  | R     | 52  | PRO  |
| 18  | R     | 61  | LYS  |
| 19  | S     | 26  | GLY  |
| 20  | T     | 28  | ALA  |
| 20  | T     | 73  | HIS  |
| 24  | Y     | 42  | PRO  |
| 24  | Y     | 200 | ARG  |
| 24  | Y     | 354 | GLY  |
| 2   | B     | 130 | ARG  |
| 2   | B     | 227 | GLY  |
| 3   | C     | 20  | SER  |
| 3   | C     | 26  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 127 | ARG  |
| 3   | C     | 180 | ALA  |
| 4   | D     | 34  | GLU  |
| 4   | D     | 104 | VAL  |
| 4   | D     | 108 | LEU  |
| 4   | D     | 162 | LEU  |
| 5   | E     | 72  | GLN  |
| 5   | E     | 105 | VAL  |
| 6   | F     | 81  | ILE  |
| 7   | G     | 149 | ARG  |
| 8   | H     | 133 | LEU  |
| 9   | I     | 10  | ARG  |
| 9   | I     | 117 | HIS  |
| 10  | J     | 84  | GLN  |
| 13  | M     | 21  | TYR  |
| 13  | M     | 28  | ALA  |
| 13  | M     | 67  | GLU  |
| 14  | N     | 16  | PHE  |
| 15  | O     | 23  | GLY  |
| 16  | P     | 44  | THR  |
| 18  | R     | 25  | THR  |
| 18  | R     | 54  | ARG  |
| 19  | S     | 17  | GLU  |
| 19  | S     | 65  | ASN  |
| 20  | T     | 97  | ALA  |
| 24  | Y     | 243 | ASN  |
| 2   | B     | 8   | LYS  |
| 2   | B     | 13  | ALA  |
| 2   | B     | 76  | GLN  |
| 2   | B     | 131 | PRO  |
| 2   | B     | 229 | VAL  |
| 3   | C     | 14  | ILE  |
| 3   | C     | 54  | ARG  |
| 3   | C     | 141 | VAL  |
| 3   | C     | 168 | ALA  |
| 3   | C     | 179 | ARG  |
| 3   | C     | 193 | TYR  |
| 3   | C     | 196 | LEU  |
| 4   | D     | 7   | PRO  |
| 4   | D     | 29  | PRO  |
| 4   | D     | 47  | ARG  |
| 5   | E     | 8   | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | F     | 16  | GLN  |
| 7   | G     | 100 | ALA  |
| 9   | I     | 121 | ARG  |
| 12  | L     | 51  | ALA  |
| 12  | L     | 71  | PRO  |
| 12  | L     | 90  | VAL  |
| 13  | M     | 31  | LYS  |
| 14  | N     | 23  | ARG  |
| 16  | P     | 59  | TRP  |
| 16  | P     | 64  | ALA  |
| 17  | Q     | 30  | PRO  |
| 17  | Q     | 77  | VAL  |
| 18  | R     | 38  | GLU  |
| 19  | S     | 42  | PRO  |
| 20  | T     | 71  | THR  |
| 24  | Y     | 158 | PRO  |
| 5   | E     | 104 | ALA  |
| 9   | I     | 77  | ILE  |
| 11  | K     | 102 | GLY  |
| 14  | N     | 14  | PRO  |
| 16  | P     | 65  | GLN  |
| 17  | Q     | 47  | PRO  |
| 18  | R     | 60  | ALA  |
| 19  | S     | 18  | LYS  |
| 20  | T     | 34  | LYS  |
| 24  | Y     | 71  | GLY  |
| 24  | Y     | 303 | ARG  |
| 19  | S     | 45  | VAL  |
| 3   | C     | 75  | VAL  |
| 4   | D     | 105 | VAL  |
| 6   | F     | 88  | VAL  |
| 15  | O     | 87  | ILE  |
| 24  | Y     | 224 | PRO  |
| 24  | Y     | 339 | GLY  |
| 2   | B     | 239 | VAL  |
| 3   | C     | 55  | VAL  |
| 5   | E     | 148 | VAL  |
| 12  | L     | 101 | VAL  |
| 17  | Q     | 33  | GLY  |
| 24  | Y     | 181 | SER  |
| 24  | Y     | 242 | VAL  |
| 7   | G     | 130 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | H     | 51  | VAL  |
| 20  | T     | 33  | ILE  |
| 24  | Y     | 333 | 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 |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 2   | B     | 202/220 (92%)   | 185 (92%)  | 17 (8%)  | 16          | 52 |
| 3   | C     | 160/188 (85%)   | 146 (91%)  | 14 (9%)  | 14          | 49 |
| 4   | D     | 180/181 (99%)   | 159 (88%)  | 21 (12%) | 8           | 29 |
| 5   | E     | 115/123 (94%)   | 110 (96%)  | 5 (4%)   | 40          | 80 |
| 6   | F     | 90/90 (100%)    | 87 (97%)   | 3 (3%)   | 50          | 86 |
| 7   | G     | 126/127 (99%)   | 121 (96%)  | 5 (4%)   | 42          | 82 |
| 8   | H     | 119/119 (100%)  | 114 (96%)  | 5 (4%)   | 40          | 81 |
| 9   | I     | 98/99 (99%)     | 89 (91%)   | 9 (9%)   | 13          | 45 |
| 10  | J     | 88/92 (96%)     | 82 (93%)   | 6 (7%)   | 22          | 62 |
| 11  | K     | 90/99 (91%)     | 86 (96%)   | 4 (4%)   | 39          | 79 |
| 12  | L     | 104/109 (95%)   | 90 (86%)   | 14 (14%) | 6           | 22 |
| 13  | M     | 99/101 (98%)    | 91 (92%)   | 8 (8%)   | 17          | 53 |
| 14  | N     | 49/50 (98%)     | 45 (92%)   | 4 (8%)   | 17          | 53 |
| 15  | O     | 79/80 (99%)     | 73 (92%)   | 6 (8%)   | 19          | 58 |
| 16  | P     | 72/74 (97%)     | 68 (94%)   | 4 (6%)   | 30          | 70 |
| 17  | Q     | 94/97 (97%)     | 92 (98%)   | 2 (2%)   | 66          | 92 |
| 18  | R     | 61/77 (79%)     | 59 (97%)   | 2 (3%)   | 50          | 86 |
| 19  | S     | 69/80 (86%)     | 59 (86%)   | 10 (14%) | 5           | 18 |
| 20  | T     | 76/82 (93%)     | 69 (91%)   | 7 (9%)   | 13          | 45 |
| 21  | U     | 19/22 (86%)     | 17 (90%)   | 2 (10%)  | 10          | 35 |
| 24  | Y     | 298/298 (100%)  | 265 (89%)  | 33 (11%) | 9           | 33 |
| All | All   | 2288/2408 (95%) | 2107 (92%) | 181 (8%) | 18          | 55 |

All (181) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 15  | VAL  |
| 2   | B     | 17  | PHE  |
| 2   | B     | 24  | TRP  |
| 2   | B     | 36  | ARG  |
| 2   | B     | 46  | LYS  |
| 2   | B     | 69  | LEU  |
| 2   | B     | 119 | GLU  |
| 2   | B     | 137 | ARG  |
| 2   | B     | 140 | HIS  |
| 2   | B     | 145 | LEU  |
| 2   | B     | 172 | ILE  |
| 2   | B     | 178 | ARG  |
| 2   | B     | 195 | ASP  |
| 2   | B     | 196 | LEU  |
| 2   | B     | 204 | ASN  |
| 2   | B     | 206 | ASP  |
| 2   | B     | 232 | PRO  |
| 3   | C     | 3   | ASN  |
| 3   | C     | 5   | ILE  |
| 3   | C     | 16  | ARG  |
| 3   | C     | 29  | TYR  |
| 3   | C     | 34  | LEU  |
| 3   | C     | 52  | LEU  |
| 3   | C     | 82  | GLU  |
| 3   | C     | 104 | GLN  |
| 3   | C     | 107 | GLN  |
| 3   | C     | 108 | ASN  |
| 3   | C     | 127 | ARG  |
| 3   | C     | 156 | ARG  |
| 3   | C     | 193 | TYR  |
| 3   | C     | 196 | LEU  |
| 4   | D     | 3   | ARG  |
| 4   | D     | 9   | CYS  |
| 4   | D     | 10  | ARG  |
| 4   | D     | 13  | ARG  |
| 4   | D     | 15  | GLU  |
| 4   | D     | 20  | TYR  |
| 4   | D     | 35  | ARG  |
| 4   | D     | 38  | TYR  |
| 4   | D     | 42  | GLN  |
| 4   | D     | 59  | ARG  |
| 4   | D     | 86  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 97  | LEU  |
| 4   | D     | 107 | ARG  |
| 4   | D     | 110 | PHE  |
| 4   | D     | 129 | ASN  |
| 4   | D     | 131 | ARG  |
| 4   | D     | 132 | ARG  |
| 4   | D     | 135 | LEU  |
| 4   | D     | 158 | ILE  |
| 4   | D     | 170 | VAL  |
| 4   | D     | 200 | GLU  |
| 5   | E     | 12  | LEU  |
| 5   | E     | 16  | THR  |
| 5   | E     | 20  | GLN  |
| 5   | E     | 79  | GLU  |
| 5   | E     | 101 | ILE  |
| 6   | F     | 16  | GLN  |
| 6   | F     | 30  | LEU  |
| 6   | F     | 69  | GLU  |
| 7   | G     | 57  | GLU  |
| 7   | G     | 62  | PHE  |
| 7   | G     | 72  | ARG  |
| 7   | G     | 113 | GLU  |
| 7   | G     | 137 | LYS  |
| 8   | H     | 1   | MET  |
| 8   | H     | 27  | PRO  |
| 8   | H     | 65  | TYR  |
| 8   | H     | 102 | ARG  |
| 8   | H     | 137 | VAL  |
| 9   | I     | 10  | ARG  |
| 9   | I     | 48  | GLU  |
| 9   | I     | 91  | ASP  |
| 9   | I     | 92  | TYR  |
| 9   | I     | 95  | LYS  |
| 9   | I     | 114 | TYR  |
| 9   | I     | 121 | ARG  |
| 9   | I     | 125 | TYR  |
| 9   | I     | 128 | ARG  |
| 10  | J     | 22  | LYS  |
| 10  | J     | 46  | ARG  |
| 10  | J     | 50  | ILE  |
| 10  | J     | 62  | HIS  |
| 10  | J     | 63  | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | J     | 96  | ILE  |
| 11  | K     | 103 | LEU  |
| 11  | K     | 117 | ASN  |
| 11  | K     | 124 | LYS  |
| 11  | K     | 125 | PHE  |
| 12  | L     | 20  | LYS  |
| 12  | L     | 27  | LEU  |
| 12  | L     | 38  | THR  |
| 12  | L     | 40  | VAL  |
| 12  | L     | 41  | ARG  |
| 12  | L     | 47  | LYS  |
| 12  | L     | 53  | ARG  |
| 12  | L     | 80  | HIS  |
| 12  | L     | 83  | VAL  |
| 12  | L     | 84  | LEU  |
| 12  | L     | 85  | ILE  |
| 12  | L     | 89  | ARG  |
| 12  | L     | 102 | ARG  |
| 12  | L     | 110 | VAL  |
| 13  | M     | 47  | ASP  |
| 13  | M     | 48  | LEU  |
| 13  | M     | 64  | TRP  |
| 13  | M     | 79  | LYS  |
| 13  | M     | 92  | HIS  |
| 13  | M     | 93  | ARG  |
| 13  | M     | 108 | ARG  |
| 13  | M     | 115 | LYS  |
| 14  | N     | 6   | LEU  |
| 14  | N     | 16  | PHE  |
| 14  | N     | 33  | VAL  |
| 14  | N     | 41  | ARG  |
| 15  | O     | 7   | GLU  |
| 15  | O     | 22  | THR  |
| 15  | O     | 39  | LEU  |
| 15  | O     | 41  | GLU  |
| 15  | O     | 65  | ARG  |
| 15  | O     | 82  | ILE  |
| 16  | P     | 1   | MET  |
| 16  | P     | 17  | TYR  |
| 16  | P     | 55  | ARG  |
| 16  | P     | 69  | THR  |
| 17  | Q     | 38  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | Q     | 52  | LYS  |
| 18  | R     | 31  | LEU  |
| 18  | R     | 32  | ARG  |
| 19  | S     | 5   | LEU  |
| 19  | S     | 6   | LYS  |
| 19  | S     | 7   | LYS  |
| 19  | S     | 15  | LEU  |
| 19  | S     | 16  | LEU  |
| 19  | S     | 27  | GLU  |
| 19  | S     | 29  | ARG  |
| 19  | S     | 37  | ARG  |
| 19  | S     | 44  | MET  |
| 19  | S     | 65  | ASN  |
| 20  | T     | 26  | ASN  |
| 20  | T     | 30  | LYS  |
| 20  | T     | 45  | GLN  |
| 20  | T     | 73  | HIS  |
| 20  | T     | 75  | ASN  |
| 20  | T     | 93  | GLU  |
| 20  | T     | 100 | ILE  |
| 21  | U     | 9   | ARG  |
| 21  | U     | 12  | LYS  |
| 24  | Y     | 8   | GLN  |
| 24  | Y     | 16  | TYR  |
| 24  | Y     | 23  | GLU  |
| 24  | Y     | 26  | LEU  |
| 24  | Y     | 29  | LEU  |
| 24  | Y     | 46  | ARG  |
| 24  | Y     | 50  | GLN  |
| 24  | Y     | 60  | ASP  |
| 24  | Y     | 66  | GLU  |
| 24  | Y     | 68  | ASP  |
| 24  | Y     | 84  | ARG  |
| 24  | Y     | 92  | GLU  |
| 24  | Y     | 93  | GLU  |
| 24  | Y     | 104 | GLN  |
| 24  | Y     | 115 | ASN  |
| 24  | Y     | 132 | TRP  |
| 24  | Y     | 147 | GLN  |
| 24  | Y     | 191 | ARG  |
| 24  | Y     | 240 | GLN  |
| 24  | Y     | 261 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | Y     | 265 | THR  |
| 24  | Y     | 266 | ARG  |
| 24  | Y     | 291 | ARG  |
| 24  | Y     | 314 | TYR  |
| 24  | Y     | 315 | VAL  |
| 24  | Y     | 316 | LEU  |
| 24  | Y     | 323 | ASP  |
| 24  | Y     | 328 | LEU  |
| 24  | Y     | 335 | ASN  |
| 24  | Y     | 340 | ASP  |
| 24  | Y     | 344 | LEU  |
| 24  | Y     | 346 | TRP  |
| 24  | Y     | 355 | ARG  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 37  | ASN  |
| 2   | B     | 40  | HIS  |
| 2   | B     | 45  | GLN  |
| 2   | B     | 78  | GLN  |
| 2   | B     | 95  | GLN  |
| 2   | B     | 110 | GLN  |
| 2   | B     | 135 | GLN  |
| 2   | B     | 146 | GLN  |
| 2   | B     | 204 | ASN  |
| 2   | B     | 212 | GLN  |
| 3   | C     | 37  | GLN  |
| 3   | C     | 69  | HIS  |
| 3   | C     | 107 | GLN  |
| 3   | C     | 170 | GLN  |
| 4   | D     | 42  | GLN  |
| 4   | D     | 62  | GLN  |
| 4   | D     | 77  | ASN  |
| 4   | D     | 123 | HIS  |
| 4   | D     | 129 | ASN  |
| 4   | D     | 161 | ASN  |
| 4   | D     | 199 | ASN  |
| 5   | E     | 20  | GLN  |
| 5   | E     | 72  | GLN  |
| 5   | E     | 73  | ASN  |
| 5   | E     | 141 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | F     | 16  | GLN  |
| 6   | F     | 18  | GLN  |
| 6   | F     | 27  | GLN  |
| 6   | F     | 32  | ASN  |
| 6   | F     | 94  | GLN  |
| 6   | F     | 100 | ASN  |
| 7   | G     | 13  | GLN  |
| 7   | G     | 28  | ASN  |
| 7   | G     | 37  | ASN  |
| 7   | G     | 64  | GLN  |
| 7   | G     | 84  | ASN  |
| 7   | G     | 86  | GLN  |
| 7   | G     | 97  | GLN  |
| 7   | G     | 106 | GLN  |
| 7   | G     | 109 | ASN  |
| 7   | G     | 148 | ASN  |
| 9   | I     | 31  | GLN  |
| 9   | I     | 124 | GLN  |
| 10  | J     | 13  | HIS  |
| 10  | J     | 56  | HIS  |
| 10  | J     | 69  | ASN  |
| 10  | J     | 84  | GLN  |
| 11  | K     | 62  | GLN  |
| 11  | K     | 78  | GLN  |
| 12  | L     | 8   | ASN  |
| 12  | L     | 9   | GLN  |
| 12  | L     | 49  | ASN  |
| 12  | L     | 75  | HIS  |
| 13  | M     | 40  | ASN  |
| 13  | M     | 77  | ASN  |
| 13  | M     | 101 | GLN  |
| 14  | N     | 52  | GLN  |
| 15  | O     | 9   | GLN  |
| 15  | O     | 37  | ASN  |
| 16  | P     | 14  | ASN  |
| 16  | P     | 16  | HIS  |
| 16  | P     | 76  | GLN  |
| 17  | Q     | 16  | GLN  |
| 17  | Q     | 93  | GLN  |
| 18  | R     | 36  | ASN  |
| 19  | S     | 23  | ASN  |
| 20  | T     | 16  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | T     | 26  | ASN  |
| 20  | T     | 42  | GLN  |
| 20  | T     | 75  | ASN  |
| 24  | Y     | 50  | GLN  |
| 24  | Y     | 147 | GLN  |
| 24  | Y     | 150 | GLN  |
| 24  | Y     | 168 | GLN  |
| 24  | Y     | 243 | ASN  |
| 24  | Y     | 324 | HIS  |
| 24  | Y     | 335 | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | A     | 1503/1522 (98%) | 207 (13%)         | 31 (2%)         |
| 22  | V     | 74/77 (96%)     | 19 (25%)          | 0               |
| 22  | W     | 74/77 (96%)     | 17 (22%)          | 1 (1%)          |
| 23  | X     | 7/8 (87%)       | 2 (28%)           | 1 (14%)         |
| All | All   | 1658/1684 (98%) | 245 (14%)         | 33 (1%)         |

