



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:16 PM GMT

PDB ID : 3T1H  
Title : Structure of the *Thermus thermophilus* 30S ribosomal subunit complexed with a human anti-codon stem loop (HASL) of transfer RNA lysine 3 (tRNA<sup>Lys</sup>3) bound to an mRNA with an AAA-codon in the A-site and Paromomycin  
Authors : Murphy, F.V.; Vendeix, F.A.P.; Cantara, W.; Leszczynska, G.; Gustilo, E.M.; Sproat, B.; Malkiewicz, A.A.P.; Agris, P.F.  
Deposited on : 2011-07-21  
Resolution : 3.11 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

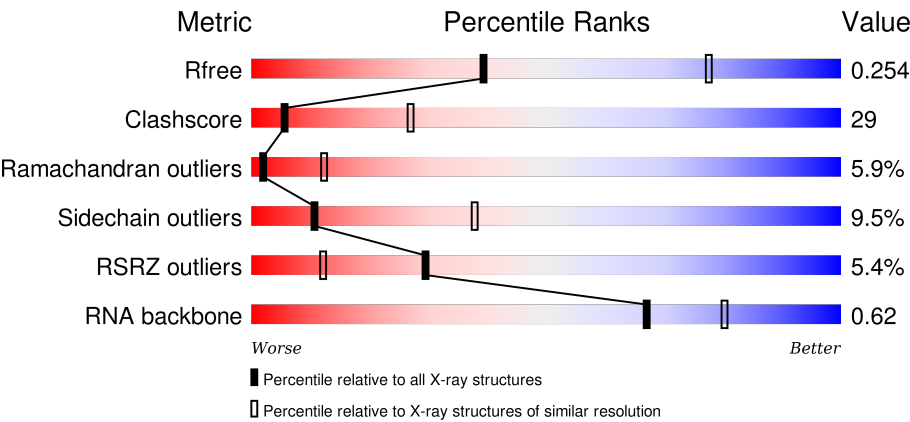
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.11 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 91344                       | 1112 (3.16-3.08)                                      |
| Clashscore            | 102246                      | 1218 (3.16-3.08)                                      |
| Ramachandran outliers | 100387                      | 1175 (3.16-3.08)                                      |
| Sidechain outliers    | 100360                      | 1175 (3.16-3.08)                                      |
| RSRZ outliers         | 91569                       | 1114 (3.16-3.08)                                      |
| RNA backbone          | 2183                        | 1010 (3.54-2.70)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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     | 1513   | <div><div>5%</div><div><div></div><div>37%</div><div>38%</div><div>19%</div><div>5%</div></div></div>             |
| 2   | B     | 256    | <div><div>7%</div><div><div></div><div>28%</div><div>53%</div><div>10%</div><div>9%</div></div></div>             |
| 3   | C     | 239    | <div><div>3%</div><div><div></div><div>35%</div><div>41%</div><div>8%</div><div>•</div><div>14%</div></div></div> |
| 4   | D     | 209    | <div><div>7%</div><div><div></div><div>45%</div><div>47%</div><div>7%</div></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     | 132    |                  |
| 13  | M     | 126    |                  |
| 14  | N     | 61     |                  |
| 15  | O     | 89     |                  |
| 16  | P     | 88     |                  |
| 17  | Q     | 105    |                  |
| 18  | R     | 88     |                  |
| 19  | S     | 93     |                  |
| 20  | T     | 106    |                  |
| 21  | V     | 27     |                  |
| 22  | W     | 3      |                  |
| 23  | X     | 11     |                  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 23  | 12A  | X     | 37   | -         | -        | X       | -                |
| 23  | PSU  | X     | 39   | -         | -        | X       | -                |
| 24  | MG   | A     | 1603 | -         | -        | -       | X                |
| 24  | MG   | A     | 1637 | -         | -        | -       | X                |
| 24  | MG   | A     | 1650 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 24  | MG   | A     | 1667 | -         | -        | -       | X                |
| 24  | MG   | A     | 1680 | -         | -        | -       | X                |
| 24  | MG   | A     | 1683 | -         | -        | -       | X                |
| 24  | MG   | A     | 1707 | -         | -        | -       | X                |
| 24  | MG   | A     | 1737 | -         | -        | -       | X                |
| 24  | MG   | A     | 1749 | -         | -        | -       | X                |
| 24  | MG   | A     | 1755 | -         | -        | -       | X                |
| 24  | MG   | A     | 1756 | -         | -        | -       | X                |
| 24  | MG   | A     | 1757 | -         | -        | -       | X                |
| 24  | MG   | A     | 1762 | -         | -        | -       | X                |
| 24  | MG   | A     | 1779 | -         | -        | -       | X                |
| 25  | ZN   | D     | 301  | -         | -        | -       | X                |

## 2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 52287 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     | 1513     | Total | C     | N    | O     | P    | 22      | 0       | 0     |
|     |       |          | 32515 | 14472 | 6016 | 10514 | 1513 |         |         |       |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference   |
|-------|---------|----------|--------|-----------|-------------|
| A     | 1517    | U        | -      | INSERTION | GB 55771382 |
| A     | 1518    | U        | -      | INSERTION | GB 55771382 |
| A     | 1519    | U        | -      | INSERTION | GB 55771382 |
| A     | 1520    | C        | -      | INSERTION | GB 55771382 |
| A     | 1521    | U        | -      | INSERTION | GB 55771382 |

- Molecule 2 is a protein called 30S 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 30S 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 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

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

- Molecule 6 is a protein called 30S ribosomal protein S6.

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

- Molecule 7 is a protein called 30S ribosomal protein S7.

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

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

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

- Molecule 11 is a protein called 30S ribosomal protein S11.

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

- Molecule 12 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | L     | 124      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 970   | 611 | 195 | 163 | 1 |         |         |       |

- Molecule 13 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | M     | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 997   | 617 | 207 | 171 | 2 |         |         |       |

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

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

- Molecule 17 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17  | Q     | 104      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 857   | 547 | 161 | 147 | 2 |         |         |       |

- Molecule 18 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 18  | R     | 73       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 597   | 380 | 118 | 99 |         |         |       |

- Molecule 19 is a protein called 30S 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 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20  | T     | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 762   | 469 | 162 | 129 | 2 |         |         |       |

- Molecule 21 is a protein called 30S ribosomal protein Thx.

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

- Molecule 22 is a RNA chain called mRNA A-site fragment.

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 22  | W     | 3        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 67    | 30 | 15 | 19 | 3 |         |         |       |

- Molecule 23 is a RNA chain called tRNA ASL human Lys3.

| Mol | Chain | Residues | Atoms |     |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---|---------|---------|-------|
| 23  | X     | 11       | Total | C   | N  | O  | P  | S | 0       | 0       | 0     |
|     |       |          | 247   | 112 | 37 | 85 | 11 | 2 |         |         |       |

- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

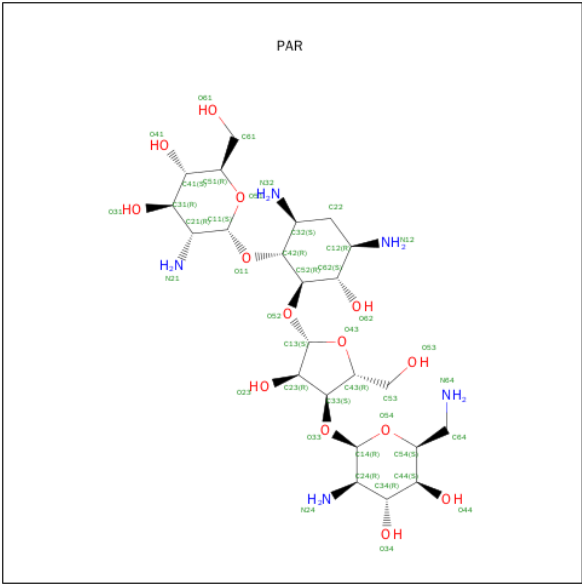
| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 24  | B     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 24  | A     | 182      | Total | Mg  | 0       | 0       |
|     |       |          | 182   | 182 |         |         |
| 24  | L     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 24  | S     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |

- Molecule 25 is ZINC ION (three-letter code: ZN) (formula: Zn).



| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 25  | D     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 25  | N     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 26 is PAROMOMYCIN (three-letter code: PAR) (formula: C<sub>23</sub>H<sub>45</sub>N<sub>5</sub>O<sub>14</sub>).

