



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:12 am GMT

PDB ID : 4JI5  
Title : Crystal Structure of 30S ribosomal subunit from *Thermus thermophilus*  
Authors : Demirci, H.; Wang, L.; Murphy IV, F.; Murphy, E.; Carr, J.; Blanchard, S.;  
Jogl, G.; Dahlberg, A.E.; Gregory, S.T.  
Deposited on : 2013-03-05  
Resolution : 3.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

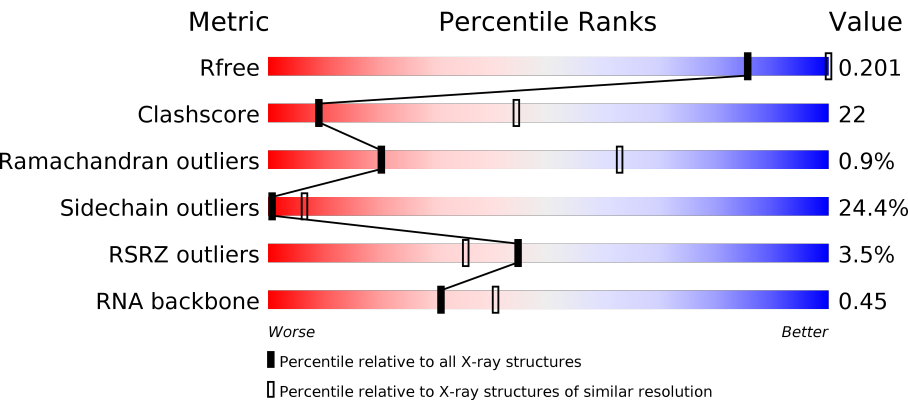
MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.85 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 <sub>free</sub>     | 100719                      | 1009 (4.16-3.56)                                      |
| Clashscore            | 112137                      | 1029 (4.12-3.60)                                      |
| Ramachandran outliers | 110173                      | 1017 (4.14-3.58)                                      |
| Sidechain outliers    | 110143                      | 1010 (4.14-3.58)                                      |
| RSRZ outliers         | 101464                      | 1023 (4.16-3.56)                                      |
| RNA backbone          | 2435                        | 1017 (4.76-2.90)                                      |

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                               |
|-----|-------|--------|--|
| 1   | A     | 1522   | <div><div>2%</div><div>19%39%33%9%</div></div> |
| 2   | B     | 256    | <div><div>%</div><div>42%33%14%9%</div></div>  |
| 3   | C     | 239    | <div><div>%</div><div>33%40%12%14%</div></div> |
| 4   | D     | 209    | <div><div>9%</div><div>41%44%15%</div></div>   |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 5   | E     | 162    |                  |
| 6   | F     | 101    |                  |
| 7   | G     | 156    |                  |
| 8   | H     | 138    |                  |
| 9   | I     | 128    |                  |
| 10  | J     | 105    |                  |
| 11  | K     | 129    |                  |
| 12  | L     | 135    |                  |
| 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     |                  |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 22  | MG   | A     | 1617 | -         | -        | -       | X                |
| 22  | MG   | A     | 1630 | -         | -        | -       | X                |
| 22  | MG   | A     | 1633 | -         | -        | -       | X                |
| 22  | MG   | A     | 1640 | -         | -        | -       | X                |
| 22  | MG   | A     | 1648 | -         | -        | -       | X                |
| 22  | MG   | A     | 1666 | -         | -        | -       | X                |
| 22  | MG   | A     | 1667 | -         | -        | -       | X                |
| 22  | MG   | A     | 1669 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 22  | MG   | A     | 1672 | -         | -        | -       | X                |
| 22  | MG   | A     | 1675 | -         | -        | -       | X                |
| 22  | MG   | A     | 1678 | -         | -        | -       | X                |
| 22  | MG   | A     | 1682 | -         | -        | -       | X                |
| 22  | MG   | A     | 1690 | -         | -        | -       | X                |
| 22  | MG   | A     | 1693 | -         | -        | -       | X                |
| 22  | MG   | A     | 1731 | -         | -        | -       | X                |

## 2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 52228 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1   | A     | 1514     | Total | C     | N    | O     | P    | 0       | 6       | 0     |
|     |       |          | 32687 | 14559 | 6046 | 10562 | 1520 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference   |
|-------|---------|----------|--------|----------|-------------|
| A     | 1534    | C        | A      | CONFLICT | GB M26923.1 |
| A     | 1535    | A        | C      | CONFLICT | GB M26923.1 |

- Molecule 2 is a protein called RIBOSOMAL PROTEIN S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | B     | 234      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1900  | 1213 | 341 | 341 | 5 |         |         |       |

- Molecule 3 is a protein called RIBOSOMAL PROTEIN S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | C     | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1612  | 1016 | 314 | 281 | 1 |         |         |       |

- Molecule 4 is a protein called 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 RIBOSOMAL PROTEIN S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | E     | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1146  | 724 | 217 | 201 | 4 |         |         |       |

- Molecule 6 is a protein called 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 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 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 RIBOSOMAL PROTEIN S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9   | I     | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1010  | 639 | 197 | 174 |   |         |         |       |

- Molecule 10 is a protein called RIBOSOMAL PROTEIN S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | J     | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 792   | 498 | 156 | 137 | 1 |         |         |       |

- Molecule 11 is a protein called RIBOSOMAL PROTEIN S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | K     | 116      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 864   | 537 | 164 | 160 | 3 |         |         |       |

- Molecule 12 is a protein called RIBOSOMAL PROTEIN S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | L     | 124      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 972   | 612 | 195 | 163 | 2 |         |         |       |

- Molecule 13 is a protein called RIBOSOMAL PROTEIN S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | M     | 118      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 937   | 579 | 193 | 163 | 2 |         |         |       |

- Molecule 14 is a protein called RIBOSOMAL PROTEIN S14.

| 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 RIBOSOMAL PROTEIN S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15  | O     | 87       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 729   | 457 | 146 | 124 | 2 |         |         |       |

- Molecule 16 is a protein called RIBOSOMAL PROTEIN S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | P     | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 700   | 443 | 139 | 117 | 1 |         |         |       |

- Molecule 17 is a protein called RIBOSOMAL PROTEIN S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17  | Q     | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 823   | 528 | 151 | 142 | 2 |         |         |       |

- Molecule 18 is a protein called 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 RIBOSOMAL PROTEIN S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | S     | 80       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 647   | 414 | 119 | 112 | 2 |         |         |       |

- Molecule 20 is a protein called 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 RIBOSOMAL PROTEIN THX.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 21  | U     | 24       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 208   | 128 | 50 | 30 |         |         |       |

- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 22  | G     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 22  | D     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 22  | K     | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 22  | E     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 22  | H     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 22  | A     | 164      | Total | Mg  | 0       | 0       |
|     |       |          | 164   | 164 |         |         |
| 22  | S     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 22  | F     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |

- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 23  | D     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 23  | N     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 24 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 24  | A     | 271      | Total | O   | 0       | 0       |
|     |       |          | 271   | 271 |         |         |

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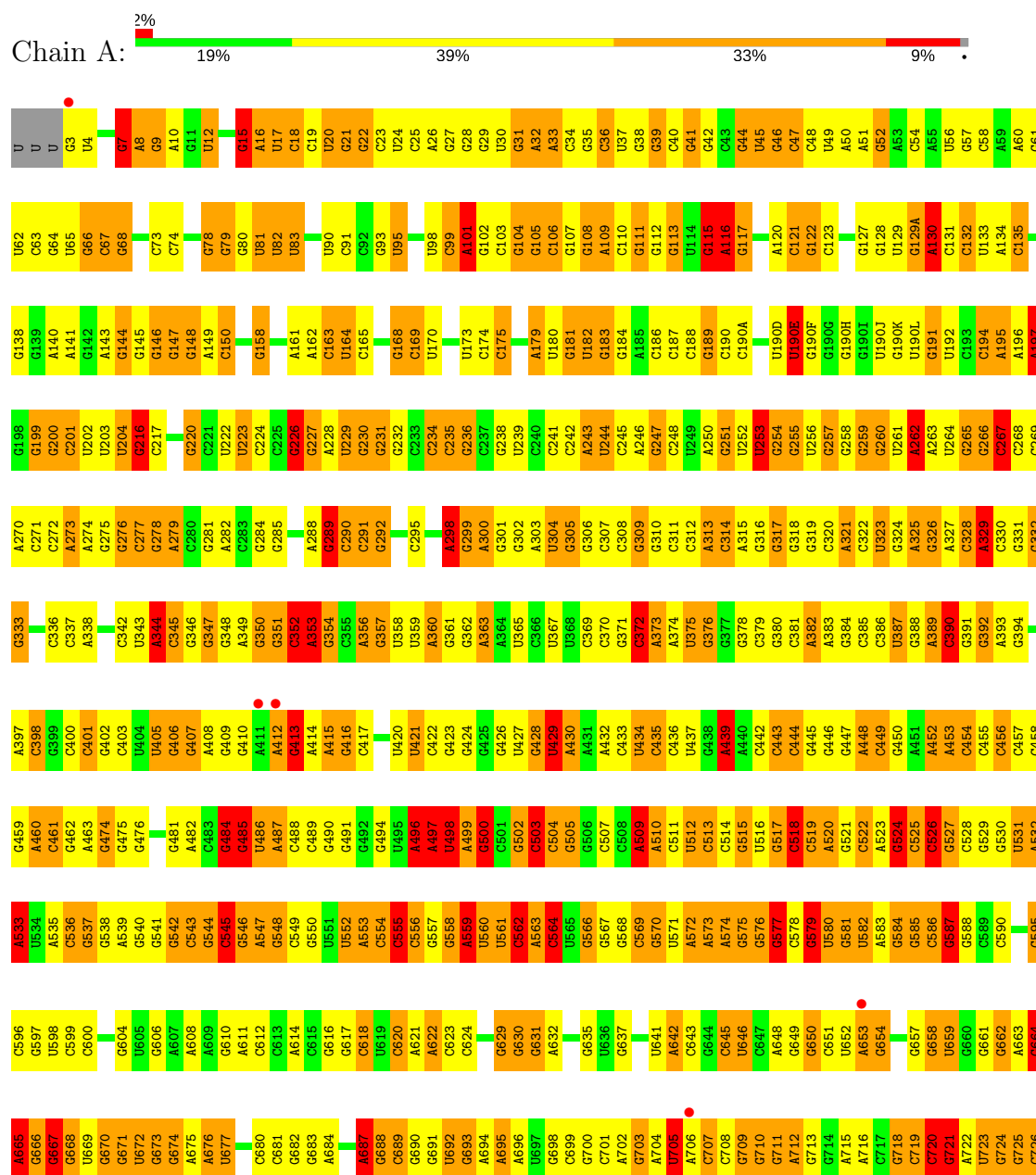
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| Mol | Chain | Residues | Atoms      |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 24  | C     | 1        | Total<br>1 | O<br>1 | 0       | 0       |
| 24  | E     | 3        | Total<br>3 | O<br>3 | 0       | 0       |
| 24  | L     | 1        | Total<br>1 | O<br>1 | 0       | 0       |
| 24  | N     | 1        | Total<br>1 | O<br>1 | 0       | 0       |
| 24  | P     | 1        | Total<br>1 | O<br>1 | 0       | 0       |
| 24  | T     | 1        | Total<br>1 | O<br>1 | 0       | 0       |

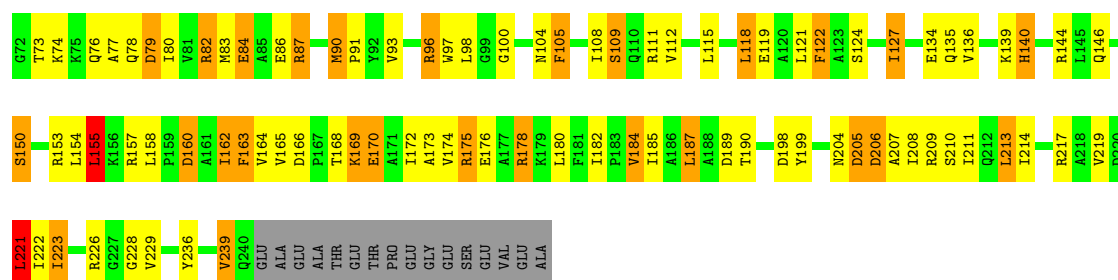
### 3 Residue-property plots

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

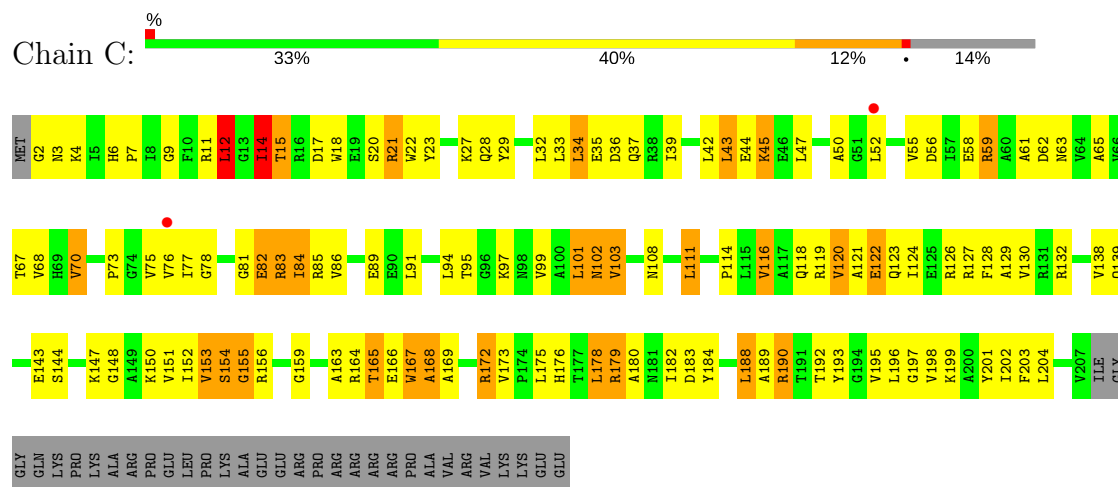
#### • Molecule 1: 16S rRNA



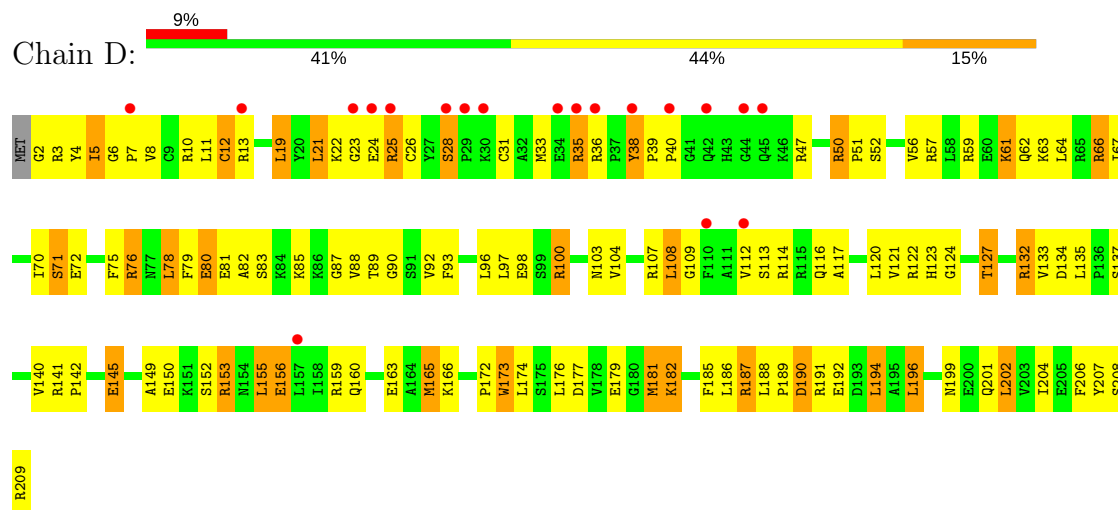
[illegible]



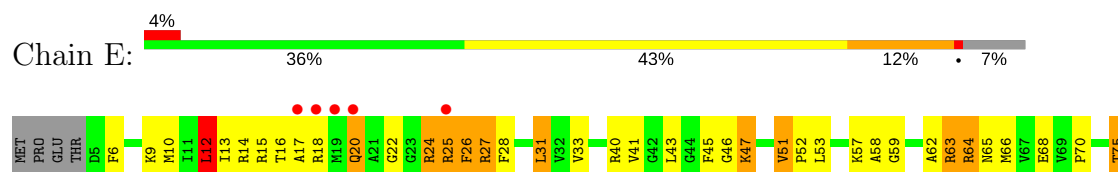
• Molecule 3: RIBOSOMAL PROTEIN S3

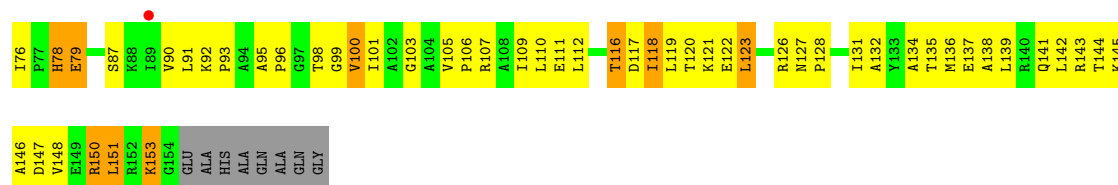


• Molecule 4: RIBOSOMAL PROTEIN S4

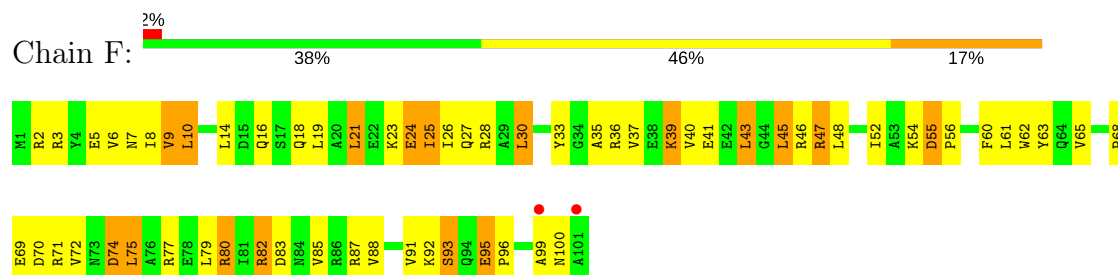


• Molecule 5: RIBOSOMAL PROTEIN S5

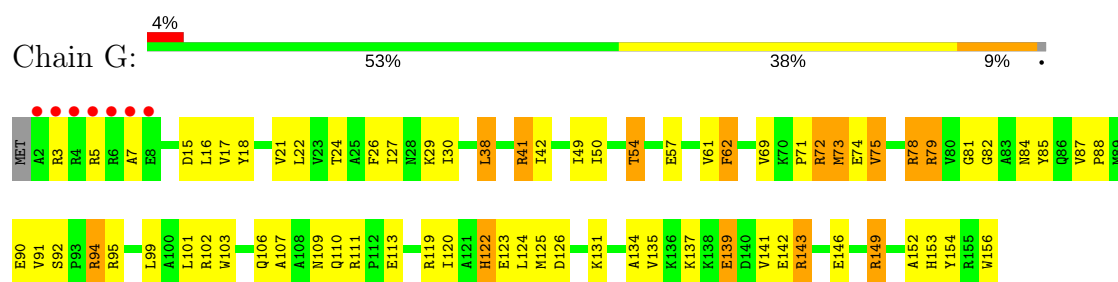




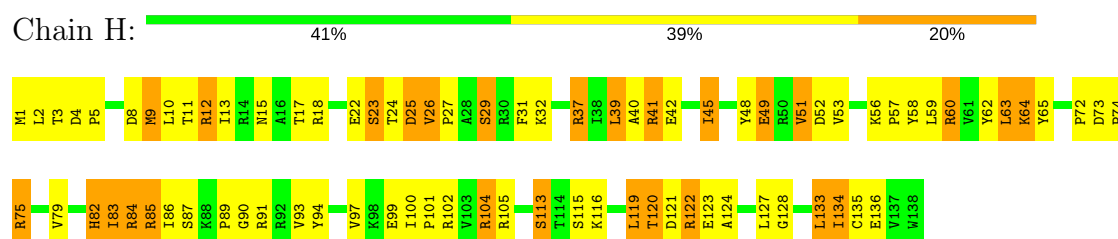
### • Molecule 6: RIBOSOMAL PROTEIN S6



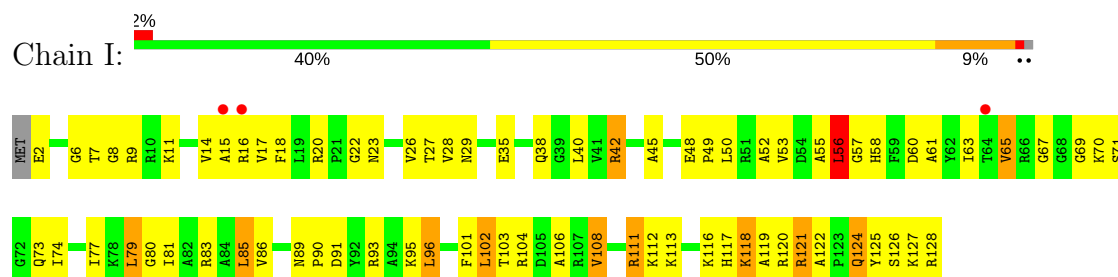
### • Molecule 7: RIBOSOMAL PROTEIN S7



### • Molecule 8: RIBOSOMAL PROTEIN S8

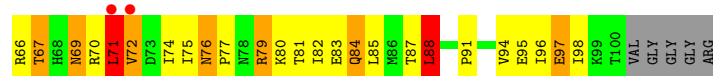
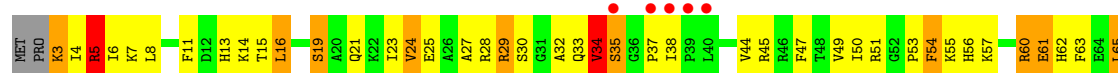


### • Molecule 9: RIBOSOMAL PROTEIN S9



### • Molecule 10: RIBOSOMAL PROTEIN S10

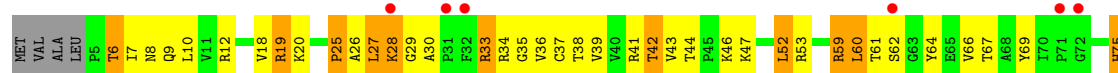




• Molecule 11: RIBOSOMAL PROTEIN S11



• Molecule 12: RIBOSOMAL PROTEIN S12



• Molecule 13: RIBOSOMAL PROTEIN S13



• Molecule 14: RIBOSOMAL PROTEIN S14

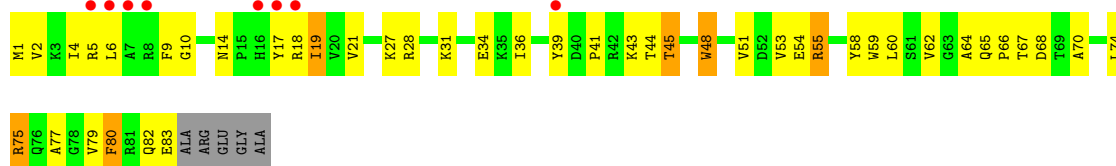
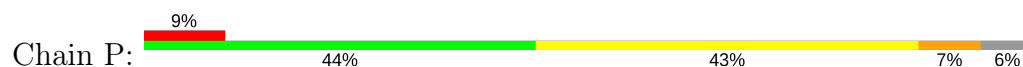


• Molecule 15: RIBOSOMAL PROTEIN S15

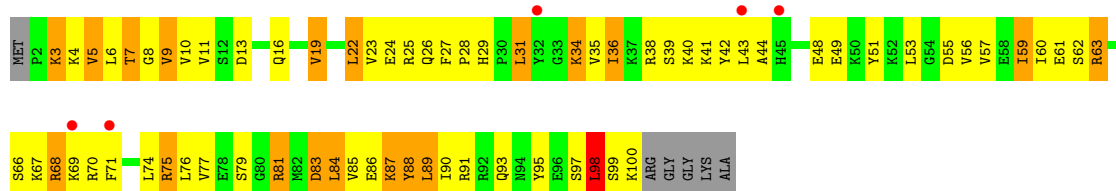




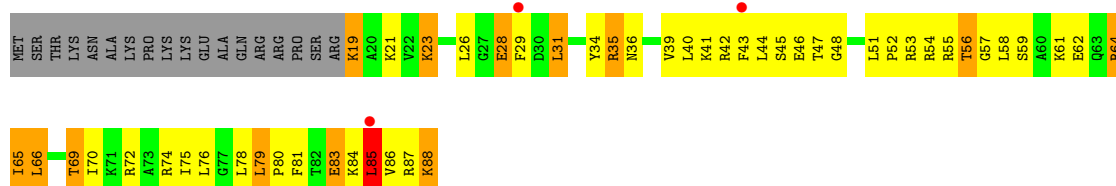
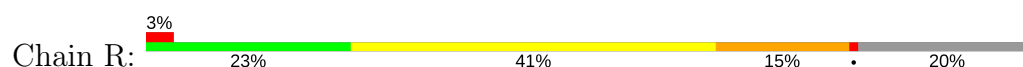
• Molecule 16: RIBOSOMAL PROTEIN S16



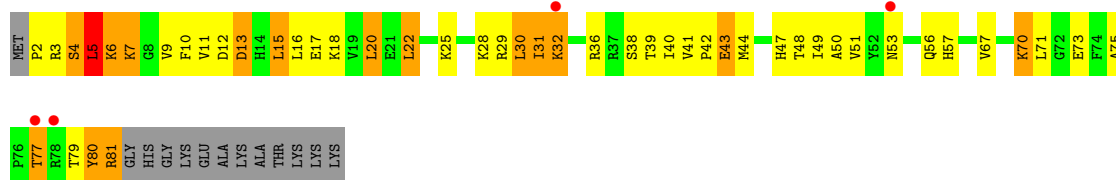
• Molecule 17: RIBOSOMAL PROTEIN S17



• Molecule 18: RIBOSOMAL PROTEIN S18

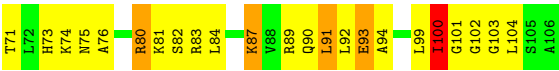


• Molecule 19: RIBOSOMAL PROTEIN S19

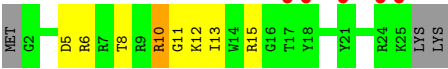


• Molecule 20: RIBOSOMAL PROTEIN S20





● Molecule 21: RIBOSOMAL PROTEIN THX





## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 41 21 2   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 399.62Å 399.62Å 216.07Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 47.29 – 3.85<br>49.67 – 3.85                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.3 (47.29-3.85)<br>99.3 (49.67-3.85)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.12  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.47 (at 3.88Å)   | Xtriage          |
| Refinement program  | PHENIX (phenix.refine: dev_1119)                            | Depositor        |
| R, $R_{free}$   | 0.153 , 0.202<br>0.152 , 0.201                              | Depositor<br>DCC |
| $R_{free}$ test set   | 8212 reflections (5.04%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 157.0   | Xtriage          |
| Anisotropy  | 0.232   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.29 , 166.7  | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.95  | EDS              |
| Total number of atoms   | 52228   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 162.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MA6, 0TD, MG, 2MG, 5MC, UR3, 4OC, M2G, 7MG, PSU

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     | 1.18         | 129/36187 (0.4%) | 2.02        | 1881/56471 (3.3%) |
| 2   | B     | 0.76         | 0/1935           | 1.00        | 6/2609 (0.2%)     |
| 3   | C     | 0.79         | 0/1636           | 0.98        | 6/2205 (0.3%)     |
| 4   | D     | 0.77         | 1/1733 (0.1%)    | 0.97        | 1/2318 (0.0%)     |
| 5   | E     | 0.82         | 0/1162           | 1.05        | 4/1564 (0.3%)     |
| 6   | F     | 0.83         | 0/856            | 1.02        | 3/1154 (0.3%)     |
| 7   | G     | 0.73         | 0/1276           | 0.87        | 1/1709 (0.1%)     |
| 8   | H     | 0.83         | 0/1136           | 0.98        | 0/1527            |
| 9   | I     | 0.63         | 0/1029           | 0.88        | 1/1379 (0.1%)     |
| 10  | J     | 0.77         | 0/805            | 1.03        | 4/1082 (0.4%)     |
| 11  | K     | 0.71         | 0/879            | 0.91        | 0/1187            |
| 12  | L     | 0.97         | 2/977 (0.2%)     | 1.15        | 2/1306 (0.2%)     |
| 13  | M     | 0.59         | 0/947            | 0.84        | 0/1270            |
| 14  | N     | 0.77         | 0/501            | 1.04        | 3/664 (0.5%)      |
| 15  | O     | 0.69         | 0/740            | 0.94        | 0/987             |
| 16  | P     | 0.74         | 0/716            | 0.92        | 0/963             |
| 17  | Q     | 0.87         | 0/836            | 1.05        | 3/1117 (0.3%)     |
| 18  | R     | 0.71         | 0/579            | 0.99        | 2/768 (0.3%)      |
| 19  | S     | 0.60         | 0/661            | 1.01        | 4/890 (0.4%)      |
| 20  | T     | 0.74         | 0/765            | 1.03        | 2/1007 (0.2%)     |
| 21  | U     | 0.71         | 0/212            | 0.83        | 0/277             |
| All | All   | 1.06         | 132/55568 (0.2%) | 1.76        | 1923/82454 (2.3%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | B     | 0                   | 2                   |
| 3   | C     | 0                   | 3                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 8   | H     | 0                   | 1                   |
| 9   | I     | 0                   | 2                   |
| 10  | J     | 0                   | 2                   |
| 13  | M     | 0                   | 3                   |
| 14  | N     | 0                   | 1                   |
| 16  | P     | 0                   | 1                   |
| 20  | T     | 0                   | 3                   |
| All | All   | 0                   | 18                  |

All (132) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | A     | 672  | U    | C4-O4 | 8.76  | 1.30        | 1.23     |
| 1   | A     | 563  | A    | N9-C4 | -7.63 | 1.33        | 1.37     |
| 1   | A     | 729  | A    | N3-C4 | -7.49 | 1.30        | 1.34     |
| 1   | A     | 1512 | U    | C4-O4 | 7.36  | 1.29        | 1.23     |
| 1   | A     | 372  | C    | C2-O2 | 7.33  | 1.31        | 1.24     |
| 1   | A     | 810  | C    | N3-C4 | -7.31 | 1.28        | 1.33     |
| 1   | A     | 1501 | C    | N1-C6 | -6.93 | 1.32        | 1.37     |
| 1   | A     | 1513 | A    | N9-C4 | -6.92 | 1.33        | 1.37     |
| 1   | A     | 802  | A    | N7-C5 | -6.88 | 1.35        | 1.39     |
| 12  | L     | 26   | ALA  | CA-CB | 6.84  | 1.66        | 1.52     |
| 1   | A     | 791  | G    | C6-O6 | 6.79  | 1.30        | 1.24     |
| 1   | A     | 481  | G    | N7-C5 | -6.78 | 1.35        | 1.39     |
| 1   | A     | 922  | G    | C6-O6 | 6.78  | 1.30        | 1.24     |
| 1   | A     | 792  | A    | N9-C4 | -6.76 | 1.33        | 1.37     |
| 1   | A     | 304  | U    | C4-O4 | 6.73  | 1.29        | 1.23     |
| 1   | A     | 558  | G    | C6-O6 | 6.69  | 1.30        | 1.24     |
| 1   | A     | 558  | G    | N3-C4 | -6.62 | 1.30        | 1.35     |
| 1   | A     | 642  | A    | N3-C4 | -6.55 | 1.30        | 1.34     |
| 1   | A     | 1392 | G    | C6-N1 | -6.55 | 1.34        | 1.39     |
| 1   | A     | 631  | G    | C6-N1 | 6.53  | 1.44        | 1.39     |
| 1   | A     | 723  | U    | C2-N3 | 6.50  | 1.42        | 1.37     |
| 1   | A     | 288  | A    | N9-C4 | -6.49 | 1.33        | 1.37     |
| 1   | A     | 523  | A    | N9-C4 | -6.47 | 1.33        | 1.37     |
| 1   | A     | 239  | U    | C4-O4 | 6.41  | 1.28        | 1.23     |
| 1   | A     | 305  | G    | C6-O6 | 6.40  | 1.29        | 1.24     |
| 1   | A     | 965  | A    | N9-C4 | -6.40 | 1.34        | 1.37     |
| 1   | A     | 790  | A    | N3-C4 | -6.36 | 1.31        | 1.34     |
| 1   | A     | 1335 | C    | N1-C2 | 6.35  | 1.46        | 1.40     |
| 1   | A     | 1394 | A    | C6-N1 | -6.33 | 1.31        | 1.35     |
| 1   | A     | 1394 | A    | N3-C4 | -6.32 | 1.31        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | A     | 715  | A    | N9-C4   | -6.28 | 1.34        | 1.37     |
| 1   | A     | 781  | A    | N9-C4   | -6.27 | 1.34        | 1.37     |
| 1   | A     | 484  | G    | C6-N1   | -6.20 | 1.35        | 1.39     |
| 1   | A     | 562  | C    | N1-C6   | -6.19 | 1.33        | 1.37     |
| 1   | A     | 509  | A    | N7-C5   | -6.17 | 1.35        | 1.39     |
| 1   | A     | 642  | A    | N9-C4   | -6.16 | 1.34        | 1.37     |
| 1   | A     | 1529 | G    | N7-C5   | -6.15 | 1.35        | 1.39     |
| 1   | A     | 32   | A    | N3-C4   | -6.14 | 1.31        | 1.34     |
| 1   | A     | 47   | C    | N3-C4   | -6.08 | 1.29        | 1.33     |
| 1   | A     | 439  | A    | N3-C4   | -6.07 | 1.31        | 1.34     |
| 1   | A     | 563  | A    | N3-C4   | -6.05 | 1.31        | 1.34     |
| 1   | A     | 238  | G    | N3-C4   | -6.01 | 1.31        | 1.35     |
| 1   | A     | 871  | U    | N1-C2   | 5.99  | 1.44        | 1.38     |
| 1   | A     | 266  | G    | N9-C4   | -5.99 | 1.33        | 1.38     |
| 1   | A     | 550  | G    | C6-N1   | -5.97 | 1.35        | 1.39     |
| 1   | A     | 1230 | C    | C2-O2   | 5.97  | 1.29        | 1.24     |
| 1   | A     | 26   | A    | N9-C4   | -5.92 | 1.34        | 1.37     |
| 1   | A     | 1005 | A    | N9-C4   | 5.91  | 1.41        | 1.37     |
| 1   | A     | 1377 | A    | N9-C4   | -5.86 | 1.34        | 1.37     |
| 1   | A     | 309  | G    | C6-N1   | 5.86  | 1.43        | 1.39     |
| 1   | A     | 50   | A    | N9-C4   | -5.84 | 1.34        | 1.37     |
| 1   | A     | 204  | U    | C2-N3   | 5.77  | 1.41        | 1.37     |
| 1   | A     | 748  | C    | N1-C2   | 5.76  | 1.46        | 1.40     |
| 1   | A     | 893  | C    | C2-O2   | 5.73  | 1.29        | 1.24     |
| 1   | A     | 622  | A    | N9-C4   | -5.73 | 1.34        | 1.37     |
| 1   | A     | 1527 | C    | N3-C4   | -5.73 | 1.29        | 1.33     |
| 1   | A     | 1392 | G    | N1-C2   | -5.72 | 1.33        | 1.37     |
| 1   | A     | 262  | A    | N9-C4   | -5.69 | 1.34        | 1.37     |
| 1   | A     | 768  | A    | N9-C4   | -5.68 | 1.34        | 1.37     |
| 12  | L     | 98   | TYR  | CD2-CE2 | 5.68  | 1.47        | 1.39     |
| 1   | A     | 267  | C    | N3-C4   | -5.67 | 1.29        | 1.33     |
| 1   | A     | 279  | A    | N9-C4   | -5.65 | 1.34        | 1.37     |
| 1   | A     | 382  | A    | C6-N1   | -5.63 | 1.31        | 1.35     |
| 1   | A     | 18   | C    | N1-C6   | -5.63 | 1.33        | 1.37     |
| 1   | A     | 250  | A    | C5-C4   | 5.62  | 1.42        | 1.38     |
| 1   | A     | 859  | A    | N9-C4   | -5.62 | 1.34        | 1.37     |
| 1   | A     | 523  | A    | N3-C4   | -5.60 | 1.31        | 1.34     |
| 1   | A     | 108  | G    | N9-C4   | -5.57 | 1.33        | 1.38     |
| 1   | A     | 828  | A    | N9-C4   | -5.55 | 1.34        | 1.37     |
| 1   | A     | 878  | G    | C6-N1   | -5.55 | 1.35        | 1.39     |
| 1   | A     | 45   | U    | C4-O4   | 5.53  | 1.28        | 1.23     |
| 1   | A     | 817  | C    | N1-C6   | -5.53 | 1.33        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | A     | 728  | A    | N3-C4 | -5.52 | 1.31        | 1.34     |
| 1   | A     | 809  | G    | C5-C4 | -5.52 | 1.34        | 1.38     |
| 1   | A     | 357  | G    | C6-O6 | 5.52  | 1.29        | 1.24     |
| 1   | A     | 32   | A    | C6-N1 | -5.51 | 1.31        | 1.35     |
| 1   | A     | 830  | G    | C6-O6 | 5.50  | 1.29        | 1.24     |
| 1   | A     | 839  | U    | N1-C2 | 5.50  | 1.43        | 1.38     |
| 1   | A     | 382  | A    | N3-C4 | -5.49 | 1.31        | 1.34     |
| 1   | A     | 108  | G    | N7-C5 | -5.48 | 1.35        | 1.39     |
| 1   | A     | 120  | A    | N7-C5 | -5.47 | 1.35        | 1.39     |
| 1   | A     | 505  | G    | C6-N1 | -5.44 | 1.35        | 1.39     |
| 1   | A     | 724  | G    | N7-C5 | -5.44 | 1.35        | 1.39     |
| 1   | A     | 969  | A    | N9-C4 | -5.42 | 1.34        | 1.37     |
| 1   | A     | 298  | A    | N3-C4 | -5.41 | 1.31        | 1.34     |
| 1   | A     | 553  | A    | N9-C4 | -5.41 | 1.34        | 1.37     |
| 1   | A     | 1531 | A    | N9-C8 | 5.40  | 1.42        | 1.37     |
| 4   | D     | 173  | TRP  | CB-CG | -5.40 | 1.40        | 1.50     |
| 1   | A     | 631  | G    | N1-C2 | 5.40  | 1.42        | 1.37     |
| 1   | A     | 1124 | G    | C6-N1 | 5.40  | 1.43        | 1.39     |
| 1   | A     | 1157 | A    | N9-C4 | 5.38  | 1.41        | 1.37     |
| 1   | A     | 27   | G    | N7-C5 | -5.38 | 1.36        | 1.39     |
| 1   | A     | 1225 | A    | N3-C4 | -5.37 | 1.31        | 1.34     |
| 1   | A     | 375  | U    | C4-O4 | 5.36  | 1.27        | 1.23     |
| 1   | A     | 703  | G    | C5-C6 | 5.36  | 1.47        | 1.42     |
| 1   | A     | 919  | A    | C5-C4 | -5.36 | 1.35        | 1.38     |
| 1   | A     | 532  | A    | N3-C4 | 5.35  | 1.38        | 1.34     |
| 1   | A     | 1493 | A    | N9-C4 | 5.33  | 1.41        | 1.37     |
| 1   | A     | 964  | A    | N3-C4 | -5.33 | 1.31        | 1.34     |
| 1   | A     | 510  | A    | N3-C4 | -5.31 | 1.31        | 1.34     |
| 1   | A     | 47   | C    | N1-C6 | -5.30 | 1.33        | 1.37     |
| 1   | A     | 729  | A    | N7-C5 | -5.30 | 1.36        | 1.39     |
| 1   | A     | 1531 | A    | C5-C4 | 5.30  | 1.42        | 1.38     |
| 1   | A     | 390  | C    | N1-C6 | -5.29 | 1.33        | 1.37     |
| 1   | A     | 9    | G    | N9-C8 | -5.28 | 1.34        | 1.37     |
| 1   | A     | 919  | A    | N7-C5 | -5.25 | 1.36        | 1.39     |
| 1   | A     | 122  | G    | C5-C4 | -5.25 | 1.34        | 1.38     |
| 1   | A     | 864  | A    | N3-C4 | -5.23 | 1.31        | 1.34     |
| 1   | A     | 325  | A    | N3-C4 | -5.23 | 1.31        | 1.34     |
| 1   | A     | 1530 | G    | C6-N1 | 5.23  | 1.43        | 1.39     |
| 1   | A     | 1393 | U    | C4-O4 | 5.20  | 1.27        | 1.23     |
| 1   | A     | 802  | A    | C5-C6 | -5.20 | 1.36        | 1.41     |
| 1   | A     | 67   | C    | N3-C4 | -5.19 | 1.30        | 1.33     |
| 1   | A     | 543  | C    | N1-C6 | -5.19 | 1.34        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | A     | 704  | A    | N9-C4 | -5.19 | 1.34        | 1.37     |
| 1   | A     | 889  | A    | N3-C4 | -5.18 | 1.31        | 1.34     |
| 1   | A     | 1403 | C    | N1-C6 | -5.18 | 1.34        | 1.37     |
| 1   | A     | 1004 | A    | N9-C4 | 5.14  | 1.41        | 1.37     |
| 1   | A     | 379  | C    | N1-C6 | -5.14 | 1.34        | 1.37     |
| 1   | A     | 357  | G    | C2-N3 | -5.12 | 1.28        | 1.32     |
| 1   | A     | 919  | A    | N9-C4 | -5.09 | 1.34        | 1.37     |
| 1   | A     | 791  | G    | N3-C4 | -5.09 | 1.31        | 1.35     |
| 1   | A     | 10   | A    | C6-N1 | -5.09 | 1.31        | 1.35     |
| 1   | A     | 728  | A    | C5-C6 | -5.09 | 1.36        | 1.41     |
| 1   | A     | 1506 | U    | N1-C2 | 5.08  | 1.43        | 1.38     |
| 1   | A     | 1084 | G    | C6-O6 | 5.07  | 1.28        | 1.24     |
| 1   | A     | 230  | G    | C6-O6 | 5.07  | 1.28        | 1.24     |
| 1   | A     | 859  | A    | N3-C4 | -5.06 | 1.31        | 1.34     |
| 1   | A     | 964  | A    | N9-C4 | -5.05 | 1.34        | 1.37     |
| 1   | A     | 1084 | G    | C5-C6 | 5.05  | 1.47        | 1.42     |
| 1   | A     | 66   | G    | N9-C4 | -5.01 | 1.33        | 1.38     |
| 1   | A     | 487  | A    | N9-C4 | -5.00 | 1.34        | 1.37     |

All (1923) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 1   | A     | 1528 | U    | O5'-P-OP2 | -17.17 | 90.09       | 110.70   |
| 1   | A     | 309  | G    | N1-C6-O6  | 16.92  | 130.05      | 119.90   |
| 1   | A     | 922  | G    | N1-C6-O6  | 15.33  | 129.10      | 119.90   |
| 1   | A     | 558  | G    | C5-C6-N1  | -15.09 | 103.95      | 111.50   |
| 1   | A     | 1335 | C    | N1-C2-O2  | 14.44  | 127.56      | 118.90   |
| 1   | A     | 117  | G    | N1-C6-O6  | 14.31  | 128.49      | 119.90   |
| 1   | A     | 791  | G    | C5-C6-N1  | -13.57 | 104.72      | 111.50   |
| 1   | A     | 325  | A    | N1-C6-N6  | -13.50 | 110.50      | 118.60   |
| 1   | A     | 922  | G    | C5-C6-N1  | -13.29 | 104.86      | 111.50   |
| 1   | A     | 970  | C    | N1-C2-O2  | 13.22  | 126.83      | 118.90   |
| 1   | A     | 672  | U    | N3-C4-C5  | -13.21 | 106.67      | 114.60   |
| 1   | A     | 305  | G    | C5-C6-N1  | -13.20 | 104.90      | 111.50   |
| 1   | A     | 239  | U    | N3-C4-C5  | -13.17 | 106.70      | 114.60   |
| 1   | A     | 1512 | U    | N3-C4-C5  | -13.00 | 106.80      | 114.60   |
| 1   | A     | 1435 | G    | N1-C6-O6  | 12.82  | 127.59      | 119.90   |
| 1   | A     | 541  | G    | N1-C6-O6  | 12.58  | 127.45      | 119.90   |
| 1   | A     | 147  | G    | N1-C6-O6  | 12.50  | 127.40      | 119.90   |
| 1   | A     | 1531 | A    | N7-C8-N9  | 12.41  | 120.01      | 113.80   |
| 1   | A     | 58   | C    | C6-N1-C2  | -12.22 | 115.41      | 120.30   |
| 1   | A     | 1531 | A    | N1-C6-N6  | 12.19  | 125.91      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 1   | A     | 1531 | A    | C5-N7-C8  | -12.04 | 97.88       | 103.90   |
| 1   | A     | 304  | U    | N3-C4-C5  | -11.95 | 107.43      | 114.60   |
| 1   | A     | 730  | G    | C4-C5-N7  | -11.91 | 106.04      | 110.80   |
| 1   | A     | 518  | C    | N1-C2-O2  | 11.81  | 125.99      | 118.90   |
| 1   | A     | 481  | G    | O5'-P-OP2 | -11.75 | 95.13       | 105.70   |
| 1   | A     | 871  | U    | N1-C2-O2  | 11.72  | 131.00      | 122.80   |
| 1   | A     | 830  | G    | C5-C6-N1  | -11.51 | 105.75      | 111.50   |
| 1   | A     | 1064 | G    | C5-C6-O6  | -11.50 | 121.70      | 128.60   |
| 1   | A     | 1050 | G    | N1-C6-O6  | 11.43  | 126.76      | 119.90   |
| 1   | A     | 1335 | C    | N3-C2-O2  | -11.43 | 113.90      | 121.90   |
| 1   | A     | 1530 | G    | N3-C4-C5  | 11.43  | 134.31      | 128.60   |
| 1   | A     | 34   | C    | C6-N1-C2  | 11.40  | 124.86      | 120.30   |
| 1   | A     | 309  | G    | C5-C6-O6  | -11.38 | 121.78      | 128.60   |
| 1   | A     | 1532 | U    | C5-C6-N1  | 11.23  | 128.32      | 122.70   |
| 1   | A     | 285  | G    | C8-N9-C4  | 11.23  | 110.89      | 106.40   |
| 1   | A     | 624  | C    | C6-N1-C2  | 11.23  | 124.79      | 120.30   |
| 1   | A     | 27   | G    | N1-C6-O6  | 11.18  | 126.61      | 119.90   |
| 1   | A     | 710  | G    | N1-C6-O6  | 11.13  | 126.58      | 119.90   |
| 1   | A     | 1397 | C    | O5'-P-OP1 | -11.08 | 95.73       | 105.70   |
| 1   | A     | 1233 | G    | N1-C6-O6  | 11.06  | 126.53      | 119.90   |
| 1   | A     | 254  | G    | O5'-P-OP1 | -11.01 | 95.79       | 105.70   |
| 1   | A     | 1124 | G    | C2-N3-C4  | 10.97  | 117.38      | 111.90   |
| 1   | A     | 117  | G    | C6-C5-N7  | -10.92 | 123.85      | 130.40   |
| 1   | A     | 897  | C    | N3-C4-C5  | 10.91  | 126.27      | 121.90   |
| 1   | A     | 769  | G    | O5'-P-OP2 | -10.88 | 95.91       | 105.70   |
| 1   | A     | 1514 | C    | C6-N1-C2  | 10.87  | 124.65      | 120.30   |
| 1   | A     | 902  | G    | N1-C6-O6  | 10.78  | 126.36      | 119.90   |
| 1   | A     | 718  | G    | C8-N9-C4  | 10.73  | 110.69      | 106.40   |
| 1   | A     | 555  | C    | O5'-P-OP2 | -10.66 | 96.11       | 105.70   |
| 1   | A     | 1277 | C    | C6-N1-C2  | -10.62 | 116.05      | 120.30   |
| 1   | A     | 1125 | U    | N3-C2-O2  | 10.61  | 129.63      | 122.20   |
| 1   | A     | 922  | G    | C4-C5-C6  | 10.61  | 125.17      | 118.80   |
| 1   | A     | 1222 | G    | C5-C6-N1  | -10.61 | 106.20      | 111.50   |
| 1   | A     | 122  | G    | C8-N9-C4  | 10.58  | 110.63      | 106.40   |
| 1   | A     | 54   | C    | C6-N1-C2  | 10.55  | 124.52      | 120.30   |
| 1   | A     | 1064 | G    | N1-C6-O6  | 10.55  | 126.23      | 119.90   |
| 1   | A     | 333  | G    | N1-C6-O6  | 10.50  | 126.20      | 119.90   |
| 1   | A     | 1256 | A    | C8-N9-C4  | 10.43  | 109.97      | 105.80   |
| 1   | A     | 1522 | U    | O5'-P-OP2 | -10.40 | 96.34       | 105.70   |
| 1   | A     | 893  | C    | N1-C2-N3  | -10.37 | 111.94      | 119.20   |
| 1   | A     | 357  | G    | C5-C6-N1  | -10.32 | 106.34      | 111.50   |
| 1   | A     | 710  | G    | C5-C6-N1  | -10.31 | 106.35      | 111.50   |

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| Mol | Chain | Res  | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1   | A     | 1227 | A    | N1-C6-N6 | 10.30  | 124.78      | 118.60   |
| 1   | A     | 251  | G    | N1-C6-O6 | 10.17  | 126.00      | 119.90   |
| 1   | A     | 314  | C    | C6-N1-C2 | 10.16  | 124.36      | 120.30   |
| 1   | A     | 108  | G    | N1-C6-O6 | 10.15  | 125.99      | 119.90   |
| 1   | A     | 975  | A    | C2-N3-C4 | -10.11 | 105.54      | 110.60   |
| 1   | A     | 300  | A    | N1-C6-N6 | -10.11 | 112.54      | 118.60   |
| 1   | A     | 522  | C    | C6-N1-C2 | 10.07  | 124.33      | 120.30   |
| 1   | A     | 234  | C    | C6-N1-C2 | 10.06  | 124.32      | 120.30   |
| 1   | A     | 1531 | A    | C4-C5-N7 | 10.04  | 115.72      | 110.70   |
| 1   | A     | 204  | U    | C5-C6-N1 | 9.88   | 127.64      | 122.70   |
| 1   | A     | 277  | C    | C6-N1-C2 | 9.84   | 124.24      | 120.30   |
| 1   | A     | 325  | A    | N9-C4-C5 | 9.80   | 109.72      | 105.80   |
| 1   | A     | 147  | G    | C5-C6-N1 | -9.79  | 106.61      | 111.50   |
| 1   | A     | 266  | G    | N3-C4-C5 | 9.78   | 133.49      | 128.60   |
| 1   | A     | 724  | G    | N3-C4-C5 | -9.77  | 123.72      | 128.60   |
| 1   | A     | 1377 | A    | C2-N3-C4 | -9.75  | 105.72      | 110.60   |
| 1   | A     | 372  | C    | C6-N1-C2 | 9.72   | 124.19      | 120.30   |
| 1   | A     | 372  | C    | N1-C2-N3 | -9.72  | 112.39      | 119.20   |
| 1   | A     | 814  | A    | C2-N3-C4 | -9.72  | 105.74      | 110.60   |
| 1   | A     | 830  | G    | N1-C6-O6 | 9.72   | 125.73      | 119.90   |
| 1   | A     | 920  | U    | N3-C4-O4 | -9.70  | 112.61      | 119.40   |
| 1   | A     | 1233 | G    | C5-C6-N1 | -9.66  | 106.67      | 111.50   |
| 1   | A     | 922  | G    | N3-C2-N2 | -9.66  | 113.14      | 119.90   |
| 1   | A     | 309  | G    | C6-C5-N7 | -9.64  | 124.61      | 130.40   |
| 1   | A     | 332  | G    | N1-C6-O6 | 9.61   | 125.67      | 119.90   |
| 1   | A     | 255  | G    | N1-C6-O6 | 9.61   | 125.66      | 119.90   |
| 1   | A     | 1084 | G    | C4-C5-N7 | -9.61  | 106.96      | 110.80   |
| 1   | A     | 32   | A    | C6-N1-C2 | -9.59  | 112.85      | 118.60   |
| 1   | A     | 1531 | A    | C8-N9-C4 | -9.51  | 101.99      | 105.80   |
| 1   | A     | 557  | G    | N1-C6-O6 | 9.51   | 125.61      | 119.90   |
| 1   | A     | 829  | G    | C8-N9-C4 | 9.50   | 110.20      | 106.40   |
| 1   | A     | 855  | G    | C5-C6-N1 | -9.50  | 106.75      | 111.50   |
| 1   | A     | 27   | G    | C6-C5-N7 | -9.49  | 124.71      | 130.40   |
| 1   | A     | 113  | G    | N1-C6-O6 | 9.44   | 125.57      | 119.90   |
| 1   | A     | 333  | G    | C5-C6-N1 | -9.41  | 106.80      | 111.50   |
| 1   | A     | 541  | G    | C5-C6-O6 | -9.41  | 122.96      | 128.60   |
| 1   | A     | 871  | U    | N3-C2-O2 | -9.40  | 115.62      | 122.20   |
| 1   | A     | 604  | G    | N1-C6-O6 | 9.39   | 125.53      | 119.90   |
| 1   | A     | 325  | A    | C5-C6-N6 | 9.37   | 131.20      | 123.70   |
| 1   | A     | 886  | G    | N1-C6-O6 | 9.36   | 125.52      | 119.90   |
| 1   | A     | 298  | A    | C2-N3-C4 | -9.34  | 105.93      | 110.60   |
| 1   | A     | 855  | G    | C2-N3-C4 | -9.29  | 107.25      | 111.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | A     | 1054 | C    | N1-C2-O2   | 9.29  | 124.48      | 118.90   |
| 1   | A     | 267  | C    | N3-C4-N4   | -9.29 | 111.50      | 118.00   |
| 1   | A     | 558  | G    | C5-C6-O6   | 9.26  | 134.16      | 128.60   |
| 1   | A     | 518  | C    | N3-C2-O2   | -9.23 | 115.44      | 121.90   |
| 1   | A     | 635  | G    | N1-C6-O6   | 9.23  | 125.44      | 119.90   |
| 1   | A     | 761  | G    | N1-C6-O6   | 9.23  | 125.44      | 119.90   |
| 1   | A     | 562  | C    | N1-C2-O2   | 9.22  | 124.43      | 118.90   |
| 1   | A     | 500  | G    | O5'-P-OP1  | -9.21 | 97.41       | 105.70   |
| 1   | A     | 893  | C    | N1-C2-O2   | 9.21  | 124.42      | 118.90   |
| 1   | A     | 830  | G    | N3-C2-N2   | -9.16 | 113.49      | 119.90   |
| 1   | A     | 31   | G    | N3-C4-N9   | 9.15  | 131.49      | 126.00   |
| 1   | A     | 313  | A    | N1-C6-N6   | 9.15  | 124.09      | 118.60   |
| 1   | A     | 28   | G    | N1-C6-O6   | 9.14  | 125.39      | 119.90   |
| 1   | A     | 398  | C    | C6-N1-C2   | 9.11  | 123.94      | 120.30   |
| 1   | A     | 887  | G    | N1-C6-O6   | 9.11  | 125.36      | 119.90   |
| 1   | A     | 610  | G    | C8-N9-C4   | -9.09 | 102.76      | 106.40   |
| 1   | A     | 1166 | G    | N3-C4-C5   | -9.09 | 124.06      | 128.60   |
| 1   | A     | 661  | G    | N1-C6-O6   | 9.08  | 125.35      | 119.90   |
| 1   | A     | 810  | C    | N3-C4-N4   | -9.08 | 111.65      | 118.00   |
| 1   | A     | 1512 | U    | C5-C4-O4   | 9.07  | 131.34      | 125.90   |
| 1   | A     | 27   | G    | O5'-P-OP1  | -9.06 | 97.55       | 105.70   |
| 3   | C     | 179  | ARG  | N-CA-C     | -9.04 | 86.59       | 111.00   |
| 1   | A     | 811  | C    | C5-C6-N1   | -9.03 | 116.49      | 121.00   |
| 1   | A     | 1426 | C    | C6-N1-C2   | 9.02  | 123.91      | 120.30   |
| 1   | A     | 228  | A    | N1-C6-N6   | -8.98 | 113.21      | 118.60   |
| 1   | A     | 901  | A    | O5'-P-OP1  | -8.98 | 97.62       | 105.70   |
| 1   | A     | 1026 | G    | N7-C8-N9   | 8.98  | 117.59      | 113.10   |
| 1   | A     | 1087 | G    | N1-C6-O6   | 8.98  | 125.29      | 119.90   |
| 1   | A     | 381  | C    | C6-N1-C2   | -8.98 | 116.71      | 120.30   |
| 1   | A     | 1057 | G    | N3-C2-N2   | -8.92 | 113.66      | 119.90   |
| 1   | A     | 535  | A    | N1-C6-N6   | -8.91 | 113.25      | 118.60   |
| 1   | A     | 1070 | U    | O5'-P-OP2  | -8.90 | 97.69       | 105.70   |
| 1   | A     | 749  | C    | C6-N1-C2   | -8.90 | 116.74      | 120.30   |
| 1   | A     | 204  | U    | C2-N1-C1'  | 8.88  | 128.36      | 117.70   |
| 1   | A     | 828  | A    | C8-N9-C4   | 8.88  | 109.35      | 105.80   |
| 1   | A     | 1530 | G    | N3-C4-N9   | -8.86 | 120.69      | 126.00   |
| 1   | A     | 372  | C    | N3-C4-C5   | 8.83  | 125.43      | 121.90   |
| 1   | A     | 19   | C    | O5'-P-OP2  | -8.82 | 97.76       | 105.70   |
| 1   | A     | 1004 | A    | O4'-C1'-N9 | 8.80  | 115.24      | 108.20   |
| 1   | A     | 1277 | C    | C5-C6-N1   | 8.78  | 125.39      | 121.00   |
| 1   | A     | 661  | G    | C5-C6-N1   | -8.77 | 107.11      | 111.50   |
| 1   | A     | 1479 | C    | C6-N1-C2   | -8.76 | 116.80      | 120.30   |

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| Mol | Chain | Res     | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 1   | A     | 113     | G    | C6-C5-N7  | -8.76 | 125.14      | 130.40   |
| 1   | A     | 400     | C    | C6-N1-C2  | 8.75  | 123.80      | 120.30   |
| 1   | A     | 251     | G    | C5-C6-O6  | -8.74 | 123.36      | 128.60   |
| 1   | A     | 817     | C    | C2-N1-C1' | 8.72  | 128.39      | 118.80   |
| 1   | A     | 811     | C    | C6-N1-C2  | 8.72  | 123.79      | 120.30   |
| 1   | A     | 544     | G    | C4-C5-N7  | 8.71  | 114.28      | 110.80   |
| 1   | A     | 387     | U    | O5'-P-OP2 | -8.71 | 97.86       | 105.70   |
| 1   | A     | 590     | C    | C6-N1-C2  | 8.71  | 123.78      | 120.30   |
| 1   | A     | 239     | U    | N3-C4-O4  | 8.70  | 125.49      | 119.40   |
| 1   | A     | 664     | G    | C5-N7-C8  | 8.70  | 108.65      | 104.30   |
| 1   | A     | 241     | C    | C6-N1-C2  | 8.70  | 123.78      | 120.30   |
| 1   | A     | 265     | G    | N3-C4-N9  | -8.70 | 120.78      | 126.00   |
| 1   | A     | 557     | G    | C6-C5-N7  | -8.70 | 125.18      | 130.40   |
| 1   | A     | 1393    | U    | C4-C5-C6  | 8.69  | 124.92      | 119.70   |
| 1   | A     | 1075    | C    | O5'-P-OP2 | -8.69 | 97.88       | 105.70   |
| 1   | A     | 1531    | A    | C6-C5-N7  | -8.68 | 126.23      | 132.30   |
| 1   | A     | 247     | G    | N1-C6-O6  | 8.66  | 125.10      | 119.90   |
| 1   | A     | 484     | G    | N1-C2-N2  | -8.65 | 108.41      | 116.20   |
| 1   | A     | 113     | G    | N3-C4-N9  | 8.65  | 131.19      | 126.00   |
| 1   | A     | 503     | C    | O5'-P-OP2 | -8.65 | 97.92       | 105.70   |
| 1   | A     | 1290    | G    | N1-C6-O6  | 8.63  | 125.08      | 119.90   |
| 1   | A     | 31      | G    | C8-N9-C1' | -8.61 | 115.81      | 127.00   |
| 1   | A     | 1516[A] | G    | N3-C4-N9  | -8.60 | 120.84      | 126.00   |
| 1   | A     | 1516[B] | G    | N3-C4-N9  | -8.60 | 120.84      | 126.00   |
| 1   | A     | 403     | C    | O5'-P-OP2 | -8.60 | 97.96       | 105.70   |
| 1   | A     | 927     | G    | O5'-P-OP1 | -8.60 | 97.96       | 105.70   |
| 1   | A     | 922     | G    | C6-C5-N7  | -8.60 | 125.24      | 130.40   |
| 1   | A     | 728     | A    | C8-N9-C4  | -8.60 | 102.36      | 105.80   |
| 1   | A     | 783     | C    | C6-N1-C2  | 8.59  | 123.73      | 120.30   |
| 1   | A     | 731     | G    | C4-C5-N7  | 8.59  | 114.23      | 110.80   |
| 1   | A     | 10      | A    | O5'-P-OP2 | -8.58 | 97.98       | 105.70   |
| 1   | A     | 113     | G    | C5-C6-O6  | -8.57 | 123.45      | 128.60   |
| 1   | A     | 1512    | U    | C6-N1-C2  | -8.57 | 115.86      | 121.00   |
| 1   | A     | 266     | G    | C5-N7-C8  | -8.56 | 100.02      | 104.30   |
| 1   | A     | 99      | C    | C6-N1-C2  | -8.54 | 116.89      | 120.30   |
| 1   | A     | 1256    | A    | N7-C8-N9  | -8.52 | 109.54      | 113.80   |
| 1   | A     | 1528    | U    | OP1-P-OP2 | 8.52  | 132.38      | 119.60   |
| 1   | A     | 46      | G    | C8-N9-C4  | -8.51 | 103.00      | 106.40   |
| 1   | A     | 794     | A    | O5'-P-OP2 | -8.51 | 98.04       | 105.70   |
| 1   | A     | 108     | G    | C6-C5-N7  | -8.49 | 125.30      | 130.40   |
| 1   | A     | 1432    | G    | C8-N9-C4  | -8.49 | 103.00      | 106.40   |
| 1   | A     | 1026    | G    | C8-N9-C4  | -8.48 | 103.01      | 106.40   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | A     | 1432 | G    | C5-C6-N1  | -8.45 | 107.27      | 111.50   |
| 1   | A     | 1305 | G    | C8-N9-C4  | -8.45 | 103.02      | 106.40   |
| 1   | A     | 47   | C    | N3-C2-O2  | -8.45 | 115.99      | 121.90   |
| 1   | A     | 277  | C    | O5'-P-OP1 | -8.44 | 98.10       | 105.70   |
| 1   | A     | 664  | G    | C4-C5-N7  | -8.44 | 107.43      | 110.80   |
| 1   | A     | 121  | C    | C6-N1-C2  | 8.43  | 123.67      | 120.30   |
| 1   | A     | 15   | G    | N1-C6-O6  | 8.42  | 124.95      | 119.90   |
| 1   | A     | 284  | G    | N1-C6-O6  | 8.42  | 124.95      | 119.90   |
| 1   | A     | 818  | G    | OP1-P-OP2 | 8.41  | 132.22      | 119.60   |
| 1   | A     | 21   | G    | C6-C5-N7  | -8.41 | 125.36      | 130.40   |
| 1   | A     | 541  | G    | C6-C5-N7  | -8.39 | 125.36      | 130.40   |
| 1   | A     | 1087 | G    | C6-C5-N7  | -8.38 | 125.37      | 130.40   |
| 1   | A     | 372  | C    | N1-C2-O2  | 8.38  | 123.92      | 118.90   |
| 1   | A     | 699  | C    | C6-N1-C2  | 8.37  | 123.65      | 120.30   |
| 1   | A     | 729  | A    | OP1-P-O3' | 8.37  | 123.62      | 105.20   |
| 1   | A     | 500  | G    | N1-C6-O6  | 8.36  | 124.91      | 119.90   |
| 1   | A     | 25   | C    | C6-N1-C2  | 8.34  | 123.64      | 120.30   |
| 1   | A     | 485  | G    | C8-N9-C4  | 8.34  | 109.74      | 106.40   |
| 1   | A     | 1205 | U    | N3-C4-C5  | -8.33 | 109.60      | 114.60   |
| 1   | A     | 526  | C    | O5'-P-OP1 | 8.32  | 120.69      | 110.70   |
| 1   | A     | 122  | G    | N7-C8-N9  | -8.30 | 108.95      | 113.10   |
| 1   | A     | 987  | G    | N1-C6-O6  | 8.30  | 124.88      | 119.90   |
| 1   | A     | 304  | U    | C4-C5-C6  | 8.29  | 124.67      | 119.70   |
| 1   | A     | 774  | G    | C6-C5-N7  | -8.28 | 125.43      | 130.40   |
| 1   | A     | 1050 | G    | C5-C6-O6  | -8.28 | 123.63      | 128.60   |
| 1   | A     | 20   | U    | C5-C4-O4  | -8.26 | 120.94      | 125.90   |
| 1   | A     | 117  | G    | C5-C6-O6  | -8.26 | 123.65      | 128.60   |
| 1   | A     | 1211 | U    | C5-C6-N1  | 8.26  | 126.83      | 122.70   |
| 1   | A     | 58   | C    | C5-C6-N1  | 8.24  | 125.12      | 121.00   |
| 1   | A     | 724  | G    | C8-N9-C4  | -8.24 | 103.11      | 106.40   |
| 1   | A     | 45   | U    | N3-C4-C5  | -8.23 | 109.66      | 114.60   |
| 1   | A     | 122  | G    | N9-C4-C5  | -8.22 | 102.11      | 105.40   |
| 1   | A     | 113  | G    | C8-N9-C1' | -8.21 | 116.32      | 127.00   |
| 1   | A     | 1393 | U    | N3-C4-C5  | -8.21 | 109.67      | 114.60   |
| 1   | A     | 408  | A    | C8-N9-C4  | -8.20 | 102.52      | 105.80   |
| 1   | A     | 906  | G    | N1-C6-O6  | 8.20  | 124.82      | 119.90   |
| 1   | A     | 133  | U    | C5-C4-O4  | 8.19  | 130.81      | 125.90   |
| 1   | A     | 239  | U    | C6-N1-C2  | -8.19 | 116.09      | 121.00   |
| 1   | A     | 766  | A    | O5'-P-OP2 | -8.18 | 98.33       | 105.70   |
| 1   | A     | 284  | G    | C2-N3-C4  | -8.18 | 107.81      | 111.90   |
| 1   | A     | 1230 | C    | C2-N3-C4  | 8.18  | 123.99      | 119.90   |
| 1   | A     | 724  | G    | C6-C5-N7  | -8.15 | 125.51      | 130.40   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | A     | 111  | G    | N3-C4-N9  | -8.14 | 121.11      | 126.00   |
| 1   | A     | 703  | G    | C8-N9-C1' | -8.14 | 116.41      | 127.00   |
| 1   | A     | 730  | G    | C5-N7-C8  | 8.14  | 108.37      | 104.30   |
| 1   | A     | 886  | G    | C2-N3-C4  | -8.13 | 107.83      | 111.90   |
| 1   | A     | 877  | C    | C6-N1-C2  | -8.13 | 117.05      | 120.30   |
| 1   | A     | 266  | G    | N3-C4-N9  | -8.12 | 121.13      | 126.00   |
| 1   | A     | 674  | G    | N1-C6-O6  | 8.12  | 124.77      | 119.90   |
| 1   | A     | 819  | A    | N1-C6-N6  | 8.12  | 123.47      | 118.60   |
| 1   | A     | 117  | G    | N9-C4-C5  | -8.10 | 102.16      | 105.40   |
| 1   | A     | 500  | G    | C8-N9-C4  | 8.09  | 109.64      | 106.40   |
| 1   | A     | 7    | G    | C5-C6-O6  | -8.09 | 123.75      | 128.60   |
| 1   | A     | 306  | G    | N1-C6-O6  | 8.08  | 124.75      | 119.90   |
| 1   | A     | 799  | G    | C6-C5-N7  | -8.07 | 125.56      | 130.40   |
| 1   | A     | 731  | G    | C5-N7-C8  | -8.05 | 100.27      | 104.30   |
| 1   | A     | 147  | G    | C6-C5-N7  | -8.05 | 125.57      | 130.40   |
| 1   | A     | 509  | A    | C8-N9-C4  | -8.05 | 102.58      | 105.80   |
| 1   | A     | 484  | G    | P-O3'-C3' | 8.05  | 129.36      | 119.70   |
| 1   | A     | 1435 | G    | C2-N3-C4  | -8.05 | 107.88      | 111.90   |
| 1   | A     | 1050 | G    | C6-C5-N7  | -8.04 | 125.57      | 130.40   |
| 1   | A     | 1064 | G    | C4-C5-N7  | 8.04  | 114.01      | 110.80   |
| 1   | A     | 893  | C    | C2-N3-C4  | 8.03  | 123.92      | 119.90   |
| 1   | A     | 1523 | G    | N1-C6-O6  | 8.03  | 124.72      | 119.90   |
| 1   | A     | 1491 | G    | C8-N9-C4  | -8.02 | 103.19      | 106.40   |
| 1   | A     | 507  | C    | C6-N1-C2  | 8.02  | 123.51      | 120.30   |
| 1   | A     | 785  | G    | N1-C6-O6  | 8.01  | 124.71      | 119.90   |
| 1   | A     | 646  | U    | N3-C4-C5  | -8.01 | 109.80      | 114.60   |
| 1   | A     | 976  | G    | C5-C6-N1  | -8.01 | 107.50      | 111.50   |
| 1   | A     | 1173 | G    | C8-N9-C4  | 8.01  | 109.60      | 106.40   |
| 1   | A     | 32   | A    | N1-C2-N3  | 8.00  | 133.30      | 129.30   |
| 1   | A     | 1539 | C    | C6-N1-C2  | -8.00 | 117.10      | 120.30   |
| 1   | A     | 484  | G    | N1-C6-O6  | -8.00 | 115.10      | 119.90   |
| 1   | A     | 1202 | G    | N9-C4-C5  | 7.99  | 108.60      | 105.40   |
| 1   | A     | 260  | G    | C8-N9-C4  | -7.99 | 103.20      | 106.40   |
| 1   | A     | 314  | C    | N3-C4-C5  | 7.99  | 125.09      | 121.90   |
| 1   | A     | 906  | G    | C6-C5-N7  | -7.99 | 125.61      | 130.40   |
| 1   | A     | 133  | U    | N3-C2-O2  | -7.98 | 116.61      | 122.20   |
| 1   | A     | 791  | G    | C4-C5-C6  | 7.98  | 123.59      | 118.80   |
| 1   | A     | 1131 | G    | N1-C6-O6  | 7.98  | 124.69      | 119.90   |
| 1   | A     | 1202 | G    | N3-C4-N9  | -7.97 | 121.22      | 126.00   |
| 1   | A     | 27   | G    | C5-C6-O6  | -7.97 | 123.82      | 128.60   |
| 1   | A     | 333  | G    | N3-C2-N2  | -7.95 | 114.33      | 119.90   |
| 17  | Q     | 98   | LEU  | CA-CB-CG  | 7.95  | 133.59      | 115.30   |