All (245) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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     | 51  | A    |
| 1   | A     | 61  | G    |
| 1   | A     | 79  | G    |
| 1   | A     | 80  | G    |
| 1   | A     | 81  | U    |
| 1   | A     | 89  | C    |
| 1   | A     | 90  | U    |
| 1   | A     | 92  | C    |
| 1   | A     | 97  | G    |
| 1   | A     | 98  | G    |
| 1   | A     | 101 | A    |
| 1   | A     | 116 | A    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 120    | A    |
| 1   | A     | 121    | C    |
| 1   | A     | 131    | C    |
| 1   | A     | 137    | C    |
| 1   | A     | 144    | G    |
| 1   | A     | 150    | C    |
| 1   | A     | 189(H) | G    |
| 1   | A     | 195    | A    |
| 1   | A     | 197    | A    |
| 1   | A     | 203    | U    |
| 1   | A     | 204    | U    |
| 1   | A     | 244    | U    |
| 1   | A     | 247    | G    |
| 1   | A     | 251    | G    |
| 1   | A     | 266    | G    |
| 1   | A     | 267    | C    |
| 1   | A     | 289    | G    |
| 1   | A     | 321    | A    |
| 1   | A     | 328    | C    |
| 1   | A     | 329    | A    |
| 1   | A     | 332    | G    |
| 1   | A     | 345    | C    |
| 1   | A     | 352    | C    |
| 1   | A     | 353    | A    |
| 1   | A     | 354    | G    |
| 1   | A     | 367    | U    |
| 1   | A     | 372    | C    |
| 1   | A     | 373    | A    |
| 1   | A     | 397    | A    |
| 1   | A     | 398    | C    |
| 1   | A     | 412    | A    |
| 1   | A     | 413    | G    |
| 1   | A     | 414    | A    |
| 1   | A     | 422    | C    |
| 1   | A     | 428    | G    |
| 1   | A     | 429    | U    |
| 1   | A     | 430    | A    |
| 1   | A     | 435    | C    |
| 1   | A     | 436    | C    |
| 1   | A     | 437    | U    |
| 1   | A     | 439    | A    |
| 1   | A     | 452    | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 461 | A    |
| 1   | A     | 484 | G    |
| 1   | A     | 485 | G    |
| 1   | A     | 496 | A    |
| 1   | A     | 498 | U    |
| 1   | A     | 509 | A    |
| 1   | A     | 510 | A    |
| 1   | A     | 511 | C    |
| 1   | A     | 512 | U    |
| 1   | A     | 518 | C    |
| 1   | A     | 527 | G    |
| 1   | A     | 532 | A    |
| 1   | A     | 533 | A    |
| 1   | A     | 534 | U    |
| 1   | A     | 547 | A    |
| 1   | A     | 559 | A    |
| 1   | A     | 561 | U    |
| 1   | A     | 572 | A    |
| 1   | A     | 573 | A    |
| 1   | A     | 575 | G    |
| 1   | A     | 576 | G    |
| 1   | A     | 577 | G    |
| 1   | A     | 630 | G    |
| 1   | A     | 631 | G    |
| 1   | A     | 632 | A    |
| 1   | A     | 653 | A    |
| 1   | A     | 687 | A    |
| 1   | A     | 688 | G    |
| 1   | A     | 724 | G    |
| 1   | A     | 731 | G    |
| 1   | A     | 749 | C    |
| 1   | A     | 755 | G    |
| 1   | A     | 777 | A    |
| 1   | A     | 794 | A    |
| 1   | A     | 816 | A    |
| 1   | A     | 817 | C    |
| 1   | A     | 818 | G    |
| 1   | A     | 819 | A    |
| 1   | A     | 828 | A    |
| 1   | A     | 833 | U    |
| 1   | A     | 839 | U    |
| 1   | A     | 840 | C    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | A     | 841     | U    |
| 1   | A     | 848     | C    |
| 1   | A     | 859     | A    |
| 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     | 960     | U    |
| 1   | A     | 961     | U    |
| 1   | A     | 966     | G    |
| 1   | A     | 968     | A    |
| 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     | 978     | A    |
| 1   | A     | 980     | C    |
| 1   | A     | 991     | U    |
| 1   | A     | 992     | U    |
| 1   | A     | 993     | G    |
| 1   | A     | 1001(A) | G    |
| 1   | A     | 1009    | G    |
| 1   | A     | 1027    | C    |
| 1   | A     | 1030    | C    |
| 1   | A     | 1050    | G    |
| 1   | A     | 1054    | C    |
| 1   | A     | 1055    | A    |
| 1   | A     | 1065    | U    |
| 1   | A     | 1066    | C    |
| 1   | A     | 1068    | G    |
| 1   | A     | 1094    | G    |
| 1   | A     | 1095    | U    |
| 1   | A     | 1101    | A    |
| 1   | A     | 1108    | G    |
| 1   | A     | 1117    | G    |
| 1   | A     | 1124    | G    |
| 1   | A     | 1126    | U    |
| 1   | A     | 1129    | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1130 | A    |
| 1   | A     | 1131 | G    |
| 1   | A     | 1136 | U    |
| 1   | A     | 1137 | C    |
| 1   | A     | 1138 | G    |
| 1   | A     | 1139 | G    |
| 1   | A     | 1146 | A    |
| 1   | A     | 1152 | A    |
| 1   | A     | 1159 | U    |
| 1   | A     | 1182 | G    |
| 1   | A     | 1196 | U    |
| 1   | A     | 1197 | G    |
| 1   | A     | 1202 | G    |
| 1   | A     | 1212 | U    |
| 1   | A     | 1213 | A    |
| 1   | A     | 1214 | C    |
| 1   | A     | 1225 | A    |
| 1   | A     | 1238 | A    |
| 1   | A     | 1249 | C    |
| 1   | A     | 1255 | G    |
| 1   | A     | 1256 | A    |
| 1   | A     | 1257 | U    |
| 1   | A     | 1280 | A    |
| 1   | A     | 1281 | U    |
| 1   | A     | 1282 | C    |
| 1   | A     | 1286 | A    |
| 1   | A     | 1287 | A    |
| 1   | A     | 1294 | G    |
| 1   | A     | 1299 | A    |
| 1   | A     | 1300 | G    |
| 1   | A     | 1301 | U    |
| 1   | A     | 1302 | U    |
| 1   | A     | 1305 | G    |
| 1   | A     | 1317 | C    |
| 1   | A     | 1322 | C    |
| 1   | A     | 1323 | G    |
| 1   | A     | 1331 | G    |
| 1   | A     | 1347 | G    |
| 1   | A     | 1363 | C    |
| 1   | A     | 1364 | U    |
| 1   | A     | 1401 | G    |
| 1   | A     | 1419 | G    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | A     | 1442    | G    |
| 1   | A     | 1442(A) | G    |
| 1   | A     | 1442(B) | A    |
| 1   | A     | 1443    | G    |
| 1   | A     | 1447    | A    |
| 1   | A     | 1452    | C    |
| 1   | A     | 1492    | A    |
| 1   | A     | 1493    | A    |
| 1   | A     | 1497    | G    |
| 1   | A     | 1498    | U    |
| 1   | A     | 1499    | A    |
| 1   | A     | 1502    | A    |
| 1   | A     | 1504    | G    |
| 1   | A     | 1505    | G    |
| 1   | A     | 1506    | U    |
| 1   | A     | 1507    | A    |
| 1   | A     | 1517    | G    |
| 1   | A     | 1520    | G    |
| 1   | A     | 1529    | G    |
| 1   | A     | 1530    | G    |
| 1   | A     | 1531    | A    |
| 22  | V     | 8       | U    |
| 22  | V     | 13      | C    |
| 22  | V     | 17      | C    |
| 22  | V     | 18      | G    |
| 22  | V     | 19      | G    |
| 22  | V     | 20      | U    |
| 22  | V     | 21      | A    |
| 22  | V     | 22      | G    |
| 22  | V     | 37      | A    |
| 22  | V     | 42      | C    |
| 22  | V     | 44      | G    |
| 22  | V     | 46      | G    |
| 22  | V     | 47      | U    |
| 22  | V     | 48      | C    |
| 22  | V     | 52      | G    |
| 22  | V     | 61      | C    |
| 22  | V     | 72      | C    |
| 22  | V     | 73      | A    |
| 22  | V     | 75      | C    |
| 22  | W     | 8       | U    |
| 22  | W     | 16      | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | W     | 17  | C    |
| 22  | W     | 18  | G    |
| 22  | W     | 19  | G    |
| 22  | W     | 21  | A    |
| 22  | W     | 22  | G    |
| 22  | W     | 23  | A    |
| 22  | W     | 39  | U    |
| 22  | W     | 40  | C    |
| 22  | W     | 43  | C    |
| 22  | W     | 44  | G    |
| 22  | W     | 47  | U    |
| 22  | W     | 51  | U    |
| 22  | W     | 52  | G    |
| 22  | W     | 61  | C    |
| 22  | W     | 71  | G    |
| 23  | X     | 15  | A    |
| 23  | X     | 21  | A    |