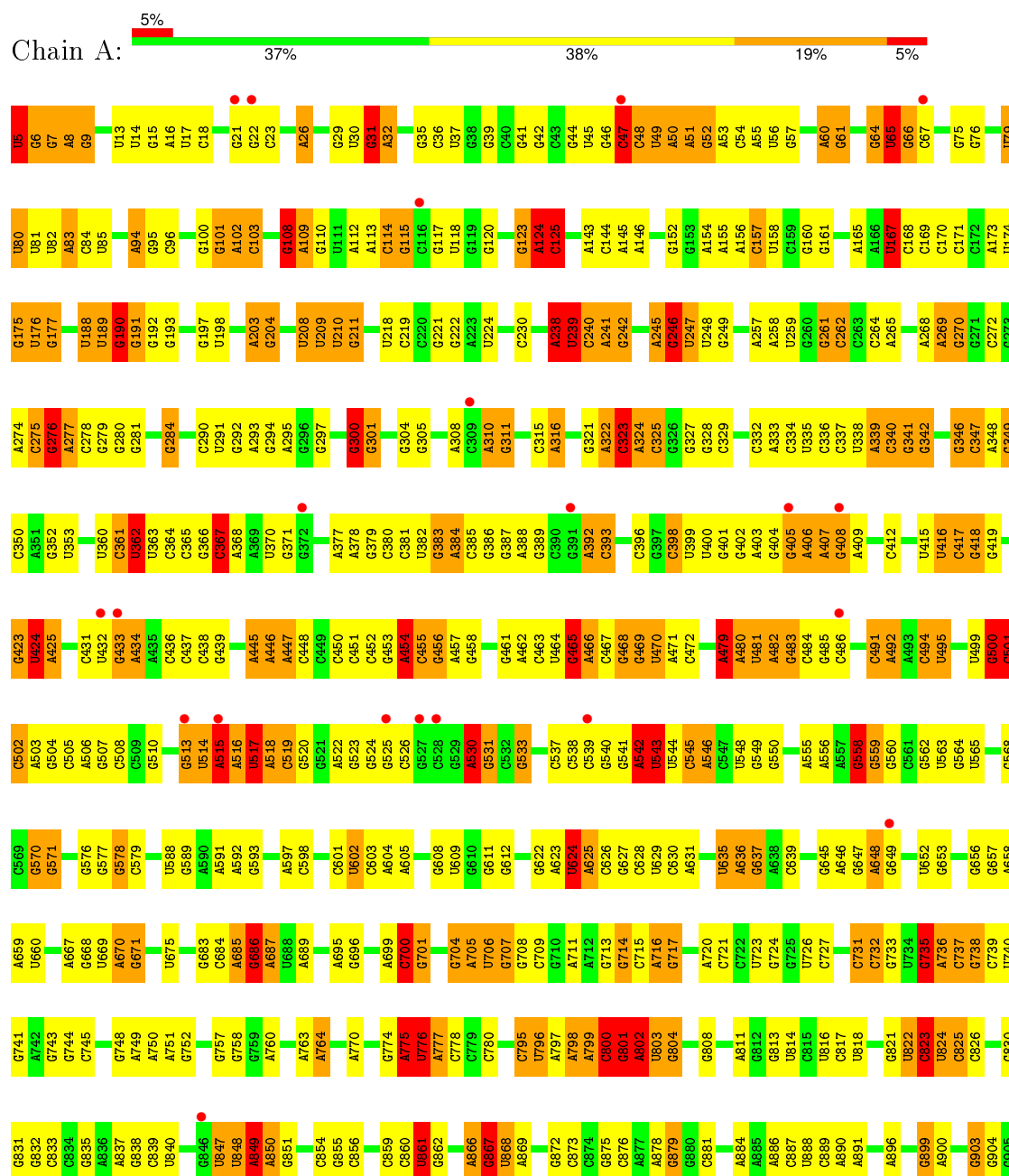


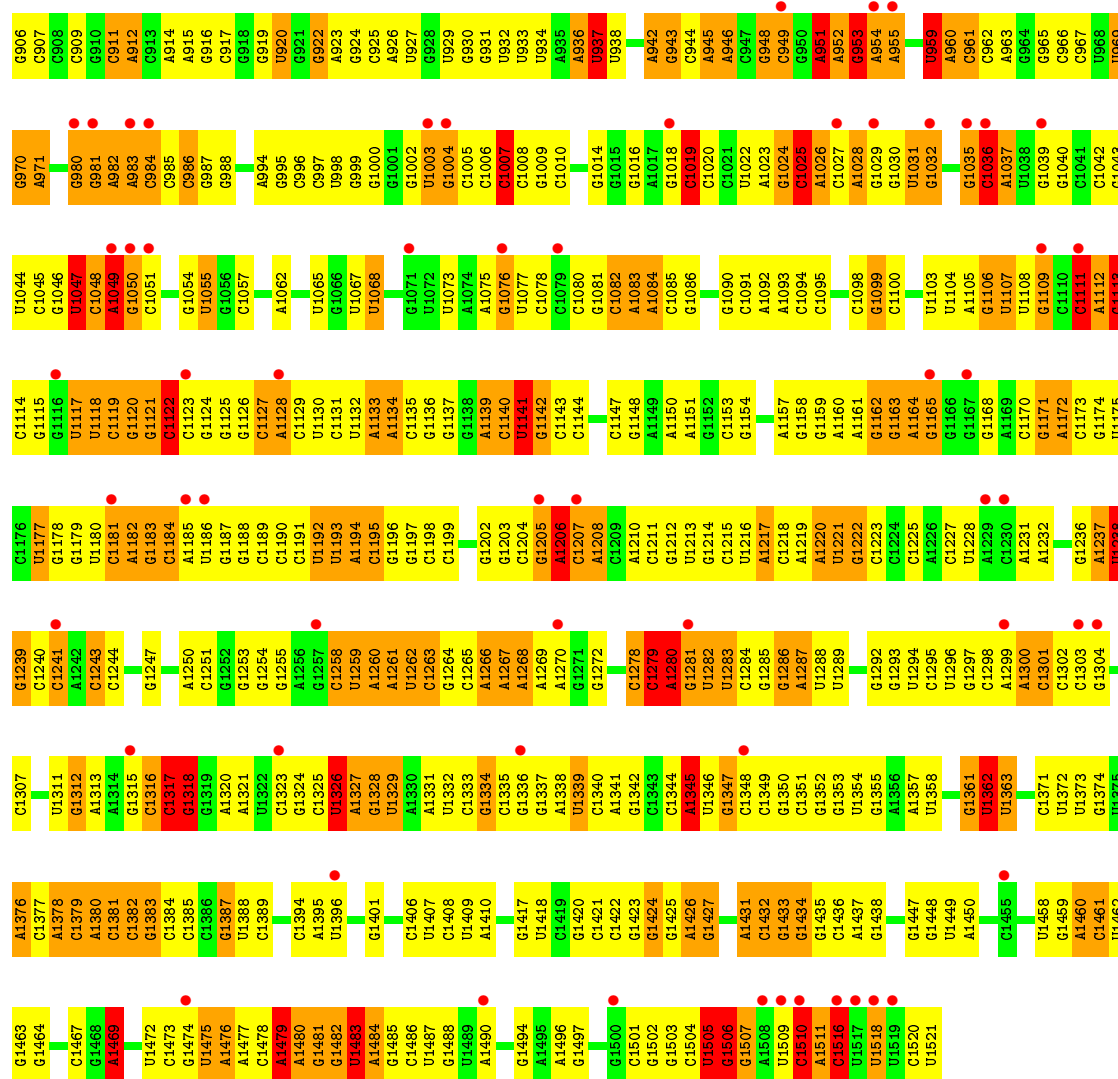
| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---------|---------|
| 26  | A     | 1        | Total | C  | N | O  | 0       | 0       |
|     |       |          | 42    | 23 | 5 | 14 |         |         |