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| Mol | Chain | Res     | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 1   | A     | 190(H)  | G    | N1-C6-O6  | 7.95  | 124.67      | 119.90   |
| 1   | A     | 290     | C    | O5'-P-OP2 | -7.93 | 98.56       | 105.70   |
| 1   | A     | 830     | G    | N3-C4-C5  | 7.93  | 132.57      | 128.60   |
| 1   | A     | 104     | G    | C5-C6-N1  | -7.93 | 107.53      | 111.50   |
| 1   | A     | 1084    | G    | C5-C6-O6  | 7.93  | 133.36      | 128.60   |
| 1   | A     | 799     | G    | N1-C6-O6  | 7.92  | 124.65      | 119.90   |
| 1   | A     | 1304    | G    | C5-C6-N1  | -7.92 | 107.54      | 111.50   |
| 1   | A     | 1211    | U    | N1-C2-O2  | 7.92  | 128.34      | 122.80   |
| 1   | A     | 257     | G    | N1-C6-O6  | 7.91  | 124.65      | 119.90   |
| 1   | A     | 936     | C    | O5'-P-OP2 | 7.91  | 120.19      | 110.70   |
| 1   | A     | 401     | C    | N3-C4-N4  | 7.91  | 123.53      | 118.00   |
| 1   | A     | 1393    | U    | N3-C4-O4  | 7.89  | 124.93      | 119.40   |
| 1   | A     | 102     | G    | C6-C5-N7  | -7.89 | 125.66      | 130.40   |
| 1   | A     | 1104    | G    | N1-C2-N3  | 7.89  | 128.63      | 123.90   |
| 1   | A     | 1257    | U    | C2-N1-C1' | 7.89  | 127.17      | 117.70   |
| 1   | A     | 852     | G    | N1-C6-O6  | 7.89  | 124.63      | 119.90   |
| 1   | A     | 481     | G    | C6-C5-N7  | -7.89 | 125.67      | 130.40   |
| 1   | A     | 1166    | G    | N3-C4-N9  | 7.89  | 130.73      | 126.00   |
| 1   | A     | 276     | G    | N1-C2-N3  | 7.88  | 128.63      | 123.90   |
| 1   | A     | 1189    | C    | C6-N1-C2  | -7.88 | 117.15      | 120.30   |
| 1   | A     | 288     | A    | C2-N3-C4  | -7.88 | 106.66      | 110.60   |
| 1   | A     | 1230    | C    | N1-C2-N3  | -7.88 | 113.69      | 119.20   |
| 1   | A     | 113     | G    | C4-N9-C1' | 7.87  | 136.74      | 126.50   |
| 1   | A     | 965     | A    | C8-N9-C4  | 7.87  | 108.95      | 105.80   |
| 1   | A     | 204     | U    | C6-N1-C2  | -7.86 | 116.28      | 121.00   |
| 1   | A     | 579     | G    | N1-C6-O6  | 7.85  | 124.61      | 119.90   |
| 1   | A     | 252     | U    | N1-C2-O2  | -7.85 | 117.30      | 122.80   |
| 1   | A     | 1079    | G    | N3-C4-C5  | -7.84 | 124.68      | 128.60   |
| 1   | A     | 674     | G    | C6-C5-N7  | -7.83 | 125.70      | 130.40   |
| 1   | A     | 329     | A    | O5'-P-OP1 | -7.81 | 98.67       | 105.70   |
| 1   | A     | 232     | G    | C6-C5-N7  | -7.81 | 125.71      | 130.40   |
| 1   | A     | 928     | G    | C5-C6-N1  | -7.81 | 107.59      | 111.50   |
| 1   | A     | 672     | U    | C4-C5-C6  | 7.80  | 124.38      | 119.70   |
| 1   | A     | 49      | U    | N3-C2-O2  | 7.80  | 127.66      | 122.20   |
| 1   | A     | 1532    | U    | C4-C5-C6  | -7.80 | 115.02      | 119.70   |
| 1   | A     | 254     | G    | OP2-P-O3' | 7.79  | 122.35      | 105.20   |
| 1   | A     | 558     | G    | N3-C4-N9  | -7.79 | 121.33      | 126.00   |
| 1   | A     | 562     | C    | C6-N1-C2  | 7.78  | 123.41      | 120.30   |
| 1   | A     | 902     | G    | N9-C4-C5  | -7.78 | 102.29      | 105.40   |
| 1   | A     | 1516[A] | G    | C2-N3-C4  | -7.78 | 108.01      | 111.90   |
| 1   | A     | 1516[B] | G    | C2-N3-C4  | -7.78 | 108.01      | 111.90   |
| 1   | A     | 928     | G    | N1-C6-O6  | 7.77  | 124.56      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | A     | 401  | C    | N1-C2-O2  | -7.77 | 114.24      | 118.90   |
| 1   | A     | 830  | G    | N3-C4-N9  | -7.77 | 121.34      | 126.00   |
| 1   | A     | 646  | U    | C6-N1-C2  | -7.77 | 116.34      | 121.00   |
| 1   | A     | 1532 | U    | N3-C2-O2  | 7.77  | 127.64      | 122.20   |
| 1   | A     | 1524 | C    | O5'-P-OP1 | -7.76 | 98.72       | 105.70   |
| 1   | A     | 761  | G    | C5-C6-N1  | -7.75 | 107.62      | 111.50   |
| 1   | A     | 789  | U    | N3-C4-C5  | -7.75 | 109.95      | 114.60   |
| 1   | A     | 902  | G    | C5-C6-O6  | -7.75 | 123.95      | 128.60   |
| 1   | A     | 976  | G    | N1-C6-O6  | 7.75  | 124.55      | 119.90   |
| 1   | A     | 703  | G    | C5-C6-O6  | 7.74  | 133.25      | 128.60   |
| 1   | A     | 1189 | C    | N3-C2-O2  | -7.74 | 116.48      | 121.90   |
| 1   | A     | 920  | U    | C5-C4-O4  | 7.73  | 130.54      | 125.90   |
| 1   | A     | 864  | A    | N9-C4-C5  | 7.73  | 108.89      | 105.80   |
| 1   | A     | 500  | G    | C5-C6-O6  | -7.72 | 123.97      | 128.60   |
| 1   | A     | 1502 | A    | C2-N3-C4  | -7.71 | 106.74      | 110.60   |
| 1   | A     | 761  | G    | C2-N3-C4  | -7.71 | 108.05      | 111.90   |
| 1   | A     | 746  | A    | C6-N1-C2  | -7.71 | 113.97      | 118.60   |
| 1   | A     | 1433 | A    | O5'-P-OP1 | -7.71 | 98.76       | 105.70   |
| 1   | A     | 372  | C    | C5-C4-N4  | -7.70 | 114.81      | 120.20   |
| 1   | A     | 1530 | G    | C4-N9-C1' | -7.70 | 116.49      | 126.50   |
| 1   | A     | 830  | G    | C2-N3-C4  | -7.70 | 108.05      | 111.90   |
| 1   | A     | 659  | U    | N1-C2-N3  | 7.69  | 119.51      | 114.90   |
| 1   | A     | 786  | G    | N1-C6-O6  | 7.68  | 124.51      | 119.90   |
| 1   | A     | 251  | G    | C4-C5-N7  | 7.66  | 113.86      | 110.80   |
| 1   | A     | 1124 | G    | N1-C2-N3  | -7.66 | 119.31      | 123.90   |
| 1   | A     | 239  | U    | C4-C5-C6  | 7.66  | 124.29      | 119.70   |
| 1   | A     | 654  | G    | N3-C4-N9  | -7.66 | 121.41      | 126.00   |
| 1   | A     | 558  | G    | C4-C5-N7  | -7.64 | 107.75      | 110.80   |
| 1   | A     | 637  | G    | N1-C6-O6  | 7.64  | 124.48      | 119.90   |
| 1   | A     | 120  | A    | C4-C5-C6  | 7.63  | 120.82      | 117.00   |
| 1   | A     | 1100 | C    | C5-C6-N1  | 7.62  | 124.81      | 121.00   |
| 1   | A     | 786  | G    | C5-C6-N1  | -7.62 | 107.69      | 111.50   |
| 1   | A     | 829  | G    | O5'-P-OP2 | -7.60 | 98.86       | 105.70   |
| 1   | A     | 1047 | G    | C5-C6-N1  | -7.59 | 107.71      | 111.50   |
| 1   | A     | 659  | U    | N3-C2-O2  | -7.57 | 116.90      | 122.20   |
| 1   | A     | 485  | G    | C5-C6-N1  | -7.56 | 107.72      | 111.50   |
| 1   | A     | 1182 | G    | N3-C4-C5  | -7.55 | 124.82      | 128.60   |
| 1   | A     | 392  | G    | C8-N9-C4  | 7.54  | 109.42      | 106.40   |
| 1   | A     | 902  | G    | C6-C5-N7  | -7.54 | 125.88      | 130.40   |
| 1   | A     | 108  | G    | C2-N3-C4  | -7.53 | 108.13      | 111.90   |
| 1   | A     | 387  | U    | N3-C4-C5  | -7.53 | 110.08      | 114.60   |
| 1   | A     | 491  | G    | C5-C6-N1  | -7.53 | 107.73      | 111.50   |

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| Mol | Chain | Res     | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 1   | A     | 1104    | G    | C2-N3-C4  | -7.53 | 108.14      | 111.90   |
| 1   | A     | 446     | G    | O5'-P-OP1 | -7.53 | 98.93       | 105.70   |
| 1   | A     | 1084    | G    | C5-N7-C8  | 7.53  | 108.06      | 104.30   |
| 1   | A     | 117     | G    | C4-C5-N7  | 7.52  | 113.81      | 110.80   |
| 1   | A     | 740     | U    | N1-C2-O2  | -7.52 | 117.54      | 122.80   |
| 1   | A     | 1129    | C    | C6-N1-C2  | -7.52 | 117.29      | 120.30   |
| 1   | A     | 1465    | C    | N1-C2-O2  | 7.51  | 123.41      | 118.90   |
| 1   | A     | 1030(C) | G    | C4-N9-C1' | 7.51  | 136.26      | 126.50   |
| 2   | B     | 71      | VAL  | CB-CA-C   | -7.51 | 97.13       | 111.40   |
| 1   | A     | 481     | G    | OP1-P-OP2 | 7.49  | 130.84      | 119.60   |
| 1   | A     | 724     | G    | N3-C4-N9  | 7.49  | 130.50      | 126.00   |
| 1   | A     | 1395    | C    | C6-N1-C2  | 7.49  | 123.30      | 120.30   |
| 1   | A     | 1516[A] | G    | N3-C4-C5  | 7.49  | 132.35      | 128.60   |
| 1   | A     | 1516[B] | G    | N3-C4-C5  | 7.49  | 132.35      | 128.60   |
| 1   | A     | 494     | G    | C8-N9-C4  | -7.49 | 103.40      | 106.40   |
| 1   | A     | 120     | A    | N1-C2-N3  | 7.49  | 133.04      | 129.30   |
| 17  | Q     | 84      | LEU  | CA-CB-CG  | -7.49 | 98.08       | 115.30   |
| 1   | A     | 833     | U    | N3-C4-C5  | -7.48 | 110.11      | 114.60   |
| 1   | A     | 1222    | G    | N1-C6-O6  | 7.48  | 124.39      | 119.90   |
| 1   | A     | 494     | G    | O5'-P-OP1 | -7.47 | 98.98       | 105.70   |
| 1   | A     | 829     | G    | N7-C8-N9  | -7.47 | 109.36      | 113.10   |
| 1   | A     | 314     | C    | C2-N1-C1' | -7.47 | 110.59      | 118.80   |
| 1   | A     | 774     | G    | N3-C4-N9  | 7.46  | 130.48      | 126.00   |
| 1   | A     | 1539    | C    | C5-C6-N1  | 7.46  | 124.73      | 121.00   |
| 1   | A     | 1075    | C    | C5-C6-N1  | -7.45 | 117.27      | 121.00   |
| 1   | A     | 1411    | C    | N1-C2-O2  | 7.45  | 123.37      | 118.90   |
| 1   | A     | 309     | G    | N3-C2-N2  | -7.44 | 114.69      | 119.90   |
| 1   | A     | 689     | C    | N3-C2-O2  | 7.44  | 127.11      | 121.90   |
| 1   | A     | 276     | G    | C2-N3-C4  | -7.43 | 108.18      | 111.90   |
| 1   | A     | 729     | A    | N9-C4-C5  | 7.43  | 108.77      | 105.80   |
| 1   | A     | 26      | A    | C2-N3-C4  | -7.43 | 106.89      | 110.60   |
| 1   | A     | 535     | A    | N9-C4-C5  | 7.42  | 108.77      | 105.80   |
| 1   | A     | 275     | G    | N1-C6-O6  | 7.42  | 124.35      | 119.90   |
| 1   | A     | 746     | A    | N1-C2-N3  | 7.42  | 133.01      | 129.30   |
| 1   | A     | 730     | G    | N9-C4-C5  | 7.42  | 108.37      | 105.40   |
| 1   | A     | 1197    | G    | C4-N9-C1' | 7.41  | 136.14      | 126.50   |
| 1   | A     | 1420    | C    | C6-N1-C2  | -7.41 | 117.34      | 120.30   |
| 1   | A     | 244     | U    | N1-C2-N3  | -7.41 | 110.45      | 114.90   |
| 1   | A     | 108     | G    | C4-C5-N7  | 7.40  | 113.76      | 110.80   |
| 1   | A     | 975     | A    | N7-C8-N9  | 7.40  | 117.50      | 113.80   |
| 2   | B     | 11      | LEU  | CA-CB-CG  | 7.40  | 132.31      | 115.30   |
| 1   | A     | 394     | G    | C5-C6-N1  | -7.39 | 107.80      | 111.50   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | A     | 29   | G    | N1-C6-O6   | 7.39  | 124.34      | 119.90   |
| 1   | A     | 715  | A    | C8-N9-C4   | 7.39  | 108.76      | 105.80   |
| 1   | A     | 83   | U    | N1-C2-N3   | -7.38 | 110.47      | 114.90   |
| 1   | A     | 1121 | U    | C5-C6-N1   | -7.38 | 119.01      | 122.70   |
| 1   | A     | 1286 | A    | N1-C6-N6   | 7.38  | 123.03      | 118.60   |
| 1   | A     | 1495 | U    | N3-C4-C5   | -7.36 | 110.18      | 114.60   |
| 1   | A     | 662  | G    | N9-C4-C5   | -7.36 | 102.46      | 105.40   |
| 1   | A     | 61   | G    | N1-C6-O6   | 7.36  | 124.31      | 119.90   |
| 1   | A     | 499  | A    | N1-C6-N6   | -7.36 | 114.19      | 118.60   |
| 1   | A     | 549  | C    | C5-C6-N1   | -7.36 | 117.32      | 121.00   |
| 1   | A     | 1092 | A    | O5'-P-OP2  | -7.35 | 99.09       | 105.70   |
| 1   | A     | 1222 | G    | C2-N3-C4   | -7.34 | 108.23      | 111.90   |
| 1   | A     | 864  | A    | N1-C6-N6   | -7.34 | 114.20      | 118.60   |
| 1   | A     | 881  | G    | C8-N9-C4   | 7.34  | 109.33      | 106.40   |
| 1   | A     | 672  | U    | C5-C4-O4   | 7.34  | 130.30      | 125.90   |
| 1   | A     | 378  | G    | N1-C6-O6   | 7.33  | 124.30      | 119.90   |
| 1   | A     | 66   | G    | N3-C4-C5   | 7.33  | 132.26      | 128.60   |
| 1   | A     | 558  | G    | C6-N1-C2   | 7.32  | 129.49      | 125.10   |
| 1   | A     | 1075 | C    | C4-C5-C6   | 7.32  | 121.06      | 117.40   |
| 1   | A     | 197  | A    | N1-C6-N6   | -7.30 | 114.22      | 118.60   |
| 1   | A     | 730  | G    | C5-C6-O6   | 7.30  | 132.98      | 128.60   |
| 1   | A     | 9    | G    | C8-N9-C4   | 7.30  | 109.32      | 106.40   |
| 1   | A     | 1530 | G    | N1-C6-O6   | 7.30  | 124.28      | 119.90   |
| 1   | A     | 818  | G    | C4-C5-N7   | -7.29 | 107.88      | 110.80   |
| 1   | A     | 741  | G    | C4-C5-N7   | -7.29 | 107.89      | 110.80   |
| 1   | A     | 446  | G    | C5-C6-O6   | -7.28 | 124.23      | 128.60   |
| 1   | A     | 122  | G    | N3-C4-N9   | 7.28  | 130.37      | 126.00   |
| 1   | A     | 556  | C    | C5-C4-N4   | -7.27 | 115.11      | 120.20   |
| 1   | A     | 1183 | A    | N1-C6-N6   | 7.27  | 122.96      | 118.60   |
| 1   | A     | 117  | G    | C5-C6-N1   | -7.27 | 107.87      | 111.50   |
| 1   | A     | 1125 | U    | C6-N1-C2   | 7.27  | 125.36      | 121.00   |
| 1   | A     | 61   | G    | N3-C4-C5   | 7.26  | 132.23      | 128.60   |
| 1   | A     | 27   | G    | C4-C5-N7   | 7.25  | 113.70      | 110.80   |
| 2   | B     | 155  | LEU  | CA-CB-CG   | 7.25  | 131.97      | 115.30   |
| 1   | A     | 300  | A    | N9-C4-C5   | 7.24  | 108.70      | 105.80   |
| 1   | A     | 524  | G    | O5'-P-OP1  | -7.24 | 99.18       | 105.70   |
| 1   | A     | 1528 | U    | O5'-P-OP1  | 7.23  | 119.38      | 110.70   |
| 1   | A     | 522  | C    | N3-C2-O2   | 7.23  | 126.96      | 121.90   |
| 1   | A     | 902  | G    | C8-N9-C4   | 7.23  | 109.29      | 106.40   |
| 1   | A     | 928  | G    | C2-N3-C4   | -7.23 | 108.28      | 111.90   |
| 1   | A     | 1212 | U    | O4'-C1'-N1 | 7.22  | 113.98      | 108.20   |
| 1   | A     | 289  | G    | N1-C6-O6   | 7.22  | 124.23      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | A     | 1490 | C    | C5-C6-N1  | 7.21  | 124.61      | 121.00   |
| 1   | A     | 31   | G    | N9-C4-C5  | -7.20 | 102.52      | 105.40   |
| 1   | A     | 1328 | C    | C6-N1-C2  | 7.20  | 123.18      | 120.30   |
| 1   | A     | 306  | G    | N3-C2-N2  | -7.20 | 114.86      | 119.90   |
| 1   | A     | 549  | C    | C6-N1-C2  | 7.20  | 123.18      | 120.30   |
| 1   | A     | 885  | G    | C5-C6-N1  | -7.20 | 107.90      | 111.50   |
| 1   | A     | 47   | C    | C5-C6-N1  | -7.19 | 117.40      | 121.00   |
| 1   | A     | 894  | G    | C2-N3-C4  | -7.19 | 108.30      | 111.90   |
| 1   | A     | 181  | G    | C4-N9-C1' | 7.18  | 135.83      | 126.50   |
| 1   | A     | 66   | G    | N3-C4-N9  | -7.17 | 121.70      | 126.00   |
| 1   | A     | 611  | A    | N1-C6-N6  | -7.17 | 114.30      | 118.60   |
| 1   | A     | 889  | A    | N9-C4-C5  | 7.17  | 108.67      | 105.80   |
| 1   | A     | 651  | C    | C6-N1-C2  | 7.17  | 123.17      | 120.30   |
| 1   | A     | 235  | C    | C6-N1-C2  | 7.16  | 123.17      | 120.30   |
| 1   | A     | 1258 | G    | C8-N9-C4  | -7.16 | 103.54      | 106.40   |
| 1   | A     | 674  | G    | C2-N3-C4  | -7.16 | 108.32      | 111.90   |
| 1   | A     | 833  | U    | C5-C4-O4  | 7.16  | 130.19      | 125.90   |
| 1   | A     | 504  | C    | C6-N1-C2  | -7.15 | 117.44      | 120.30   |
| 1   | A     | 1435 | G    | C5-C6-O6  | -7.14 | 124.32      | 128.60   |
| 1   | A     | 1166 | G    | C4-N9-C1' | 7.14  | 135.78      | 126.50   |
| 4   | D     | 12   | CYS  | CA-CB-SG  | 7.14  | 126.85      | 114.00   |
| 1   | A     | 584  | G    | N7-C8-N9  | -7.14 | 109.53      | 113.10   |
| 1   | A     | 729  | A    | C8-N9-C4  | -7.14 | 102.94      | 105.80   |
| 1   | A     | 1526 | G    | N3-C2-N2  | -7.14 | 114.90      | 119.90   |
| 1   | A     | 672  | U    | C2-N3-C4  | 7.13  | 131.28      | 127.00   |
| 1   | A     | 522  | C    | C2-N1-C1' | -7.12 | 110.96      | 118.80   |
| 1   | A     | 1513 | A    | C8-N9-C4  | 7.12  | 108.65      | 105.80   |
| 1   | A     | 1432 | G    | N3-C4-N9  | -7.11 | 121.73      | 126.00   |
| 1   | A     | 299  | G    | C4-C5-C6  | 7.11  | 123.07      | 118.80   |
| 1   | A     | 803  | G    | OP2-P-O3' | 7.11  | 120.83      | 105.20   |
| 1   | A     | 285  | G    | N9-C4-C5  | -7.11 | 102.56      | 105.40   |
| 1   | A     | 1104 | G    | N1-C2-N2  | -7.11 | 109.81      | 116.20   |
| 1   | A     | 735  | C    | C6-N1-C2  | 7.10  | 123.14      | 120.30   |
| 1   | A     | 765  | G    | C8-N9-C4  | 7.10  | 109.24      | 106.40   |
| 1   | A     | 20   | U    | C6-N1-C2  | 7.09  | 125.26      | 121.00   |
| 1   | A     | 1392 | G    | N1-C6-O6  | -7.09 | 115.64      | 119.90   |
| 1   | A     | 789  | U    | N1-C2-N3  | 7.09  | 119.15      | 114.90   |
| 1   | A     | 817  | C    | C6-N1-C1' | -7.08 | 112.30      | 120.80   |
| 1   | A     | 230  | G    | C5-C6-N1  | -7.08 | 107.96      | 111.50   |
| 1   | A     | 630  | G    | C8-N9-C4  | 7.08  | 109.23      | 106.40   |
| 1   | A     | 1155 | G    | C8-N9-C1' | -7.07 | 117.81      | 127.00   |
| 1   | A     | 586  | C    | C5-C4-N4  | -7.07 | 115.25      | 120.20   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | A     | 21   | G    | N3-C2-N2  | 7.07  | 124.85      | 119.90   |
| 1   | A     | 1126 | U    | C5-C6-N1  | 7.07  | 126.23      | 122.70   |
| 1   | A     | 1155 | G    | C5-C6-N1  | -7.07 | 107.97      | 111.50   |
| 1   | A     | 566  | G    | C8-N9-C4  | 7.07  | 109.23      | 106.40   |
| 1   | A     | 494  | G    | O5'-P-OP2 | 7.06  | 119.17      | 110.70   |
| 1   | A     | 497  | A    | N1-C6-N6  | -7.06 | 114.37      | 118.60   |
| 1   | A     | 748  | C    | C2-N1-C1' | 7.05  | 126.56      | 118.80   |
| 1   | A     | 1397 | C    | OP1-P-OP2 | 7.05  | 130.18      | 119.60   |
| 1   | A     | 1155 | G    | C4-C5-C6  | 7.05  | 123.03      | 118.80   |
| 1   | A     | 1257 | U    | C5-C6-N1  | 7.04  | 126.22      | 122.70   |
| 1   | A     | 578  | C    | N3-C2-O2  | -7.04 | 116.97      | 121.90   |
| 1   | A     | 44   | G    | C6-C5-N7  | -7.03 | 126.18      | 130.40   |
| 1   | A     | 703  | G    | C4-N9-C1' | 7.03  | 135.64      | 126.50   |
| 1   | A     | 484  | G    | C5-C6-O6  | 7.03  | 132.82      | 128.60   |
| 1   | A     | 299  | G    | C6-C5-N7  | -7.03 | 126.18      | 130.40   |
| 1   | A     | 22   | G    | N1-C6-O6  | 7.02  | 124.11      | 119.90   |
| 1   | A     | 353  | A    | O5'-P-OP2 | -7.01 | 99.39       | 105.70   |
| 1   | A     | 1529 | G    | O5'-P-OP1 | -7.01 | 99.39       | 105.70   |
| 1   | A     | 674  | G    | N9-C4-C5  | -7.01 | 102.60      | 105.40   |
| 1   | A     | 1478 | C    | C5-C6-N1  | 7.00  | 124.50      | 121.00   |
| 1   | A     | 95   | U    | N3-C4-C5  | -7.00 | 110.40      | 114.60   |
| 1   | A     | 734  | G    | C5-C6-O6  | -7.00 | 124.40      | 128.60   |
| 1   | A     | 746  | A    | N1-C6-N6  | -7.00 | 114.40      | 118.60   |
| 1   | A     | 232  | G    | N1-C6-O6  | 6.99  | 124.09      | 119.90   |
| 1   | A     | 862  | C    | O5'-P-OP1 | -6.99 | 99.41       | 105.70   |
| 1   | A     | 949  | A    | N1-C6-N6  | 6.97  | 122.78      | 118.60   |
| 1   | A     | 67   | C    | N3-C4-C5  | 6.97  | 124.69      | 121.90   |
| 1   | A     | 523  | A    | C2-N3-C4  | -6.96 | 107.12      | 110.60   |
| 1   | A     | 854  | G    | C6-C5-N7  | -6.96 | 126.22      | 130.40   |
| 1   | A     | 308  | C    | N3-C4-N4  | 6.96  | 122.87      | 118.00   |
| 1   | A     | 168  | G    | C5-C6-N1  | -6.96 | 108.02      | 111.50   |
| 1   | A     | 382  | A    | N1-C2-N3  | 6.96  | 132.78      | 129.30   |
| 1   | A     | 940  | C    | C6-N1-C2  | 6.96  | 123.08      | 120.30   |
| 1   | A     | 277  | C    | C2-N1-C1' | -6.95 | 111.15      | 118.80   |
| 1   | A     | 784  | C    | O5'-P-OP2 | -6.95 | 99.44       | 105.70   |
| 1   | A     | 577  | G    | N3-C4-C5  | 6.95  | 132.07      | 128.60   |
| 1   | A     | 859  | A    | C8-N9-C4  | 6.94  | 108.58      | 105.80   |
| 1   | A     | 279  | A    | N7-C8-N9  | 6.94  | 117.27      | 113.80   |
| 1   | A     | 1394 | A    | N1-C6-N6  | -6.93 | 114.44      | 118.60   |
| 1   | A     | 550  | G    | C2-N3-C4  | -6.93 | 108.43      | 111.90   |
| 1   | A     | 703  | G    | C4-C5-N7  | -6.92 | 108.03      | 110.80   |
| 1   | A     | 645  | C    | N3-C4-C5  | 6.92  | 124.67      | 121.90   |

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| Mol | Chain | Res    | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 1   | A     | 955    | U    | N3-C4-C5   | -6.92 | 110.45      | 114.60   |
| 1   | A     | 587    | G    | C5-C6-N1   | 6.92  | 114.96      | 111.50   |
| 1   | A     | 724    | G    | C4-C5-C6   | 6.91  | 122.94      | 118.80   |
| 1   | A     | 880    | C    | C6-N1-C2   | 6.91  | 123.06      | 120.30   |
| 1   | A     | 216    | G    | N3-C4-C5   | 6.90  | 132.05      | 128.60   |
| 1   | A     | 667    | G    | N1-C6-O6   | 6.90  | 124.04      | 119.90   |
| 20  | T     | 94     | ALA  | N-CA-C     | -6.90 | 92.37       | 111.00   |
| 1   | A     | 20     | U    | C5-C6-N1   | -6.90 | 119.25      | 122.70   |
| 1   | A     | 253    | U    | O5'-P-OP2  | -6.89 | 99.50       | 105.70   |
| 1   | A     | 584    | G    | C5-N7-C8   | 6.89  | 107.74      | 104.30   |
| 1   | A     | 774    | G    | N9-C4-C5   | -6.89 | 102.64      | 105.40   |
| 1   | A     | 859    | A    | N1-C6-N6   | 6.89  | 122.73      | 118.60   |
| 1   | A     | 734    | G    | C4-C5-N7   | 6.88  | 113.55      | 110.80   |
| 1   | A     | 190(H) | G    | C6-C5-N7   | -6.88 | 126.27      | 130.40   |
| 1   | A     | 1237   | C    | N3-C2-O2   | -6.88 | 117.08      | 121.90   |
| 1   | A     | 1373   | G    | N3-C4-C5   | -6.88 | 125.16      | 128.60   |
| 1   | A     | 817    | C    | C4-C5-C6   | 6.87  | 120.83      | 117.40   |
| 1   | A     | 200    | G    | N1-C6-O6   | 6.86  | 124.02      | 119.90   |
| 1   | A     | 873    | A    | O5'-P-OP2  | -6.86 | 99.52       | 105.70   |
| 1   | A     | 306    | G    | N3-C4-C5   | 6.86  | 132.03      | 128.60   |
| 9   | I     | 56     | LEU  | CA-CB-CG   | 6.86  | 131.07      | 115.30   |
| 1   | A     | 326    | G    | C5-C6-N1   | -6.85 | 108.07      | 111.50   |
| 1   | A     | 763    | G    | C5-C6-O6   | -6.85 | 124.49      | 128.60   |
| 1   | A     | 1432   | G    | N9-C4-C5   | 6.85  | 108.14      | 105.40   |
| 1   | A     | 893    | C    | C4-C5-C6   | -6.85 | 113.97      | 117.40   |
| 1   | A     | 1094   | G    | N3-C4-C5   | -6.85 | 125.18      | 128.60   |
| 1   | A     | 555    | C    | O5'-P-OP1  | 6.85  | 118.92      | 110.70   |
| 1   | A     | 1390   | U    | N3-C4-C5   | -6.84 | 110.49      | 114.60   |
| 1   | A     | 518    | C    | O5'-P-OP2  | 6.84  | 118.91      | 110.70   |
| 1   | A     | 884    | U    | C4-C5-C6   | 6.84  | 123.80      | 119.70   |
| 1   | A     | 1100   | C    | C2-N1-C1'  | 6.84  | 126.32      | 118.80   |
| 1   | A     | 1197   | G    | O5'-P-OP2  | 6.83  | 118.90      | 110.70   |
| 1   | A     | 481    | G    | C5-C6-O6   | -6.83 | 124.50      | 128.60   |
| 1   | A     | 799    | G    | C2-N3-C4   | -6.83 | 108.48      | 111.90   |
| 1   | A     | 1411   | C    | N3-C2-O2   | -6.83 | 117.12      | 121.90   |
| 1   | A     | 1155   | G    | C4-N9-C1'  | 6.83  | 135.38      | 126.50   |
| 1   | A     | 1189   | C    | C2-N1-C1'  | 6.83  | 126.31      | 118.80   |
| 1   | A     | 370    | C    | N1-C2-O2   | 6.83  | 123.00      | 118.90   |
| 1   | A     | 429    | U    | O4'-C1'-N1 | 6.82  | 113.66      | 108.20   |
| 1   | A     | 759    | A    | N1-C6-N6   | -6.82 | 114.51      | 118.60   |
| 1   | A     | 975    | A    | C5-C6-N1   | -6.82 | 114.29      | 117.70   |
| 1   | A     | 1435   | G    | C5-C6-N1   | -6.82 | 108.09      | 111.50   |

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| Mol | Chain | Res     | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 1   | A     | 544     | G    | C5-C6-O6  | -6.82 | 124.51      | 128.60   |
| 1   | A     | 1287    | A    | C8-N9-C4  | -6.82 | 103.07      | 105.80   |
| 1   | A     | 216     | G    | C4-N9-C1' | -6.81 | 117.65      | 126.50   |
| 1   | A     | 230     | G    | C8-N9-C4  | 6.81  | 109.12      | 106.40   |
| 1   | A     | 147     | G    | C4-C5-C6  | 6.81  | 122.89      | 118.80   |
| 1   | A     | 758     | G    | N9-C4-C5  | -6.80 | 102.68      | 105.40   |
| 1   | A     | 548     | G    | N1-C6-O6  | 6.80  | 123.98      | 119.90   |
| 1   | A     | 376     | G    | N7-C8-N9  | -6.78 | 109.71      | 113.10   |
| 1   | A     | 944     | G    | N3-C4-C5  | -6.78 | 125.21      | 128.60   |
| 1   | A     | 579     | G    | C6-C5-N7  | -6.78 | 126.33      | 130.40   |
| 1   | A     | 1088    | G    | C5-C6-O6  | -6.78 | 124.53      | 128.60   |
| 1   | A     | 688     | G    | C5-C6-N1  | -6.77 | 108.11      | 111.50   |
| 1   | A     | 308     | C    | C5-C4-N4  | -6.77 | 115.46      | 120.20   |
| 1   | A     | 190(L)  | U    | O5'-P-OP2 | 6.76  | 118.81      | 110.70   |
| 1   | A     | 45      | U    | C4-C5-C6  | 6.76  | 123.75      | 119.70   |
| 1   | A     | 579     | G    | C2-N3-C4  | -6.76 | 108.52      | 111.90   |
| 1   | A     | 1227    | A    | C6-C5-N7  | -6.76 | 127.57      | 132.30   |
| 1   | A     | 276     | G    | N1-C6-O6  | 6.75  | 123.95      | 119.90   |
| 1   | A     | 357     | G    | C8-N9-C4  | 6.75  | 109.10      | 106.40   |
| 1   | A     | 661     | G    | C2-N3-C4  | -6.75 | 108.52      | 111.90   |
| 1   | A     | 32      | A    | C5-C6-N1  | 6.75  | 121.08      | 117.70   |
| 1   | A     | 174     | C    | OP2-P-O3' | 6.75  | 120.05      | 105.20   |
| 1   | A     | 729     | A    | C4-C5-C6  | 6.75  | 120.37      | 117.00   |
| 1   | A     | 47      | C    | C2-N3-C4  | -6.74 | 116.53      | 119.90   |
| 1   | A     | 31      | G    | C4-N9-C1' | 6.74  | 135.26      | 126.50   |
| 1   | A     | 266     | G    | C4-C5-N7  | 6.74  | 113.50      | 110.80   |
| 1   | A     | 289     | G    | C6-C5-N7  | -6.74 | 126.36      | 130.40   |
| 1   | A     | 783     | C    | N3-C2-O2  | 6.74  | 126.61      | 121.90   |
| 1   | A     | 833     | U    | C4-C5-C6  | 6.74  | 123.74      | 119.70   |
| 1   | A     | 899     | C    | C6-N1-C2  | 6.74  | 122.99      | 120.30   |
| 1   | A     | 1435    | G    | C6-C5-N7  | -6.73 | 126.36      | 130.40   |
| 1   | A     | 1053    | G    | N3-C4-N9  | -6.73 | 121.96      | 126.00   |
| 1   | A     | 557     | G    | C4-C5-C6  | 6.72  | 122.83      | 118.80   |
| 1   | A     | 718     | G    | N7-C8-N9  | -6.72 | 109.74      | 113.10   |
| 1   | A     | 1168    | A    | C2-N3-C4  | 6.72  | 113.96      | 110.60   |
| 1   | A     | 1516[A] | G    | N3-C2-N2  | -6.72 | 115.19      | 119.90   |
| 1   | A     | 1516[B] | G    | N3-C2-N2  | -6.72 | 115.19      | 119.90   |
| 1   | A     | 1053    | G    | C4-N9-C1' | -6.72 | 117.77      | 126.50   |
| 1   | A     | 260     | G    | N9-C4-C5  | 6.72  | 108.09      | 105.40   |
| 1   | A     | 662     | G    | N1-C6-O6  | 6.71  | 123.93      | 119.90   |
| 19  | S     | 81      | ARG  | NE-CZ-NH1 | 6.71  | 123.66      | 120.30   |
| 1   | A     | 1527    | C    | C5-C6-N1  | -6.71 | 117.64      | 121.00   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | A     | 46   | G    | C5-C6-N1  | -6.71 | 108.14      | 111.50   |
| 1   | A     | 791  | G    | C2-N3-C4  | -6.71 | 108.55      | 111.90   |
| 1   | A     | 789  | U    | C6-N1-C2  | -6.71 | 116.98      | 121.00   |
| 1   | A     | 144  | G    | N1-C6-O6  | 6.70  | 123.92      | 119.90   |
| 1   | A     | 361  | G    | C8-N9-C4  | 6.70  | 109.08      | 106.40   |
| 1   | A     | 631  | G    | N3-C4-C5  | 6.70  | 131.95      | 128.60   |
| 1   | A     | 774  | G    | C4-C5-N7  | 6.70  | 113.48      | 110.80   |
| 1   | A     | 1236 | A    | C8-N9-C4  | 6.70  | 108.48      | 105.80   |
| 1   | A     | 906  | G    | C4-C5-N7  | 6.69  | 113.48      | 110.80   |
| 1   | A     | 587  | G    | N1-C6-O6  | -6.69 | 115.89      | 119.90   |
| 1   | A     | 1498 | UR3  | P-O3'-C3' | 6.69  | 127.73      | 119.70   |
| 1   | A     | 50   | A    | C8-N9-C4  | 6.69  | 108.47      | 105.80   |
| 1   | A     | 1286 | A    | C5-N7-C8  | -6.68 | 100.56      | 103.90   |
| 1   | A     | 922  | G    | C4-N9-C1' | 6.67  | 135.18      | 126.50   |
| 1   | A     | 1195 | C    | C6-N1-C2  | -6.67 | 117.63      | 120.30   |
| 1   | A     | 1370 | G    | C5-C6-N1  | -6.67 | 108.16      | 111.50   |
| 1   | A     | 169  | C    | C6-N1-C2  | -6.67 | 117.63      | 120.30   |
| 1   | A     | 304  | U    | N3-C4-O4  | 6.67  | 124.07      | 119.40   |
| 1   | A     | 1442 | G    | C8-N9-C1' | -6.67 | 118.33      | 127.00   |
| 1   | A     | 285  | G    | N3-C4-C5  | 6.67  | 131.93      | 128.60   |
| 1   | A     | 736  | C    | N3-C2-O2  | -6.66 | 117.24      | 121.90   |
| 1   | A     | 309  | G    | C5-C6-N1  | -6.66 | 108.17      | 111.50   |
| 1   | A     | 257  | G    | C2-N3-C4  | -6.65 | 108.57      | 111.90   |
| 1   | A     | 1442 | G    | C4-N9-C1' | 6.65  | 135.14      | 126.50   |
| 1   | A     | 1487 | G    | N3-C4-N9  | 6.65  | 129.99      | 126.00   |
| 1   | A     | 810  | C    | C5-C4-N4  | 6.64  | 124.85      | 120.20   |
| 1   | A     | 317  | G    | C5-C6-O6  | -6.64 | 124.62      | 128.60   |
| 1   | A     | 376  | G    | C8-N9-C4  | 6.64  | 109.06      | 106.40   |
| 1   | A     | 111  | G    | C5-C6-O6  | 6.64  | 132.58      | 128.60   |
| 1   | A     | 407  | G    | O5'-P-OP1 | -6.63 | 99.73       | 105.70   |
| 1   | A     | 799  | G    | C4-C5-N7  | 6.63  | 113.45      | 110.80   |
| 1   | A     | 1530 | G    | C8-N9-C1' | 6.63  | 135.62      | 127.00   |
| 1   | A     | 200  | G    | C2-N3-C4  | -6.63 | 108.58      | 111.90   |
| 1   | A     | 595  | G    | N3-C4-N9  | 6.63  | 129.98      | 126.00   |
| 1   | A     | 731  | G    | N7-C8-N9  | 6.62  | 116.41      | 113.10   |
| 1   | A     | 1394 | A    | N9-C4-C5  | 6.62  | 108.45      | 105.80   |
| 1   | A     | 24   | U    | C5-C6-N1  | -6.62 | 119.39      | 122.70   |
| 1   | A     | 279  | A    | C5-N7-C8  | -6.62 | 100.59      | 103.90   |
| 1   | A     | 766  | A    | C5-N7-C8  | -6.62 | 100.59      | 103.90   |
| 1   | A     | 855  | G    | N1-C6-O6  | 6.62  | 123.87      | 119.90   |
| 1   | A     | 120  | A    | C2-N3-C4  | -6.61 | 107.29      | 110.60   |
| 1   | A     | 721  | G    | C5-C6-N1  | -6.61 | 108.19      | 111.50   |

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| Mol | Chain | Res    | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1   | A     | 1228   | C    | N1-C2-O2  | 6.61  | 122.87      | 118.90   |
| 1   | A     | 28     | G    | C6-C5-N7  | -6.61 | 126.44      | 130.40   |
| 1   | A     | 732    | C    | N3-C2-O2  | -6.61 | 117.28      | 121.90   |
| 1   | A     | 712    | A    | C6-N1-C2  | -6.61 | 114.64      | 118.60   |
| 1   | A     | 445    | G    | C8-N9-C4  | -6.60 | 103.76      | 106.40   |
| 1   | A     | 693    | G    | N3-C2-N2  | -6.60 | 115.28      | 119.90   |
| 1   | A     | 1512   | U    | N1-C2-N3  | 6.60  | 118.86      | 114.90   |
| 1   | A     | 21     | G    | N9-C4-C5  | -6.60 | 102.76      | 105.40   |
| 1   | A     | 922    | G    | C8-N9-C1' | -6.60 | 118.42      | 127.00   |
| 1   | A     | 1124   | G    | C5-C6-O6  | -6.60 | 124.64      | 128.60   |
| 1   | A     | 584    | G    | C8-N9-C4  | 6.59  | 109.04      | 106.40   |
| 1   | A     | 570    | G    | C4-N9-C1' | 6.59  | 135.07      | 126.50   |
| 1   | A     | 1125   | U    | O5'-P-OP1 | -6.59 | 99.77       | 105.70   |
| 1   | A     | 1415   | G    | OP1-P-O3' | 6.59  | 119.69      | 105.20   |
| 1   | A     | 190(E) | U    | N3-C2-O2  | -6.59 | 117.59      | 122.20   |
| 1   | A     | 288    | A    | N3-C4-C5  | 6.59  | 131.41      | 126.80   |
| 1   | A     | 1527   | C    | O5'-P-OP2 | -6.59 | 99.77       | 105.70   |
| 1   | A     | 285    | G    | C2-N3-C4  | -6.58 | 108.61      | 111.90   |
| 1   | A     | 298    | A    | N1-C2-N3  | 6.58  | 132.59      | 129.30   |
| 1   | A     | 428    | G    | P-O3'-C3' | 6.58  | 127.59      | 119.70   |
| 1   | A     | 1392   | G    | N1-C2-N2  | -6.58 | 110.28      | 116.20   |
| 1   | A     | 353    | A    | O5'-P-OP1 | 6.58  | 118.59      | 110.70   |
| 1   | A     | 608    | A    | N1-C6-N6  | -6.58 | 114.66      | 118.60   |
| 1   | A     | 610    | G    | N7-C8-N9  | 6.57  | 116.38      | 113.10   |
| 1   | A     | 616    | G    | C5-C6-N1  | -6.57 | 108.22      | 111.50   |
| 1   | A     | 1166   | G    | C6-C5-N7  | -6.57 | 126.46      | 130.40   |
| 1   | A     | 147    | G    | C2-N3-C4  | -6.56 | 108.62      | 111.90   |
| 1   | A     | 735    | C    | N3-C4-C5  | 6.56  | 124.53      | 121.90   |
| 1   | A     | 761    | G    | C6-C5-N7  | -6.56 | 126.46      | 130.40   |
| 1   | A     | 46     | G    | O5'-P-OP1 | -6.56 | 99.80       | 105.70   |
| 1   | A     | 401    | C    | N3-C4-C5  | -6.56 | 119.28      | 121.90   |
| 1   | A     | 387    | U    | C5-C4-O4  | 6.56  | 129.83      | 125.90   |
| 1   | A     | 757    | U    | C5-C4-O4  | 6.56  | 129.83      | 125.90   |
| 1   | A     | 95     | U    | C5-C4-O4  | 6.55  | 129.83      | 125.90   |
| 1   | A     | 200    | G    | C5-C6-N1  | -6.55 | 108.22      | 111.50   |
| 1   | A     | 955    | U    | C4-C5-C6  | 6.55  | 123.63      | 119.70   |
| 1   | A     | 1452   | C    | C6-N1-C2  | 6.55  | 122.92      | 120.30   |
| 1   | A     | 247    | G    | N3-C2-N2  | -6.55 | 115.32      | 119.90   |
| 1   | A     | 1092   | A    | C8-N9-C4  | -6.55 | 103.18      | 105.80   |
| 1   | A     | 158    | G    | C8-N9-C4  | -6.55 | 103.78      | 106.40   |
| 1   | A     | 403    | C    | C5-C6-N1  | -6.55 | 117.73      | 121.00   |
| 1   | A     | 618    | C    | C6-N1-C2  | 6.54  | 122.92      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | A     | 720  | C    | C5-C4-N4   | -6.54 | 115.62      | 120.20   |
| 1   | A     | 102  | G    | N1-C6-O6   | 6.53  | 123.82      | 119.90   |
| 1   | A     | 741  | G    | C5-N7-C8   | 6.53  | 107.56      | 104.30   |
| 1   | A     | 1075 | C    | C5-C4-N4   | 6.53  | 124.77      | 120.20   |
| 1   | A     | 108  | G    | N3-C4-C5   | 6.52  | 131.86      | 128.60   |
| 1   | A     | 26   | A    | N3-C4-C5   | 6.52  | 131.37      | 126.80   |
| 1   | A     | 812  | C    | N1-C2-O2   | 6.52  | 122.81      | 118.90   |
| 1   | A     | 1512 | U    | C4-C5-C6   | 6.52  | 123.61      | 119.70   |
| 1   | A     | 849  | C    | C6-N1-C2   | -6.52 | 117.69      | 120.30   |
| 1   | A     | 631  | G    | C4-N9-C1'  | -6.52 | 118.03      | 126.50   |
| 1   | A     | 1231 | G    | N1-C6-O6   | 6.52  | 123.81      | 119.90   |
| 1   | A     | 949  | A    | C4-C5-N7   | 6.51  | 113.96      | 110.70   |
| 1   | A     | 1108 | G    | C5-C6-O6   | 6.51  | 132.51      | 128.60   |
| 3   | C     | 14   | ILE  | CB-CA-C    | -6.51 | 98.57       | 111.60   |
| 1   | A     | 975  | A    | N1-C2-N3   | 6.51  | 132.56      | 129.30   |
| 1   | A     | 529  | G    | O5'-P-OP2  | -6.51 | 99.84       | 105.70   |
| 1   | A     | 707  | C    | N1-C2-O2   | 6.51  | 122.81      | 118.90   |
| 1   | A     | 1338 | G    | C4-N9-C1'  | 6.51  | 134.96      | 126.50   |
| 1   | A     | 150  | C    | C6-N1-C2   | 6.51  | 122.90      | 120.30   |
| 1   | A     | 248  | C    | C5-C6-N1   | -6.51 | 117.75      | 121.00   |
| 1   | A     | 1506 | U    | N1-C2-O2   | 6.51  | 127.36      | 122.80   |
| 1   | A     | 1104 | G    | C6-C5-N7   | -6.50 | 126.50      | 130.40   |
| 1   | A     | 614  | A    | N1-C6-N6   | 6.50  | 122.50      | 118.60   |
| 1   | A     | 413  | G    | O4'-C1'-N9 | 6.49  | 113.39      | 108.20   |
| 1   | A     | 703  | G    | N3-C4-C5   | -6.49 | 125.36      | 128.60   |
| 1   | A     | 106  | C    | OP2-P-O3'  | 6.49  | 119.47      | 105.20   |
| 1   | A     | 917  | G    | N1-C6-O6   | -6.48 | 116.01      | 119.90   |
| 1   | A     | 1531 | A    | C5-C6-N6   | -6.48 | 118.52      | 123.70   |
| 1   | A     | 724  | G    | C4-N9-C1'  | 6.48  | 134.93      | 126.50   |
| 1   | A     | 677  | U    | O5'-P-OP2  | -6.48 | 99.87       | 105.70   |
| 1   | A     | 289  | G    | O5'-P-OP2  | -6.47 | 99.87       | 105.70   |
| 1   | A     | 579  | G    | N9-C4-C5   | -6.47 | 102.81      | 105.40   |
| 1   | A     | 577  | G    | C2-N3-C4   | -6.47 | 108.67      | 111.90   |
| 1   | A     | 1093 | A    | C5-C6-N1   | 6.47  | 120.94      | 117.70   |
| 1   | A     | 21   | G    | N3-C4-N9   | 6.46  | 129.88      | 126.00   |
| 1   | A     | 703  | G    | C5-N7-C8   | 6.46  | 107.53      | 104.30   |
| 1   | A     | 710  | G    | C4-C5-C6   | 6.46  | 122.68      | 118.80   |
| 1   | A     | 902  | G    | N1-C2-N3   | 6.46  | 127.78      | 123.90   |
| 1   | A     | 1526 | G    | N1-C6-O6   | 6.46  | 123.78      | 119.90   |
| 1   | A     | 809  | G    | C5-C6-N1   | 6.46  | 114.73      | 111.50   |
| 1   | A     | 481  | G    | C4-C5-N7   | 6.45  | 113.38      | 110.80   |
| 1   | A     | 975  | A    | C5-N7-C8   | -6.45 | 100.67      | 103.90   |

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| Mol | Chain | Res    | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1   | A     | 1166   | G    | C4-C5-C6  | 6.45  | 122.67      | 118.80   |
| 1   | A     | 520    | A    | O5'-P-OP2 | -6.45 | 99.89       | 105.70   |
| 1   | A     | 535    | A    | O5'-P-OP2 | -6.45 | 99.89       | 105.70   |
| 1   | A     | 1432   | G    | O5'-P-OP2 | -6.45 | 99.90       | 105.70   |
| 1   | A     | 111    | G    | C5-C6-N1  | -6.44 | 108.28      | 111.50   |
| 1   | A     | 833    | U    | N1-C2-N3  | 6.44  | 118.77      | 114.90   |
| 1   | A     | 893    | C    | C6-N1-C2  | 6.44  | 122.88      | 120.30   |
| 1   | A     | 190(E) | U    | O5'-P-OP2 | -6.44 | 99.91       | 105.70   |
| 1   | A     | 135    | C    | O5'-P-OP2 | -6.43 | 99.91       | 105.70   |
| 1   | A     | 314    | C    | N1-C2-O2  | -6.43 | 115.04      | 118.90   |
| 1   | A     | 517    | G    | C4-C5-N7  | -6.43 | 108.23      | 110.80   |
| 1   | A     | 723    | U    | N3-C4-C5  | -6.43 | 110.74      | 114.60   |
| 1   | A     | 726    | C    | O5'-P-OP1 | -6.43 | 99.92       | 105.70   |
| 1   | A     | 1050   | G    | C4-C5-N7  | 6.43  | 113.37      | 110.80   |
| 1   | A     | 122    | G    | N3-C2-N2  | 6.42  | 124.40      | 119.90   |
| 1   | A     | 484    | G    | N1-C2-N3  | 6.42  | 127.75      | 123.90   |
| 1   | A     | 885    | G    | C4-C5-N7  | -6.42 | 108.23      | 110.80   |
| 1   | A     | 579    | G    | C8-N9-C4  | 6.42  | 108.97      | 106.40   |
| 1   | A     | 1465   | C    | N3-C4-C5  | 6.41  | 124.46      | 121.90   |
| 1   | A     | 1502   | A    | C5-N7-C8  | -6.41 | 100.69      | 103.90   |
| 1   | A     | 1525   | G    | C2-N3-C4  | -6.41 | 108.69      | 111.90   |
| 1   | A     | 631    | G    | N1-C2-N2  | 6.41  | 121.97      | 116.20   |
| 1   | A     | 307    | C    | O5'-P-OP2 | -6.41 | 99.93       | 105.70   |
| 1   | A     | 1485   | U    | N1-C2-N3  | 6.41  | 118.74      | 114.90   |
| 1   | A     | 449    | C    | N3-C4-C5  | -6.40 | 119.34      | 121.90   |
| 1   | A     | 617    | G    | N1-C2-N3  | 6.40  | 127.74      | 123.90   |
| 1   | A     | 1512   | U    | C6-N1-C1' | 6.40  | 130.15      | 121.20   |
| 1   | A     | 255    | G    | C6-C5-N7  | -6.39 | 126.56      | 130.40   |
| 1   | A     | 981    | U    | N3-C4-O4  | 6.39  | 123.88      | 119.40   |
| 1   | A     | 900    | A    | N1-C6-N6  | 6.39  | 122.44      | 118.60   |
| 1   | A     | 857    | C    | N3-C2-O2  | -6.39 | 117.43      | 121.90   |
| 1   | A     | 285    | G    | N7-C8-N9  | -6.39 | 109.91      | 113.10   |
| 1   | A     | 871    | U    | C5-C6-N1  | -6.39 | 119.51      | 122.70   |
| 1   | A     | 910    | C    | N1-C2-O2  | -6.39 | 115.07      | 118.90   |
| 1   | A     | 313    | A    | N9-C4-C5  | -6.39 | 103.25      | 105.80   |
| 1   | A     | 1502   | A    | C4-C5-N7  | 6.38  | 113.89      | 110.70   |
| 1   | A     | 232    | G    | C4-N9-C1' | 6.38  | 134.79      | 126.50   |
| 1   | A     | 265    | G    | N9-C4-C5  | 6.38  | 107.95      | 105.40   |
| 1   | A     | 49     | U    | C6-N1-C2  | 6.38  | 124.83      | 121.00   |
| 19  | S     | 81     | ARG  | NE-CZ-NH2 | -6.38 | 117.11      | 120.30   |
| 1   | A     | 535    | A    | C4-C5-N7  | -6.37 | 107.52      | 110.70   |
| 1   | A     | 657    | G    | N1-C6-O6  | 6.37  | 123.72      | 119.90   |

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| Mol | Chain | Res     | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 1   | A     | 1240    | U    | C5-C6-N1  | -6.36 | 119.52      | 122.70   |
| 1   | A     | 1341    | U    | C5-C4-O4  | 6.36  | 129.72      | 125.90   |
| 1   | A     | 36      | C    | O5'-P-OP2 | -6.36 | 99.98       | 105.70   |
| 1   | A     | 1057    | G    | N1-C2-N2  | 6.36  | 121.92      | 116.20   |
| 1   | A     | 1030(C) | G    | C8-N9-C1' | -6.36 | 118.74      | 127.00   |
| 1   | A     | 654     | G    | N3-C4-C5  | 6.35  | 131.78      | 128.60   |
| 1   | A     | 190(L)  | U    | O5'-P-OP1 | -6.35 | 99.98       | 105.70   |
| 1   | A     | 779     | C    | C5-C6-N1  | -6.35 | 117.83      | 121.00   |
| 1   | A     | 927     | G    | N1-C6-O6  | 6.35  | 123.71      | 119.90   |
| 1   | A     | 1087    | G    | C4-C5-C6  | 6.35  | 122.61      | 118.80   |
| 1   | A     | 1442    | G    | N3-C4-N9  | 6.35  | 129.81      | 126.00   |
| 1   | A     | 799     | G    | O5'-P-OP2 | -6.34 | 99.99       | 105.70   |
| 1   | A     | 700     | G    | C5-C6-N1  | -6.34 | 108.33      | 111.50   |
| 1   | A     | 965     | A    | N3-C4-C5  | 6.34  | 131.24      | 126.80   |
| 1   | A     | 1058    | G    | C8-N9-C4  | 6.34  | 108.94      | 106.40   |
| 1   | A     | 104     | G    | N1-C6-O6  | 6.34  | 123.70      | 119.90   |
| 1   | A     | 1542    | U    | N1-C2-N3  | -6.34 | 111.10      | 114.90   |
| 1   | A     | 635     | G    | C6-C5-N7  | -6.33 | 126.60      | 130.40   |
| 1   | A     | 1197    | G    | C8-N9-C1' | -6.33 | 118.77      | 127.00   |
| 1   | A     | 1374    | A    | N1-C2-N3  | 6.33  | 132.47      | 129.30   |
| 1   | A     | 630     | G    | C6-C5-N7  | 6.33  | 134.20      | 130.40   |
| 1   | A     | 725     | G    | C5-C6-O6  | -6.33 | 124.80      | 128.60   |
| 1   | A     | 1030(B) | C    | C6-N1-C2  | -6.33 | 117.77      | 120.30   |
| 1   | A     | 507     | C    | N3-C4-C5  | 6.32  | 124.43      | 121.90   |
| 1   | A     | 834     | C    | C6-N1-C2  | 6.32  | 122.83      | 120.30   |
| 1   | A     | 1514    | C    | N3-C4-C5  | 6.32  | 124.43      | 121.90   |
| 1   | A     | 1227    | A    | C5-N7-C8  | -6.32 | 100.74      | 103.90   |
| 1   | A     | 1506    | U    | O5'-P-OP2 | -6.32 | 100.01      | 105.70   |
| 1   | A     | 1512    | U    | C2-N3-C4  | 6.32  | 130.79      | 127.00   |
| 1   | A     | 488     | C    | N3-C4-C5  | 6.31  | 124.43      | 121.90   |
| 1   | A     | 517     | G    | C4-C5-C6  | 6.31  | 122.59      | 118.80   |
| 1   | A     | 834     | C    | O5'-P-OP2 | -6.31 | 100.02      | 105.70   |
| 1   | A     | 950     | U    | C5-C4-O4  | 6.31  | 129.69      | 125.90   |
| 1   | A     | 1197    | G    | O5'-P-OP1 | -6.31 | 100.02      | 105.70   |
| 1   | A     | 1338    | G    | N3-C4-C5  | -6.31 | 125.44      | 128.60   |
| 1   | A     | 1528    | U    | C6-N1-C2  | 6.31  | 124.79      | 121.00   |
| 1   | A     | 703     | G    | N3-C4-N9  | 6.31  | 129.78      | 126.00   |
| 1   | A     | 1390    | U    | C4-C5-C6  | 6.31  | 123.48      | 119.70   |
| 1   | A     | 758     | G    | OP2-P-O3' | 6.30  | 119.07      | 105.20   |
| 1   | A     | 1544    | U    | C6-N1-C2  | -6.30 | 117.22      | 121.00   |
| 1   | A     | 816     | A    | N1-C6-N6  | -6.30 | 114.82      | 118.60   |
| 1   | A     | 309     | G    | C4-C5-C6  | 6.30  | 122.58      | 118.80   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | A     | 1323 | G    | N1-C6-O6  | 6.30  | 123.68      | 119.90   |
| 1   | A     | 654  | G    | C2-N3-C4  | -6.29 | 108.75      | 111.90   |
| 1   | A     | 1432 | G    | N3-C2-N2  | -6.29 | 115.50      | 119.90   |
| 1   | A     | 133  | U    | N1-C2-O2  | 6.29  | 127.20      | 122.80   |
| 1   | A     | 314  | C    | C5-C6-N1  | -6.29 | 117.86      | 121.00   |
| 1   | A     | 314  | C    | N3-C4-N4  | -6.29 | 113.60      | 118.00   |
| 1   | A     | 266  | G    | C2-N3-C4  | -6.29 | 108.76      | 111.90   |
| 1   | A     | 1126 | U    | C6-N1-C2  | -6.29 | 117.23      | 121.00   |
| 1   | A     | 599  | C    | C6-N1-C2  | 6.28  | 122.81      | 120.30   |
| 1   | A     | 535  | A    | C2-N3-C4  | 6.28  | 113.74      | 110.60   |
| 1   | A     | 817  | C    | N3-C4-C5  | -6.28 | 119.39      | 121.90   |
| 1   | A     | 723  | U    | C6-N1-C2  | -6.27 | 117.24      | 121.00   |
| 1   | A     | 765  | G    | O5'-P-OP1 | -6.27 | 100.06      | 105.70   |
| 1   | A     | 835  | U    | N3-C2-O2  | -6.27 | 117.81      | 122.20   |
| 1   | A     | 890  | G    | C5-C6-O6  | 6.27  | 132.36      | 128.60   |
| 1   | A     | 1397 | C    | N1-C2-O2  | 6.27  | 122.66      | 118.90   |
| 1   | A     | 1525 | G    | N1-C2-N3  | 6.27  | 127.66      | 123.90   |
| 1   | A     | 662  | G    | C8-N9-C1' | -6.26 | 118.86      | 127.00   |
| 1   | A     | 1124 | G    | N1-C2-N2  | 6.26  | 121.84      | 116.20   |
| 1   | A     | 710  | G    | C6-C5-N7  | -6.25 | 126.65      | 130.40   |
| 1   | A     | 916  | G    | N1-C6-O6  | -6.25 | 116.15      | 119.90   |
| 1   | A     | 1394 | A    | C5-C6-N6  | 6.24  | 128.69      | 123.70   |
| 1   | A     | 113  | G    | N9-C4-C5  | -6.24 | 102.90      | 105.40   |
| 1   | A     | 818  | G    | O5'-P-OP1 | -6.24 | 100.08      | 105.70   |
| 1   | A     | 790  | A    | N1-C2-N3  | 6.24  | 132.42      | 129.30   |
| 3   | C     | 155  | GLY  | N-CA-C    | 6.24  | 128.70      | 113.10   |
| 1   | A     | 498  | U    | O5'-P-OP2 | -6.24 | 100.09      | 105.70   |
| 1   | A     | 889  | A    | N1-C6-N6  | -6.24 | 114.86      | 118.60   |
| 1   | A     | 401  | C    | N3-C2-O2  | 6.23  | 126.26      | 121.90   |
| 1   | A     | 544  | G    | N9-C4-C5  | -6.23 | 102.91      | 105.40   |
| 1   | A     | 542  | G    | N3-C4-C5  | -6.23 | 125.49      | 128.60   |
| 1   | A     | 1334 | G    | C8-N9-C4  | -6.22 | 103.91      | 106.40   |
| 1   | A     | 117  | G    | C2-N3-C4  | -6.22 | 108.79      | 111.90   |
| 1   | A     | 192  | U    | N3-C2-O2  | -6.22 | 117.84      | 122.20   |
| 1   | A     | 975  | A    | C6-C5-N7  | -6.22 | 127.94      | 132.30   |
| 1   | A     | 504  | C    | C2-N1-C1' | 6.22  | 125.64      | 118.80   |
| 1   | A     | 815  | A    | OP1-P-OP2 | -6.22 | 110.27      | 119.60   |
| 1   | A     | 392  | G    | N7-C8-N9  | -6.22 | 109.99      | 113.10   |
| 1   | A     | 29   | G    | C5-C6-N1  | -6.22 | 108.39      | 111.50   |
| 1   | A     | 631  | G    | C8-N9-C1' | 6.21  | 135.08      | 127.00   |
| 1   | A     | 731  | G    | C8-N9-C4  | -6.21 | 103.92      | 106.40   |
| 1   | A     | 38   | G    | C5-C6-N1  | -6.21 | 108.39      | 111.50   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | A     | 1286 | A    | C4-C5-N7  | 6.21  | 113.81      | 110.70   |
| 1   | A     | 497  | A    | C5-C6-N6  | 6.21  | 128.66      | 123.70   |
| 1   | A     | 1401 | G    | C8-N9-C4  | 6.21  | 108.88      | 106.40   |
| 1   | A     | 1513 | A    | N7-C8-N9  | -6.21 | 110.70      | 113.80   |
| 1   | A     | 641  | U    | C2-N1-C1' | 6.20  | 125.14      | 117.70   |
| 1   | A     | 1305 | G    | N7-C8-N9  | 6.20  | 116.20      | 113.10   |
| 1   | A     | 385  | C    | O5'-P-OP1 | -6.19 | 100.13      | 105.70   |
| 1   | A     | 115  | G    | P-O3'-C3' | 6.19  | 127.13      | 119.70   |
| 1   | A     | 101  | A    | C2-N3-C4  | -6.19 | 107.51      | 110.60   |
| 1   | A     | 610  | G    | N9-C4-C5  | 6.19  | 107.88      | 105.40   |
| 1   | A     | 832  | C    | OP2-P-O3' | 6.19  | 118.81      | 105.20   |
| 1   | A     | 1239 | A    | C8-N9-C4  | 6.18  | 108.27      | 105.80   |
| 1   | A     | 148  | G    | N3-C4-N9  | 6.18  | 129.71      | 126.00   |
| 1   | A     | 305  | G    | C4-C5-C6  | 6.18  | 122.51      | 118.80   |
| 1   | A     | 733  | A    | N1-C2-N3  | 6.18  | 132.39      | 129.30   |
| 1   | A     | 435  | C    | O5'-P-OP1 | -6.18 | 100.14      | 105.70   |
| 1   | A     | 836  | G    | N1-C6-O6  | 6.18  | 123.61      | 119.90   |
| 1   | A     | 331  | G    | C6-C5-N7  | -6.17 | 126.69      | 130.40   |
| 1   | A     | 536  | C    | C6-N1-C2  | -6.17 | 117.83      | 120.30   |
| 1   | A     | 1094 | G    | N3-C4-N9  | 6.17  | 129.71      | 126.00   |
| 1   | A     | 267  | C    | C5-C4-N4  | 6.17  | 124.52      | 120.20   |
| 1   | A     | 652  | U    | N3-C4-C5  | 6.16  | 118.30      | 114.60   |
| 1   | A     | 161  | A    | C5-C6-N6  | 6.16  | 128.63      | 123.70   |
| 1   | A     | 104  | G    | C4-C5-C6  | 6.16  | 122.49      | 118.80   |
| 1   | A     | 284  | G    | N3-C2-N2  | -6.16 | 115.59      | 119.90   |
| 1   | A     | 925  | G    | C2-N3-C4  | -6.16 | 108.82      | 111.90   |
| 1   | A     | 1079 | G    | N3-C4-N9  | 6.16  | 129.69      | 126.00   |
| 1   | A     | 1341 | U    | N3-C4-O4  | -6.16 | 115.09      | 119.40   |
| 1   | A     | 232  | G    | C8-N9-C1' | -6.15 | 119.00      | 127.00   |
| 1   | A     | 1259 | C    | N1-C2-O2  | 6.15  | 122.59      | 118.90   |
| 1   | A     | 587  | G    | C2-N3-C4  | 6.15  | 114.97      | 111.90   |
| 1   | A     | 774  | G    | C8-N9-C1' | -6.15 | 119.01      | 127.00   |
| 1   | A     | 187  | C    | N3-C4-C5  | -6.14 | 119.44      | 121.90   |
| 1   | A     | 1206 | G    | C2-N3-C4  | -6.14 | 108.83      | 111.90   |
| 1   | A     | 1478 | C    | C6-N1-C2  | -6.14 | 117.84      | 120.30   |
| 1   | A     | 105  | G    | N1-C6-O6  | 6.14  | 123.59      | 119.90   |
| 1   | A     | 255  | G    | C2-N3-C4  | -6.14 | 108.83      | 111.90   |
| 1   | A     | 1058 | G    | N1-C6-O6  | 6.14  | 123.59      | 119.90   |
| 1   | A     | 1227 | A    | N9-C4-C5  | -6.14 | 103.34      | 105.80   |
| 1   | A     | 944  | G    | C4-N9-C1' | 6.14  | 134.48      | 126.50   |
| 1   | A     | 26   | A    | N3-C4-N9  | -6.14 | 122.49      | 127.40   |
| 1   | A     | 357  | G    | N1-C6-O6  | 6.14  | 123.58      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | A     | 406  | G    | C8-N9-C4  | -6.14 | 103.94      | 106.40   |
| 1   | A     | 564  | C    | C6-N1-C2  | 6.13  | 122.75      | 120.30   |
| 1   | A     | 570  | G    | C8-N9-C4  | -6.13 | 103.95      | 106.40   |
| 1   | A     | 705  | U    | O5'-P-OP2 | -6.13 | 100.18      | 105.70   |
| 1   | A     | 375  | U    | N3-C4-C5  | -6.13 | 110.92      | 114.60   |
| 1   | A     | 352  | C    | N3-C4-C5  | -6.12 | 119.45      | 121.90   |
| 1   | A     | 1069 | C    | N3-C2-O2  | 6.12  | 126.19      | 121.90   |
| 1   | A     | 1131 | G    | C5-C6-N1  | -6.12 | 108.44      | 111.50   |
| 1   | A     | 1125 | U    | N1-C2-N3  | -6.12 | 111.23      | 114.90   |
| 1   | A     | 61   | G    | O5'-P-OP1 | -6.11 | 100.20      | 105.70   |
| 1   | A     | 976  | G    | C8-N9-C4  | 6.11  | 108.84      | 106.40   |
| 1   | A     | 631  | G    | N1-C2-N3  | -6.11 | 120.23      | 123.90   |
| 1   | A     | 776  | G    | OP1-P-O3' | 6.10  | 118.63      | 105.20   |
| 1   | A     | 1435 | G    | N3-C2-N2  | -6.10 | 115.63      | 119.90   |
| 1   | A     | 1490 | C    | C4-C5-C6  | -6.10 | 114.35      | 117.40   |
| 1   | A     | 562  | C    | C5-C6-N1  | -6.10 | 117.95      | 121.00   |
| 1   | A     | 1341 | U    | C5-C6-N1  | -6.10 | 119.65      | 122.70   |
| 1   | A     | 1530 | G    | O5'-P-OP2 | -6.09 | 100.22      | 105.70   |
| 1   | A     | 47   | C    | C4-C5-C6  | 6.09  | 120.44      | 117.40   |
| 1   | A     | 773  | G    | N1-C2-N3  | 6.09  | 127.55      | 123.90   |
| 1   | A     | 941  | G    | C8-N9-C4  | 6.08  | 108.83      | 106.40   |
| 1   | A     | 1202 | G    | C8-N9-C4  | -6.08 | 103.97      | 106.40   |
| 1   | A     | 1342 | C    | N3-C4-C5  | 6.08  | 124.33      | 121.90   |
| 1   | A     | 67   | C    | C2-N3-C4  | -6.08 | 116.86      | 119.90   |
| 1   | A     | 1528 | U    | OP1-P-O3' | 6.08  | 118.57      | 105.20   |
| 1   | A     | 517  | G    | N3-C4-C5  | -6.08 | 125.56      | 128.60   |
| 1   | A     | 819  | A    | N9-C4-C5  | -6.07 | 103.37      | 105.80   |
| 1   | A     | 1342 | C    | C6-N1-C2  | 6.07  | 122.73      | 120.30   |
| 1   | A     | 1188 | A    | N1-C2-N3  | 6.07  | 132.34      | 129.30   |
| 1   | A     | 945  | G    | C5-C6-N1  | 6.07  | 114.53      | 111.50   |
| 1   | A     | 1454 | G    | C2-N3-C4  | -6.07 | 108.87      | 111.90   |
| 1   | A     | 778  | G    | C4-C5-C6  | 6.06  | 122.44      | 118.80   |
| 1   | A     | 641  | U    | C6-N1-C1' | -6.06 | 112.72      | 121.20   |
| 1   | A     | 707  | C    | N3-C2-O2  | -6.06 | 117.66      | 121.90   |
| 1   | A     | 774  | G    | C4-N9-C1' | 6.05  | 134.37      | 126.50   |
| 1   | A     | 652  | U    | C6-N1-C2  | 6.05  | 124.63      | 121.00   |
| 1   | A     | 1054 | C    | C2-N1-C1' | 6.05  | 125.45      | 118.80   |
| 1   | A     | 710  | G    | C2-N3-C4  | -6.05 | 108.88      | 111.90   |
| 1   | A     | 513  | C    | C6-N1-C2  | 6.04  | 122.72      | 120.30   |
| 1   | A     | 66   | G    | N3-C2-N2  | -6.04 | 115.67      | 119.90   |
| 1   | A     | 642  | A    | N1-C2-N3  | 6.04  | 132.32      | 129.30   |
| 1   | A     | 105  | G    | C6-C5-N7  | -6.04 | 126.78      | 130.40   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | A     | 1227 | A    | O4'-C1'-N9 | -6.04 | 103.37      | 108.20   |
| 1   | A     | 10   | A    | C6-N1-C2   | -6.03 | 114.98      | 118.60   |
| 1   | A     | 698  | G    | N1-C6-O6   | 6.03  | 123.52      | 119.90   |
| 1   | A     | 1491 | G    | N7-C8-N9   | 6.03  | 116.12      | 113.10   |
| 1   | A     | 28   | G    | C4-C5-C6   | 6.03  | 122.42      | 118.80   |
| 1   | A     | 325  | A    | C4-C5-N7   | -6.03 | 107.69      | 110.70   |
| 1   | A     | 1100 | C    | N1-C2-O2   | 6.03  | 122.52      | 118.90   |
| 1   | A     | 1479 | C    | N3-C4-C5   | -6.03 | 119.49      | 121.90   |
| 1   | A     | 1530 | G    | N1-C2-N2   | 6.03  | 121.62      | 116.20   |
| 1   | A     | 16   | A    | O5'-P-OP1  | -6.02 | 100.28      | 105.70   |
| 1   | A     | 1227 | A    | C5-C6-N6   | -6.02 | 118.88      | 123.70   |
| 1   | A     | 809  | G    | C2-N3-C4   | 6.02  | 114.91      | 111.90   |
| 1   | A     | 234  | C    | C5-C6-N1   | -6.02 | 117.99      | 121.00   |
| 1   | A     | 584  | G    | C4-C5-N7   | -6.02 | 108.39      | 110.80   |
| 1   | A     | 811  | C    | C2-N3-C4   | -6.02 | 116.89      | 119.90   |
| 1   | A     | 1227 | A    | C4-C5-N7   | 6.02  | 113.71      | 110.70   |
| 1   | A     | 1424 | C    | C6-N1-C2   | 6.02  | 122.71      | 120.30   |
| 1   | A     | 1054 | C    | N3-C2-O2   | -6.02 | 117.69      | 121.90   |
| 1   | A     | 24   | U    | C2-N3-C4   | -6.01 | 123.39      | 127.00   |
| 1   | A     | 635  | G    | C5-C6-N1   | -6.01 | 108.49      | 111.50   |
| 1   | A     | 658  | G    | N1-C2-N3   | 6.01  | 127.50      | 123.90   |
| 1   | A     | 1253 | G    | C8-N9-C4   | -6.01 | 104.00      | 106.40   |
| 1   | A     | 1437 | C    | C6-N1-C2   | 6.01  | 122.70      | 120.30   |
| 1   | A     | 563  | A    | C2-N3-C4   | -6.01 | 107.60      | 110.60   |
| 1   | A     | 1053 | G    | C8-N9-C1'  | 6.00  | 134.81      | 127.00   |
| 1   | A     | 1392 | G    | N3-C4-C5   | -6.00 | 125.60      | 128.60   |
| 1   | A     | 111  | G    | N9-C4-C5   | 6.00  | 107.80      | 105.40   |
| 1   | A     | 234  | C    | N3-C4-C5   | 6.00  | 124.30      | 121.90   |
| 3   | C     | 12   | LEU  | CA-CB-CG   | -6.00 | 101.51      | 115.30   |
| 1   | A     | 1453 | G    | N9-C4-C5   | -6.00 | 103.00      | 105.40   |
| 1   | A     | 1064 | G    | N9-C4-C5   | -5.99 | 103.00      | 105.40   |
| 1   | A     | 1167 | A    | C2-N3-C4   | -5.99 | 107.61      | 110.60   |
| 1   | A     | 22   | G    | C6-C5-N7   | -5.99 | 126.81      | 130.40   |
| 1   | A     | 864  | A    | C5-C6-N6   | 5.99  | 128.49      | 123.70   |
| 1   | A     | 791  | G    | C8-N9-C1'  | -5.99 | 119.22      | 127.00   |
| 1   | A     | 1302 | U    | N3-C4-O4   | -5.99 | 115.21      | 119.40   |
| 1   | A     | 1054 | C    | O4'-C1'-N1 | 5.98  | 112.98      | 108.20   |
| 1   | A     | 1522 | U    | O5'-P-OP1  | 5.98  | 117.88      | 110.70   |
| 1   | A     | 549  | C    | C2-N3-C4   | -5.98 | 116.91      | 119.90   |
| 1   | A     | 557  | G    | C5-C6-N1   | -5.98 | 108.51      | 111.50   |
| 1   | A     | 228  | A    | C6-N1-C2   | -5.97 | 115.02      | 118.60   |
| 1   | A     | 553  | A    | C8-N9-C4   | 5.97  | 108.19      | 105.80   |