All (33) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 30  | U    |
| 1   | A     | 60  | A    |
| 1   | A     | 115 | G    |
| 1   | A     | 119 | A    |
| 1   | A     | 243 | A    |
| 1   | A     | 250 | A    |
| 1   | A     | 266 | G    |
| 1   | A     | 328 | C    |
| 1   | A     | 366 | C    |
| 1   | A     | 428 | G    |
| 1   | A     | 429 | U    |
| 1   | A     | 438 | G    |
| 1   | A     | 484 | G    |
| 1   | A     | 509 | A    |
| 1   | A     | 533 | A    |
| 1   | A     | 560 | U    |
| 1   | A     | 575 | G    |
| 1   | A     | 687 | A    |
| 1   | A     | 748 | C    |
| 1   | A     | 793 | U    |
| 1   | A     | 913 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 992  | U    |
| 1   | A     | 1049 | U    |
| 1   | A     | 1065 | U    |
| 1   | A     | 1067 | A    |
| 1   | A     | 1201 | A    |
| 1   | A     | 1281 | U    |
| 1   | A     | 1285 | A    |
| 1   | A     | 1300 | G    |
| 1   | A     | 1498 | U    |
| 1   | A     | 1504 | G    |
| 22  | W     | 70   | G    |
| 23  | X     | 15   | A    |

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

| Mol | Type | Chain | Res | Link  | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|-------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |       | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 22  | 8AN  | V     | 76  | 25,22 | 24,24,25     | 0.69 | 0           | 34,35,38    | 1.03 | 3 (8%)      |
| 22  | PHA  | V     | 77  | 22    | 11,11,11     | 1.70 | 1 (9%)      | 13,13,13    | 0.98 | 1 (7%)      |
| 22  | 8AN  | W     | 76  | 22    | 24,24,25     | 0.67 | 0           | 34,35,38    | 1.15 | 2 (5%)      |
| 22  | PHA  | W     | 77  | 22    | 11,11,11     | 2.04 | 1 (9%)      | 13,13,13    | 0.78 | 1 (7%)      |

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   |
|-----|------|-------|-----|-------|---------|-----------|---------|
| 22  | 8AN  | V     | 76  | 25,22 | -       | 0/9/25/26 | 0/1/3/3 |
| 22  | PHA  | V     | 77  | 22    | -       | 0/5/6/6   | 0/1/1/1 |
| 22  | 8AN  | W     | 76  | 22    | -       | 0/9/25/26 | 0/1/3/3 |
| 22  | PHA  | W     | 77  | 22    | -       | 0/5/6/6   | 0/1/1/1 |



All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 22  | W     | 77  | PHA  | CA-C  | 6.14 | 1.56        | 1.50     |
| 22  | V     | 77  | PHA  | CA-C  | 4.96 | 1.55        | 1.50     |

All (7) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | W     | 76  | 8AN  | C2'-C1'-N9  | 3.52  | 122.30      | 113.27   |
| 22  | W     | 77  | PHA  | O-C-CA      | -2.55 | 119.41      | 125.12   |
| 22  | V     | 77  | PHA  | C-CA-N      | 2.32  | 117.11      | 110.42   |
| 22  | V     | 76  | 8AN  | O4'-C4'-C3' | 2.10  | 107.13      | 104.00   |
| 22  | V     | 76  | 8AN  | O1P-P-O5'   | -2.09 | 106.80      | 113.42   |
| 22  | W     | 76  | 8AN  | O1P-P-O5'   | -2.04 | 106.97      | 113.42   |
| 22  | V     | 76  | 8AN  | C4'-C3'-N3' | -2.01 | 109.18      | 113.46   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 549 ligands modelled in this entry, 549 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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     | 1504/1522 (98%) | -0.10  | 16 (1%) 77 22 | 34, 96, 178, 201      | 0     |
| 2   | B     | 235/256 (91%)   | 0.07   | 1 (0%) 90 45  | 34, 118, 174, 201     | 0     |
| 3   | C     | 207/239 (86%)   | 0.02   | 4 (1%) 64 13  | 62, 113, 157, 198     | 0     |
| 4   | D     | 208/209 (99%)   | 0.08   | 3 (1%) 72 17  | 63, 108, 157, 201     | 0     |
| 5   | E     | 151/162 (93%)   | -0.10  | 2 (1%) 74 19  | 52, 84, 132, 163      | 0     |
| 6   | F     | 101/101 (100%)  | -0.25  | 1 (0%) 79 23  | 51, 88, 141, 168      | 0     |
| 7   | G     | 155/156 (99%)   | 0.05   | 5 (3%) 45 7   | 60, 106, 163, 201     | 0     |
| 8   | H     | 138/138 (100%)  | -0.07  | 1 (0%) 84 32  | 48, 83, 125, 157      | 0     |
| 9   | I     | 127/128 (99%)   | 0.32   | 3 (2%) 56 9   | 57, 123, 185, 200     | 0     |
| 10  | J     | 99/105 (94%)    | 0.22   | 3 (3%) 48 7   | 66, 133, 186, 201     | 0     |
| 11  | K     | 119/129 (92%)   | -0.11  | 1 (0%) 83 28  | 38, 81, 138, 181      | 0     |
| 12  | L     | 125/132 (94%)   | 0.23   | 5 (4%) 36 5   | 40, 90, 142, 200      | 0     |
| 13  | M     | 125/126 (99%)   | 0.14   | 4 (3%) 45 7   | 40, 112, 176, 201     | 0     |
| 14  | N     | 60/61 (98%)     | 0.26   | 0 100 100     | 63, 102, 144, 167     | 0     |
| 15  | O     | 88/89 (98%)     | -0.15  | 0 100 100     | 45, 82, 126, 162      | 0     |
| 16  | P     | 84/88 (95%)     | 0.09   | 2 (2%) 56 9   | 63, 105, 145, 168     | 0     |
| 17  | Q     | 100/105 (95%)   | -0.12  | 0 100 100     | 49, 86, 121, 161      | 0     |
| 18  | R     | 70/88 (79%)     | 0.00   | 0 100 100     | 61, 85, 129, 150      | 0     |
| 19  | S     | 79/93 (84%)     | 0.44   | 4 (5%) 27 4   | 69, 126, 187, 201     | 0     |
| 20  | T     | 99/106 (93%)    | 0.05   | 0 100 100     | 49, 101, 152, 192     | 0     |
| 21  | U     | 25/27 (92%)     | 0.90   | 3 (12%) 5 1   | 77, 106, 145, 200     | 0     |
| 22  | V     | 77/77 (100%)    | -0.30  | 1 (1%) 74 19  | 61, 106, 152, 192     | 0     |
| 22  | W     | 77/77 (100%)    | 0.46   | 10 (12%) 4 1  | 64, 163, 200, 201     | 0     |
| 23  | X     | 8/8 (100%)      | 0.31   | 1 (12%) 5 1   | 46, 77, 146, 167      | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 24  | Y     | 351/351 (100%)  | 0.27   | 20 (5%) 23 3  | 66, 142, 191, 201     | 0     |
| All | All   | 4412/4573 (96%) | 0.03   | 90 (2%) 59 12 | 34, 104, 177, 201     | 0     |

All (90) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 12  | L     | 129  | ALA  | 10.6 |
| 19  | S     | 69   | HIS  | 9.1  |
| 22  | W     | 33   | U    | 8.2  |
| 3   | C     | 208  | ILE  | 7.8  |
| 22  | W     | 34   | G    | 6.4  |
| 22  | W     | 36   | A    | 6.2  |
| 22  | W     | 47   | U    | 5.9  |
| 10  | J     | 100  | THR  | 5.7  |
| 19  | S     | 82   | GLY  | 5.0  |
| 21  | U     | 26   | LYS  | 4.7  |
| 22  | V     | 17   | C    | 4.6  |
| 10  | J     | 5    | ARG  | 4.3  |
| 3   | C     | 207  | VAL  | 4.3  |
| 13  | M     | 126  | LYS  | 4.1  |
| 22  | W     | 37   | A    | 4.1  |
| 22  | W     | 32   | U    | 4.0  |
| 24  | Y     | 298  | LEU  | 3.9  |
| 7   | G     | 12   | LEU  | 3.9  |
| 16  | P     | 84   | ALA  | 3.8  |
| 7   | G     | 5    | ARG  | 3.8  |
| 24  | Y     | 161  | GLU  | 3.6  |
| 12  | L     | 73   | GLU  | 3.6  |
| 12  | L     | 128  | ALA  | 3.4  |
| 5   | E     | 155  | GLU  | 3.3  |
| 19  | S     | 68   | GLY  | 3.3  |
| 9   | I     | 2    | GLU  | 3.0  |
| 21  | U     | 25   | LYS  | 3.0  |
| 7   | G     | 84   | ASN  | 2.9  |
| 1   | A     | 1149 | C    | 2.9  |
| 10  | J     | 99   | LYS  | 2.8  |
| 24  | Y     | 244  | THR  | 2.8  |
| 24  | Y     | 217  | GLU  | 2.8  |
| 24  | Y     | 197  | ALA  | 2.8  |
| 1   | A     | 1019 | C    | 2.8  |
| 1   | A     | 182  | U    | 2.7  |
| 8   | H     | 54   | ASP  | 2.7  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 4   | D     | 84      | LYS  | 2.7  |
| 12  | L     | 127     | GLU  | 2.7  |
| 23  | X     | 14      | A    | 2.7  |
| 2   | B     | 36      | ARG  | 2.6  |
| 24  | Y     | 216     | GLU  | 2.6  |
| 7   | G     | 115     | ARG  | 2.6  |
| 12  | L     | 65      | GLU  | 2.6  |
| 4   | D     | 118     | ARG  | 2.6  |
| 3   | C     | 2       | GLY  | 2.6  |
| 13  | M     | 2       | ALA  | 2.5  |
| 6   | F     | 101     | ALA  | 2.5  |
| 1   | A     | 1040    | U    | 2.5  |
| 24  | Y     | 300     | GLY  | 2.4  |
| 1   | A     | 181     | G    | 2.4  |
| 22  | W     | 38      | A    | 2.3  |
| 1   | A     | 1394    | A    | 2.3  |
| 24  | Y     | 95      | ALA  | 2.3  |
| 1   | A     | 531     | U    | 2.3  |
| 24  | Y     | 15      | GLY  | 2.3  |
| 3   | C     | 3       | ASN  | 2.3  |
| 1   | A     | 488     | C    | 2.2  |
| 24  | Y     | 14      | ARG  | 2.2  |
| 24  | Y     | 42      | PRO  | 2.2  |
| 1   | A     | 1442(B) | A    | 2.2  |
| 22  | W     | 17      | C    | 2.2  |
| 24  | Y     | 301     | GLU  | 2.2  |
| 24  | Y     | 16      | TYR  | 2.2  |
| 9   | I     | 102     | LEU  | 2.2  |
| 13  | M     | 84      | ILE  | 2.2  |
| 1   | A     | 840     | C    | 2.2  |
| 24  | Y     | 66      | GLU  | 2.2  |
| 24  | Y     | 338     | ASP  | 2.2  |
| 11  | K     | 129     | SER  | 2.2  |
| 4   | D     | 115     | ARG  | 2.2  |
| 1   | A     | 1119    | C    | 2.1  |
| 13  | M     | 99      | ARG  | 2.1  |
| 1   | A     | 140     | A    | 2.1  |
| 24  | Y     | 145     | GLU  | 2.1  |
| 24  | Y     | 157     | THR  | 2.1  |
| 16  | P     | 83      | GLU  | 2.1  |
| 7   | G     | 83      | ALA  | 2.1  |
| 24  | Y     | 82      | GLU  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 24  | Y     | 63   | ARG  | 2.1  |
| 22  | W     | 35   | A    | 2.1  |
| 1   | A     | 381  | C    | 2.1  |
| 21  | U     | 16   | GLY  | 2.1  |
| 1   | A     | 135  | C    | 2.0  |
| 1   | A     | 1447 | A    | 2.0  |
| 19  | S     | 61   | TYR  | 2.0  |
| 22  | W     | 44   | G    | 2.0  |
| 1   | A     | 1257 | U    | 2.0  |
| 5   | E     | 154  | GLY  | 2.0  |
| 24  | Y     | 160  | PRO  | 2.0  |
| 9   | I     | 56   | LEU  | 2.0  |