### 3 Residue-property plots

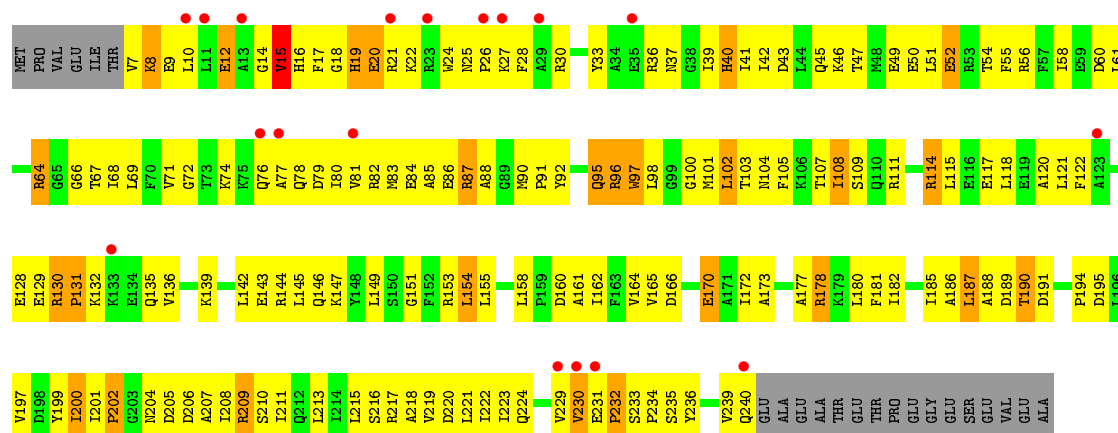
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

#### • Molecule 1: 16s rRNA

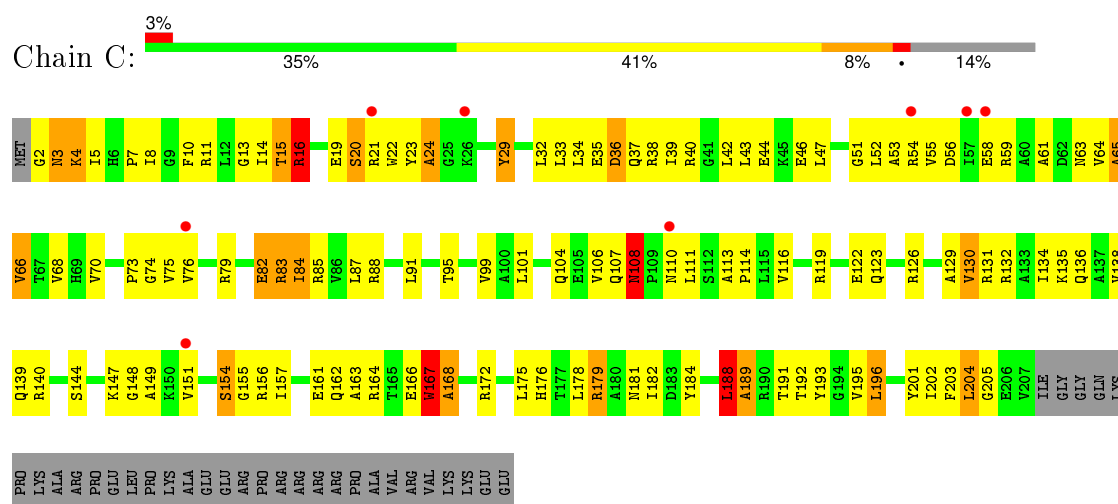




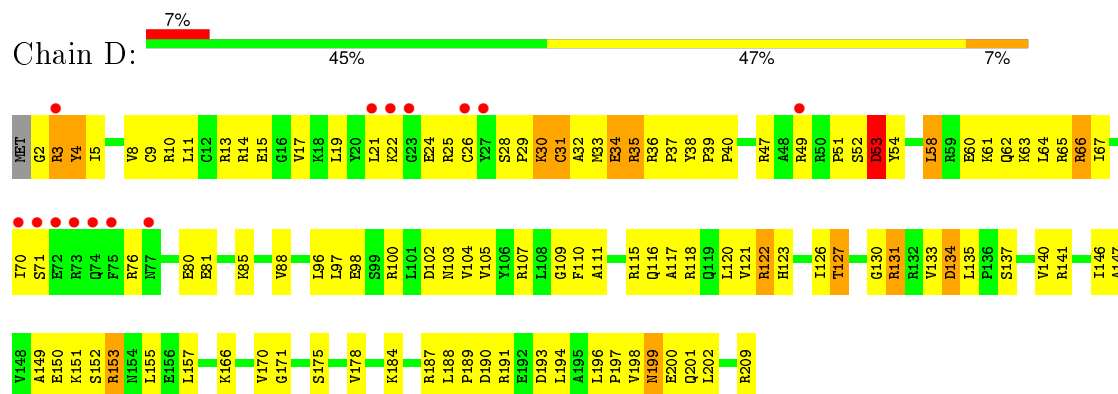
• Molecule 2: 30S ribosomal protein S2



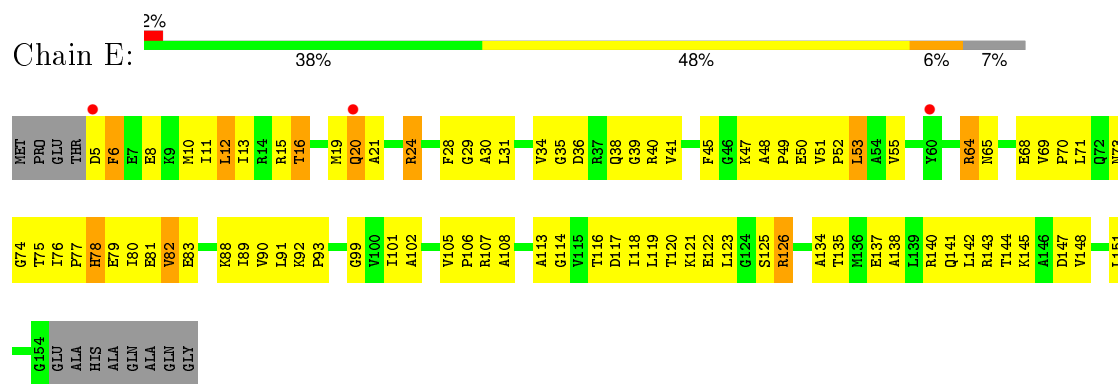
• Molecule 3: 30S ribosomal protein S3



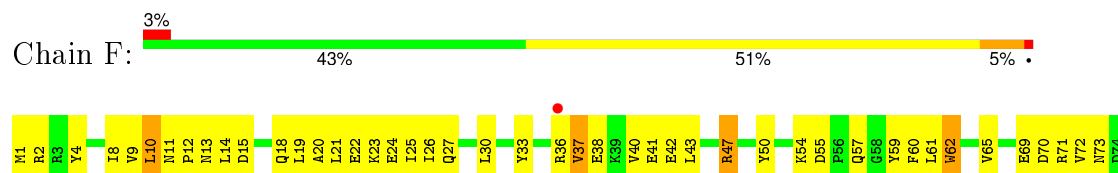
• Molecule 4: 30S ribosomal protein S4



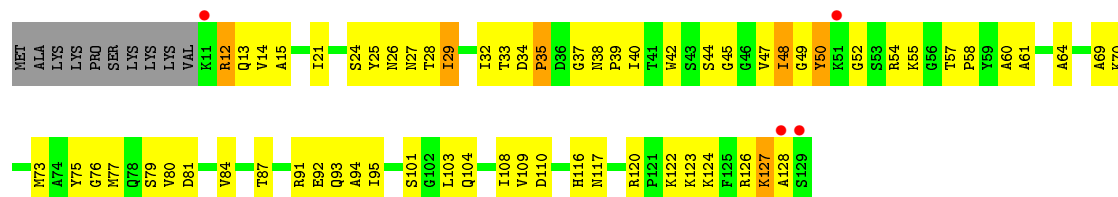
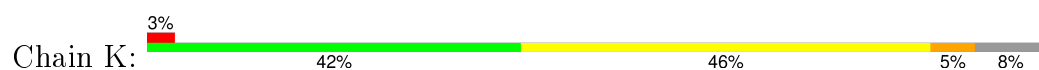
• Molecule 5: 30S ribosomal protein S5