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| Mol | Chain | Res     | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 1   | A     | 1387    | G    | OP1-P-O3' | 5.97  | 118.34      | 105.20   |
| 1   | A     | 761     | G    | N1-C2-N3  | 5.97  | 127.48      | 123.90   |
| 1   | A     | 385     | C    | O5'-P-OP2 | 5.97  | 117.86      | 110.70   |
| 1   | A     | 970     | C    | C6-N1-C2  | 5.97  | 122.69      | 120.30   |
| 1   | A     | 748     | C    | C6-N1-C2  | -5.96 | 117.91      | 120.30   |
| 1   | A     | 251     | G    | N9-C4-C5  | -5.96 | 103.02      | 105.40   |
| 1   | A     | 9       | G    | N7-C8-N9  | -5.96 | 110.12      | 113.10   |
| 1   | A     | 181     | G    | C8-N9-C1' | -5.96 | 119.25      | 127.00   |
| 1   | A     | 724     | G    | N7-C8-N9  | 5.96  | 116.08      | 113.10   |
| 1   | A     | 1149    | C    | N1-C2-O2  | -5.96 | 115.33      | 118.90   |
| 1   | A     | 474     | G    | N1-C6-O6  | 5.96  | 123.47      | 119.90   |
| 1   | A     | 1211    | U    | C5-C4-O4  | -5.96 | 122.33      | 125.90   |
| 1   | A     | 1333    | A    | N1-C2-N3  | 5.95  | 132.28      | 129.30   |
| 1   | A     | 1502    | A    | OP2-P-O3' | 5.95  | 118.30      | 105.20   |
| 1   | A     | 498     | U    | N1-C2-O2  | -5.95 | 118.63      | 122.80   |
| 1   | A     | 132     | C    | C5-C6-N1  | -5.95 | 118.03      | 121.00   |
| 1   | A     | 575     | G    | OP1-P-O3' | 5.95  | 118.28      | 105.20   |
| 1   | A     | 243     | A    | O5'-P-OP2 | -5.95 | 100.35      | 105.70   |
| 1   | A     | 481     | G    | N1-C6-O6  | 5.95  | 123.47      | 119.90   |
| 1   | A     | 31      | G    | C6-C5-N7  | -5.94 | 126.83      | 130.40   |
| 1   | A     | 365     | U    | N3-C2-O2  | -5.94 | 118.04      | 122.20   |
| 1   | A     | 242     | C    | C5-C6-N1  | -5.94 | 118.03      | 121.00   |
| 1   | A     | 805     | C    | C5-C4-N4  | -5.94 | 116.04      | 120.20   |
| 1   | A     | 1396    | A    | OP1-P-OP2 | 5.94  | 128.51      | 119.60   |
| 12  | L     | 27      | LEU  | CA-CB-CG  | 5.93  | 128.95      | 115.30   |
| 18  | R     | 85      | LEU  | CA-CB-CG  | 5.93  | 128.94      | 115.30   |
| 1   | A     | 1309    | G    | N1-C6-O6  | -5.93 | 116.34      | 119.90   |
| 1   | A     | 1061    | G    | N1-C6-O6  | 5.93  | 123.46      | 119.90   |
| 1   | A     | 196     | A    | C4-C5-C6  | -5.92 | 114.04      | 117.00   |
| 1   | A     | 1026    | G    | C5-N7-C8  | -5.92 | 101.34      | 104.30   |
| 1   | A     | 168     | G    | N1-C6-O6  | 5.92  | 123.45      | 119.90   |
| 1   | A     | 388     | G    | C8-N9-C4  | 5.92  | 108.77      | 106.40   |
| 1   | A     | 957     | U    | N1-C2-N3  | 5.92  | 118.45      | 114.90   |
| 1   | A     | 300     | A    | C5-C6-N6  | 5.92  | 128.43      | 123.70   |
| 1   | A     | 1200    | C    | N1-C2-O2  | -5.91 | 115.35      | 118.90   |
| 1   | A     | 1516[A] | G    | C8-N9-C1' | 5.91  | 134.69      | 127.00   |
| 1   | A     | 1516[B] | G    | C8-N9-C1' | 5.91  | 134.69      | 127.00   |
| 1   | A     | 719     | C    | N3-C4-C5  | -5.91 | 119.53      | 121.90   |
| 1   | A     | 970     | C    | N3-C2-O2  | -5.91 | 117.76      | 121.90   |
| 1   | A     | 113     | G    | C4-C5-C6  | 5.91  | 122.35      | 118.80   |
| 1   | A     | 381     | C    | C5-C6-N1  | 5.91  | 123.95      | 121.00   |
| 1   | A     | 553     | A    | C2-N3-C4  | -5.91 | 107.65      | 110.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | A     | 554  | C    | C4-C5-C6   | 5.91  | 120.35      | 117.40   |
| 1   | A     | 174  | C    | C6-N1-C2   | -5.90 | 117.94      | 120.30   |
| 1   | A     | 886  | G    | C6-C5-N7   | -5.90 | 126.86      | 130.40   |
| 1   | A     | 1502 | A    | C6-C5-N7   | -5.90 | 128.17      | 132.30   |
| 1   | A     | 117  | G    | C4-C5-C6   | 5.90  | 122.34      | 118.80   |
| 1   | A     | 641  | U    | N1-C2-O2   | 5.90  | 126.93      | 122.80   |
| 1   | A     | 766  | A    | C4-C5-N7   | 5.90  | 113.65      | 110.70   |
| 1   | A     | 650  | G    | C5-C6-O6   | -5.89 | 125.06      | 128.60   |
| 1   | A     | 133  | U    | N3-C4-C5   | -5.89 | 111.06      | 114.60   |
| 1   | A     | 357  | G    | N7-C8-N9   | -5.89 | 110.15      | 113.10   |
| 1   | A     | 791  | G    | C4-C5-N7   | -5.89 | 108.44      | 110.80   |
| 1   | A     | 858  | G    | N3-C4-N9   | 5.89  | 129.54      | 126.00   |
| 1   | A     | 61   | G    | C5-N7-C8   | -5.89 | 101.36      | 104.30   |
| 1   | A     | 861  | G    | C4-C5-N7   | 5.89  | 113.16      | 110.80   |
| 1   | A     | 313  | A    | C5-C6-N6   | -5.89 | 118.99      | 123.70   |
| 1   | A     | 712  | A    | N1-C2-N3   | 5.89  | 132.24      | 129.30   |
| 1   | A     | 116  | A    | C2-N3-C4   | -5.89 | 107.66      | 110.60   |
| 1   | A     | 807  | A    | N1-C6-N6   | 5.89  | 122.13      | 118.60   |
| 1   | A     | 216  | G    | N3-C4-N9   | -5.88 | 122.47      | 126.00   |
| 1   | A     | 630  | G    | N7-C8-N9   | -5.88 | 110.16      | 113.10   |
| 1   | A     | 1453 | G    | N3-C4-N9   | 5.88  | 129.53      | 126.00   |
| 1   | A     | 485  | G    | O4'-C1'-N9 | 5.88  | 112.90      | 108.20   |
| 1   | A     | 491  | G    | C4-C5-C6   | 5.87  | 122.32      | 118.80   |
| 1   | A     | 993  | G    | C4-C5-N7   | 5.87  | 113.15      | 110.80   |
| 1   | A     | 1054 | C    | C6-N1-C1'  | -5.87 | 113.75      | 120.80   |
| 1   | A     | 25   | C    | O5'-P-OP1  | 5.87  | 117.75      | 110.70   |
| 1   | A     | 216  | G    | C8-N9-C4   | 5.87  | 108.75      | 106.40   |
| 1   | A     | 1005 | A    | C4-C5-C6   | 5.87  | 119.94      | 117.00   |
| 1   | A     | 45   | U    | N1-C2-N3   | 5.87  | 118.42      | 114.90   |
| 1   | A     | 102  | G    | C5-C6-O6   | -5.87 | 125.08      | 128.60   |
| 1   | A     | 173  | U    | N3-C4-O4   | -5.87 | 115.29      | 119.40   |
| 1   | A     | 41   | G    | N1-C6-O6   | 5.87  | 123.42      | 119.90   |
| 1   | A     | 400  | C    | N3-C2-O2   | 5.87  | 126.01      | 121.90   |
| 1   | A     | 1287 | A    | N7-C8-N9   | 5.87  | 116.73      | 113.80   |
| 1   | A     | 1463 | C    | C6-N1-C2   | 5.86  | 122.65      | 120.30   |
| 1   | A     | 578  | C    | C2-N3-C4   | -5.86 | 116.97      | 119.90   |
| 1   | A     | 505  | G    | N1-C6-O6   | -5.86 | 116.38      | 119.90   |
| 1   | A     | 362  | G    | C5-C6-N1   | -5.86 | 108.57      | 111.50   |
| 1   | A     | 388  | G    | C5-C6-N1   | -5.86 | 108.57      | 111.50   |
| 1   | A     | 405  | U    | C5-C4-O4   | 5.86  | 129.41      | 125.90   |
| 1   | A     | 657  | G    | N3-C2-N2   | -5.86 | 115.80      | 119.90   |
| 1   | A     | 778  | G    | C5-C6-N1   | -5.86 | 108.57      | 111.50   |

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| Mol | Chain | Res     | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 1   | A     | 1524    | C    | N1-C2-O2   | -5.86 | 115.39      | 118.90   |
| 1   | A     | 887     | G    | N3-C2-N2   | -5.85 | 115.80      | 119.90   |
| 1   | A     | 1129    | C    | O4'-C1'-N1 | 5.85  | 112.88      | 108.20   |
| 1   | A     | 15      | G    | C6-C5-N7   | -5.85 | 126.89      | 130.40   |
| 1   | A     | 251     | G    | C6-C5-N7   | -5.85 | 126.89      | 130.40   |
| 1   | A     | 1030(A) | G    | C2-N3-C4   | 5.85  | 114.82      | 111.90   |
| 1   | A     | 780     | A    | C5-C6-N1   | 5.84  | 120.62      | 117.70   |
| 1   | A     | 317     | G    | N1-C6-O6   | 5.84  | 123.40      | 119.90   |
| 1   | A     | 553     | A    | N1-C6-N6   | 5.84  | 122.10      | 118.60   |
| 1   | A     | 1333    | A    | C6-N1-C2   | -5.84 | 115.10      | 118.60   |
| 1   | A     | 595     | G    | C8-N9-C1'  | -5.83 | 119.42      | 127.00   |
| 1   | A     | 719     | C    | N3-C4-N4   | 5.83  | 122.08      | 118.00   |
| 1   | A     | 1198    | G    | C2-N3-C4   | -5.83 | 108.98      | 111.90   |
| 1   | A     | 188     | C    | N3-C4-C5   | -5.83 | 119.57      | 121.90   |
| 1   | A     | 284     | G    | N3-C4-C5   | 5.83  | 131.51      | 128.60   |
| 1   | A     | 190(D)  | U    | C5-C6-N1   | -5.83 | 119.79      | 122.70   |
| 1   | A     | 1528    | U    | C5-C6-N1   | -5.82 | 119.79      | 122.70   |
| 1   | A     | 23      | C    | OP2-P-O3'  | 5.82  | 118.00      | 105.20   |
| 1   | A     | 1205    | U    | N3-C4-O4   | 5.82  | 123.47      | 119.40   |
| 1   | A     | 305     | G    | N1-C6-O6   | 5.82  | 123.39      | 119.90   |
| 6   | F     | 21      | LEU  | CA-CB-CG   | -5.82 | 101.92      | 115.30   |
| 1   | A     | 572     | A    | N1-C6-N6   | -5.81 | 115.11      | 118.60   |
| 1   | A     | 1157    | A    | C8-N9-C4   | -5.81 | 103.48      | 105.80   |
| 1   | A     | 378     | G    | C5-C6-O6   | -5.81 | 125.11      | 128.60   |
| 1   | A     | 859     | A    | C5-C6-N1   | -5.81 | 114.80      | 117.70   |
| 1   | A     | 189     | G    | C8-N9-C4   | 5.80  | 108.72      | 106.40   |
| 1   | A     | 810     | C    | N3-C2-O2   | -5.80 | 117.84      | 121.90   |
| 1   | A     | 260     | G    | C5-C6-N1   | -5.80 | 108.60      | 111.50   |
| 1   | A     | 1100    | C    | C5-C4-N4   | -5.80 | 116.14      | 120.20   |
| 1   | A     | 631     | G    | N3-C4-N9   | -5.80 | 122.52      | 126.00   |
| 1   | A     | 728     | A    | N7-C8-N9   | 5.80  | 116.70      | 113.80   |
| 1   | A     | 877     | C    | N3-C4-N4   | 5.80  | 122.06      | 118.00   |
| 1   | A     | 1205    | U    | C4-C5-C6   | 5.79  | 123.18      | 119.70   |
| 1   | A     | 25      | C    | O5'-P-OP2  | -5.79 | 100.49      | 105.70   |
| 1   | A     | 1079    | G    | C8-N9-C4   | -5.79 | 104.08      | 106.40   |
| 1   | A     | 305     | G    | C2-N3-C4   | -5.79 | 109.00      | 111.90   |
| 1   | A     | 571     | U    | C6-N1-C2   | -5.79 | 117.53      | 121.00   |
| 1   | A     | 885     | G    | N3-C2-N2   | -5.79 | 115.85      | 119.90   |
| 1   | A     | 1220    | G    | N1-C6-O6   | 5.79  | 123.37      | 119.90   |
| 1   | A     | 769     | G    | OP2-P-O3'  | 5.78  | 117.92      | 105.20   |
| 1   | A     | 907     | A    | N1-C6-N6   | -5.78 | 115.13      | 118.60   |
| 19  | S     | 4       | SER  | N-CA-C     | 5.78  | 126.61      | 111.00   |

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| Mol | Chain | Res     | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 1   | A     | 670     | G    | O5'-P-OP2 | -5.78 | 100.50      | 105.70   |
| 1   | A     | 720     | C    | N3-C4-C5  | 5.78  | 124.21      | 121.90   |
| 1   | A     | 1470    | G    | C8-N9-C1' | -5.78 | 119.49      | 127.00   |
| 1   | A     | 108     | G    | C5-C6-O6  | -5.78 | 125.14      | 128.60   |
| 1   | A     | 194     | C    | C6-N1-C2  | 5.78  | 122.61      | 120.30   |
| 1   | A     | 548     | G    | C5-C6-O6  | -5.78 | 125.14      | 128.60   |
| 1   | A     | 562     | C    | C6-N1-C1' | -5.78 | 113.87      | 120.80   |
| 1   | A     | 1182    | G    | N3-C4-N9  | 5.77  | 129.46      | 126.00   |
| 1   | A     | 448     | A    | O5'-P-OP2 | -5.77 | 100.51      | 105.70   |
| 1   | A     | 703     | G    | N3-C2-N2  | 5.77  | 123.94      | 119.90   |
| 1   | A     | 943     | U    | N3-C2-O2  | 5.77  | 126.24      | 122.20   |
| 1   | A     | 1377    | A    | N1-C2-N3  | 5.77  | 132.18      | 129.30   |
| 1   | A     | 79      | G    | C6-C5-N7  | -5.76 | 126.94      | 130.40   |
| 1   | A     | 485     | G    | N7-C8-N9  | -5.76 | 110.22      | 113.10   |
| 1   | A     | 1426    | C    | C5-C6-N1  | -5.76 | 118.12      | 121.00   |
| 1   | A     | 533     | A    | O5'-P-OP2 | -5.76 | 100.52      | 105.70   |
| 1   | A     | 122     | G    | O5'-P-OP1 | -5.75 | 100.52      | 105.70   |
| 1   | A     | 314     | C    | N3-C2-O2  | 5.75  | 125.93      | 121.90   |
| 1   | A     | 1432    | G    | N7-C8-N9  | 5.75  | 115.98      | 113.10   |
| 1   | A     | 821     | G    | C2-N3-C4  | -5.75 | 109.03      | 111.90   |
| 1   | A     | 1030(B) | C    | C5-C6-N1  | 5.75  | 123.87      | 121.00   |
| 1   | A     | 1053    | G    | C6-C5-N7  | 5.75  | 133.85      | 130.40   |
| 1   | A     | 255     | G    | C5-C6-O6  | -5.75 | 125.15      | 128.60   |
| 1   | A     | 712     | A    | O5'-P-OP1 | -5.74 | 100.53      | 105.70   |
| 1   | A     | 637     | G    | C8-N9-C4  | 5.74  | 108.70      | 106.40   |
| 1   | A     | 21      | G    | C4-C5-N7  | 5.74  | 113.10      | 110.80   |
| 1   | A     | 1542    | U    | N1-C2-O2  | 5.74  | 126.82      | 122.80   |
| 1   | A     | 664     | G    | N7-C8-N9  | -5.74 | 110.23      | 113.10   |
| 1   | A     | 562     | C    | N3-C2-O2  | -5.74 | 117.89      | 121.90   |
| 1   | A     | 61      | G    | C4-C5-N7  | 5.73  | 113.09      | 110.80   |
| 1   | A     | 295     | C    | N3-C4-C5  | 5.73  | 124.19      | 121.90   |
| 1   | A     | 1257    | U    | N1-C2-O2  | 5.73  | 126.81      | 122.80   |
| 1   | A     | 104     | G    | C6-C5-N7  | -5.72 | 126.97      | 130.40   |
| 1   | A     | 566     | G    | N7-C8-N9  | -5.72 | 110.24      | 113.10   |
| 1   | A     | 817     | C    | N3-C2-O2  | -5.72 | 117.89      | 121.90   |
| 1   | A     | 31      | G    | N3-C2-N2  | 5.72  | 123.91      | 119.90   |
| 1   | A     | 1487    | G    | N3-C4-C5  | -5.72 | 125.74      | 128.60   |
| 1   | A     | 791     | G    | N1-C6-O6  | 5.72  | 123.33      | 119.90   |
| 1   | A     | 502     | G    | O5'-P-OP2 | -5.72 | 100.55      | 105.70   |
| 1   | A     | 164     | U    | O5'-P-OP1 | -5.72 | 100.56      | 105.70   |
| 1   | A     | 304     | U    | C6-N1-C2  | -5.72 | 117.57      | 121.00   |
| 1   | A     | 50      | A    | C2-N3-C4  | -5.71 | 107.74      | 110.60   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | A     | 181  | G    | C6-C5-N7  | -5.71 | 126.97      | 130.40   |
| 1   | A     | 816  | A    | C4-C5-N7  | -5.71 | 107.84      | 110.70   |
| 1   | A     | 1100 | C    | C6-N1-C1' | -5.71 | 113.95      | 120.80   |
| 1   | A     | 1230 | C    | C5-C6-N1  | 5.71  | 123.86      | 121.00   |
| 1   | A     | 1083 | U    | C4-C5-C6  | 5.71  | 123.13      | 119.70   |
| 1   | A     | 1193 | G    | C4-C5-C6  | 5.71  | 122.23      | 118.80   |
| 1   | A     | 502  | G    | N3-C4-N9  | -5.71 | 122.58      | 126.00   |
| 1   | A     | 1514 | C    | C5-C6-N1  | -5.71 | 118.15      | 121.00   |
| 1   | A     | 381  | C    | N3-C4-C5  | -5.70 | 119.62      | 121.90   |
| 1   | A     | 541  | G    | N3-C2-N2  | -5.70 | 115.91      | 119.90   |
| 1   | A     | 1523 | G    | N3-C2-N2  | -5.70 | 115.91      | 119.90   |
| 1   | A     | 1125 | U    | N3-C4-O4  | 5.70  | 123.39      | 119.40   |
| 1   | A     | 169  | C    | C5-C6-N1  | 5.70  | 123.85      | 121.00   |
| 1   | A     | 1055 | A    | C4-C5-C6  | 5.70  | 119.85      | 117.00   |
| 1   | A     | 1240 | U    | C2-N1-C1' | -5.70 | 110.87      | 117.70   |
| 1   | A     | 381  | C    | C2-N1-C1' | 5.69  | 125.06      | 118.80   |
| 1   | A     | 146  | G    | O5'-P-OP1 | -5.69 | 100.58      | 105.70   |
| 1   | A     | 859  | A    | C2-N3-C4  | -5.69 | 107.75      | 110.60   |
| 1   | A     | 897  | C    | C2-N3-C4  | -5.69 | 117.05      | 119.90   |
| 1   | A     | 1470 | G    | C4-C5-C6  | 5.69  | 122.22      | 118.80   |
| 1   | A     | 299  | G    | C8-N9-C1' | -5.69 | 119.60      | 127.00   |
| 1   | A     | 729  | A    | N3-C4-C5  | -5.69 | 122.82      | 126.80   |
| 1   | A     | 558  | G    | N3-C4-C5  | 5.69  | 131.44      | 128.60   |
| 1   | A     | 380  | G    | O5'-P-OP2 | -5.69 | 100.58      | 105.70   |
| 1   | A     | 555  | C    | N3-C4-C5  | 5.68  | 124.17      | 121.90   |
| 1   | A     | 917  | G    | C8-N9-C4  | -5.68 | 104.13      | 106.40   |
| 1   | A     | 1139 | G    | N3-C4-C5  | -5.68 | 125.76      | 128.60   |
| 1   | A     | 229  | U    | C4-C5-C6  | 5.68  | 123.11      | 119.70   |
| 1   | A     | 604  | G    | N3-C2-N2  | -5.68 | 115.92      | 119.90   |
| 1   | A     | 227  | G    | C6-C5-N7  | -5.68 | 126.99      | 130.40   |
| 1   | A     | 854  | G    | N1-C6-O6  | 5.68  | 123.31      | 119.90   |
| 1   | A     | 1157 | A    | C2-N3-C4  | 5.68  | 113.44      | 110.60   |
| 1   | A     | 1394 | A    | O5'-P-OP1 | -5.67 | 100.59      | 105.70   |
| 1   | A     | 1109 | C    | N3-C2-O2  | -5.67 | 117.93      | 121.90   |
| 1   | A     | 1232 | U    | N3-C4-O4  | 5.67  | 123.37      | 119.40   |
| 10  | J     | 65   | LEU  | CA-CB-CG  | 5.67  | 128.34      | 115.30   |
| 1   | A     | 7    | G    | N9-C4-C5  | -5.67 | 103.13      | 105.40   |
| 1   | A     | 830  | G    | N1-C2-N2  | 5.67  | 121.30      | 116.20   |
| 1   | A     | 1432 | G    | C5-C6-O6  | 5.67  | 132.00      | 128.60   |
| 1   | A     | 12   | U    | C2-N1-C1' | 5.67  | 124.50      | 117.70   |
| 1   | A     | 789  | U    | C5-C4-O4  | 5.67  | 129.30      | 125.90   |
| 1   | A     | 1023 | G    | N9-C4-C5  | -5.67 | 103.13      | 105.40   |

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| Mol | Chain | Res     | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 1   | A     | 993     | G    | C6-C5-N7  | -5.66 | 127.00      | 130.40   |
| 1   | A     | 1286    | A    | N7-C8-N9  | 5.66  | 116.63      | 113.80   |
| 1   | A     | 45      | U    | C5-C4-O4  | 5.66  | 129.30      | 125.90   |
| 1   | A     | 485     | G    | OP2-P-O3' | 5.66  | 117.65      | 105.20   |
| 1   | A     | 1090    | U    | N3-C2-O2  | -5.66 | 118.24      | 122.20   |
| 1   | A     | 292     | G    | N1-C6-O6  | 5.66  | 123.30      | 119.90   |
| 1   | A     | 289     | G    | C4-N9-C1' | 5.66  | 133.85      | 126.50   |
| 1   | A     | 902     | G    | C4-C5-N7  | 5.66  | 113.06      | 110.80   |
| 1   | A     | 23      | C    | C2-N1-C1' | -5.66 | 112.58      | 118.80   |
| 1   | A     | 242     | C    | C2-N3-C4  | -5.66 | 117.07      | 119.90   |
| 1   | A     | 709     | G    | N1-C6-O6  | 5.65  | 123.29      | 119.90   |
| 1   | A     | 862     | C    | C6-N1-C2  | 5.65  | 122.56      | 120.30   |
| 1   | A     | 790     | A    | C2-N3-C4  | -5.65 | 107.78      | 110.60   |
| 1   | A     | 499     | A    | OP1-P-O3' | 5.65  | 117.63      | 105.20   |
| 1   | A     | 566     | G    | C2-N3-C4  | -5.65 | 109.08      | 111.90   |
| 1   | A     | 635     | G    | C2-N3-C4  | -5.65 | 109.08      | 111.90   |
| 1   | A     | 752     | G    | C8-N9-C4  | 5.65  | 108.66      | 106.40   |
| 18  | R     | 66      | LEU  | CA-CB-CG  | -5.65 | 102.31      | 115.30   |
| 1   | A     | 372     | C    | C6-N1-C1' | -5.65 | 114.03      | 120.80   |
| 1   | A     | 1098    | C    | C6-N1-C2  | 5.64  | 122.56      | 120.30   |
| 1   | A     | 265     | G    | C8-N9-C1' | 5.64  | 134.33      | 127.00   |
| 1   | A     | 394     | G    | N1-C6-O6  | 5.64  | 123.28      | 119.90   |
| 1   | A     | 456     | C    | O5'-P-OP1 | 5.64  | 117.47      | 110.70   |
| 1   | A     | 120     | A    | C8-N9-C4  | -5.64 | 103.55      | 105.80   |
| 1   | A     | 828     | A    | N9-C4-C5  | -5.64 | 103.55      | 105.80   |
| 1   | A     | 239     | U    | C2-N3-C4  | 5.63  | 130.38      | 127.00   |
| 1   | A     | 911     | U    | C5-C4-O4  | 5.63  | 129.28      | 125.90   |
| 1   | A     | 1204    | A    | N1-C6-N6  | 5.63  | 121.98      | 118.60   |
| 1   | A     | 884     | U    | C5-C6-N1  | -5.63 | 119.89      | 122.70   |
| 1   | A     | 28      | G    | C5-C6-N1  | -5.63 | 108.69      | 111.50   |
| 1   | A     | 279     | A    | C8-N9-C4  | -5.63 | 103.55      | 105.80   |
| 1   | A     | 44      | G    | C4-C5-N7  | 5.63  | 113.05      | 110.80   |
| 1   | A     | 1139    | G    | C4-C5-N7  | -5.63 | 108.55      | 110.80   |
| 1   | A     | 292     | G    | C4-C5-C6  | 5.62  | 122.17      | 118.80   |
| 1   | A     | 484     | G    | N3-C2-N2  | 5.62  | 123.84      | 119.90   |
| 1   | A     | 676     | A    | C8-N9-C4  | 5.62  | 108.05      | 105.80   |
| 1   | A     | 1516[A] | G    | C5-C6-N1  | -5.62 | 108.69      | 111.50   |
| 1   | A     | 1516[B] | G    | C5-C6-N1  | -5.62 | 108.69      | 111.50   |
| 1   | A     | 1396    | A    | C2-N3-C4  | -5.62 | 107.79      | 110.60   |
| 1   | A     | 1462    | G    | N1-C6-O6  | 5.62  | 123.27      | 119.90   |
| 1   | A     | 1461    | G    | N3-C4-C5  | 5.62  | 131.41      | 128.60   |
| 1   | A     | 484     | G    | C4-N9-C1' | 5.62  | 133.80      | 126.50   |

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| Mol | Chain | Res    | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 1   | A     | 1322   | C    | N3-C2-O2   | 5.62  | 125.83      | 121.90   |
| 14  | N     | 39     | LEU  | CA-CB-CG   | -5.62 | 102.38      | 115.30   |
| 1   | A     | 34     | C    | N3-C2-O2   | 5.61  | 125.83      | 121.90   |
| 1   | A     | 509    | A    | N7-C8-N9   | 5.61  | 116.61      | 113.80   |
| 1   | A     | 662    | G    | C6-C5-N7   | -5.61 | 127.03      | 130.40   |
| 1   | A     | 752    | G    | N7-C8-N9   | -5.61 | 110.29      | 113.10   |
| 1   | A     | 774    | G    | N1-C6-O6   | 5.61  | 123.27      | 119.90   |
| 1   | A     | 859    | A    | OP1-P-O3'  | -5.61 | 92.85       | 105.20   |
| 1   | A     | 347    | G    | N1-C6-O6   | 5.61  | 123.27      | 119.90   |
| 1   | A     | 575    | G    | N1-C6-O6   | -5.61 | 116.53      | 119.90   |
| 1   | A     | 864    | A    | C8-N9-C4   | -5.61 | 103.56      | 105.80   |
| 1   | A     | 1451   | A    | N1-C6-N6   | -5.61 | 115.23      | 118.60   |
| 1   | A     | 22     | G    | OP2-P-O3'  | 5.61  | 117.53      | 105.20   |
| 1   | A     | 672    | U    | C6-N1-C2   | -5.61 | 117.64      | 121.00   |
| 1   | A     | 945    | G    | O5'-P-OP2  | -5.61 | 100.66      | 105.70   |
| 1   | A     | 577    | G    | N3-C2-N2   | -5.60 | 115.98      | 119.90   |
| 1   | A     | 1530   | G    | C6-N1-C2   | 5.60  | 128.46      | 125.10   |
| 1   | A     | 281    | G    | N1-C6-O6   | 5.60  | 123.26      | 119.90   |
| 1   | A     | 361    | G    | N7-C8-N9   | -5.60 | 110.30      | 113.10   |
| 1   | A     | 579    | G    | C5-C6-N1   | -5.60 | 108.70      | 111.50   |
| 1   | A     | 815    | A    | C6-N1-C2   | -5.60 | 115.24      | 118.60   |
| 1   | A     | 888    | G    | C4-C5-N7   | -5.60 | 108.56      | 110.80   |
| 1   | A     | 1014   | A    | C2-N3-C4   | 5.60  | 113.40      | 110.60   |
| 1   | A     | 1180   | A    | C8-N9-C4   | -5.60 | 103.56      | 105.80   |
| 1   | A     | 17     | U    | N3-C4-O4   | 5.60  | 123.32      | 119.40   |
| 1   | A     | 574    | A    | C2-N3-C4   | -5.60 | 107.80      | 110.60   |
| 1   | A     | 802    | A    | N1-C6-N6   | 5.60  | 121.96      | 118.60   |
| 1   | A     | 190(H) | G    | C5-C6-O6   | -5.60 | 125.24      | 128.60   |
| 1   | A     | 1493   | A    | O4'-C1'-N9 | 5.60  | 112.68      | 108.20   |
| 1   | A     | 552    | U    | C2-N3-C4   | -5.59 | 123.64      | 127.00   |
| 1   | A     | 901    | A    | C2-N3-C4   | -5.59 | 107.80      | 110.60   |
| 1   | A     | 928    | G    | N3-C2-N2   | -5.59 | 115.98      | 119.90   |
| 1   | A     | 949    | A    | C5-C6-N6   | -5.59 | 119.23      | 123.70   |
| 1   | A     | 1211   | U    | C2-N1-C1'  | 5.59  | 124.41      | 117.70   |
| 1   | A     | 890    | G    | O4'-C1'-N9 | 5.59  | 112.67      | 108.20   |
| 1   | A     | 266    | G    | N7-C8-N9   | 5.58  | 115.89      | 113.10   |
| 1   | A     | 344    | A    | N7-C8-N9   | 5.58  | 116.59      | 113.80   |
| 1   | A     | 791    | G    | C5-C6-O6   | 5.58  | 131.95      | 128.60   |
| 1   | A     | 1485   | U    | C6-N1-C1'  | 5.58  | 129.02      | 121.20   |
| 1   | A     | 488    | C    | C5-C4-N4   | -5.58 | 116.29      | 120.20   |
| 1   | A     | 550    | G    | C8-N9-C4   | 5.58  | 108.63      | 106.40   |
| 1   | A     | 600    | C    | OP2-P-O3'  | 5.58  | 117.47      | 105.20   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | A     | 830  | G    | C6-N1-C2  | 5.58  | 128.44      | 125.10   |
| 1   | A     | 360  | A    | C6-N1-C2  | -5.57 | 115.26      | 118.60   |
| 1   | A     | 1121 | U    | C2-N3-C4  | -5.57 | 123.66      | 127.00   |
| 1   | A     | 1373 | G    | C4-C5-C6  | 5.57  | 122.14      | 118.80   |
| 1   | A     | 559  | A    | P-O3'-C3' | 5.57  | 126.39      | 119.70   |
| 1   | A     | 715  | A    | OP1-P-O3' | 5.57  | 117.46      | 105.20   |
| 1   | A     | 31   | G    | C8-N9-C4  | 5.57  | 108.63      | 106.40   |
| 1   | A     | 362  | G    | C4-C5-N7  | -5.57 | 108.57      | 110.80   |
| 1   | A     | 805  | C    | C5-C6-N1  | 5.57  | 123.78      | 121.00   |
| 1   | A     | 299  | G    | N1-C2-N2  | -5.57 | 111.19      | 116.20   |
| 1   | A     | 21   | G    | C4-N9-C1' | 5.57  | 133.73      | 126.50   |
| 1   | A     | 1117 | G    | N3-C4-N9  | 5.56  | 129.34      | 126.00   |
| 1   | A     | 1166 | G    | C8-N9-C4  | -5.56 | 104.17      | 106.40   |
| 1   | A     | 575  | G    | C5-C6-N1  | 5.56  | 114.28      | 111.50   |
| 1   | A     | 785  | G    | N9-C4-C5  | -5.56 | 103.18      | 105.40   |
| 1   | A     | 839  | U    | N1-C2-O2  | 5.56  | 126.69      | 122.80   |
| 1   | A     | 872  | A    | N1-C2-N3  | 5.56  | 132.08      | 129.30   |
| 1   | A     | 1134 | G    | C4-C5-N7  | -5.56 | 108.58      | 110.80   |
| 1   | A     | 27   | G    | C5-N7-C8  | -5.56 | 101.52      | 104.30   |
| 1   | A     | 279  | A    | O5'-P-OP2 | -5.56 | 100.70      | 105.70   |
| 1   | A     | 741  | G    | N3-C4-C5  | -5.56 | 125.82      | 128.60   |
| 1   | A     | 899  | C    | C2-N1-C1' | -5.56 | 112.69      | 118.80   |
| 1   | A     | 733  | A    | C2-N3-C4  | -5.56 | 107.82      | 110.60   |
| 1   | A     | 604  | G    | C5-C6-N1  | -5.55 | 108.72      | 111.50   |
| 1   | A     | 761  | G    | N3-C2-N2  | -5.55 | 116.01      | 119.90   |
| 1   | A     | 783  | C    | N3-C4-C5  | 5.55  | 124.12      | 121.90   |
| 1   | A     | 893  | C    | C5-C6-N1  | 5.55  | 123.78      | 121.00   |
| 1   | A     | 1076 | C    | N3-C4-C5  | 5.55  | 124.12      | 121.90   |
| 17  | Q     | 31   | LEU  | CA-CB-CG  | -5.55 | 102.53      | 115.30   |
| 1   | A     | 658  | G    | O5'-P-OP2 | -5.55 | 100.70      | 105.70   |
| 1   | A     | 1405 | G    | N1-C6-O6  | 5.55  | 123.23      | 119.90   |
| 1   | A     | 299  | G    | C4-N9-C1' | 5.55  | 133.71      | 126.50   |
| 1   | A     | 1399 | C    | N3-C4-C5  | -5.54 | 119.68      | 121.90   |
| 1   | A     | 788  | U    | N3-C4-O4  | 5.54  | 123.28      | 119.40   |
| 1   | A     | 1479 | C    | C5-C6-N1  | 5.54  | 123.77      | 121.00   |
| 19  | S     | 5    | LEU  | N-CA-C    | 5.54  | 125.96      | 111.00   |
| 1   | A     | 711  | G    | N1-C6-O6  | 5.54  | 123.22      | 119.90   |
| 1   | A     | 332  | G    | N3-C2-N2  | -5.53 | 116.03      | 119.90   |
| 1   | A     | 1093 | A    | C6-N1-C2  | -5.53 | 115.28      | 118.60   |
| 1   | A     | 1124 | G    | C5-C6-N1  | 5.53  | 114.27      | 111.50   |
| 1   | A     | 1147 | C    | C4-C5-C6  | 5.53  | 120.17      | 117.40   |
| 1   | A     | 944  | G    | N3-C4-N9  | 5.53  | 129.32      | 126.00   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | A     | 66   | G    | O5'-P-OP1 | -5.53 | 100.72      | 105.70   |
| 1   | A     | 421  | U    | N1-C2-O2  | 5.53  | 126.67      | 122.80   |
| 1   | A     | 905  | U    | C6-N1-C2  | 5.53  | 124.32      | 121.00   |
| 1   | A     | 1380 | U    | P-O3'-C3' | 5.53  | 126.33      | 119.70   |
| 1   | A     | 1435 | G    | N3-C4-C5  | 5.53  | 131.36      | 128.60   |
| 1   | A     | 1501 | C    | N3-C4-C5  | 5.53  | 124.11      | 121.90   |
| 7   | G     | 120  | ILE  | CB-CA-C   | -5.53 | 100.55      | 111.60   |
| 1   | A     | 1323 | G    | C6-C5-N7  | -5.52 | 127.09      | 130.40   |
| 1   | A     | 121  | C    | O5'-P-OP2 | -5.52 | 100.73      | 105.70   |
| 1   | A     | 814  | A    | N1-C2-N3  | 5.52  | 132.06      | 129.30   |
| 1   | A     | 1352 | C    | O5'-P-OP2 | -5.52 | 100.73      | 105.70   |
| 1   | A     | 21   | G    | C8-N9-C1' | -5.52 | 119.83      | 127.00   |
| 1   | A     | 1188 | A    | C2-N3-C4  | -5.52 | 107.84      | 110.60   |
| 1   | A     | 1259 | C    | N3-C2-O2  | -5.52 | 118.04      | 121.90   |
| 1   | A     | 1053 | G    | N3-C4-C5  | 5.51  | 131.36      | 128.60   |
| 1   | A     | 1529 | G    | C4-C5-C6  | 5.51  | 122.11      | 118.80   |
| 1   | A     | 443  | C    | C6-N1-C2  | 5.51  | 122.50      | 120.30   |
| 1   | A     | 23   | C    | N1-C2-O2  | -5.51 | 115.59      | 118.90   |
| 1   | A     | 1193 | G    | C4-N9-C1' | 5.51  | 133.66      | 126.50   |
| 1   | A     | 1160 | G    | N1-C6-O6  | 5.51  | 123.20      | 119.90   |
| 1   | A     | 235  | C    | C5-C6-N1  | -5.50 | 118.25      | 121.00   |
| 1   | A     | 314  | C    | C2-N3-C4  | -5.50 | 117.15      | 119.90   |
| 1   | A     | 1197 | G    | C6-C5-N7  | -5.50 | 127.10      | 130.40   |
| 1   | A     | 1376 | U    | N3-C2-O2  | -5.50 | 118.35      | 122.20   |
| 1   | A     | 617  | G    | C2-N3-C4  | -5.50 | 109.15      | 111.90   |
| 1   | A     | 922  | G    | N1-C2-N3  | 5.50  | 127.20      | 123.90   |
| 1   | A     | 829  | G    | OP1-P-OP2 | 5.50  | 127.84      | 119.60   |
| 1   | A     | 1087 | G    | C4-N9-C1' | 5.50  | 133.65      | 126.50   |
| 1   | A     | 1121 | U    | C6-N1-C2  | 5.49  | 124.30      | 121.00   |
| 1   | A     | 1139 | G    | C5-C6-O6  | 5.49  | 131.90      | 128.60   |
| 1   | A     | 504  | C    | C5-C6-N1  | 5.49  | 123.75      | 121.00   |
| 1   | A     | 445  | G    | C4-C5-N7  | 5.49  | 113.00      | 110.80   |
| 1   | A     | 692  | U    | C6-N1-C2  | 5.49  | 124.30      | 121.00   |
| 1   | A     | 902  | G    | C8-N9-C1' | -5.49 | 119.86      | 127.00   |
| 10  | J     | 71   | LEU  | CA-CB-CG  | -5.49 | 102.67      | 115.30   |
| 1   | A     | 148  | G    | C6-C5-N7  | -5.49 | 127.11      | 130.40   |
| 1   | A     | 290  | C    | C5-C4-N4  | -5.49 | 116.36      | 120.20   |
| 1   | A     | 855  | G    | N1-C2-N3  | 5.49  | 127.19      | 123.90   |
| 1   | A     | 1146 | A    | N1-C6-N6  | 5.49  | 121.89      | 118.60   |
| 1   | A     | 1501 | C    | C6-N1-C1' | -5.49 | 114.21      | 120.80   |
| 1   | A     | 780  | A    | C4-C5-C6  | -5.49 | 114.26      | 117.00   |
| 1   | A     | 928  | G    | N1-C2-N3  | 5.49  | 127.19      | 123.90   |

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| Mol | Chain | Res     | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 1   | A     | 1118    | C    | C6-N1-C2  | -5.49 | 118.11      | 120.30   |
| 1   | A     | 1388    | C    | N3-C4-C5  | 5.49  | 124.09      | 121.90   |
| 1   | A     | 1485    | U    | C6-N1-C2  | -5.49 | 117.71      | 121.00   |
| 1   | A     | 732     | C    | C6-N1-C2  | -5.48 | 118.11      | 120.30   |
| 1   | A     | 284     | G    | C5-C6-N1  | -5.48 | 108.76      | 111.50   |
| 1   | A     | 323     | U    | O5'-P-OP2 | -5.48 | 100.77      | 105.70   |
| 1   | A     | 860     | A    | C8-N9-C4  | 5.48  | 107.99      | 105.80   |
| 1   | A     | 748     | C    | P-O3'-C3' | 5.47  | 126.27      | 119.70   |
| 1   | A     | 975     | A    | C4-C5-C6  | 5.47  | 119.74      | 117.00   |
| 1   | A     | 741     | G    | C8-N9-C1' | -5.47 | 119.89      | 127.00   |
| 1   | A     | 325     | A    | N3-C4-N9  | -5.47 | 123.03      | 127.40   |
| 1   | A     | 1030(C) | G    | N3-C4-C5  | -5.47 | 125.86      | 128.60   |
| 1   | A     | 1507    | A    | O5'-P-OP1 | -5.47 | 100.78      | 105.70   |
| 5   | E     | 12      | LEU  | CB-CG-CD1 | -5.47 | 101.70      | 111.00   |
| 1   | A     | 856     | C    | N1-C2-O2  | -5.47 | 115.62      | 118.90   |
| 1   | A     | 325     | A    | C6-C5-N7  | 5.47  | 136.13      | 132.30   |
| 1   | A     | 975     | A    | C8-N9-C4  | -5.47 | 103.61      | 105.80   |
| 1   | A     | 33      | A    | O5'-P-OP2 | -5.46 | 100.78      | 105.70   |
| 1   | A     | 102     | G    | N3-C4-N9  | 5.46  | 129.28      | 126.00   |
| 1   | A     | 1068    | G    | OP2-P-O3' | 5.46  | 117.22      | 105.20   |
| 1   | A     | 1256    | A    | C5-N7-C8  | 5.46  | 106.63      | 103.90   |
| 1   | A     | 29      | G    | OP1-P-OP2 | 5.46  | 127.80      | 119.60   |
| 1   | A     | 376     | G    | C5-N7-C8  | 5.46  | 107.03      | 104.30   |
| 1   | A     | 668     | G    | C2-N3-C4  | -5.46 | 109.17      | 111.90   |
| 1   | A     | 251     | G    | C5-N7-C8  | -5.46 | 101.57      | 104.30   |
| 1   | A     | 434     | U    | C6-N1-C2  | -5.46 | 117.72      | 121.00   |
| 1   | A     | 538     | G    | N1-C6-O6  | -5.46 | 116.62      | 119.90   |
| 1   | A     | 1416    | G    | C8-N9-C4  | -5.46 | 104.22      | 106.40   |
| 1   | A     | 317     | G    | C4-C5-N7  | 5.46  | 112.98      | 110.80   |
| 1   | A     | 542     | G    | N1-C6-O6  | -5.46 | 116.62      | 119.90   |
| 1   | A     | 814     | A    | OP1-P-O3' | 5.46  | 117.21      | 105.20   |
| 1   | A     | 728     | A    | C5-N7-C8  | -5.46 | 101.17      | 103.90   |
| 1   | A     | 867     | G    | O5'-P-OP2 | -5.46 | 100.79      | 105.70   |
| 1   | A     | 904     | C    | O5'-P-OP2 | 5.46  | 117.25      | 110.70   |
| 1   | A     | 1193    | G    | N1-C2-N3  | 5.46  | 127.17      | 123.90   |
| 1   | A     | 35      | G    | C8-N9-C4  | 5.45  | 108.58      | 106.40   |
| 1   | A     | 1399    | C    | C4-C5-C6  | 5.45  | 120.13      | 117.40   |
| 1   | A     | 957     | U    | C5-C4-O4  | 5.45  | 129.17      | 125.90   |
| 1   | A     | 332     | G    | C5-C6-O6  | -5.45 | 125.33      | 128.60   |
| 1   | A     | 1131    | G    | C6-C5-N7  | -5.45 | 127.13      | 130.40   |
| 1   | A     | 1063    | C    | C4-C5-C6  | 5.45  | 120.12      | 117.40   |
| 1   | A     | 570     | G    | N7-C8-N9  | 5.45  | 115.82      | 113.10   |

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| Mol | Chain | Res    | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 1   | A     | 47     | C    | N1-C2-N3   | 5.45  | 123.01      | 119.20   |
| 1   | A     | 108    | G    | C5-N7-C8   | -5.45 | 101.58      | 104.30   |
| 1   | A     | 199    | G    | C8-N9-C4   | 5.45  | 108.58      | 106.40   |
| 1   | A     | 1350   | A    | O5'-P-OP2  | -5.45 | 100.80      | 105.70   |
| 1   | A     | 1511   | G    | C8-N9-C1'  | -5.44 | 119.92      | 127.00   |
| 1   | A     | 239    | U    | N1-C2-O2   | -5.44 | 118.99      | 122.80   |
| 1   | A     | 976    | G    | C2-N3-C4   | -5.44 | 109.18      | 111.90   |
| 1   | A     | 1230   | C    | N1-C2-O2   | 5.44  | 122.17      | 118.90   |
| 6   | F     | 75     | LEU  | CA-CB-CG   | 5.44  | 127.81      | 115.30   |
| 1   | A     | 871    | U    | C6-N1-C2   | 5.44  | 124.26      | 121.00   |
| 1   | A     | 1467   | G    | C2-N3-C4   | 5.44  | 114.62      | 111.90   |
| 1   | A     | 278    | G    | N3-C4-N9   | -5.44 | 122.74      | 126.00   |
| 1   | A     | 852    | G    | C2-N3-C4   | -5.44 | 109.18      | 111.90   |
| 1   | A     | 961    | U    | N3-C4-O4   | 5.44  | 123.20      | 119.40   |
| 1   | A     | 935    | A    | OP1-P-OP2  | 5.43  | 127.75      | 119.60   |
| 1   | A     | 234    | C    | C2-N1-C1'  | -5.43 | 112.82      | 118.80   |
| 1   | A     | 374    | A    | C8-N9-C4   | 5.43  | 107.97      | 105.80   |
| 1   | A     | 976    | G    | O5'-P-OP1  | -5.43 | 100.81      | 105.70   |
| 1   | A     | 117    | G    | C8-N9-C1'  | -5.43 | 119.94      | 127.00   |
| 1   | A     | 1396   | A    | C8-N9-C4   | 5.43  | 107.97      | 105.80   |
| 1   | A     | 564    | C    | C6-N1-C1'  | -5.43 | 114.28      | 120.80   |
| 1   | A     | 190(E) | U    | N1-C2-O2   | 5.43  | 126.60      | 122.80   |
| 1   | A     | 336    | C    | C6-N1-C2   | 5.43  | 122.47      | 120.30   |
| 1   | A     | 224    | C    | N1-C2-O2   | 5.43  | 122.16      | 118.90   |
| 1   | A     | 672    | U    | O4'-C1'-N1 | 5.43  | 112.54      | 108.20   |
| 1   | A     | 839    | U    | N3-C2-O2   | -5.43 | 118.40      | 122.20   |
| 1   | A     | 1064   | G    | C6-C5-N7   | -5.42 | 127.15      | 130.40   |
| 1   | A     | 1249   | C    | C6-N1-C2   | 5.42  | 122.47      | 120.30   |
| 1   | A     | 970    | C    | N1-C2-N3   | -5.42 | 115.40      | 119.20   |
| 1   | A     | 886    | G    | N3-C4-C5   | 5.42  | 131.31      | 128.60   |
| 1   | A     | 947    | G    | N1-C6-O6   | 5.42  | 123.15      | 119.90   |
| 1   | A     | 955    | U    | N1-C2-N3   | 5.42  | 118.15      | 114.90   |
| 14  | N     | 7      | ILE  | CB-CA-C    | 5.42  | 122.44      | 111.60   |
| 1   | A     | 877    | C    | C5-C6-N1   | 5.42  | 123.71      | 121.00   |
| 1   | A     | 1377   | A    | N3-C4-C5   | 5.42  | 130.59      | 126.80   |
| 1   | A     | 36     | C    | O5'-P-OP1  | 5.42  | 117.20      | 110.70   |
| 1   | A     | 504    | C    | N3-C4-N4   | 5.42  | 121.79      | 118.00   |
| 1   | A     | 820    | U    | C6-N1-C2   | 5.42  | 124.25      | 121.00   |
| 1   | A     | 936    | C    | O5'-P-OP1  | -5.42 | 100.82      | 105.70   |
| 1   | A     | 170    | U    | N3-C4-O4   | 5.42  | 123.19      | 119.40   |
| 1   | A     | 509    | A    | C4-C5-C6   | 5.42  | 119.71      | 117.00   |
| 1   | A     | 785    | G    | C5-C6-O6   | -5.42 | 125.35      | 128.60   |

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| Mol | Chain | Res     | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 1   | A     | 902     | G    | C2-N3-C4   | -5.41 | 109.19      | 111.90   |
| 1   | A     | 41      | G    | C8-N9-C4   | -5.41 | 104.23      | 106.40   |
| 1   | A     | 1494    | G    | C4-N9-C1'  | 5.41  | 133.53      | 126.50   |
| 1   | A     | 820     | U    | N3-C2-O2   | 5.41  | 125.98      | 122.20   |
| 1   | A     | 113     | G    | N3-C4-C5   | -5.40 | 125.90      | 128.60   |
| 1   | A     | 316     | G    | C5-C6-O6   | -5.40 | 125.36      | 128.60   |
| 1   | A     | 1490    | C    | C2-N3-C4   | 5.40  | 122.60      | 119.90   |
| 1   | A     | 161     | A    | N1-C6-N6   | -5.40 | 115.36      | 118.60   |
| 1   | A     | 661     | G    | N3-C2-N2   | -5.40 | 116.12      | 119.90   |
| 1   | A     | 819     | A    | C6-C5-N7   | -5.40 | 128.52      | 132.30   |
| 1   | A     | 1166    | G    | C8-N9-C1'  | -5.40 | 119.98      | 127.00   |
| 1   | A     | 590     | C    | C5-C6-N1   | -5.40 | 118.30      | 121.00   |
| 1   | A     | 234     | C    | N3-C4-N4   | -5.40 | 114.22      | 118.00   |
| 1   | A     | 102     | G    | C4-C5-C6   | 5.39  | 122.04      | 118.80   |
| 1   | A     | 281     | G    | C6-C5-N7   | -5.39 | 127.16      | 130.40   |
| 1   | A     | 729     | A    | C6-N1-C2   | -5.39 | 115.37      | 118.60   |
| 1   | A     | 651     | C    | N3-C2-O2   | 5.39  | 125.67      | 121.90   |
| 1   | A     | 817     | C    | O4'-C1'-N1 | -5.39 | 103.89      | 108.20   |
| 1   | A     | 890     | G    | OP2-P-O3'  | 5.39  | 117.05      | 105.20   |
| 1   | A     | 54      | C    | OP1-P-O3'  | 5.38  | 117.05      | 105.20   |
| 1   | A     | 792     | A    | C2-N3-C4   | -5.38 | 107.91      | 110.60   |
| 1   | A     | 1234    | C    | C6-N1-C2   | 5.38  | 122.45      | 120.30   |
| 1   | A     | 276     | G    | C6-C5-N7   | -5.38 | 127.17      | 130.40   |
| 1   | A     | 445     | G    | C5-C6-O6   | -5.38 | 125.37      | 128.60   |
| 1   | A     | 1240    | U    | C5-C4-O4   | 5.38  | 129.13      | 125.90   |
| 1   | A     | 444     | C    | N3-C2-O2   | -5.38 | 118.13      | 121.90   |
| 1   | A     | 934     | C    | C6-N1-C2   | -5.38 | 118.15      | 120.30   |
| 1   | A     | 525     | C    | C5-C6-N1   | 5.38  | 123.69      | 121.00   |
| 1   | A     | 250     | A    | N1-C2-N3   | 5.37  | 131.99      | 129.30   |
| 1   | A     | 659     | U    | C6-N1-C2   | -5.37 | 117.78      | 121.00   |
| 1   | A     | 1516[A] | G    | C4-N9-C1'  | -5.37 | 119.52      | 126.50   |
| 1   | A     | 1516[B] | G    | C4-N9-C1'  | -5.37 | 119.52      | 126.50   |
| 1   | A     | 175     | C    | O5'-P-OP1  | 5.37  | 117.14      | 110.70   |
| 1   | A     | 1201    | A    | P-O3'-C3'  | 5.37  | 126.14      | 119.70   |
| 1   | A     | 313     | A    | C6-C5-N7   | -5.37 | 128.54      | 132.30   |
| 1   | A     | 1239    | A    | N1-C6-N6   | 5.37  | 121.82      | 118.60   |
| 1   | A     | 1304    | G    | C4-C5-C6   | 5.37  | 122.02      | 118.80   |
| 1   | A     | 970     | C    | C6-N1-C1'  | -5.37 | 114.36      | 120.80   |
| 1   | A     | 1117    | G    | N3-C2-N2   | 5.37  | 123.66      | 119.90   |
| 20  | T     | 13      | LEU  | CB-CG-CD1  | 5.37  | 120.12      | 111.00   |
| 1   | A     | 161     | A    | N1-C2-N3   | 5.36  | 131.98      | 129.30   |
| 1   | A     | 861     | G    | C5-N7-C8   | -5.36 | 101.62      | 104.30   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | A     | 133  | U    | C4-C5-C6  | 5.36  | 122.92      | 119.70   |
| 1   | A     | 517  | G    | C8-N9-C4  | -5.36 | 104.25      | 106.40   |
| 1   | A     | 496  | A    | O5'-P-OP2 | 5.36  | 117.13      | 110.70   |
| 1   | A     | 1373 | G    | N3-C4-N9  | 5.36  | 129.22      | 126.00   |
| 1   | A     | 769  | G    | O5'-P-OP1 | 5.36  | 117.13      | 110.70   |
| 1   | A     | 1418 | A    | C8-N9-C4  | -5.36 | 103.66      | 105.80   |
| 1   | A     | 228  | A    | N9-C4-C5  | 5.36  | 107.94      | 105.80   |
| 1   | A     | 284  | G    | OP2-P-O3' | 5.36  | 116.98      | 105.20   |
| 1   | A     | 446  | G    | N1-C6-O6  | 5.36  | 123.11      | 119.90   |
| 1   | A     | 1118 | C    | C5-C6-N1  | 5.36  | 123.68      | 121.00   |
| 1   | A     | 1440 | C    | N3-C4-N4  | 5.36  | 121.75      | 118.00   |
| 1   | A     | 275  | G    | C6-C5-N7  | -5.35 | 127.19      | 130.40   |
| 1   | A     | 899  | C    | N3-C2-O2  | 5.35  | 125.65      | 121.90   |
| 1   | A     | 216  | G    | N7-C8-N9  | -5.35 | 110.42      | 113.10   |
| 1   | A     | 497  | A    | N9-C4-C5  | 5.35  | 107.94      | 105.80   |
| 1   | A     | 1139 | G    | C8-N9-C4  | -5.35 | 104.26      | 106.40   |
| 1   | A     | 1464 | G    | N1-C6-O6  | 5.35  | 123.11      | 119.90   |
| 1   | A     | 148  | G    | C8-N9-C1' | -5.35 | 120.05      | 127.00   |
| 1   | A     | 292  | G    | C5-C6-N1  | -5.34 | 108.83      | 111.50   |
| 1   | A     | 900  | A    | OP1-P-OP2 | -5.34 | 111.58      | 119.60   |
| 1   | A     | 446  | G    | N3-C2-N2  | -5.34 | 116.16      | 119.90   |
| 1   | A     | 818  | G    | C5-C6-O6  | 5.34  | 131.81      | 128.60   |
| 14  | N     | 39   | LEU  | CB-CG-CD2 | -5.34 | 101.92      | 111.00   |
| 1   | A     | 238  | G    | O5'-P-OP2 | -5.34 | 100.89      | 105.70   |
| 1   | A     | 541  | G    | C4-C5-N7  | 5.34  | 112.94      | 110.80   |
| 1   | A     | 886  | G    | C5-C6-N1  | -5.34 | 108.83      | 111.50   |
| 2   | B     | 122  | PHE  | N-CA-C    | 5.34  | 125.41      | 111.00   |
| 1   | A     | 299  | G    | N1-C2-N3  | 5.34  | 127.10      | 123.90   |
| 1   | A     | 1142 | G    | O5'-P-OP1 | -5.34 | 100.90      | 105.70   |
| 1   | A     | 1230 | C    | N3-C4-N4  | 5.34  | 121.74      | 118.00   |
| 1   | A     | 853  | G    | C4-C5-C6  | 5.33  | 122.00      | 118.80   |
| 1   | A     | 1233 | G    | C6-C5-N7  | -5.33 | 127.20      | 130.40   |
| 1   | A     | 265  | G    | C4-N9-C1' | -5.33 | 119.56      | 126.50   |
| 1   | A     | 321  | A    | C8-N9-C4  | 5.33  | 107.93      | 105.80   |
| 1   | A     | 1522 | U    | OP2-P-O3' | 5.33  | 116.94      | 105.20   |
| 1   | A     | 61   | G    | C2-N3-C4  | -5.33 | 109.23      | 111.90   |
| 1   | A     | 306  | G    | N1-C2-N2  | 5.33  | 121.00      | 116.20   |
| 1   | A     | 363  | A    | C5-N7-C8  | -5.33 | 101.23      | 103.90   |
| 1   | A     | 148  | G    | C4-N9-C1' | 5.33  | 133.43      | 126.50   |
| 1   | A     | 573  | A    | OP2-P-O3' | 5.33  | 116.92      | 105.20   |
| 1   | A     | 893  | C    | C5-C4-N4  | -5.33 | 116.47      | 120.20   |
| 1   | A     | 197  | A    | C5-C6-N6  | 5.33  | 127.96      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | A     | 759  | A    | C2-N3-C4   | 5.33  | 113.26      | 110.60   |
| 1   | A     | 1083 | U    | N3-C4-C5   | -5.33 | 111.41      | 114.60   |
| 1   | A     | 624  | C    | N1-C2-N3   | -5.32 | 115.47      | 119.20   |
| 1   | A     | 1353 | G    | C4-C5-N7   | 5.32  | 112.93      | 110.80   |
| 1   | A     | 1507 | A    | OP1-P-O3'  | 5.32  | 116.91      | 105.20   |
| 10  | J     | 54   | PHE  | N-CA-C     | 5.32  | 125.37      | 111.00   |
| 1   | A     | 748  | C    | N3-C2-O2   | -5.32 | 118.18      | 121.90   |
| 1   | A     | 987  | G    | C5-C6-N1   | -5.32 | 108.84      | 111.50   |
| 1   | A     | 1478 | C    | C2-N3-C4   | 5.32  | 122.56      | 119.90   |
| 2   | B     | 221  | LEU  | CA-CB-CG   | 5.32  | 127.54      | 115.30   |
| 1   | A     | 436  | C    | O5'-P-OP1  | -5.32 | 100.91      | 105.70   |
| 1   | A     | 487  | A    | C2-N3-C4   | -5.32 | 107.94      | 110.60   |
| 1   | A     | 204  | U    | C2-N3-C4   | 5.32  | 130.19      | 127.00   |
| 1   | A     | 265  | G    | N3-C4-C5   | 5.32  | 131.26      | 128.60   |
| 1   | A     | 913  | A    | N1-C6-N6   | -5.32 | 115.41      | 118.60   |
| 1   | A     | 1440 | C    | C5-C4-N4   | -5.32 | 116.48      | 120.20   |
| 1   | A     | 52   | G    | N3-C4-N9   | -5.31 | 122.81      | 126.00   |
| 1   | A     | 120  | A    | N9-C4-C5   | 5.31  | 107.92      | 105.80   |
| 1   | A     | 242  | C    | C6-N1-C2   | 5.31  | 122.42      | 120.30   |
| 1   | A     | 299  | G    | C5-C6-N1   | -5.31 | 108.85      | 111.50   |
| 1   | A     | 583  | A    | C4-C5-C6   | 5.31  | 119.65      | 117.00   |
| 1   | A     | 1005 | A    | C4-N9-C1'  | 5.31  | 135.85      | 126.30   |
| 1   | A     | 1034 | G    | O4'-C1'-N9 | 5.31  | 112.44      | 108.20   |
| 1   | A     | 1533 | C    | C5-C6-N1   | 5.31  | 123.65      | 121.00   |
| 1   | A     | 313  | A    | O4'-C1'-N9 | -5.31 | 103.95      | 108.20   |
| 1   | A     | 1302 | U    | N3-C2-O2   | -5.30 | 118.49      | 122.20   |
| 1   | A     | 1369 | C    | N3-C4-C5   | -5.30 | 119.78      | 121.90   |
| 1   | A     | 66   | G    | N1-C2-N2   | 5.30  | 120.97      | 116.20   |
| 1   | A     | 265  | G    | C4-C5-N7   | -5.30 | 108.68      | 110.80   |
| 1   | A     | 1077 | G    | N3-C4-C5   | 5.30  | 131.25      | 128.60   |
| 1   | A     | 531  | U    | N3-C2-O2   | -5.30 | 118.49      | 122.20   |
| 1   | A     | 241  | C    | N3-C4-C5   | 5.30  | 124.02      | 121.90   |
| 1   | A     | 515  | G    | C6-C5-N7   | -5.30 | 127.22      | 130.40   |
| 1   | A     | 1206 | G    | N1-C6-O6   | 5.30  | 123.08      | 119.90   |
| 1   | A     | 1443 | G    | O4'-C1'-N9 | -5.29 | 103.97      | 108.20   |
| 1   | A     | 1497 | G    | N1-C2-N3   | 5.29  | 127.08      | 123.90   |
| 1   | A     | 546  | G    | C8-N9-C4   | -5.29 | 104.28      | 106.40   |
| 1   | A     | 1393 | U    | O5'-P-OP1  | 5.29  | 117.05      | 110.70   |
| 1   | A     | 243  | A    | O4'-C1'-N9 | -5.29 | 103.97      | 108.20   |
| 1   | A     | 676  | A    | N7-C8-N9   | -5.29 | 111.16      | 113.80   |
| 6   | F     | 9    | VAL  | CB-CA-C    | -5.29 | 101.36      | 111.40   |
| 1   | A     | 41   | G    | C5-C6-O6   | -5.28 | 125.43      | 128.60   |