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

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 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 22  | 8AN  | W     | 76  | 22/23 | 0.19 | -    | 71,74,82,82                | 0     |
| 22  | 8AN  | V     | 76  | 22/23 | 0.12 | -    | 59,59,59,104               | 0     |
| 22  | PHA  | V     | 77  | 11/11 | 0.50 | -    | 70,70,72,73                | 0     |
| 22  | PHA  | W     | 77  | 11/11 | 0.33 | -    | 77,77,79,80                | 0     |

## 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( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 25  | MG   | Z     | 379 | 1/1   | 0.09 | -    | 51,51,51,51                 | 0     |
| 25  | MG   | Z     | 61  | 1/1   | 0.12 | -    | 11,11,11,11                 | 0     |
| 25  | MG   | Z     | 18  | 1/1   | 0.16 | -    | 58,58,58,58                 | 0     |
| 25  | MG   | Z     | 469 | 1/1   | 0.48 | -    | 63,63,63,63                 | 0     |
| 25  | MG   | Z     | 372 | 1/1   | 0.07 | -    | 18,18,18,18                 | 0     |
| 25  | MG   | Z     | 458 | 1/1   | 0.06 | -    | 15,15,15,15                 | 0     |
| 25  | MG   | Z     | 299 | 1/1   | 0.20 | -    | 16,16,16,16                 | 0     |
| 25  | MG   | Z     | 528 | 1/1   | 0.11 | -    | 48,48,48,48                 | 0     |
| 25  | MG   | Z     | 232 | 1/1   | 0.13 | -    | 75,75,75,75                 | 0     |
| 25  | MG   | Z     | 263 | 1/1   | 0.40 | -    | 31,31,31,31                 | 0     |
| 25  | MG   | Z     | 423 | 1/1   | 0.14 | -    | 37,37,37,37                 | 0     |
| 25  | MG   | Z     | 473 | 1/1   | 0.47 | -    | 85,85,85,85                 | 0     |
| 25  | MG   | Z     | 119 | 1/1   | 0.17 | -    | 33,33,33,33                 | 0     |
| 25  | MG   | Z     | 417 | 1/1   | 0.24 | -    | 58,58,58,58                 | 0     |
| 25  | MG   | Z     | 157 | 1/1   | 0.30 | -    | 46,46,46,46                 | 0     |
| 25  | MG   | Z     | 419 | 1/1   | 0.54 | -    | 1,1,1,1                     | 1     |
| 25  | MG   | Z     | 125 | 1/1   | 0.12 | -    | 13,13,13,13                 | 0     |
| 25  | MG   | Z     | 98  | 1/1   | 0.12 | -    | 10,10,10,10                 | 0     |
| 25  | MG   | Z     | 155 | 1/1   | 0.22 | -    | 57,57,57,57                 | 0     |
| 25  | MG   | Z     | 365 | 1/1   | 0.23 | -    | 44,44,44,44                 | 1     |
| 25  | MG   | Z     | 218 | 1/1   | 0.14 | -    | 54,54,54,54                 | 0     |
| 25  | MG   | Z     | 123 | 1/1   | 0.16 | -    | 56,56,56,56                 | 0     |
| 25  | MG   | Z     | 82  | 1/1   | 0.26 | -    | 17,17,17,17                 | 0     |
| 25  | MG   | Z     | 79  | 1/1   | 0.12 | -    | 20,20,20,20                 | 0     |
| 25  | MG   | Z     | 402 | 1/1   | 0.25 | -    | 58,58,58,58                 | 0     |
| 25  | MG   | Z     | 115 | 1/1   | 0.17 | -    | 24,24,24,24                 | 0     |
| 25  | MG   | Z     | 478 | 1/1   | 0.25 | -    | 48,48,48,48                 | 0     |
| 25  | MG   | Z     | 12  | 1/1   | 0.07 | -    | 44,44,44,44                 | 0     |
| 25  | MG   | Z     | 55  | 1/1   | 0.10 | -    | 37,37,37,37                 | 0     |
| 25  | MG   | Z     | 220 | 1/1   | 0.34 | -    | 73,73,73,73                 | 0     |
| 25  | MG   | Z     | 180 | 1/1   | 0.15 | -    | 21,21,21,21                 | 0     |
| 25  | MG   | Z     | 321 | 1/1   | 0.19 | -    | 95,95,95,95                 | 0     |
| 25  | MG   | Z     | 103 | 1/1   | 0.10 | -    | 1,1,1,1                     | 0     |
| 25  | MG   | Z     | 326 | 1/1   | 0.98 | -    | 129,129,129,129             | 0     |
| 25  | MG   | Z     | 110 | 1/1   | 0.04 | -    | 19,19,19,19                 | 0     |
| 25  | MG   | Z     | 519 | 1/1   | 0.68 | -    | 88,88,88,88                 | 0     |
| 25  | MG   | Z     | 485 | 1/1   | 0.36 | -    | 53,53,53,53                 | 0     |
| 25  | MG   | Z     | 300 | 1/1   | 0.36 | -    | 34,34,34,34                 | 0     |
| 25  | MG   | Z     | 272 | 1/1   | 0.21 | -    | 27,27,27,27                 | 0     |
| 25  | MG   | Z     | 142 | 1/1   | 0.27 | -    | 46,46,46,46                 | 0     |
| 25  | MG   | Z     | 435 | 1/1   | 0.19 | -    | 17,17,17,17                 | 0     |
| 25  | MG   | Z     | 57  | 1/1   | 0.10 | -    | 16,16,16,16                 | 0     |
| 25  | MG   | Z     | 444 | 1/1   | 3.03 | -    | 51,51,51,51                 | 1     |

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| Mol | Type | Chain | Res | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 25  | MG   | Z     | 245 | 1/1   | 0.38 | -    | 38,38,38,38                 | 0     |
| 25  | MG   | Z     | 317 | 1/1   | 0.17 | -    | 57,57,57,57                 | 0     |
| 25  | MG   | Z     | 7   | 1/1   | 0.08 | -    | 8,8,8,8                     | 1     |
| 25  | MG   | Z     | 353 | 1/1   | 0.13 | -    | 43,43,43,43                 | 0     |
| 25  | MG   | Z     | 289 | 1/1   | 0.11 | -    | 11,11,11,11                 | 0     |
| 25  | MG   | Z     | 139 | 1/1   | 0.12 | -    | 84,84,84,84                 | 0     |
| 25  | MG   | Z     | 395 | 1/1   | 0.23 | -    | 58,58,58,58                 | 0     |
| 25  | MG   | Z     | 450 | 1/1   | 0.37 | -    | 78,78,78,78                 | 0     |
| 25  | MG   | Z     | 189 | 1/1   | 0.10 | -    | 12,12,12,12                 | 0     |
| 25  | MG   | Z     | 292 | 1/1   | 0.13 | -    | 45,45,45,45                 | 0     |
| 25  | MG   | Z     | 383 | 1/1   | 1.50 | -    | 11,11,11,11                 | 1     |
| 25  | MG   | Z     | 521 | 1/1   | 0.33 | -    | 22,22,22,22                 | 1     |
| 25  | MG   | Z     | 294 | 1/1   | 0.24 | -    | 39,39,39,39                 | 0     |
| 25  | MG   | Z     | 323 | 1/1   | 0.28 | -    | 59,59,59,59                 | 0     |
| 25  | MG   | Z     | 351 | 1/1   | 0.10 | -    | 40,40,40,40                 | 1     |
| 25  | MG   | Z     | 36  | 1/1   | 0.16 | -    | 51,51,51,51                 | 0     |
| 25  | MG   | Z     | 158 | 1/1   | 0.84 | -    | 59,59,59,59                 | 0     |
| 25  | MG   | Z     | 24  | 1/1   | 0.17 | -    | 65,65,65,65                 | 0     |
| 25  | MG   | Z     | 197 | 1/1   | 0.27 | -    | 31,31,31,31                 | 0     |
| 25  | MG   | Z     | 200 | 1/1   | 0.24 | -    | 46,46,46,46                 | 0     |
| 25  | MG   | Z     | 541 | 1/1   | 0.29 | -    | 74,74,74,74                 | 0     |
| 25  | MG   | Z     | 226 | 1/1   | 0.22 | -    | 20,20,20,20                 | 1     |
| 25  | MG   | Z     | 403 | 1/1   | 0.15 | -    | 31,31,31,31                 | 0     |
| 25  | MG   | Z     | 287 | 1/1   | 0.29 | -    | 51,51,51,51                 | 0     |
| 25  | MG   | Z     | 132 | 1/1   | 0.27 | -    | 43,43,43,43                 | 0     |
| 25  | MG   | Z     | 71  | 1/1   | 0.19 | -    | 34,34,34,34                 | 0     |
| 25  | MG   | Z     | 501 | 1/1   | 0.35 | -    | 61,61,61,61                 | 0     |
| 25  | MG   | Z     | 258 | 1/1   | 0.37 | -    | 43,43,43,43                 | 0     |
| 25  | MG   | Z     | 306 | 1/1   | 0.45 | -    | 41,41,41,41                 | 0     |
| 25  | MG   | Z     | 68  | 1/1   | 0.05 | -    | 1,1,1,1                     | 0     |
| 25  | MG   | Z     | 462 | 1/1   | 0.13 | -    | 51,51,51,51                 | 0     |
| 25  | MG   | Z     | 331 | 1/1   | 0.18 | -    | 29,29,29,29                 | 0     |
| 25  | MG   | Z     | 27  | 1/1   | 0.16 | -    | 26,26,26,26                 | 0     |
| 25  | MG   | Z     | 255 | 1/1   | 0.16 | -    | 27,27,27,27                 | 0     |
| 25  | MG   | Z     | 301 | 1/1   | 0.13 | -    | 35,35,35,35                 | 0     |
| 25  | MG   | Z     | 20  | 1/1   | 0.33 | -    | 60,60,60,60                 | 0     |
| 25  | MG   | Z     | 484 | 1/1   | 0.08 | -    | 30,30,30,30                 | 0     |
| 25  | MG   | Z     | 242 | 1/1   | 0.42 | -    | 13,13,13,13                 | 1     |
| 25  | MG   | Z     | 441 | 1/1   | 0.32 | -    | 13,13,13,13                 | 1     |
| 25  | MG   | Z     | 217 | 1/1   | 0.11 | -    | 57,57,57,57                 | 0     |
| 25  | MG   | Z     | 153 | 1/1   | 0.79 | -    | 83,83,83,83                 | 0     |
| 25  | MG   | Z     | 279 | 1/1   | 0.19 | -    | 25,25,25,25                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 25  | MG   | Z     | 410 | 1/1   | 0.06 | -    | 27,27,27,27                 | 0     |
| 25  | MG   | Z     | 539 | 1/1   | 0.06 | -    | 21,21,21,21                 | 0     |
| 25  | MG   | Z     | 169 | 1/1   | 0.24 | -    | 46,46,46,46                 | 1     |
| 25  | MG   | Z     | 524 | 1/1   | 0.65 | -    | 89,89,89,89                 | 0     |
| 25  | MG   | Z     | 122 | 1/1   | 0.05 | -    | 16,16,16,16                 | 0     |
| 25  | MG   | Z     | 199 | 1/1   | 0.14 | -    | 6,6,6,6                     | 1     |
| 25  | MG   | Z     | 17  | 1/1   | 0.04 | -    | 10,10,10,10                 | 0     |
| 25  | MG   | Z     | 161 | 1/1   | 0.09 | -    | 33,33,33,33                 | 0     |
| 25  | MG   | Z     | 192 | 1/1   | 0.08 | -    | 1,1,1,1                     | 0     |
| 25  | MG   | Z     | 124 | 1/1   | 0.15 | -    | 11,11,11,11                 | 0     |
| 25  | MG   | Z     | 187 | 1/1   | 0.35 | -    | 15,15,15,15                 | 0     |
| 25  | MG   | Z     | 434 | 1/1   | 0.42 | -    | 61,61,61,61                 | 0     |
| 25  | MG   | Z     | 345 | 1/1   | 0.22 | -    | 27,27,27,27                 | 0     |
| 25  | MG   | Z     | 531 | 1/1   | 0.05 | -    | 42,42,42,42                 | 0     |
| 25  | MG   | Z     | 19  | 1/1   | 0.06 | -    | 15,15,15,15                 | 0     |
| 25  | MG   | Z     | 540 | 1/1   | 0.38 | -    | 68,68,68,68                 | 0     |
| 25  | MG   | Z     | 178 | 1/1   | 0.11 | -    | 21,21,21,21                 | 1     |
| 25  | MG   | Z     | 106 | 1/1   | 0.39 | -    | 65,65,65,65                 | 0     |
| 25  | MG   | Z     | 527 | 1/1   | 0.11 | -    | 61,61,61,61                 | 0     |
| 25  | MG   | Z     | 140 | 1/1   | 0.80 | -    | 72,72,72,72                 | 0     |
| 25  | MG   | Z     | 363 | 1/1   | 0.18 | -    | 50,50,50,50                 | 0     |
| 25  | MG   | Z     | 296 | 1/1   | 0.07 | -    | 44,44,44,44                 | 0     |
| 25  | MG   | Z     | 360 | 1/1   | 0.59 | -    | 94,94,94,94                 | 0     |
| 25  | MG   | Z     | 100 | 1/1   | 0.09 | -    | 13,13,13,13                 | 0     |
| 25  | MG   | Z     | 114 | 1/1   | 0.07 | -    | 15,15,15,15                 | 0     |
| 25  | MG   | Z     | 209 | 1/1   | 0.26 | -    | 40,40,40,40                 | 0     |
| 25  | MG   | Z     | 475 | 1/1   | 0.05 | -    | 38,38,38,38                 | 0     |
| 25  | MG   | Z     | 149 | 1/1   | 0.17 | -    | 52,52,52,52                 | 0     |
| 25  | MG   | Z     | 303 | 1/1   | 0.31 | -    | 32,32,32,32                 | 0     |
| 25  | MG   | Z     | 254 | 1/1   | 0.35 | -    | 43,43,43,43                 | 0     |
| 25  | MG   | Z     | 77  | 1/1   | 0.10 | -    | 39,39,39,39                 | 0     |
| 25  | MG   | Z     | 551 | 1/1   | 0.35 | -    | 1,1,1,1                     | 1     |
| 25  | MG   | Z     | 324 | 1/1   | 0.17 | -    | 17,17,17,17                 | 0     |
| 25  | MG   | Z     | 416 | 1/1   | 0.12 | -    | 30,30,30,30                 | 0     |
| 25  | MG   | Z     | 421 | 1/1   | 0.27 | -    | 28,28,28,28                 | 1     |
| 25  | MG   | Z     | 41  | 1/1   | 0.07 | -    | 51,51,51,51                 | 0     |
| 25  | MG   | Z     | 182 | 1/1   | 0.18 | -    | 18,18,18,18                 | 0     |
| 25  | MG   | Z     | 244 | 1/1   | 0.09 | -    | 33,33,33,33                 | 0     |
| 25  | MG   | Z     | 316 | 1/1   | 0.26 | -    | 46,46,46,46                 | 0     |
| 25  | MG   | Z     | 21  | 1/1   | 0.43 | -    | 54,54,54,54                 | 0     |
| 25  | MG   | Z     | 146 | 1/1   | 0.27 | -    | 48,48,48,48                 | 0     |
| 25  | MG   | Z     | 185 | 1/1   | 0.41 | -    | 111,111,111,111             | 0     |