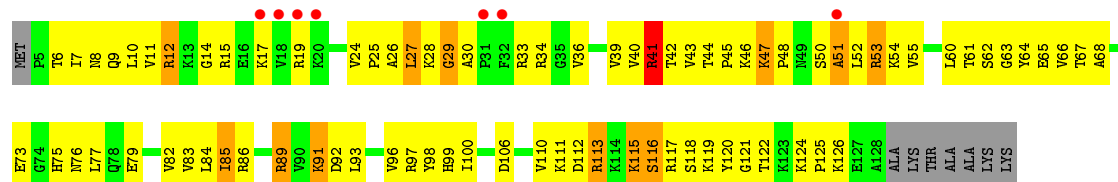
• Molecule 6: 30S ribosomal protein S6



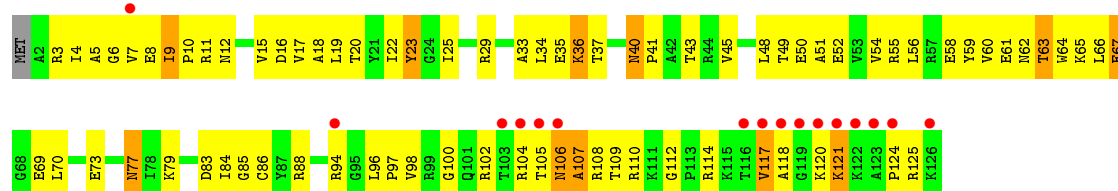




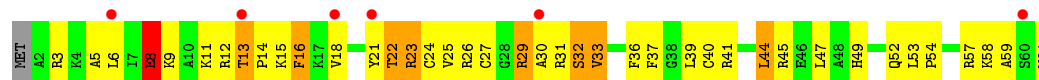
- Molecule 12: 30S ribosomal protein S12



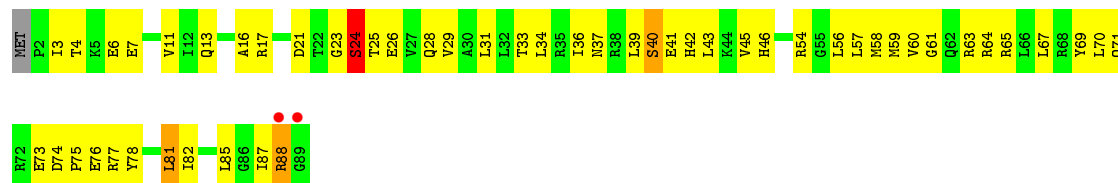
- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 15: 30S ribosomal protein S15

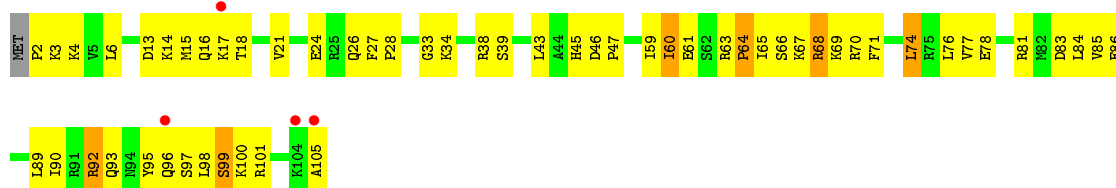


- Molecule 16: 30S ribosomal protein S16

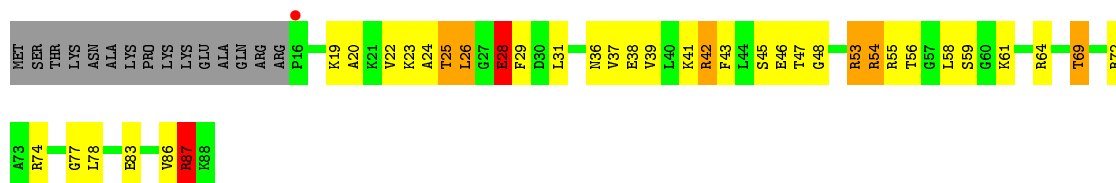




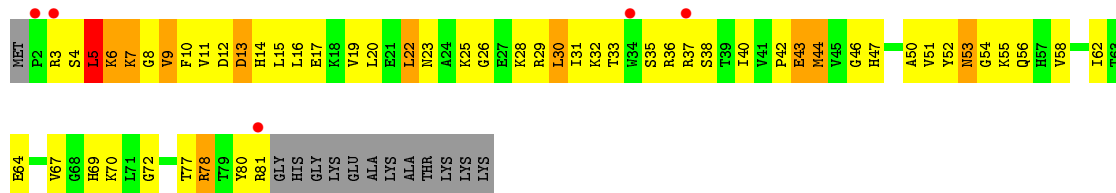
• Molecule 17: 30S ribosomal protein S17



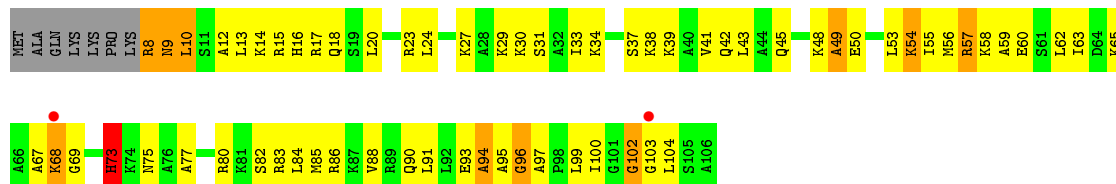
• Molecule 18: 30S ribosomal protein S18



• Molecule 19: 30S ribosomal protein S19



• Molecule 20: 30S ribosomal protein S20



• Molecule 21: 30S ribosomal protein Thx

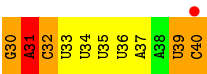




● Molecule 22: mRNA A-site fragment



● Molecule 23: tRNA ASL human Lys3





## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 41 21 2   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 402.30Å 402.30Å 175.25Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 29.72 – 3.11<br>284.47 – 2.98                               | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.0 (29.72-3.11)<br>98.9 (284.47-2.98)                     | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 0.00 (at 2.96Å)   | Xtriage          |
| Refinement program  | CNS 1.3   | Depositor        |
| R, $R_{free}$   | 0.247 , 0.276<br>0.251 , 0.254                              | Depositor<br>DCC |
| $R_{free}$ test set   | 12791 reflections (5.07%)                                   | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 61.5  | Xtriage          |
| Anisotropy  | 0.264   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.26 , 63.3   | EDS              |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$ | Xtriage          |
| Outliers  | 0 of 288591 reflections                                     | Xtriage          |
| $F_o, F_c$ correlation  | 0.86  | EDS              |
| Total number of atoms   | 52287   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 68.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.77% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: 12A, MG, ZN, 70U, PAR, 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     | 0.58         | 6/36395 (0.0%) | 0.87        | 90/56801 (0.2%) |
| 2   | B     | 0.38         | 0/1935         | 0.63        | 0/2609          |
| 3   | C     | 0.40         | 0/1636         | 0.64        | 0/2205          |
| 4   | D     | 0.37         | 0/1733         | 0.59        | 0/2318          |
| 5   | E     | 0.47         | 0/1162         | 0.70        | 1/1564 (0.1%)   |
| 6   | F     | 0.37         | 0/856          | 0.62        | 0/1154          |
| 7   | G     | 0.40         | 0/1276         | 0.59        | 0/1709          |
| 8   | H     | 0.45         | 0/1136         | 0.76        | 0/1527          |
| 9   | I     | 0.40         | 0/1029         | 0.63        | 0/1378          |
| 10  | J     | 0.40         | 0/805          | 0.66        | 0/1082          |
| 11  | K     | 0.44         | 0/900          | 0.68        | 1/1213 (0.1%)   |
| 12  | L     | 0.47         | 0/986          | 0.77        | 0/1320          |
| 13  | M     | 0.41         | 0/1008         | 0.63        | 0/1347          |
| 14  | N     | 0.43         | 0/501          | 0.66        | 0/664           |
| 15  | O     | 0.39         | 0/745          | 0.65        | 0/992           |
| 16  | P     | 0.44         | 0/716          | 0.73        | 0/963           |
| 17  | Q     | 0.43         | 0/870          | 0.74        | 0/1159          |
| 18  | R     | 0.43         | 0/603          | 0.63        | 0/799           |
| 19  | S     | 0.35         | 0/661          | 0.64        | 0/890           |
| 20  | T     | 0.46         | 0/764          | 0.74        | 0/1006          |
| 21  | V     | 0.46         | 0/212          | 0.65        | 0/277           |
| 22  | W     | 0.99         | 1/75 (1.3%)    | 0.80        | 1/113 (0.9%)    |
| 23  | X     | 0.98         | 1/184 (0.5%)   | 1.27        | 1/277 (0.4%)    |
| All | All   | 0.53         | 8/56188 (0.0%) | 0.81        | 94/83367 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 46                  |

All (8) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 1   | A     | 517  | U    | O3'-P   | -15.24 | 1.42        | 1.61     |
| 23  | X     | 30   | G    | OP3-P   | -7.09  | 1.52        | 1.61     |
| 1   | A     | 980  | G    | P-OP1   | 6.37   | 1.59        | 1.49     |
| 1   | A     | 5    | U    | OP3-P   | -6.35  | 1.53        | 1.61     |
| 22  | W     | 1    | A    | OP3-P   | -6.00  | 1.53        | 1.61     |
| 1   | A     | 1511 | A    | O3'-P   | 5.25   | 1.67        | 1.61     |
| 1   | A     | 1511 | A    | C3'-O3' | 5.08   | 1.49        | 1.42     |
| 1   | A     | 79   | U    | N3-C4   | 5.02   | 1.43        | 1.38     |