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| Mol | Chain | Res    | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1   | A     | 95     | U    | C4-C5-C6  | 5.28  | 122.87      | 119.70   |
| 1   | A     | 1100   | C    | C4-C5-C6  | -5.28 | 114.76      | 117.40   |
| 1   | A     | 1215   | G    | N1-C6-O6  | 5.28  | 123.07      | 119.90   |
| 1   | A     | 1530   | G    | C5-C6-N1  | -5.28 | 108.86      | 111.50   |
| 1   | A     | 190(A) | C    | C5-C4-N4  | -5.28 | 116.50      | 120.20   |
| 1   | A     | 320    | C    | C6-N1-C2  | 5.28  | 122.41      | 120.30   |
| 1   | A     | 1328   | C    | N3-C4-C5  | 5.28  | 124.01      | 121.90   |
| 1   | A     | 763    | G    | C4-C5-N7  | 5.28  | 112.91      | 110.80   |
| 1   | A     | 1125   | U    | N1-C2-O2  | -5.28 | 119.11      | 122.80   |
| 1   | A     | 1073   | U    | C6-N1-C2  | -5.28 | 117.83      | 121.00   |
| 1   | A     | 330    | C    | OP2-P-O3' | 5.27  | 116.80      | 105.20   |
| 1   | A     | 1099   | G    | N3-C4-N9  | -5.27 | 122.84      | 126.00   |
| 1   | A     | 1389   | C    | C6-N1-C2  | -5.27 | 118.19      | 120.30   |
| 1   | A     | 415    | A    | C8-N9-C4  | -5.27 | 103.69      | 105.80   |
| 1   | A     | 1084   | G    | C4-C5-C6  | 5.27  | 121.96      | 118.80   |
| 1   | A     | 1172   | C    | C6-N1-C2  | 5.27  | 122.41      | 120.30   |
| 1   | A     | 31     | G    | N3-C4-C5  | -5.26 | 125.97      | 128.60   |
| 1   | A     | 321    | A    | O5'-P-OP2 | -5.26 | 100.96      | 105.70   |
| 1   | A     | 687    | A    | OP1-P-O3' | 5.26  | 116.78      | 105.20   |
| 1   | A     | 36     | C    | C5-C6-N1  | -5.26 | 118.37      | 121.00   |
| 1   | A     | 282    | A    | C4-C5-N7  | 5.26  | 113.33      | 110.70   |
| 1   | A     | 900    | A    | C5-C6-N6  | -5.26 | 119.49      | 123.70   |
| 1   | A     | 1508   | G    | N1-C2-N2  | 5.26  | 120.94      | 116.20   |
| 1   | A     | 1396   | A    | C5-C6-N1  | -5.26 | 115.07      | 117.70   |
| 1   | A     | 200    | G    | C6-C5-N7  | -5.26 | 127.25      | 130.40   |
| 1   | A     | 1338   | G    | C4-C5-C6  | 5.26  | 121.95      | 118.80   |
| 1   | A     | 108    | G    | C5-C6-N1  | -5.25 | 108.87      | 111.50   |
| 1   | A     | 344    | A    | C8-N9-C4  | -5.25 | 103.70      | 105.80   |
| 1   | A     | 348    | G    | C5-C6-O6  | -5.25 | 125.45      | 128.60   |
| 1   | A     | 387    | U    | C4-C5-C6  | 5.25  | 122.85      | 119.70   |
| 1   | A     | 885    | G    | OP1-P-OP2 | 5.25  | 127.48      | 119.60   |
| 1   | A     | 1358   | U    | C5-C6-N1  | -5.25 | 120.07      | 122.70   |
| 1   | A     | 127    | G    | N1-C6-O6  | 5.25  | 123.05      | 119.90   |
| 1   | A     | 799    | G    | OP1-P-OP2 | 5.25  | 127.48      | 119.60   |
| 1   | A     | 405    | U    | N3-C2-O2  | -5.25 | 118.53      | 122.20   |
| 1   | A     | 791    | G    | C4-N9-C1' | 5.25  | 133.32      | 126.50   |
| 1   | A     | 1304   | G    | N1-C6-O6  | 5.25  | 123.05      | 119.90   |
| 1   | A     | 10     | A    | N1-C2-N3  | 5.25  | 131.92      | 129.30   |
| 1   | A     | 587    | G    | C8-N9-C4  | -5.25 | 104.30      | 106.40   |
| 1   | A     | 1222   | G    | C4-C5-C6  | 5.24  | 121.95      | 118.80   |
| 1   | A     | 689    | C    | N1-C2-O2  | -5.24 | 115.76      | 118.90   |
| 1   | A     | 993    | G    | C5-C6-O6  | -5.24 | 125.46      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | A     | 908  | A    | N1-C6-N6   | -5.24 | 115.46      | 118.60   |
| 1   | A     | 977  | A    | C2-N3-C4   | 5.24  | 113.22      | 110.60   |
| 1   | A     | 1391 | U    | C6-N1-C2   | 5.24  | 124.14      | 121.00   |
| 1   | A     | 10   | A    | C5-C6-N1   | 5.24  | 120.32      | 117.70   |
| 1   | A     | 348  | G    | N1-C6-O6   | 5.23  | 123.04      | 119.90   |
| 1   | A     | 537  | G    | C8-N9-C4   | 5.23  | 108.49      | 106.40   |
| 1   | A     | 1193 | G    | C5-C6-N1   | -5.23 | 108.88      | 111.50   |
| 1   | A     | 1261 | A    | N9-C4-C5   | -5.23 | 103.71      | 105.80   |
| 2   | B     | 41   | ILE  | CB-CA-C    | -5.23 | 101.13      | 111.60   |
| 5   | E     | 12   | LEU  | CA-CB-CG   | 5.23  | 127.33      | 115.30   |
| 1   | A     | 254  | G    | C2-N3-C4   | -5.23 | 109.28      | 111.90   |
| 1   | A     | 853  | G    | C4-N9-C1'  | 5.23  | 133.30      | 126.50   |
| 1   | A     | 1069 | C    | C5-C4-N4   | -5.23 | 116.54      | 120.20   |
| 1   | A     | 140  | A    | N1-C6-N6   | 5.23  | 121.74      | 118.60   |
| 1   | A     | 1532 | U    | N1-C2-N3   | -5.23 | 111.76      | 114.90   |
| 1   | A     | 509  | A    | C6-C5-N7   | -5.23 | 128.64      | 132.30   |
| 1   | A     | 748  | C    | N1-C2-O2   | 5.23  | 122.04      | 118.90   |
| 1   | A     | 1084 | G    | N3-C4-C5   | -5.23 | 125.99      | 128.60   |
| 1   | A     | 78   | G    | C5-C6-N1   | -5.22 | 108.89      | 111.50   |
| 1   | A     | 1359 | C    | N1-C2-O2   | 5.22  | 122.03      | 118.90   |
| 1   | A     | 8    | A    | C2-N3-C4   | -5.22 | 107.99      | 110.60   |
| 1   | A     | 578  | C    | C5-C6-N1   | -5.22 | 118.39      | 121.00   |
| 1   | A     | 183  | G    | C6-C5-N7   | -5.22 | 127.27      | 130.40   |
| 1   | A     | 944  | G    | OP2-P-O3'  | 5.22  | 116.68      | 105.20   |
| 1   | A     | 50   | A    | C5-C6-N6   | 5.22  | 127.88      | 123.70   |
| 1   | A     | 597  | G    | C2-N3-C4   | -5.22 | 109.29      | 111.90   |
| 1   | A     | 712  | A    | N1-C6-N6   | -5.22 | 115.47      | 118.60   |
| 1   | A     | 673  | G    | C6-C5-N7   | 5.22  | 133.53      | 130.40   |
| 1   | A     | 715  | A    | N7-C8-N9   | -5.22 | 111.19      | 113.80   |
| 1   | A     | 949  | A    | C6-C5-N7   | -5.22 | 128.65      | 132.30   |
| 1   | A     | 1124 | G    | O4'-C1'-N9 | 5.22  | 112.37      | 108.20   |
| 1   | A     | 1125 | U    | OP2-P-O3'  | 5.22  | 116.68      | 105.20   |
| 1   | A     | 1511 | G    | C8-N9-C4   | 5.22  | 108.49      | 106.40   |
| 1   | A     | 61   | G    | C5-C6-O6   | -5.21 | 125.47      | 128.60   |
| 1   | A     | 267  | C    | N3-C4-C5   | 5.21  | 123.99      | 121.90   |
| 1   | A     | 352  | C    | C2-N3-C4   | 5.21  | 122.51      | 119.90   |
| 1   | A     | 284  | G    | N1-C2-N3   | 5.21  | 127.03      | 123.90   |
| 1   | A     | 1195 | C    | N3-C4-C5   | -5.21 | 119.81      | 121.90   |
| 1   | A     | 1452 | C    | N1-C2-N3   | -5.21 | 115.55      | 119.20   |
| 1   | A     | 764  | C    | C2-N1-C1'  | 5.21  | 124.53      | 118.80   |
| 1   | A     | 403  | C    | C4-C5-C6   | 5.21  | 120.00      | 117.40   |
| 1   | A     | 1290 | G    | C6-C5-N7   | -5.21 | 127.27      | 130.40   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | A     | 289  | G    | C8-N9-C1' | -5.21 | 120.23      | 127.00   |
| 1   | A     | 852  | G    | C5-C6-N1  | -5.21 | 108.90      | 111.50   |
| 1   | A     | 791  | G    | N1-C2-N3  | 5.20  | 127.02      | 123.90   |
| 1   | A     | 1055 | A    | C6-C5-N7  | -5.20 | 128.66      | 132.30   |
| 1   | A     | 1058 | G    | C2-N3-C4  | -5.20 | 109.30      | 111.90   |
| 1   | A     | 1079 | G    | C6-C5-N7  | -5.20 | 127.28      | 130.40   |
| 1   | A     | 1098 | C    | C5-C6-N1  | -5.20 | 118.40      | 121.00   |
| 1   | A     | 229  | U    | N3-C4-O4  | 5.20  | 123.04      | 119.40   |
| 1   | A     | 144  | G    | C5-C6-N1  | -5.20 | 108.90      | 111.50   |
| 1   | A     | 255  | G    | N1-C2-N3  | 5.20  | 127.02      | 123.90   |
| 1   | A     | 610  | G    | N3-C2-N2  | -5.20 | 116.26      | 119.90   |
| 1   | A     | 1087 | G    | N7-C8-N9  | 5.20  | 115.70      | 113.10   |
| 1   | A     | 1119 | C    | N1-C2-O2  | 5.20  | 122.02      | 118.90   |
| 1   | A     | 1143 | G    | C8-N9-C4  | 5.20  | 108.48      | 106.40   |
| 1   | A     | 949  | A    | C5-N7-C8  | -5.20 | 101.30      | 103.90   |
| 1   | A     | 1129 | C    | C6-N1-C1' | 5.20  | 127.04      | 120.80   |
| 1   | A     | 1410 | G    | C8-N9-C4  | 5.20  | 108.48      | 106.40   |
| 1   | A     | 513  | C    | N3-C4-C5  | 5.20  | 123.98      | 121.90   |
| 1   | A     | 650  | G    | N1-C6-O6  | 5.20  | 123.02      | 119.90   |
| 1   | A     | 1102 | A    | C8-N9-C4  | -5.20 | 103.72      | 105.80   |
| 1   | A     | 1190 | G    | C4-C5-N7  | -5.20 | 108.72      | 110.80   |
| 1   | A     | 1239 | A    | N9-C4-C5  | -5.20 | 103.72      | 105.80   |
| 1   | A     | 252  | U    | N3-C2-O2  | 5.19  | 125.84      | 122.20   |
| 1   | A     | 1353 | G    | C6-C5-N7  | -5.19 | 127.28      | 130.40   |
| 1   | A     | 809  | G    | N1-C2-N3  | -5.19 | 120.78      | 123.90   |
| 1   | A     | 818  | G    | N9-C4-C5  | 5.19  | 107.48      | 105.40   |
| 1   | A     | 1450 | U    | O5'-P-OP2 | -5.19 | 101.03      | 105.70   |
| 1   | A     | 439  | A    | N9-C4-C5  | 5.19  | 107.88      | 105.80   |
| 1   | A     | 869  | G    | N1-C6-O6  | -5.19 | 116.78      | 119.90   |
| 5   | E     | 12   | LEU  | CB-CG-CD2 | 5.19  | 119.82      | 111.00   |
| 1   | A     | 262  | A    | N3-C4-C5  | 5.19  | 130.43      | 126.80   |
| 1   | A     | 556  | C    | N3-C4-N4  | 5.19  | 121.63      | 118.00   |
| 1   | A     | 1229 | A    | C2-N3-C4  | -5.19 | 108.01      | 110.60   |
| 1   | A     | 1467 | G    | N3-C4-C5  | -5.19 | 126.01      | 128.60   |
| 1   | A     | 658  | G    | N1-C2-N2  | -5.18 | 111.53      | 116.20   |
| 1   | A     | 1087 | G    | C5-C6-N1  | -5.18 | 108.91      | 111.50   |
| 1   | A     | 305  | G    | C5-C6-O6  | 5.18  | 131.71      | 128.60   |
| 1   | A     | 620  | C    | C6-N1-C2  | 5.18  | 122.37      | 120.30   |
| 1   | A     | 672  | U    | N3-C4-O4  | 5.18  | 123.03      | 119.40   |
| 1   | A     | 369  | C    | O5'-P-OP1 | 5.18  | 116.92      | 110.70   |
| 1   | A     | 416  | G    | C8-N9-C4  | -5.18 | 104.33      | 106.40   |
| 1   | A     | 855  | G    | C4-C5-C6  | 5.18  | 121.91      | 118.80   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | A     | 1158 | C    | N3-C2-O2  | -5.18 | 118.28      | 121.90   |
| 1   | A     | 1495 | U    | C6-N1-C2  | -5.18 | 117.89      | 121.00   |
| 1   | A     | 629  | G    | OP2-P-O3' | 5.17  | 116.58      | 105.20   |
| 1   | A     | 1128 | C    | N3-C4-C5  | -5.17 | 119.83      | 121.90   |
| 1   | A     | 247  | G    | C5-C6-O6  | -5.17 | 125.50      | 128.60   |
| 1   | A     | 20   | U    | C6-N1-C1' | -5.17 | 113.96      | 121.20   |
| 1   | A     | 228  | A    | N1-C2-N3  | 5.17  | 131.89      | 129.30   |
| 1   | A     | 244  | U    | N1-C2-O2  | 5.17  | 126.42      | 122.80   |
| 1   | A     | 1261 | A    | C8-N9-C4  | 5.17  | 107.87      | 105.80   |
| 1   | A     | 1155 | G    | N1-C2-N3  | 5.17  | 127.00      | 123.90   |
| 1   | A     | 50   | A    | C5-C6-N1  | -5.17 | 115.12      | 117.70   |
| 1   | A     | 762  | C    | C2-N3-C4  | -5.17 | 117.32      | 119.90   |
| 1   | A     | 259  | G    | N1-C6-O6  | 5.17  | 123.00      | 119.90   |
| 1   | A     | 668  | G    | N1-C6-O6  | 5.17  | 123.00      | 119.90   |
| 1   | A     | 798  | G    | N1-C2-N3  | -5.17 | 120.80      | 123.90   |
| 1   | A     | 841  | U    | C5-C6-N1  | 5.16  | 125.28      | 122.70   |
| 1   | A     | 910  | C    | N3-C2-O2  | 5.16  | 125.52      | 121.90   |
| 1   | A     | 360  | A    | N1-C2-N3  | 5.16  | 131.88      | 129.30   |
| 1   | A     | 444  | C    | N1-C2-O2  | 5.16  | 122.00      | 118.90   |
| 1   | A     | 895  | G    | N1-C2-N3  | 5.16  | 127.00      | 123.90   |
| 1   | A     | 147  | G    | N3-C2-N2  | -5.16 | 116.29      | 119.90   |
| 1   | A     | 254  | G    | C8-N9-C4  | 5.16  | 108.46      | 106.40   |
| 1   | A     | 281  | G    | C2-N3-C4  | -5.16 | 109.32      | 111.90   |
| 1   | A     | 965  | A    | C4-C5-C6  | -5.16 | 114.42      | 117.00   |
| 1   | A     | 528  | C    | O5'-P-OP1 | -5.16 | 101.06      | 105.70   |
| 1   | A     | 818  | G    | C5-N7-C8  | 5.16  | 106.88      | 104.30   |
| 1   | A     | 614  | A    | C4-C5-N7  | 5.15  | 113.28      | 110.70   |
| 1   | A     | 226  | G    | N1-C6-O6  | 5.15  | 122.99      | 119.90   |
| 1   | A     | 1099 | G    | C4-N9-C1' | -5.15 | 119.80      | 126.50   |
| 1   | A     | 1522 | U    | C4-C5-C6  | 5.15  | 122.79      | 119.70   |
| 1   | A     | 303  | A    | C8-N9-C4  | -5.15 | 103.74      | 105.80   |
| 1   | A     | 499  | A    | N9-C4-C5  | 5.14  | 107.86      | 105.80   |
| 1   | A     | 553  | A    | OP2-P-O3' | 5.14  | 116.52      | 105.20   |
| 1   | A     | 590  | C    | N3-C4-C5  | 5.14  | 123.96      | 121.90   |
| 1   | A     | 731  | G    | C5-C6-O6  | -5.14 | 125.51      | 128.60   |
| 1   | A     | 866  | C    | C5-C4-N4  | 5.14  | 123.80      | 120.20   |
| 1   | A     | 1136 | U    | C5-C6-N1  | 5.14  | 125.27      | 122.70   |
| 1   | A     | 257  | G    | C6-C5-N7  | -5.14 | 127.31      | 130.40   |
| 1   | A     | 1075 | C    | C2-N1-C1' | -5.14 | 113.14      | 118.80   |
| 1   | A     | 1532 | U    | C2-N3-C4  | 5.14  | 130.09      | 127.00   |
| 1   | A     | 273  | A    | C2-N3-C4  | -5.14 | 108.03      | 110.60   |
| 1   | A     | 570  | G    | C6-C5-N7  | -5.14 | 127.32      | 130.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 502  | G    | C4-N9-C1'   | -5.14 | 119.82      | 126.50   |
| 1   | A     | 894  | G    | C5-C6-N1    | -5.14 | 108.93      | 111.50   |
| 1   | A     | 1084 | G    | C5-C6-N1    | -5.14 | 108.93      | 111.50   |
| 1   | A     | 382  | A    | N9-C4-C5    | 5.14  | 107.86      | 105.80   |
| 1   | A     | 1510 | U    | O5'-P-OP1   | -5.14 | 101.08      | 105.70   |
| 1   | A     | 34   | C    | N1-C2-N3    | -5.13 | 115.61      | 119.20   |
| 1   | A     | 1394 | A    | C2-N3-C4    | -5.13 | 108.03      | 110.60   |
| 1   | A     | 577  | G    | N3-C4-N9    | -5.13 | 122.92      | 126.00   |
| 1   | A     | 799  | G    | C5-N7-C8    | -5.13 | 101.73      | 104.30   |
| 1   | A     | 612  | C    | C5-C4-N4    | 5.13  | 123.79      | 120.20   |
| 1   | A     | 779  | C    | O5'-P-OP2   | -5.13 | 101.08      | 105.70   |
| 1   | A     | 908  | A    | N9-C4-C5    | 5.13  | 107.85      | 105.80   |
| 1   | A     | 641  | U    | C5-C4-O4    | -5.13 | 122.82      | 125.90   |
| 1   | A     | 1278 | U    | O5'-P-OP2   | -5.13 | 101.08      | 105.70   |
| 1   | A     | 658  | G    | C6-N1-C2    | -5.13 | 122.03      | 125.10   |
| 1   | A     | 912  | C    | N1-C2-O2    | -5.13 | 115.82      | 118.90   |
| 1   | A     | 532  | A    | C8-N9-C4    | 5.12  | 107.85      | 105.80   |
| 1   | A     | 734  | G    | C6-C5-N7    | -5.12 | 127.33      | 130.40   |
| 1   | A     | 821  | G    | N1-C2-N3    | 5.12  | 126.97      | 123.90   |
| 1   | A     | 1453 | G    | C6-C5-N7    | -5.12 | 127.33      | 130.40   |
| 1   | A     | 792  | A    | C5-C6-N1    | -5.12 | 115.14      | 117.70   |
| 1   | A     | 1290 | G    | C5-C6-O6    | -5.12 | 125.53      | 128.60   |
| 12  | L     | 27   | LEU  | CB-CG-CD2   | 5.12  | 119.70      | 111.00   |
| 1   | A     | 7    | G    | C8-N9-C4    | 5.12  | 108.45      | 106.40   |
| 1   | A     | 740  | U    | C2-N1-C1'   | -5.12 | 111.56      | 117.70   |
| 1   | A     | 111  | G    | OP1-P-OP2   | 5.12  | 127.27      | 119.60   |
| 1   | A     | 382  | A    | N1-C6-N6    | -5.12 | 115.53      | 118.60   |
| 1   | A     | 794  | A    | N1-C6-N6    | -5.12 | 115.53      | 118.60   |
| 1   | A     | 897  | C    | C6-N1-C2    | 5.12  | 122.35      | 120.30   |
| 1   | A     | 453  | A    | C8-N9-C4    | -5.11 | 103.75      | 105.80   |
| 1   | A     | 851  | G    | N1-C6-O6    | 5.11  | 122.97      | 119.90   |
| 1   | A     | 665  | A    | C2-N3-C4    | 5.11  | 113.16      | 110.60   |
| 1   | A     | 1232 | U    | C2-N1-C1'   | 5.11  | 123.83      | 117.70   |
| 1   | A     | 329  | A    | C5-C6-N6    | 5.11  | 127.79      | 123.70   |
| 1   | A     | 1085 | U    | N1-C2-N3    | -5.11 | 111.84      | 114.90   |
| 1   | A     | 46   | G    | N9-C4-C5    | 5.11  | 107.44      | 105.40   |
| 1   | A     | 631  | G    | C6-N1-C2    | 5.11  | 128.16      | 125.10   |
| 1   | A     | 665  | A    | C5-C6-N1    | 5.11  | 120.25      | 117.70   |
| 1   | A     | 512  | U    | C5-C4-O4    | -5.10 | 122.84      | 125.90   |
| 1   | A     | 130  | A    | N1-C6-N6    | 5.10  | 121.66      | 118.60   |
| 1   | A     | 292  | G    | C6-C5-N7    | -5.10 | 127.34      | 130.40   |
| 1   | A     | 509  | A    | C2'-C3'-O3' | 5.10  | 121.86      | 113.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | A     | 870  | U    | C5-C6-N1   | -5.10 | 120.15      | 122.70   |
| 1   | A     | 1257 | U    | C6-N1-C2   | -5.10 | 117.94      | 121.00   |
| 1   | A     | 68   | G    | N3-C4-N9   | -5.10 | 122.94      | 126.00   |
| 1   | A     | 674  | G    | C4-C5-N7   | 5.10  | 112.84      | 110.80   |
| 1   | A     | 816  | A    | OP1-P-O3'  | 5.10  | 116.42      | 105.20   |
| 1   | A     | 1128 | C    | C6-N1-C2   | -5.10 | 118.26      | 120.30   |
| 1   | A     | 1198 | G    | C5-C6-N1   | -5.10 | 108.95      | 111.50   |
| 1   | A     | 191  | G    | N3-C4-C5   | -5.09 | 126.05      | 128.60   |
| 1   | A     | 500  | G    | N9-C4-C5   | -5.09 | 103.36      | 105.40   |
| 1   | A     | 1399 | C    | N1-C2-N3   | 5.09  | 122.77      | 119.20   |
| 1   | A     | 1525 | G    | N9-C1'-C2' | -5.09 | 106.40      | 112.00   |
| 1   | A     | 1531 | A    | C2-N3-C4   | -5.09 | 108.05      | 110.60   |
| 1   | A     | 362  | G    | C5-N7-C8   | 5.09  | 106.85      | 104.30   |
| 1   | A     | 585  | G    | N3-C4-C5   | 5.09  | 131.15      | 128.60   |
| 1   | A     | 1299 | A    | N7-C8-N9   | 5.09  | 116.35      | 113.80   |
| 1   | A     | 397  | A    | C8-N9-C4   | -5.09 | 103.76      | 105.80   |
| 1   | A     | 407  | G    | C2-N3-C4   | -5.09 | 109.35      | 111.90   |
| 1   | A     | 507  | C    | N3-C2-O2   | 5.09  | 125.46      | 121.90   |
| 1   | A     | 1023 | G    | N3-C4-N9   | 5.09  | 129.06      | 126.00   |
| 1   | A     | 148  | G    | N3-C4-C5   | -5.09 | 126.06      | 128.60   |
| 1   | A     | 184  | G    | C5-N7-C8   | 5.09  | 106.84      | 104.30   |
| 1   | A     | 389  | A    | C8-N9-C4   | -5.09 | 103.76      | 105.80   |
| 1   | A     | 499  | A    | C5-C6-N6   | 5.09  | 127.77      | 123.70   |
| 1   | A     | 900  | A    | C4-C5-N7   | 5.09  | 113.25      | 110.70   |
| 1   | A     | 1529 | G    | C8-N9-C4   | -5.09 | 104.36      | 106.40   |
| 1   | A     | 872  | A    | C4-C5-C6   | 5.09  | 119.54      | 117.00   |
| 1   | A     | 46   | G    | N7-C8-N9   | 5.09  | 115.64      | 113.10   |
| 1   | A     | 889  | A    | C8-N9-C4   | -5.09 | 103.77      | 105.80   |
| 1   | A     | 331  | G    | N7-C8-N9   | 5.08  | 115.64      | 113.10   |
| 1   | A     | 728  | A    | C6-C5-N7   | -5.08 | 128.74      | 132.30   |
| 1   | A     | 833  | U    | C6-N1-C1'  | 5.08  | 128.32      | 121.20   |
| 1   | A     | 9    | G    | O5'-P-OP2  | -5.08 | 101.12      | 105.70   |
| 1   | A     | 747  | C    | C4-C5-C6   | 5.08  | 119.94      | 117.40   |
| 1   | A     | 667  | G    | C5-C6-N1   | -5.08 | 108.96      | 111.50   |
| 1   | A     | 1379 | G    | C6-C5-N7   | -5.08 | 127.35      | 130.40   |
| 1   | A     | 502  | G    | N3-C4-C5   | 5.08  | 131.14      | 128.60   |
| 1   | A     | 1079 | G    | C4-N9-C1'  | 5.08  | 133.10      | 126.50   |
| 1   | A     | 1138 | G    | N3-C2-N2   | -5.08 | 116.35      | 119.90   |
| 1   | A     | 497  | A    | C4-C5-N7   | -5.08 | 108.16      | 110.70   |
| 1   | A     | 1416 | G    | N7-C8-N9   | 5.08  | 115.64      | 113.10   |
| 1   | A     | 880  | C    | N1-C2-N3   | -5.07 | 115.65      | 119.20   |
| 1   | A     | 1322 | C    | OP1-P-OP2  | -5.07 | 111.99      | 119.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | A     | 904  | C    | C6-N1-C2   | 5.07  | 122.33      | 120.30   |
| 1   | A     | 223  | U    | C5-C6-N1   | -5.07 | 120.17      | 122.70   |
| 1   | A     | 917  | G    | C2-N3-C4   | 5.07  | 114.43      | 111.90   |
| 1   | A     | 363  | A    | C5-C6-N6   | -5.07 | 119.65      | 123.70   |
| 1   | A     | 1502 | A    | N7-C8-N9   | 5.07  | 116.33      | 113.80   |
| 1   | A     | 58   | C    | N3-C4-N4   | 5.07  | 121.55      | 118.00   |
| 1   | A     | 60   | A    | C8-N9-C4   | -5.07 | 103.77      | 105.80   |
| 1   | A     | 435  | C    | O5'-P-OP2  | 5.07  | 116.78      | 110.70   |
| 1   | A     | 887  | G    | C5-C6-N1   | -5.07 | 108.97      | 111.50   |
| 3   | C     | 14   | ILE  | CG1-CB-CG2 | 5.07  | 122.54      | 111.40   |
| 3   | C     | 21   | ARG  | NE-CZ-NH1  | 5.07  | 122.83      | 120.30   |
| 1   | A     | 116  | A    | OP1-P-OP2  | 5.06  | 127.20      | 119.60   |
| 1   | A     | 857  | C    | OP2-P-O3'  | 5.06  | 116.34      | 105.20   |
| 1   | A     | 881  | G    | N9-C4-C5   | -5.06 | 103.37      | 105.40   |
| 1   | A     | 612  | C    | N3-C4-N4   | -5.06 | 114.46      | 118.00   |
| 1   | A     | 820  | U    | C5-C6-N1   | -5.06 | 120.17      | 122.70   |
| 1   | A     | 148  | G    | C4-C5-C6   | 5.06  | 121.84      | 118.80   |
| 1   | A     | 231  | G    | O5'-P-OP2  | 5.06  | 116.77      | 110.70   |
| 1   | A     | 1240 | U    | N3-C4-O4   | -5.06 | 115.86      | 119.40   |
| 1   | A     | 248  | C    | C2-N3-C4   | -5.06 | 117.37      | 119.90   |
| 1   | A     | 504  | C    | N3-C4-C5   | -5.06 | 119.88      | 121.90   |
| 1   | A     | 934  | C    | O5'-P-OP2  | -5.06 | 101.15      | 105.70   |
| 1   | A     | 277  | C    | N3-C4-C5   | 5.06  | 123.92      | 121.90   |
| 1   | A     | 406  | G    | N7-C8-N9   | 5.06  | 115.63      | 113.10   |
| 1   | A     | 599  | C    | N3-C2-O2   | 5.06  | 125.44      | 121.90   |
| 1   | A     | 300  | A    | C4-C5-N7   | -5.06 | 108.17      | 110.70   |
| 1   | A     | 595  | G    | N3-C2-N2   | 5.05  | 123.44      | 119.90   |
| 10  | J     | 5    | ARG  | CG-CD-NE   | 5.05  | 122.41      | 111.80   |
| 1   | A     | 564  | C    | N1-C2-O2   | 5.05  | 121.93      | 118.90   |
| 1   | A     | 788  | U    | N3-C4-C5   | -5.05 | 111.57      | 114.60   |
| 1   | A     | 1193 | G    | OP1-P-OP2  | 5.05  | 127.18      | 119.60   |
| 1   | A     | 1373 | G    | C4-N9-C1'  | 5.05  | 133.06      | 126.50   |
| 1   | A     | 688  | G    | N1-C6-O6   | 5.05  | 122.93      | 119.90   |
| 1   | A     | 993  | G    | N3-C4-N9   | 5.05  | 129.03      | 126.00   |
| 1   | A     | 382  | A    | C5-C6-N6   | 5.05  | 127.74      | 123.70   |
| 1   | A     | 500  | G    | C2-N3-C4   | -5.05 | 109.38      | 111.90   |
| 1   | A     | 546  | G    | N7-C8-N9   | 5.05  | 115.62      | 113.10   |
| 1   | A     | 1125 | U    | C2-N1-C1'  | -5.05 | 111.64      | 117.70   |
| 1   | A     | 1494 | G    | C8-N9-C1'  | -5.04 | 120.44      | 127.00   |
| 1   | A     | 316  | G    | N3-C4-N9   | 5.04  | 129.03      | 126.00   |
| 1   | A     | 224  | C    | N3-C2-O2   | -5.04 | 118.37      | 121.90   |
| 1   | A     | 535  | A    | C5-N7-C8   | 5.04  | 106.42      | 103.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | A     | 1166 | G    | N7-C8-N9   | 5.04  | 115.62      | 113.10   |
| 1   | A     | 1338 | G    | C8-N9-C1'  | -5.04 | 120.45      | 127.00   |
| 1   | A     | 1397 | C    | N3-C4-C5   | 5.04  | 123.92      | 121.90   |
| 1   | A     | 1304 | G    | C4-N9-C1'  | 5.04  | 133.05      | 126.50   |
| 1   | A     | 1391 | U    | C2-N1-C1'  | -5.04 | 111.65      | 117.70   |
| 1   | A     | 585  | G    | N3-C4-N9   | -5.04 | 122.98      | 126.00   |
| 1   | A     | 879  | C    | C2-N1-C1'  | -5.04 | 113.26      | 118.80   |
| 1   | A     | 918  | A    | C5-C6-N6   | -5.04 | 119.67      | 123.70   |
| 1   | A     | 232  | G    | N3-C4-N9   | 5.04  | 129.02      | 126.00   |
| 1   | A     | 787  | A    | C6-N1-C2   | -5.04 | 115.58      | 118.60   |
| 1   | A     | 1370 | G    | C2-N3-C4   | -5.04 | 109.38      | 111.90   |
| 1   | A     | 1524 | C    | OP2-P-O3'  | 5.04  | 116.28      | 105.20   |
| 1   | A     | 517  | G    | C5-C6-N1   | -5.03 | 108.98      | 111.50   |
| 1   | A     | 580  | U    | N3-C4-C5   | -5.03 | 111.58      | 114.60   |
| 1   | A     | 834  | C    | N3-C4-C5   | 5.03  | 123.91      | 121.90   |
| 1   | A     | 1227 | A    | O5'-P-OP1  | -5.03 | 101.17      | 105.70   |
| 1   | A     | 375  | U    | N3-C4-O4   | 5.03  | 122.92      | 119.40   |
| 1   | A     | 918  | A    | C5-C6-N1   | 5.03  | 120.22      | 117.70   |
| 1   | A     | 79   | G    | N1-C6-O6   | 5.03  | 122.92      | 119.90   |
| 1   | A     | 545  | C    | OP1-P-OP2  | 5.03  | 127.14      | 119.60   |
| 5   | E     | 123  | LEU  | CB-CG-CD2  | -5.03 | 102.45      | 111.00   |
| 1   | A     | 951  | G    | N1-C6-O6   | 5.03  | 122.92      | 119.90   |
| 1   | A     | 1386 | G    | O5'-P-OP2  | -5.03 | 101.18      | 105.70   |
| 1   | A     | 575  | G    | N3-C2-N2   | 5.02  | 123.42      | 119.90   |
| 1   | A     | 542  | G    | C5-C6-N1   | 5.02  | 114.01      | 111.50   |
| 1   | A     | 28   | G    | O5'-P-OP1  | -5.02 | 101.18      | 105.70   |
| 1   | A     | 42   | G    | N3-C2-N2   | -5.02 | 116.39      | 119.90   |
| 1   | A     | 1397 | C    | N3-C2-O2   | -5.02 | 118.39      | 121.90   |
| 1   | A     | 1526 | G    | C2-N3-C4   | -5.02 | 109.39      | 111.90   |
| 1   | A     | 352  | C    | C5-C6-N1   | 5.02  | 123.51      | 121.00   |
| 1   | A     | 1148 | U    | N3-C2-O2   | -5.02 | 118.69      | 122.20   |
| 1   | A     | 1395 | C    | N3-C2-O2   | 5.02  | 125.41      | 121.90   |
| 1   | A     | 582  | U    | C4-C5-C6   | 5.02  | 122.71      | 119.70   |
| 1   | A     | 406  | G    | C6-C5-N7   | -5.01 | 127.39      | 130.40   |
| 1   | A     | 517  | G    | N9-C4-C5   | 5.01  | 107.41      | 105.40   |
| 1   | A     | 786  | G    | C4-C5-C6   | 5.01  | 121.81      | 118.80   |
| 1   | A     | 1202 | G    | C8-N9-C1'  | 5.01  | 133.52      | 127.00   |
| 1   | A     | 886  | G    | C4-C5-N7   | 5.01  | 112.80      | 110.80   |
| 1   | A     | 906  | G    | C5-C6-O6   | -5.01 | 125.59      | 128.60   |
| 1   | A     | 646  | U    | C2-N3-C4   | 5.01  | 130.00      | 127.00   |
| 1   | A     | 1417 | G    | O4'-C1'-N9 | 5.01  | 112.21      | 108.20   |
| 1   | A     | 1435 | G    | C4-C5-N7   | 5.01  | 112.80      | 110.80   |

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| Mol | Chain | Res    | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1   | A     | 710    | G    | N3-C2-N2  | -5.01 | 116.39      | 119.90   |
| 1   | A     | 1494   | G    | N3-C4-N9  | 5.01  | 129.00      | 126.00   |
| 1   | A     | 1495   | U    | C2-N3-C4  | 5.01  | 130.00      | 127.00   |
| 1   | A     | 357    | G    | C6-N1-C2  | 5.00  | 128.10      | 125.10   |
| 1   | A     | 654    | G    | OP2-P-O3' | 5.00  | 116.21      | 105.20   |
| 1   | A     | 190(H) | G    | C8-N9-C1' | -5.00 | 120.49      | 127.00   |
| 1   | A     | 869    | G    | N3-C4-N9  | 5.00  | 129.00      | 126.00   |
| 1   | A     | 332    | G    | C5-C6-N1  | -5.00 | 109.00      | 111.50   |
| 1   | A     | 518    | C    | C2-N1-C1' | 5.00  | 124.30      | 118.80   |
| 1   | A     | 662    | G    | C5-C6-N1  | -5.00 | 109.00      | 111.50   |
| 1   | A     | 770    | C    | N1-C2-O2  | 5.00  | 121.90      | 118.90   |
| 1   | A     | 786    | G    | C8-N9-C1' | -5.00 | 120.50      | 127.00   |
| 1   | A     | 1079   | G    | C6-N1-C2  | -5.00 | 122.10      | 125.10   |

There are no chirality outliers.

All (18) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 2   | B     | 8   | LYS  | Peptide |
| 2   | B     | 9   | GLU  | Peptide |
| 3   | C     | 154 | SER  | Peptide |
| 3   | C     | 166 | GLU  | Peptide |
| 3   | C     | 168 | ALA  | Peptide |
| 8   | H     | 90  | GLY  | Peptide |
| 9   | I     | 56  | LEU  | Peptide |
| 9   | I     | 57  | GLY  | Peptide |
| 10  | J     | 34  | VAL  | Peptide |
| 10  | J     | 88  | LEU  | Peptide |
| 13  | M     | 105 | THR  | Peptide |
| 13  | M     | 107 | ALA  | Peptide |
| 13  | M     | 62  | ASN  | Peptide |
| 14  | N     | 7   | ILE  | Peptide |
| 16  | P     | 19  | ILE  | Peptide |
| 20  | T     | 12  | ALA  | Peptide |
| 20  | T     | 92  | LEU  | Peptide |
| 20  | T     | 93  | GLU  | Peptide |

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 32687 | 0        | 16528    | 920     | 0            |
| 2   | B     | 1900  | 0        | 1951     | 96      | 0            |
| 3   | C     | 1612  | 0        | 1677     | 97      | 0            |
| 4   | D     | 1703  | 0        | 1763     | 104     | 0            |
| 5   | E     | 1146  | 0        | 1207     | 78      | 0            |
| 6   | F     | 843   | 0        | 857      | 62      | 0            |
| 7   | G     | 1257  | 0        | 1296     | 69      | 0            |
| 8   | H     | 1116  | 0        | 1177     | 74      | 0            |
| 9   | I     | 1010  | 0        | 1037     | 65      | 0            |
| 10  | J     | 792   | 0        | 835      | 73      | 0            |
| 11  | K     | 864   | 0        | 881      | 44      | 0            |
| 12  | L     | 972   | 0        | 1058     | 59      | 0            |
| 13  | M     | 937   | 0        | 995      | 59      | 0            |
| 14  | N     | 492   | 0        | 529      | 47      | 0            |
| 15  | O     | 729   | 0        | 768      | 49      | 0            |
| 16  | P     | 700   | 0        | 720      | 34      | 0            |
| 17  | Q     | 823   | 0        | 891      | 55      | 0            |
| 18  | R     | 574   | 0        | 644      | 49      | 0            |
| 19  | S     | 647   | 0        | 673      | 48      | 0            |
| 20  | T     | 763   | 0        | 861      | 51      | 0            |
| 21  | U     | 208   | 0        | 221      | 9       | 0            |
| 22  | A     | 164   | 0        | 0        | 0       | 0            |
| 22  | D     | 1     | 0        | 0        | 0       | 0            |
| 22  | E     | 1     | 0        | 0        | 0       | 0            |
| 22  | F     | 1     | 0        | 0        | 0       | 0            |
| 22  | G     | 1     | 0        | 0        | 0       | 0            |
| 22  | H     | 1     | 0        | 0        | 0       | 0            |
| 22  | K     | 2     | 0        | 0        | 0       | 0            |
| 22  | S     | 1     | 0        | 0        | 0       | 0            |
| 23  | D     | 1     | 0        | 0        | 0       | 0            |
| 23  | N     | 1     | 0        | 0        | 0       | 0            |
| 24  | A     | 271   | 0        | 0        | 14      | 0            |
| 24  | C     | 1     | 0        | 0        | 0       | 0            |
| 24  | E     | 3     | 0        | 0        | 0       | 0            |
| 24  | L     | 1     | 0        | 0        | 0       | 0            |
| 24  | N     | 1     | 0        | 0        | 0       | 0            |
| 24  | P     | 1     | 0        | 0        | 0       | 0            |
| 24  | T     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 52228 | 0        | 36569    | 1946    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 22.