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| Mol | Type | Chain | Res | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 25  | MG   | Z     | 482 | 1/1   | 0.30 | -    | 47,47,47,47                 | 0     |
| 25  | MG   | Z     | 97  | 1/1   | 0.21 | -    | 26,26,26,26                 | 0     |
| 25  | MG   | Z     | 141 | 1/1   | 0.23 | -    | 22,22,22,22                 | 0     |
| 25  | MG   | Z     | 447 | 1/1   | 0.20 | -    | 37,37,37,37                 | 1     |
| 25  | MG   | Z     | 38  | 1/1   | 0.23 | -    | 52,52,52,52                 | 0     |
| 25  | MG   | Z     | 526 | 1/1   | 0.58 | -    | 36,36,36,36                 | 1     |
| 25  | MG   | Z     | 194 | 1/1   | 0.17 | -    | 35,35,35,35                 | 0     |
| 25  | MG   | Z     | 95  | 1/1   | 0.07 | -    | 22,22,22,22                 | 0     |
| 25  | MG   | Z     | 511 | 1/1   | 0.19 | -    | 84,84,84,84                 | 0     |
| 25  | MG   | Z     | 30  | 1/1   | 0.29 | -    | 38,38,38,38                 | 0     |
| 25  | MG   | Z     | 414 | 1/1   | 0.23 | -    | 30,30,30,30                 | 0     |
| 25  | MG   | Z     | 166 | 1/1   | 0.20 | -    | 15,15,15,15                 | 0     |
| 25  | MG   | Z     | 28  | 1/1   | 0.55 | -    | 65,65,65,65                 | 0     |
| 25  | MG   | Z     | 286 | 1/1   | 0.19 | -    | 53,53,53,53                 | 0     |
| 25  | MG   | Z     | 396 | 1/1   | 0.26 | -    | 51,51,51,51                 | 0     |
| 25  | MG   | Z     | 491 | 1/1   | 0.94 | -    | 72,72,72,72                 | 1     |
| 25  | MG   | Z     | 227 | 1/1   | 0.78 | -    | 84,84,84,84                 | 0     |
| 25  | MG   | Z     | 507 | 1/1   | 0.29 | -    | 65,65,65,65                 | 0     |
| 25  | MG   | Z     | 64  | 1/1   | 0.21 | -    | 20,20,20,20                 | 0     |
| 25  | MG   | Z     | 342 | 1/1   | 0.14 | -    | 56,56,56,56                 | 0     |
| 25  | MG   | Z     | 208 | 1/1   | 0.20 | -    | 15,15,15,15                 | 0     |
| 25  | MG   | Z     | 488 | 1/1   | 0.24 | -    | 69,69,69,69                 | 0     |
| 25  | MG   | Z     | 459 | 1/1   | 0.05 | -    | 14,14,14,14                 | 0     |
| 25  | MG   | Z     | 534 | 1/1   | 0.21 | -    | 18,18,18,18                 | 1     |
| 25  | MG   | Z     | 319 | 1/1   | 0.17 | -    | 26,26,26,26                 | 0     |
| 25  | MG   | Z     | 266 | 1/1   | 0.35 | -    | 26,26,26,26                 | 0     |
| 25  | MG   | Z     | 1   | 1/1   | 0.28 | -    | 59,59,59,59                 | 0     |
| 25  | MG   | Z     | 236 | 1/1   | 0.06 | -    | 6,6,6,6                     | 0     |
| 25  | MG   | Z     | 313 | 1/1   | 0.16 | -    | 37,37,37,37                 | 0     |
| 25  | MG   | Z     | 538 | 1/1   | 0.14 | -    | 43,43,43,43                 | 0     |
| 25  | MG   | Z     | 47  | 1/1   | 0.16 | -    | 69,69,69,69                 | 0     |
| 25  | MG   | Z     | 422 | 1/1   | 0.18 | -    | 57,57,57,57                 | 0     |
| 25  | MG   | Z     | 260 | 1/1   | 0.26 | -    | 25,25,25,25                 | 0     |
| 25  | MG   | Z     | 552 | 1/1   | 0.36 | -    | 97,97,97,97                 | 1     |
| 25  | MG   | Z     | 13  | 1/1   | 0.35 | -    | 58,58,58,58                 | 0     |
| 25  | MG   | Z     | 297 | 1/1   | 0.08 | -    | 7,7,7,7                     | 0     |
| 25  | MG   | Z     | 168 | 1/1   | 0.28 | -    | 64,64,64,64                 | 0     |
| 25  | MG   | Z     | 270 | 1/1   | 0.20 | -    | 44,44,44,44                 | 0     |
| 25  | MG   | Z     | 461 | 1/1   | 0.22 | -    | 61,61,61,61                 | 0     |
| 25  | MG   | Z     | 96  | 1/1   | 0.17 | -    | 23,23,23,23                 | 0     |
| 25  | MG   | Z     | 59  | 1/1   | 0.13 | -    | 16,16,16,16                 | 0     |
| 25  | MG   | Z     | 338 | 1/1   | 0.30 | -    | 34,34,34,34                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 25  | MG   | Z     | 275 | 1/1   | 0.14 | -    | 29,29,29,29                 | 0     |
| 25  | MG   | Z     | 443 | 1/1   | 0.45 | -    | 42,42,42,42                 | 1     |
| 25  | MG   | Z     | 361 | 1/1   | 0.29 | -    | 62,62,62,62                 | 0     |
| 25  | MG   | Z     | 88  | 1/1   | 0.11 | -    | 20,20,20,20                 | 0     |
| 25  | MG   | Z     | 205 | 1/1   | 0.45 | -    | 44,44,44,44                 | 0     |
| 25  | MG   | Z     | 512 | 1/1   | 0.25 | -    | 67,67,67,67                 | 0     |
| 25  | MG   | Z     | 151 | 1/1   | 0.42 | -    | 69,69,69,69                 | 0     |
| 25  | MG   | Z     | 118 | 1/1   | 0.13 | -    | 9,9,9,9                     | 0     |
| 25  | MG   | Z     | 238 | 1/1   | 0.39 | -    | 46,46,46,46                 | 0     |
| 25  | MG   | Z     | 411 | 1/1   | 0.07 | -    | 27,27,27,27                 | 0     |
| 25  | MG   | Z     | 380 | 1/1   | 0.24 | -    | 50,50,50,50                 | 1     |
| 25  | MG   | Z     | 378 | 1/1   | 0.33 | -    | 96,96,96,96                 | 0     |
| 25  | MG   | Z     | 368 | 1/1   | 0.26 | -    | 74,74,74,74                 | 0     |
| 25  | MG   | Z     | 85  | 1/1   | 0.28 | -    | 62,62,62,62                 | 0     |
| 25  | MG   | Z     | 167 | 1/1   | 0.42 | -    | 35,35,35,35                 | 1     |
| 25  | MG   | Z     | 468 | 1/1   | 0.26 | -    | 33,33,33,33                 | 1     |
| 25  | MG   | Z     | 127 | 1/1   | 0.07 | -    | 18,18,18,18                 | 0     |
| 25  | MG   | Z     | 433 | 1/1   | 0.11 | -    | 28,28,28,28                 | 0     |
| 25  | MG   | Z     | 476 | 1/1   | 0.18 | -    | 45,45,45,45                 | 0     |
| 25  | MG   | Z     | 240 | 1/1   | 0.11 | -    | 18,18,18,18                 | 0     |
| 25  | MG   | Z     | 344 | 1/1   | 0.19 | -    | 41,41,41,41                 | 0     |
| 25  | MG   | Z     | 431 | 1/1   | 0.54 | -    | 48,48,48,48                 | 0     |
| 25  | MG   | Z     | 75  | 1/1   | 0.25 | -    | 32,32,32,32                 | 0     |
| 25  | MG   | Z     | 212 | 1/1   | 0.80 | -    | 73,73,73,73                 | 0     |
| 25  | MG   | Z     | 505 | 1/1   | 0.17 | -    | 21,21,21,21                 | 1     |
| 25  | MG   | Z     | 193 | 1/1   | 0.05 | -    | 12,12,12,12                 | 0     |
| 25  | MG   | Z     | 343 | 1/1   | 0.06 | -    | 42,42,42,42                 | 0     |
| 25  | MG   | Z     | 375 | 1/1   | 0.32 | -    | 47,47,47,47                 | 0     |
| 25  | MG   | Z     | 107 | 1/1   | 0.19 | -    | 14,14,14,14                 | 0     |
| 25  | MG   | Z     | 73  | 1/1   | 0.13 | -    | 32,32,32,32                 | 0     |
| 25  | MG   | Z     | 373 | 1/1   | 0.29 | -    | 43,43,43,43                 | 0     |
| 25  | MG   | Z     | 474 | 1/1   | 0.35 | -    | 1,1,1,1                     | 1     |
| 25  | MG   | Z     | 78  | 1/1   | 0.09 | -    | 7,7,7,7                     | 0     |
| 25  | MG   | Z     | 237 | 1/1   | 0.10 | -    | 56,56,56,56                 | 0     |
| 25  | MG   | Z     | 154 | 1/1   | 0.17 | -    | 49,49,49,49                 | 0     |
| 25  | MG   | Z     | 112 | 1/1   | 0.15 | -    | 18,18,18,18                 | 0     |
| 25  | MG   | Z     | 90  | 1/1   | 0.11 | -    | 15,15,15,15                 | 0     |
| 25  | MG   | Z     | 546 | 1/1   | 0.59 | -    | 1,1,1,1                     | 1     |
| 25  | MG   | Z     | 269 | 1/1   | 0.06 | -    | 18,18,18,18                 | 0     |
| 25  | MG   | Z     | 305 | 1/1   | 0.22 | -    | 102,102,102,102             | 0     |
| 25  | MG   | Z     | 54  | 1/1   | 0.20 | -    | 51,51,51,51                 | 0     |
| 25  | MG   | Z     | 445 | 1/1   | 0.19 | -    | 15,15,15,15                 | 1     |