All (94) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 515  | A    | P-O3'-C3'   | 11.33 | 133.29      | 119.70   |
| 1   | A     | 800  | C    | N1-C1'-C2'  | 9.64  | 126.53      | 114.00   |
| 23  | X     | 31   | A    | C2'-C3'-O3' | 9.56  | 130.54      | 109.50   |
| 1   | A     | 800  | C    | C2'-C3'-O3' | 8.78  | 128.81      | 109.50   |
| 1   | A     | 1479 | A    | N9-C1'-C2'  | 8.27  | 124.75      | 114.00   |
| 1   | A     | 367  | C    | C2'-C3'-O3' | 8.05  | 127.22      | 109.50   |
| 1   | A     | 211  | G    | N9-C1'-C2'  | 7.98  | 124.38      | 114.00   |
| 1   | A     | 1113 | G    | N9-C1'-C2'  | -7.66 | 103.57      | 112.00   |
| 1   | A     | 801  | G    | C2'-C3'-O3' | 7.56  | 126.14      | 109.50   |
| 1   | A     | 1516 | C    | O4'-C4'-C3' | -7.51 | 96.49       | 104.00   |
| 1   | A     | 1025 | C    | C4'-C3'-O3' | 7.45  | 127.90      | 113.00   |
| 1   | A     | 1280 | A    | N9-C1'-C2'  | 7.40  | 123.62      | 114.00   |
| 1   | A     | 1036 | C    | N1-C1'-C2'  | -7.36 | 103.90      | 112.00   |
| 1   | A     | 937  | U    | N1-C1'-C2'  | 7.36  | 123.57      | 114.00   |
| 1   | A     | 479  | A    | N9-C1'-C2'  | 7.36  | 123.56      | 114.00   |
| 1   | A     | 1483 | U    | C2'-C3'-O3' | 7.32  | 125.61      | 109.50   |
| 1   | A     | 491  | C    | C2'-C3'-O3' | 7.31  | 125.58      | 109.50   |
| 1   | A     | 238  | A    | N9-C1'-C2'  | 7.06  | 123.18      | 114.00   |
| 1   | A     | 867  | G    | N9-C1'-C2'  | 6.97  | 123.07      | 114.00   |
| 1   | A     | 47   | C    | C2'-C3'-O3' | 6.97  | 124.85      | 113.70   |
| 1   | A     | 700  | C    | C2'-C3'-O3' | 6.93  | 124.79      | 113.70   |
| 1   | A     | 558  | G    | N9-C1'-C2'  | 6.89  | 122.96      | 114.00   |
| 1   | A     | 108  | G    | C2'-C3'-O3' | 6.87  | 124.70      | 113.70   |
| 1   | A     | 1141 | U    | N1-C1'-C2'  | 6.83  | 122.88      | 114.00   |
| 1   | A     | 1483 | U    | N1-C1'-C2'  | 6.72  | 122.74      | 114.00   |
| 1   | A     | 239  | U    | C5'-C4'-C3' | -6.70 | 105.29      | 116.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 1122 | C    | N1-C1'-C2'  | -6.62 | 104.72      | 112.00   |
| 1   | A     | 1047 | U    | N1-C1'-C2'  | 6.61  | 122.60      | 114.00   |
| 1   | A     | 1141 | U    | C2'-C3'-O3' | 6.56  | 124.19      | 113.70   |
| 1   | A     | 515  | A    | O3'-P-O5'   | 6.55  | 116.44      | 104.00   |
| 1   | A     | 239  | U    | C2'-C3'-O3' | 6.42  | 123.98      | 113.70   |
| 1   | A     | 323  | C    | N1-C1'-C2'  | 6.42  | 122.35      | 114.00   |
| 1   | A     | 246  | G    | N9-C1'-C2'  | 6.39  | 122.31      | 114.00   |
| 1   | A     | 1279 | C    | C2'-C3'-O3' | 6.37  | 123.89      | 113.70   |
| 1   | A     | 1111 | C    | N1-C1'-C2'  | 6.30  | 122.19      | 114.00   |
| 1   | A     | 31   | G    | C2'-C3'-O3' | 6.27  | 123.73      | 113.70   |
| 1   | A     | 1292 | G    | O5'-P-OP2   | -6.23 | 100.09      | 105.70   |
| 1   | A     | 1326 | U    | C2'-C3'-O3' | 6.21  | 123.64      | 113.70   |
| 1   | A     | 47   | C    | N1-C1'-C2'  | 6.13  | 121.97      | 114.00   |
| 1   | A     | 65   | U    | C2'-C3'-O3' | 6.10  | 123.46      | 113.70   |
| 1   | A     | 500  | G    | C2'-C3'-O3' | 6.05  | 123.38      | 113.70   |
| 1   | A     | 1345 | A    | N9-C1'-C2'  | 6.03  | 121.84      | 114.00   |
| 1   | A     | 108  | G    | N9-C1'-C2'  | 6.01  | 121.81      | 114.00   |
| 1   | A     | 1035 | G    | O4'-C1'-N9  | 6.01  | 113.01      | 108.20   |
| 1   | A     | 124  | A    | C2'-C3'-O3' | 6.00  | 123.31      | 113.70   |
| 1   | A     | 1278 | C    | N1-C1'-C2'  | 5.89  | 121.66      | 114.00   |
| 1   | A     | 861  | U    | C2'-C3'-O3' | 5.88  | 123.11      | 113.70   |
| 1   | A     | 542  | A    | C2'-C3'-O3' | 5.83  | 123.03      | 113.70   |
| 1   | A     | 686  | G    | C2'-C3'-O3' | 5.78  | 122.95      | 113.70   |
| 1   | A     | 775  | A    | N9-C1'-C2'  | 5.77  | 121.50      | 114.00   |
| 1   | A     | 238  | A    | C2'-C3'-O3' | 5.74  | 122.89      | 113.70   |
| 1   | A     | 515  | A    | C2'-C3'-O3' | 5.72  | 122.86      | 113.70   |
| 1   | A     | 300  | G    | C2'-C3'-O3' | 5.71  | 122.84      | 113.70   |
| 1   | A     | 959  | U    | N1-C1'-C2'  | 5.70  | 121.41      | 114.00   |
| 1   | A     | 802  | A    | N9-C1'-C2'  | 5.69  | 121.39      | 114.00   |
| 1   | A     | 1345 | A    | C2'-C3'-O3' | 5.66  | 122.76      | 113.70   |
| 1   | A     | 1479 | A    | O4'-C1'-N9  | 5.65  | 112.72      | 108.20   |
| 1   | A     | 797  | A    | C5'-C4'-C3' | -5.64 | 106.98      | 116.00   |
| 1   | A     | 1479 | A    | C1'-O4'-C4' | -5.59 | 105.42      | 109.90   |
| 22  | W     | 1    | A    | OP1-P-OP2   | -5.58 | 111.22      | 119.60   |
| 1   | A     | 735  | G    | N9-C1'-C2'  | 5.58  | 121.26      | 114.00   |
| 1   | A     | 124  | A    | N9-C1'-C2'  | 5.58  | 121.25      | 114.00   |
| 1   | A     | 1238 | U    | N1-C1'-C2'  | 5.56  | 121.23      | 114.00   |
| 1   | A     | 776  | U    | N1-C1'-C2'  | 5.53  | 121.19      | 114.00   |
| 1   | A     | 1019 | C    | N1-C1'-C2'  | -5.50 | 105.95      | 112.00   |
| 1   | A     | 1362 | U    | C2'-C3'-O3' | 5.49  | 122.49      | 113.70   |
| 5   | E     | 64   | ARG  | N-CA-C      | -5.48 | 96.22       | 111.00   |
| 1   | A     | 1206 | A    | C2'-C3'-O3' | 5.44  | 122.40      | 113.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 468  | G    | N9-C1'-C2'  | 5.40  | 121.02      | 114.00   |
| 1   | A     | 125  | C    | O5'-P-OP1   | 5.40  | 117.18      | 110.70   |
| 1   | A     | 953  | G    | C5'-C4'-O4' | -5.38 | 102.65      | 109.10   |
| 1   | A     | 1505 | U    | C2'-C3'-O3' | 5.37  | 122.30      | 113.70   |
| 1   | A     | 775  | A    | C2'-C3'-O3' | 5.36  | 122.28      | 113.70   |
| 1   | A     | 5    | U    | OP2-P-O3'   | 5.28  | 116.81      | 105.20   |
| 1   | A     | 1024 | G    | OP2-P-O3'   | 5.26  | 116.78      | 105.20   |
| 1   | A     | 454  | A    | C2'-C3'-O3' | 5.26  | 122.11      | 113.70   |
| 1   | A     | 1376 | A    | C5'-C4'-C3' | -5.23 | 107.63      | 116.00   |
| 1   | A     | 1036 | C    | C4'-C3'-O3' | 5.22  | 123.45      | 113.00   |
| 1   | A     | 823  | C    | N1-C1'-C2'  | 5.21  | 120.77      | 114.00   |
| 1   | A     | 1506 | G    | N9-C1'-C2'  | 5.21  | 120.78      | 114.00   |
| 1   | A     | 239  | U    | N1-C1'-C2'  | 5.17  | 120.72      | 114.00   |
| 1   | A     | 849  | A    | O4'-C1'-N9  | 5.17  | 112.33      | 108.20   |
| 1   | A     | 445  | A    | N9-C1'-C2'  | 5.15  | 120.70      | 114.00   |
| 1   | A     | 322  | A    | OP1-P-O3'   | 5.15  | 116.53      | 105.20   |
| 1   | A     | 1510 | C    | N1-C1'-C2'  | 5.13  | 120.67      | 114.00   |
| 11  | K     | 37   | GLY  | N-CA-C      | 5.08  | 125.79      | 113.10   |
| 1   | A     | 1317 | C    | N1-C1'-C2'  | 5.08  | 120.60      | 114.00   |
| 1   | A     | 360  | U    | N1-C1'-C2'  | 5.07  | 120.60      | 114.00   |
| 1   | A     | 530  | A    | N9-C1'-C2'  | 5.07  | 120.59      | 114.00   |
| 1   | A     | 424  | U    | N1-C1'-C2'  | 5.06  | 120.58      | 114.00   |
| 1   | A     | 1326 | U    | N1-C1'-C2'  | 5.04  | 120.56      | 114.00   |
| 1   | A     | 83   | A    | N9-C1'-C2'  | -5.03 | 106.46      | 112.00   |
| 1   | A     | 276  | G    | C2'-C3'-O3' | 5.03  | 121.75      | 113.70   |
| 1   | A     | 861  | U    | N1-C1'-C2'  | 5.01  | 120.52      | 114.00   |