All (1946) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:I:8:GLY:HA2    | 9:I:79:LEU:HD13  | 1.48                     | 0.95              |
| 8:H:10:LEU:HD22  | 8:H:83:ILE:HD11  | 1.49                     | 0.94              |
| 1:A:664:G:H22    | 1:A:741:G:H1     | 1.17                     | 0.92              |
| 1:A:1002:G:N1    | 1:A:1003(A):G:O6 | 2.04                     | 0.91              |
| 4:D:187:ARG:HH22 | 4:D:188:LEU:HD12 | 1.36                     | 0.91              |
| 1:A:1026:G:H8    | 1:A:1027:C:H5''  | 1.34                     | 0.90              |
| 1:A:1003:G:O2'   | 1:A:1003(A):G:N7 | 2.04                     | 0.90              |
| 1:A:1366:C:O2'   | 10:J:60:ARG:NH2  | 2.05                     | 0.89              |
| 15:O:5:LYS:HZ3   | 15:O:5:LYS:H     | 1.18                     | 0.88              |
| 13:M:48:LEU:HD12 | 13:M:53:VAL:HG22 | 1.55                     | 0.88              |
| 19:S:18:LYS:HG2  | 19:S:31:ILE:HD11 | 1.55                     | 0.87              |
| 7:G:85:TYR:HD1   | 7:G:154:TYR:HE1  | 1.23                     | 0.87              |
| 8:H:113:SER:HB3  | 8:H:134:ILE:HD11 | 1.56                     | 0.87              |
| 11:K:57:THR:HG22 | 11:K:59:TYR:H    | 1.40                     | 0.85              |
| 2:B:17:PHE:HD1   | 2:B:18:GLY:H     | 1.22                     | 0.85              |
| 1:A:1443:G:H4'   | 1:A:1446:A:H5'   | 1.59                     | 0.85              |
| 1:A:677:U:H3     | 1:A:713:G:H22    | 1.23                     | 0.85              |
| 7:G:122:HIS:HA   | 7:G:125:MET:HB2  | 1.57                     | 0.84              |
| 1:A:1028:C:H6    | 1:A:1033:G:H22   | 1.25                     | 0.84              |
| 10:J:55:LYS:HG2  | 10:J:56:HIS:H    | 1.44                     | 0.83              |
| 1:A:598:U:H4'    | 8:H:94:TYR:CD1   | 2.13                     | 0.82              |
| 8:H:9:MET:HG3    | 8:H:26:VAL:HG21  | 1.60                     | 0.82              |
| 4:D:187:ARG:CZ   | 4:D:188:LEU:H    | 1.93                     | 0.82              |
| 1:A:1026:G:C8    | 1:A:1027:C:H5''  | 2.15                     | 0.81              |
| 15:O:70:LEU:HD11 | 15:O:77:ARG:HB2  | 1.61                     | 0.81              |
| 15:O:32:LEU:HD12 | 15:O:63:ARG:HB3  | 1.63                     | 0.81              |
| 1:A:1543:C:H2'   | 1:A:1544:U:H5''  | 1.63                     | 0.80              |
| 19:S:39:THR:HG22 | 19:S:70:LYS:HD2  | 1.61                     | 0.80              |
| 1:A:1238:A:H5'   | 1:A:1336:C:H41   | 1.47                     | 0.79              |
| 1:A:1425:U:H3    | 1:A:1475:G:H1    | 1.26                     | 0.79              |
| 6:F:2:ARG:HH11   | 6:F:69:GLU:HG2   | 1.47                     | 0.79              |
| 1:A:1527:C:H2'   | 1:A:1528:U:C6    | 2.17                     | 0.79              |
| 1:A:103:C:OP1    | 20:T:17:ARG:NH1  | 2.15                     | 0.79              |
| 12:L:27:LEU:O    | 12:L:29:GLY:N    | 2.16                     | 0.79              |
| 1:A:1178:G:OP1   | 9:I:93:ARG:NH1   | 2.16                     | 0.78              |
| 4:D:98:GLU:OE1   | 4:D:103:ASN:ND2  | 2.16                     | 0.78              |
| 3:C:155:GLY:HA3  | 3:C:163:ALA:HB1  | 1.65                     | 0.78              |
| 2:B:16:HIS:HB3   | 2:B:210:SER:HB2  | 1.65                     | 0.78              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:123:GLN:HB2  | 3:C:128:PHE:HD1   | 1.47                     | 0.78              |
| 11:K:85:ARG:HD3  | 11:K:113:PRO:HD3  | 1.65                     | 0.78              |
| 1:A:298:A:N6     | 24:A:1868:HOH:O   | 2.18                     | 0.77              |
| 1:A:254:G:H2'    | 1:A:255:G:H8      | 1.48                     | 0.77              |
| 1:A:758:G:N7     | 24:A:2070:HOH:O   | 2.17                     | 0.77              |
| 3:C:95:THR:HB    | 3:C:97:LYS:HG2    | 1.67                     | 0.77              |
| 4:D:153:ARG:HD3  | 4:D:181:MET:HG3   | 1.67                     | 0.76              |
| 1:A:677:U:O4     | 1:A:713:G:N1      | 2.15                     | 0.76              |
| 19:S:80:TYR:CE1  | 19:S:81:ARG:HD3   | 2.20                     | 0.76              |
| 1:A:1262:C:H42   | 1:A:1273:G:H1     | 1.31                     | 0.76              |
| 2:B:91:PRO:HG3   | 2:B:155:LEU:HB3   | 1.67                     | 0.76              |
| 18:R:79:LEU:HD23 | 18:R:80:PRO:HD2   | 1.66                     | 0.76              |
| 1:A:1001:A:H61   | 1:A:1039:C:H42    | 1.34                     | 0.76              |
| 3:C:35:GLU:OE1   | 3:C:59:ARG:NH1    | 2.18                     | 0.76              |
| 7:G:27:ILE:HA    | 7:G:30:ILE:HD12   | 1.66                     | 0.76              |
| 1:A:1073:U:OP2   | 5:E:57:LYS:NZ     | 2.18                     | 0.75              |
| 1:A:1249:C:O2'   | 9:I:73:GLN:NE2    | 2.20                     | 0.75              |
| 15:O:62:GLN:HG2  | 15:O:65:ARG:HH21  | 1.52                     | 0.75              |
| 1:A:673:G:H2'    | 1:A:674:G:C8      | 2.21                     | 0.75              |
| 1:A:902:G:H2'    | 1:A:903:G:H8      | 1.50                     | 0.75              |
| 5:E:64:ARG:HE    | 5:E:65:ASN:HB2    | 1.51                     | 0.75              |
| 20:T:40:ALA:HB2  | 20:T:55:ILE:HG22  | 1.68                     | 0.75              |
| 18:R:34:TYR:HB3  | 18:R:69:THR:HG22  | 1.69                     | 0.75              |
| 1:A:695:A:H2'    | 1:A:696:A:C8      | 2.21                     | 0.74              |
| 4:D:57:ARG:HG3   | 4:D:202:LEU:HD12  | 1.68                     | 0.74              |
| 8:H:40:ALA:HB2   | 8:H:45:ILE:HD13   | 1.68                     | 0.74              |
| 1:A:967:5MC:O2'  | 9:I:128:ARG:NH1   | 2.20                     | 0.74              |
| 16:P:9:PHE:CD1   | 16:P:18:ARG:HD2   | 2.23                     | 0.74              |
| 7:G:85:TYR:HD1   | 7:G:154:TYR:CE1   | 2.05                     | 0.74              |
| 1:A:299:G:N1     | 24:A:1868:HOH:O   | 2.19                     | 0.74              |
| 4:D:149:ALA:HB3  | 4:D:152:SER:HB3   | 1.69                     | 0.74              |
| 11:K:92:GLU:HB3  | 11:K:96:ARG:HH21  | 1.52                     | 0.74              |
| 1:A:1236:A:H4'   | 1:A:1304:G:H4'    | 1.70                     | 0.73              |
| 1:A:1423:G:N2    | 1:A:1477:C:O2     | 2.19                     | 0.73              |
| 1:A:669:U:H2'    | 1:A:670:G:C8      | 2.24                     | 0.73              |
| 1:A:1367:C:H5'   | 10:J:60:ARG:HH21  | 1.53                     | 0.73              |
| 1:A:1026:G:OP1   | 1:A:1030(D):A:O2' | 2.07                     | 0.73              |
| 1:A:562:C:H4'    | 1:A:563:A:H5''    | 1.71                     | 0.73              |
| 1:A:1316:G:H4'   | 14:N:18:VAL:HG11  | 1.71                     | 0.73              |
| 9:I:29:ASN:HD21  | 9:I:65:VAL:HB     | 1.52                     | 0.73              |
| 1:A:925:G:O2'    | 1:A:927:G:OP1     | 2.07                     | 0.73              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:F:5:GLU:HB3    | 6:F:62:TRP:HE1    | 1.53                     | 0.73              |
| 12:L:25:PRO:C    | 12:L:27:LEU:H     | 1.91                     | 0.73              |
| 1:A:920:U:H2'    | 1:A:921:U:C6      | 2.23                     | 0.72              |
| 6:F:14:LEU:HD13  | 6:F:19:LEU:HA     | 1.71                     | 0.72              |
| 8:H:11:THR:O     | 8:H:15:ASN:ND2    | 2.21                     | 0.72              |
| 20:T:53:LEU:HD13 | 20:T:103:GLY:H    | 1.55                     | 0.72              |
| 1:A:1033:G:H3'   | 1:A:1034:G:H5'    | 1.70                     | 0.72              |
| 3:C:50:ALA:HB2   | 3:C:75:VAL:HB     | 1.71                     | 0.72              |
| 1:A:669:U:OP1    | 15:O:48:LYS:NZ    | 2.15                     | 0.72              |
| 2:B:15:VAL:HG13  | 2:B:209:ARG:HG3   | 1.72                     | 0.72              |
| 1:A:413:G:H8     | 1:A:428:G:H21     | 1.35                     | 0.72              |
| 1:A:62:U:H2'     | 1:A:63:C:H6       | 1.55                     | 0.72              |
| 2:B:178:ARG:HB2  | 2:B:178:ARG:HH11  | 1.55                     | 0.71              |
| 5:E:79:GLU:HG3   | 8:H:105:ARG:HG2   | 1.72                     | 0.71              |
| 15:O:56:LEU:O    | 15:O:60:VAL:HG23  | 1.90                     | 0.71              |
| 1:A:1258:G:H2'   | 1:A:1259:C:H5'    | 1.72                     | 0.71              |
| 1:A:1316:G:N1    | 1:A:1319:A:OP2    | 2.22                     | 0.71              |
| 20:T:50:GLU:HB2  | 20:T:99:LEU:HD23  | 1.70                     | 0.71              |
| 1:A:108:G:H5'    | 1:A:109:A:H5'     | 1.72                     | 0.71              |
| 1:A:45:U:H2'     | 1:A:46:G:C8       | 2.25                     | 0.71              |
| 1:A:1348:U:H4'   | 9:I:120:ARG:HG3   | 1.71                     | 0.71              |
| 20:T:57:ARG:HH22 | 20:T:100:ILE:HD12 | 1.55                     | 0.71              |
| 1:A:1288:A:N3    | 1:A:1352:C:O2'    | 2.24                     | 0.71              |
| 7:G:113:GLU:HG2  | 7:G:119:ARG:HG2   | 1.73                     | 0.71              |
| 7:G:111:ARG:HH21 | 7:G:123:GLU:HA    | 1.56                     | 0.70              |
| 3:C:77:ILE:HG22  | 3:C:81:GLY:HA2    | 1.73                     | 0.70              |
| 4:D:155:LEU:HD23 | 4:D:156:GLU:H     | 1.56                     | 0.70              |
| 11:K:85:ARG:HE   | 11:K:111:ASP:HB3  | 1.55                     | 0.70              |
| 1:A:390:C:H2'    | 1:A:391:G:C8      | 2.26                     | 0.70              |
| 1:A:975:A:H4'    | 1:A:976:G:H5''    | 1.71                     | 0.70              |
| 8:H:41:ARG:HH12  | 8:H:42:GLU:HG2    | 1.56                     | 0.70              |
| 4:D:186:LEU:H    | 4:D:186:LEU:HD23  | 1.56                     | 0.70              |
| 6:F:77:ARG:HA    | 6:F:80:ARG:HG2    | 1.74                     | 0.70              |
| 1:A:337:C:H2'    | 1:A:338:A:H8      | 1.57                     | 0.70              |
| 1:A:981:U:H5'    | 14:N:21:TYR:CE1   | 2.27                     | 0.70              |
| 8:H:124:ALA:O    | 8:H:128:GLY:N     | 2.25                     | 0.70              |
| 10:J:57:LYS:HG3  | 10:J:60:ARG:HH12  | 1.57                     | 0.69              |
| 1:A:1005:A:N7    | 1:A:1025:U:H1'    | 2.07                     | 0.69              |
| 17:Q:3:LYS:NZ    | 17:Q:61:GLU:O     | 2.24                     | 0.69              |
| 1:A:337:C:H2'    | 1:A:338:A:C8      | 2.27                     | 0.69              |
| 4:D:23:GLY:HA3   | 4:D:112:VAL:HG12  | 1.73                     | 0.69              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 11:K:44:SER:H      | 11:K:47:VAL:HB    | 1.55                     | 0.69              |
| 1:A:343:U:O2'      | 1:A:346:G:O6      | 2.09                     | 0.69              |
| 1:A:878:G:H5'      | 8:H:89:PRO:HG2    | 1.74                     | 0.69              |
| 14:N:32:SER:O      | 14:N:40:CYS:HA    | 1.91                     | 0.69              |
| 1:A:1320:C:O2      | 19:S:36:ARG:NH1   | 2.26                     | 0.69              |
| 11:K:86:GLY:N      | 11:K:112:THR:OG1  | 2.20                     | 0.69              |
| 16:P:60:LEU:HD23   | 16:P:64:ALA:HB3   | 1.75                     | 0.69              |
| 1:A:948:C:H42      | 1:A:1233:G:H1     | 1.41                     | 0.69              |
| 6:F:33:TYR:HB2     | 6:F:75:LEU:HD23   | 1.75                     | 0.69              |
| 1:A:253:U:H2'      | 1:A:254:G:H8      | 1.59                     | 0.68              |
| 1:A:1391:U:H2'     | 1:A:1392:G:C8     | 2.28                     | 0.68              |
| 2:B:136:VAL:HA     | 2:B:139:LYS:HZ2   | 1.58                     | 0.68              |
| 10:J:34:VAL:HG13   | 10:J:74:ILE:HA    | 1.75                     | 0.68              |
| 13:M:12:ASN:H      | 13:M:45:VAL:CG1   | 2.05                     | 0.68              |
| 15:O:16:ALA:HB1    | 15:O:21:ASP:HB3   | 1.73                     | 0.68              |
| 17:Q:9:VAL:HG23    | 17:Q:56:VAL:HG22  | 1.74                     | 0.68              |
| 9:I:50:LEU:HA      | 9:I:53:VAL:HG22   | 1.75                     | 0.68              |
| 1:A:1128:C:O2'     | 1:A:1130:A:OP1    | 2.09                     | 0.68              |
| 2:B:79:ASP:HA      | 2:B:82:ARG:HG2    | 1.75                     | 0.68              |
| 1:A:1147:C:O2      | 9:I:16:ARG:NH1    | 2.26                     | 0.68              |
| 1:A:259:G:H1       | 1:A:267:C:H42     | 1.42                     | 0.68              |
| 17:Q:61:GLU:HA     | 17:Q:71:PHE:CE2   | 2.29                     | 0.68              |
| 1:A:1366:C:H2'     | 1:A:1367:C:C6     | 2.28                     | 0.68              |
| 1:A:770:C:H1'      | 1:A:899:C:H42     | 1.57                     | 0.68              |
| 19:S:49:ILE:HG21   | 19:S:71:LEU:HD11  | 1.74                     | 0.68              |
| 2:B:77:ALA:HB2     | 2:B:211:ILE:HD13  | 1.74                     | 0.68              |
| 4:D:76:ARG:HB2     | 4:D:207:TYR:HE2   | 1.59                     | 0.68              |
| 6:F:14:LEU:HD22    | 6:F:18:GLN:HB3    | 1.76                     | 0.67              |
| 1:A:1030(D):A:H5'' | 1:A:1031:G:H5''   | 1.77                     | 0.67              |
| 2:B:90:MET:SD      | 2:B:90:MET:N      | 2.67                     | 0.67              |
| 1:A:310:G:H2'      | 1:A:311:C:H6      | 1.59                     | 0.67              |
| 2:B:96:ARG:HG3     | 2:B:97:TRP:N      | 2.09                     | 0.67              |
| 1:A:17:U:H2'       | 1:A:18:C:C6       | 2.30                     | 0.67              |
| 1:A:527:7MG:H81    | 1:A:527:7MG:H5''  | 1.76                     | 0.67              |
| 1:A:669:U:H2'      | 1:A:670:G:H8      | 1.56                     | 0.67              |
| 2:B:76:GLN:HE22    | 2:B:206:ASP:HB3   | 1.58                     | 0.67              |
| 1:A:664:G:N2       | 1:A:741:G:H1      | 1.92                     | 0.67              |
| 11:K:80:VAL:HG13   | 11:K:103:LEU:HD21 | 1.76                     | 0.67              |
| 1:A:1367:C:H5'     | 10:J:60:ARG:NH2   | 2.10                     | 0.66              |
| 3:C:14:ILE:HB      | 3:C:15:THR:HG23   | 1.76                     | 0.66              |
| 1:A:967:5MC:H4'    | 9:I:128:ARG:HG3   | 1.76                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1427:U:H2'   | 1:A:1428:A:C8    | 2.29                     | 0.66              |
| 15:O:29:VAL:HG11 | 15:O:81:LEU:HD11 | 1.77                     | 0.66              |
| 2:B:119:GLU:OE2  | 2:B:153:ARG:NH2  | 2.29                     | 0.66              |
| 1:A:1343:G:H4'   | 9:I:122:ALA:HB3  | 1.75                     | 0.66              |
| 1:A:1326:C:H5''  | 21:U:12:LYS:HE3  | 1.78                     | 0.66              |
| 1:A:720:C:H5''   | 1:A:721:G:H5''   | 1.77                     | 0.66              |
| 8:H:29:SER:HG    | 8:H:32:LYS:H     | 1.43                     | 0.66              |
| 5:E:31:LEU:HG    | 5:E:45:PHE:HD1   | 1.61                     | 0.66              |
| 13:M:4:ILE:HD12  | 13:M:22:ILE:HD11 | 1.78                     | 0.66              |
| 20:T:53:LEU:HD22 | 20:T:56:MET:HG2  | 1.77                     | 0.66              |
| 1:A:1127:G:H1    | 1:A:1145:C:H42   | 1.40                     | 0.66              |
| 6:F:30:LEU:HA    | 6:F:75:LEU:HD21  | 1.77                     | 0.66              |
| 1:A:514:C:H2'    | 1:A:515:G:H8     | 1.60                     | 0.66              |
| 8:H:11:THR:HG23  | 8:H:15:ASN:HD21  | 1.60                     | 0.66              |
| 13:M:96:LEU:HB3  | 13:M:97:PRO:HD2  | 1.78                     | 0.66              |
| 17:Q:6:LEU:H     | 17:Q:59:ILE:HG22 | 1.59                     | 0.66              |
| 1:A:1035:A:H2'   | 1:A:1036:G:H8    | 1.59                     | 0.66              |
| 13:M:8:GLU:OE2   | 13:M:8:GLU:N     | 2.29                     | 0.66              |
| 6:F:91:VAL:HG13  | 18:R:72:ARG:HH22 | 1.61                     | 0.65              |
| 6:F:8:ILE:HD11   | 6:F:79:LEU:HD13  | 1.78                     | 0.65              |
| 8:H:4:ASP:OD2    | 8:H:85:ARG:NH1   | 2.29                     | 0.65              |
| 6:F:91:VAL:HG12  | 6:F:92:LYS:O     | 1.95                     | 0.65              |
| 7:G:95:ARG:HG3   | 7:G:99:LEU:HD12  | 1.77                     | 0.65              |
| 16:P:74:LEU:HD22 | 16:P:79:VAL:HG21 | 1.79                     | 0.65              |
| 1:A:1527:C:H2'   | 1:A:1528:U:H6    | 1.58                     | 0.65              |
| 4:D:206:PHE:HD2  | 4:D:207:TYR:CE1  | 2.15                     | 0.65              |
| 3:C:164:ARG:HG2  | 3:C:165:THR:H    | 1.61                     | 0.65              |
| 5:E:99:GLY:N     | 5:E:117:ASP:OD1  | 2.29                     | 0.65              |
| 1:A:1332:A:H2'   | 1:A:1333:A:H8    | 1.61                     | 0.65              |
| 1:A:259:G:OP2    | 20:T:83:ARG:NH1  | 2.29                     | 0.65              |
| 1:A:1226:C:OP2   | 13:M:91:ARG:NH2  | 2.30                     | 0.65              |
| 9:I:118:LYS:O    | 9:I:120:ARG:N    | 2.30                     | 0.65              |
| 8:H:25:ASP:OD1   | 8:H:25:ASP:N     | 2.30                     | 0.64              |
| 10:J:29:ARG:NH2  | 10:J:84:GLN:OE1  | 2.30                     | 0.64              |
| 1:A:1130:A:OP1   | 1:A:1130:A:H8    | 1.79                     | 0.64              |
| 11:K:17:GLY:HA2  | 11:K:35:PRO:HD3  | 1.80                     | 0.64              |
| 15:O:26:GLU:O    | 15:O:29:VAL:HG12 | 1.97                     | 0.64              |
| 1:A:1320:C:H4'   | 19:S:73:GLU:HG3  | 1.80                     | 0.64              |
| 1:A:1541:PSU:H5' | 1:A:1542:U:OP1   | 1.97                     | 0.64              |
| 9:I:6:GLY:HA3    | 9:I:83:ARG:HG3   | 1.79                     | 0.64              |
| 10:J:4:ILE:HB    | 10:J:74:ILE:CG1  | 2.27                     | 0.64              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 17:Q:7:THR:O     | 17:Q:23:VAL:HG13  | 1.97                     | 0.64              |
| 17:Q:88:TYR:HA   | 17:Q:91:ARG:HD3   | 1.79                     | 0.64              |
| 1:A:312:C:H2'    | 1:A:313:A:C8      | 2.32                     | 0.64              |
| 1:A:537:G:OP1    | 12:L:113:ARG:NH2  | 2.30                     | 0.64              |
| 13:M:22:ILE:HG21 | 13:M:66:LEU:HD13  | 1.79                     | 0.64              |
| 14:N:25:VAL:HG12 | 14:N:38:GLY:O     | 1.97                     | 0.64              |
| 5:E:116:THR:OG1  | 5:E:117:ASP:OD2   | 2.16                     | 0.64              |
| 6:F:45:LEU:O     | 6:F:46:ARG:NH1    | 2.31                     | 0.64              |
| 14:N:47:LEU:O    | 14:N:50:LYS:N     | 2.31                     | 0.64              |
| 1:A:579:G:H4'    | 15:O:54:ARG:HH21  | 1.63                     | 0.64              |
| 1:A:793:U:O2     | 1:A:1516[A]:G:H4' | 1.96                     | 0.64              |
| 4:D:199:ASN:HB3  | 4:D:202:LEU:HD23  | 1.78                     | 0.64              |
| 12:L:27:LEU:HG   | 12:L:28:LYS:H     | 1.62                     | 0.64              |
| 1:A:352:C:H5'    | 24:A:2004:HOH:O   | 1.97                     | 0.64              |
| 1:A:1125:U:O2'   | 1:A:1126:U:OP2    | 2.12                     | 0.64              |
| 1:A:1258:G:OP2   | 1:A:1258:G:H8     | 1.80                     | 0.64              |
| 1:A:426:G:OP1    | 4:D:36:ARG:NH1    | 2.31                     | 0.64              |
| 1:A:62:U:H2'     | 1:A:63:C:C6       | 2.33                     | 0.64              |
| 2:B:68:ILE:H     | 2:B:90:MET:HG3    | 1.63                     | 0.64              |
| 7:G:78:ARG:HH12  | 7:G:156:TRP:HB2   | 1.63                     | 0.64              |
| 15:O:15:PHE:CE2  | 15:O:84:LYS:HG2   | 2.33                     | 0.64              |
| 1:A:1121:U:H2'   | 1:A:1122:U:C6     | 2.33                     | 0.63              |
| 1:A:937:A:H5''   | 1:A:938:A:OP2     | 1.98                     | 0.63              |
| 3:C:76:VAL:O     | 3:C:83:ARG:HG2    | 1.98                     | 0.63              |
| 7:G:15:ASP:OD2   | 7:G:18:TYR:N      | 2.29                     | 0.63              |
| 9:I:77:ILE:O     | 9:I:81:ILE:HG12   | 1.98                     | 0.63              |
| 1:A:1146:A:H2'   | 1:A:1147:C:O4'    | 1.98                     | 0.63              |
| 1:A:1418:A:H2'   | 1:A:1419:G:O4'    | 1.99                     | 0.63              |
| 14:N:42:ILE:O    | 14:N:46:GLU:HG3   | 1.99                     | 0.63              |
| 15:O:18:PHE:CE2  | 15:O:21:ASP:HB2   | 2.32                     | 0.63              |
| 18:R:26:LEU:HD11 | 18:R:42:ARG:HD3   | 1.81                     | 0.63              |
| 18:R:56:THR:OG1  | 18:R:57:GLY:N     | 2.28                     | 0.63              |
| 1:A:1171:G:O2'   | 1:A:1172:C:H5'    | 1.98                     | 0.63              |
| 1:A:1366:C:H2'   | 1:A:1367:C:H6     | 1.62                     | 0.63              |
| 1:A:1510:U:H2'   | 1:A:1511:G:C8     | 2.32                     | 0.63              |
| 4:D:31:CYS:C     | 4:D:33:MET:H      | 2.02                     | 0.63              |
| 12:L:66:VAL:HG21 | 12:L:98:TYR:CE1   | 2.33                     | 0.63              |
| 19:S:13:ASP:N    | 19:S:13:ASP:OD2   | 2.28                     | 0.63              |
| 1:A:444:C:O2     | 1:A:490:G:N2      | 2.27                     | 0.63              |
| 1:A:940:C:OP1    | 7:G:29:LYS:NZ     | 2.31                     | 0.63              |
| 1:A:115:G:O2'    | 1:A:116:A:OP2     | 2.13                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1342:C:H2'   | 1:A:1343:G:C8    | 2.33                     | 0.63              |
| 10:J:88:LEU:HD22 | 10:J:88:LEU:N    | 2.12                     | 0.63              |
| 1:A:711:G:H2'    | 1:A:712:A:H8     | 1.64                     | 0.63              |
| 4:D:71:SER:OG    | 4:D:72:GLU:N     | 2.32                     | 0.63              |
| 5:E:151:LEU:HD11 | 8:H:79:VAL:HA    | 1.80                     | 0.63              |
| 10:J:4:ILE:HG13  | 10:J:77:PRO:HG2  | 1.81                     | 0.63              |
| 20:T:49:ALA:O    | 20:T:53:LEU:HB2  | 1.99                     | 0.63              |
| 1:A:782:A:OP1    | 1:A:1521:G:N2    | 2.31                     | 0.63              |
| 7:G:72:ARG:NE    | 7:G:142:GLU:OE1  | 2.20                     | 0.63              |
| 20:T:63:ILE:HD13 | 20:T:80:ARG:HB3  | 1.81                     | 0.63              |
| 1:A:664:G:OP1    | 18:R:64:ARG:HD2  | 1.99                     | 0.63              |
| 10:J:53:PRO:HA   | 14:N:41:ARG:HH21 | 1.64                     | 0.63              |
| 1:A:1057:G:H4'   | 3:C:197:GLY:H    | 1.64                     | 0.62              |
| 2:B:16:HIS:CB    | 2:B:210:SER:HB2  | 2.28                     | 0.62              |
| 7:G:85:TYR:CD1   | 7:G:154:TYR:HE1  | 2.10                     | 0.62              |
| 1:A:1523:G:OP1   | 11:K:123:LYS:NZ  | 2.18                     | 0.62              |
| 6:F:9:VAL:HG22   | 6:F:60:PHE:CD2   | 2.34                     | 0.62              |
| 1:A:881:G:OP2    | 12:L:12:ARG:NH2  | 2.30                     | 0.62              |
| 13:M:5:ALA:HA    | 13:M:61:GLU:HG3  | 1.80                     | 0.62              |
| 3:C:91:LEU:HB3   | 3:C:99:VAL:HG21  | 1.81                     | 0.62              |
| 7:G:41:ARG:HB2   | 7:G:41:ARG:NH1   | 2.15                     | 0.62              |
| 2:B:236:TYR:O    | 2:B:239:VAL:HG23 | 2.00                     | 0.62              |
| 1:A:1388:C:H2'   | 1:A:1389:C:H6    | 1.64                     | 0.62              |
| 1:A:1481:U:H2'   | 1:A:1482:G:C8    | 2.35                     | 0.62              |
| 1:A:750:G:H1'    | 15:O:23:GLY:H    | 1.65                     | 0.62              |
| 4:D:36:ARG:HD2   | 4:D:38:TYR:CE2   | 2.33                     | 0.62              |
| 1:A:489:C:H2'    | 1:A:490:G:H8     | 1.63                     | 0.62              |
| 1:A:880:C:OP1    | 12:L:8:ASN:ND2   | 2.33                     | 0.62              |
| 21:U:10:ARG:HA   | 21:U:13:ILE:HB   | 1.82                     | 0.62              |
| 3:C:153:VAL:HG23 | 3:C:198:VAL:HG22 | 1.81                     | 0.62              |
| 5:E:33:VAL:HG11  | 5:E:109:ILE:HA   | 1.81                     | 0.62              |
| 10:J:88:LEU:HD22 | 10:J:88:LEU:H    | 1.65                     | 0.62              |
| 11:K:26:ASN:ND2  | 11:K:26:ASN:O    | 2.30                     | 0.62              |
| 1:A:390:C:O3'    | 16:P:28:ARG:NH2  | 2.32                     | 0.62              |
| 2:B:19:HIS:CE1   | 2:B:206:ASP:HB2  | 2.35                     | 0.62              |
| 2:B:80:ILE:HG21  | 2:B:211:ILE:HG22 | 1.80                     | 0.62              |
| 3:C:121:ALA:HA   | 3:C:124:ILE:HD12 | 1.81                     | 0.62              |
| 5:E:18:ARG:HG2   | 5:E:25:ARG:O     | 1.99                     | 0.61              |
| 10:J:8:LEU:HD22  | 10:J:96:ILE:HG22 | 1.81                     | 0.61              |
| 1:A:1196:U:H3'   | 24:A:1871:HOH:O  | 1.99                     | 0.61              |
| 2:B:9:GLU:OE2    | 2:B:12:GLU:N     | 2.33                     | 0.61              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:H:116:LYS:HG3  | 8:H:127:LEU:HD11  | 1.82                     | 0.61              |
| 1:A:861:G:HO2'   | 1:A:874:G:HO2'    | 1.47                     | 0.61              |
| 4:D:21:LEU:HD12  | 4:D:22:LYS:H      | 1.65                     | 0.61              |
| 9:I:50:LEU:HD11  | 9:I:81:ILE:HG21   | 1.81                     | 0.61              |
| 1:A:1228:C:OP1   | 13:M:108:ARG:NH2  | 2.33                     | 0.61              |
| 1:A:1258:G:C2'   | 1:A:1259:C:H5'    | 2.30                     | 0.61              |
| 1:A:1060:C:C5    | 3:C:2:GLY:HA2     | 2.35                     | 0.61              |
| 1:A:1368:G:OP2   | 9:I:112:LYS:NZ    | 2.27                     | 0.61              |
| 1:A:1504:G:OP1   | 1:A:1507:A:H4'    | 2.00                     | 0.61              |
| 7:G:146:GLU:HA   | 7:G:149:ARG:HB2   | 1.80                     | 0.61              |
| 13:M:4:ILE:HD11  | 13:M:10:PRO:HG3   | 1.81                     | 0.61              |
| 15:O:18:PHE:CD2  | 15:O:21:ASP:HB2   | 2.35                     | 0.61              |
| 15:O:5:LYS:NZ    | 15:O:5:LYS:H      | 1.97                     | 0.61              |
| 18:R:87:ARG:O    | 18:R:88:LYS:HB2   | 2.00                     | 0.61              |
| 1:A:322:C:H4'    | 20:T:23:ARG:HD2   | 1.82                     | 0.61              |
| 1:A:955:U:H1'    | 1:A:1227:A:H61    | 1.66                     | 0.61              |
| 13:M:5:ALA:N     | 13:M:8:GLU:OE1    | 2.34                     | 0.61              |
| 1:A:1060:C:OP1   | 14:N:45:ARG:NH2   | 2.33                     | 0.61              |
| 1:A:643:C:H5'    | 8:H:31:PHE:CD1    | 2.36                     | 0.61              |
| 8:H:85:ARG:NE    | 8:H:87:SER:O      | 2.34                     | 0.61              |
| 14:N:29:ARG:HH22 | 14:N:41:ARG:HH12  | 1.49                     | 0.61              |
| 1:A:1127:G:O6    | 1:A:1144:G:N1     | 2.30                     | 0.61              |
| 1:A:1505:G:H4'   | 1:A:1506:U:H5''   | 1.82                     | 0.61              |
| 1:A:1511:G:H2'   | 1:A:1512:U:O4'    | 2.01                     | 0.61              |
| 1:A:264:U:H2'    | 1:A:265:G:O4'     | 2.00                     | 0.61              |
| 1:A:737:A:H2'    | 1:A:738:C:C6      | 2.36                     | 0.61              |
| 3:C:6:HIS:CD2    | 3:C:9:GLY:H       | 2.19                     | 0.61              |
| 19:S:47:HIS:HB3  | 19:S:49:ILE:HD11  | 1.82                     | 0.61              |
| 1:A:1243:C:H2'   | 1:A:1244:C:C6     | 2.36                     | 0.61              |
| 1:A:1321:C:H5''  | 1:A:1322:C:H5''   | 1.82                     | 0.61              |
| 12:L:83:VAL:HG21 | 12:L:100:ILE:HD13 | 1.83                     | 0.61              |
| 15:O:22:THR:O    | 15:O:27:VAL:HG11  | 2.00                     | 0.61              |
| 1:A:1491:G:C6    | 1:A:1493:A:H2     | 2.19                     | 0.60              |
| 3:C:150:LYS:HB3  | 3:C:201:TYR:HB2   | 1.82                     | 0.60              |
| 12:L:77:LEU:HD21 | 12:L:107:ALA:HA   | 1.82                     | 0.60              |
| 6:F:91:VAL:HG13  | 18:R:72:ARG:NH2   | 2.17                     | 0.60              |
| 1:A:1425:U:H2'   | 1:A:1426:C:C6     | 2.36                     | 0.60              |
| 8:H:23:SER:HB2   | 8:H:62:TYR:HA     | 1.82                     | 0.60              |
| 1:A:1435:G:H2'   | 1:A:1436:U:C6     | 2.36                     | 0.60              |
| 1:A:310:G:OP2    | 16:P:27:LYS:NZ    | 2.35                     | 0.60              |
| 1:A:1103:C:H5''  | 2:B:98:LEU:HD22   | 1.84                     | 0.60              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 4:D:155:LEU:HD23    | 4:D:156:GLU:N      | 2.16                     | 0.60              |
| 3:C:18:TRP:CD1      | 14:N:54:PRO:HA     | 2.36                     | 0.60              |
| 18:R:39:VAL:HG13    | 18:R:40:LEU:HD23   | 1.84                     | 0.60              |
| 1:A:1307:U:H2'      | 1:A:1308:U:C6      | 2.37                     | 0.60              |
| 1:A:976:G:H5'       | 1:A:1358:U:O2'     | 2.02                     | 0.60              |
| 1:A:253:U:H2'       | 1:A:254:G:C8       | 2.35                     | 0.60              |
| 11:K:48:ILE:HG22    | 11:K:49:GLY:H      | 1.66                     | 0.60              |
| 1:A:1124:G:H5'      | 10:J:35:SER:HB2    | 1.83                     | 0.60              |
| 3:C:188:LEU:HD11    | 3:C:195:VAL:HG13   | 1.84                     | 0.60              |
| 2:B:178:ARG:HD3     | 8:H:72:PRO:HA      | 1.82                     | 0.60              |
| 1:A:1134:G:H2'      | 1:A:1135:U:O4'     | 2.01                     | 0.60              |
| 1:A:448:A:OP2       | 1:A:485:G:N2       | 2.31                     | 0.60              |
| 1:A:499:A:H4'       | 1:A:500:G:OP1      | 2.01                     | 0.60              |
| 5:E:64:ARG:NE       | 5:E:65:ASN:HB2     | 2.16                     | 0.60              |
| 6:F:2:ARG:HD2       | 6:F:69:GLU:HG2     | 1.83                     | 0.60              |
| 1:A:1255:G:H2'      | 1:A:1258:G:H21     | 1.67                     | 0.60              |
| 1:A:197:A:H5''      | 24:A:1993:HOH:O    | 2.01                     | 0.60              |
| 2:B:213:LEU:HD23    | 2:B:214:ILE:HD13   | 1.84                     | 0.60              |
| 7:G:38:LEU:O        | 7:G:42:ILE:HG13    | 2.02                     | 0.60              |
| 10:J:61:GLU:OE2     | 14:N:49:HIS:NE2    | 2.34                     | 0.60              |
| 20:T:87:LYS:O       | 20:T:91:LEU:HB2    | 2.02                     | 0.60              |
| 1:A:1144:G:H2'      | 1:A:1145:C:C5      | 2.36                     | 0.60              |
| 10:J:24:VAL:HG21    | 10:J:37:PRO:HG3    | 1.84                     | 0.60              |
| 11:K:92:GLU:HB3     | 11:K:96:ARG:NH2    | 2.16                     | 0.60              |
| 17:Q:87:LYS:HE3     | 17:Q:88:TYR:N      | 2.16                     | 0.60              |
| 1:A:1518[B]:MA6:O5' | 1:A:1518[B]:MA6:H8 | 2.01                     | 0.59              |
| 1:A:434:U:H2'       | 1:A:435:C:H6       | 1.66                     | 0.59              |
| 2:B:9:GLU:HG2       | 2:B:10:LEU:N       | 2.16                     | 0.59              |
| 7:G:102:ARG:O       | 7:G:106:GLN:HG3    | 2.01                     | 0.59              |
| 1:A:447:G:H2'       | 1:A:485:G:N2       | 2.17                     | 0.59              |
| 20:T:10:LEU:HD22    | 20:T:11:SER:N      | 2.16                     | 0.59              |
| 20:T:33:ILE:HG13    | 20:T:62:LEU:HD13   | 1.83                     | 0.59              |
| 3:C:12:LEU:HD21     | 14:N:51:GLY:HA2    | 1.83                     | 0.59              |
| 1:A:1096:C:H2'      | 1:A:1097:C:H6      | 1.66                     | 0.59              |
| 10:J:50:ILE:N       | 10:J:50:ILE:HD12   | 2.17                     | 0.59              |
| 4:D:104:VAL:HG21    | 4:D:140:VAL:HG21   | 1.85                     | 0.59              |
| 1:A:1338:G:H2'      | 1:A:1339:A:C8      | 2.38                     | 0.59              |
| 1:A:447:G:H1        | 1:A:485:G:HO2'     | 1.50                     | 0.59              |
| 3:C:6:HIS:CD2       | 14:N:49:HIS:HB3    | 2.38                     | 0.59              |
| 4:D:187:ARG:NH2     | 4:D:188:LEU:HB2    | 2.16                     | 0.59              |
| 13:M:50:GLU:HA      | 13:M:53:VAL:HB     | 1.85                     | 0.59              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:8:A:N7       | 4:D:208:SER:OG    | 2.36                     | 0.59              |
| 4:D:206:PHE:HD2  | 4:D:207:TYR:CD1   | 2.20                     | 0.59              |
| 1:A:514:C:O2'    | 1:A:515:G:H5'     | 2.03                     | 0.59              |
| 2:B:180:LEU:HB2  | 2:B:182:ILE:HG13  | 1.84                     | 0.59              |
| 9:I:26:VAL:HG13  | 9:I:61:ALA:HB3    | 1.83                     | 0.59              |
| 9:I:65:VAL:HG11  | 9:I:73:GLN:OE1    | 2.03                     | 0.59              |
| 1:A:1399:C:H4'   | 1:A:1400:5MC:H5'' | 1.84                     | 0.59              |
| 1:A:948:C:H5'    | 1:A:1306:A:O2'    | 2.02                     | 0.59              |
| 2:B:189:ASP:OD1  | 2:B:190:THR:N     | 2.30                     | 0.59              |
| 4:D:196:LEU:H    | 4:D:196:LEU:HD23  | 1.67                     | 0.59              |
| 16:P:19:ILE:HG22 | 16:P:36:ILE:HG13  | 1.85                     | 0.59              |
| 1:A:579:G:H5'    | 1:A:728:A:H1'     | 1.84                     | 0.58              |
| 1:A:1190:G:H5'   | 3:C:176:HIS:CE1   | 2.38                     | 0.58              |
| 6:F:5:GLU:HB3    | 6:F:62:TRP:NE1    | 2.18                     | 0.58              |
| 8:H:64:LYS:HG2   | 8:H:79:VAL:HG21   | 1.84                     | 0.58              |
| 1:A:1099:G:H2'   | 1:A:1100:C:C6     | 2.38                     | 0.58              |
| 8:H:51:VAL:HG12  | 8:H:58:TYR:O      | 2.03                     | 0.58              |
| 2:B:74:LYS:NZ    | 2:B:74:LYS:HB3    | 2.18                     | 0.58              |
| 6:F:39:LYS:HD3   | 6:F:40:VAL:N      | 2.18                     | 0.58              |
| 6:F:77:ARG:O     | 6:F:77:ARG:HG2    | 2.04                     | 0.58              |
| 6:F:41:GLU:OE1   | 18:R:35:ARG:NH2   | 2.36                     | 0.58              |
| 1:A:1027:C:O2    | 1:A:1028:C:N4     | 2.36                     | 0.58              |
| 1:A:1332:A:H2'   | 1:A:1333:A:C8     | 2.38                     | 0.58              |
| 1:A:234:C:H2'    | 1:A:235:C:C6      | 2.39                     | 0.58              |
| 1:A:243:A:C2     | 1:A:246:A:C8      | 2.91                     | 0.58              |
| 1:A:457:C:H2'    | 1:A:458:C:H6      | 1.68                     | 0.58              |
| 18:R:87:ARG:HG2  | 18:R:88:LYS:H     | 1.67                     | 0.58              |
| 1:A:437:U:HO2'   | 4:D:123:HIS:HD1   | 1.50                     | 0.58              |
| 2:B:121:LEU:O    | 2:B:124:SER:OG    | 2.21                     | 0.58              |
| 2:B:170:GLU:O    | 2:B:173:ALA:N     | 2.37                     | 0.58              |
| 6:F:33:TYR:HD2   | 6:F:71:ARG:HD2    | 1.68                     | 0.58              |
| 17:Q:22:LEU:HD11 | 17:Q:39:SER:HB2   | 1.85                     | 0.58              |
| 20:T:14:LYS:HA   | 20:T:17:ARG:HG3   | 1.86                     | 0.58              |
| 1:A:1003(A):G:N2 | 1:A:1038:C:O2     | 2.36                     | 0.58              |
| 1:A:1234:C:H1'   | 1:A:1364:U:O2     | 2.03                     | 0.58              |
| 21:U:5:ASP:O     | 21:U:11:GLY:HA3   | 2.02                     | 0.58              |
| 2:B:158:LEU:H    | 2:B:158:LEU:HD12  | 1.69                     | 0.58              |
| 3:C:21:ARG:HH11  | 3:C:21:ARG:HG3    | 1.69                     | 0.58              |
| 4:D:21:LEU:O     | 4:D:113:SER:HB2   | 2.04                     | 0.58              |
| 1:A:426:G:OP1    | 4:D:38:TYR:OH     | 2.14                     | 0.58              |
| 3:C:28:GLN:HB3   | 3:C:32:LEU:HD13   | 1.86                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:I:35:GLU:HA    | 9:I:38:GLN:HB2   | 1.85                     | 0.58              |
| 10:J:53:PRO:HA   | 14:N:41:ARG:NH2  | 2.18                     | 0.58              |
| 18:R:51:LEU:HD13 | 18:R:55:ARG:HE   | 1.69                     | 0.58              |
| 1:A:190(J):U:H2' | 1:A:190(K):G:C8  | 2.39                     | 0.58              |
| 3:C:9:GLY:HA2    | 3:C:12:LEU:HD13  | 1.84                     | 0.58              |
| 13:M:23:TYR:HB3  | 13:M:67:GLU:HA   | 1.85                     | 0.58              |
| 13:M:40:ASN:HB3  | 13:M:43:THR:HG23 | 1.86                     | 0.58              |
| 1:A:132:C:O3'    | 20:T:74:LYS:NZ   | 2.37                     | 0.58              |
| 1:A:390:C:H2'    | 1:A:391:G:H8     | 1.65                     | 0.57              |
| 1:A:1005:A:H3'   | 1:A:1006:C:C6    | 2.39                     | 0.57              |
| 1:A:811:C:H4'    | 1:A:900:A:N6     | 2.19                     | 0.57              |
| 6:F:100:ASN:ND2  | 18:R:23:LYS:O    | 2.36                     | 0.57              |
| 8:H:65:TYR:HA    | 8:H:79:VAL:HG23  | 1.86                     | 0.57              |
| 2:B:122:PHE:CD2  | 2:B:127:ILE:HG21 | 2.38                     | 0.57              |
| 11:K:62:GLN:HG2  | 11:K:63:LEU:HD23 | 1.86                     | 0.57              |
| 12:L:19:ARG:H    | 12:L:19:ARG:CZ   | 2.16                     | 0.57              |
| 15:O:25:THR:HG21 | 15:O:70:LEU:HD23 | 1.87                     | 0.57              |
| 19:S:12:ASP:O    | 19:S:15:LEU:HD23 | 2.04                     | 0.57              |
| 1:A:1310:G:OP2   | 13:M:88:ARG:NH2  | 2.24                     | 0.57              |
| 1:A:1531:A:O5'   | 1:A:1531:A:H8    | 1.87                     | 0.57              |
| 1:A:353:A:H5'    | 1:A:353:A:H8     | 1.70                     | 0.57              |
| 4:D:78:LEU:HD21  | 4:D:96:LEU:HB3   | 1.86                     | 0.57              |
| 9:I:102:LEU:HD12 | 9:I:102:LEU:H    | 1.69                     | 0.57              |
| 12:L:66:VAL:HG22 | 12:L:67:THR:N    | 2.20                     | 0.57              |
| 1:A:1412:C:H2'   | 1:A:1413:A:C8    | 2.40                     | 0.57              |
| 1:A:606:G:H1'    | 1:A:632:A:H61    | 1.69                     | 0.57              |
| 1:A:665:A:H3'    | 1:A:725:G:N2     | 2.18                     | 0.57              |
| 5:E:107:ARG:HG3  | 5:E:111:GLU:HG3  | 1.85                     | 0.57              |
| 15:O:18:PHE:HB2  | 15:O:19:PRO:HD2  | 1.87                     | 0.57              |
| 17:Q:83:ASP:N    | 17:Q:83:ASP:OD2  | 2.36                     | 0.57              |
| 1:A:1392:G:H21   | 1:A:1502:A:H8    | 1.50                     | 0.57              |
| 1:A:509:A:H3'    | 1:A:509:A:C8     | 2.40                     | 0.57              |
| 8:H:82:HIS:NE2   | 8:H:84:ARG:HD2   | 2.19                     | 0.57              |
| 9:I:106:ALA:O    | 9:I:108:VAL:HG22 | 2.04                     | 0.57              |
| 12:L:7:ILE:O     | 12:L:10:LEU:N    | 2.37                     | 0.57              |
| 17:Q:74:LEU:HG   | 17:Q:75:ARG:HG2  | 1.85                     | 0.57              |
| 1:A:1314:C:H5    | 19:S:6:LYS:HZ2   | 1.52                     | 0.57              |
| 2:B:97:TRP:HH2   | 2:B:176:GLU:CD   | 2.07                     | 0.57              |
| 2:B:33:TYR:CD2   | 2:B:43:ASP:HA    | 2.40                     | 0.57              |
| 3:C:17:ASP:OD1   | 3:C:18:TRP:N     | 2.37                     | 0.57              |
| 6:F:46:ARG:HB2   | 6:F:60:PHE:CE1   | 2.40                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:7:VAL:N      | 2:B:8:LYS:HD2    | 2.19                     | 0.57              |
| 1:A:922:G:H4'    | 5:E:20:GLN:HA    | 1.87                     | 0.57              |
| 18:R:45:SER:OG   | 18:R:46:GLU:N    | 2.38                     | 0.57              |
| 16:P:34:GLU:OE1  | 16:P:55:ARG:NH1  | 2.38                     | 0.57              |
| 17:Q:10:VAL:HG23 | 17:Q:55:ASP:O    | 2.05                     | 0.57              |
| 1:A:1118:C:H1'   | 1:A:1179:A:C4    | 2.40                     | 0.57              |
| 1:A:1226:C:H4'   | 1:A:1227:A:OP1   | 2.05                     | 0.57              |
| 1:A:517:G:N2     | 1:A:533:A:OP2    | 2.33                     | 0.57              |
| 1:A:807:A:H2'    | 1:A:808:C:C6     | 2.39                     | 0.57              |
| 1:A:201:C:H42    | 1:A:216:G:H1     | 1.53                     | 0.56              |
| 1:A:527:7MG:H5'' | 1:A:527:7MG:C8   | 2.40                     | 0.56              |
| 16:P:10:GLY:HA3  | 16:P:14:ASN:O    | 2.05                     | 0.56              |
| 1:A:1032:G:H2'   | 1:A:1033:G:H5'   | 1.86                     | 0.56              |
| 1:A:1280:A:O2'   | 1:A:1281:U:H5'   | 2.05                     | 0.56              |
| 4:D:52:SER:O     | 4:D:56:VAL:HG23  | 2.04                     | 0.56              |
| 10:J:5:ARG:O     | 10:J:98:ILE:HA   | 2.04                     | 0.56              |
| 18:R:29:PHE:HZ   | 18:R:43:PHE:HE1  | 1.52                     | 0.56              |
| 1:A:1041:A:H2'   | 1:A:1042:G:O4'   | 2.05                     | 0.56              |
| 1:A:922:G:H2'    | 1:A:923:A:C8     | 2.39                     | 0.56              |
| 4:D:8:VAL:HG12   | 4:D:21:LEU:HD22  | 1.87                     | 0.56              |
| 6:F:41:GLU:HB3   | 6:F:43:LEU:HD11  | 1.87                     | 0.56              |
| 1:A:1033:G:N3    | 1:A:1033:G:H2'   | 2.20                     | 0.56              |
| 2:B:21:ARG:HA    | 2:B:39:ILE:HA    | 1.86                     | 0.56              |
| 2:B:80:ILE:O     | 2:B:84:GLU:HB2   | 2.06                     | 0.56              |
| 20:T:37:SER:HB3  | 20:T:84:LEU:HD13 | 1.87                     | 0.56              |
| 2:B:84:GLU:OE1   | 2:B:87:ARG:NH2   | 2.37                     | 0.56              |
| 4:D:176:LEU:HD12 | 4:D:177:ASP:N    | 2.20                     | 0.56              |
| 6:F:47:ARG:NH1   | 6:F:48:LEU:O     | 2.37                     | 0.56              |
| 7:G:73:MET:HG3   | 7:G:90:GLU:HA    | 1.86                     | 0.56              |
| 1:A:269:C:H2'    | 1:A:270:A:C8     | 2.40                     | 0.56              |
| 1:A:485:G:O2'    | 1:A:486:U:P      | 2.63                     | 0.56              |
| 1:A:693:G:H2'    | 1:A:694:A:C8     | 2.41                     | 0.56              |
| 1:A:838:G:H1     | 1:A:848:C:H42    | 1.54                     | 0.56              |
| 9:I:50:LEU:HD23  | 9:I:55:ALA:HB3   | 1.87                     | 0.56              |
| 9:I:79:LEU:O     | 9:I:83:ARG:HG2   | 2.06                     | 0.56              |
| 6:F:80:ARG:NE    | 6:F:88:VAL:HB    | 2.20                     | 0.56              |
| 1:A:129:U:O3'    | 1:A:129(A):G:H3' | 2.05                     | 0.56              |
| 1:A:676:A:H1'    | 11:K:115:PRO:HB3 | 1.88                     | 0.56              |
| 2:B:208:ILE:HD12 | 2:B:208:ILE:H    | 1.71                     | 0.56              |
| 5:E:138:ALA:O    | 5:E:141:GLN:HB2  | 2.06                     | 0.56              |
| 6:F:75:LEU:HD13  | 6:F:79:LEU:HD11  | 1.86                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 15:O:33:THR:OG1   | 15:O:63:ARG:NH1    | 2.39                     | 0.56              |
| 16:P:74:LEU:O     | 16:P:77:ALA:HB3    | 2.06                     | 0.56              |
| 17:Q:19:VAL:HG22  | 17:Q:44:ALA:HB3    | 1.85                     | 0.56              |
| 1:A:277:C:H5'     | 17:Q:68:ARG:NH1    | 2.21                     | 0.56              |
| 1:A:254:G:H2'     | 1:A:255:G:C8       | 2.36                     | 0.56              |
| 1:A:40:C:H2'      | 1:A:41:G:O4'       | 2.06                     | 0.56              |
| 1:A:691:G:H2'     | 1:A:692:U:H6       | 1.71                     | 0.56              |
| 1:A:841:U:C6      | 1:A:848:C:H5'      | 2.41                     | 0.56              |
| 12:L:27:LEU:C     | 12:L:29:GLY:H      | 2.04                     | 0.56              |
| 2:B:118:LEU:O     | 2:B:121:LEU:HB3    | 2.06                     | 0.56              |
| 16:P:58:TYR:O     | 16:P:62:VAL:HG13   | 2.06                     | 0.56              |
| 20:T:74:LYS:HB2   | 20:T:76:ALA:H      | 1.69                     | 0.56              |
| 1:A:496:A:H4'     | 1:A:497:A:H5'      | 1.87                     | 0.55              |
| 1:A:680:C:H42     | 1:A:710:G:H1       | 1.55                     | 0.55              |
| 2:B:22:LYS:HE2    | 2:B:40:HIS:HE1     | 1.71                     | 0.55              |
| 4:D:82:ALA:HB1    | 4:D:92:VAL:HG13    | 1.87                     | 0.55              |
| 15:O:50:HIS:O     | 15:O:53:HIS:HB3    | 2.06                     | 0.55              |
| 1:A:1030(A):G:H2' | 1:A:1030(B):C:H5'' | 1.89                     | 0.55              |
| 1:A:1414:U:H2'    | 1:A:1415:G:C8      | 2.41                     | 0.55              |
| 1:A:141:A:H1'     | 1:A:182:U:O2       | 2.06                     | 0.55              |
| 1:A:1501:C:N4     | 1:A:1504:G:C2      | 2.73                     | 0.55              |
| 1:A:975:A:H5'     | 1:A:975:A:H8       | 1.71                     | 0.55              |
| 2:B:82:ARG:NH2    | 2:B:86:GLU:OE2     | 2.39                     | 0.55              |
| 2:B:9:GLU:HG2     | 2:B:10:LEU:H       | 1.70                     | 0.55              |
| 4:D:159:ARG:O     | 4:D:163:GLU:HB2    | 2.06                     | 0.55              |
| 18:R:36:ASN:OD1   | 18:R:39:VAL:HG12   | 2.06                     | 0.55              |
| 18:R:52:PRO:HG3   | 18:R:54:ARG:NH2    | 2.20                     | 0.55              |
| 1:A:1060:C:H5''   | 10:J:51:ARG:HG2    | 1.88                     | 0.55              |
| 1:A:553:A:O2'     | 12:L:29:GLY:O      | 2.23                     | 0.55              |
| 7:G:79:ARG:HA     | 7:G:84:ASN:HB3     | 1.88                     | 0.55              |
| 1:A:922:G:H1      | 1:A:1395:C:H42     | 1.53                     | 0.55              |
| 3:C:77:ILE:HD11   | 3:C:103:VAL:HG21   | 1.88                     | 0.55              |
| 10:J:49:VAL:HG13  | 14:N:41:ARG:HG3    | 1.88                     | 0.55              |
| 16:P:59:TRP:HB3   | 16:P:64:ALA:HB2    | 1.89                     | 0.55              |
| 1:A:1211:U:O2'    | 1:A:1213:A:N3      | 2.34                     | 0.55              |
| 3:C:36:ASP:HA     | 3:C:39:ILE:HD12    | 1.88                     | 0.55              |
| 9:I:79:LEU:HD22   | 9:I:83:ARG:NE      | 2.22                     | 0.55              |
| 1:A:1118:C:OP1    | 9:I:9:ARG:HD2      | 2.06                     | 0.55              |
| 12:L:75:HIS:HA    | 12:L:102:ARG:HH22  | 1.72                     | 0.55              |
| 18:R:51:LEU:HD22  | 18:R:52:PRO:HD2    | 1.88                     | 0.55              |
| 18:R:85:LEU:HD11  | 18:R:88:LYS:HG2    | 1.89                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 19:S:31:ILE:HA   | 19:S:32:LYS:HZ3   | 1.70                     | 0.55              |
| 19:S:7:LYS:O     | 19:S:7:LYS:HE2    | 2.06                     | 0.55              |
| 1:A:1040:U:O4    | 1:A:1041:A:N6     | 2.40                     | 0.55              |
| 1:A:1194:U:H4'   | 5:E:22:GLY:HA2    | 1.89                     | 0.55              |
| 6:F:75:LEU:O     | 6:F:79:LEU:HG     | 2.06                     | 0.55              |
| 1:A:106:C:O2'    | 1:A:107:G:H5'     | 2.07                     | 0.55              |
| 1:A:1275:A:H2'   | 1:A:1276:G:O4'    | 2.07                     | 0.55              |
| 1:A:1287:A:H2'   | 1:A:1288:A:C8     | 2.42                     | 0.55              |
| 4:D:12:CYS:HA    | 4:D:19:LEU:HG     | 1.89                     | 0.55              |
| 4:D:174:LEU:HD23 | 4:D:185:PHE:HA    | 1.89                     | 0.55              |
| 5:E:20:GLN:OE1   | 5:E:25:ARG:NH2    | 2.28                     | 0.55              |
| 5:E:27:ARG:HB2   | 5:E:27:ARG:NH1    | 2.22                     | 0.55              |
| 1:A:1089:G:C5    | 1:A:1090:U:C5     | 2.95                     | 0.55              |
| 1:A:1322:C:H4'   | 1:A:1323:G:OP1    | 2.06                     | 0.55              |
| 1:A:20:U:H1'     | 1:A:916:G:N2      | 2.22                     | 0.55              |
| 1:A:706:A:H1'    | 11:K:29:ILE:HD11  | 1.89                     | 0.55              |
| 3:C:95:THR:C     | 3:C:97:LYS:H      | 2.10                     | 0.55              |
| 4:D:4:TYR:OH     | 4:D:7:PRO:O       | 2.21                     | 0.55              |
| 7:G:26:PHE:HA    | 7:G:101:LEU:HD23  | 1.89                     | 0.55              |
| 9:I:28:VAL:HG12  | 9:I:29:ASN:HD22   | 1.72                     | 0.55              |
| 1:A:976:G:OP2    | 1:A:1358:U:O2'    | 2.24                     | 0.54              |
| 1:A:881:G:P      | 12:L:12:ARG:HH22  | 2.30                     | 0.54              |
| 15:O:15:PHE:HE2  | 15:O:84:LYS:HG2   | 1.72                     | 0.54              |
| 15:O:15:PHE:HD1  | 15:O:30:ALA:HB2   | 1.72                     | 0.54              |
| 1:A:325:A:H2'    | 1:A:326:G:O4'     | 2.07                     | 0.54              |
| 1:A:563:A:H2'    | 1:A:567:G:C8      | 2.42                     | 0.54              |
| 4:D:70:ILE:HG22  | 4:D:71:SER:N      | 2.21                     | 0.54              |
| 12:L:28:LYS:HD2  | 12:L:33:ARG:CZ    | 2.37                     | 0.54              |
| 12:L:93:LEU:HB3  | 12:L:96:VAL:HG21  | 1.88                     | 0.54              |
| 21:U:5:ASP:HB3   | 21:U:8:THR:HG23   | 1.90                     | 0.54              |
| 1:A:1443:G:C4'   | 1:A:1446:A:H5'    | 2.34                     | 0.54              |
| 4:D:100:ARG:HD2  | 4:D:137:SER:HA    | 1.90                     | 0.54              |
| 1:A:299:G:C6     | 1:A:300:A:C6      | 2.96                     | 0.54              |
| 4:D:70:ILE:HG22  | 4:D:71:SER:H      | 1.72                     | 0.54              |
| 2:B:79:ASP:OD2   | 2:B:79:ASP:N      | 2.31                     | 0.54              |
| 4:D:187:ARG:NH2  | 4:D:188:LEU:HD12  | 2.15                     | 0.54              |
| 4:D:196:LEU:N    | 4:D:196:LEU:HD23  | 2.22                     | 0.54              |
| 7:G:139:GLU:HG3  | 7:G:143:ARG:HH22  | 1.71                     | 0.54              |
| 9:I:96:LEU:HG    | 9:I:101:PHE:HD1   | 1.72                     | 0.54              |
| 19:S:40:ILE:HB   | 19:S:67:VAL:O     | 2.08                     | 0.54              |
| 1:A:1499:A:H1'   | 1:A:1520[B]:G:OP1 | 2.07                     | 0.54              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:375:U:C2     | 1:A:376:G:C8      | 2.96                     | 0.54              |
| 1:A:668:G:O4'    | 15:O:49:ASP:HB2   | 2.08                     | 0.54              |
| 2:B:71:VAL:O     | 2:B:164:VAL:HA    | 2.06                     | 0.54              |
| 5:E:93:PRO:HG2   | 8:H:105:ARG:NH1   | 2.22                     | 0.54              |
| 10:J:4:ILE:HB    | 10:J:74:ILE:HD11  | 1.90                     | 0.54              |
| 1:A:1286:A:H2'   | 1:A:1287:A:H4'    | 1.88                     | 0.54              |
| 1:A:560:U:H4'    | 1:A:561:U:H5''    | 1.88                     | 0.54              |
| 12:L:76:ASN:OD1  | 12:L:108:ALA:N    | 2.38                     | 0.54              |
| 13:M:11:ARG:HA   | 13:M:45:VAL:HG11  | 1.90                     | 0.54              |
| 1:A:216:G:O2'    | 1:A:217:C:O5'     | 2.26                     | 0.54              |
| 1:A:292:G:N2     | 1:A:309:G:C4      | 2.76                     | 0.54              |
| 1:A:620:C:H2'    | 1:A:621:A:O4'     | 2.08                     | 0.54              |
| 1:A:986:A:C2     | 1:A:1220:G:C2     | 2.96                     | 0.54              |
| 2:B:19:HIS:NE2   | 2:B:206:ASP:HB2   | 2.22                     | 0.54              |
| 16:P:6:LEU:HD23  | 16:P:17:TYR:CG    | 2.42                     | 0.54              |
| 1:A:1016:A:H2'   | 1:A:1017:G:O4'    | 2.07                     | 0.54              |
| 1:A:1496:C:O2    | 1:A:1517[A]:G:N2  | 2.41                     | 0.54              |
| 1:A:691:G:O2'    | 1:A:797:C:H4'     | 2.08                     | 0.54              |
| 1:A:81:U:H2'     | 1:A:82:U:H5''     | 1.89                     | 0.54              |
| 3:C:156:ARG:H    | 3:C:163:ALA:HA    | 1.73                     | 0.54              |
| 7:G:109:ASN:OD1  | 7:G:119:ARG:NH2   | 2.40                     | 0.54              |
| 13:M:91:ARG:NH2  | 13:M:103:THR:HG21 | 2.23                     | 0.54              |
| 21:U:6:ARG:HG2   | 21:U:15:ARG:HH21  | 1.73                     | 0.54              |
| 1:A:182:U:H5'    | 1:A:182:U:H6      | 1.72                     | 0.53              |
| 1:A:950:U:H2'    | 1:A:951:G:C8      | 2.43                     | 0.53              |
| 7:G:50:ILE:HD11  | 7:G:124:LEU:HD11  | 1.89                     | 0.53              |
| 10:J:84:GLN:HA   | 10:J:84:GLN:HE21  | 1.73                     | 0.53              |
| 1:A:356:A:H2'    | 1:A:357:G:O4'     | 2.09                     | 0.53              |
| 3:C:73:PRO:O     | 3:C:77:ILE:HG12   | 2.08                     | 0.53              |
| 5:E:137:GLU:O    | 5:E:141:GLN:HG2   | 2.08                     | 0.53              |
| 1:A:1465:C:H2'   | 1:A:1466:C:O4'    | 2.08                     | 0.53              |
| 3:C:68:VAL:HG12  | 3:C:70:VAL:HG22   | 1.91                     | 0.53              |
| 5:E:15:ARG:HG3   | 5:E:15:ARG:HH11   | 1.72                     | 0.53              |
| 10:J:76:ASN:N    | 10:J:77:PRO:HD3   | 2.22                     | 0.53              |
| 11:K:85:ARG:NE   | 11:K:111:ASP:HB3  | 2.21                     | 0.53              |
| 12:L:90:VAL:HG23 | 12:L:93:LEU:HB2   | 1.90                     | 0.53              |
| 13:M:2:ALA:O     | 13:M:10:PRO:HD2   | 2.09                     | 0.53              |
| 13:M:2:ALA:N     | 13:M:9:ILE:HG23   | 2.23                     | 0.53              |
| 1:A:1095:U:N3    | 1:A:1096:C:C4     | 2.77                     | 0.53              |
| 1:A:1361:G:H2'   | 1:A:1361(A):C:C6  | 2.43                     | 0.53              |
| 12:L:28:LYS:HB2  | 12:L:33:ARG:HE    | 1.74                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1190:G:H5'   | 3:C:176:HIS:NE2   | 2.24                     | 0.53              |
| 1:A:1202:G:N2    | 14:N:43:CYS:SG    | 2.81                     | 0.53              |
| 1:A:1425:U:H2'   | 1:A:1426:C:H6     | 1.74                     | 0.53              |
| 1:A:547:A:OP2    | 4:D:2:GLY:N       | 2.42                     | 0.53              |
| 4:D:152:SER:OG   | 4:D:152:SER:O     | 2.25                     | 0.53              |
| 4:D:36:ARG:HD2   | 4:D:38:TYR:HE2    | 1.71                     | 0.53              |
| 7:G:113:GLU:CG   | 7:G:119:ARG:HG2   | 2.38                     | 0.53              |
| 12:L:84:LEU:HD23 | 12:L:101:VAL:HG21 | 1.90                     | 0.53              |
| 1:A:147:G:C2     | 1:A:148:G:C8      | 2.96                     | 0.53              |
| 1:A:1502:A:H2    | 1:A:1505:G:H1     | 1.57                     | 0.53              |
| 1:A:44:G:H5''    | 1:A:44:G:H8       | 1.73                     | 0.53              |
| 8:H:23:SER:HA    | 8:H:63:LEU:HD13   | 1.89                     | 0.53              |
| 9:I:71:SER:O     | 9:I:74:ILE:HB     | 2.08                     | 0.53              |
| 10:J:79:ARG:O    | 10:J:82:ILE:N     | 2.42                     | 0.53              |
| 18:R:51:LEU:HD11 | 18:R:55:ARG:HH21  | 1.74                     | 0.53              |
| 20:T:33:ILE:HD11 | 20:T:63:ILE:HA    | 1.91                     | 0.53              |
| 1:A:1119:C:H42   | 1:A:1154:G:H1     | 1.55                     | 0.53              |
| 1:A:1163:C:H2'   | 1:A:1164:G:O4'    | 2.09                     | 0.53              |
| 1:A:258:G:H2'    | 1:A:259:G:H8      | 1.73                     | 0.53              |
| 1:A:514:C:H2'    | 1:A:515:G:C8      | 2.42                     | 0.53              |
| 4:D:127:THR:HG21 | 4:D:150:GLU:OE1   | 2.08                     | 0.53              |
| 5:E:43:LEU:HB2   | 5:E:136:MET:HG3   | 1.91                     | 0.53              |
| 5:E:27:ARG:HH11  | 5:E:27:ARG:HB2    | 1.74                     | 0.53              |
| 16:P:6:LEU:HB3   | 16:P:17:TYR:CD2   | 2.44                     | 0.53              |
| 1:A:658:G:H2'    | 1:A:659:U:O4'     | 2.08                     | 0.53              |
| 1:A:734:G:N2     | 18:R:75:ILE:HD11  | 2.23                     | 0.53              |
| 1:A:770:C:O2'    | 1:A:899:C:N3      | 2.39                     | 0.53              |
| 1:A:965:A:C2     | 1:A:969:A:C2      | 2.96                     | 0.53              |
| 2:B:84:GLU:O     | 2:B:219:VAL:HG21  | 2.09                     | 0.53              |
| 13:M:62:ASN:OD1  | 13:M:62:ASN:N     | 2.41                     | 0.53              |
| 1:A:130:A:H1'    | 1:A:263:A:O2'     | 2.09                     | 0.53              |
| 1:A:375:U:H2'    | 1:A:376:G:H8      | 1.74                     | 0.53              |
| 1:A:671:G:C2     | 1:A:672:U:H1'     | 2.44                     | 0.53              |
| 1:A:778:G:H8     | 1:A:778:G:O5'     | 1.91                     | 0.53              |
| 5:E:144:THR:HB   | 5:E:147:ASP:H     | 1.74                     | 0.53              |
| 5:E:40:ARG:HH21  | 5:E:66:MET:HG3    | 1.73                     | 0.53              |
| 9:I:17:VAL:HG21  | 9:I:80:GLY:HA3    | 1.91                     | 0.53              |
| 12:L:25:PRO:C    | 12:L:27:LEU:N     | 2.61                     | 0.53              |
| 20:T:20:LEU:HD22 | 20:T:20:LEU:H     | 1.73                     | 0.53              |
| 1:A:1241:G:H2'   | 1:A:1242:C:H6     | 1.73                     | 0.53              |
| 5:E:103:GLY:O    | 5:E:106:PRO:HD2   | 2.09                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:276:G:O2'    | 17:Q:68:ARG:NH1  | 2.42                     | 0.53              |
| 1:A:123:C:OP1    | 1:A:311:C:O2'    | 2.25                     | 0.52              |
| 1:A:569:C:H42    | 1:A:881:G:H1     | 1.55                     | 0.52              |
| 4:D:187:ARG:HH22 | 4:D:188:LEU:CD1  | 2.17                     | 0.52              |
| 5:E:150:ARG:NH1  | 5:E:150:ARG:HB2  | 2.25                     | 0.52              |
| 6:F:30:LEU:HD23  | 6:F:35:ALA:HB3   | 1.90                     | 0.52              |
| 12:L:84:LEU:HB3  | 12:L:101:VAL:CG2 | 2.39                     | 0.52              |
| 13:M:108:ARG:O   | 13:M:111:LYS:N   | 2.42                     | 0.52              |
| 1:A:1144:G:H2'   | 1:A:1145:C:C6    | 2.44                     | 0.52              |
| 1:A:414:A:H3'    | 24:A:1969:HOH:O  | 2.10                     | 0.52              |
| 1:A:881:G:H2'    | 1:A:882:C:O4'    | 2.09                     | 0.52              |
| 1:A:975:A:H5'    | 1:A:975:A:C8     | 2.43                     | 0.52              |
| 5:E:144:THR:HG22 | 5:E:146:ALA:H    | 1.74                     | 0.52              |
| 9:I:48:GLU:N     | 9:I:49:PRO:HD2   | 2.24                     | 0.52              |
| 10:J:34:VAL:HG13 | 10:J:74:ILE:HG22 | 1.90                     | 0.52              |
| 20:T:53:LEU:HD12 | 20:T:101:GLY:H   | 1.74                     | 0.52              |
| 1:A:1491:G:C6    | 1:A:1493:A:C2    | 2.98                     | 0.52              |
| 7:G:99:LEU:O     | 7:G:103:TRP:HB2  | 2.10                     | 0.52              |
| 10:J:65:LEU:HD12 | 14:N:56:VAL:HG22 | 1.91                     | 0.52              |
| 17:Q:97:SER:O    | 17:Q:98:LEU:HD12 | 2.09                     | 0.52              |
| 1:A:254:G:OP1    | 17:Q:67:LYS:O    | 2.27                     | 0.52              |
| 2:B:60:ASP:O     | 2:B:64:ARG:HG3   | 2.10                     | 0.52              |
| 21:U:10:ARG:HA   | 21:U:13:ILE:HD12 | 1.92                     | 0.52              |
| 1:A:1031:G:O2'   | 1:A:1032:G:N2    | 2.43                     | 0.52              |
| 1:A:1476:G:C2'   | 1:A:1477:C:H5'   | 2.39                     | 0.52              |
| 1:A:279:A:OP2    | 17:Q:95:TYR:OH   | 2.17                     | 0.52              |
| 1:A:946:A:H2'    | 1:A:947:G:C8     | 2.45                     | 0.52              |
| 2:B:93:VAL:HG21  | 2:B:97:TRP:CD1   | 2.44                     | 0.52              |
| 4:D:142:PRO:HA   | 4:D:185:PHE:HD2  | 1.74                     | 0.52              |
| 9:I:18:PHE:HB3   | 9:I:20:ARG:HH12  | 1.74                     | 0.52              |
| 1:A:1148:U:H2'   | 1:A:1149:C:O4'   | 2.10                     | 0.52              |
| 1:A:1313:U:H5    | 19:S:4:SER:HB2   | 1.74                     | 0.52              |
| 1:A:926:G:C6     | 1:A:1505:G:C6    | 2.97                     | 0.52              |
| 2:B:47:THR:O     | 2:B:51:LEU:HB2   | 2.10                     | 0.52              |
| 6:F:47:ARG:HB2   | 6:F:47:ARG:CZ    | 2.33                     | 0.52              |
| 16:P:58:TYR:CZ   | 16:P:62:VAL:HG11 | 2.45                     | 0.52              |
| 1:A:474:G:O2'    | 1:A:475:G:H5'    | 2.09                     | 0.52              |
| 1:A:562:C:H4'    | 1:A:563:A:C5'    | 2.40                     | 0.52              |
| 1:A:78:G:C2      | 1:A:79:G:C8      | 2.97                     | 0.52              |
| 1:A:877:C:O2     | 8:H:3:THR:HG21   | 2.09                     | 0.52              |
| 17:Q:34:LYS:HG2  | 17:Q:35:VAL:H    | 1.74                     | 0.52              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 18:R:58:LEU:HB3     | 18:R:62:GLU:HB3     | 1.91                     | 0.52              |
| 1:A:1313:U:OP2      | 19:S:6:LYS:HA       | 2.09                     | 0.52              |
| 1:A:1451:A:H5''     | 1:A:1452:C:C5       | 2.45                     | 0.52              |
| 1:A:1483:A:H2'      | 1:A:1483:A:N3       | 2.23                     | 0.52              |
| 1:A:1518[B]:MA6:O2' | 1:A:1519[B]:MA6:OP1 | 2.27                     | 0.52              |
| 1:A:164:U:H2'       | 1:A:165:C:C6        | 2.44                     | 0.52              |
| 1:A:563:A:H5'       | 1:A:564:C:OP1       | 2.09                     | 0.52              |
| 5:E:40:ARG:HE       | 5:E:66:MET:HE2      | 1.75                     | 0.52              |
| 7:G:41:ARG:HH11     | 7:G:41:ARG:HB2      | 1.74                     | 0.52              |
| 12:L:6:THR:HG23     | 12:L:9:GLN:OE1      | 2.09                     | 0.52              |
| 15:O:72:ARG:HB3     | 15:O:72:ARG:NH1     | 2.25                     | 0.52              |
| 1:A:1234:C:H2'      | 1:A:1235:U:H6       | 1.74                     | 0.52              |
| 1:A:1324:A:H2'      | 1:A:1325:C:O4'      | 2.09                     | 0.52              |
| 1:A:143:A:O3'       | 1:A:144:G:H8        | 1.93                     | 0.52              |
| 1:A:924:C:O2'       | 1:A:1502:A:N6       | 2.43                     | 0.52              |
| 2:B:189:ASP:HB2     | 2:B:205:ASP:H       | 1.75                     | 0.52              |
| 1:A:1192:C:OP2      | 3:C:4:LYS:NZ        | 2.42                     | 0.52              |
| 1:A:1124:G:OP1      | 10:J:33:GLN:NE2     | 2.43                     | 0.52              |
| 14:N:33:VAL:HA      | 14:N:39:LEU:O       | 2.10                     | 0.52              |
| 1:A:1277:C:C6       | 1:A:1277:C:H3'      | 2.44                     | 0.52              |
| 1:A:1342:C:H2'      | 1:A:1343:G:H8       | 1.75                     | 0.52              |
| 1:A:474:G:OP2       | 16:P:75:ARG:HD2     | 2.10                     | 0.52              |
| 5:E:43:LEU:O        | 5:E:62:ALA:HA       | 2.10                     | 0.52              |
| 7:G:99:LEU:HD22     | 7:G:103:TRP:CH2     | 2.45                     | 0.52              |
| 14:N:26:ARG:HH22    | 14:N:47:LEU:HD13    | 1.74                     | 0.52              |
| 18:R:36:ASN:O       | 18:R:40:LEU:HG      | 2.10                     | 0.52              |
| 19:S:18:LYS:O       | 19:S:22:LEU:HG      | 2.10                     | 0.52              |
| 1:A:17:U:H2'        | 1:A:18:C:H6         | 1.73                     | 0.51              |
| 1:A:924:C:O2'       | 1:A:925:G:H5'       | 2.09                     | 0.51              |
| 6:F:69:GLU:O        | 6:F:72:VAL:HG23     | 2.10                     | 0.51              |
| 5:E:78:HIS:HB2      | 8:H:104:ARG:HG2     | 1.91                     | 0.51              |
| 12:L:25:PRO:HB2     | 12:L:64:TYR:CE2     | 2.45                     | 0.51              |
| 1:A:1023:G:H3'      | 1:A:1024:G:H5''     | 1.91                     | 0.51              |
| 1:A:1134:G:H1       | 1:A:1140:C:H42      | 1.57                     | 0.51              |
| 1:A:1321:C:C5'      | 1:A:1322:C:H5''     | 2.39                     | 0.51              |
| 1:A:671:G:N2        | 1:A:672:U:H1'       | 2.25                     | 0.51              |
| 1:A:814:A:N7        | 1:A:816:A:C4        | 2.79                     | 0.51              |
| 1:A:830:G:C6        | 1:A:831:U:C4        | 2.98                     | 0.51              |
| 2:B:97:TRP:CH2      | 2:B:173:ALA:HA      | 2.46                     | 0.51              |
| 10:J:85:LEU:HA      | 10:J:88:LEU:HD11    | 1.92                     | 0.51              |
| 11:K:57:THR:HB      | 11:K:60:ALA:H       | 1.76                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 14:N:14:PRO:O    | 14:N:15:LYS:HB3   | 2.09                     | 0.51              |
| 1:A:279:A:C6     | 17:Q:98:LEU:HD13  | 2.45                     | 0.51              |
| 19:S:31:ILE:HG22 | 19:S:49:ILE:HA    | 1.92                     | 0.51              |
| 1:A:1005:A:H1'   | 1:A:1026:G:H1     | 1.75                     | 0.51              |
| 1:A:168:G:C2     | 1:A:169:C:C5      | 2.98                     | 0.51              |
| 1:A:39:G:O2'     | 1:A:40:C:H5'      | 2.10                     | 0.51              |
| 1:A:547:A:H4'    | 1:A:548:G:O5'     | 2.09                     | 0.51              |
| 1:A:667:G:C2     | 1:A:740:U:O2      | 2.63                     | 0.51              |
| 1:A:839:U:O2     | 1:A:839:U:H3'     | 2.11                     | 0.51              |
| 2:B:105:PHE:CE1  | 2:B:109:SER:HB3   | 2.45                     | 0.51              |
| 1:A:1323:G:H2'   | 1:A:1324:A:C8     | 2.45                     | 0.51              |
| 1:A:1366:C:O3'   | 10:J:60:ARG:NH2   | 2.42                     | 0.51              |
| 1:A:1403:C:C2    | 1:A:1404:5MC:HM52 | 2.45                     | 0.51              |
| 1:A:181:G:H4'    | 1:A:182:U:C5'     | 2.41                     | 0.51              |
| 12:L:110:VAL:O   | 12:L:122:THR:HG21 | 2.11                     | 0.51              |
| 19:S:11:VAL:HG12 | 19:S:15:LEU:HD21  | 1.92                     | 0.51              |
| 20:T:43:LEU:HA   | 20:T:46:GLU:HB2   | 1.93                     | 0.51              |
| 1:A:1169:A:C5    | 1:A:1171:G:H1'    | 2.45                     | 0.51              |
| 1:A:1216:G:H5''  | 14:N:5:ALA:CB     | 2.40                     | 0.51              |
| 1:A:1493:A:HO2'  | 1:A:1494:G:H8     | 1.58                     | 0.51              |
| 1:A:734:G:H21    | 18:R:75:ILE:HD11  | 1.76                     | 0.51              |
| 1:A:951:G:OP2    | 13:M:102:ARG:NH2  | 2.44                     | 0.51              |
| 1:A:956:U:H2'    | 1:A:957:U:O4'     | 2.11                     | 0.51              |
| 8:H:86:ILE:HG22  | 8:H:93:VAL:HG21   | 1.92                     | 0.51              |
| 13:M:10:PRO:O    | 13:M:45:VAL:HG21  | 2.11                     | 0.51              |
| 18:R:47:THR:HB   | 18:R:83:GLU:O     | 2.10                     | 0.51              |
| 1:A:708:C:H2'    | 1:A:709:G:H8      | 1.76                     | 0.51              |
| 1:A:781:A:H2'    | 1:A:782:A:H5'     | 1.92                     | 0.51              |
| 10:J:50:ILE:H    | 10:J:50:ILE:HD12  | 1.76                     | 0.51              |
| 10:J:55:LYS:HG2  | 10:J:56:HIS:N     | 2.22                     | 0.51              |
| 18:R:61:LYS:O    | 18:R:65:ILE:HG12  | 2.09                     | 0.51              |
| 19:S:50:ALA:HB1  | 19:S:57:HIS:HB3   | 1.92                     | 0.51              |
| 20:T:43:LEU:HB2  | 20:T:52:ALA:HB2   | 1.93                     | 0.51              |
| 1:A:143:A:H2     | 1:A:220:G:H22     | 1.58                     | 0.51              |
| 2:B:160:ASP:N    | 2:B:160:ASP:OD2   | 2.37                     | 0.51              |
| 2:B:22:LYS:HE2   | 2:B:40:HIS:CE1    | 2.46                     | 0.51              |
| 4:D:145:GLU:OE2  | 4:D:182:LYS:NZ    | 2.43                     | 0.51              |
| 1:A:8:A:N6       | 4:D:209:ARG:HB2   | 2.26                     | 0.51              |
| 1:A:825:G:H21    | 8:H:11:THR:HG21   | 1.76                     | 0.51              |
| 1:A:1403:C:H2'   | 1:A:1403:C:O2     | 2.11                     | 0.51              |
| 1:A:710:G:H2'    | 1:A:711:G:H8      | 1.75                     | 0.51              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:860:A:H2'     | 1:A:861:G:O4'    | 2.10                     | 0.51              |
| 2:B:53:ARG:HG3    | 2:B:54:THR:N     | 2.25                     | 0.51              |
| 1:A:1057:G:H5''   | 3:C:154:SER:HB2  | 1.93                     | 0.51              |
| 4:D:57:ARG:HB3    | 4:D:206:PHE:HB2  | 1.91                     | 0.51              |
| 1:A:546:G:P       | 4:D:72:GLU:HB3   | 2.51                     | 0.51              |
| 5:E:131:ILE:O     | 5:E:134:ALA:HB3  | 2.11                     | 0.51              |
| 8:H:73:ASP:OD2    | 8:H:75:ARG:HG3   | 2.11                     | 0.51              |
| 1:A:439:A:C4      | 1:A:497:A:C2     | 2.99                     | 0.51              |
| 2:B:17:PHE:CD1    | 2:B:18:GLY:N     | 2.77                     | 0.51              |
| 3:C:159:GLY:HA2   | 3:C:193:TYR:CD1  | 2.46                     | 0.51              |
| 17:Q:89:LEU:O     | 17:Q:93:GLN:HG3  | 2.11                     | 0.51              |
| 1:A:1070:U:H2'    | 1:A:1071:C:C6    | 2.46                     | 0.51              |
| 1:A:1064:G:H1'    | 1:A:1190:G:N2    | 2.25                     | 0.51              |
| 1:A:748:C:O5'     | 1:A:748:C:H6     | 1.93                     | 0.51              |
| 1:A:858:G:O6      | 1:A:869:G:H3'    | 2.10                     | 0.51              |
| 4:D:156:GLU:O     | 4:D:160:GLN:HG3  | 2.10                     | 0.51              |
| 5:E:101:ILE:O     | 5:E:120:THR:HB   | 2.11                     | 0.51              |
| 10:J:19:SER:HB2   | 10:J:91:PRO:HG2  | 1.93                     | 0.51              |
| 16:P:48:TRP:CD1   | 16:P:48:TRP:N    | 2.79                     | 0.51              |
| 1:A:1313:U:C5     | 19:S:4:SER:HB2   | 2.46                     | 0.51              |
| 20:T:93:GLU:OE2   | 20:T:93:GLU:N    | 2.44                     | 0.51              |
| 1:A:1299:A:C8     | 1:A:1301:U:H1'   | 2.46                     | 0.50              |
| 1:A:1238:A:OP2    | 1:A:1335:C:O2    | 2.29                     | 0.50              |
| 1:A:1372:U:OP2    | 9:I:11:LYS:NZ    | 2.35                     | 0.50              |
| 2:B:105:PHE:O     | 2:B:108:ILE:N    | 2.44                     | 0.50              |
| 8:H:27:PRO:HG3    | 8:H:58:TYR:CE2   | 2.46                     | 0.50              |
| 1:A:1133:G:H1     | 1:A:1141:C:H42   | 1.59                     | 0.50              |
| 1:A:1189:C:H5'    | 14:N:58:LYS:HZ1  | 1.77                     | 0.50              |
| 3:C:130:VAL:HG11  | 3:C:153:VAL:HG11 | 1.93                     | 0.50              |
| 12:L:113:ARG:HH11 | 12:L:116:SER:H   | 1.58                     | 0.50              |
| 19:S:41:VAL:HG23  | 19:S:43:GLU:HG2  | 1.92                     | 0.50              |
| 1:A:1029:C:N3     | 1:A:1030:C:N4    | 2.55                     | 0.50              |
| 1:A:1122:U:O2'    | 1:A:1123:A:H5'   | 2.11                     | 0.50              |
| 1:A:116:A:O5'     | 1:A:116:A:H8     | 1.94                     | 0.50              |
| 1:A:1223:C:H3'    | 1:A:1224:G:H5''  | 1.92                     | 0.50              |
| 1:A:235:C:O2'     | 1:A:236:G:H5'    | 2.11                     | 0.50              |
| 3:C:150:LYS:HA    | 3:C:169:ALA:HA   | 1.94                     | 0.50              |
| 10:J:16:LEU:HD22  | 10:J:94:VAL:HG23 | 1.93                     | 0.50              |
| 13:M:14:ARG:HB2   | 13:M:17:VAL:HG22 | 1.92                     | 0.50              |
| 1:A:1001:A:H61    | 1:A:1039:C:N4    | 2.06                     | 0.50              |
| 1:A:1238:A:N7     | 1:A:1303:C:H1'   | 2.26                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1426:C:H2'   | 1:A:1427:U:C6    | 2.46                     | 0.50              |
| 1:A:836:G:C6     | 1:A:851:G:C6     | 3.00                     | 0.50              |
| 4:D:12:CYS:SG    | 4:D:21:LEU:HD11  | 2.51                     | 0.50              |
| 8:H:51:VAL:HG22  | 8:H:52:ASP:H     | 1.76                     | 0.50              |
| 19:S:31:ILE:HG21 | 19:S:49:ILE:HD12 | 1.93                     | 0.50              |
| 1:A:1194:U:H2'   | 1:A:1195:C:C6    | 2.46                     | 0.50              |
| 1:A:1504:G:H4'   | 1:A:1505:G:O5'   | 2.11                     | 0.50              |
| 1:A:512:U:H2'    | 1:A:513:C:H6     | 1.76                     | 0.50              |
| 1:A:665:A:H1'    | 1:A:733:A:O4'    | 2.12                     | 0.50              |
| 1:A:811:C:H4'    | 1:A:900:A:H61    | 1.76                     | 0.50              |
| 3:C:7:PRO:O      | 3:C:11:ARG:HD2   | 2.11                     | 0.50              |
| 3:C:139:GLN:HG3  | 3:C:143:GLU:OE1  | 2.10                     | 0.50              |
| 3:C:85:ARG:HH11  | 3:C:86:VAL:HG23  | 1.77                     | 0.50              |
| 11:K:11:LYS:NZ   | 11:K:11:LYS:HB2  | 2.27                     | 0.50              |
| 16:P:9:PHE:HD1   | 16:P:18:ARG:HD2  | 1.72                     | 0.50              |
| 18:R:19:LYS:O    | 18:R:21:LYS:NZ   | 2.45                     | 0.50              |
| 1:A:1221:G:H4'   | 19:S:77:THR:HG21 | 1.93                     | 0.50              |
| 1:A:774:G:C4     | 1:A:775:G:C8     | 2.99                     | 0.50              |
| 1:A:804:U:H5''   | 1:A:805:C:OP2    | 2.11                     | 0.50              |
| 3:C:184:TYR:OH   | 3:C:199:LYS:HD3  | 2.11                     | 0.50              |
| 16:P:51:VAL:HG11 | 16:P:77:ALA:HB1  | 1.93                     | 0.50              |
| 1:A:134:A:H2'    | 1:A:135:C:O4'    | 2.12                     | 0.50              |
| 1:A:1451:A:H5''  | 1:A:1452:C:H5    | 1.77                     | 0.50              |
| 1:A:227:G:O2'    | 24:A:1959:HOH:O  | 2.20                     | 0.50              |
| 1:A:310:G:H2'    | 1:A:311:C:C6     | 2.43                     | 0.50              |
| 4:D:163:GLU:OE1  | 4:D:166:LYS:HE2  | 2.11                     | 0.50              |
| 1:A:1073:U:P     | 5:E:57:LYS:HZ1   | 2.34                     | 0.50              |
| 6:F:33:TYR:CD2   | 6:F:71:ARG:HD2   | 2.46                     | 0.50              |
| 9:I:22:GLY:HA3   | 9:I:60:ASP:N     | 2.26                     | 0.50              |
| 9:I:79:LEU:HD22  | 9:I:83:ARG:HE    | 1.77                     | 0.50              |
| 12:L:19:ARG:NE   | 12:L:19:ARG:H    | 2.09                     | 0.50              |
| 12:L:6:THR:O     | 12:L:9:GLN:HB2   | 2.12                     | 0.50              |
| 16:P:58:TYR:CE2  | 16:P:62:VAL:HG11 | 2.46                     | 0.50              |
| 17:Q:83:ASP:OD2  | 17:Q:84:LEU:HG   | 2.12                     | 0.50              |
| 1:A:179:A:H2'    | 1:A:180:U:C6     | 2.47                     | 0.50              |
| 1:A:350:G:H5''   | 1:A:350:G:H8     | 1.77                     | 0.50              |
| 1:A:410:G:C2     | 1:A:429:U:C2     | 3.00                     | 0.50              |
| 1:A:681:C:N4     | 1:A:682:G:O6     | 2.45                     | 0.50              |
| 2:B:204:ASN:HB3  | 2:B:206:ASP:O    | 2.12                     | 0.50              |
| 4:D:172:PRO:HD2  | 4:D:173:TRP:CE3  | 2.47                     | 0.50              |
| 6:F:39:LYS:HD3   | 6:F:40:VAL:H     | 1.77                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1349:A:H1'   | 1:A:1374:A:N6    | 2.27                     | 0.50              |
| 1:A:1410:G:H2'   | 1:A:1411:C:C6    | 2.46                     | 0.50              |
| 1:A:138:G:C2     | 1:A:226:G:N3     | 2.80                     | 0.50              |
| 1:A:736:C:H2'    | 1:A:737:A:C8     | 2.46                     | 0.50              |
| 5:E:99:GLY:O     | 5:E:101:ILE:HG13 | 2.11                     | 0.50              |
| 9:I:124:GLN:HG3  | 9:I:125:TYR:N    | 2.26                     | 0.50              |
| 9:I:50:LEU:H     | 9:I:50:LEU:HD12  | 1.77                     | 0.50              |
| 18:R:74:ARG:HB3  | 18:R:81:PHE:CE2  | 2.46                     | 0.50              |
| 1:A:1502:A:H2    | 1:A:1505:G:H22   | 1.54                     | 0.49              |
| 1:A:259:G:H2'    | 1:A:260:G:O4'    | 2.12                     | 0.49              |
| 6:F:82:ARG:HB2   | 6:F:85:VAL:HG23  | 1.93                     | 0.49              |
| 9:I:81:ILE:HG22  | 9:I:85:LEU:HD22  | 1.94                     | 0.49              |
| 1:A:1133:G:H1    | 1:A:1141:C:N4    | 2.10                     | 0.49              |
| 1:A:1352:C:H2'   | 1:A:1353:G:C8    | 2.47                     | 0.49              |
| 1:A:763:G:H2'    | 1:A:764:C:H6     | 1.77                     | 0.49              |
| 1:A:966:M2G:HM22 | 1:A:967:5MC:O2   | 2.12                     | 0.49              |
| 1:A:975:A:N6     | 1:A:1366:C:O2'   | 2.41                     | 0.49              |
| 12:L:35:GLY:HA3  | 12:L:59:ARG:O    | 2.12                     | 0.49              |
| 17:Q:26:GLN:HA   | 17:Q:36:ILE:O    | 2.13                     | 0.49              |
| 1:A:346:G:H2'    | 1:A:347:G:O4'    | 2.13                     | 0.49              |
| 1:A:727:G:N2     | 1:A:730:G:OP2    | 2.45                     | 0.49              |
| 2:B:146:GLN:O    | 2:B:150:SER:HB2  | 2.11                     | 0.49              |
| 13:M:11:ARG:HD2  | 13:M:45:VAL:HG11 | 1.94                     | 0.49              |
| 1:A:278:G:C6     | 17:Q:95:TYR:CD2  | 3.00                     | 0.49              |
| 1:A:1095:U:C4    | 1:A:1096:C:N4    | 2.80                     | 0.49              |
| 1:A:1400:5MC:H3' | 1:A:1401:G:H5'   | 1.93                     | 0.49              |
| 1:A:260:G:H2'    | 1:A:261:U:C6     | 2.47                     | 0.49              |
| 12:L:66:VAL:HG21 | 12:L:98:TYR:HE1  | 1.75                     | 0.49              |
| 13:M:34:LEU:HD13 | 13:M:41:PRO:HA   | 1.94                     | 0.49              |
| 15:O:18:PHE:N    | 15:O:18:PHE:CD2  | 2.80                     | 0.49              |
| 20:T:57:ARG:HH22 | 20:T:100:ILE:CD1 | 2.25                     | 0.49              |
| 1:A:1112:C:O2    | 3:C:179:ARG:HB2  | 2.13                     | 0.49              |
| 1:A:191:G:O2'    | 20:T:101:GLY:O   | 2.30                     | 0.49              |
| 1:A:270:A:H2'    | 1:A:271:C:O4'    | 2.13                     | 0.49              |
| 1:A:767:A:H2'    | 1:A:768:A:O4'    | 2.13                     | 0.49              |
| 1:A:1112:C:N3    | 3:C:178:LEU:HD12 | 2.27                     | 0.49              |
| 3:C:116:VAL:HG21 | 3:C:202:ILE:HD11 | 1.94                     | 0.49              |
| 4:D:31:CYS:O     | 4:D:31:CYS:SG    | 2.71                     | 0.49              |
| 5:E:15:ARG:HG3   | 5:E:15:ARG:NH1   | 2.27                     | 0.49              |
| 10:J:3:LYS:HB3   | 10:J:3:LYS:NZ    | 2.27                     | 0.49              |
| 15:O:18:PHE:N    | 15:O:18:PHE:HD2  | 2.11                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:927:G:O2'    | 1:A:1503:A:N7     | 2.44                     | 0.49              |
| 1:A:460:A:O2'    | 1:A:461:C:H5'     | 2.13                     | 0.49              |
| 1:A:522:C:OP2    | 12:L:69:TYR:OH    | 2.24                     | 0.49              |
| 1:A:62:U:C2      | 1:A:63:C:C5       | 3.01                     | 0.49              |
| 3:C:150:LYS:HG3  | 3:C:169:ALA:HB2   | 1.93                     | 0.49              |
| 4:D:173:TRP:O    | 4:D:186:LEU:HD23  | 2.13                     | 0.49              |
| 5:E:76:ILE:N     | 5:E:76:ILE:HD13   | 2.27                     | 0.49              |
| 3:C:67:THR:HA    | 3:C:102:ASN:OD1   | 2.13                     | 0.49              |
| 5:E:14:ARG:O     | 5:E:28:PHE:HD2    | 1.95                     | 0.49              |
| 9:I:118:LYS:C    | 9:I:120:ARG:H     | 2.16                     | 0.49              |
| 10:J:15:THR:O    | 10:J:19:SER:HB3   | 2.13                     | 0.49              |
| 10:J:61:GLU:OE1  | 14:N:58:LYS:HD2   | 2.13                     | 0.49              |
| 11:K:48:ILE:HD13 | 11:K:63:LEU:HB2   | 1.93                     | 0.49              |
| 13:M:10:PRO:HB2  | 13:M:18:ALA:HB1   | 1.95                     | 0.49              |
| 13:M:50:GLU:HG3  | 13:M:53:VAL:HB    | 1.93                     | 0.49              |
| 19:S:11:VAL:HG13 | 19:S:38:SER:HB3   | 1.95                     | 0.49              |
| 1:A:933:G:N2     | 1:A:1384:C:O2     | 2.40                     | 0.49              |
| 1:A:1442:G:N1    | 1:A:1446:A:N6     | 2.60                     | 0.49              |
| 1:A:680:C:N3     | 1:A:710:G:N2      | 2.46                     | 0.49              |
| 1:A:718:G:O6     | 18:R:74:ARG:NH1   | 2.46                     | 0.49              |
| 1:A:770:C:N4     | 24:A:1934:HOH:O   | 2.18                     | 0.49              |
| 11:K:80:VAL:HG22 | 11:K:103:LEU:HD22 | 1.93                     | 0.49              |
| 20:T:16:HIS:O    | 20:T:20:LEU:HD22  | 2.13                     | 0.49              |
| 1:A:106:C:C2'    | 1:A:107:G:H5'     | 2.43                     | 0.49              |
| 1:A:1505:G:H5'   | 24:A:1809:HOH:O   | 2.12                     | 0.49              |
| 1:A:116:A:H61    | 1:A:313:A:H1'     | 1.77                     | 0.49              |
| 1:A:432:A:H2'    | 1:A:433:C:O4'     | 2.13                     | 0.49              |
| 13:M:19:LEU:HD11 | 13:M:56:LEU:HD11  | 1.94                     | 0.49              |
| 1:A:1345:U:C4    | 1:A:1377:A:C2     | 3.01                     | 0.49              |
| 1:A:642:A:H2'    | 1:A:643:C:C6      | 2.48                     | 0.49              |
| 1:A:725:G:C5     | 1:A:726:C:C5      | 3.01                     | 0.49              |
| 1:A:939:G:C6     | 1:A:940:C:N4      | 2.81                     | 0.49              |
| 5:E:92:LYS:HB3   | 5:E:119:LEU:HB2   | 1.94                     | 0.49              |
| 8:H:116:LYS:CG   | 8:H:127:LEU:HD11  | 2.43                     | 0.49              |
| 14:N:35:ARG:HH11 | 14:N:35:ARG:HG2   | 1.77                     | 0.49              |
| 16:P:53:VAL:HG23 | 16:P:54:GLU:H     | 1.77                     | 0.49              |
| 17:Q:5:VAL:HB    | 17:Q:60:ILE:CD1   | 2.43                     | 0.49              |
| 18:R:29:PHE:HZ   | 18:R:43:PHE:CE1   | 2.30                     | 0.49              |
| 18:R:46:GLU:OE2  | 18:R:46:GLU:N     | 2.37                     | 0.49              |
| 1:A:350:G:O2'    | 1:A:351:G:H5'     | 2.13                     | 0.48              |
| 1:A:358:U:H2'    | 1:A:359:U:H6      | 1.78                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:642:A:N7     | 8:H:115:SER:HA    | 2.28                     | 0.48              |
| 3:C:164:ARG:HG2  | 3:C:165:THR:N     | 2.27                     | 0.48              |
| 13:M:91:ARG:HH21 | 13:M:103:THR:HG21 | 1.77                     | 0.48              |
| 1:A:7:G:C5       | 1:A:298:A:C2      | 3.01                     | 0.48              |
| 3:C:121:ALA:O    | 3:C:124:ILE:HB    | 2.13                     | 0.48              |
| 6:F:30:LEU:HD21  | 6:F:65:VAL:HG11   | 1.95                     | 0.48              |
| 7:G:69:VAL:HG11  | 7:G:134:ALA:HB1   | 1.95                     | 0.48              |
| 7:G:78:ARG:NH1   | 7:G:154:TYR:O     | 2.46                     | 0.48              |
| 10:J:13:HIS:CD2  | 10:J:14:LYS:N     | 2.80                     | 0.48              |
| 17:Q:40:LYS:HD3  | 17:Q:42:TYR:CZ    | 2.48                     | 0.48              |
| 1:A:1461:G:H2'   | 1:A:1462:G:H8     | 1.77                     | 0.48              |
| 1:A:291:C:H2'    | 1:A:291:C:O2      | 2.12                     | 0.48              |
| 1:A:730:G:N2     | 1:A:765:G:H5''    | 2.27                     | 0.48              |
| 1:A:826:C:H2'    | 1:A:827:U:H6      | 1.78                     | 0.48              |
| 2:B:76:GLN:NE2   | 2:B:206:ASP:HB3   | 2.27                     | 0.48              |
| 5:E:51:VAL:N     | 5:E:52:PRO:HD2    | 2.28                     | 0.48              |
| 13:M:87:TYR:HA   | 13:M:90:LEU:HD22  | 1.95                     | 0.48              |
| 6:F:99:ALA:HB2   | 18:R:31:LEU:HG    | 1.94                     | 0.48              |
| 1:A:1118:C:OP1   | 9:I:104:ARG:NE    | 2.45                     | 0.48              |
| 1:A:1378:C:N4    | 1:A:1379:G:N3     | 2.62                     | 0.48              |
| 1:A:1378:C:C5    | 1:A:1379:G:C8     | 3.02                     | 0.48              |
| 1:A:1481:U:H2'   | 1:A:1482:G:H8     | 1.76                     | 0.48              |
| 2:B:69:LEU:HB3   | 2:B:162:ILE:HD11  | 1.95                     | 0.48              |
| 3:C:147:LYS:NZ   | 3:C:172:ARG:HE    | 2.10                     | 0.48              |
| 5:E:121:LYS:HG3  | 5:E:122:GLU:O     | 2.13                     | 0.48              |
| 6:F:25:ILE:HA    | 6:F:28:ARG:HG2    | 1.94                     | 0.48              |
| 7:G:88:PRO:HG2   | 7:G:152:ALA:HA    | 1.95                     | 0.48              |
| 2:B:178:ARG:CD   | 8:H:72:PRO:HA     | 2.44                     | 0.48              |
| 13:M:12:ASN:H    | 13:M:45:VAL:HG12  | 1.76                     | 0.48              |
| 15:O:3:ILE:HA    | 15:O:7:GLU:OE1    | 2.13                     | 0.48              |
| 16:P:19:ILE:HD11 | 16:P:39:TYR:HB2   | 1.95                     | 0.48              |
| 1:A:1025:U:H5    | 1:A:1034:G:H1     | 1.62                     | 0.48              |
| 1:A:1168:A:H2'   | 1:A:1169:A:C8     | 2.48                     | 0.48              |
| 1:A:1371:G:O3'   | 9:I:69:GLY:HA3    | 2.13                     | 0.48              |
| 1:A:15:G:H5'     | 1:A:1396:A:O2'    | 2.14                     | 0.48              |
| 1:A:414:A:H2'    | 1:A:415:A:C8      | 2.48                     | 0.48              |
| 1:A:44:G:H2'     | 1:A:45:U:O4'      | 2.13                     | 0.48              |
| 2:B:28:PHE:CE2   | 2:B:190:THR:HG22  | 2.49                     | 0.48              |
| 1:A:1026:G:C8    | 1:A:1026:G:H3'    | 2.49                     | 0.48              |
| 1:A:1508:G:C5    | 1:A:1509:C:C5     | 3.02                     | 0.48              |
| 1:A:389:A:C6     | 1:A:390:C:H1'     | 2.49                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:648:A:H2'    | 1:A:649:G:O4'     | 2.14                     | 0.48              |
| 5:E:78:HIS:CE1   | 5:E:143:ARG:H     | 2.31                     | 0.48              |
| 20:T:55:ILE:HD13 | 20:T:55:ILE:HA    | 1.72                     | 0.48              |
| 1:A:1029:C:OP1   | 1:A:1033:G:N2     | 2.47                     | 0.48              |
| 1:A:1138:G:N3    | 1:A:1138:G:H3'    | 2.29                     | 0.48              |
| 1:A:323:U:H2'    | 1:A:324:G:O4'     | 2.12                     | 0.48              |
| 1:A:539:A:H2'    | 1:A:540:G:C8      | 2.49                     | 0.48              |
| 1:A:806:C:O2'    | 1:A:807:A:H5'     | 2.13                     | 0.48              |
| 1:A:745:C:H5''   | 1:A:851:G:O2'     | 2.13                     | 0.48              |
| 2:B:93:VAL:HG21  | 2:B:97:TRP:HD1    | 1.79                     | 0.48              |
| 3:C:108:ASN:ND2  | 3:C:111:LEU:HD22  | 2.29                     | 0.48              |
| 1:A:1096:C:H2'   | 1:A:1097:C:C6     | 2.48                     | 0.48              |
| 1:A:1152:A:H5''  | 10:J:13:HIS:HB2   | 1.94                     | 0.48              |
| 1:A:1374:A:C4    | 1:A:1375:A:C8     | 3.01                     | 0.48              |
| 1:A:109:A:C6     | 1:A:326:G:C6      | 3.02                     | 0.48              |
| 1:A:463:A:O2'    | 16:P:82:GLN:HG2   | 2.14                     | 0.48              |
| 1:A:780:A:OP2    | 11:K:122:LYS:HE3  | 2.13                     | 0.48              |
| 2:B:10:LEU:O     | 2:B:12:GLU:N      | 2.47                     | 0.48              |
| 4:D:72:GLU:O     | 4:D:75:PHE:N      | 2.47                     | 0.48              |
| 12:L:113:ARG:NH1 | 12:L:116:SER:H    | 2.11                     | 0.48              |
| 13:M:101:GLN:OE1 | 13:M:101:GLN:N    | 2.46                     | 0.48              |
| 1:A:1070:U:H2'   | 1:A:1071:C:H6     | 1.77                     | 0.48              |
| 1:A:1150:U:C2'   | 1:A:1151:A:H5'    | 2.43                     | 0.48              |
| 1:A:1195:C:O3'   | 1:A:1196:U:H4'    | 2.14                     | 0.48              |
| 1:A:1238:A:H5'   | 1:A:1336:C:N4     | 2.23                     | 0.48              |
| 1:A:1224:G:O2'   | 1:A:1322:C:OP1    | 2.20                     | 0.48              |
| 1:A:485:G:O2'    | 1:A:486:U:OP2     | 2.29                     | 0.48              |
| 1:A:586:C:C2'    | 1:A:587:G:H5'     | 2.44                     | 0.48              |
| 1:A:662:G:H2'    | 1:A:663:A:C8      | 2.49                     | 0.48              |
| 1:A:683:G:H3'    | 1:A:684:A:H8      | 1.78                     | 0.48              |
| 1:A:691:G:H2'    | 1:A:692:U:C6      | 2.48                     | 0.48              |
| 4:D:201:GLN:HG2  | 4:D:204:ILE:HD12  | 1.96                     | 0.48              |
| 5:E:9:LYS:HG2    | 5:E:112:LEU:HD11  | 1.95                     | 0.48              |
| 7:G:17:VAL:HG12  | 7:G:18:TYR:CD1    | 2.49                     | 0.48              |
| 9:I:90:PRO:O     | 9:I:93:ARG:HG3    | 2.14                     | 0.48              |
| 16:P:6:LEU:HD23  | 16:P:17:TYR:CD2   | 2.49                     | 0.48              |
| 17:Q:75:ARG:HB2  | 17:Q:75:ARG:NH1   | 2.29                     | 0.48              |
| 19:S:11:VAL:HG12 | 19:S:12:ASP:H     | 1.79                     | 0.48              |
| 20:T:57:ARG:NH1  | 20:T:100:ILE:HG21 | 2.29                     | 0.48              |
| 1:A:1044:A:C6    | 1:A:1045:C:H1'    | 2.49                     | 0.48              |
| 1:A:949:A:C2     | 1:A:1233:G:N3     | 2.82                     | 0.48              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:558:G:H3'     | 1:A:559:A:H3'    | 1.96                     | 0.48              |
| 1:A:682:G:C2      | 1:A:683:G:C8     | 3.02                     | 0.48              |
| 3:C:120:VAL:HG12  | 3:C:198:VAL:HG11 | 1.95                     | 0.48              |
| 3:C:20:SER:HB3    | 3:C:22:TRP:HE1   | 1.79                     | 0.48              |
| 7:G:50:ILE:O      | 7:G:54:THR:OG1   | 2.23                     | 0.48              |
| 1:A:716:A:N3      | 11:K:118:GLY:HA2 | 2.29                     | 0.48              |
| 16:P:44:THR:OG1   | 16:P:45:THR:HG22 | 2.13                     | 0.48              |
| 18:R:45:SER:HB2   | 18:R:51:LEU:HD21 | 1.96                     | 0.48              |
| 1:A:1137:C:O2     | 1:A:1138:G:N1    | 2.45                     | 0.47              |
| 1:A:429:U:H1'     | 1:A:430:A:H5''   | 1.96                     | 0.47              |
| 1:A:512:U:H2'     | 1:A:513:C:C6     | 2.49                     | 0.47              |
| 1:A:622:A:C8      | 1:A:623:C:C5     | 3.02                     | 0.47              |
| 1:A:910:C:C4      | 1:A:911:U:C5     | 3.03                     | 0.47              |
| 1:A:918:A:H2'     | 1:A:919:A:C8     | 2.48                     | 0.47              |
| 1:A:98:U:O2'      | 1:A:99:C:H5'     | 2.14                     | 0.47              |
| 3:C:43:LEU:HD13   | 3:C:47:LEU:HD22  | 1.95                     | 0.47              |
| 4:D:38:TYR:HD2    | 4:D:38:TYR:H     | 1.62                     | 0.47              |
| 17:Q:66:SER:OG    | 17:Q:69:LYS:HB2  | 2.14                     | 0.47              |
| 19:S:5:LEU:HD22   | 19:S:6:LYS:NZ    | 2.29                     | 0.47              |
| 1:A:1086:U:O5'    | 1:A:1086:U:H6    | 1.96                     | 0.47              |
| 1:A:1381:U:O2'    | 1:A:1382:C:H5'   | 2.14                     | 0.47              |
| 1:A:416:G:C6      | 1:A:417:C:N3     | 2.82                     | 0.47              |
| 1:A:705:U:H5''    | 1:A:706:A:OP2    | 2.14                     | 0.47              |
| 5:E:40:ARG:HB3    | 5:E:66:MET:CE    | 2.43                     | 0.47              |
| 2:B:178:ARG:HH21  | 8:H:74:PRO:HG3   | 1.78                     | 0.47              |
| 7:G:16:LEU:HD22   | 9:I:42:ARG:HA    | 1.96                     | 0.47              |
| 11:K:126:ARG:HH11 | 11:K:126:ARG:HG3 | 1.79                     | 0.47              |
| 18:R:46:GLU:OE2   | 18:R:55:ARG:NH2  | 2.47                     | 0.47              |
| 1:A:1075:C:O3'    | 2:B:175:ARG:NH2  | 2.47                     | 0.47              |
| 1:A:1304:G:C6     | 1:A:1305:G:N1    | 2.82                     | 0.47              |
| 1:A:149:A:H2'     | 1:A:150:C:C6     | 2.49                     | 0.47              |
| 1:A:344:A:C5'     | 1:A:345:C:H5     | 2.28                     | 0.47              |
| 1:A:454:C:H5''    | 1:A:455:C:C5     | 2.49                     | 0.47              |
| 1:A:709:G:H2'     | 1:A:710:G:H8     | 1.79                     | 0.47              |
| 1:A:725:G:H2'     | 1:A:726:C:H6     | 1.79                     | 0.47              |
| 10:J:6:ILE:HB     | 10:J:72:VAL:CG2  | 2.44                     | 0.47              |
| 13:M:48:LEU:HG    | 13:M:48:LEU:H    | 1.42                     | 0.47              |
| 3:C:34:LEU:HD23   | 14:N:25:VAL:HG21 | 1.96                     | 0.47              |
| 15:O:11:VAL:HG21  | 15:O:34:LEU:HD22 | 1.95                     | 0.47              |
| 19:S:39:THR:HA    | 19:S:70:LYS:HA   | 1.95                     | 0.47              |
| 1:A:1233:G:N2     | 1:A:1234:C:N3    | 2.62                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:A:1519[B]:MA6:C5 | 1:A:1520[B]:G:H1' | 2.44                     | 0.47              |
| 1:A:434:U:H2'      | 1:A:435:C:C6      | 2.48                     | 0.47              |
| 1:A:737:A:H2'      | 1:A:738:C:H6      | 1.79                     | 0.47              |
| 2:B:54:THR:OG1     | 2:B:199:TYR:HB3   | 2.13                     | 0.47              |
| 14:N:9:LYS:HD3     | 14:N:10:ALA:N     | 2.29                     | 0.47              |
| 18:R:69:THR:O      | 18:R:72:ARG:HB2   | 2.14                     | 0.47              |
| 1:A:107:G:C2       | 1:A:108:G:H1'     | 2.50                     | 0.47              |
| 1:A:1191:A:H2'     | 1:A:1192:C:C6     | 2.49                     | 0.47              |
| 1:A:109:A:C4       | 1:A:327:A:C2      | 3.02                     | 0.47              |
| 1:A:448:A:C4       | 1:A:487:A:C2      | 3.03                     | 0.47              |
| 1:A:452:A:C2       | 1:A:453:A:C4      | 3.03                     | 0.47              |
| 2:B:109:SER:O      | 2:B:112:VAL:HB    | 2.14                     | 0.47              |
| 3:C:148:GLY:HA3    | 3:C:172:ARG:O     | 2.14                     | 0.47              |
| 4:D:190:ASP:OD2    | 4:D:192:GLU:N     | 2.39                     | 0.47              |
| 9:I:52:ALA:O       | 9:I:95:LYS:HD3    | 2.15                     | 0.47              |
| 10:J:6:ILE:HB      | 10:J:72:VAL:HG23  | 1.96                     | 0.47              |
| 11:K:62:GLN:O      | 11:K:66:LEU:HB2   | 2.14                     | 0.47              |
| 13:M:49:THR:OG1    | 13:M:52:GLU:HG3   | 2.14                     | 0.47              |
| 1:A:1309:G:C6      | 1:A:1329:A:C2     | 3.02                     | 0.47              |
| 1:A:37:U:O2'       | 1:A:500:G:H4'     | 2.14                     | 0.47              |
| 2:B:112:VAL:O      | 2:B:115:LEU:HB3   | 2.15                     | 0.47              |
| 3:C:151:VAL:O      | 3:C:152:ILE:HD13  | 2.14                     | 0.47              |
| 12:L:117:ARG:NH2   | 12:L:124:LYS:HB2  | 2.29                     | 0.47              |
| 13:M:108:ARG:NH2   | 13:M:111:LYS:HG2  | 2.30                     | 0.47              |
| 13:M:23:TYR:CE2    | 13:M:70:LEU:HD13  | 2.50                     | 0.47              |
| 21:U:8:THR:HG1     | 21:U:11:GLY:H     | 1.61                     | 0.47              |
| 1:A:1057:G:O6      | 1:A:1203:C:N4     | 2.44                     | 0.47              |
| 1:A:375:U:H2'      | 1:A:376:G:C8      | 2.50                     | 0.47              |
| 1:A:729:A:C2'      | 1:A:730:G:H5'     | 2.44                     | 0.47              |
| 3:C:20:SER:O       | 14:N:54:PRO:HB3   | 2.15                     | 0.47              |
| 8:H:10:LEU:O       | 8:H:13:ILE:HB     | 2.15                     | 0.47              |
| 8:H:39:LEU:HD22    | 8:H:39:LEU:HA     | 1.54                     | 0.47              |
| 15:O:15:PHE:HD1    | 15:O:30:ALA:CB    | 2.27                     | 0.47              |
| 1:A:1127:G:N2      | 1:A:1145:C:N3     | 2.62                     | 0.47              |
| 1:A:1315:U:H2'     | 1:A:1316:G:O4'    | 2.15                     | 0.47              |
| 1:A:1327:C:H2'     | 1:A:1328:C:C6     | 2.50                     | 0.47              |
| 1:A:975:A:H4'      | 1:A:976:G:C5'     | 2.40                     | 0.47              |
| 3:C:126:ARG:O      | 3:C:127:ARG:HG2   | 2.15                     | 0.47              |
| 3:C:182:ILE:HD12   | 3:C:203:PHE:HB2   | 1.96                     | 0.47              |
| 10:J:87:THR:C      | 10:J:88:LEU:HD13  | 2.34                     | 0.47              |
| 11:K:120:ARG:HH22  | 11:K:126:ARG:HH12 | 1.62                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1508:G:H2'   | 1:A:1509:C:O4'   | 2.15                     | 0.47              |
| 1:A:292:G:C2     | 1:A:309:G:C2     | 3.03                     | 0.47              |
| 1:A:710:G:H5''   | 6:F:54:LYS:HE3   | 1.97                     | 0.47              |
| 2:B:18:GLY:H     | 2:B:41:ILE:HG23  | 1.80                     | 0.47              |
| 3:C:167:TRP:HE3  | 3:C:168:ALA:H    | 1.59                     | 0.47              |
| 12:L:36:VAL:HG12 | 12:L:37:CYS:O    | 2.15                     | 0.47              |
| 1:A:376:G:H5''   | 16:P:5:ARG:HD2   | 1.96                     | 0.47              |
| 1:A:564:C:C5     | 17:Q:31:LEU:HD21 | 2.50                     | 0.47              |
| 1:A:475:G:H2'    | 1:A:476:G:H8     | 1.80                     | 0.47              |
| 1:A:674:G:H2'    | 1:A:675:A:C8     | 2.49                     | 0.47              |
| 1:A:902:G:O2'    | 1:A:903:G:H5'    | 2.15                     | 0.47              |
| 3:C:23:TYR:HD1   | 10:J:11:PHE:CE2  | 2.33                     | 0.47              |
| 5:E:59:GLY:C     | 5:E:63:ARG:HH21  | 2.18                     | 0.47              |
| 6:F:14:LEU:HA    | 6:F:18:GLN:OE1   | 2.14                     | 0.47              |
| 8:H:51:VAL:HG11  | 8:H:60:ARG:NH1   | 2.30                     | 0.47              |
| 11:K:27:ASN:OD1  | 11:K:28:THR:N    | 2.47                     | 0.47              |
| 13:M:53:VAL:O    | 13:M:57:ARG:HB2  | 2.14                     | 0.47              |
| 14:N:6:LEU:HD13  | 14:N:23:ARG:HH22 | 1.80                     | 0.47              |
| 1:A:263:A:O2'    | 1:A:264:U:H5'    | 2.15                     | 0.47              |
| 1:A:500:G:C5     | 1:A:546:G:N2     | 2.83                     | 0.47              |
| 4:D:206:PHE:CD2  | 4:D:207:TYR:CE1  | 2.99                     | 0.47              |
| 5:E:100:VAL:HA   | 5:E:118:ILE:HG22 | 1.97                     | 0.47              |
| 5:E:106:PRO:O    | 5:E:110:LEU:HG   | 2.14                     | 0.47              |
| 7:G:62:PHE:HD1   | 7:G:124:LEU:HD22 | 1.80                     | 0.47              |
| 11:K:19:ALA:HB2  | 11:K:32:ILE:HG23 | 1.96                     | 0.47              |
| 13:M:4:ILE:CD1   | 13:M:22:ILE:HD11 | 2.44                     | 0.47              |
| 16:P:67:THR:O    | 16:P:70:ALA:HB3  | 2.15                     | 0.47              |
| 1:A:1377:A:N6    | 7:G:5:ARG:HH22   | 2.14                     | 0.46              |
| 1:A:405:U:C2     | 1:A:498:U:C5     | 3.03                     | 0.46              |
| 1:A:530:G:N3     | 1:A:530:G:H2'    | 2.30                     | 0.46              |
| 2:B:163:PHE:CE2  | 2:B:185:ILE:HG22 | 2.50                     | 0.46              |
| 6:F:52:ILE:O     | 6:F:55:ASP:HB2   | 2.15                     | 0.46              |
| 11:K:17:GLY:O    | 11:K:80:VAL:HA   | 2.15                     | 0.46              |
| 19:S:51:VAL:O    | 19:S:57:HIS:HA   | 2.16                     | 0.46              |
| 1:A:1172:C:H2'   | 1:A:1173:G:H8    | 1.80                     | 0.46              |
| 1:A:1057:G:N2    | 1:A:1204:A:H1'   | 2.30                     | 0.46              |
| 1:A:595:G:H1'    | 1:A:596:C:H5     | 1.80                     | 0.46              |
| 1:A:750:G:N3     | 15:O:23:GLY:HA3  | 2.30                     | 0.46              |
| 3:C:102:ASN:OD1  | 3:C:102:ASN:N    | 2.48                     | 0.46              |
| 3:C:18:TRP:O     | 3:C:21:ARG:NH1   | 2.49                     | 0.46              |
| 6:F:26:ILE:O     | 6:F:30:LEU:HB2   | 2.15                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:H:49:GLU:HB2   | 8:H:62:TYR:CE2    | 2.50                     | 0.46              |
| 12:L:123:LYS:H   | 12:L:123:LYS:HG2  | 1.27                     | 0.46              |
| 1:A:1226:C:C5    | 13:M:104:ARG:HA   | 2.50                     | 0.46              |
| 19:S:53:ASN:O    | 19:S:77:THR:HG22  | 2.15                     | 0.46              |
| 20:T:50:GLU:CB   | 20:T:99:LEU:HD23  | 2.42                     | 0.46              |
| 1:A:1310:G:C2    | 1:A:1328:C:N3     | 2.84                     | 0.46              |
| 1:A:949:A:H1'    | 1:A:1364:U:N3     | 2.30                     | 0.46              |
| 1:A:1487:G:C5    | 1:A:1488:G:C8     | 3.03                     | 0.46              |
| 1:A:17:U:C2      | 1:A:18:C:C5       | 3.04                     | 0.46              |
| 1:A:3:G:H1       | 4:D:87:GLY:H      | 1.64                     | 0.46              |
| 1:A:66:G:N3      | 1:A:66:G:H2'      | 2.29                     | 0.46              |
| 1:A:710:G:C2     | 1:A:711:G:C5      | 3.03                     | 0.46              |
| 2:B:223:ILE:CD1  | 2:B:228:GLY:HA3   | 2.45                     | 0.46              |
| 5:E:33:VAL:HG22  | 5:E:43:LEU:HD13   | 1.98                     | 0.46              |
| 1:A:1539:C:H5''  | 7:G:82:GLY:CA     | 2.46                     | 0.46              |
| 8:H:1:MET:HG2    | 8:H:2:LEU:H       | 1.79                     | 0.46              |
| 9:I:63:ILE:HG21  | 9:I:77:ILE:HD11   | 1.96                     | 0.46              |
| 16:P:21:VAL:HG21 | 16:P:59:TRP:CD1   | 2.50                     | 0.46              |
| 1:A:128:G:H4'    | 17:Q:3:LYS:HG2    | 1.97                     | 0.46              |
| 1:A:1310:G:N7    | 19:S:2:PRO:HD3    | 2.30                     | 0.46              |
| 1:A:138:G:C2     | 1:A:226:G:C2      | 3.03                     | 0.46              |
| 1:A:442:C:H2'    | 1:A:443:C:C6      | 2.50                     | 0.46              |
| 1:A:452:A:O2'    | 1:A:453:A:H8      | 1.97                     | 0.46              |
| 1:A:948:C:OP2    | 13:M:108:ARG:HB2  | 2.16                     | 0.46              |
| 2:B:223:ILE:HD12 | 2:B:228:GLY:HA3   | 1.97                     | 0.46              |
| 3:C:11:ARG:HH12  | 3:C:180:ALA:HB3   | 1.81                     | 0.46              |
| 6:F:43:LEU:H     | 6:F:43:LEU:HD22   | 1.80                     | 0.46              |
| 8:H:87:SER:HB2   | 8:H:93:VAL:HG22   | 1.95                     | 0.46              |
| 11:K:66:LEU:HD23 | 11:K:97:ALA:HB1   | 1.97                     | 0.46              |
| 20:T:43:LEU:HD13 | 20:T:51:GLU:HB3   | 1.97                     | 0.46              |
| 1:A:1048:G:H1    | 1:A:1209:C:H42    | 1.63                     | 0.46              |
| 1:A:1248:A:O2'   | 9:I:70:LYS:NZ     | 2.28                     | 0.46              |
| 1:A:1438:G:H2'   | 1:A:1439:C:H6     | 1.80                     | 0.46              |
| 1:A:1491:G:C2'   | 1:A:1492:A:H5'    | 2.45                     | 0.46              |
| 1:A:448:A:P      | 1:A:485:G:H22     | 2.38                     | 0.46              |
| 2:B:69:LEU:HD23  | 2:B:91:PRO:O      | 2.15                     | 0.46              |
| 7:G:95:ARG:CZ    | 7:G:99:LEU:HD11   | 2.46                     | 0.46              |
| 13:M:90:LEU:HA   | 13:M:93:ARG:HB3   | 1.98                     | 0.46              |
| 1:A:1499:A:H1'   | 1:A:1520[A]:G:H5' | 1.98                     | 0.46              |
| 1:A:463:A:H2'    | 1:A:474:G:O4'     | 2.15                     | 0.46              |
| 1:A:500:G:C6     | 1:A:546:G:C2      | 3.04                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:544:G:OP1    | 4:D:59:ARG:NH2   | 2.33                     | 0.46              |
| 1:A:833:U:H2'    | 1:A:834:C:C6     | 2.50                     | 0.46              |
| 1:A:992:U:H3     | 1:A:1044:A:H62   | 1.63                     | 0.46              |
| 2:B:36:ARG:HB3   | 2:B:41:ILE:HD11  | 1.96                     | 0.46              |
| 3:C:129:ALA:HB3  | 3:C:132:ARG:HD2  | 1.97                     | 0.46              |
| 3:C:195:VAL:C    | 3:C:196:LEU:HD12 | 2.35                     | 0.46              |
| 1:A:935:A:N6     | 7:G:3:ARG:HG3    | 2.31                     | 0.46              |
| 10:J:4:ILE:HB    | 10:J:74:ILE:CD1  | 2.46                     | 0.46              |
| 1:A:502:G:OP1    | 12:L:117:ARG:N   | 2.47                     | 0.46              |
| 14:N:23:ARG:HD3  | 14:N:29:ARG:O    | 2.16                     | 0.46              |
| 14:N:41:ARG:HG2  | 14:N:42:ILE:HG23 | 1.97                     | 0.46              |
| 15:O:50:HIS:O    | 15:O:53:HIS:N    | 2.48                     | 0.46              |
| 20:T:53:LEU:CD2  | 20:T:56:MET:HG2  | 2.46                     | 0.46              |
| 21:U:6:ARG:HG2   | 21:U:15:ARG:NH2  | 2.31                     | 0.46              |
| 1:A:1079:G:C6    | 1:A:1080:A:N6    | 2.84                     | 0.46              |
| 1:A:1333:A:H2'   | 1:A:1334:G:O4'   | 2.15                     | 0.46              |
| 1:A:229:U:H2'    | 1:A:230:G:H8     | 1.81                     | 0.46              |
| 1:A:542:G:H2'    | 1:A:543:C:H6     | 1.80                     | 0.46              |
| 1:A:867:G:O2'    | 1:A:868:C:H5'    | 2.15                     | 0.46              |
| 1:A:869:G:C8     | 24:A:2036:HOH:O  | 2.68                     | 0.46              |
| 3:C:81:GLY:O     | 3:C:84:ILE:HG22  | 2.16                     | 0.46              |
| 4:D:202:LEU:HD13 | 4:D:202:LEU:HA   | 1.80                     | 0.46              |
| 7:G:101:LEU:HD12 | 7:G:101:LEU:N    | 2.31                     | 0.46              |
| 1:A:693:G:O2'    | 7:G:81:GLY:O     | 2.25                     | 0.46              |
| 10:J:32:ALA:HB3  | 10:J:75:ILE:HB   | 1.97                     | 0.46              |
| 13:M:12:ASN:H    | 13:M:45:VAL:HG11 | 1.79                     | 0.46              |
| 15:O:85:LEU:HD23 | 15:O:85:LEU:HA   | 1.54                     | 0.46              |
| 1:A:1443:G:H5''  | 1:A:1443:G:H8    | 1.81                     | 0.46              |
| 1:A:1502:A:H5''  | 1:A:1504:G:N7    | 2.31                     | 0.46              |
| 1:A:310:G:C5     | 1:A:311:C:C5     | 3.04                     | 0.46              |
| 1:A:448:A:C2     | 1:A:449:C:C2     | 3.03                     | 0.46              |
| 1:A:872:A:C5     | 1:A:874:G:C8     | 3.04                     | 0.46              |
| 4:D:19:LEU:HB2   | 4:D:21:LEU:HD23  | 1.98                     | 0.46              |
| 7:G:50:ILE:HD13  | 7:G:61:VAL:HG11  | 1.98                     | 0.46              |
| 7:G:87:VAL:HA    | 7:G:88:PRO:HD2   | 1.75                     | 0.46              |
| 9:I:86:VAL:HA    | 9:I:89:ASN:O     | 2.16                     | 0.46              |
| 18:R:66:LEU:O    | 18:R:70:ILE:HG13 | 2.15                     | 0.46              |
| 19:S:53:ASN:HB2  | 19:S:56:GLN:O    | 2.15                     | 0.46              |
| 1:A:1035:A:C4    | 1:A:1036:G:N7    | 2.84                     | 0.46              |
| 1:A:920:U:O4'    | 1:A:1080:A:C2    | 2.68                     | 0.46              |
| 1:A:1367:C:N3    | 1:A:1368:G:C8    | 2.84                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1486:G:H2'   | 1:A:1487:G:O4'    | 2.16                     | 0.46              |
| 1:A:690:G:N7     | 11:K:55:LYS:NZ    | 2.63                     | 0.46              |
| 1:A:839:U:H5''   | 1:A:840:C:OP2     | 2.16                     | 0.46              |
| 1:A:93:G:H2'     | 1:A:95:U:O4'      | 2.16                     | 0.46              |
| 3:C:150:LYS:HD2  | 3:C:173:VAL:HG21  | 1.98                     | 0.46              |
| 5:E:135:THR:O    | 5:E:138:ALA:HB3   | 2.16                     | 0.46              |
| 5:E:12:LEU:HD23  | 5:E:13:ILE:CA     | 2.46                     | 0.46              |
| 7:G:75:VAL:HA    | 7:G:87:VAL:O      | 2.16                     | 0.46              |
| 12:L:10:LEU:HA   | 12:L:10:LEU:HD23  | 1.57                     | 0.46              |
| 12:L:117:ARG:HB3 | 12:L:122:THR:OG1  | 2.16                     | 0.46              |
| 17:Q:31:LEU:HA   | 17:Q:31:LEU:HD12  | 1.65                     | 0.46              |
| 18:R:53:ARG:HA   | 18:R:56:THR:HG23  | 1.98                     | 0.46              |
| 20:T:89:ARG:HH21 | 20:T:104:LEU:HD22 | 1.81                     | 0.46              |
| 1:A:1151:A:H1'   | 1:A:1152:A:C8     | 2.51                     | 0.46              |
| 1:A:1487:G:H2'   | 1:A:1488:G:H5'    | 1.97                     | 0.46              |
| 1:A:401:C:H2'    | 1:A:402:G:H8      | 1.81                     | 0.46              |
| 1:A:499:A:N6     | 1:A:547:A:C8      | 2.84                     | 0.46              |
| 1:A:800:G:O2'    | 1:A:801:U:H5'     | 2.16                     | 0.46              |
| 1:A:520:A:OP1    | 12:L:52:LEU:HD12  | 2.16                     | 0.46              |
| 17:Q:60:ILE:HA   | 17:Q:60:ILE:HD12  | 1.68                     | 0.46              |
| 17:Q:8:GLY:HA3   | 17:Q:22:LEU:O     | 2.16                     | 0.46              |
| 1:A:1491:G:N1    | 1:A:1493:A:H2     | 2.14                     | 0.45              |
| 1:A:130:A:H4'    | 1:A:190(F):G:C2   | 2.51                     | 0.45              |
| 1:A:515:G:H2'    | 1:A:516:PSU:O4'   | 2.16                     | 0.45              |
| 1:A:56:U:O2'     | 1:A:57:G:H5'      | 2.16                     | 0.45              |
| 1:A:645:C:H2'    | 1:A:646:U:O4'     | 2.15                     | 0.45              |
| 1:A:7:G:H5'      | 1:A:298:A:O4'     | 2.16                     | 0.45              |
| 5:E:12:LEU:HD21  | 5:E:14:ARG:HB3    | 1.98                     | 0.45              |
| 8:H:120:THR:HG23 | 8:H:123:GLU:HG3   | 1.99                     | 0.45              |
| 10:J:3:LYS:N     | 10:J:74:ILE:O     | 2.50                     | 0.45              |
| 19:S:25:LYS:HE3  | 19:S:25:LYS:HB3   | 1.75                     | 0.45              |
| 1:A:1171:G:H2'   | 1:A:1172:C:C6     | 2.51                     | 0.45              |
| 1:A:1309:G:N2    | 1:A:1329:A:H1'    | 2.31                     | 0.45              |
| 1:A:942:G:C2     | 1:A:1342:C:C2     | 3.05                     | 0.45              |
| 1:A:1378:C:N4    | 1:A:1379:G:C4     | 2.85                     | 0.45              |
| 1:A:352:C:H5''   | 1:A:352:C:H6      | 1.81                     | 0.45              |
| 1:A:401:C:H2'    | 1:A:402:G:C8      | 2.51                     | 0.45              |
| 1:A:452:A:HO2'   | 1:A:453:A:H8      | 1.64                     | 0.45              |
| 1:A:728:A:H2'    | 1:A:729:A:O4'     | 2.16                     | 0.45              |
| 1:A:938:A:C6     | 1:A:939:G:C5      | 3.04                     | 0.45              |
| 1:A:689:C:P      | 11:K:46:GLY:HA3   | 2.56                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 13:M:80:ARG:HB3   | 13:M:80:ARG:CZ   | 2.45                     | 0.45              |
| 17:Q:70:ARG:O     | 17:Q:71:PHE:HD2  | 1.99                     | 0.45              |
| 1:A:1126:U:C4     | 1:A:1127:G:C2    | 3.04                     | 0.45              |
| 1:A:1402:4OC:O2   | 1:A:1500:A:N1    | 2.49                     | 0.45              |
| 1:A:496:A:C2      | 1:A:497:A:C5     | 3.04                     | 0.45              |
| 1:A:581:G:C2      | 1:A:582:U:C5     | 3.04                     | 0.45              |
| 1:A:665:A:C5      | 1:A:733:A:C5     | 3.04                     | 0.45              |
| 1:A:682:G:H1      | 1:A:708:C:H42    | 1.65                     | 0.45              |
| 1:A:581:G:N2      | 1:A:760:G:N7     | 2.63                     | 0.45              |
| 1:A:993:G:H2'     | 1:A:995:C:H41    | 1.81                     | 0.45              |
| 3:C:122:GLU:OE1   | 3:C:126:ARG:HD2  | 2.16                     | 0.45              |
| 6:F:23:LYS:O      | 6:F:26:ILE:HB    | 2.17                     | 0.45              |
| 17:Q:81:ARG:HE    | 17:Q:81:ARG:HB3  | 1.45                     | 0.45              |
| 17:Q:85:VAL:O     | 17:Q:89:LEU:HB2  | 2.17                     | 0.45              |
| 18:R:83:GLU:OE1   | 18:R:84:LYS:HG3  | 2.16                     | 0.45              |
| 1:A:1234:C:H2'    | 1:A:1235:U:C6    | 2.49                     | 0.45              |
| 1:A:1461:G:H2'    | 1:A:1462:G:C8    | 2.51                     | 0.45              |
| 1:A:665:A:H3'     | 1:A:725:G:H21    | 1.82                     | 0.45              |
| 7:G:5:ARG:HE      | 7:G:7:ALA:HA     | 1.81                     | 0.45              |
| 8:H:100:ILE:HA    | 8:H:101:PRO:HD2  | 1.77                     | 0.45              |
| 8:H:9:MET:O       | 8:H:13:ILE:HD12  | 2.17                     | 0.45              |
| 8:H:29:SER:OG     | 8:H:32:LYS:N     | 2.31                     | 0.45              |
| 10:J:8:LEU:CD2    | 10:J:96:ILE:HG22 | 2.44                     | 0.45              |
| 17:Q:4:LYS:HE2    | 17:Q:6:LEU:HD21  | 1.98                     | 0.45              |
| 1:A:1119:C:N4     | 1:A:1154:G:H1    | 2.13                     | 0.45              |
| 1:A:1256:A:H4'    | 1:A:1257:U:O5'   | 2.16                     | 0.45              |
| 1:A:222:U:H2'     | 1:A:223:U:C6     | 2.51                     | 0.45              |
| 1:A:342:C:H42     | 1:A:347:G:H1     | 1.62                     | 0.45              |
| 1:A:561:U:HO2'    | 1:A:562:C:P      | 2.40                     | 0.45              |
| 1:A:584:G:H2'     | 1:A:585:G:C8     | 2.51                     | 0.45              |
| 1:A:709:G:H2'     | 1:A:710:G:C8     | 2.52                     | 0.45              |
| 6:F:40:VAL:HG22   | 6:F:63:TYR:HD2   | 1.80                     | 0.45              |
| 8:H:121:ASP:OD2   | 8:H:122:ARG:N    | 2.49                     | 0.45              |
| 10:J:6:ILE:HA     | 10:J:97:GLU:O    | 2.17                     | 0.45              |
| 11:K:18:ARG:HG3   | 11:K:33:THR:HG23 | 1.99                     | 0.45              |
| 15:O:70:LEU:HD22  | 15:O:70:LEU:HA   | 1.68                     | 0.45              |
| 17:Q:95:TYR:O     | 17:Q:98:LEU:HD12 | 2.17                     | 0.45              |
| 20:T:100:ILE:HG22 | 20:T:102:GLY:H   | 1.81                     | 0.45              |
| 20:T:53:LEU:HA    | 20:T:53:LEU:HD23 | 1.82                     | 0.45              |
| 21:U:6:ARG:H      | 21:U:6:ARG:HG3   | 1.57                     | 0.45              |
| 1:A:1510:U:H2'    | 1:A:1511:G:N7    | 2.32                     | 0.45              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 1:A:1518[B]:MA6:HO2' | 1:A:1519[B]:MA6:P    | 2.40                     | 0.45              |
| 1:A:629:G:H2'        | 1:A:630:G:O4'        | 2.16                     | 0.45              |
| 1:A:710:G:H2'        | 1:A:711:G:C8         | 2.50                     | 0.45              |
| 1:A:899:C:H2'        | 1:A:900:A:O4'        | 2.16                     | 0.45              |
| 2:B:184:VAL:O        | 2:B:198:ASP:HB2      | 2.16                     | 0.45              |
| 7:G:107:ALA:HA       | 7:G:110:GLN:HG2      | 1.99                     | 0.45              |
| 7:G:139:GLU:CG       | 7:G:143:ARG:HH22     | 2.28                     | 0.45              |
| 7:G:71:PRO:HG3       | 7:G:103:TRP:HZ3      | 1.81                     | 0.45              |
| 8:H:86:ILE:HG21      | 8:H:133:LEU:HD13     | 1.99                     | 0.45              |
| 9:I:111:ARG:HG3      | 9:I:111:ARG:O        | 2.16                     | 0.45              |
| 16:P:41:PRO:O        | 16:P:43:LYS:HD2      | 2.17                     | 0.45              |
| 19:S:16:LEU:HD11     | 19:S:20:LEU:HD23     | 1.98                     | 0.45              |
| 1:A:1414:U:H2'       | 1:A:1415:G:H8        | 1.82                     | 0.45              |
| 1:A:1503:A:N6        | 1:A:1532:U:O2'       | 2.49                     | 0.45              |
| 1:A:1403:C:N4        | 1:A:1544:U:OP1       | 2.50                     | 0.45              |
| 1:A:509:A:C3'        | 1:A:509:A:C8         | 3.00                     | 0.45              |
| 1:A:542:G:O2'        | 1:A:543:C:H5'        | 2.16                     | 0.45              |
| 1:A:725:G:C4         | 1:A:726:C:C5         | 3.05                     | 0.45              |
| 1:A:782:A:H2'        | 1:A:783:C:O4'        | 2.17                     | 0.45              |
| 3:C:182:ILE:HG22     | 3:C:183:ASP:O        | 2.16                     | 0.45              |
| 4:D:35:ARG:O         | 4:D:36:ARG:HG2       | 2.15                     | 0.45              |
| 4:D:63:LYS:O         | 4:D:67:ILE:HG13      | 2.17                     | 0.45              |
| 5:E:17:ALA:HB2       | 5:E:26:PHE:CD2       | 2.52                     | 0.45              |
| 5:E:79:GLU:HG3       | 8:H:105:ARG:CG       | 2.45                     | 0.45              |
| 10:J:6:ILE:O         | 10:J:72:VAL:HG23     | 2.17                     | 0.45              |
| 15:O:41:GLU:OE2      | 15:O:44:LYS:HD3      | 2.16                     | 0.45              |
| 1:A:112:G:H21        | 1:A:354:G:C4'        | 2.30                     | 0.45              |
| 1:A:1233:G:C2        | 1:A:1234:C:C4        | 3.05                     | 0.45              |
| 1:A:1514:C:H2'       | 1:A:1515[A]:C:O4'    | 2.16                     | 0.45              |
| 1:A:502:G:H2'        | 1:A:503:C:O4'        | 2.16                     | 0.45              |
| 1:A:933:G:N1         | 1:A:935:A:H1'        | 2.32                     | 0.45              |
| 1:A:966:M2G:C8       | 1:A:967:5MC:HM52     | 2.52                     | 0.45              |
| 4:D:10:ARG:HG3       | 4:D:40:PRO:HG3       | 1.98                     | 0.45              |
| 8:H:51:VAL:HG11      | 8:H:60:ARG:HH12      | 1.82                     | 0.45              |
| 1:A:1015:A:H2'       | 1:A:1016:A:C8        | 2.52                     | 0.45              |
| 1:A:1518[A]:MA6:N6   | 1:A:1519[A]:MA6:H103 | 2.32                     | 0.45              |
| 1:A:950:U:H2'        | 1:A:951:G:H8         | 1.82                     | 0.45              |
| 3:C:150:LYS:CG       | 3:C:169:ALA:HB2      | 2.46                     | 0.45              |
| 5:E:75:THR:C         | 5:E:76:ILE:HD13      | 2.37                     | 0.45              |
| 6:F:7:ASN:HD22       | 6:F:7:ASN:N          | 2.14                     | 0.45              |
| 1:A:1539:C:H5''      | 7:G:82:GLY:HA2       | 1.99                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1349:A:OP1   | 9:I:120:ARG:HB2  | 2.16                     | 0.45              |
| 20:T:10:LEU:HD22 | 20:T:11:SER:H    | 1.82                     | 0.45              |
| 1:A:1377:A:OP2   | 7:G:94:ARG:NE    | 2.50                     | 0.45              |
| 1:A:499:A:C6     | 1:A:547:A:C8     | 3.05                     | 0.45              |
| 1:A:711:G:N3     | 1:A:712:A:C8     | 2.85                     | 0.45              |
| 7:G:99:LEU:HD22  | 7:G:103:TRP:CZ3  | 2.52                     | 0.45              |
| 14:N:31:ARG:O    | 14:N:33:VAL:HG22 | 2.17                     | 0.45              |
| 14:N:6:LEU:HD23  | 14:N:6:LEU:HA    | 1.63                     | 0.45              |
| 1:A:1392:G:O5'   | 1:A:1392:G:H8    | 2.01                     | 0.44              |
| 1:A:1481:U:O2'   | 1:A:1482:G:H5'   | 2.17                     | 0.44              |
| 1:A:73:C:O2'     | 1:A:74:C:H5'     | 2.17                     | 0.44              |
| 1:A:874:G:C6     | 1:A:875:C:C4     | 3.04                     | 0.44              |
| 1:A:936:C:H2'    | 1:A:937:A:O4'    | 2.17                     | 0.44              |
| 4:D:107:ARG:NH1  | 4:D:114:ARG:HH22 | 2.15                     | 0.44              |
| 5:E:46:GLY:N     | 5:E:58:ALA:HB2   | 2.31                     | 0.44              |
| 11:K:33:THR:OG1  | 11:K:34:ASP:N    | 2.49                     | 0.44              |
| 12:L:111:LYS:O   | 12:L:112:ASP:HB2 | 2.17                     | 0.44              |
| 12:L:38:THR:HB   | 12:L:39:VAL:H    | 1.66                     | 0.44              |
| 14:N:32:SER:HB2  | 14:N:41:ARG:HB3  | 1.98                     | 0.44              |
| 15:O:49:ASP:OD1  | 15:O:52:SER:OG   | 2.22                     | 0.44              |
| 17:Q:29:HIS:HB2  | 17:Q:36:ILE:HD12 | 2.00                     | 0.44              |
| 19:S:5:LEU:C     | 19:S:6:LYS:HZ3   | 2.20                     | 0.44              |
| 1:A:1307:U:H2'   | 1:A:1308:U:H6    | 1.82                     | 0.44              |
| 1:A:1416:G:H2'   | 1:A:1417:G:H5'   | 1.99                     | 0.44              |
| 1:A:1506:U:N3    | 1:A:1522:U:OP1   | 2.29                     | 0.44              |
| 1:A:226:G:C2     | 1:A:227:G:C8     | 3.05                     | 0.44              |
| 1:A:489:C:H2'    | 1:A:490:G:C8     | 2.48                     | 0.44              |
| 1:A:711:G:H2'    | 1:A:712:A:C8     | 2.49                     | 0.44              |
| 1:A:792:A:H4'    | 1:A:793:U:H5''   | 1.99                     | 0.44              |
| 2:B:221:LEU:HD13 | 2:B:222:ILE:N    | 2.32                     | 0.44              |
| 5:E:127:ASN:HA   | 5:E:128:PRO:HD2  | 1.81                     | 0.44              |
| 5:E:28:PHE:O     | 5:E:47:LYS:HA    | 2.16                     | 0.44              |
| 5:E:91:LEU:HA    | 5:E:91:LEU:HD23  | 1.59                     | 0.44              |
| 6:F:3:ARG:HG2    | 6:F:93:SER:HB2   | 1.99                     | 0.44              |
| 8:H:119:LEU:HD12 | 8:H:119:LEU:N    | 2.33                     | 0.44              |
| 9:I:48:GLU:HB3   | 9:I:101:PHE:CZ   | 2.52                     | 0.44              |
| 1:A:1250:A:H4'   | 9:I:67:GLY:HA2   | 2.00                     | 0.44              |
| 12:L:28:LYS:HD2  | 12:L:33:ARG:NE   | 2.32                     | 0.44              |
| 15:O:51:HIS:O    | 15:O:54:ARG:HB3  | 2.18                     | 0.44              |
| 15:O:74:ASP:HA   | 15:O:75:PRO:HD2  | 1.85                     | 0.44              |
| 17:Q:27:PHE:HA   | 17:Q:28:PRO:HD3  | 1.66                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 19:S:7:LYS:HZ3   | 19:S:7:LYS:H      | 1.65                     | 0.44              |
| 20:T:36:LEU:HA   | 20:T:36:LEU:HD22  | 1.83                     | 0.44              |
| 20:T:65:LYS:O    | 20:T:68:LYS:HB2   | 2.18                     | 0.44              |
| 1:A:106:C:H2'    | 1:A:107:G:H8      | 1.81                     | 0.44              |
| 1:A:1086:U:O2'   | 1:A:1087:G:H5'    | 2.18                     | 0.44              |
| 1:A:1143:G:H2'   | 1:A:1144:G:C8     | 2.53                     | 0.44              |
| 1:A:1254:C:O4'   | 1:A:1356:G:H5''   | 2.17                     | 0.44              |
| 1:A:1356:G:H2'   | 1:A:1357:A:C8     | 2.52                     | 0.44              |
| 1:A:1539:C:H2'   | 1:A:1540:PSU:H5'' | 1.98                     | 0.44              |
| 1:A:414:A:OP2    | 1:A:428:G:N2      | 2.43                     | 0.44              |
| 1:A:785:G:C2     | 1:A:786:G:C8      | 3.06                     | 0.44              |
| 1:A:929:G:C5     | 1:A:930:C:C5      | 3.05                     | 0.44              |
| 3:C:123:GLN:HB2  | 3:C:128:PHE:CD1   | 2.37                     | 0.44              |
| 4:D:177:ASP:OD2  | 4:D:179:GLU:HG2   | 2.17                     | 0.44              |
| 4:D:61:LYS:HG3   | 4:D:62:GLN:N      | 2.27                     | 0.44              |
| 9:I:28:VAL:HG22  | 9:I:63:ILE:HB     | 1.98                     | 0.44              |
| 10:J:38:ILE:HG13 | 10:J:71:LEU:HB2   | 1.99                     | 0.44              |
| 17:Q:57:VAL:HG12 | 17:Q:76:LEU:HA    | 1.98                     | 0.44              |
| 1:A:1053:G:C3'   | 1:A:1054:C:H5'    | 2.47                     | 0.44              |
| 1:A:1438:G:H2'   | 1:A:1439:C:C6     | 2.52                     | 0.44              |
| 1:A:1476:G:O2'   | 1:A:1477:C:H5'    | 2.17                     | 0.44              |
| 1:A:147:G:H1     | 1:A:175:C:H42     | 1.65                     | 0.44              |
| 1:A:1496:C:H2'   | 1:A:1497:G:O4'    | 2.18                     | 0.44              |
| 1:A:486:U:H2'    | 1:A:487:A:H8      | 1.82                     | 0.44              |
| 1:A:484:G:H5'    | 1:A:486:U:O4'     | 2.17                     | 0.44              |
| 1:A:762:C:H2'    | 1:A:763:G:H8      | 1.83                     | 0.44              |
| 2:B:71:VAL:HG13  | 2:B:93:VAL:HB     | 2.00                     | 0.44              |
| 4:D:172:PRO:HD2  | 4:D:173:TRP:CZ3   | 2.53                     | 0.44              |
| 1:A:412:A:N6     | 4:D:35:ARG:HB3    | 2.33                     | 0.44              |
| 6:F:40:VAL:HG22  | 6:F:63:TYR:CD2    | 2.52                     | 0.44              |
| 6:F:68:PRO:HG2   | 6:F:71:ARG:NH2    | 2.33                     | 0.44              |
| 14:N:23:ARG:HA   | 14:N:29:ARG:O     | 2.16                     | 0.44              |
| 1:A:1387:G:C6    | 1:A:1388:C:N4     | 2.85                     | 0.44              |
| 1:A:138:G:N2     | 1:A:226:G:N3      | 2.66                     | 0.44              |
| 1:A:255:G:C2     | 1:A:256:U:C4      | 3.05                     | 0.44              |
| 1:A:372:C:H4'    | 1:A:373:A:OP1     | 2.17                     | 0.44              |
| 2:B:136:VAL:O    | 2:B:140:HIS:HB2   | 2.17                     | 0.44              |
| 4:D:190:ASP:OD2  | 4:D:190:ASP:C     | 2.56                     | 0.44              |
| 6:F:10:LEU:HD12  | 6:F:10:LEU:H      | 1.82                     | 0.44              |
| 7:G:74:GLU:HG2   | 7:G:91:VAL:HG11   | 2.00                     | 0.44              |
| 8:H:52:ASP:OD1   | 8:H:56:LYS:N      | 2.51                     | 0.44              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 10:J:7:LYS:O    | 10:J:8:LEU:HD23  | 2.18                     | 0.44              |
| 13:M:91:ARG:HA  | 13:M:91:ARG:HD2  | 1.81                     | 0.44              |
| 1:A:1072:G:C5   | 1:A:1073:U:C4    | 3.06                     | 0.44              |
| 1:A:1241:G:H2'  | 1:A:1242:C:C6    | 2.52                     | 0.44              |
| 1:A:1484:C:H2'  | 1:A:1485:U:O4'   | 2.17                     | 0.44              |
| 1:A:194:C:H2'   | 1:A:195:A:H5''   | 1.99                     | 0.44              |
| 1:A:386:C:H2'   | 1:A:387:U:H5'    | 1.99                     | 0.44              |
| 1:A:693:G:H2'   | 1:A:694:A:H8     | 1.82                     | 0.44              |
| 1:A:764:C:H5''  | 1:A:765:G:OP2    | 2.18                     | 0.44              |
| 1:A:79:G:C2     | 1:A:80:G:C8      | 3.06                     | 0.44              |
| 2:B:166:ASP:HB3 | 2:B:169:LYS:HB3  | 2.00                     | 0.44              |
| 9:I:7:THR:HG22  | 9:I:8:GLY:N      | 2.32                     | 0.44              |
| 10:J:25:GLU:HA  | 10:J:28:ARG:HB2  | 2.00                     | 0.44              |
| 17:Q:59:ILE:HA  | 17:Q:59:ILE:HD13 | 1.77                     | 0.44              |
| 1:A:1221:G:H4'  | 19:S:77:THR:CG2  | 2.48                     | 0.44              |
| 1:A:1417:G:H2'  | 1:A:1482:G:N2    | 2.33                     | 0.44              |
| 1:A:1484:C:C4   | 1:A:1485:U:O2    | 2.71                     | 0.44              |
| 1:A:622:A:C8    | 1:A:623:C:C6     | 3.05                     | 0.44              |
| 3:C:11:ARG:O    | 3:C:14:ILE:O     | 2.34                     | 0.44              |
| 5:E:116:THR:OG1 | 5:E:117:ASP:N    | 2.51                     | 0.44              |
| 1:A:826:C:H5'   | 8:H:12:ARG:CZ    | 2.47                     | 0.44              |
| 8:H:86:ILE:HG21 | 8:H:133:LEU:HD22 | 1.99                     | 0.44              |
| 9:I:48:GLU:HB3  | 9:I:101:PHE:HZ   | 1.83                     | 0.44              |
| 17:Q:29:HIS:HB2 | 17:Q:36:ILE:CD1  | 2.48                     | 0.44              |
| 1:A:932:C:H2'   | 1:A:933:G:C8     | 2.52                     | 0.44              |
| 3:C:35:GLU:HG3  | 3:C:95:THR:HG21  | 1.99                     | 0.44              |
| 1:A:544:G:P     | 4:D:59:ARG:HH22  | 2.39                     | 0.44              |
| 7:G:17:VAL:HG12 | 7:G:18:TYR:HD1   | 1.83                     | 0.44              |
| 8:H:56:LYS:HA   | 8:H:57:PRO:HD3   | 1.80                     | 0.44              |
| 13:M:14:ARG:HB3 | 13:M:41:PRO:O    | 2.17                     | 0.44              |
| 13:M:86:CYS:O   | 13:M:90:LEU:HD22 | 2.18                     | 0.44              |
| 15:O:57:LEU:HA  | 15:O:57:LEU:HD13 | 1.45                     | 0.44              |
| 1:A:1459:C:H2'  | 1:A:1460:A:O4'   | 2.18                     | 0.44              |
| 1:A:1478:C:H2'  | 1:A:1479:C:O4'   | 2.18                     | 0.44              |
| 1:A:254:G:N3    | 1:A:255:G:C8     | 2.86                     | 0.44              |
| 1:A:427:U:C4    | 1:A:428:G:C6     | 3.06                     | 0.44              |
| 1:A:803:G:H2'   | 1:A:804:U:O4'    | 2.18                     | 0.44              |
| 4:D:104:VAL:O   | 4:D:108:LEU:HB2  | 2.18                     | 0.44              |
| 8:H:13:ILE:O    | 8:H:17:THR:HG23  | 2.18                     | 0.44              |
| 8:H:40:ALA:O    | 8:H:42:GLU:N     | 2.51                     | 0.44              |
| 11:K:59:TYR:CE2 | 11:K:63:LEU:HD11 | 2.52                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 14:N:15:LYS:HE2  | 14:N:15:LYS:HB3  | 1.74                     | 0.44              |
| 17:Q:26:GLN:O    | 17:Q:27:PHE:HB3  | 2.18                     | 0.44              |
| 20:T:87:LYS:HE2  | 20:T:87:LYS:HB2  | 1.91                     | 0.44              |
| 1:A:113:G:H1     | 1:A:314:C:H42    | 1.66                     | 0.43              |
| 1:A:67:C:H2'     | 1:A:68:G:C8      | 2.53                     | 0.43              |
| 1:A:670:G:H1     | 1:A:736:C:H42    | 1.66                     | 0.43              |
| 1:A:967:5MC:H2'  | 1:A:968:A:C8     | 2.53                     | 0.43              |
| 4:D:194:LEU:HB3  | 4:D:196:LEU:CD2  | 2.48                     | 0.43              |
| 8:H:86:ILE:HG21  | 8:H:133:LEU:HB3  | 1.99                     | 0.43              |
| 10:J:57:LYS:O    | 10:J:57:LYS:HG3  | 2.18                     | 0.43              |
| 13:M:29:ARG:HB3  | 13:M:64:TRP:CZ3  | 2.53                     | 0.43              |
| 19:S:39:THR:HG22 | 19:S:70:LYS:CD   | 2.42                     | 0.43              |
| 1:A:1104:G:H5''  | 1:A:1104:G:H8    | 1.82                     | 0.43              |
| 1:A:1399:C:O2    | 1:A:1401:G:C5    | 2.71                     | 0.43              |
| 1:A:235:C:N4     | 24:A:1842:HOH:O  | 2.51                     | 0.43              |
| 1:A:518:C:H2'    | 1:A:530:G:C8     | 2.53                     | 0.43              |
| 1:A:954:G:H2'    | 1:A:955:U:C6     | 2.54                     | 0.43              |
| 2:B:57:PHE:CG    | 2:B:199:TYR:CE1  | 3.06                     | 0.43              |
| 8:H:63:LEU:HD13  | 8:H:63:LEU:H     | 1.83                     | 0.43              |
| 10:J:57:LYS:HG3  | 10:J:60:ARG:NH1  | 2.29                     | 0.43              |
| 1:A:707:C:OP1    | 11:K:85:ARG:NH1  | 2.51                     | 0.43              |
| 12:L:33:ARG:HG2  | 12:L:62:SER:HB3  | 2.00                     | 0.43              |
| 13:M:94:ARG:HB3  | 13:M:96:LEU:HD12 | 2.00                     | 0.43              |
| 14:N:11:LYS:HE2  | 14:N:11:LYS:HB3  | 1.78                     | 0.43              |
| 17:Q:43:LEU:HD23 | 17:Q:68:ARG:NH2  | 2.32                     | 0.43              |
| 1:A:104:G:C2     | 1:A:105:G:C8     | 3.06                     | 0.43              |
| 1:A:1297:C:H4'   | 1:A:1298:C:H5'   | 2.00                     | 0.43              |
| 1:A:277:C:OP2    | 17:Q:41:LYS:HE3  | 2.19                     | 0.43              |
| 1:A:382:A:C2     | 1:A:383:A:C4     | 3.06                     | 0.43              |
| 1:A:64:G:H4'     | 1:A:65:U:H3'     | 2.00                     | 0.43              |
| 1:A:841:U:H6     | 1:A:848:C:H5'    | 1.82                     | 0.43              |
| 4:D:117:ALA:O    | 4:D:121:VAL:HG23 | 2.18                     | 0.43              |
| 5:E:142:LEU:O    | 5:E:143:ARG:HD3  | 2.17                     | 0.43              |
| 1:A:673:G:H5''   | 6:F:87:ARG:NH1   | 2.33                     | 0.43              |
| 9:I:117:HIS:HB2  | 9:I:121:ARG:HG2  | 2.00                     | 0.43              |
| 9:I:65:VAL:HG11  | 9:I:73:GLN:CD    | 2.38                     | 0.43              |
| 12:L:33:ARG:HB3  | 12:L:60:LEU:CD1  | 2.49                     | 0.43              |
| 1:A:1005:A:C2    | 1:A:1006:C:C2    | 3.07                     | 0.43              |
| 1:A:1022:G:H2'   | 1:A:1023:G:O4'   | 2.17                     | 0.43              |
| 1:A:1198:G:C6    | 1:A:1199:U:C4    | 3.07                     | 0.43              |
| 1:A:1052:U:O4    | 1:A:1200:C:C2    | 2.71                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:A:1468:A:O5'     | 1:A:1468:A:H8     | 2.02                     | 0.43              |
| 1:A:1519[B]:MA6:N7 | 1:A:1520[B]:G:H1' | 2.33                     | 0.43              |
| 1:A:392:G:H2'      | 1:A:393:A:C8      | 2.54                     | 0.43              |
| 1:A:949:A:N1       | 1:A:1233:G:N3     | 2.67                     | 0.43              |
| 4:D:5:ILE:HG12     | 4:D:5:ILE:O       | 2.19                     | 0.43              |
| 8:H:23:SER:HA      | 8:H:63:LEU:CD1    | 2.48                     | 0.43              |
| 13:M:87:TYR:HA     | 13:M:90:LEU:CD2   | 2.48                     | 0.43              |
| 15:O:79:ARG:HB2    | 15:O:79:ARG:HE    | 1.56                     | 0.43              |
| 16:P:34:GLU:OE2    | 16:P:55:ARG:HD2   | 2.18                     | 0.43              |
| 17:Q:24:GLU:HA     | 17:Q:38:ARG:O     | 2.18                     | 0.43              |
| 17:Q:68:ARG:N      | 17:Q:70:ARG:HH12  | 2.16                     | 0.43              |
| 18:R:23:LYS:HE3    | 18:R:57:GLY:O     | 2.17                     | 0.43              |
| 1:A:186:C:O3'      | 20:T:82:SER:HB2   | 2.19                     | 0.43              |
| 1:A:947:G:H1       | 1:A:1234:C:H42    | 1.65                     | 0.43              |
| 1:A:1124:G:H22     | 1:A:1280:A:N6     | 2.17                     | 0.43              |
| 1:A:261:U:O2       | 1:A:263:A:C8      | 2.71                     | 0.43              |
| 1:A:358:U:H2'      | 1:A:359:U:C6      | 2.53                     | 0.43              |
| 1:A:778:G:H1       | 1:A:804:U:H3      | 1.67                     | 0.43              |
| 3:C:114:PRO:O      | 3:C:118:GLN:HG3   | 2.19                     | 0.43              |
| 4:D:31:CYS:C       | 4:D:33:MET:N      | 2.71                     | 0.43              |
| 4:D:79:PHE:HA      | 4:D:93:PHE:CE2    | 2.53                     | 0.43              |
| 9:I:49:PRO:HG2     | 9:I:50:LEU:HD12   | 1.99                     | 0.43              |
| 11:K:77:MET:O      | 11:K:78:GLN:NE2   | 2.43                     | 0.43              |
| 1:A:1213:A:C4      | 1:A:1215:G:C8     | 3.07                     | 0.43              |
| 1:A:1256:A:O4'     | 1:A:1256:A:N3     | 2.51                     | 0.43              |
| 1:A:200:G:H2'      | 1:A:201:C:O4'     | 2.19                     | 0.43              |
| 1:A:352:C:O2'      | 1:A:354:G:OP1     | 2.33                     | 0.43              |
| 1:A:585:G:H8       | 1:A:585:G:O5'     | 2.00                     | 0.43              |
| 1:A:674:G:H2'      | 1:A:675:A:H8      | 1.83                     | 0.43              |
| 3:C:101:LEU:HA     | 3:C:101:LEU:HD23  | 1.77                     | 0.43              |
| 6:F:99:ALA:O       | 18:R:28:GLU:HG3   | 2.19                     | 0.43              |
| 7:G:111:ARG:HB3    | 7:G:113:GLU:OE2   | 2.19                     | 0.43              |
| 10:J:50:ILE:CD1    | 10:J:50:ILE:H     | 2.31                     | 0.43              |
| 20:T:48:LYS:H      | 20:T:48:LYS:HG2   | 1.39                     | 0.43              |
| 1:A:110:C:H2'      | 1:A:111:G:O4'     | 2.19                     | 0.43              |
| 1:A:1172:C:H2'     | 1:A:1173:G:C8     | 2.53                     | 0.43              |
| 1:A:1220:G:H2'     | 1:A:1221:G:H8     | 1.84                     | 0.43              |
| 1:A:1427:U:H2'     | 1:A:1428:A:H8     | 1.80                     | 0.43              |
| 1:A:229:U:H2'      | 1:A:230:G:C8      | 2.54                     | 0.43              |
| 1:A:332:G:H2'      | 1:A:333:G:H8      | 1.83                     | 0.43              |
| 1:A:429:U:O3'      | 4:D:22:LYS:HE3    | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:443:C:H2'    | 1:A:444:C:H6     | 1.82                     | 0.43              |
| 1:A:925:G:O2'    | 1:A:926:G:H5''   | 2.18                     | 0.43              |
| 3:C:188:LEU:CD1  | 3:C:195:VAL:HG13 | 2.49                     | 0.43              |
| 1:A:1192:C:P     | 3:C:4:LYS:HZ1    | 2.41                     | 0.43              |
| 4:D:25:ARG:HA    | 4:D:28:SER:HB3   | 2.00                     | 0.43              |
| 11:K:91:ARG:HB3  | 11:K:92:GLU:OE1  | 2.19                     | 0.43              |
| 12:L:28:LYS:HB3  | 12:L:30:ALA:CB   | 2.49                     | 0.43              |
| 15:O:32:LEU:HD22 | 15:O:32:LEU:HA   | 1.64                     | 0.43              |
| 20:T:10:LEU:HD13 | 20:T:13:LEU:H    | 1.84                     | 0.43              |
| 1:A:1095:U:C4    | 1:A:1096:C:C4    | 3.06                     | 0.43              |
| 1:A:1179:A:O3'   | 9:I:103:THR:HG23 | 2.19                     | 0.43              |
| 1:A:1196:U:O2'   | 1:A:1197:G:OP1   | 2.33                     | 0.43              |
| 1:A:1233:G:N2    | 1:A:1234:C:C2    | 2.87                     | 0.43              |
| 1:A:1480:G:C6    | 1:A:1481:U:C4    | 3.06                     | 0.43              |
| 1:A:1485:U:C6    | 1:A:1486:G:N7    | 2.87                     | 0.43              |
| 1:A:162:A:C5     | 1:A:163:C:H1'    | 2.54                     | 0.43              |
| 4:D:90:GLY:N     | 4:D:204:ILE:HD11 | 2.34                     | 0.43              |
| 5:E:79:GLU:H     | 5:E:79:GLU:HG3   | 1.48                     | 0.43              |
| 6:F:21:LEU:HD12  | 6:F:21:LEU:HA    | 1.78                     | 0.43              |
| 3:C:23:TYR:CD1   | 10:J:11:PHE:CE2  | 3.07                     | 0.43              |
| 10:J:69:ASN:O    | 10:J:70:ARG:HG3  | 2.18                     | 0.43              |
| 17:Q:29:HIS:O    | 17:Q:31:LEU:N    | 2.51                     | 0.43              |
| 1:A:1525:G:H3'   | 1:A:1525:G:C8    | 2.54                     | 0.43              |
| 1:A:262:A:C6     | 1:A:263:A:C6     | 3.06                     | 0.43              |
| 1:A:349:A:H2'    | 1:A:350:G:H5''   | 2.00                     | 0.43              |
| 1:A:429:U:H4'    | 1:A:430:A:O5'    | 2.18                     | 0.43              |
| 1:A:869:G:N7     | 24:A:2036:HOH:O  | 2.36                     | 0.43              |
| 3:C:91:LEU:HD23  | 3:C:99:VAL:HG21  | 2.00                     | 0.43              |
| 10:J:50:ILE:N    | 10:J:50:ILE:CD1  | 2.81                     | 0.43              |
| 12:L:84:LEU:HD13 | 12:L:105:TYR:HE1 | 1.84                     | 0.43              |
| 16:P:80:PHE:CD1  | 16:P:80:PHE:N    | 2.87                     | 0.43              |
| 1:A:1124:G:H4'   | 1:A:1125:U:OP1   | 2.19                     | 0.43              |
| 1:A:1152:A:H2'   | 1:A:1153:C:C6    | 2.54                     | 0.43              |
| 1:A:1233:G:OP2   | 9:I:124:GLN:HB3  | 2.18                     | 0.43              |
| 1:A:449:C:C5     | 1:A:450:G:C5     | 3.06                     | 0.43              |
| 1:A:695:A:H2'    | 1:A:696:A:H8     | 1.78                     | 0.43              |
| 1:A:780:A:P      | 11:K:122:LYS:HG3 | 2.58                     | 0.43              |
| 1:A:947:G:H2'    | 1:A:948:C:O4'    | 2.19                     | 0.43              |
| 1:A:973:G:OP1    | 10:J:57:LYS:HD3  | 2.19                     | 0.43              |
| 3:C:33:LEU:HD21  | 14:N:53:LEU:HD22 | 1.99                     | 0.43              |
| 3:C:78:GLY:HA3   | 3:C:83:ARG:HB3   | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:80:GLU:O     | 4:D:83:SER:N     | 2.50                     | 0.43              |
| 6:F:8:ILE:HG21   | 6:F:26:ILE:HD11  | 2.01                     | 0.43              |
| 12:L:28:LYS:HB3  | 12:L:30:ALA:H    | 1.84                     | 0.43              |
| 14:N:26:ARG:HH12 | 14:N:47:LEU:HD22 | 1.82                     | 0.43              |
| 15:O:8:LYS:O     | 15:O:12:ILE:HG13 | 2.19                     | 0.43              |
| 18:R:64:ARG:HE   | 18:R:64:ARG:HB2  | 1.50                     | 0.43              |
| 1:A:1023:G:N3    | 1:A:1023:G:H2'   | 2.33                     | 0.42              |
| 1:A:1361:G:H2'   | 1:A:1361(A):C:H6 | 1.84                     | 0.42              |
| 1:A:554:C:C2'    | 1:A:555:C:H5'    | 2.49                     | 0.42              |
| 1:A:788:U:H2'    | 1:A:789:U:C6     | 2.54                     | 0.42              |
| 2:B:49:GLU:O     | 2:B:52:GLU:HB3   | 2.19                     | 0.42              |
| 4:D:67:ILE:O     | 4:D:114:ARG:HD2  | 2.18                     | 0.42              |
| 10:J:47:PHE:HB2  | 10:J:63:PHE:HB2  | 2.01                     | 0.42              |
| 13:M:22:ILE:HB   | 13:M:25:ILE:HB   | 2.01                     | 0.42              |
| 14:N:22:THR:OG1  | 14:N:33:VAL:HG21 | 2.19                     | 0.42              |
| 14:N:24:CYS:HB3  | 14:N:29:ARG:HB2  | 2.01                     | 0.42              |
| 18:R:58:LEU:HD22 | 18:R:62:GLU:HB3  | 2.00                     | 0.42              |
| 19:S:41:VAL:HB   | 19:S:42:PRO:HD2  | 2.01                     | 0.42              |
| 1:A:1029:C:H1'   | 1:A:1033:G:H1'   | 2.01                     | 0.42              |
| 1:A:1039:C:H2'   | 1:A:1040:U:C6    | 2.54                     | 0.42              |
| 1:A:1063:C:N4    | 1:A:1064:G:C2    | 2.87                     | 0.42              |
| 1:A:1188:A:N7    | 1:A:1189:C:C5    | 2.87                     | 0.42              |
| 1:A:267:C:H2'    | 1:A:268:C:H6     | 1.85                     | 0.42              |
| 1:A:576:G:H3'    | 1:A:577:G:H5''   | 2.01                     | 0.42              |
| 3:C:152:ILE:HB   | 3:C:199:LYS:HB2  | 2.01                     | 0.42              |
| 4:D:13:ARG:NH1   | 4:D:38:TYR:O     | 2.52                     | 0.42              |
| 8:H:119:LEU:H    | 8:H:119:LEU:HD12 | 1.83                     | 0.42              |
| 9:I:17:VAL:HG22  | 9:I:63:ILE:HD12  | 2.01                     | 0.42              |
| 11:K:29:ILE:HD12 | 11:K:30:VAL:N    | 2.34                     | 0.42              |
| 12:L:102:ARG:HE  | 12:L:102:ARG:HB3 | 1.52                     | 0.42              |
| 17:Q:89:LEU:HD22 | 17:Q:89:LEU:HA   | 1.78                     | 0.42              |
| 18:R:44:LEU:HD12 | 18:R:48:GLY:O    | 2.18                     | 0.42              |
| 18:R:53:ARG:NH1  | 18:R:59:SER:HA   | 2.33                     | 0.42              |
| 19:S:30:LEU:O    | 19:S:31:ILE:HB   | 2.18                     | 0.42              |
| 1:A:1178:G:N2    | 1:A:1180:A:H3'   | 2.34                     | 0.42              |
| 1:A:148:G:H2'    | 1:A:149:A:H8     | 1.85                     | 0.42              |
| 1:A:304:U:O2'    | 1:A:305:G:H5'    | 2.18                     | 0.42              |
| 1:A:575:G:O2'    | 1:A:821:G:OP2    | 2.24                     | 0.42              |
| 6:F:95:GLU:HA    | 6:F:96:PRO:HD3   | 1.79                     | 0.42              |
| 7:G:57:GLU:O     | 7:G:61:VAL:HG23  | 2.19                     | 0.42              |
| 7:G:95:ARG:HG3   | 7:G:99:LEU:CD1   | 2.46                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 12:L:28:LYS:HB3   | 12:L:30:ALA:HB2  | 2.01                     | 0.42              |
| 19:S:10:PHE:O     | 19:S:39:THR:HG23 | 2.18                     | 0.42              |
| 20:T:20:LEU:N     | 20:T:20:LEU:HD13 | 2.34                     | 0.42              |
| 20:T:60:GLU:HG3   | 20:T:81:LYS:HD2  | 2.01                     | 0.42              |
| 1:A:134:A:C6      | 1:A:135:C:C2     | 3.08                     | 0.42              |
| 1:A:1502:A:C2     | 1:A:1504:G:C2    | 3.07                     | 0.42              |
| 1:A:328:C:H4'     | 1:A:329:A:H5'    | 2.00                     | 0.42              |
| 1:A:526:C:H3'     | 1:A:527:7MG:O4'  | 2.19                     | 0.42              |
| 1:A:52:G:C5       | 1:A:360:A:C2     | 3.07                     | 0.42              |
| 1:A:561:U:O2'     | 1:A:562:C:P      | 2.78                     | 0.42              |
| 2:B:17:PHE:HA     | 2:B:44:LEU:HD21  | 2.01                     | 0.42              |
| 4:D:187:ARG:HD2   | 4:D:187:ARG:HA   | 1.35                     | 0.42              |
| 5:E:63:ARG:HE     | 5:E:63:ARG:HB2   | 1.53                     | 0.42              |
| 8:H:83:ILE:HA     | 8:H:136:GLU:O    | 2.18                     | 0.42              |
| 9:I:40:LEU:CD1    | 9:I:70:LYS:HD2   | 2.50                     | 0.42              |
| 12:L:66:VAL:HG22  | 12:L:67:THR:H    | 1.82                     | 0.42              |
| 14:N:40:CYS:O     | 14:N:44:LEU:HB3  | 2.20                     | 0.42              |
| 1:A:122:G:O2'     | 1:A:123:C:H5'    | 2.19                     | 0.42              |
| 2:B:21:ARG:HG2    | 2:B:21:ARG:H     | 1.51                     | 0.42              |
| 3:C:61:ALA:O      | 3:C:63:ASN:N     | 2.53                     | 0.42              |
| 4:D:109:GLY:HA3   | 4:D:165:MET:SD   | 2.59                     | 0.42              |
| 4:D:24:GLU:O      | 4:D:25:ARG:HB3   | 2.19                     | 0.42              |
| 5:E:139:LEU:HA    | 5:E:142:LEU:HG   | 2.02                     | 0.42              |
| 5:E:24:ARG:O      | 5:E:25:ARG:HG2   | 2.20                     | 0.42              |
| 6:F:9:VAL:HG22    | 6:F:60:PHE:CE2   | 2.55                     | 0.42              |
| 8:H:120:THR:OG1   | 8:H:122:ARG:HG3  | 2.20                     | 0.42              |
| 9:I:124:GLN:HE21  | 9:I:124:GLN:HB2  | 1.57                     | 0.42              |
| 20:T:13:LEU:HD12  | 20:T:14:LYS:N    | 2.34                     | 0.42              |
| 1:A:1130:A:C8     | 1:A:1130:A:OP1   | 2.67                     | 0.42              |
| 1:A:115:G:H1'     | 1:A:116:A:N7     | 2.34                     | 0.42              |
| 1:A:1532:U:H3'    | 1:A:1532:U:H6    | 1.83                     | 0.42              |
| 1:A:719:C:C5      | 1:A:720:C:C4     | 3.07                     | 0.42              |
| 1:A:749:C:O2'     | 1:A:750:G:H5'    | 2.20                     | 0.42              |
| 1:A:986:A:H2'     | 1:A:987:G:O4'    | 2.19                     | 0.42              |
| 5:E:78:HIS:NE2    | 5:E:142:LEU:HA   | 2.35                     | 0.42              |
| 6:F:16:GLN:OE1    | 6:F:16:GLN:HA    | 2.18                     | 0.42              |
| 14:N:57:ARG:HG2   | 14:N:58:LYS:N    | 2.34                     | 0.42              |
| 15:O:70:LEU:HD12  | 15:O:78:TYR:N    | 2.34                     | 0.42              |
| 17:Q:87:LYS:O     | 17:Q:90:ILE:N    | 2.52                     | 0.42              |
| 20:T:100:ILE:HG22 | 20:T:102:GLY:N   | 2.34                     | 0.42              |
| 1:A:99:C:H2'      | 1:A:101:A:C8     | 2.54                     | 0.42              |