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| Mol | Type | Chain | Res | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 25  | MG   | Z     | 14  | 1/1   | 0.07 | -    | 4,4,4,4                     | 0     |
| 25  | MG   | Z     | 172 | 1/1   | 0.19 | -    | 60,60,60,60                 | 0     |
| 25  | MG   | Z     | 137 | 1/1   | 0.10 | -    | 37,37,37,37                 | 0     |
| 25  | MG   | Z     | 99  | 1/1   | 0.09 | -    | 23,23,23,23                 | 0     |
| 25  | MG   | Z     | 211 | 1/1   | 0.25 | -    | 14,14,14,14                 | 1     |
| 25  | MG   | Z     | 454 | 1/1   | 0.07 | -    | 1,1,1,1                     | 0     |
| 25  | MG   | Z     | 442 | 1/1   | 0.36 | -    | 34,34,34,34                 | 0     |
| 25  | MG   | Z     | 11  | 1/1   | 0.39 | -    | 52,52,52,52                 | 0     |
| 25  | MG   | Z     | 387 | 1/1   | 0.08 | -    | 38,38,38,38                 | 0     |
| 25  | MG   | Z     | 281 | 1/1   | 0.07 | -    | 3,3,3,3                     | 0     |
| 25  | MG   | Z     | 83  | 1/1   | 0.06 | -    | 12,12,12,12                 | 0     |
| 25  | MG   | Z     | 533 | 1/1   | 0.14 | -    | 18,18,18,18                 | 0     |
| 25  | MG   | Z     | 290 | 1/1   | 0.17 | -    | 26,26,26,26                 | 0     |
| 25  | MG   | Z     | 121 | 1/1   | 0.17 | -    | 32,32,32,32                 | 0     |
| 26  | ZN   | Z     | 549 | 1/1   | 0.04 | -    | 59,59,59,59                 | 0     |
| 25  | MG   | Z     | 261 | 1/1   | 0.24 | -    | 38,38,38,38                 | 0     |
| 25  | MG   | Z     | 329 | 1/1   | 0.56 | -    | 44,44,44,44                 | 0     |
| 25  | MG   | Z     | 333 | 1/1   | 0.14 | -    | 51,51,51,51                 | 0     |
| 25  | MG   | Z     | 369 | 1/1   | 0.72 | -    | 69,69,69,69                 | 0     |
| 25  | MG   | Z     | 222 | 1/1   | 0.16 | -    | 37,37,37,37                 | 1     |
| 25  | MG   | Z     | 234 | 1/1   | 0.13 | -    | 18,18,18,18                 | 0     |
| 25  | MG   | Z     | 267 | 1/1   | 0.06 | -    | 37,37,37,37                 | 0     |
| 25  | MG   | Z     | 310 | 1/1   | 0.16 | -    | 18,18,18,18                 | 0     |
| 25  | MG   | Z     | 513 | 1/1   | 1.11 | -    | 68,68,68,68                 | 1     |
| 25  | MG   | Z     | 406 | 1/1   | 0.19 | -    | 33,33,33,33                 | 0     |
| 25  | MG   | Z     | 298 | 1/1   | 0.06 | -    | 21,21,21,21                 | 0     |
| 25  | MG   | Z     | 67  | 1/1   | 0.31 | -    | 21,21,21,21                 | 0     |
| 25  | MG   | Z     | 249 | 1/1   | 0.28 | -    | 57,57,57,57                 | 0     |
| 25  | MG   | Z     | 207 | 1/1   | 0.09 | -    | 16,16,16,16                 | 0     |
| 25  | MG   | Z     | 424 | 1/1   | 0.15 | -    | 40,40,40,40                 | 0     |
| 25  | MG   | Z     | 371 | 1/1   | 0.56 | -    | 45,45,45,45                 | 1     |
| 25  | MG   | Z     | 449 | 1/1   | 0.23 | -    | 44,44,44,44                 | 0     |
| 25  | MG   | Z     | 486 | 1/1   | 0.21 | -    | 33,33,33,33                 | 1     |
| 25  | MG   | Z     | 427 | 1/1   | 0.85 | -    | 59,59,59,59                 | 0     |
| 25  | MG   | Z     | 239 | 1/1   | 0.21 | -    | 45,45,45,45                 | 0     |
| 25  | MG   | Z     | 357 | 1/1   | 0.13 | -    | 120,120,120,120             | 0     |
| 25  | MG   | Z     | 271 | 1/1   | 0.07 | -    | 1,1,1,1                     | 0     |
| 25  | MG   | Z     | 126 | 1/1   | 0.06 | -    | 5,5,5,5                     | 0     |
| 25  | MG   | Z     | 32  | 1/1   | 0.14 | -    | 48,48,48,48                 | 0     |
| 25  | MG   | Z     | 399 | 1/1   | 0.18 | -    | 13,13,13,13                 | 0     |
| 25  | MG   | Z     | 463 | 1/1   | 0.54 | -    | 75,75,75,75                 | 0     |
| 25  | MG   | Z     | 285 | 1/1   | 0.09 | -    | 7,7,7,7                     | 0     |

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| Mol | Type | Chain | Res | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 25  | MG   | Z     | 116 | 1/1   | 0.10 | -    | 26,26,26,26                 | 0     |
| 25  | MG   | Z     | 388 | 1/1   | 0.23 | -    | 28,28,28,28                 | 0     |
| 25  | MG   | Z     | 367 | 1/1   | 0.56 | -    | 93,93,93,93                 | 1     |
| 25  | MG   | Z     | 111 | 1/1   | 0.08 | -    | 11,11,11,11                 | 0     |
| 25  | MG   | Z     | 440 | 1/1   | 0.13 | -    | 33,33,33,33                 | 0     |
| 25  | MG   | Z     | 283 | 1/1   | 0.22 | -    | 46,46,46,46                 | 0     |
| 25  | MG   | Z     | 535 | 1/1   | 0.12 | -    | 37,37,37,37                 | 0     |
| 25  | MG   | Z     | 490 | 1/1   | 0.14 | -    | 50,50,50,50                 | 0     |
| 25  | MG   | Z     | 354 | 1/1   | 0.07 | -    | 57,57,57,57                 | 0     |
| 25  | MG   | Z     | 430 | 1/1   | 0.07 | -    | 1,1,1,1                     | 0     |
| 25  | MG   | Z     | 72  | 1/1   | 0.44 | -    | 52,52,52,52                 | 0     |
| 25  | MG   | Z     | 16  | 1/1   | 0.10 | -    | 35,35,35,35                 | 0     |
| 25  | MG   | Z     | 381 | 1/1   | 0.30 | -    | 69,69,69,69                 | 0     |
| 25  | MG   | Z     | 358 | 1/1   | 0.12 | -    | 40,40,40,40                 | 0     |
| 25  | MG   | Z     | 108 | 1/1   | 0.14 | -    | 13,13,13,13                 | 0     |
| 25  | MG   | Z     | 282 | 1/1   | 0.06 | -    | 12,12,12,12                 | 0     |
| 25  | MG   | Z     | 201 | 1/1   | 0.10 | -    | 33,33,33,33                 | 0     |
| 25  | MG   | Z     | 509 | 1/1   | 0.05 | -    | 69,69,69,69                 | 0     |
| 25  | MG   | Z     | 336 | 1/1   | 0.17 | -    | 32,32,32,32                 | 0     |
| 25  | MG   | Z     | 206 | 1/1   | 0.04 | -    | 7,7,7,7                     | 0     |
| 25  | MG   | Z     | 428 | 1/1   | 0.17 | -    | 41,41,41,41                 | 0     |
| 25  | MG   | Z     | 105 | 1/1   | 0.07 | -    | 18,18,18,18                 | 0     |
| 25  | MG   | Z     | 81  | 1/1   | 0.07 | -    | 27,27,27,27                 | 0     |
| 25  | MG   | Z     | 309 | 1/1   | 0.10 | -    | 14,14,14,14                 | 0     |
| 25  | MG   | Z     | 499 | 1/1   | 0.16 | -    | 34,34,34,34                 | 0     |
| 25  | MG   | Z     | 500 | 1/1   | 0.41 | -    | 32,32,32,32                 | 1     |
| 25  | MG   | Z     | 537 | 1/1   | 0.20 | -    | 46,46,46,46                 | 0     |
| 25  | MG   | Z     | 225 | 1/1   | 0.15 | -    | 58,58,58,58                 | 0     |
| 25  | MG   | Z     | 145 | 1/1   | 0.07 | -    | 44,44,44,44                 | 0     |
| 25  | MG   | Z     | 243 | 1/1   | 0.15 | -    | 28,28,28,28                 | 0     |
| 25  | MG   | Z     | 148 | 1/1   | 0.11 | -    | 29,29,29,29                 | 0     |
| 25  | MG   | Z     | 413 | 1/1   | 0.19 | -    | 9,9,9,9                     | 0     |
| 25  | MG   | Z     | 25  | 1/1   | 0.34 | -    | 58,58,58,58                 | 0     |
| 25  | MG   | Z     | 362 | 1/1   | 0.88 | -    | 50,50,50,50                 | 1     |
| 25  | MG   | Z     | 91  | 1/1   | 0.07 | -    | 13,13,13,13                 | 0     |
| 25  | MG   | Z     | 352 | 1/1   | 0.51 | -    | 37,37,37,37                 | 0     |
| 25  | MG   | Z     | 401 | 1/1   | 0.29 | -    | 35,35,35,35                 | 0     |
| 25  | MG   | Z     | 40  | 1/1   | 0.24 | -    | 75,75,75,75                 | 0     |
| 25  | MG   | Z     | 86  | 1/1   | 0.15 | -    | 34,34,34,34                 | 0     |
| 25  | MG   | Z     | 293 | 1/1   | 0.26 | -    | 46,46,46,46                 | 0     |
| 25  | MG   | Z     | 322 | 1/1   | 0.56 | -    | 69,69,69,69                 | 0     |
| 25  | MG   | Z     | 135 | 1/1   | 0.20 | -    | 64,64,64,64                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 25  | MG   | Z     | 330 | 1/1   | 0.06 | -    | 29,29,29,29                 | 0     |
| 25  | MG   | Z     | 291 | 1/1   | 0.53 | -    | 42,42,42,42                 | 0     |
| 25  | MG   | Z     | 10  | 1/1   | 0.16 | -    | 21,21,21,21                 | 0     |
| 25  | MG   | Z     | 370 | 1/1   | 1.53 | -    | 74,74,74,74                 | 1     |
| 25  | MG   | Z     | 481 | 1/1   | 0.07 | -    | 32,32,32,32                 | 0     |
| 25  | MG   | Z     | 4   | 1/1   | 0.41 | -    | 39,39,39,39                 | 1     |
| 25  | MG   | Z     | 393 | 1/1   | 0.50 | -    | 68,68,68,68                 | 0     |
| 25  | MG   | Z     | 183 | 1/1   | 0.12 | -    | 11,11,11,11                 | 0     |
| 25  | MG   | Z     | 334 | 1/1   | 0.84 | -    | 63,63,63,63                 | 0     |
| 25  | MG   | Z     | 174 | 1/1   | 0.14 | -    | 58,58,58,58                 | 0     |
| 25  | MG   | Z     | 134 | 1/1   | 0.32 | -    | 10,10,10,10                 | 1     |
| 25  | MG   | Z     | 483 | 1/1   | 0.09 | -    | 23,23,23,23                 | 0     |
| 25  | MG   | Z     | 52  | 1/1   | 0.91 | -    | 77,77,77,77                 | 0     |
| 25  | MG   | Z     | 144 | 1/1   | 0.21 | -    | 71,71,71,71                 | 0     |
| 25  | MG   | Z     | 389 | 1/1   | 0.09 | -    | 45,45,45,45                 | 0     |
| 25  | MG   | Z     | 5   | 1/1   | 0.13 | -    | 35,35,35,35                 | 0     |
| 25  | MG   | Z     | 259 | 1/1   | 0.24 | -    | 48,48,48,48                 | 0     |
| 25  | MG   | Z     | 426 | 1/1   | 0.12 | -    | 54,54,54,54                 | 0     |
| 25  | MG   | Z     | 496 | 1/1   | 0.52 | -    | 15,15,15,15                 | 1     |
| 25  | MG   | Z     | 497 | 1/1   | 1.83 | -    | 94,94,94,94                 | 1     |
| 25  | MG   | Z     | 48  | 1/1   | 0.21 | -    | 35,35,35,35                 | 0     |
| 25  | MG   | Z     | 532 | 1/1   | 1.02 | -    | 24,24,24,24                 | 1     |
| 25  | MG   | Z     | 188 | 1/1   | 0.17 | -    | 6,6,6,6                     | 0     |
| 25  | MG   | Z     | 415 | 1/1   | 0.07 | -    | 7,7,7,7                     | 0     |
| 25  | MG   | Z     | 191 | 1/1   | 0.07 | -    | 16,16,16,16                 | 0     |
| 25  | MG   | Z     | 43  | 1/1   | 0.12 | -    | 55,55,55,55                 | 0     |
| 25  | MG   | Z     | 224 | 1/1   | 0.90 | -    | 17,17,17,17                 | 1     |
| 25  | MG   | Z     | 264 | 1/1   | 0.27 | -    | 50,50,50,50                 | 0     |
| 25  | MG   | Z     | 150 | 1/1   | 0.15 | -    | 53,53,53,53                 | 0     |
| 25  | MG   | Z     | 173 | 1/1   | 0.43 | -    | 67,67,67,67                 | 0     |
| 25  | MG   | Z     | 210 | 1/1   | 0.12 | -    | 9,9,9,9                     | 0     |
| 25  | MG   | Z     | 514 | 1/1   | 0.19 | -    | 52,52,52,52                 | 1     |
| 25  | MG   | Z     | 9   | 1/1   | 0.07 | -    | 25,25,25,25                 | 0     |
| 25  | MG   | Z     | 495 | 1/1   | 0.31 | -    | 59,59,59,59                 | 0     |
| 25  | MG   | Z     | 45  | 1/1   | 0.15 | -    | 24,24,24,24                 | 0     |
| 25  | MG   | Z     | 359 | 1/1   | 0.35 | -    | 67,67,67,67                 | 0     |
| 25  | MG   | Z     | 385 | 1/1   | 0.27 | -    | 27,27,27,27                 | 1     |
| 25  | MG   | Z     | 407 | 1/1   | 0.15 | -    | 32,32,32,32                 | 0     |
| 25  | MG   | Z     | 152 | 1/1   | 0.15 | -    | 69,69,69,69                 | 0     |
| 25  | MG   | Z     | 113 | 1/1   | 0.11 | -    | 20,20,20,20                 | 0     |
| 25  | MG   | Z     | 516 | 1/1   | 0.98 | -    | 26,26,26,26                 | 1     |
| 25  | MG   | Z     | 400 | 1/1   | 0.37 | -    | 49,49,49,49                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 25  | MG   | Z     | 418 | 1/1   | 0.12 | -    | 19,19,19,19                 | 0     |
| 25  | MG   | Z     | 109 | 1/1   | 0.09 | -    | 6,6,6,6                     | 0     |
| 25  | MG   | Z     | 248 | 1/1   | 0.11 | -    | 23,23,23,23                 | 0     |
| 25  | MG   | Z     | 177 | 1/1   | 0.42 | -    | 50,50,50,50                 | 0     |
| 25  | MG   | Z     | 437 | 1/1   | 0.12 | -    | 49,49,49,49                 | 0     |
| 25  | MG   | Z     | 60  | 1/1   | 0.14 | -    | 17,17,17,17                 | 0     |
| 25  | MG   | Z     | 33  | 1/1   | 0.11 | -    | 19,19,19,19                 | 0     |
| 25  | MG   | Z     | 320 | 1/1   | 0.36 | -    | 47,47,47,47                 | 0     |
| 25  | MG   | Z     | 277 | 1/1   | 0.05 | -    | 18,18,18,18                 | 0     |
| 25  | MG   | Z     | 311 | 1/1   | 0.10 | -    | 29,29,29,29                 | 0     |
| 25  | MG   | Z     | 347 | 1/1   | 0.28 | -    | 47,47,47,47                 | 0     |
| 25  | MG   | Z     | 284 | 1/1   | 0.23 | -    | 59,59,59,59                 | 0     |
| 25  | MG   | Z     | 409 | 1/1   | 0.23 | -    | 58,58,58,58                 | 1     |
| 25  | MG   | Z     | 65  | 1/1   | 0.08 | -    | 10,10,10,10                 | 0     |
| 25  | MG   | Z     | 489 | 1/1   | 0.71 | -    | 70,70,70,70                 | 0     |
| 25  | MG   | Z     | 446 | 1/1   | 0.57 | -    | 72,72,72,72                 | 0     |
| 25  | MG   | Z     | 465 | 1/1   | 0.31 | -    | 74,74,74,74                 | 0     |
| 25  | MG   | Z     | 257 | 1/1   | 0.18 | -    | 7,7,7,7                     | 0     |
| 25  | MG   | Z     | 8   | 1/1   | 0.11 | -    | 51,51,51,51                 | 0     |
| 25  | MG   | Z     | 84  | 1/1   | 0.11 | -    | 2,2,2,2                     | 0     |
| 25  | MG   | Z     | 328 | 1/1   | 0.15 | -    | 7,7,7,7                     | 0     |
| 25  | MG   | Z     | 184 | 1/1   | 0.13 | -    | 9,9,9,9                     | 0     |
| 25  | MG   | Z     | 355 | 1/1   | 0.16 | -    | 2,2,2,2                     | 1     |
| 25  | MG   | Z     | 143 | 1/1   | 0.14 | -    | 40,40,40,40                 | 0     |
| 25  | MG   | Z     | 377 | 1/1   | 0.30 | -    | 58,58,58,58                 | 0     |
| 25  | MG   | Z     | 262 | 1/1   | 0.99 | -    | 94,94,94,94                 | 0     |
| 25  | MG   | Z     | 215 | 1/1   | 0.50 | -    | 20,20,20,20                 | 1     |
| 25  | MG   | Z     | 179 | 1/1   | 0.16 | -    | 53,53,53,53                 | 0     |
| 25  | MG   | Z     | 159 | 1/1   | 0.28 | -    | 57,57,57,57                 | 0     |
| 25  | MG   | Z     | 456 | 1/1   | 0.35 | -    | 18,18,18,18                 | 1     |
| 25  | MG   | Z     | 432 | 1/1   | 0.10 | -    | 41,41,41,41                 | 0     |
| 25  | MG   | Z     | 94  | 1/1   | 0.23 | -    | 50,50,50,50                 | 0     |
| 25  | MG   | Z     | 314 | 1/1   | 0.35 | -    | 37,37,37,37                 | 0     |
| 25  | MG   | Z     | 104 | 1/1   | 0.11 | -    | 17,17,17,17                 | 0     |
| 25  | MG   | Z     | 543 | 1/1   | 0.16 | -    | 30,30,30,30                 | 0     |
| 25  | MG   | Z     | 346 | 1/1   | 0.14 | -    | 37,37,37,37                 | 1     |
| 25  | MG   | Z     | 35  | 1/1   | 0.15 | -    | 53,53,53,53                 | 0     |
| 25  | MG   | Z     | 337 | 1/1   | 0.14 | -    | 44,44,44,44                 | 0     |
| 25  | MG   | Z     | 529 | 1/1   | 0.04 | -    | 43,43,43,43                 | 0     |
| 26  | ZN   | Z     | 547 | 1/1   | 0.13 | -    | 80,80,80,80                 | 0     |
| 25  | MG   | Z     | 520 | 1/1   | 0.19 | -    | 48,48,48,48                 | 0     |
| 25  | MG   | Z     | 56  | 1/1   | 0.06 | -    | 9,9,9,9                     | 0     |