There are no chirality outliers.

All (46) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | A     | 1007 | C    | Sidechain |
| 1   | A     | 1019 | C    | Sidechain |
| 1   | A     | 1036 | C    | Sidechain |
| 1   | A     | 1047 | U    | Sidechain |
| 1   | A     | 1049 | A    | Sidechain |
| 1   | A     | 1055 | U    | Sidechain |
| 1   | A     | 1065 | U    | Sidechain |
| 1   | A     | 1113 | G    | Sidechain |
| 1   | A     | 1122 | C    | Sidechain |
| 1   | A     | 1141 | U    | Sidechain |
| 1   | A     | 1142 | G    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | A     | 1162 | G    | Sidechain |
| 1   | A     | 1177 | U    | Sidechain |
| 1   | A     | 1258 | C    | Sidechain |
| 1   | A     | 1280 | A    | Sidechain |
| 1   | A     | 1318 | G    | Sidechain |
| 1   | A     | 1339 | U    | Sidechain |
| 1   | A     | 1387 | G    | Sidechain |
| 1   | A     | 1401 | G    | Sidechain |
| 1   | A     | 1434 | G    | Sidechain |
| 1   | A     | 1469 | A    | Sidechain |
| 1   | A     | 1479 | A    | Sidechain |
| 1   | A     | 1518 | U    | Sidechain |
| 1   | A     | 167  | U    | Sidechain |
| 1   | A     | 190  | G    | Sidechain |
| 1   | A     | 246  | G    | Sidechain |
| 1   | A     | 272  | C    | Sidechain |
| 1   | A     | 362  | U    | Sidechain |
| 1   | A     | 37   | U    | Sidechain |
| 1   | A     | 381  | C    | Sidechain |
| 1   | A     | 382  | U    | Sidechain |
| 1   | A     | 398  | C    | Sidechain |
| 1   | A     | 465  | G    | Sidechain |
| 1   | A     | 47   | C    | Sidechain |
| 1   | A     | 479  | A    | Sidechain |
| 1   | A     | 501  | C    | Sidechain |
| 1   | A     | 543  | U    | Sidechain |
| 1   | A     | 558  | G    | Sidechain |
| 1   | A     | 624  | U    | Sidechain |
| 1   | A     | 800  | C    | Sidechain |
| 1   | A     | 840  | U    | Sidechain |
| 1   | A     | 861  | U    | Sidechain |
| 1   | A     | 875  | G    | Sidechain |
| 1   | A     | 920  | U    | Sidechain |
| 1   | A     | 951  | A    | Sidechain |
| 1   | A     | 959  | U    | Sidechain |

## 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     | 32515 | 0        | 16409    | 1151    | 0            |
| 2   | B     | 1900  | 0        | 1951     | 182     | 0            |
| 3   | C     | 1612  | 0        | 1677     | 157     | 0            |
| 4   | D     | 1703  | 0        | 1764     | 129     | 0            |
| 5   | E     | 1146  | 0        | 1207     | 94      | 0            |
| 6   | F     | 843   | 0        | 857      | 65      | 0            |
| 7   | G     | 1257  | 0        | 1296     | 81      | 0            |
| 8   | H     | 1116  | 0        | 1177     | 64      | 0            |
| 9   | I     | 1011  | 0        | 1043     | 109     | 0            |
| 10  | J     | 792   | 0        | 835      | 110     | 0            |
| 11  | K     | 885   | 0        | 904      | 57      | 0            |
| 12  | L     | 970   | 0        | 1056     | 98      | 0            |
| 13  | M     | 997   | 0        | 1072     | 90      | 0            |
| 14  | N     | 492   | 0        | 530      | 70      | 0            |
| 15  | O     | 734   | 0        | 771      | 49      | 0            |
| 16  | P     | 700   | 0        | 720      | 53      | 0            |
| 17  | Q     | 857   | 0        | 930      | 65      | 0            |
| 18  | R     | 597   | 0        | 668      | 45      | 0            |
| 19  | S     | 647   | 0        | 673      | 68      | 0            |
| 20  | T     | 762   | 0        | 859      | 66      | 0            |
| 21  | V     | 208   | 0        | 221      | 24      | 0            |
| 22  | W     | 67    | 0        | 34       | 5       | 0            |
| 23  | X     | 247   | 0        | 129      | 32      | 0            |
| 24  | A     | 182   | 0        | 0        | 0       | 0            |
| 24  | B     | 1     | 0        | 0        | 0       | 0            |
| 24  | L     | 1     | 0        | 0        | 0       | 0            |
| 24  | S     | 1     | 0        | 0        | 0       | 0            |
| 25  | D     | 1     | 0        | 0        | 0       | 0            |
| 25  | N     | 1     | 0        | 0        | 0       | 0            |
| 26  | A     | 42    | 0        | 45       | 5       | 0            |
| All | All   | 52287 | 0        | 36828    | 2600    | 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 29.