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| Atom-1             | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|----------------------|--------------------------|-------------------|
| 1:A:289:G:P        | 24:A:1801:HOH:O      | 2.77                     | 0.42              |
| 1:A:687:A:H2'      | 1:A:701:C:H41        | 1.84                     | 0.42              |
| 1:A:620:C:C2       | 4:D:135:LEU:HD22     | 2.54                     | 0.42              |
| 1:A:437:U:H5''     | 4:D:155:LEU:HD11     | 2.01                     | 0.42              |
| 4:D:186:LEU:N      | 4:D:186:LEU:HD23     | 2.30                     | 0.42              |
| 5:E:153:LYS:HG2    | 5:E:153:LYS:O        | 2.20                     | 0.42              |
| 5:E:43:LEU:HD21    | 5:E:132:ALA:HB1      | 2.01                     | 0.42              |
| 7:G:38:LEU:O       | 7:G:41:ARG:HB3       | 2.18                     | 0.42              |
| 8:H:40:ALA:HB2     | 8:H:45:ILE:CD1       | 2.44                     | 0.42              |
| 11:K:126:ARG:HG3   | 11:K:126:ARG:NH1     | 2.35                     | 0.42              |
| 13:M:3:ARG:O       | 13:M:57:ARG:NE       | 2.50                     | 0.42              |
| 14:N:43:CYS:O      | 14:N:46:GLU:N        | 2.53                     | 0.42              |
| 16:P:36:ILE:HG21   | 16:P:36:ILE:HD13     | 1.76                     | 0.42              |
| 20:T:74:LYS:HE2    | 20:T:74:LYS:HA       | 2.02                     | 0.42              |
| 1:A:1251:A:H2'     | 1:A:1252:A:C8        | 2.55                     | 0.42              |
| 1:A:1239:A:C4      | 1:A:1298:C:N4        | 2.88                     | 0.42              |
| 1:A:642:A:H2'      | 1:A:643:C:H6         | 1.84                     | 0.42              |
| 1:A:807:A:C6       | 1:A:808:C:N4         | 2.87                     | 0.42              |
| 4:D:108:LEU:HA     | 4:D:108:LEU:HD23     | 1.89                     | 0.42              |
| 4:D:89:THR:O       | 4:D:92:VAL:HG12      | 2.20                     | 0.42              |
| 5:E:64:ARG:O       | 5:E:65:ASN:HB3       | 2.19                     | 0.42              |
| 6:F:47:ARG:HH22    | 6:F:56:PRO:HB3       | 1.85                     | 0.42              |
| 7:G:5:ARG:HH21     | 7:G:7:ALA:HA         | 1.84                     | 0.42              |
| 1:A:653:A:O4'      | 8:H:56:LYS:HD3       | 2.19                     | 0.42              |
| 9:I:69:GLY:O       | 9:I:73:GLN:HG3       | 2.19                     | 0.42              |
| 10:J:23:ILE:HD12   | 10:J:72:VAL:HG21     | 2.01                     | 0.42              |
| 10:J:88:LEU:CD2    | 10:J:88:LEU:N        | 2.80                     | 0.42              |
| 19:S:70:LYS:HE3    | 19:S:70:LYS:HB3      | 1.76                     | 0.42              |
| 1:A:1309:G:N1      | 1:A:1329:A:C4        | 2.88                     | 0.42              |
| 1:A:1518[A]:MA6:C6 | 1:A:1519[A]:MA6:H103 | 2.50                     | 0.42              |
| 1:A:514:C:C2'      | 1:A:515:G:H5'        | 2.49                     | 0.42              |
| 1:A:849:C:H2'      | 1:A:850:U:H6         | 1.84                     | 0.42              |
| 5:E:26:PHE:N       | 5:E:26:PHE:CD1       | 2.88                     | 0.42              |
| 5:E:15:ARG:HA      | 5:E:28:PHE:CE2       | 2.55                     | 0.42              |
| 7:G:38:LEU:HD23    | 7:G:38:LEU:HA        | 1.85                     | 0.42              |
| 1:A:363:A:OP2      | 12:L:34:ARG:NH1      | 2.52                     | 0.42              |
| 14:N:14:PRO:C      | 14:N:16:PHE:H        | 2.23                     | 0.42              |
| 1:A:390:C:H4'      | 16:P:28:ARG:HH21     | 1.85                     | 0.42              |
| 1:A:1097:C:H2'     | 1:A:1098:C:C6        | 2.54                     | 0.42              |
| 1:A:1127:G:H8      | 1:A:1127:G:H3'       | 1.83                     | 0.42              |
| 1:A:36:C:O2'       | 12:L:117:ARG:NH2     | 2.53                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:519:C:H2'    | 1:A:520:A:C8     | 2.55                     | 0.42              |
| 2:B:69:LEU:HB3   | 2:B:162:ILE:CD1  | 2.50                     | 0.42              |
| 5:E:98:THR:N     | 5:E:117:ASP:OD1  | 2.53                     | 0.42              |
| 6:F:37:VAL:HG12  | 6:F:39:LYS:O     | 2.20                     | 0.42              |
| 15:O:4:THR:OG1   | 15:O:7:GLU:HG3   | 2.20                     | 0.42              |
| 18:R:78:LEU:H    | 18:R:78:LEU:HG   | 1.60                     | 0.42              |
| 1:A:1316:G:O6    | 19:S:5:LEU:HD21  | 2.20                     | 0.42              |
| 1:A:1108:G:H2'   | 1:A:1109:C:H5'   | 2.02                     | 0.41              |
| 1:A:1112:C:C4    | 3:C:178:LEU:HD12 | 2.55                     | 0.41              |
| 1:A:1326:C:H2'   | 1:A:1327:C:C6    | 2.55                     | 0.41              |
| 1:A:1350:A:H2'   | 1:A:1351:U:C6    | 2.55                     | 0.41              |
| 1:A:579:G:H2'    | 1:A:580:U:C6     | 2.55                     | 0.41              |
| 2:B:209:ARG:HD3  | 2:B:239:VAL:HG11 | 2.02                     | 0.41              |
| 5:E:95:ALA:HB1   | 5:E:96:PRO:HD2   | 2.01                     | 0.41              |
| 9:I:7:THR:O      | 9:I:15:ALA:O     | 2.38                     | 0.41              |
| 1:A:1226:C:H5''  | 19:S:80:TYR:CE2  | 2.54                     | 0.41              |
| 20:T:89:ARG:HG2  | 20:T:90:GLN:N    | 2.35                     | 0.41              |
| 1:A:1107:C:OP1   | 3:C:172:ARG:HB2  | 2.20                     | 0.41              |
| 1:A:1136:U:H2'   | 1:A:1136:U:H6    | 1.61                     | 0.41              |
| 1:A:1453:G:H2'   | 1:A:1454:G:O4'   | 2.20                     | 0.41              |
| 1:A:1497:G:C2'   | 1:A:1498:UR3:H5' | 2.50                     | 0.41              |
| 1:A:257:G:C2     | 1:A:270:A:C2     | 3.08                     | 0.41              |
| 1:A:373:A:C2     | 1:A:482:A:C6     | 3.08                     | 0.41              |
| 1:A:671:G:H2'    | 1:A:671:G:N3     | 2.34                     | 0.41              |
| 1:A:801:U:H2'    | 1:A:802:A:C8     | 2.55                     | 0.41              |
| 1:A:829:G:N2     | 1:A:830:G:H1'    | 2.35                     | 0.41              |
| 2:B:100:GLY:O    | 2:B:104:ASN:N    | 2.50                     | 0.41              |
| 2:B:213:LEU:O    | 2:B:217:ARG:HG2  | 2.20                     | 0.41              |
| 2:B:74:LYS:NZ    | 2:B:76:GLN:HG3   | 2.35                     | 0.41              |
| 5:E:90:VAL:O     | 5:E:120:THR:HA   | 2.20                     | 0.41              |
| 8:H:5:PRO:O      | 8:H:8:ASP:HB3    | 2.19                     | 0.41              |
| 15:O:29:VAL:HG21 | 15:O:67:LEU:HG   | 2.03                     | 0.41              |
| 1:A:1026:G:C3'   | 1:A:1026:G:C8    | 3.02                     | 0.41              |
| 1:A:146:G:C2     | 1:A:147:G:C8     | 3.09                     | 0.41              |
| 1:A:273:A:N6     | 1:A:274:A:C6     | 2.89                     | 0.41              |
| 1:A:289:G:N2     | 1:A:290:C:C2     | 2.88                     | 0.41              |
| 1:A:33:A:O2'     | 1:A:363:A:H1'    | 2.20                     | 0.41              |
| 1:A:672:U:H2'    | 1:A:673:G:H8     | 1.86                     | 0.41              |
| 6:F:74:ASP:HA    | 6:F:77:ARG:HH11  | 1.85                     | 0.41              |
| 8:H:99:GLU:O     | 8:H:101:PRO:HD3  | 2.19                     | 0.41              |
| 10:J:80:LYS:HG2  | 10:J:83:GLU:OE2  | 2.21                     | 0.41              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 1:A:552:U:O2'     | 12:L:86:ARG:O       | 2.34                     | 0.41              |
| 13:M:37:THR:HG21  | 13:M:56:LEU:HA      | 2.01                     | 0.41              |
| 13:M:90:LEU:O     | 13:M:93:ARG:HB3     | 2.21                     | 0.41              |
| 1:A:1071:C:H2'    | 1:A:1072:G:C8       | 2.55                     | 0.41              |
| 1:A:1516[A]:G:H2' | 1:A:1518[A]:MA6:OP2 | 2.20                     | 0.41              |
| 1:A:563:A:N7      | 1:A:567:G:H1'       | 2.36                     | 0.41              |
| 1:A:670:G:C4      | 1:A:671:G:C8        | 3.08                     | 0.41              |
| 3:C:75:VAL:O      | 3:C:83:ARG:HD3      | 2.21                     | 0.41              |
| 4:D:124:GLY:HA3   | 4:D:132:ARG:NH1     | 2.35                     | 0.41              |
| 4:D:13:ARG:HD2    | 4:D:36:ARG:O        | 2.21                     | 0.41              |
| 5:E:110:LEU:HD13  | 5:E:118:ILE:HD13    | 2.01                     | 0.41              |
| 5:E:43:LEU:HD12   | 5:E:43:LEU:HA       | 1.72                     | 0.41              |
| 7:G:101:LEU:HD12  | 7:G:101:LEU:H       | 1.84                     | 0.41              |
| 8:H:101:PRO:HG3   | 8:H:133:LEU:HD11    | 2.00                     | 0.41              |
| 1:A:688:G:H5'     | 11:K:46:GLY:O       | 2.19                     | 0.41              |
| 12:L:98:TYR:CD1   | 12:L:98:TYR:N       | 2.89                     | 0.41              |
| 1:A:486:U:C2      | 1:A:487:A:C8        | 3.08                     | 0.41              |
| 1:A:524:G:C6      | 1:A:525:C:N4        | 2.89                     | 0.41              |
| 1:A:667:G:H4'     | 15:O:51:HIS:CE1     | 2.55                     | 0.41              |
| 1:A:996:A:N1      | 1:A:1045:C:O2'      | 2.47                     | 0.41              |
| 1:A:1104:G:H4'    | 2:B:111:ARG:HD3     | 2.03                     | 0.41              |
| 2:B:187:LEU:HD23  | 2:B:187:LEU:HA      | 1.81                     | 0.41              |
| 3:C:77:ILE:CG2    | 3:C:81:GLY:HA2      | 2.47                     | 0.41              |
| 3:C:95:THR:O      | 3:C:97:LYS:N        | 2.53                     | 0.41              |
| 4:D:4:TYR:CE2     | 4:D:11:LEU:HD11     | 2.54                     | 0.41              |
| 6:F:24:GLU:O      | 6:F:27:GLN:N        | 2.53                     | 0.41              |
| 10:J:34:VAL:CG1   | 10:J:74:ILE:HG22    | 2.49                     | 0.41              |
| 10:J:75:ILE:HG22  | 10:J:76:ASN:OD1     | 2.21                     | 0.41              |
| 13:M:105:THR:O    | 13:M:107:ALA:N      | 2.53                     | 0.41              |
| 19:S:36:ARG:HG2   | 19:S:51:VAL:HG12    | 2.02                     | 0.41              |
| 1:A:1417:G:N2     | 1:A:1484:C:N4       | 2.69                     | 0.41              |
| 1:A:179:A:H2'     | 1:A:180:U:H6        | 1.86                     | 0.41              |
| 4:D:6:GLY:O       | 4:D:8:VAL:HG23      | 2.20                     | 0.41              |
| 7:G:26:PHE:CA     | 7:G:101:LEU:HD23    | 2.50                     | 0.41              |
| 1:A:103:C:P       | 20:T:17:ARG:HH12    | 2.41                     | 0.41              |
| 1:A:1220:G:H2'    | 1:A:1221:G:C8       | 2.55                     | 0.41              |
| 1:A:1367:C:C2     | 1:A:1368:G:C8       | 3.08                     | 0.41              |
| 1:A:1469:G:H8     | 1:A:1469:G:O5'      | 2.03                     | 0.41              |
| 1:A:21:G:H2'      | 1:A:22:G:C8         | 2.55                     | 0.41              |
| 1:A:344:A:H5'     | 1:A:345:C:H5        | 1.85                     | 0.41              |
| 1:A:682:G:N1      | 1:A:709:G:C6        | 2.89                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:666:G:C2     | 1:A:741:G:C4      | 3.08                     | 0.41              |
| 1:A:833:U:O2     | 1:A:854:G:C2      | 2.73                     | 0.41              |
| 2:B:52:GLU:HG3   | 2:B:53:ARG:N      | 2.35                     | 0.41              |
| 3:C:45:LYS:NZ    | 3:C:45:LYS:HA     | 2.36                     | 0.41              |
| 4:D:206:PHE:CD2  | 4:D:207:TYR:CD1   | 3.07                     | 0.41              |
| 7:G:18:TYR:N     | 7:G:18:TYR:CD1    | 2.88                     | 0.41              |
| 12:L:42:THR:HA   | 12:L:53:ARG:O     | 2.21                     | 0.41              |
| 18:R:87:ARG:CG   | 18:R:88:LYS:H     | 2.30                     | 0.41              |
| 19:S:18:LYS:HE3  | 19:S:31:ILE:HG12  | 2.01                     | 0.41              |
| 1:A:1023:G:H3'   | 1:A:1024:G:C5'    | 2.49                     | 0.41              |
| 1:A:1134:G:N2    | 1:A:1140:C:N3     | 2.54                     | 0.41              |
| 1:A:1189:C:H5'   | 14:N:58:LYS:NZ    | 2.35                     | 0.41              |
| 1:A:1277:C:H3'   | 1:A:1277:C:H6     | 1.84                     | 0.41              |
| 1:A:1403:C:H3'   | 1:A:1404:5MC:HM51 | 2.02                     | 0.41              |
| 1:A:1464:G:O2'   | 1:A:1465:C:H5'    | 2.21                     | 0.41              |
| 1:A:254:G:C4     | 1:A:255:G:C8      | 3.09                     | 0.41              |
| 1:A:353:A:H5'    | 1:A:353:A:C8      | 2.52                     | 0.41              |
| 1:A:682:G:N3     | 1:A:683:G:C8      | 2.88                     | 0.41              |
| 1:A:806:C:H2'    | 1:A:807:A:C8      | 2.56                     | 0.41              |
| 10:J:23:ILE:HD13 | 10:J:23:ILE:HG21  | 1.86                     | 0.41              |
| 10:J:55:LYS:CG   | 10:J:56:HIS:H     | 2.19                     | 0.41              |
| 1:A:264:U:O2'    | 17:Q:63:ARG:HG2   | 2.20                     | 0.41              |
| 18:R:36:ASN:CG   | 18:R:39:VAL:HG12  | 2.41                     | 0.41              |
| 20:T:45:GLN:HB2  | 20:T:91:LEU:HG    | 2.01                     | 0.41              |
| 1:A:199:G:O2'    | 1:A:200:G:H5'     | 2.21                     | 0.41              |
| 1:A:420:U:O2'    | 1:A:423:G:O6      | 2.30                     | 0.41              |
| 1:A:475:G:H2'    | 1:A:476:G:C8      | 2.56                     | 0.41              |
| 1:A:794:A:H2'    | 1:A:795:C:C6      | 2.55                     | 0.41              |
| 2:B:76:GLN:OE1   | 2:B:207:ALA:N     | 2.54                     | 0.41              |
| 3:C:85:ARG:NH1   | 3:C:86:VAL:HG23   | 2.35                     | 0.41              |
| 7:G:149:ARG:HD2  | 11:K:59:TYR:CD1   | 2.55                     | 0.41              |
| 7:G:15:ASP:HB3   | 7:G:24:THR:HG23   | 2.02                     | 0.41              |
| 7:G:22:LEU:HD23  | 7:G:62:PHE:HE2    | 1.85                     | 0.41              |
| 8:H:24:THR:O     | 8:H:24:THR:HG23   | 2.21                     | 0.41              |
| 10:J:57:LYS:O    | 10:J:60:ARG:NH1   | 2.53                     | 0.41              |
| 10:J:8:LEU:O     | 10:J:69:ASN:HA    | 2.20                     | 0.41              |
| 13:M:15:VAL:CG1  | 13:M:34:LEU:HD21  | 2.51                     | 0.41              |
| 13:M:64:TRP:CD1  | 13:M:64:TRP:N     | 2.84                     | 0.41              |
| 17:Q:51:TYR:N    | 17:Q:51:TYR:CD1   | 2.89                     | 0.41              |
| 1:A:1068:G:N3    | 1:A:1191:A:C2     | 2.89                     | 0.41              |
| 1:A:1326:C:H2'   | 1:A:1327:C:H6     | 1.86                     | 0.41              |