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| Mol | Type | Chain | Res | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 25  | MG   | Z     | 390 | 1/1   | 0.16 | -    | 44,44,44,44                 | 0     |
| 25  | MG   | Z     | 472 | 1/1   | 0.28 | -    | 56,56,56,56                 | 0     |
| 25  | MG   | Z     | 392 | 1/1   | 0.64 | -    | 27,27,27,27                 | 1     |
| 25  | MG   | Z     | 42  | 1/1   | 0.14 | -    | 49,49,49,49                 | 0     |
| 25  | MG   | Z     | 265 | 1/1   | 0.14 | -    | 31,31,31,31                 | 0     |
| 25  | MG   | Z     | 460 | 1/1   | 0.33 | -    | 41,41,41,41                 | 0     |
| 25  | MG   | Z     | 348 | 1/1   | 0.69 | -    | 53,53,53,53                 | 0     |
| 25  | MG   | Z     | 273 | 1/1   | 0.15 | -    | 44,44,44,44                 | 0     |
| 25  | MG   | Z     | 231 | 1/1   | 0.39 | -    | 62,62,62,62                 | 0     |
| 25  | MG   | Z     | 420 | 1/1   | 0.42 | -    | 69,69,69,69                 | 0     |
| 25  | MG   | Z     | 274 | 1/1   | 0.18 | -    | 45,45,45,45                 | 0     |
| 25  | MG   | Z     | 46  | 1/1   | 0.40 | -    | 88,88,88,88                 | 0     |
| 25  | MG   | Z     | 228 | 1/1   | 0.34 | -    | 58,58,58,58                 | 0     |
| 25  | MG   | Z     | 467 | 1/1   | 0.11 | -    | 15,15,15,15                 | 0     |
| 25  | MG   | Z     | 471 | 1/1   | 0.32 | -    | 71,71,71,71                 | 0     |
| 25  | MG   | Z     | 214 | 1/1   | 0.49 | -    | 76,76,76,76                 | 0     |
| 25  | MG   | Z     | 176 | 1/1   | 0.14 | -    | 35,35,35,35                 | 0     |
| 25  | MG   | Z     | 517 | 1/1   | 0.24 | -    | 55,55,55,55                 | 0     |
| 25  | MG   | Z     | 175 | 1/1   | 0.15 | -    | 60,60,60,60                 | 0     |
| 25  | MG   | Z     | 318 | 1/1   | 0.35 | -    | 40,40,40,40                 | 0     |
| 25  | MG   | Z     | 190 | 1/1   | 0.10 | -    | 3,3,3,3                     | 0     |
| 25  | MG   | Z     | 247 | 1/1   | 0.34 | -    | 58,58,58,58                 | 0     |
| 25  | MG   | Z     | 339 | 1/1   | 0.23 | -    | 64,64,64,64                 | 0     |
| 25  | MG   | Z     | 332 | 1/1   | 0.17 | -    | 32,32,32,32                 | 0     |
| 25  | MG   | Z     | 39  | 1/1   | 0.06 | -    | 36,36,36,36                 | 0     |
| 25  | MG   | Z     | 241 | 1/1   | 0.57 | -    | 62,62,62,62                 | 0     |
| 25  | MG   | Z     | 453 | 1/1   | 0.06 | -    | 21,21,21,21                 | 0     |
| 25  | MG   | Z     | 162 | 1/1   | 0.86 | -    | 77,77,77,77                 | 0     |
| 25  | MG   | Z     | 133 | 1/1   | 2.03 | -    | 67,67,67,67                 | 1     |
| 25  | MG   | Z     | 525 | 1/1   | 0.15 | -    | 25,25,25,25                 | 0     |
| 25  | MG   | Z     | 3   | 1/1   | 0.21 | -    | 16,16,16,16                 | 1     |
| 25  | MG   | Z     | 312 | 1/1   | 0.25 | -    | 35,35,35,35                 | 0     |
| 25  | MG   | Z     | 160 | 1/1   | 0.20 | -    | 50,50,50,50                 | 0     |
| 25  | MG   | Z     | 129 | 1/1   | 0.04 | -    | 8,8,8,8                     | 0     |
| 25  | MG   | Z     | 186 | 1/1   | 0.13 | -    | 50,50,50,50                 | 0     |
| 25  | MG   | Z     | 136 | 1/1   | 0.13 | -    | 45,45,45,45                 | 1     |
| 25  | MG   | Z     | 93  | 1/1   | 0.07 | -    | 25,25,25,25                 | 0     |
| 25  | MG   | Z     | 202 | 1/1   | 0.16 | -    | 42,42,42,42                 | 0     |
| 25  | MG   | Z     | 386 | 1/1   | 1.30 | -    | 1,1,1,1                     | 1     |
| 25  | MG   | Z     | 408 | 1/1   | 0.10 | -    | 53,53,53,53                 | 0     |
| 25  | MG   | Z     | 131 | 1/1   | 0.09 | -    | 20,20,20,20                 | 0     |
| 25  | MG   | Z     | 295 | 1/1   | 0.08 | -    | 17,17,17,17                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 25  | MG   | Z     | 58  | 1/1   | 0.09 | -    | 22,22,22,22                 | 0     |
| 25  | MG   | Z     | 530 | 1/1   | 0.26 | -    | 46,46,46,46                 | 0     |
| 25  | MG   | Z     | 425 | 1/1   | 0.13 | -    | 16,16,16,16                 | 0     |
| 25  | MG   | Z     | 63  | 1/1   | 0.06 | -    | 16,16,16,16                 | 0     |
| 25  | MG   | Z     | 466 | 1/1   | 0.13 | -    | 31,31,31,31                 | 0     |
| 25  | MG   | Z     | 477 | 1/1   | 0.20 | -    | 25,25,25,25                 | 1     |
| 25  | MG   | Z     | 120 | 1/1   | 0.08 | -    | 10,10,10,10                 | 0     |
| 25  | MG   | Z     | 364 | 1/1   | 0.31 | -    | 63,63,63,63                 | 1     |
| 25  | MG   | Z     | 356 | 1/1   | 0.26 | -    | 66,66,66,66                 | 0     |
| 25  | MG   | Z     | 544 | 1/1   | 0.25 | -    | 23,23,23,23                 | 0     |
| 25  | MG   | Z     | 493 | 1/1   | 0.17 | -    | 55,55,55,55                 | 0     |
| 25  | MG   | Z     | 101 | 1/1   | 0.04 | -    | 17,17,17,17                 | 0     |
| 25  | MG   | Z     | 70  | 1/1   | 0.13 | -    | 49,49,49,49                 | 0     |
| 25  | MG   | Z     | 374 | 1/1   | 0.27 | -    | 39,39,39,39                 | 0     |
| 25  | MG   | Z     | 506 | 1/1   | 0.87 | -    | 1,1,1,1                     | 1     |
| 25  | MG   | Z     | 235 | 1/1   | 0.08 | -    | 6,6,6,6                     | 0     |
| 25  | MG   | Z     | 62  | 1/1   | 0.14 | -    | 20,20,20,20                 | 0     |
| 25  | MG   | Z     | 51  | 1/1   | 0.44 | -    | 65,65,65,65                 | 0     |
| 25  | MG   | Z     | 455 | 1/1   | 0.25 | -    | 25,25,25,25                 | 0     |
| 25  | MG   | Z     | 195 | 1/1   | 0.17 | -    | 1,1,1,1                     | 0     |
| 25  | MG   | Z     | 376 | 1/1   | 0.06 | -    | 29,29,29,29                 | 0     |
| 25  | MG   | Z     | 325 | 1/1   | 1.57 | -    | 117,117,117,117             | 0     |
| 25  | MG   | Z     | 278 | 1/1   | 0.34 | -    | 47,47,47,47                 | 0     |
| 25  | MG   | Z     | 341 | 1/1   | 0.18 | -    | 41,41,41,41                 | 0     |
| 25  | MG   | Z     | 69  | 1/1   | 0.07 | -    | 24,24,24,24                 | 0     |
| 25  | MG   | Z     | 50  | 1/1   | 0.15 | -    | 52,52,52,52                 | 0     |
| 25  | MG   | Z     | 163 | 1/1   | 0.11 | -    | 44,44,44,44                 | 0     |
| 25  | MG   | Z     | 451 | 1/1   | 0.27 | -    | 49,49,49,49                 | 0     |
| 25  | MG   | Z     | 251 | 1/1   | 0.16 | -    | 17,17,17,17                 | 0     |
| 25  | MG   | Z     | 203 | 1/1   | 0.09 | -    | 16,16,16,16                 | 0     |
| 25  | MG   | Z     | 229 | 1/1   | 0.27 | -    | 55,55,55,55                 | 1     |
| 25  | MG   | Z     | 117 | 1/1   | 0.11 | -    | 11,11,11,11                 | 0     |
| 25  | MG   | Z     | 439 | 1/1   | 0.34 | -    | 63,63,63,63                 | 0     |
| 25  | MG   | Z     | 502 | 1/1   | 0.18 | -    | 38,38,38,38                 | 0     |
| 25  | MG   | Z     | 87  | 1/1   | 0.12 | -    | 11,11,11,11                 | 0     |
| 25  | MG   | Z     | 487 | 1/1   | 0.16 | -    | 72,72,72,72                 | 0     |
| 25  | MG   | Z     | 307 | 1/1   | 0.86 | -    | 94,94,94,94                 | 0     |
| 25  | MG   | Z     | 492 | 1/1   | 0.15 | -    | 21,21,21,21                 | 0     |
| 25  | MG   | Z     | 156 | 1/1   | 0.11 | -    | 28,28,28,28                 | 0     |
| 25  | MG   | Z     | 504 | 1/1   | 0.32 | -    | 10,10,10,10                 | 1     |
| 25  | MG   | Z     | 536 | 1/1   | 0.32 | -    | 70,70,70,70                 | 0     |
| 25  | MG   | Z     | 522 | 1/1   | 0.30 | -    | 102,102,102,102             | 0     |