All (2600) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:981:G:N2    | 1:A:982:A:H1'   | 1.44                     | 1.31              |
| 1:A:515:A:H5''  | 3:C:161:GLU:OE1 | 1.36                     | 1.21              |
| 23:X:39:PSU:C2' | 23:X:40:C:H5'   | 1.74                     | 1.18              |
| 1:A:1036:C:H3'  | 1:A:1036:C:C6   | 1.80                     | 1.15              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:984:C:H2'    | 1:A:985:C:C6     | 1.82                     | 1.14              |
| 1:A:513:G:H4'    | 1:A:513:G:OP1    | 1.35                     | 1.13              |
| 2:B:80:ILE:HD11  | 2:B:208:ILE:HG23 | 1.28                     | 1.09              |
| 23:X:37:12A:H8   | 23:X:37:12A:H5'  | 1.32                     | 1.09              |
| 9:I:53:VAL:HG21  | 9:I:85:LEU:HD21  | 1.36                     | 1.08              |
| 1:A:246:G:H4'    | 1:A:247:U:C5'    | 1.84                     | 1.07              |
| 1:A:980:G:H2'    | 1:A:981:G:C8     | 1.87                     | 1.07              |
| 20:T:8:ARG:HB2   | 20:T:8:ARG:HH11  | 1.14                     | 1.06              |
| 1:A:1303:C:H4'   | 1:A:1304:G:OP1   | 1.56                     | 1.04              |
| 1:A:346:G:H4'    | 1:A:347:C:OP1    | 1.57                     | 1.04              |
| 1:A:1237:A:C2'   | 1:A:1238:U:H4'   | 1.87                     | 1.04              |
| 19:S:33:THR:HG22 | 19:S:35:SER:H    | 1.18                     | 1.03              |
| 1:A:515:A:C5'    | 3:C:161:GLU:OE1  | 2.07                     | 1.03              |
| 1:A:1237:A:H2'   | 1:A:1238:U:H4'   | 1.03                     | 1.02              |
| 1:A:542:A:H4'    | 1:A:543:U:H5'    | 1.36                     | 1.02              |
| 1:A:1237:A:H2'   | 1:A:1238:U:C4'   | 1.89                     | 1.02              |
| 10:J:8:LEU:HB2   | 10:J:70:ARG:HB2  | 1.39                     | 1.01              |
| 12:L:41:ARG:HB3  | 12:L:41:ARG:NH1  | 1.76                     | 1.00              |
| 4:D:189:PRO:HB2  | 4:D:194:LEU:HD21 | 1.43                     | 0.99              |
| 1:A:513:G:C8     | 23:X:35:U:O2'    | 2.13                     | 0.99              |
| 1:A:241:A:H4'    | 1:A:242:G:OP1    | 1.58                     | 0.99              |
| 1:A:515:A:H4'    | 1:A:515:A:OP2    | 1.62                     | 0.99              |
| 13:M:94:ARG:HH12 | 19:S:81:ARG:HD3  | 1.28                     | 0.99              |
| 1:A:936:A:H3'    | 1:A:937:U:H5''   | 1.43                     | 0.98              |
| 1:A:984:C:C5     | 1:A:985:C:N4     | 2.30                     | 0.98              |
| 23:X:39:PSU:C3'  | 23:X:40:C:H5'    | 1.94                     | 0.97              |
| 6:F:2:ARG:HE     | 6:F:69:GLU:HG2   | 1.26                     | 0.97              |
| 1:A:465:G:H4'    | 1:A:466:A:OP1    | 1.61                     | 0.97              |
| 19:S:7:LYS:HD2   | 19:S:7:LYS:O     | 1.65                     | 0.96              |
| 10:J:90:LEU:H    | 10:J:91:PRO:HD2  | 1.25                     | 0.96              |
| 1:A:981:G:N2     | 1:A:982:A:C1'    | 2.30                     | 0.95              |
| 11:K:54:ARG:O    | 11:K:57:THR:HG22 | 1.65                     | 0.95              |
| 1:A:1036:C:C3'   | 1:A:1036:C:C6    | 2.50                     | 0.95              |
| 1:A:1035:G:H5'   | 1:A:1036:C:H5'   | 1.49                     | 0.94              |
| 15:O:17:ARG:HH11 | 15:O:17:ARG:HG3  | 1.32                     | 0.94              |
| 4:D:3:ARG:HD3    | 4:D:118:ARG:NH1  | 1.82                     | 0.94              |
| 1:A:245:A:H4'    | 1:A:246:G:O5'    | 1.64                     | 0.94              |
| 1:A:981:G:H21    | 1:A:982:A:H1'    | 1.29                     | 0.94              |
| 17:Q:97:SER:O    | 17:Q:98:LEU:HD23 | 1.68                     | 0.94              |
| 1:A:1286:G:H5''  | 21:V:4:GLY:HA3   | 1.49                     | 0.93              |
| 4:D:151:LYS:H    | 4:D:151:LYS:HD2  | 1.31                     | 0.93              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:542:A:H4'    | 1:A:543:U:C5'    | 1.99                     | 0.93              |
| 17:Q:67:LYS:HA   | 17:Q:70:ARG:HH12 | 1.33                     | 0.92              |
| 10:J:34:VAL:HG12 | 10:J:36:GLY:H    | 1.34                     | 0.92              |
| 1:A:1243:C:H2'   | 1:A:1244:C:H5'   | 1.51                     | 0.92              |
| 1:A:982:A:H3'    | 1:A:983:A:H4'    | 1.51                     | 0.92              |
| 12:L:75:HIS:HD2  | 12:L:77:LEU:H    | 1.17                     | 0.92              |
| 8:H:103:VAL:HG21 | 8:H:109:ILE:O    | 1.68                     | 0.91              |
| 2:B:132:LYS:HA   | 2:B:135:GLN:HB3  | 1.52                     | 0.91              |
| 6:F:54:LYS:HE2   | 6:F:54:LYS:N     | 1.86                     | 0.91              |
| 1:A:669:U:H1'    | 11:K:42:TRP:HE1  | 1.35                     | 0.91              |
| 2:B:7:VAL:HG23   | 2:B:8:LYS:H      | 1.36                     | 0.90              |
| 1:A:955:A:O2'    | 1:A:1303:C:N3    | 2.02                     | 0.90              |
| 1:A:647:G:H22    | 1:A:724:G:H1     | 1.13                     | 0.90              |
| 1:A:1121:G:H4'   | 1:A:1122:C:OP1   | 1.71                     | 0.90              |
| 14:N:57:ARG:HG2  | 14:N:58:LYS:H    | 1.37                     | 0.90              |
| 1:A:936:A:H5'    | 1:A:937:U:OP2    | 1.73                     | 0.89              |
| 1:A:1227:C:H2'   | 1:A:1228:U:H5'   | 1.52                     | 0.89              |
| 4:D:104:VAL:HG11 | 4:D:146:ILE:HD12 | 1.53                     | 0.89              |
| 1:A:1243:C:H42   | 1:A:1254:G:H1    | 1.17                     | 0.89              |
| 2:B:91:PRO:HG3   | 2:B:154:LEU:HB3  | 1.54                     | 0.88              |
| 1:A:1286:G:HO2'  | 1:A:1287:A:H8    | 0.90                     | 0.88              |
| 2:B:197:VAL:HB   | 2:B:200:ILE:HG12 | 1.55                     | 0.88              |
| 1:A:501:C:C5     | 1:A:513:G:H5''   | 2.09                     | 0.88              |
| 1:A:1124:G:H2'   | 1:A:1125:G:H5'   | 1.56                     | 0.88              |
| 6:F:11:ASN:HD22  | 6:F:13:ASN:H     | 1.21                     | 0.88              |
| 1:A:985:C:H2'    | 1:A:986:C:C6     | 2.09                     | 0.88              |
| 1:A:1083:A:H4'   | 1:A:1084:A:O5'   | 1.72                     | 0.87              |
| 4:D:19:LEU:CD2   | 4:D:67:ILE:HG12  | 2.04                     | 0.87              |
| 1:A:1262:U:H5'   | 1:A:1263:C:C5    | 2.08                     | 0.87              |
| 19:S:29:ARG:H    | 19:S:29:ARG:HD2  | 1.37                     | 0.87              |
| 9:I:125:TYR:HE1  | 9:I:128:ARG:HB3  | 1.39                     | 0.87              |
| 8:H:68:ARG:HB3   | 8:H:68:ARG:HH11  | 1.40                     | 0.87              |
| 20:T:39:LYS:HD2  | 20:T:55:ILE:CD1  | 2.05                     | 0.86              |
| 6:F:54:LYS:HE2   | 6:F:54:LYS:H     | 1.38                     | 0.86              |
| 1:A:984:C:H2'    | 1:A:985:C:C5     | 2.09                     | 0.86              |
| 1:A:736:A:H4'    | 1:A:737:C:O5'    | 1.74                     | 0.86              |
| 10:J:39:PRO:O    | 10:J:40:LEU:HB2  | 1.76                     | 0.86              |