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| Atom-1           | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|---------------------|--------------------------|-------------------|
| 1:A:1428:A:H2'   | 1:A:1429:C:C6       | 2.55                     | 0.41              |
| 1:A:1442:G:N1    | 1:A:1446:A:C6       | 2.89                     | 0.41              |
| 1:A:190(J):U:H2' | 1:A:190(K):G:H8     | 1.84                     | 0.41              |
| 1:A:519:C:H41    | 1:A:533:A:N6        | 2.18                     | 0.41              |
| 1:A:587:G:O2'    | 1:A:588:G:OP2       | 2.32                     | 0.41              |
| 1:A:665:A:C2     | 1:A:732:C:C2        | 3.09                     | 0.41              |
| 2:B:74:LYS:HZ2   | 2:B:74:LYS:HB3      | 1.84                     | 0.41              |
| 5:E:123:LEU:HD23 | 5:E:123:LEU:HA      | 1.73                     | 0.41              |
| 5:E:68:GLU:OE1   | 5:E:68:GLU:N        | 2.54                     | 0.41              |
| 1:A:939:G:H5'    | 7:G:102:ARG:NH1     | 2.36                     | 0.41              |
| 1:A:875:C:H1'    | 8:H:15:ASN:OD1      | 2.21                     | 0.41              |
| 8:H:4:ASP:HA     | 8:H:5:PRO:HD2       | 1.91                     | 0.41              |
| 13:M:59:TYR:O    | 13:M:60:VAL:C       | 2.59                     | 0.41              |
| 1:A:1039:C:O2'   | 1:A:1040:U:O4'      | 2.36                     | 0.41              |
| 1:A:1350:A:OP2   | 9:I:118:LYS:NZ      | 2.35                     | 0.41              |
| 1:A:1415:G:O6    | 1:A:1485:U:C4       | 2.74                     | 0.41              |
| 1:A:1424:C:C4    | 1:A:1425:U:C5       | 3.08                     | 0.41              |
| 1:A:1406:U:H4'   | 1:A:1518[B]:MA6:H1' | 2.03                     | 0.41              |
| 1:A:189:G:H2'    | 1:A:190:C:O4'       | 2.21                     | 0.41              |
| 1:A:696:A:H8     | 1:A:696:A:O5'       | 2.04                     | 0.41              |
| 2:B:60:ASP:OD2   | 2:B:64:ARG:HD2      | 2.21                     | 0.41              |
| 3:C:190:ARG:HG2  | 3:C:190:ARG:H       | 1.65                     | 0.41              |
| 4:D:11:LEU:HD13  | 4:D:66:ARG:HG2      | 2.03                     | 0.41              |
| 6:F:6:VAL:HB     | 6:F:63:TYR:HB2      | 2.03                     | 0.41              |
| 10:J:27:ALA:O    | 10:J:30:SER:N       | 2.54                     | 0.41              |
| 10:J:11:PHE:HE2  | 10:J:67:THR:HG23    | 1.86                     | 0.41              |
| 12:L:111:LYS:HB2 | 12:L:111:LYS:HE2    | 1.83                     | 0.41              |
| 19:S:36:ARG:NH2  | 19:S:75:ALA:O       | 2.54                     | 0.41              |
| 20:T:52:ALA:O    | 20:T:56:MET:HB3     | 2.20                     | 0.41              |
| 1:A:1014:A:H2'   | 1:A:1015:A:C8       | 2.56                     | 0.40              |
| 1:A:1084:G:H5'   | 1:A:1102:A:OP2      | 2.22                     | 0.40              |
| 1:A:1116:C:C2'   | 1:A:1117:G:H5'      | 2.51                     | 0.40              |
| 1:A:459:G:H8     | 1:A:459:G:O5'       | 2.04                     | 0.40              |
| 1:A:569:C:H1'    | 1:A:574:A:C4        | 2.56                     | 0.40              |
| 1:A:855:G:C6     | 1:A:856:C:C4        | 3.09                     | 0.40              |
| 1:A:901:A:C5     | 1:A:902:G:H1'       | 2.57                     | 0.40              |
| 1:A:90:U:H2'     | 1:A:91:C:C6         | 2.56                     | 0.40              |
| 1:A:939:G:OP1    | 7:G:102:ARG:NH1     | 2.50                     | 0.40              |
| 3:C:121:ALA:HB1  | 3:C:189:ALA:HB2     | 2.02                     | 0.40              |
| 5:E:12:LEU:HD23  | 5:E:13:ILE:C        | 2.41                     | 0.40              |
| 13:M:70:LEU:O    | 13:M:74:VAL:HG23    | 2.21                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:755:G:OP2    | 15:O:65:ARG:HD2   | 2.21                     | 0.40              |
| 17:Q:56:VAL:O    | 17:Q:77:VAL:HB    | 2.21                     | 0.40              |
| 1:A:1096:C:C2    | 1:A:1097:C:C5     | 3.10                     | 0.40              |
| 1:A:1116:C:C2    | 1:A:1185:G:C2     | 3.09                     | 0.40              |
| 1:A:1253:G:H1'   | 1:A:1355:G:O2'    | 2.21                     | 0.40              |
| 1:A:1434:A:H61   | 1:A:1467:G:H1'    | 1.86                     | 0.40              |
| 1:A:544:G:C6     | 1:A:545:C:C4      | 3.09                     | 0.40              |
| 1:A:993:G:H4'    | 1:A:994:A:OP2     | 2.20                     | 0.40              |
| 2:B:41:ILE:HG22  | 2:B:42:ILE:N      | 2.36                     | 0.40              |
| 3:C:58:GLU:HB2   | 3:C:65:ALA:HB2    | 2.03                     | 0.40              |
| 4:D:189:PRO:HB2  | 4:D:194:LEU:HD22  | 2.03                     | 0.40              |
| 6:F:77:ARG:O     | 6:F:80:ARG:HB2    | 2.21                     | 0.40              |
| 7:G:26:PHE:CD2   | 7:G:62:PHE:HE1    | 2.39                     | 0.40              |
| 11:K:33:THR:HB   | 11:K:39:PRO:HA    | 2.03                     | 0.40              |
| 12:L:120:TYR:O   | 12:L:122:THR:HG23 | 2.22                     | 0.40              |
| 20:T:73:HIS:HB3  | 20:T:74:LYS:H     | 1.66                     | 0.40              |
| 1:A:1375:A:H4'   | 7:G:29:LYS:HE2    | 2.02                     | 0.40              |
| 1:A:1440:C:H5''  | 1:A:1441:G:OP2    | 2.21                     | 0.40              |
| 1:A:1416:G:N2    | 1:A:1485:U:O2'    | 2.55                     | 0.40              |
| 1:A:1515[B]:C:N4 | 1:A:1520[B]:G:O6  | 2.51                     | 0.40              |
| 1:A:725:G:O2'    | 1:A:726:C:H5'     | 2.20                     | 0.40              |
| 1:A:763:G:H2'    | 1:A:764:C:C6      | 2.57                     | 0.40              |
| 2:B:54:THR:O     | 2:B:58:ILE:HG13   | 2.21                     | 0.40              |
| 3:C:152:ILE:HA   | 3:C:152:ILE:HD13  | 1.70                     | 0.40              |
| 4:D:50:ARG:HA    | 4:D:51:PRO:HD3    | 1.59                     | 0.40              |
| 7:G:16:LEU:HD23  | 9:I:45:ALA:HB2    | 2.02                     | 0.40              |
| 9:I:8:GLY:N      | 9:I:83:ARG:HD2    | 2.36                     | 0.40              |
| 15:O:43:LEU:HA   | 15:O:43:LEU:HD23  | 1.83                     | 0.40              |
| 6:F:62:TRP:HB2   | 18:R:35:ARG:NH1   | 2.36                     | 0.40              |
| 1:A:1133:G:H2'   | 1:A:1134:G:O4'    | 2.21                     | 0.40              |
| 1:A:190(E):U:C2  | 17:Q:63:ARG:NH1   | 2.89                     | 0.40              |
| 1:A:317:G:C2'    | 1:A:318:G:H5'     | 2.51                     | 0.40              |
| 1:A:721:G:O5'    | 1:A:721:G:H8      | 2.04                     | 0.40              |
| 3:C:44:GLU:HA    | 3:C:52:LEU:HD21   | 2.03                     | 0.40              |
| 3:C:82:GLU:OE2   | 3:C:83:ARG:N      | 2.54                     | 0.40              |
| 1:A:407:G:H4'    | 4:D:116:GLN:HA    | 2.04                     | 0.40              |
| 5:E:118:ILE:O    | 5:E:119:LEU:HD23  | 2.21                     | 0.40              |
| 5:E:53:LEU:HD13  | 5:E:53:LEU:HA     | 1.63                     | 0.40              |
| 7:G:74:GLU:OE2   | 7:G:95:ARG:NH2    | 2.49                     | 0.40              |
| 8:H:37:ARG:HH11  | 8:H:37:ARG:HB3    | 1.86                     | 0.40              |
| 8:H:41:ARG:NH1   | 8:H:42:GLU:HG2    | 2.27                     | 0.40              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 10:J:54:PHE:O     | 10:J:55:LYS:HB3  | 2.21                     | 0.40              |
| 14:N:8:GLU:O      | 14:N:11:LYS:HB3  | 2.21                     | 0.40              |
| 15:O:27:VAL:HG12  | 15:O:31:LEU:HD22 | 2.04                     | 0.40              |
| 15:O:5:LYS:O      | 15:O:9:GLN:HB2   | 2.22                     | 0.40              |
| 17:Q:66:SER:O     | 17:Q:70:ARG:NH1  | 2.54                     | 0.40              |
| 19:S:31:ILE:HA    | 19:S:32:LYS:NZ   | 2.36                     | 0.40              |
| 19:S:40:ILE:HG23  | 19:S:44:MET:SD   | 2.62                     | 0.40              |
| 1:A:1072:G:C6     | 1:A:1073:U:N3    | 2.89                     | 0.40              |
| 1:A:1127:G:C8     | 1:A:1127:G:H3'   | 2.57                     | 0.40              |
| 1:A:965:A:OP1     | 1:A:1198:G:H5''  | 2.21                     | 0.40              |
| 1:A:134:A:C6      | 1:A:135:C:N3     | 2.89                     | 0.40              |
| 1:A:148:G:C2      | 1:A:149:A:C5     | 3.10                     | 0.40              |
| 1:A:392:G:H2'     | 1:A:393:A:H8     | 1.85                     | 0.40              |
| 1:A:302:G:N3      | 1:A:556:C:H4'    | 2.37                     | 0.40              |
| 1:A:745:C:H6      | 1:A:745:C:O5'    | 2.04                     | 0.40              |
| 1:A:673:G:H5''    | 6:F:87:ARG:CZ    | 2.51                     | 0.40              |
| 10:J:91:PRO:O     | 10:J:94:VAL:HG12 | 2.21                     | 0.40              |
| 11:K:120:ARG:HH22 | 11:K:126:ARG:NH1 | 2.19                     | 0.40              |
| 14:N:12:ARG:NH1   | 14:N:21:TYR:O    | 2.55                     | 0.40              |
| 16:P:4:ILE:H      | 16:P:66:PRO:HA   | 1.86                     | 0.40              |
| 1:A:463:A:OP2     | 16:P:75:ARG:NH1  | 2.54                     | 0.40              |
| 18:R:46:GLU:CD    | 18:R:55:ARG:HH22 | 2.24                     | 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     | 232/256 (91%) | 198 (85%) | 29 (12%) | 5 (2%)   | 8 47        |
| 3   | C     | 204/239 (85%) | 175 (86%) | 27 (13%) | 2 (1%)   | 18 61       |
| 4   | D     | 206/209 (99%) | 190 (92%) | 16 (8%)  | 0        | 100 100     |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 5   | E     | 148/162 (91%)   | 139 (94%)  | 6 (4%)    | 3 (2%)   | 9           | 50  |
| 6   | F     | 99/101 (98%)    | 97 (98%)   | 2 (2%)    | 0        | 100         | 100 |
| 7   | G     | 153/156 (98%)   | 137 (90%)  | 16 (10%)  | 0        | 100         | 100 |
| 8   | H     | 136/138 (99%)   | 127 (93%)  | 9 (7%)    | 0        | 100         | 100 |
| 9   | I     | 125/128 (98%)   | 111 (89%)  | 12 (10%)  | 2 (2%)   | 11          | 53  |
| 10  | J     | 96/105 (91%)    | 81 (84%)   | 13 (14%)  | 2 (2%)   | 8           | 48  |
| 11  | K     | 114/129 (88%)   | 99 (87%)   | 15 (13%)  | 0        | 100         | 100 |
| 12  | L     | 121/135 (90%)   | 106 (88%)  | 12 (10%)  | 3 (2%)   | 6           | 45  |
| 13  | M     | 116/126 (92%)   | 94 (81%)   | 21 (18%)  | 1 (1%)   | 20          | 63  |
| 14  | N     | 58/61 (95%)     | 48 (83%)   | 10 (17%)  | 0        | 100         | 100 |
| 15  | O     | 85/89 (96%)     | 78 (92%)   | 7 (8%)    | 0        | 100         | 100 |
| 16  | P     | 81/88 (92%)     | 70 (86%)   | 11 (14%)  | 0        | 100         | 100 |
| 17  | Q     | 97/105 (92%)    | 89 (92%)   | 8 (8%)    | 0        | 100         | 100 |
| 18  | R     | 68/88 (77%)     | 59 (87%)   | 9 (13%)   | 0        | 100         | 100 |
| 19  | S     | 78/93 (84%)     | 67 (86%)   | 9 (12%)   | 2 (3%)   | 6           | 44  |
| 20  | T     | 97/106 (92%)    | 79 (81%)   | 16 (16%)  | 2 (2%)   | 8           | 48  |
| 21  | U     | 22/27 (82%)     | 21 (96%)   | 1 (4%)    | 0        | 100         | 100 |
| All | All   | 2336/2541 (92%) | 2065 (88%) | 249 (11%) | 22 (1%)  | 20          | 63  |

All (22) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 21  | ARG  |
| 12  | L     | 28  | LYS  |
| 19  | S     | 31  | ILE  |
| 2   | B     | 9   | GLU  |
| 3   | C     | 62  | ASP  |
| 9   | I     | 58  | HIS  |
| 2   | B     | 11  | LEU  |
| 5   | E     | 16  | THR  |
| 9   | I     | 119 | ALA  |
| 12  | L     | 25  | PRO  |
| 2   | B     | 78  | GLN  |
| 3   | C     | 27  | LYS  |
| 5   | E     | 118 | ILE  |
| 10  | J     | 35  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | T     | 71  | THR  |
| 12  | L     | 79  | GLU  |
| 19  | S     | 30  | LEU  |
| 10  | J     | 34  | VAL  |
| 13  | M     | 7   | VAL  |
| 5   | E     | 70  | PRO  |
| 2   | B     | 229 | VAL  |
| 20  | T     | 100 | ILE  |

### 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%)  | 150 (74%) | 52 (26%) | 0           | 6  |
| 3   | C     | 160/188 (85%)  | 121 (76%) | 39 (24%) | 1           | 6  |
| 4   | D     | 180/181 (99%)  | 135 (75%) | 45 (25%) | 1           | 6  |
| 5   | E     | 115/123 (94%)  | 88 (76%)  | 27 (24%) | 1           | 7  |
| 6   | F     | 90/90 (100%)   | 72 (80%)  | 18 (20%) | 1           | 12 |
| 7   | G     | 126/127 (99%)  | 103 (82%) | 23 (18%) | 2           | 14 |
| 8   | H     | 119/119 (100%) | 83 (70%)  | 36 (30%) | 0           | 3  |
| 9   | I     | 98/99 (99%)    | 77 (79%)  | 21 (21%) | 1           | 10 |
| 10  | J     | 87/92 (95%)    | 63 (72%)  | 24 (28%) | 0           | 4  |
| 11  | K     | 88/99 (89%)    | 69 (78%)  | 19 (22%) | 1           | 9  |
| 12  | L     | 103/110 (94%)  | 78 (76%)  | 25 (24%) | 1           | 6  |
| 13  | M     | 94/101 (93%)   | 71 (76%)  | 23 (24%) | 1           | 6  |
| 14  | N     | 49/50 (98%)    | 34 (69%)  | 15 (31%) | 0           | 3  |
| 15  | O     | 79/80 (99%)    | 61 (77%)  | 18 (23%) | 1           | 8  |
| 16  | P     | 72/74 (97%)    | 61 (85%)  | 11 (15%) | 3           | 22 |
| 17  | Q     | 94/97 (97%)    | 64 (68%)  | 30 (32%) | 0           | 3  |
| 18  | R     | 61/77 (79%)    | 45 (74%)  | 16 (26%) | 0           | 5  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 19  | S     | 71/80 (89%)     | 52 (73%)   | 19 (27%)  | 0           | 4  |
| 20  | T     | 76/82 (93%)     | 54 (71%)   | 22 (29%)  | 0           | 3  |
| 21  | U     | 19/22 (86%)     | 18 (95%)   | 1 (5%)    | 26          | 64 |
| All | All   | 1983/2111 (94%) | 1499 (76%) | 484 (24%) | 1           | 6  |

All (484) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 8   | LYS  |
| 2   | B     | 12  | GLU  |
| 2   | B     | 19  | HIS  |
| 2   | B     | 20  | GLU  |
| 2   | B     | 21  | ARG  |
| 2   | B     | 24  | TRP  |
| 2   | B     | 33  | TYR  |
| 2   | B     | 51  | LEU  |
| 2   | B     | 52  | GLU  |
| 2   | B     | 53  | ARG  |
| 2   | B     | 67  | THR  |
| 2   | B     | 69  | LEU  |
| 2   | B     | 73  | THR  |
| 2   | B     | 79  | ASP  |
| 2   | B     | 82  | ARG  |
| 2   | B     | 83  | MET  |
| 2   | B     | 84  | GLU  |
| 2   | B     | 87  | ARG  |
| 2   | B     | 90  | MET  |
| 2   | B     | 96  | ARG  |
| 2   | B     | 105 | PHE  |
| 2   | B     | 109 | SER  |
| 2   | B     | 118 | LEU  |
| 2   | B     | 127 | ILE  |
| 2   | B     | 134 | GLU  |
| 2   | B     | 135 | GLN  |
| 2   | B     | 140 | HIS  |
| 2   | B     | 144 | ARG  |
| 2   | B     | 150 | SER  |
| 2   | B     | 154 | LEU  |
| 2   | B     | 155 | LEU  |
| 2   | B     | 157 | ARG  |
| 2   | B     | 160 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 162 | ILE  |
| 2   | B     | 163 | PHE  |
| 2   | B     | 165 | VAL  |
| 2   | B     | 168 | THR  |
| 2   | B     | 169 | LYS  |
| 2   | B     | 170 | GLU  |
| 2   | B     | 172 | ILE  |
| 2   | B     | 174 | VAL  |
| 2   | B     | 175 | ARG  |
| 2   | B     | 178 | ARG  |
| 2   | B     | 184 | VAL  |
| 2   | B     | 187 | LEU  |
| 2   | B     | 205 | ASP  |
| 2   | B     | 206 | ASP  |
| 2   | B     | 213 | LEU  |
| 2   | B     | 221 | LEU  |
| 2   | B     | 223 | ILE  |
| 2   | B     | 226 | ARG  |
| 2   | B     | 239 | VAL  |
| 3   | C     | 3   | ASN  |
| 3   | C     | 12  | LEU  |
| 3   | C     | 14  | ILE  |
| 3   | C     | 15  | THR  |
| 3   | C     | 29  | TYR  |
| 3   | C     | 34  | LEU  |
| 3   | C     | 37  | GLN  |
| 3   | C     | 42  | LEU  |
| 3   | C     | 43  | LEU  |
| 3   | C     | 45  | LYS  |
| 3   | C     | 55  | VAL  |
| 3   | C     | 56  | ASP  |
| 3   | C     | 59  | ARG  |
| 3   | C     | 70  | VAL  |
| 3   | C     | 82  | GLU  |
| 3   | C     | 83  | ARG  |
| 3   | C     | 84  | ILE  |
| 3   | C     | 89  | GLU  |
| 3   | C     | 94  | LEU  |
| 3   | C     | 101 | LEU  |
| 3   | C     | 102 | ASN  |
| 3   | C     | 103 | VAL  |
| 3   | C     | 111 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 116 | VAL  |
| 3   | C     | 119 | ARG  |
| 3   | C     | 120 | VAL  |
| 3   | C     | 122 | GLU  |
| 3   | C     | 138 | VAL  |
| 3   | C     | 144 | SER  |
| 3   | C     | 153 | VAL  |
| 3   | C     | 165 | THR  |
| 3   | C     | 167 | TRP  |
| 3   | C     | 172 | ARG  |
| 3   | C     | 175 | LEU  |
| 3   | C     | 178 | LEU  |
| 3   | C     | 188 | LEU  |
| 3   | C     | 190 | ARG  |
| 3   | C     | 192 | THR  |
| 3   | C     | 204 | LEU  |
| 4   | D     | 3   | ARG  |
| 4   | D     | 5   | ILE  |
| 4   | D     | 19  | LEU  |
| 4   | D     | 21  | LEU  |
| 4   | D     | 25  | ARG  |
| 4   | D     | 26  | CYS  |
| 4   | D     | 28  | SER  |
| 4   | D     | 35  | ARG  |
| 4   | D     | 38  | TYR  |
| 4   | D     | 39  | PRO  |
| 4   | D     | 47  | ARG  |
| 4   | D     | 50  | ARG  |
| 4   | D     | 61  | LYS  |
| 4   | D     | 64  | LEU  |
| 4   | D     | 66  | ARG  |
| 4   | D     | 71  | SER  |
| 4   | D     | 76  | ARG  |
| 4   | D     | 78  | LEU  |
| 4   | D     | 80  | GLU  |
| 4   | D     | 81  | GLU  |
| 4   | D     | 85  | LYS  |
| 4   | D     | 88  | VAL  |
| 4   | D     | 97  | LEU  |
| 4   | D     | 100 | ARG  |
| 4   | D     | 108 | LEU  |
| 4   | D     | 120 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 122 | ARG  |
| 4   | D     | 127 | THR  |
| 4   | D     | 132 | ARG  |
| 4   | D     | 133 | VAL  |
| 4   | D     | 134 | ASP  |
| 4   | D     | 141 | ARG  |
| 4   | D     | 145 | GLU  |
| 4   | D     | 153 | ARG  |
| 4   | D     | 155 | LEU  |
| 4   | D     | 156 | GLU  |
| 4   | D     | 165 | MET  |
| 4   | D     | 181 | MET  |
| 4   | D     | 182 | LYS  |
| 4   | D     | 187 | ARG  |
| 4   | D     | 190 | ASP  |
| 4   | D     | 191 | ARG  |
| 4   | D     | 194 | LEU  |
| 4   | D     | 196 | LEU  |
| 4   | D     | 202 | LEU  |
| 5   | E     | 6   | PHE  |
| 5   | E     | 10  | MET  |
| 5   | E     | 12  | LEU  |
| 5   | E     | 20  | GLN  |
| 5   | E     | 24  | ARG  |
| 5   | E     | 25  | ARG  |
| 5   | E     | 26  | PHE  |
| 5   | E     | 27  | ARG  |
| 5   | E     | 31  | LEU  |
| 5   | E     | 41  | VAL  |
| 5   | E     | 47  | LYS  |
| 5   | E     | 51  | VAL  |
| 5   | E     | 63  | ARG  |
| 5   | E     | 64  | ARG  |
| 5   | E     | 75  | THR  |
| 5   | E     | 78  | HIS  |
| 5   | E     | 79  | GLU  |
| 5   | E     | 87  | SER  |
| 5   | E     | 100 | VAL  |
| 5   | E     | 105 | VAL  |
| 5   | E     | 116 | THR  |
| 5   | E     | 126 | ARG  |
| 5   | E     | 145 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | E     | 148 | VAL  |
| 5   | E     | 150 | ARG  |
| 5   | E     | 151 | LEU  |
| 5   | E     | 153 | LYS  |
| 6   | F     | 10  | LEU  |
| 6   | F     | 24  | GLU  |
| 6   | F     | 25  | ILE  |
| 6   | F     | 30  | LEU  |
| 6   | F     | 36  | ARG  |
| 6   | F     | 39  | LYS  |
| 6   | F     | 43  | LEU  |
| 6   | F     | 45  | LEU  |
| 6   | F     | 47  | ARG  |
| 6   | F     | 55  | ASP  |
| 6   | F     | 61  | LEU  |
| 6   | F     | 70  | ASP  |
| 6   | F     | 74  | ASP  |
| 6   | F     | 80  | ARG  |
| 6   | F     | 82  | ARG  |
| 6   | F     | 83  | ASP  |
| 6   | F     | 93  | SER  |
| 6   | F     | 95  | GLU  |
| 7   | G     | 21  | VAL  |
| 7   | G     | 38  | LEU  |
| 7   | G     | 41  | ARG  |
| 7   | G     | 49  | ILE  |
| 7   | G     | 54  | THR  |
| 7   | G     | 62  | PHE  |
| 7   | G     | 72  | ARG  |
| 7   | G     | 73  | MET  |
| 7   | G     | 75  | VAL  |
| 7   | G     | 78  | ARG  |
| 7   | G     | 79  | ARG  |
| 7   | G     | 92  | SER  |
| 7   | G     | 94  | ARG  |
| 7   | G     | 122 | HIS  |
| 7   | G     | 126 | ASP  |
| 7   | G     | 131 | LYS  |
| 7   | G     | 135 | VAL  |
| 7   | G     | 137 | LYS  |
| 7   | G     | 139 | GLU  |
| 7   | G     | 141 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | G     | 143 | ARG  |
| 7   | G     | 149 | ARG  |
| 7   | G     | 153 | HIS  |
| 8   | H     | 9   | MET  |
| 8   | H     | 12  | ARG  |
| 8   | H     | 18  | ARG  |
| 8   | H     | 22  | GLU  |
| 8   | H     | 23  | SER  |
| 8   | H     | 25  | ASP  |
| 8   | H     | 26  | VAL  |
| 8   | H     | 29  | SER  |
| 8   | H     | 37  | ARG  |
| 8   | H     | 39  | LEU  |
| 8   | H     | 41  | ARG  |
| 8   | H     | 45  | ILE  |
| 8   | H     | 48  | TYR  |
| 8   | H     | 49  | GLU  |
| 8   | H     | 51  | VAL  |
| 8   | H     | 53  | VAL  |
| 8   | H     | 59  | LEU  |
| 8   | H     | 60  | ARG  |
| 8   | H     | 63  | LEU  |
| 8   | H     | 64  | LYS  |
| 8   | H     | 75  | ARG  |
| 8   | H     | 82  | HIS  |
| 8   | H     | 83  | ILE  |
| 8   | H     | 84  | ARG  |
| 8   | H     | 85  | ARG  |
| 8   | H     | 91  | ARG  |
| 8   | H     | 97  | VAL  |
| 8   | H     | 102 | ARG  |
| 8   | H     | 104 | ARG  |
| 8   | H     | 113 | SER  |
| 8   | H     | 119 | LEU  |
| 8   | H     | 120 | THR  |
| 8   | H     | 122 | ARG  |
| 8   | H     | 133 | LEU  |
| 8   | H     | 134 | ILE  |
| 8   | H     | 135 | CYS  |
| 9   | I     | 2   | GLU  |
| 9   | I     | 14  | VAL  |
| 9   | I     | 23  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | I     | 27  | THR  |
| 9   | I     | 42  | ARG  |
| 9   | I     | 56  | LEU  |
| 9   | I     | 65  | VAL  |
| 9   | I     | 79  | LEU  |
| 9   | I     | 85  | LEU  |
| 9   | I     | 91  | ASP  |
| 9   | I     | 96  | LEU  |
| 9   | I     | 102 | LEU  |
| 9   | I     | 108 | VAL  |
| 9   | I     | 111 | ARG  |
| 9   | I     | 113 | LYS  |
| 9   | I     | 116 | LYS  |
| 9   | I     | 118 | LYS  |
| 9   | I     | 121 | ARG  |
| 9   | I     | 124 | GLN  |
| 9   | I     | 126 | SER  |
| 9   | I     | 127 | LYS  |
| 10  | J     | 3   | LYS  |
| 10  | J     | 5   | ARG  |
| 10  | J     | 16  | LEU  |
| 10  | J     | 19  | SER  |
| 10  | J     | 21  | GLN  |
| 10  | J     | 24  | VAL  |
| 10  | J     | 29  | ARG  |
| 10  | J     | 44  | VAL  |
| 10  | J     | 45  | ARG  |
| 10  | J     | 60  | ARG  |
| 10  | J     | 61  | GLU  |
| 10  | J     | 62  | HIS  |
| 10  | J     | 66  | ARG  |
| 10  | J     | 67  | THR  |
| 10  | J     | 69  | ASN  |
| 10  | J     | 71  | LEU  |
| 10  | J     | 72  | VAL  |
| 10  | J     | 76  | ASN  |
| 10  | J     | 79  | ARG  |
| 10  | J     | 81  | THR  |
| 10  | J     | 84  | GLN  |
| 10  | J     | 88  | LEU  |
| 10  | J     | 95  | GLU  |
| 10  | J     | 97  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | K     | 11  | LYS  |
| 11  | K     | 26  | ASN  |
| 11  | K     | 29  | ILE  |
| 11  | K     | 33  | THR  |
| 11  | K     | 36  | ASP  |
| 11  | K     | 47  | VAL  |
| 11  | K     | 51  | LYS  |
| 11  | K     | 62  | GLN  |
| 11  | K     | 66  | LEU  |
| 11  | K     | 67  | ASP  |
| 11  | K     | 75  | TYR  |
| 11  | K     | 82  | VAL  |
| 11  | K     | 83  | ILE  |
| 11  | K     | 87  | THR  |
| 11  | K     | 92  | GLU  |
| 11  | K     | 101 | SER  |
| 11  | K     | 105 | VAL  |
| 11  | K     | 112 | THR  |
| 11  | K     | 119 | CYS  |
| 12  | L     | 6   | THR  |
| 12  | L     | 18  | VAL  |
| 12  | L     | 19  | ARG  |
| 12  | L     | 20  | LYS  |
| 12  | L     | 33  | ARG  |
| 12  | L     | 41  | ARG  |
| 12  | L     | 42  | THR  |
| 12  | L     | 43  | VAL  |
| 12  | L     | 44  | THR  |
| 12  | L     | 46  | LYS  |
| 12  | L     | 47  | LYS  |
| 12  | L     | 52  | LEU  |
| 12  | L     | 59  | ARG  |
| 12  | L     | 60  | LEU  |
| 12  | L     | 61  | THR  |
| 12  | L     | 75  | HIS  |
| 12  | L     | 76  | ASN  |
| 12  | L     | 81  | SER  |
| 12  | L     | 82  | VAL  |
| 12  | L     | 89  | ARG  |
| 12  | L     | 97  | ARG  |
| 12  | L     | 111 | LYS  |
| 12  | L     | 114 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | L     | 123 | LYS  |
| 12  | L     | 126 | LYS  |
| 13  | M     | 3   | ARG  |
| 13  | M     | 4   | ILE  |
| 13  | M     | 29  | ARG  |
| 13  | M     | 35  | GLU  |
| 13  | M     | 45  | VAL  |
| 13  | M     | 46  | LYS  |
| 13  | M     | 48  | LEU  |
| 13  | M     | 50  | GLU  |
| 13  | M     | 54  | VAL  |
| 13  | M     | 63  | THR  |
| 13  | M     | 64  | TRP  |
| 13  | M     | 65  | LYS  |
| 13  | M     | 66  | LEU  |
| 13  | M     | 70  | LEU  |
| 13  | M     | 81  | LEU  |
| 13  | M     | 90  | LEU  |
| 13  | M     | 102 | ARG  |
| 13  | M     | 105 | THR  |
| 13  | M     | 108 | ARG  |
| 13  | M     | 109 | THR  |
| 13  | M     | 115 | LYS  |
| 13  | M     | 116 | THR  |
| 13  | M     | 117 | VAL  |
| 14  | N     | 3   | ARG  |
| 14  | N     | 7   | ILE  |
| 14  | N     | 8   | GLU  |
| 14  | N     | 9   | LYS  |
| 14  | N     | 22  | THR  |
| 14  | N     | 24  | CYS  |
| 14  | N     | 25  | VAL  |
| 14  | N     | 26  | ARG  |
| 14  | N     | 29  | ARG  |
| 14  | N     | 33  | VAL  |
| 14  | N     | 41  | ARG  |
| 14  | N     | 42  | ILE  |
| 14  | N     | 44  | LEU  |
| 14  | N     | 47  | LEU  |
| 14  | N     | 50  | LYS  |
| 15  | O     | 18  | PHE  |
| 15  | O     | 22  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | O     | 29  | VAL  |
| 15  | O     | 31  | LEU  |
| 15  | O     | 32  | LEU  |
| 15  | O     | 38  | ARG  |
| 15  | O     | 39  | LEU  |
| 15  | O     | 47  | LYS  |
| 15  | O     | 49  | ASP  |
| 15  | O     | 57  | LEU  |
| 15  | O     | 62  | GLN  |
| 15  | O     | 63  | ARG  |
| 15  | O     | 66  | LEU  |
| 15  | O     | 70  | LEU  |
| 15  | O     | 76  | GLU  |
| 15  | O     | 77  | ARG  |
| 15  | O     | 79  | ARG  |
| 15  | O     | 82  | ILE  |
| 16  | P     | 1   | MET  |
| 16  | P     | 2   | VAL  |
| 16  | P     | 31  | LYS  |
| 16  | P     | 45  | THR  |
| 16  | P     | 48  | TRP  |
| 16  | P     | 55  | ARG  |
| 16  | P     | 65  | GLN  |
| 16  | P     | 68  | ASP  |
| 16  | P     | 75  | ARG  |
| 16  | P     | 80  | PHE  |
| 16  | P     | 83  | GLU  |
| 17  | Q     | 3   | LYS  |
| 17  | Q     | 5   | VAL  |
| 17  | Q     | 7   | THR  |
| 17  | Q     | 9   | VAL  |
| 17  | Q     | 11  | VAL  |
| 17  | Q     | 13  | ASP  |
| 17  | Q     | 16  | GLN  |
| 17  | Q     | 19  | VAL  |
| 17  | Q     | 22  | LEU  |
| 17  | Q     | 25  | ARG  |
| 17  | Q     | 34  | LYS  |
| 17  | Q     | 36  | ILE  |
| 17  | Q     | 48  | GLU  |
| 17  | Q     | 49  | GLU  |
| 17  | Q     | 53  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | Q     | 59  | ILE  |
| 17  | Q     | 62  | SER  |
| 17  | Q     | 63  | ARG  |
| 17  | Q     | 68  | ARG  |
| 17  | Q     | 75  | ARG  |
| 17  | Q     | 79  | SER  |
| 17  | Q     | 81  | ARG  |
| 17  | Q     | 83  | ASP  |
| 17  | Q     | 86  | GLU  |
| 17  | Q     | 87  | LYS  |
| 17  | Q     | 88  | TYR  |
| 17  | Q     | 89  | LEU  |
| 17  | Q     | 98  | LEU  |
| 17  | Q     | 99  | SER  |
| 17  | Q     | 100 | LYS  |
| 18  | R     | 19  | LYS  |
| 18  | R     | 23  | LYS  |
| 18  | R     | 28  | GLU  |
| 18  | R     | 31  | LEU  |
| 18  | R     | 35  | ARG  |
| 18  | R     | 41  | LYS  |
| 18  | R     | 56  | THR  |
| 18  | R     | 64  | ARG  |
| 18  | R     | 65  | ILE  |
| 18  | R     | 69  | THR  |
| 18  | R     | 76  | LEU  |
| 18  | R     | 79  | LEU  |
| 18  | R     | 83  | GLU  |
| 18  | R     | 85  | LEU  |
| 18  | R     | 86  | VAL  |
| 18  | R     | 88  | LYS  |
| 19  | S     | 3   | ARG  |
| 19  | S     | 5   | LEU  |
| 19  | S     | 6   | LYS  |
| 19  | S     | 7   | LYS  |
| 19  | S     | 9   | VAL  |
| 19  | S     | 13  | ASP  |
| 19  | S     | 15  | LEU  |
| 19  | S     | 17  | GLU  |
| 19  | S     | 20  | LEU  |
| 19  | S     | 22  | LEU  |
| 19  | S     | 28  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19  | S     | 29  | ARG  |
| 19  | S     | 32  | LYS  |
| 19  | S     | 43  | GLU  |
| 19  | S     | 48  | THR  |
| 19  | S     | 70  | LYS  |
| 19  | S     | 77  | THR  |
| 19  | S     | 79  | THR  |
| 19  | S     | 80  | TYR  |
| 20  | T     | 10  | LEU  |
| 20  | T     | 14  | LYS  |
| 20  | T     | 17  | ARG  |
| 20  | T     | 19  | SER  |
| 20  | T     | 20  | LEU  |
| 20  | T     | 22  | ARG  |
| 20  | T     | 24  | LEU  |
| 20  | T     | 27  | LYS  |
| 20  | T     | 36  | LEU  |
| 20  | T     | 41  | ILE  |
| 20  | T     | 45  | GLN  |
| 20  | T     | 46  | GLU  |
| 20  | T     | 48  | LYS  |
| 20  | T     | 50  | GLU  |
| 20  | T     | 53  | LEU  |
| 20  | T     | 56  | MET  |
| 20  | T     | 62  | LEU  |
| 20  | T     | 75  | ASN  |
| 20  | T     | 80  | ARG  |
| 20  | T     | 87  | LYS  |
| 20  | T     | 91  | LEU  |
| 20  | T     | 100 | ILE  |
| 21  | U     | 10  | ARG  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 19  | HIS  |
| 2   | B     | 40  | HIS  |
| 3   | C     | 6   | HIS  |
| 7   | G     | 110 | GLN  |
| 9   | I     | 29  | ASN  |
| 9   | I     | 73  | GLN  |
| 9   | I     | 124 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | J     | 13  | HIS  |
| 10  | J     | 33  | GLN  |
| 15  | O     | 62  | GLN  |
| 20  | T     | 16  | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | A     | 1505/1522 (98%) | 357 (23%)         | 0               |