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| Mol | Type | Chain | Res | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 25  | MG   | Z     | 92  | 1/1   | 0.10 | -    | 23,23,23,23                 | 0     |
| 25  | MG   | Z     | 256 | 1/1   | 0.08 | -    | 52,52,52,52                 | 0     |
| 25  | MG   | Z     | 542 | 1/1   | 0.07 | -    | 55,55,55,55                 | 0     |
| 25  | MG   | Z     | 76  | 1/1   | 0.09 | -    | 19,19,19,19                 | 0     |
| 25  | MG   | Z     | 37  | 1/1   | 0.14 | -    | 16,16,16,16                 | 0     |
| 25  | MG   | Z     | 276 | 1/1   | 0.05 | -    | 46,46,46,46                 | 0     |
| 25  | MG   | Z     | 550 | 1/1   | 0.24 | -    | 50,50,50,50                 | 0     |
| 25  | MG   | Z     | 335 | 1/1   | 0.14 | -    | 15,15,15,15                 | 0     |
| 25  | MG   | Z     | 315 | 1/1   | 0.32 | -    | 59,59,59,59                 | 0     |
| 25  | MG   | Z     | 498 | 1/1   | 0.12 | -    | 56,56,56,56                 | 0     |
| 25  | MG   | Z     | 308 | 1/1   | 0.20 | -    | 52,52,52,52                 | 0     |
| 25  | MG   | Z     | 545 | 1/1   | 0.11 | -    | 20,20,20,20                 | 0     |
| 25  | MG   | Z     | 44  | 1/1   | 0.24 | -    | 68,68,68,68                 | 0     |
| 25  | MG   | Z     | 246 | 1/1   | 0.13 | -    | 11,11,11,11                 | 0     |
| 25  | MG   | Z     | 252 | 1/1   | 0.25 | -    | 48,48,48,48                 | 0     |
| 25  | MG   | Z     | 219 | 1/1   | 0.27 | -    | 33,33,33,33                 | 0     |
| 25  | MG   | Z     | 510 | 1/1   | 0.24 | -    | 62,62,62,62                 | 0     |
| 25  | MG   | Z     | 480 | 1/1   | 0.28 | -    | 38,38,38,38                 | 0     |
| 25  | MG   | Z     | 53  | 1/1   | 0.18 | -    | 20,20,20,20                 | 0     |
| 25  | MG   | Z     | 394 | 1/1   | 0.85 | -    | 18,18,18,18                 | 1     |
| 25  | MG   | Z     | 147 | 1/1   | 0.54 | -    | 37,37,37,37                 | 0     |
| 25  | MG   | Z     | 404 | 1/1   | 1.40 | -    | 1,1,1,1                     | 1     |
| 25  | MG   | Z     | 349 | 1/1   | 0.12 | -    | 65,65,65,65                 | 0     |
| 25  | MG   | Z     | 34  | 1/1   | 0.24 | -    | 77,77,77,77                 | 0     |
| 25  | MG   | Z     | 165 | 1/1   | 0.19 | -    | 52,52,52,52                 | 1     |
| 25  | MG   | Z     | 340 | 1/1   | 0.10 | -    | 22,22,22,22                 | 0     |
| 25  | MG   | Z     | 49  | 1/1   | 0.06 | -    | 31,31,31,31                 | 0     |
| 25  | MG   | Z     | 448 | 1/1   | 0.41 | -    | 48,48,48,48                 | 0     |
| 25  | MG   | Z     | 216 | 1/1   | 0.14 | -    | 56,56,56,56                 | 0     |
| 25  | MG   | Z     | 31  | 1/1   | 0.15 | -    | 41,41,41,41                 | 0     |
| 25  | MG   | Z     | 130 | 1/1   | 0.17 | -    | 5,5,5,5                     | 0     |
| 25  | MG   | Z     | 22  | 1/1   | 0.27 | -    | 51,51,51,51                 | 0     |
| 25  | MG   | Z     | 128 | 1/1   | 0.04 | -    | 1,1,1,1                     | 0     |
| 25  | MG   | Z     | 26  | 1/1   | 0.22 | -    | 44,44,44,44                 | 0     |
| 25  | MG   | Z     | 280 | 1/1   | 0.21 | -    | 3,3,3,3                     | 0     |
| 25  | MG   | Z     | 518 | 1/1   | 0.23 | -    | 63,63,63,63                 | 0     |
| 25  | MG   | Z     | 508 | 1/1   | 0.60 | -    | 76,76,76,76                 | 0     |
| 25  | MG   | Z     | 29  | 1/1   | 0.19 | -    | 61,61,61,61                 | 0     |
| 25  | MG   | Z     | 170 | 1/1   | 0.18 | -    | 46,46,46,46                 | 1     |
| 25  | MG   | Z     | 470 | 1/1   | 0.22 | -    | 49,49,49,49                 | 0     |
| 25  | MG   | Z     | 204 | 1/1   | 0.05 | -    | 15,15,15,15                 | 0     |
| 25  | MG   | Z     | 302 | 1/1   | 0.24 | -    | 61,61,61,61                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 25  | MG   | Z     | 230 | 1/1   | 0.12 | -    | 57,57,57,57                 | 0     |
| 25  | MG   | Z     | 391 | 1/1   | 0.28 | -    | 2,2,2,2                     | 1     |
| 25  | MG   | Z     | 429 | 1/1   | 0.10 | -    | 35,35,35,35                 | 0     |
| 25  | MG   | Z     | 80  | 1/1   | 0.54 | -    | 97,97,97,97                 | 0     |
| 25  | MG   | Z     | 66  | 1/1   | 0.17 | -    | 29,29,29,29                 | 0     |
| 25  | MG   | Z     | 523 | 1/1   | 0.20 | -    | 58,58,58,58                 | 0     |
| 25  | MG   | Z     | 515 | 1/1   | 1.78 | -    | 79,79,79,79                 | 0     |
| 25  | MG   | Z     | 196 | 1/1   | 0.13 | -    | 23,23,23,23                 | 0     |
| 25  | MG   | Z     | 288 | 1/1   | 0.47 | -    | 49,49,49,49                 | 0     |
| 25  | MG   | Z     | 412 | 1/1   | 0.25 | -    | 13,13,13,13                 | 0     |
| 25  | MG   | Z     | 405 | 1/1   | 0.14 | -    | 43,43,43,43                 | 0     |
| 25  | MG   | Z     | 15  | 1/1   | 0.16 | -    | 32,32,32,32                 | 0     |
| 25  | MG   | Z     | 138 | 1/1   | 0.14 | -    | 44,44,44,44                 | 0     |
| 25  | MG   | Z     | 213 | 1/1   | 0.18 | -    | 25,25,25,25                 | 0     |
| 25  | MG   | Z     | 452 | 1/1   | 0.07 | -    | 10,10,10,10                 | 0     |
| 25  | MG   | Z     | 23  | 1/1   | 0.09 | -    | 10,10,10,10                 | 0     |
| 26  | ZN   | Z     | 548 | 1/1   | 0.11 | -    | 101,101,101,101             | 0     |
| 25  | MG   | Z     | 479 | 1/1   | 0.23 | -    | 35,35,35,35                 | 0     |
| 25  | MG   | Z     | 398 | 1/1   | 0.39 | -    | 50,50,50,50                 | 1     |
| 25  | MG   | Z     | 350 | 1/1   | 0.26 | -    | 104,104,104,104             | 0     |
| 25  | MG   | Z     | 89  | 1/1   | 0.23 | -    | 22,22,22,22                 | 0     |
| 25  | MG   | Z     | 102 | 1/1   | 0.10 | -    | 10,10,10,10                 | 0     |
| 25  | MG   | Z     | 397 | 1/1   | 1.32 | -    | 18,18,18,18                 | 1     |
| 25  | MG   | Z     | 171 | 1/1   | 0.38 | -    | 101,101,101,101             | 0     |
| 25  | MG   | Z     | 464 | 1/1   | 0.23 | -    | 65,65,65,65                 | 0     |
| 25  | MG   | Z     | 268 | 1/1   | 0.50 | -    | 68,68,68,68                 | 0     |
| 25  | MG   | Z     | 366 | 1/1   | 0.32 | -    | 98,98,98,98                 | 0     |
| 25  | MG   | Z     | 253 | 1/1   | 0.20 | -    | 56,56,56,56                 | 0     |
| 25  | MG   | Z     | 2   | 1/1   | 0.34 | -    | 29,29,29,29                 | 1     |
| 25  | MG   | Z     | 250 | 1/1   | 0.12 | -    | 56,56,56,56                 | 0     |
| 25  | MG   | Z     | 382 | 1/1   | 0.33 | -    | 46,46,46,46                 | 1     |
| 25  | MG   | Z     | 6   | 1/1   | 1.41 | -    | 130,130,130,130             | 0     |
| 25  | MG   | Z     | 74  | 1/1   | 0.12 | -    | 16,16,16,16                 | 0     |
| 25  | MG   | Z     | 494 | 1/1   | 0.96 | -    | 80,80,80,80                 | 0     |
| 25  | MG   | Z     | 457 | 1/1   | 0.20 | -    | 39,39,39,39                 | 0     |
| 25  | MG   | Z     | 384 | 1/1   | 0.24 | -    | 54,54,54,54                 | 1     |
| 25  | MG   | Z     | 221 | 1/1   | 0.18 | -    | 56,56,56,56                 | 0     |
| 25  | MG   | Z     | 327 | 1/1   | 0.44 | -    | 11,11,11,11                 | 1     |
| 25  | MG   | Z     | 438 | 1/1   | 0.10 | -    | 40,40,40,40                 | 0     |
| 25  | MG   | Z     | 198 | 1/1   | 0.13 | -    | 16,16,16,16                 | 0     |
| 25  | MG   | Z     | 223 | 1/1   | 1.24 | -    | 46,46,46,46                 | 1     |
| 25  | MG   | Z     | 181 | 1/1   | 0.18 | -    | 64,64,64,64                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 25  | MG   | Z     | 503 | 1/1   | 0.22 | -    | 37,37,37,37                 | 0     |
| 25  | MG   | Z     | 436 | 1/1   | 0.32 | -    | 1,1,1,1                     | 1     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.