All (357) RNA backbone outliers are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 4      | U    |
| 1   | A     | 7      | G    |
| 1   | A     | 9      | G    |
| 1   | A     | 12     | U    |
| 1   | A     | 15     | G    |
| 1   | A     | 16     | A    |
| 1   | A     | 30     | U    |
| 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     | 81     | U    |
| 1   | A     | 82     | U    |
| 1   | A     | 83     | U    |
| 1   | A     | 101    | A    |
| 1   | A     | 109    | A    |
| 1   | A     | 115    | G    |
| 1   | A     | 116    | A    |
| 1   | A     | 117    | G    |
| 1   | A     | 121    | C    |
| 1   | A     | 129(A) | G    |
| 1   | A     | 130    | A    |
| 1   | A     | 131    | C    |
| 1   | A     | 145    | G    |
| 1   | A     | 158    | G    |
| 1   | A     | 163    | C    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 179    | A    |
| 1   | A     | 182    | U    |
| 1   | A     | 183    | G    |
| 1   | A     | 190(E) | U    |
| 1   | A     | 195    | A    |
| 1   | A     | 197    | A    |
| 1   | A     | 201    | C    |
| 1   | A     | 202    | U    |
| 1   | A     | 203    | U    |
| 1   | A     | 204    | U    |
| 1   | A     | 216    | G    |
| 1   | A     | 220    | G    |
| 1   | A     | 226    | G    |
| 1   | A     | 231    | G    |
| 1   | A     | 236    | G    |
| 1   | A     | 244    | U    |
| 1   | A     | 245    | C    |
| 1   | A     | 247    | G    |
| 1   | A     | 251    | G    |
| 1   | A     | 253    | U    |
| 1   | A     | 262    | A    |
| 1   | A     | 266    | G    |
| 1   | A     | 267    | C    |
| 1   | A     | 272    | C    |
| 1   | A     | 289    | G    |
| 1   | A     | 291    | C    |
| 1   | A     | 298    | A    |
| 1   | A     | 301    | G    |
| 1   | A     | 315    | A    |
| 1   | A     | 319    | G    |
| 1   | A     | 321    | A    |
| 1   | A     | 328    | C    |
| 1   | A     | 329    | A    |
| 1   | A     | 344    | A    |
| 1   | A     | 345    | C    |
| 1   | A     | 350    | G    |
| 1   | A     | 351    | G    |
| 1   | A     | 352    | C    |
| 1   | A     | 353    | A    |
| 1   | A     | 354    | G    |
| 1   | A     | 356    | A    |
| 1   | A     | 367    | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 371 | G    |
| 1   | A     | 372 | C    |
| 1   | A     | 373 | A    |
| 1   | A     | 384 | G    |
| 1   | A     | 390 | C    |
| 1   | A     | 398 | C    |
| 1   | A     | 406 | G    |
| 1   | A     | 409 | G    |
| 1   | A     | 412 | A    |
| 1   | A     | 413 | G    |
| 1   | A     | 421 | U    |
| 1   | A     | 422 | C    |
| 1   | A     | 424 | G    |
| 1   | A     | 429 | U    |
| 1   | A     | 430 | A    |
| 1   | A     | 439 | A    |
| 1   | A     | 452 | A    |
| 1   | A     | 454 | C    |
| 1   | A     | 456 | C    |
| 1   | A     | 460 | A    |
| 1   | A     | 461 | C    |
| 1   | A     | 462 | G    |
| 1   | A     | 484 | G    |
| 1   | A     | 485 | G    |
| 1   | A     | 486 | U    |
| 1   | A     | 496 | A    |
| 1   | A     | 497 | A    |
| 1   | A     | 498 | U    |
| 1   | A     | 500 | G    |
| 1   | A     | 503 | C    |
| 1   | A     | 504 | C    |
| 1   | A     | 505 | G    |
| 1   | A     | 509 | A    |
| 1   | A     | 510 | A    |
| 1   | A     | 511 | C    |
| 1   | A     | 518 | C    |
| 1   | A     | 519 | C    |
| 1   | A     | 521 | G    |
| 1   | A     | 524 | G    |
| 1   | A     | 526 | C    |
| 1   | A     | 527 | 7MG  |
| 1   | A     | 531 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 532 | A    |
| 1   | A     | 533 | A    |
| 1   | A     | 536 | C    |
| 1   | A     | 545 | C    |
| 1   | A     | 547 | A    |
| 1   | A     | 555 | C    |
| 1   | A     | 559 | A    |
| 1   | A     | 560 | U    |
| 1   | A     | 561 | U    |
| 1   | A     | 562 | C    |
| 1   | A     | 564 | C    |
| 1   | A     | 566 | G    |
| 1   | A     | 568 | G    |
| 1   | A     | 569 | C    |
| 1   | A     | 570 | G    |
| 1   | A     | 572 | A    |
| 1   | A     | 573 | A    |
| 1   | A     | 576 | G    |
| 1   | A     | 577 | G    |
| 1   | A     | 579 | G    |
| 1   | A     | 581 | G    |
| 1   | A     | 587 | G    |
| 1   | A     | 618 | C    |
| 1   | A     | 631 | G    |
| 1   | A     | 650 | G    |
| 1   | A     | 653 | A    |
| 1   | A     | 654 | G    |
| 1   | A     | 664 | G    |
| 1   | A     | 665 | A    |
| 1   | A     | 666 | G    |
| 1   | A     | 667 | G    |
| 1   | A     | 671 | G    |
| 1   | A     | 687 | A    |
| 1   | A     | 695 | A    |
| 1   | A     | 702 | A    |
| 1   | A     | 703 | G    |
| 1   | A     | 705 | U    |
| 1   | A     | 720 | C    |
| 1   | A     | 721 | G    |
| 1   | A     | 722 | A    |
| 1   | A     | 723 | U    |
| 1   | A     | 724 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 730 | G    |
| 1   | A     | 734 | G    |
| 1   | A     | 741 | G    |
| 1   | A     | 749 | C    |
| 1   | A     | 751 | U    |
| 1   | A     | 753 | A    |
| 1   | A     | 755 | G    |
| 1   | A     | 760 | G    |
| 1   | A     | 766 | A    |
| 1   | A     | 774 | G    |
| 1   | A     | 777 | A    |
| 1   | A     | 781 | A    |
| 1   | A     | 782 | A    |
| 1   | A     | 783 | C    |
| 1   | A     | 784 | C    |
| 1   | A     | 787 | A    |
| 1   | A     | 789 | U    |
| 1   | A     | 793 | U    |
| 1   | A     | 794 | A    |
| 1   | A     | 798 | G    |
| 1   | A     | 801 | U    |
| 1   | A     | 802 | A    |
| 1   | A     | 815 | A    |
| 1   | A     | 817 | C    |
| 1   | A     | 818 | G    |
| 1   | A     | 821 | G    |
| 1   | A     | 827 | U    |
| 1   | A     | 828 | A    |
| 1   | A     | 839 | U    |
| 1   | A     | 840 | C    |
| 1   | A     | 841 | U    |
| 1   | A     | 848 | C    |
| 1   | A     | 852 | G    |
| 1   | A     | 858 | G    |
| 1   | A     | 870 | U    |
| 1   | A     | 872 | A    |
| 1   | A     | 873 | A    |
| 1   | A     | 874 | G    |
| 1   | A     | 885 | G    |
| 1   | A     | 922 | G    |
| 1   | A     | 926 | G    |
| 1   | A     | 927 | G    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | A     | 934     | C    |
| 1   | A     | 935     | A    |
| 1   | A     | 937     | A    |
| 1   | A     | 939     | G    |
| 1   | A     | 960     | U    |
| 1   | A     | 965     | A    |
| 1   | A     | 966     | M2G  |
| 1   | A     | 969     | A    |
| 1   | A     | 971     | G    |
| 1   | A     | 972     | C    |
| 1   | A     | 974     | A    |
| 1   | A     | 975     | A    |
| 1   | A     | 976     | G    |
| 1   | A     | 977     | A    |
| 1   | A     | 982     | U    |
| 1   | A     | 993     | G    |
| 1   | A     | 998     | G    |
| 1   | A     | 999     | C    |
| 1   | A     | 1003    | G    |
| 1   | A     | 1003(A) | G    |
| 1   | A     | 1004    | A    |
| 1   | A     | 1005    | A    |
| 1   | A     | 1007    | C    |
| 1   | A     | 1009    | G    |
| 1   | A     | 1016    | A    |
| 1   | A     | 1021    | G    |
| 1   | A     | 1022    | G    |
| 1   | A     | 1024    | G    |
| 1   | A     | 1025    | U    |
| 1   | A     | 1026    | G    |
| 1   | A     | 1027    | C    |
| 1   | A     | 1028    | C    |
| 1   | A     | 1029    | C    |
| 1   | A     | 1030    | C    |
| 1   | A     | 1030(A) | G    |
| 1   | A     | 1030(B) | C    |
| 1   | A     | 1030(C) | G    |
| 1   | A     | 1030(D) | A    |
| 1   | A     | 1031    | G    |
| 1   | A     | 1032    | G    |
| 1   | A     | 1034    | G    |
| 1   | A     | 1035    | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1039 | C    |
| 1   | A     | 1045 | C    |
| 1   | A     | 1050 | G    |
| 1   | A     | 1053 | G    |
| 1   | A     | 1054 | C    |
| 1   | A     | 1055 | A    |
| 1   | A     | 1056 | U    |
| 1   | A     | 1065 | U    |
| 1   | A     | 1079 | G    |
| 1   | A     | 1094 | G    |
| 1   | A     | 1095 | U    |
| 1   | A     | 1100 | C    |
| 1   | A     | 1101 | A    |
| 1   | A     | 1108 | G    |
| 1   | A     | 1118 | C    |
| 1   | A     | 1125 | U    |
| 1   | A     | 1126 | U    |
| 1   | A     | 1127 | G    |
| 1   | A     | 1129 | C    |
| 1   | A     | 1130 | A    |
| 1   | A     | 1131 | G    |
| 1   | A     | 1134 | G    |
| 1   | A     | 1135 | U    |
| 1   | A     | 1136 | U    |
| 1   | A     | 1137 | C    |
| 1   | A     | 1139 | G    |
| 1   | A     | 1140 | C    |
| 1   | A     | 1141 | C    |
| 1   | A     | 1145 | C    |
| 1   | A     | 1146 | A    |
| 1   | A     | 1151 | A    |
| 1   | A     | 1159 | U    |
| 1   | A     | 1160 | G    |
| 1   | A     | 1171 | G    |
| 1   | A     | 1172 | C    |
| 1   | A     | 1174 | G    |
| 1   | A     | 1182 | G    |
| 1   | A     | 1190 | G    |
| 1   | A     | 1196 | U    |
| 1   | A     | 1197 | G    |
| 1   | A     | 1198 | G    |
| 1   | A     | 1201 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1202 | G    |
| 1   | A     | 1203 | C    |
| 1   | A     | 1205 | U    |
| 1   | A     | 1211 | U    |
| 1   | A     | 1212 | U    |
| 1   | A     | 1213 | A    |
| 1   | A     | 1214 | C    |
| 1   | A     | 1224 | G    |
| 1   | A     | 1225 | A    |
| 1   | A     | 1227 | A    |
| 1   | A     | 1233 | G    |
| 1   | A     | 1238 | A    |
| 1   | A     | 1253 | G    |
| 1   | A     | 1256 | A    |
| 1   | A     | 1257 | U    |
| 1   | A     | 1258 | G    |
| 1   | A     | 1259 | C    |
| 1   | A     | 1270 | C    |
| 1   | A     | 1277 | C    |
| 1   | A     | 1278 | U    |
| 1   | A     | 1279 | A    |
| 1   | A     | 1280 | A    |
| 1   | A     | 1286 | A    |
| 1   | A     | 1287 | A    |
| 1   | A     | 1296 | C    |
| 1   | A     | 1298 | C    |
| 1   | A     | 1300 | G    |
| 1   | A     | 1302 | U    |
| 1   | A     | 1307 | U    |
| 1   | A     | 1320 | C    |
| 1   | A     | 1322 | C    |
| 1   | A     | 1323 | G    |
| 1   | A     | 1336 | C    |
| 1   | A     | 1338 | G    |
| 1   | A     | 1353 | G    |
| 1   | A     | 1363 | A    |
| 1   | A     | 1370 | G    |
| 1   | A     | 1379 | G    |
| 1   | A     | 1381 | U    |
| 1   | A     | 1394 | A    |
| 1   | A     | 1398 | A    |
| 1   | A     | 1399 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1400 | 5MC  |
| 1   | A     | 1403 | C    |
| 1   | A     | 1418 | A    |
| 1   | A     | 1428 | A    |
| 1   | A     | 1432 | G    |
| 1   | A     | 1440 | C    |
| 1   | A     | 1442 | G    |
| 1   | A     | 1443 | G    |
| 1   | A     | 1447 | G    |
| 1   | A     | 1451 | A    |
| 1   | A     | 1453 | G    |
| 1   | A     | 1474 | G    |
| 1   | A     | 1475 | G    |
| 1   | A     | 1477 | C    |
| 1   | A     | 1478 | C    |
| 1   | A     | 1479 | C    |
| 1   | A     | 1481 | U    |
| 1   | A     | 1482 | G    |
| 1   | A     | 1485 | U    |
| 1   | A     | 1486 | G    |
| 1   | A     | 1487 | G    |
| 1   | A     | 1491 | G    |
| 1   | A     | 1493 | A    |
| 1   | A     | 1497 | G    |
| 1   | A     | 1498 | UR3  |
| 1   | A     | 1499 | A    |
| 1   | A     | 1502 | A    |
| 1   | A     | 1506 | U    |
| 1   | A     | 1529 | G    |
| 1   | A     | 1530 | G    |
| 1   | A     | 1533 | C    |
| 1   | A     | 1540 | PSU  |
| 1   | A     | 1541 | PSU  |
| 1   | A     | 1542 | U    |
| 1   | A     | 1544 | U    |

There are no RNA pucker outliers to report.

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

17 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 |
| 1   | 2MG  | A     | 1207    | 1,22 | 19,26,27     | 1.60 | 2 (10%)  | 20,38,41    | 2.07 | 3 (15%)  |
| 1   | 5MC  | A     | 1400    | 1    | 15,22,23     | 0.95 | 1 (6%)   | 17,32,35    | 0.86 | 0        |
| 1   | 4OC  | A     | 1402    | 1    | 16,23,24     | 1.12 | 2 (12%)  | 19,32,35    | 0.96 | 1 (5%)   |
| 1   | 5MC  | A     | 1404    | 1    | 15,22,23     | 1.18 | 1 (6%)   | 17,32,35    | 1.01 | 1 (5%)   |
| 1   | 5MC  | A     | 1407    | 1    | 15,22,23     | 1.07 | 1 (6%)   | 17,32,35    | 1.09 | 1 (5%)   |
| 1   | UR3  | A     | 1498    | 1    | 14,22,23     | 1.34 | 2 (14%)  | 16,32,35    | 1.45 | 3 (18%)  |
| 1   | MA6  | A     | 1518[A] | 1    | 16,26,27     | 0.59 | 0        | 18,38,41    | 1.08 | 2 (11%)  |
| 1   | MA6  | A     | 1518[B] | 1    | 16,26,27     | 1.08 | 2 (12%)  | 18,38,41    | 1.03 | 1 (5%)   |
| 1   | MA6  | A     | 1519[A] | 1    | 16,26,27     | 1.08 | 2 (12%)  | 18,38,41    | 1.22 | 2 (11%)  |
| 1   | MA6  | A     | 1519[B] | 1    | 16,26,27     | 1.47 | 4 (25%)  | 18,38,41    | 1.03 | 2 (11%)  |
| 1   | PSU  | A     | 1540    | 1    | 16,21,22     | 0.96 | 1 (6%)   | 20,30,33    | 3.65 | 6 (30%)  |
| 1   | PSU  | A     | 1541    | 1    | 16,21,22     | 1.35 | 3 (18%)  | 20,30,33    | 3.99 | 8 (40%)  |
| 1   | PSU  | A     | 516     | 1,22 | 16,21,22     | 1.27 | 2 (12%)  | 20,30,33    | 4.71 | 6 (30%)  |
| 1   | 7MG  | A     | 527     | 1    | 20,26,27     | 2.32 | 6 (30%)  | 22,39,42    | 1.66 | 6 (27%)  |
| 1   | M2G  | A     | 966     | 1    | 20,27,28     | 1.94 | 5 (25%)  | 21,40,43    | 2.35 | 4 (19%)  |
| 1   | 5MC  | A     | 967     | 1    | 15,22,23     | 0.85 | 1 (6%)   | 17,32,35    | 1.10 | 1 (5%)   |
| 12  | 0TD  | L     | 92      | 12   | 5,9,10       | 2.71 | 1 (20%)  | 3,11,13     | 2.76 | 1 (33%)  |

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

| Mol | Type | Chain | Res     | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|---------|------|---------|-----------|---------|
| 1   | 2MG  | A     | 1207    | 1,22 | -       | 0/5/27/28 | 0/3/3/3 |
| 1   | 5MC  | A     | 1400    | 1    | -       | 0/3/25/26 | 0/2/2/2 |
| 1   | 4OC  | A     | 1402    | 1    | -       | 0/7/29/30 | 0/2/2/2 |
| 1   | 5MC  | A     | 1404    | 1    | -       | 0/3/25/26 | 0/2/2/2 |
| 1   | 5MC  | A     | 1407    | 1    | -       | 0/3/25/26 | 0/2/2/2 |
| 1   | UR3  | A     | 1498    | 1    | -       | 0/3/25/26 | 0/2/2/2 |
| 1   | MA6  | A     | 1518[A] | 1    | -       | 0/7/29/30 | 0/3/3/3 |
| 1   | MA6  | A     | 1518[B] | 1    | -       | 0/7/29/30 | 0/3/3/3 |

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| Mol | Type | Chain | Res     | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|---------|------|---------|-----------|---------|
| 1   | MA6  | A     | 1519[A] | 1    | -       | 0/7/29/30 | 0/3/3/3 |
| 1   | MA6  | A     | 1519[B] | 1    | -       | 0/7/29/30 | 0/3/3/3 |
| 1   | PSU  | A     | 1540    | 1    | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | PSU  | A     | 1541    | 1    | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | PSU  | A     | 516     | 1,22 | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | 7MG  | A     | 527     | 1    | -       | 0/7/37/38 | 0/3/3/3 |
| 1   | M2G  | A     | 966     | 1    | -       | 0/7/29/30 | 0/3/3/3 |
| 1   | 5MC  | A     | 967     | 1    | -       | 0/3/25/26 | 0/2/2/2 |
| 12  | 0TD  | L     | 92      | 12   | -       | 0/2/12/14 | 0/0/0/0 |

All (36) bond length outliers are listed below:

| Mol | Chain | Res     | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|---------|-------|-------------|----------|
| 1   | A     | 527     | 7MG  | C8-N9   | -7.07 | 1.35        | 1.45     |
| 1   | A     | 1541    | PSU  | C5-C1'  | -3.64 | 1.49        | 1.52     |
| 1   | A     | 527     | 7MG  | C2-N1   | -3.42 | 1.29        | 1.35     |
| 1   | A     | 527     | 7MG  | C2-N3   | -3.33 | 1.29        | 1.35     |
| 1   | A     | 1402    | 4OC  | C6-N1   | -3.06 | 1.31        | 1.35     |
| 1   | A     | 966     | M2G  | O5'-C5' | -2.82 | 1.40        | 1.44     |
| 1   | A     | 1407    | 5MC  | C6-C5   | -2.58 | 1.33        | 1.40     |
| 1   | A     | 1402    | 4OC  | O5'-C5' | -2.55 | 1.41        | 1.44     |
| 1   | A     | 516     | PSU  | O4'-C1' | -2.55 | 1.40        | 1.44     |
| 1   | A     | 1498    | UR3  | C3U-N3  | -2.52 | 1.41        | 1.47     |
| 1   | A     | 1404    | 5MC  | O5'-C5' | -2.46 | 1.41        | 1.44     |
| 1   | A     | 1541    | PSU  | O4'-C1' | -2.45 | 1.40        | 1.44     |
| 1   | A     | 527     | 7MG  | C8-N7   | -2.45 | 1.32        | 1.43     |
| 1   | A     | 527     | 7MG  | CM7-N7  | -2.24 | 1.42        | 1.46     |
| 1   | A     | 1498    | UR3  | O5'-C5' | -2.06 | 1.41        | 1.44     |
| 1   | A     | 967     | 5MC  | C6-C5   | -2.00 | 1.34        | 1.40     |
| 1   | A     | 1518[B] | MA6  | C2-N3   | 2.00  | 1.35        | 1.32     |
| 1   | A     | 1518[B] | MA6  | C2-N1   | 2.13  | 1.37        | 1.33     |
| 1   | A     | 966     | M2G  | CM2-N2  | 2.21  | 1.50        | 1.45     |
| 1   | A     | 1400    | 5MC  | C2-N3   | 2.29  | 1.42        | 1.38     |
| 1   | A     | 1519[A] | MA6  | C5-C4   | 2.29  | 1.45        | 1.40     |
| 1   | A     | 1519[B] | MA6  | C4-N3   | 2.41  | 1.39        | 1.35     |
| 1   | A     | 1519[A] | MA6  | C2-N1   | 2.52  | 1.38        | 1.33     |
| 1   | A     | 1519[B] | MA6  | C2-N3   | 2.68  | 1.36        | 1.32     |
| 1   | A     | 1541    | PSU  | C4-N3   | 2.84  | 1.38        | 1.33     |
| 1   | A     | 1540    | PSU  | C4-N3   | 2.91  | 1.38        | 1.33     |
| 1   | A     | 1519[B] | MA6  | C5-C4   | 2.96  | 1.47        | 1.40     |
| 1   | A     | 966     | M2G  | C2-N1   | 3.06  | 1.40        | 1.34     |
| 1   | A     | 1519[B] | MA6  | C2-N1   | 3.09  | 1.39        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 1   | A     | 527  | 7MG  | C2-N2 | 3.51 | 1.41        | 1.34     |
| 1   | A     | 516  | PSU  | C4-N3 | 3.54 | 1.39        | 1.33     |
| 1   | A     | 966  | M2G  | C6-N1 | 4.06 | 1.40        | 1.33     |
| 1   | A     | 1207 | 2MG  | C6-N1 | 4.26 | 1.40        | 1.33     |
| 1   | A     | 1207 | 2MG  | C2-N2 | 4.47 | 1.38        | 1.34     |
| 1   | A     | 966  | M2G  | C2-N2 | 4.98 | 1.42        | 1.34     |
| 12  | L     | 92   | 0TD  | CA-C  | 5.71 | 1.57        | 1.50     |

All (48) bond angle outliers are listed below:

| Mol | Chain | Res     | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-------------|--------|-------------|----------|
| 1   | A     | 516     | PSU  | N1-C2-N3    | -17.36 | 115.92      | 128.40   |
| 1   | A     | 1540    | PSU  | N1-C2-N3    | -12.84 | 119.16      | 128.40   |
| 1   | A     | 1541    | PSU  | N1-C2-N3    | -12.59 | 119.34      | 128.40   |
| 1   | A     | 1541    | PSU  | C5-C4-N3    | -8.42  | 118.52      | 125.43   |
| 1   | A     | 966     | M2G  | C5-C6-N1    | -7.94  | 112.18      | 123.48   |
| 1   | A     | 1207    | 2MG  | C5-C6-N1    | -7.19  | 113.25      | 123.48   |
| 1   | A     | 516     | PSU  | C5-C4-N3    | -6.12  | 120.41      | 125.43   |
| 1   | A     | 1540    | PSU  | C5-C4-N3    | -5.77  | 120.70      | 125.43   |
| 12  | L     | 92      | 0TD  | CSB-SB-CB   | -4.09  | 93.96       | 101.60   |
| 1   | A     | 527     | 7MG  | C5-C4-N3    | -3.99  | 119.81      | 126.47   |
| 1   | A     | 1402    | 4OC  | CM4-N4-C4   | -3.53  | 119.89      | 122.94   |
| 1   | A     | 1541    | PSU  | C5-C1'-C2'  | -3.52  | 109.47      | 115.55   |
| 1   | A     | 1541    | PSU  | C5-C6-N1    | -2.96  | 120.55      | 124.39   |
| 1   | A     | 1540    | PSU  | C5-C1'-C2'  | -2.79  | 110.73      | 115.55   |
| 1   | A     | 1498    | UR3  | C5-C4-N3    | -2.42  | 112.36      | 117.34   |
| 1   | A     | 1518[A] | MA6  | N1-C6-N6    | -2.41  | 114.45      | 117.00   |
| 1   | A     | 516     | PSU  | C5-C6-N1    | -2.27  | 121.45      | 124.39   |
| 1   | A     | 1540    | PSU  | C5-C6-N1    | -2.26  | 121.46      | 124.39   |
| 1   | A     | 527     | 7MG  | C5-C6-N1    | -2.25  | 119.84      | 123.37   |
| 1   | A     | 1404    | 5MC  | CM5-C5-C4   | -2.21  | 119.38      | 121.65   |
| 1   | A     | 1541    | PSU  | O5'-C5'-C4' | 2.00   | 116.06      | 109.01   |
| 1   | A     | 1498    | UR3  | C4'-O4'-C1' | 2.05   | 111.95      | 109.77   |
| 1   | A     | 967     | 5MC  | CM5-C5-C6   | 2.07   | 122.80      | 118.67   |
| 1   | A     | 1518[A] | MA6  | C2-N1-C6    | 2.11   | 116.99      | 111.82   |
| 1   | A     | 1519[B] | MA6  | C2-N1-C6    | 2.11   | 116.99      | 111.82   |
| 1   | A     | 1407    | 5MC  | CM5-C5-C6   | 2.15   | 122.97      | 118.67   |
| 1   | A     | 527     | 7MG  | O5'-C5'-C4' | 2.19   | 116.72      | 109.01   |
| 1   | A     | 527     | 7MG  | C2-N3-C4    | 2.20   | 120.12      | 113.95   |
| 1   | A     | 966     | M2G  | CM2-N2-C2   | 2.26   | 123.49      | 121.34   |
| 1   | A     | 516     | PSU  | O4'-C1'-C2' | 2.31   | 108.16      | 104.45   |
| 1   | A     | 1519[A] | MA6  | C2-N1-C6    | 2.36   | 117.62      | 111.82   |

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| Mol | Chain | Res     | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-------------|------|-------------|----------|
| 1   | A     | 1519[A] | MA6  | N3-C2-N1    | 2.42 | 130.96      | 128.86   |
| 1   | A     | 1541    | PSU  | O4'-C1'-C2' | 2.47 | 108.42      | 104.45   |
| 1   | A     | 1518[B] | MA6  | N3-C2-N1    | 2.50 | 131.03      | 128.86   |
| 1   | A     | 1519[B] | MA6  | N3-C2-N1    | 2.55 | 131.07      | 128.86   |
| 1   | A     | 527     | 7MG  | C6-N1-C2    | 2.64 | 119.86      | 116.06   |
| 1   | A     | 1207    | 2MG  | C4-C5-N7    | 2.82 | 112.13      | 109.41   |
| 1   | A     | 966     | M2G  | C1'-N9-C4   | 2.95 | 131.73      | 126.64   |
| 1   | A     | 1498    | UR3  | O3'-C3'-C2' | 3.08 | 121.69      | 111.83   |
| 1   | A     | 1541    | PSU  | C6-N1-C2    | 3.22 | 120.52      | 115.36   |
| 1   | A     | 1540    | PSU  | C6-N1-C2    | 3.29 | 120.62      | 115.36   |
| 1   | A     | 1207    | 2MG  | C6-N1-C2    | 3.48 | 121.41      | 115.18   |
| 1   | A     | 527     | 7MG  | N3-C4-N9    | 3.83 | 131.87      | 126.98   |
| 1   | A     | 516     | PSU  | C6-N1-C2    | 4.34 | 122.31      | 115.36   |
| 1   | A     | 966     | M2G  | C6-N1-C2    | 5.00 | 122.14      | 116.18   |
| 1   | A     | 1540    | PSU  | C4-N3-C2    | 5.86 | 120.28      | 115.16   |
| 1   | A     | 1541    | PSU  | C4-N3-C2    | 6.28 | 120.65      | 115.16   |
| 1   | A     | 516     | PSU  | C4-N3-C2    | 8.26 | 122.38      | 115.16   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 26 short contacts:

| Mol | Chain | Res     | Type | Clashes | Symm-Clashes |
|-----|-------|---------|------|---------|--------------|
| 1   | A     | 1400    | 5MC  | 2       | 0            |
| 1   | A     | 1402    | 4OC  | 1       | 0            |
| 1   | A     | 1404    | 5MC  | 2       | 0            |
| 1   | A     | 1498    | UR3  | 1       | 0            |
| 1   | A     | 1518[A] | MA6  | 3       | 0            |
| 1   | A     | 1518[B] | MA6  | 4       | 0            |
| 1   | A     | 1519[A] | MA6  | 2       | 0            |
| 1   | A     | 1519[B] | MA6  | 4       | 0            |
| 1   | A     | 1540    | PSU  | 1       | 0            |
| 1   | A     | 1541    | PSU  | 1       | 0            |
| 1   | A     | 516     | PSU  | 1       | 0            |
| 1   | A     | 527     | 7MG  | 3       | 0            |
| 1   | A     | 966     | M2G  | 2       | 0            |
| 1   | A     | 967     | 5MC  | 5       | 0            |



## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 174 ligands modelled in this entry, 174 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.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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     | 1500/1522 (98%) | 0.01   | 28 (1%) 67 58  | 107, 152, 229, 333    | 0     |
| 2   | B     | 234/256 (91%)   | -0.15  | 2 (0%) 84 77   | 122, 170, 240, 274    | 0     |
| 3   | C     | 206/239 (86%)   | -0.05  | 2 (0%) 82 74   | 121, 156, 199, 229    | 0     |
| 4   | D     | 208/209 (99%)   | 0.13   | 19 (9%) 10 8   | 104, 151, 206, 237    | 0     |
| 5   | E     | 150/162 (92%)   | -0.01  | 6 (4%) 39 30   | 93, 132, 172, 216     | 0     |
| 6   | F     | 101/101 (100%)  | -0.43  | 2 (1%) 65 56   | 135, 171, 201, 254    | 0     |
| 7   | G     | 155/156 (99%)   | -0.37  | 7 (4%) 34 27   | 145, 183, 228, 254    | 0     |
| 8   | H     | 138/138 (100%)  | -0.24  | 0 100 100      | 114, 143, 181, 226    | 0     |
| 9   | I     | 127/128 (99%)   | -0.35  | 3 (2%) 59 49   | 149, 182, 222, 246    | 0     |
| 10  | J     | 98/105 (93%)    | 0.10   | 7 (7%) 17 12   | 136, 186, 225, 252    | 0     |
| 11  | K     | 116/129 (89%)   | 0.35   | 11 (9%) 9 8    | 134, 168, 207, 226    | 0     |
| 12  | L     | 123/135 (91%)   | 0.38   | 10 (8%) 13 10  | 106, 137, 168, 224    | 0     |
| 13  | M     | 118/126 (93%)   | 0.48   | 12 (10%) 7 7   | 149, 192, 225, 299    | 0     |
| 14  | N     | 60/61 (98%)     | -0.41  | 0 100 100      | 133, 161, 214, 240    | 0     |
| 15  | O     | 87/89 (97%)     | -0.16  | 0 100 100      | 128, 160, 194, 201    | 0     |
| 16  | P     | 83/88 (94%)     | 0.61   | 8 (9%) 9 8     | 126, 148, 181, 205    | 0     |
| 17  | Q     | 99/105 (94%)    | 0.06   | 5 (5%) 29 23   | 120, 144, 178, 199    | 0     |
| 18  | R     | 70/88 (79%)     | 0.20   | 3 (4%) 36 28   | 131, 165, 237, 266    | 0     |
| 19  | S     | 80/93 (86%)     | 0.39   | 4 (5%) 30 24   | 157, 197, 240, 268    | 0     |
| 20  | T     | 99/106 (93%)    | -0.32  | 1 (1%) 82 74   | 123, 154, 196, 214    | 0     |
| 21  | U     | 24/27 (88%)     | 1.28   | 5 (20%) 1 2    | 172, 194, 241, 254    | 0     |
| All | All   | 3876/4063 (95%) | 0.01   | 135 (3%) 44 35 | 93, 159, 221, 333     | 0     |

All (135) RSRZ outliers are listed below:

| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 1   | A     | 1129    | C    | 5.9  |
| 4   | D     | 35      | ARG  | 5.7  |
| 1   | A     | 1030(D) | A    | 5.6  |
| 1   | A     | 1003    | G    | 5.3  |
| 6   | F     | 101     | ALA  | 4.6  |
| 13  | M     | 2       | ALA  | 4.6  |
| 11  | K     | 31      | THR  | 4.5  |
| 1   | A     | 412     | A    | 4.2  |
| 21  | U     | 18      | TYR  | 4.2  |
| 7   | G     | 2       | ALA  | 4.2  |
| 5   | E     | 19      | MET  | 4.1  |
| 7   | G     | 3       | ARG  | 4.1  |
| 4   | D     | 45      | GLN  | 4.1  |
| 1   | A     | 1283    | G    | 4.0  |
| 1   | A     | 1003(A) | G    | 3.9  |
| 5   | E     | 20      | GLN  | 3.8  |
| 11  | K     | 19      | ALA  | 3.8  |
| 1   | A     | 1031    | G    | 3.7  |
| 16  | P     | 39      | TYR  | 3.7  |
| 10  | J     | 71      | LEU  | 3.6  |
| 12  | L     | 72      | GLY  | 3.5  |
| 13  | M     | 3       | ARG  | 3.5  |
| 11  | K     | 21      | ILE  | 3.5  |
| 13  | M     | 4       | ILE  | 3.4  |
| 4   | D     | 25      | ARG  | 3.4  |
| 4   | D     | 42      | GLN  | 3.4  |
| 4   | D     | 24      | GLU  | 3.3  |
| 1   | A     | 1024    | G    | 3.3  |
| 4   | D     | 40      | PRO  | 3.3  |
| 11  | K     | 118     | GLY  | 3.3  |
| 4   | D     | 29      | PRO  | 3.2  |
| 13  | M     | 10      | PRO  | 3.2  |
| 10  | J     | 39      | PRO  | 3.2  |
| 21  | U     | 17      | THR  | 3.2  |
| 16  | P     | 17      | TYR  | 3.1  |
| 10  | J     | 72      | VAL  | 3.1  |
| 5   | E     | 18      | ARG  | 3.0  |
| 1   | A     | 1002    | G    | 3.0  |
| 5   | E     | 25      | ARG  | 3.0  |
| 10  | J     | 38      | ILE  | 3.0  |
| 16  | P     | 16      | HIS  | 3.0  |
| 19  | S     | 53      | ASN  | 3.0  |
| 11  | K     | 42      | TRP  | 2.9  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 7   | G     | 7       | ALA  | 2.8  |
| 4   | D     | 30      | LYS  | 2.8  |
| 1   | A     | 1027    | C    | 2.8  |
| 12  | L     | 62      | SER  | 2.8  |
| 4   | D     | 13      | ARG  | 2.8  |
| 16  | P     | 6       | LEU  | 2.8  |
| 21  | U     | 24      | ARG  | 2.8  |
| 19  | S     | 77      | THR  | 2.8  |
| 4   | D     | 38      | TYR  | 2.7  |
| 7   | G     | 6       | ARG  | 2.7  |
| 6   | F     | 99      | ALA  | 2.7  |
| 1   | A     | 1282    | C    | 2.7  |
| 12  | L     | 71      | PRO  | 2.7  |
| 1   | A     | 1030(C) | G    | 2.6  |
| 16  | P     | 7       | ALA  | 2.6  |
| 1   | A     | 653     | A    | 2.6  |
| 12  | L     | 28      | LYS  | 2.6  |
| 1   | A     | 1128    | C    | 2.6  |
| 1   | A     | 1334    | G    | 2.6  |
| 4   | D     | 36      | ARG  | 2.6  |
| 16  | P     | 18      | ARG  | 2.5  |
| 1   | A     | 1040    | U    | 2.5  |
| 1   | A     | 1030    | C    | 2.5  |
| 1   | A     | 706     | A    | 2.5  |
| 19  | S     | 78      | ARG  | 2.5  |
| 1   | A     | 1032    | G    | 2.5  |
| 17  | Q     | 45      | HIS  | 2.5  |
| 18  | R     | 29      | PHE  | 2.5  |
| 12  | L     | 31      | PRO  | 2.4  |
| 17  | Q     | 43      | LEU  | 2.4  |
| 3   | C     | 76      | VAL  | 2.4  |
| 5   | E     | 89      | ILE  | 2.4  |
| 11  | K     | 30      | VAL  | 2.4  |
| 9   | I     | 16      | ARG  | 2.4  |
| 7   | G     | 4       | ARG  | 2.4  |
| 13  | M     | 96      | LEU  | 2.4  |
| 4   | D     | 28      | SER  | 2.4  |
| 4   | D     | 110     | PHE  | 2.4  |
| 1   | A     | 1398    | A    | 2.4  |
| 4   | D     | 23      | GLY  | 2.4  |
| 1   | A     | 1026    | G    | 2.4  |
| 7   | G     | 8       | GLU  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 4   | D     | 44   | GLY  | 2.3  |
| 10  | J     | 37   | PRO  | 2.3  |
| 10  | J     | 35   | SER  | 2.3  |
| 13  | M     | 9    | ILE  | 2.3  |
| 12  | L     | 102  | ARG  | 2.3  |
| 1   | A     | 1039 | C    | 2.3  |
| 19  | S     | 32   | LYS  | 2.3  |
| 4   | D     | 34   | GLU  | 2.3  |
| 1   | A     | 1124 | G    | 2.3  |
| 13  | M     | 97   | PRO  | 2.3  |
| 21  | U     | 25   | LYS  | 2.3  |
| 1   | A     | 1127 | G    | 2.3  |
| 1   | A     | 1034 | G    | 2.3  |
| 2   | B     | 28   | PHE  | 2.3  |
| 11  | K     | 111  | ASP  | 2.3  |
| 11  | K     | 29   | ILE  | 2.3  |
| 13  | M     | 19   | LEU  | 2.3  |
| 5   | E     | 17   | ALA  | 2.2  |
| 11  | K     | 28   | THR  | 2.2  |
| 1   | A     | 411  | A    | 2.2  |
| 12  | L     | 120  | TYR  | 2.2  |
| 4   | D     | 112  | VAL  | 2.2  |
| 11  | K     | 20   | TYR  | 2.2  |
| 3   | C     | 52   | LEU  | 2.2  |
| 1   | A     | 3    | G    | 2.2  |
| 1   | A     | 1067 | A    | 2.2  |
| 10  | J     | 40   | LEU  | 2.2  |
| 13  | M     | 15   | VAL  | 2.2  |
| 21  | U     | 21   | TYR  | 2.1  |
| 12  | L     | 87   | GLY  | 2.1  |
| 13  | M     | 11   | ARG  | 2.1  |
| 13  | M     | 45   | VAL  | 2.1  |
| 12  | L     | 32   | PHE  | 2.1  |
| 4   | D     | 157  | LEU  | 2.1  |
| 17  | Q     | 32   | TYR  | 2.1  |
| 20  | T     | 65   | LYS  | 2.1  |
| 7   | G     | 5    | ARG  | 2.1  |
| 13  | M     | 101  | GLN  | 2.1  |
| 9   | I     | 15   | ALA  | 2.1  |
| 17  | Q     | 69   | LYS  | 2.1  |
| 16  | P     | 5    | ARG  | 2.1  |
| 17  | Q     | 71   | PHE  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | B     | 31  | TYR  | 2.0  |
| 18  | R     | 85  | LEU  | 2.0  |
| 9   | I     | 64  | THR  | 2.0  |
| 12  | L     | 100 | ILE  | 2.0  |
| 18  | R     | 43  | PHE  | 2.0  |
| 16  | P     | 8   | ARG  | 2.0  |
| 4   | D     | 7   | PRO  | 2.0  |
| 11  | K     | 50  | TYR  | 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 | RSCC | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|---------|-------|------|------|------|----------------------------|-------|
| 1   | MA6  | A     | 1518[A] | 24/25 | 0.90 | 0.28 | -    | 109,121,135,142            | 24    |
| 1   | 5MC  | A     | 967     | 21/22 | 0.97 | 0.15 | -    | 134,149,157,162            | 0     |
| 1   | MA6  | A     | 1518[B] | 24/25 | 0.90 | 0.28 | -    | 126,134,140,141            | 24    |
| 1   | 4OC  | A     | 1402    | 22/23 | 0.91 | 0.26 | -    | 117,134,153,154            | 0     |
| 1   | PSU  | A     | 516     | 20/21 | 0.91 | 0.15 | -    | 143,152,163,165            | 0     |
| 1   | 2MG  | A     | 1207    | 24/25 | 0.97 | 0.10 | -    | 148,156,161,163            | 0     |
| 1   | 5MC  | A     | 1404    | 21/22 | 0.89 | 0.36 | -    | 132,137,141,146            | 0     |
| 1   | PSU  | A     | 1541    | 20/21 | 0.89 | 0.21 | -    | 232,243,250,252            | 0     |
| 1   | M2G  | A     | 966     | 25/26 | 0.95 | 0.21 | -    | 120,145,181,186            | 0     |
| 1   | MA6  | A     | 1519[B] | 24/25 | 0.94 | 0.38 | -    | 105,117,131,134            | 24    |
| 1   | 7MG  | A     | 527     | 24/25 | 0.88 | 0.25 | -    | 127,137,152,160            | 0     |
| 1   | 5MC  | A     | 1407    | 21/22 | 0.95 | 0.19 | -    | 140,145,154,161            | 0     |
| 12  | 0TD  | L     | 92      | 10/11 | 0.98 | 0.39 | -    | 130,141,148,274            | 0     |
| 1   | MA6  | A     | 1519[A] | 24/25 | 0.94 | 0.38 | -    | 104,118,124,129            | 24    |
| 1   | UR3  | A     | 1498    | 21/22 | 0.95 | 0.32 | -    | 115,130,138,144            | 0     |
| 1   | 5MC  | A     | 1400    | 21/22 | 0.94 | 0.16 | -    | 106,127,151,157            | 0     |
| 1   | PSU  | A     | 1540    | 20/21 | 0.87 | 0.34 | -    | 234,259,275,280            | 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 | RSCC | RSR  | LLDF   | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|--------|----------------------------|-------|
| 22  | MG   | A     | 1675 | 1/1   | 0.24 | 1.45 | 231.56 | 95,95,95,95                | 0     |
| 22  | MG   | A     | 1731 | 1/1   | 0.89 | 1.35 | 33.62  | 185,185,185,185            | 0     |
| 22  | MG   | A     | 1667 | 1/1   | 0.96 | 0.51 | 22.15  | 93,93,93,93                | 0     |
| 22  | MG   | A     | 1617 | 1/1   | 0.79 | 0.53 | 20.65  | 109,109,109,109            | 0     |
| 22  | MG   | A     | 1630 | 1/1   | 0.81 | 1.23 | 20.26  | 127,127,127,127            | 0     |
| 22  | MG   | A     | 1693 | 1/1   | 0.92 | 0.81 | 19.76  | 94,94,94,94                | 0     |
| 22  | MG   | A     | 1678 | 1/1   | 0.89 | 0.99 | 18.60  | 79,79,79,79                | 0     |
| 22  | MG   | A     | 1669 | 1/1   | 0.93 | 0.80 | 13.05  | 89,89,89,89                | 0     |
| 22  | MG   | A     | 1672 | 1/1   | 0.84 | 0.43 | 11.65  | 129,129,129,129            | 0     |
| 22  | MG   | A     | 1690 | 1/1   | 0.95 | 0.42 | 11.00  | 96,96,96,96                | 0     |
| 22  | MG   | A     | 1640 | 1/1   | 0.97 | 0.35 | 7.38   | 141,141,141,141            | 0     |
| 22  | MG   | A     | 1633 | 1/1   | 0.92 | 0.17 | 2.95   | 171,171,171,171            | 0     |
| 22  | MG   | A     | 1666 | 1/1   | 0.96 | 0.32 | 2.82   | 97,97,97,97                | 0     |
| 22  | MG   | A     | 1648 | 1/1   | 0.99 | 0.30 | 2.54   | 227,227,227,227            | 0     |
| 22  | MG   | A     | 1665 | 1/1   | 0.94 | 0.21 | 1.44   | 102,102,102,102            | 0     |
| 22  | MG   | A     | 1700 | 1/1   | 0.99 | 0.18 | 1.29   | 129,129,129,129            | 0     |
| 22  | MG   | A     | 1657 | 1/1   | 0.94 | 0.26 | 1.10   | 95,95,95,95                | 0     |
| 22  | MG   | A     | 1621 | 1/1   | 0.93 | 0.20 | 0.97   | 107,107,107,107            | 0     |
| 22  | MG   | A     | 1685 | 1/1   | 0.90 | 0.18 | 0.76   | 136,136,136,136            | 0     |
| 22  | MG   | A     | 1609 | 1/1   | 0.94 | 0.21 | 0.55   | 140,140,140,140            | 0     |
| 22  | MG   | A     | 1610 | 1/1   | 0.95 | 0.27 | 0.53   | 87,87,87,87                | 0     |
| 22  | MG   | A     | 1652 | 1/1   | 0.87 | 0.39 | 0.49   | 127,127,127,127            | 0     |
| 22  | MG   | A     | 1668 | 1/1   | 0.96 | 0.21 | 0.42   | 115,115,115,115            | 0     |
| 22  | MG   | A     | 1706 | 1/1   | 0.80 | 0.16 | 0.28   | 400,400,400,400            | 0     |
| 22  | MG   | A     | 1722 | 1/1   | 0.59 | 0.34 | 0.23   | 73,73,73,73                | 0     |
| 23  | ZN   | N     | 101  | 1/1   | 1.00 | 0.20 | 0.18   | 148,148,148,148            | 0     |
| 22  | MG   | A     | 1692 | 1/1   | 0.95 | 0.11 | 0.10   | 126,126,126,126            | 0     |
| 22  | MG   | A     | 1661 | 1/1   | 0.88 | 0.14 | -0.31  | 105,105,105,105            | 0     |
| 22  | MG   | D     | 302  | 1/1   | 0.94 | 0.19 | -0.34  | 130,130,130,130            | 0     |
| 22  | MG   | A     | 1682 | 1/1   | 1.00 | 0.40 | -0.36  | 126,126,126,126            | 0     |
| 22  | MG   | A     | 1687 | 1/1   | 0.97 | 0.31 | -0.38  | 157,157,157,157            | 0     |
| 22  | MG   | A     | 1637 | 1/1   | 0.97 | 0.17 | -0.67  | 235,235,235,235            | 0     |
| 23  | ZN   | D     | 301  | 1/1   | 0.99 | 0.23 | -1.13  | 136,136,136,136            | 0     |
| 22  | MG   | A     | 1662 | 1/1   | 0.94 | 0.24 | -1.24  | 110,110,110,110            | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 22  | MG   | K     | 202  | 1/1   | 0.90 | 0.07 | -1.38 | 110,110,110,110             | 0     |
| 22  | MG   | A     | 1710 | 1/1   | 0.91 | 0.07 | -1.43 | 470,470,470,470             | 0     |
| 22  | MG   | A     | 1711 | 1/1   | 0.94 | 0.13 | -1.70 | 398,398,398,398             | 0     |
| 22  | MG   | A     | 1654 | 1/1   | 0.96 | 0.09 | -1.73 | 105,105,105,105             | 0     |
| 22  | MG   | A     | 1655 | 1/1   | 0.98 | 0.14 | -1.92 | 96,96,96,96                 | 0     |
| 22  | MG   | A     | 1713 | 1/1   | 0.96 | 0.13 | -1.99 | 192,192,192,192             | 0     |
| 22  | MG   | A     | 1746 | 1/1   | 0.88 | 0.07 | -2.59 | 185,185,185,185             | 0     |
| 22  | MG   | A     | 1604 | 1/1   | 0.99 | 0.11 | -2.74 | 90,90,90,90                 | 0     |
| 22  | MG   | A     | 1618 | 1/1   | 0.98 | 0.19 | -2.87 | 147,147,147,147             | 0     |
| 22  | MG   | A     | 1697 | 1/1   | 0.97 | 0.09 | -3.08 | 411,411,411,411             | 0     |
| 22  | MG   | A     | 1724 | 1/1   | 0.97 | 0.11 | -3.09 | 290,290,290,290             | 0     |
| 22  | MG   | A     | 1723 | 1/1   | 0.99 | 0.10 | -3.10 | 181,181,181,181             | 0     |
| 22  | MG   | A     | 1626 | 1/1   | 0.97 | 0.14 | -3.73 | 108,108,108,108             | 0     |
| 22  | MG   | A     | 1673 | 1/1   | 0.84 | 0.32 | -     | 121,121,121,121             | 0     |
| 22  | MG   | A     | 1716 | 1/1   | 0.86 | 0.25 | -     | 497,497,497,497             | 0     |
| 22  | MG   | A     | 1696 | 1/1   | 0.92 | 0.19 | -     | 390,390,390,390             | 0     |
| 22  | MG   | A     | 1718 | 1/1   | 1.00 | 0.18 | -     | 111,111,111,111             | 0     |
| 22  | MG   | A     | 1683 | 1/1   | 0.91 | 0.06 | -     | 264,264,264,264             | 0     |
| 22  | MG   | A     | 1632 | 1/1   | 0.33 | 0.58 | -     | 161,161,161,161             | 0     |
| 22  | MG   | A     | 1625 | 1/1   | 0.98 | 0.30 | -     | 123,123,123,123             | 0     |
| 22  | MG   | A     | 1751 | 1/1   | 0.57 | 1.18 | -     | 170,170,170,170             | 0     |
| 22  | MG   | A     | 1749 | 1/1   | 0.78 | 1.28 | -     | 134,134,134,134             | 0     |
| 22  | MG   | A     | 1664 | 1/1   | 0.97 | 0.12 | -     | 101,101,101,101             | 0     |
| 22  | MG   | A     | 1734 | 1/1   | 0.77 | 0.19 | -     | 136,136,136,136             | 0     |
| 22  | MG   | A     | 1622 | 1/1   | 0.82 | 0.53 | -     | 88,88,88,88                 | 0     |
| 22  | MG   | A     | 1613 | 1/1   | 0.83 | 0.80 | -     | 88,88,88,88                 | 0     |
| 22  | MG   | A     | 1744 | 1/1   | 0.80 | 0.15 | -     | 115,115,115,115             | 0     |
| 22  | MG   | A     | 1624 | 1/1   | 0.96 | 0.10 | -     | 114,114,114,114             | 0     |
| 22  | MG   | A     | 1760 | 1/1   | 0.68 | 0.47 | -     | 121,121,121,121             | 0     |
| 22  | MG   | A     | 1645 | 1/1   | 0.99 | 0.17 | -     | 141,141,141,141             | 0     |
| 22  | MG   | A     | 1759 | 1/1   | 0.93 | 1.01 | -     | 132,132,132,132             | 0     |
| 22  | MG   | A     | 1608 | 1/1   | 0.97 | 0.11 | -     | 143,143,143,143             | 0     |
| 22  | MG   | A     | 1628 | 1/1   | 0.64 | 0.28 | -     | 127,127,127,127             | 0     |
| 22  | MG   | A     | 1607 | 1/1   | 0.91 | 0.11 | -     | 134,134,134,134             | 0     |
| 22  | MG   | A     | 1647 | 1/1   | 0.94 | 0.97 | -     | 141,141,141,141             | 0     |
| 22  | MG   | A     | 1708 | 1/1   | 0.94 | 0.09 | -     | 262,262,262,262             | 0     |
| 22  | MG   | A     | 1679 | 1/1   | 0.88 | 0.52 | -     | 140,140,140,140             | 0     |
| 22  | MG   | A     | 1677 | 1/1   | 0.97 | 0.79 | -     | 89,89,89,89                 | 0     |
| 22  | MG   | A     | 1764 | 1/1   | 0.79 | 0.51 | -     | 132,132,132,132             | 0     |
| 22  | MG   | A     | 1727 | 1/1   | 0.90 | 0.29 | -     | 92,92,92,92                 | 0     |
| 22  | MG   | G     | 201  | 1/1   | 0.09 | 1.05 | -     | 157,157,157,157             | 0     |
| 22  | MG   | A     | 1753 | 1/1   | 0.79 | 0.71 | -     | 118,118,118,118             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 22  | MG   | A     | 1686 | 1/1   | 0.98 | 0.12 | -    | 118,118,118,118             | 0     |
| 22  | MG   | A     | 1733 | 1/1   | 0.95 | 0.14 | -    | 143,143,143,143             | 0     |
| 22  | MG   | A     | 1741 | 1/1   | 0.71 | 0.29 | -    | 111,111,111,111             | 0     |
| 22  | MG   | A     | 1620 | 1/1   | 0.97 | 0.15 | -    | 114,114,114,114             | 0     |
| 22  | MG   | A     | 1736 | 1/1   | 0.52 | 0.53 | -    | 112,112,112,112             | 0     |
| 22  | MG   | A     | 1650 | 1/1   | 0.74 | 0.43 | -    | 120,120,120,120             | 0     |
| 22  | MG   | A     | 1763 | 1/1   | 0.92 | 0.20 | -    | 148,148,148,148             | 0     |
| 22  | MG   | A     | 1717 | 1/1   | 0.99 | 0.19 | -    | 254,254,254,254             | 0     |
| 22  | MG   | A     | 1699 | 1/1   | 0.97 | 0.09 | -    | 426,426,426,426             | 0     |
| 22  | MG   | A     | 1671 | 1/1   | 0.91 | 0.84 | -    | 108,108,108,108             | 0     |
| 22  | MG   | A     | 1656 | 1/1   | 0.98 | 0.14 | -    | 68,68,68,68                 | 0     |
| 22  | MG   | A     | 1735 | 1/1   | 0.77 | 0.32 | -    | 143,143,143,143             | 0     |
| 22  | MG   | A     | 1635 | 1/1   | 0.92 | 0.06 | -    | 129,129,129,129             | 0     |
| 22  | MG   | A     | 1623 | 1/1   | 0.95 | 0.42 | -    | 90,90,90,90                 | 0     |
| 22  | MG   | A     | 1643 | 1/1   | 0.85 | 0.19 | -    | 245,245,245,245             | 0     |
| 22  | MG   | A     | 1739 | 1/1   | 0.98 | 0.46 | -    | 96,96,96,96                 | 0     |
| 22  | MG   | A     | 1761 | 1/1   | 0.88 | 0.10 | -    | 148,148,148,148             | 0     |
| 22  | MG   | K     | 201  | 1/1   | 0.92 | 0.44 | -    | 93,93,93,93                 | 0     |
| 22  | MG   | A     | 1704 | 1/1   | 0.97 | 0.08 | -    | 436,436,436,436             | 0     |
| 22  | MG   | A     | 1743 | 1/1   | 0.95 | 0.35 | -    | 104,104,104,104             | 0     |
| 22  | MG   | A     | 1659 | 1/1   | 0.89 | 0.17 | -    | 100,100,100,100             | 0     |
| 22  | MG   | A     | 1644 | 1/1   | 0.91 | 0.20 | -    | 279,279,279,279             | 0     |
| 22  | MG   | A     | 1740 | 1/1   | 0.95 | 0.18 | -    | 130,130,130,130             | 0     |
| 22  | MG   | A     | 1603 | 1/1   | 0.94 | 0.09 | -    | 184,184,184,184             | 0     |
| 22  | MG   | A     | 1688 | 1/1   | 0.99 | 0.37 | -    | 84,84,84,84                 | 0     |
| 22  | MG   | A     | 1691 | 1/1   | 0.94 | 0.08 | -    | 109,109,109,109             | 0     |
| 22  | MG   | A     | 1642 | 1/1   | 0.94 | 0.08 | -    | 191,191,191,191             | 0     |
| 22  | MG   | A     | 1602 | 1/1   | 0.99 | 0.13 | -    | 114,114,114,114             | 0     |
| 22  | MG   | A     | 1732 | 1/1   | 0.11 | 0.14 | -    | 161,161,161,161             | 0     |
| 22  | MG   | A     | 1627 | 1/1   | 0.99 | 0.23 | -    | 121,121,121,121             | 0     |
| 22  | MG   | A     | 1660 | 1/1   | 0.91 | 0.45 | -    | 107,107,107,107             | 0     |
| 22  | MG   | A     | 1695 | 1/1   | 0.90 | 0.08 | -    | 184,184,184,184             | 0     |
| 22  | MG   | A     | 1663 | 1/1   | 0.95 | 0.41 | -    | 122,122,122,122             | 0     |
| 22  | MG   | F     | 201  | 1/1   | 0.87 | 0.26 | -    | 127,127,127,127             | 0     |
| 22  | MG   | H     | 201  | 1/1   | 0.84 | 0.21 | -    | 83,83,83,83                 | 0     |
| 22  | MG   | A     | 1681 | 1/1   | 0.88 | 0.70 | -    | 107,107,107,107             | 0     |
| 22  | MG   | A     | 1725 | 1/1   | 0.99 | 0.24 | -    | 114,114,114,114             | 0     |
| 22  | MG   | A     | 1702 | 1/1   | 0.95 | 0.08 | -    | 259,259,259,259             | 0     |
| 22  | MG   | A     | 1601 | 1/1   | 0.62 | 0.64 | -    | 96,96,96,96                 | 0     |
| 22  | MG   | A     | 1726 | 1/1   | 0.89 | 0.15 | -    | 127,127,127,127             | 0     |
| 22  | MG   | A     | 1715 | 1/1   | 0.83 | 0.09 | -    | 167,167,167,167             | 0     |
| 22  | MG   | A     | 1754 | 1/1   | 0.47 | 0.35 | -    | 121,121,121,121             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 22  | MG   | A     | 1742 | 1/1   | 0.75 | 0.32 | -    | 97,97,97,97                 | 0     |
| 22  | MG   | A     | 1709 | 1/1   | 0.99 | 0.08 | -    | 354,354,354,354             | 0     |
| 22  | MG   | A     | 1658 | 1/1   | 0.92 | 0.26 | -    | 130,130,130,130             | 0     |
| 22  | MG   | A     | 1674 | 1/1   | 0.77 | 0.31 | -    | 114,114,114,114             | 0     |
| 22  | MG   | A     | 1719 | 1/1   | 0.98 | 0.09 | -    | 320,320,320,320             | 0     |
| 22  | MG   | A     | 1653 | 1/1   | 0.60 | 1.57 | -    | 100,100,100,100             | 0     |
| 22  | MG   | A     | 1721 | 1/1   | 0.94 | 0.12 | -    | 259,259,259,259             | 0     |
| 22  | MG   | A     | 1646 | 1/1   | 0.79 | 0.19 | -    | 153,153,153,153             | 0     |
| 22  | MG   | A     | 1680 | 1/1   | 0.98 | 0.13 | -    | 134,134,134,134             | 0     |
| 22  | MG   | A     | 1605 | 1/1   | 0.77 | 0.24 | -    | 293,293,293,293             | 0     |
| 22  | MG   | A     | 1714 | 1/1   | 0.96 | 0.13 | -    | 200,200,200,200             | 0     |
| 22  | MG   | A     | 1676 | 1/1   | 0.88 | 0.20 | -    | 153,153,153,153             | 0     |
| 22  | MG   | A     | 1638 | 1/1   | 0.78 | 0.56 | -    | 95,95,95,95                 | 0     |
| 22  | MG   | A     | 1670 | 1/1   | 0.96 | 0.94 | -    | 111,111,111,111             | 0     |
| 22  | MG   | A     | 1651 | 1/1   | 0.96 | 0.27 | -    | 95,95,95,95                 | 0     |
| 22  | MG   | A     | 1615 | 1/1   | 0.88 | 0.54 | -    | 92,92,92,92                 | 0     |
| 22  | MG   | A     | 1737 | 1/1   | 0.62 | 0.60 | -    | 143,143,143,143             | 0     |
| 22  | MG   | S     | 101  | 1/1   | 0.63 | 0.24 | -    | 137,137,137,137             | 0     |
| 22  | MG   | A     | 1748 | 1/1   | 0.97 | 1.40 | -    | 97,97,97,97                 | 0     |
| 22  | MG   | A     | 1747 | 1/1   | 0.56 | 0.83 | -    | 102,102,102,102             | 0     |
| 22  | MG   | A     | 1616 | 1/1   | 0.97 | 0.21 | -    | 127,127,127,127             | 0     |
| 22  | MG   | A     | 1752 | 1/1   | 0.57 | 0.61 | -    | 156,156,156,156             | 0     |
| 22  | MG   | A     | 1758 | 1/1   | 0.84 | 1.46 | -    | 139,139,139,139             | 0     |
| 22  | MG   | A     | 1730 | 1/1   | 0.90 | 0.22 | -    | 181,181,181,181             | 0     |
| 22  | MG   | A     | 1694 | 1/1   | 0.91 | 0.09 | -    | 244,244,244,244             | 0     |
| 22  | MG   | A     | 1639 | 1/1   | 0.89 | 0.13 | -    | 133,133,133,133             | 0     |
| 22  | MG   | A     | 1689 | 1/1   | 0.75 | 1.29 | -    | 107,107,107,107             | 0     |
| 22  | MG   | A     | 1701 | 1/1   | 0.83 | 0.24 | -    | 383,383,383,383             | 0     |
| 22  | MG   | A     | 1629 | 1/1   | 0.92 | 0.13 | -    | 192,192,192,192             | 0     |
| 22  | MG   | A     | 1745 | 1/1   | 0.89 | 1.42 | -    | 107,107,107,107             | 0     |
| 22  | MG   | A     | 1611 | 1/1   | 0.95 | 0.19 | -    | 153,153,153,153             | 0     |
| 22  | MG   | A     | 1684 | 1/1   | 0.94 | 0.66 | -    | 128,128,128,128             | 0     |
| 22  | MG   | A     | 1712 | 1/1   | 0.99 | 0.64 | -    | 376,376,376,376             | 0     |
| 22  | MG   | A     | 1738 | 1/1   | 0.71 | 0.73 | -    | 126,126,126,126             | 0     |
| 22  | MG   | A     | 1612 | 1/1   | 0.98 | 0.20 | -    | 104,104,104,104             | 0     |
| 22  | MG   | A     | 1707 | 1/1   | 0.80 | 0.11 | -    | 411,411,411,411             | 0     |
| 22  | MG   | A     | 1728 | 1/1   | 0.42 | 0.15 | -    | 120,120,120,120             | 0     |
| 22  | MG   | A     | 1762 | 1/1   | 0.73 | 0.27 | -    | 136,136,136,136             | 0     |
| 22  | MG   | A     | 1614 | 1/1   | 0.81 | 0.87 | -    | 113,113,113,113             | 0     |
| 22  | MG   | A     | 1641 | 1/1   | 0.99 | 0.27 | -    | 96,96,96,96                 | 0     |
| 22  | MG   | A     | 1705 | 1/1   | 0.89 | 0.10 | -    | 310,310,310,310             | 0     |
| 22  | MG   | A     | 1720 | 1/1   | 0.92 | 0.06 | -    | 324,324,324,324             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 22  | MG   | A     | 1698 | 1/1   | 0.80 | 0.12 | -    | 424,424,424,424             | 0     |
| 22  | MG   | A     | 1636 | 1/1   | 0.98 | 0.59 | -    | 186,186,186,186             | 0     |
| 22  | MG   | A     | 1756 | 1/1   | 0.45 | 0.17 | -    | 132,132,132,132             | 0     |
| 22  | MG   | A     | 1757 | 1/1   | 0.95 | 0.93 | -    | 121,121,121,121             | 0     |
| 22  | MG   | A     | 1631 | 1/1   | 0.90 | 0.11 | -    | 277,277,277,277             | 0     |
| 22  | MG   | A     | 1750 | 1/1   | 0.53 | 1.45 | -    | 137,137,137,137             | 0     |
| 22  | MG   | A     | 1606 | 1/1   | 0.99 | 0.28 | -    | 154,154,154,154             | 0     |
| 22  | MG   | A     | 1649 | 1/1   | 0.91 | 0.28 | -    | 102,102,102,102             | 0     |
| 22  | MG   | A     | 1703 | 1/1   | 0.89 | 0.37 | -    | 475,475,475,475             | 0     |
| 22  | MG   | A     | 1755 | 1/1   | 0.75 | 0.21 | -    | 148,148,148,148             | 0     |
| 22  | MG   | A     | 1619 | 1/1   | 0.78 | 0.16 | -    | 132,132,132,132             | 0     |
| 22  | MG   | A     | 1729 | 1/1   | 0.68 | 0.77 | -    | 94,94,94,94                 | 0     |
| 22  | MG   | E     | 201  | 1/1   | 0.74 | 0.42 | -    | 95,95,95,95                 | 0     |
| 22  | MG   | A     | 1634 | 1/1   | 0.62 | 0.56 | -    | 113,113,113,113             | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.