| 5:E:148:VAL:HG21 | 8:H:107:LEU:HD22 | 1.57                     | 0.86              |
| 1:A:1479:A:H2    | 1:A:1482:G:H1    | 1.24                     | 0.85              |
| 23:X:36:U:H2'    | 23:X:37:12A:H5'' | 1.59                     | 0.85              |
| 1:A:102:A:H2'    | 1:A:321:G:N2     | 1.91                     | 0.85              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 12:L:41:ARG:HG2  | 12:L:42:THR:H    | 1.41                     | 0.85              |
| 1:A:984:C:C4     | 1:A:985:C:N4     | 2.45                     | 0.85              |
| 1:A:1301:C:H5'   | 19:S:70:LYS:HD2  | 1.56                     | 0.85              |
| 13:M:49:THR:HG22 | 13:M:51:ALA:H    | 1.42                     | 0.85              |
| 1:A:983:A:OP2    | 1:A:984:C:C4     | 2.30                     | 0.84              |
| 1:A:1286:G:O2'   | 1:A:1287:A:H8    | 1.60                     | 0.84              |
| 11:K:84:VAL:HG23 | 11:K:110:ASP:HA  | 1.59                     | 0.84              |
| 3:C:88:ARG:HG3   | 3:C:101:LEU:HD12 | 1.60                     | 0.84              |
| 20:T:8:ARG:HB2   | 20:T:8:ARG:NH1   | 1.92                     | 0.84              |
| 1:A:716:A:H4'    | 1:A:717:G:OP1    | 1.76                     | 0.84              |
| 1:A:1004:G:H1    | 1:A:1018:G:H1    | 1.25                     | 0.84              |
| 1:A:1231:A:H4'   | 9:I:68:GLY:H     | 1.41                     | 0.84              |
| 1:A:1098:C:H2'   | 1:A:1099:G:H5''  | 1.58                     | 0.84              |
| 1:A:1119:C:OP2   | 1:A:1120:G:H5''  | 1.78                     | 0.83              |
| 2:B:60:ASP:HB3   | 2:B:64:ARG:NH2   | 1.92                     | 0.83              |
| 1:A:1409:U:H2'   | 1:A:1410:A:C8    | 2.13                     | 0.83              |
| 3:C:75:VAL:O     | 3:C:83:ARG:HG2   | 1.77                     | 0.83              |
| 1:A:1417:G:H2'   | 1:A:1418:U:C6    | 2.14                     | 0.83              |
| 1:A:980:G:C6     | 1:A:981:G:O6     | 2.32                     | 0.82              |
| 12:L:41:ARG:HB3  | 12:L:41:ARG:HH11 | 1.41                     | 0.82              |
| 1:A:1036:C:H6    | 1:A:1036:C:H3'   | 1.38                     | 0.82              |
| 1:A:246:G:H4'    | 1:A:247:U:H5''   | 1.62                     | 0.82              |
| 4:D:19:LEU:HD21  | 4:D:67:ILE:HG12  | 1.59                     | 0.82              |
| 9:I:112:LYS:HE2  | 9:I:117:HIS:O    | 1.80                     | 0.82              |
| 5:E:88:LYS:HB3   | 5:E:123:LEU:HB2  | 1.62                     | 0.82              |
| 3:C:16:ARG:HG3   | 3:C:16:ARG:HH11  | 1.44                     | 0.82              |
| 3:C:195:VAL:C    | 3:C:196:LEU:HD23 | 1.99                     | 0.82              |
| 1:A:1206:A:H3'   | 1:A:1207:C:C6    | 2.14                     | 0.82              |
| 5:E:81:GLU:HG3   | 5:E:90:VAL:HG22  | 1.62                     | 0.81              |
| 1:A:689:A:H1'    | 11:K:29:ILE:HD11 | 1.59                     | 0.81              |
| 2:B:80:ILE:HD11  | 2:B:208:ILE:CG2  | 2.09                     | 0.81              |
| 1:A:341:G:H2'    | 1:A:342:G:H5'    | 1.62                     | 0.81              |
| 1:A:980:G:H2'    | 1:A:981:G:H8     | 1.42                     | 0.81              |
| 5:E:13:ILE:HD12  | 5:E:13:ILE:O     | 1.80                     | 0.81              |
| 13:M:49:THR:HB   | 13:M:52:GLU:HG3  | 1.63                     | 0.81              |
| 11:K:84:VAL:HG11 | 11:K:95:ILE:HD11 | 1.61                     | 0.81              |
| 9:I:48:GLU:HA    | 9:I:51:ARG:HH11  | 1.44                     | 0.81              |
| 1:A:501:C:H5     | 1:A:513:G:H5''   | 1.43                     | 0.81              |
| 1:A:505:C:H41    | 12:L:53:ARG:NH2  | 1.79                     | 0.80              |
| 16:P:74:LEU:HG   | 16:P:79:VAL:HG21 | 1.62                     | 0.80              |
| 13:M:40:ASN:HD22 | 13:M:41:PRO:CD   | 1.94                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1207:C:H4'    | 1:A:1208:A:OP1    | 1.81                     | 0.80              |
| 1:A:530:A:H4'     | 1:A:531:G:O5'     | 1.81                     | 0.80              |
| 1:A:1170:C:H5'    | 1:A:1171:G:OP2    | 1.81                     | 0.80              |
| 20:T:68:LYS:HA    | 20:T:68:LYS:HE3   | 1.64                     | 0.80              |
| 3:C:15:THR:O      | 3:C:16:ARG:HB2    | 1.80                     | 0.80              |
| 2:B:83:MET:HG3    | 2:B:235:SER:OG    | 1.81                     | 0.80              |
| 2:B:84:GLU:HB3    | 2:B:219:VAL:HG21  | 1.62                     | 0.80              |
| 13:M:117:VAL:HG12 | 13:M:118:ALA:H    | 1.46                     | 0.80              |
| 1:A:1006:C:H42    | 1:A:1016:G:N2     | 1.79                     | 0.79              |
| 1:A:955:A:H1'     | 1:A:1303:C:O2     | 1.81                     | 0.79              |
| 16:P:28:ARG:HH11  | 16:P:28:ARG:HG2   | 1.47                     | 0.79              |
| 8:H:113:SER:HB2   | 8:H:134:ILE:HD11  | 1.64                     | 0.79              |
| 14:N:3:ARG:NH2    | 14:N:6:LEU:HD11   | 1.98                     | 0.79              |
| 2:B:14:GLY:O      | 2:B:15:VAL:HG13   | 1.82                     | 0.79              |
| 2:B:178:ARG:HG3   | 2:B:178:ARG:HH11  | 1.46                     | 0.79              |
| 13:M:40:ASN:HD22  | 13:M:41:PRO:HD2   | 1.47                     | 0.79              |
| 1:A:499:U:O2      | 1:A:516:A:N6      | 2.16                     | 0.79              |
| 1:A:849:A:H4'     | 1:A:850:A:OP1     | 1.82                     | 0.79              |
| 23:X:39:PSU:H6    | 23:X:39:PSU:H5'   | 1.48                     | 0.79              |
| 1:A:1049:A:H4'    | 1:A:1050:G:O5'    | 1.82                     | 0.79              |
| 2:B:105:PHE:O     | 2:B:109:SER:HB2   | 1.82                     | 0.79              |
| 1:A:562:G:H5'     | 1:A:711:A:H1'     | 1.63                     | 0.79              |
| 8:H:120:THR:OG1   | 8:H:123:GLU:HG3   | 1.82                     | 0.79              |
| 8:H:64:LYS:HG2    | 8:H:79:VAL:HG21   | 1.63                     | 0.79              |
| 23:X:39:PSU:H2'   | 23:X:40:C:H5'     | 1.62                     | 0.79              |
| 1:A:1228:U:H3'    | 1:A:1228:U:H6     | 1.47                     | 0.79              |
| 1:A:1106:G:H2'    | 1:A:1127:C:C5     | 2.17                     | 0.79              |
| 1:A:516:A:H4'     | 1:A:517:U:OP1     | 1.81                     | 0.79              |
| 1:A:35:G:H2'      | 1:A:36:C:C6       | 2.17                     | 0.79              |
| 1:A:1267:A:H8     | 1:A:1268:A:H4'    | 1.48                     | 0.79              |
| 1:A:246:G:H4'     | 1:A:247:U:H5'     | 1.62                     | 0.78              |
| 2:B:60:ASP:HB3    | 2:B:64:ARG:HH22   | 1.47                     | 0.78              |
| 2:B:21:ARG:HG3    | 2:B:22:LYS:H      | 1.46                     | 0.78              |
| 1:A:347:C:H4'     | 1:A:349:G:OP1     | 1.82                     | 0.78              |
| 1:A:1123:C:H2'    | 1:A:1124:G:H5'    | 1.64                     | 0.78              |
| 1:A:1098:C:H2'    | 1:A:1099:G:C5'    | 2.12                     | 0.78              |
| 3:C:14:ILE:HG22   | 3:C:15:THR:H      | 1.49                     | 0.78              |
| 10:J:64:GLU:HG2   | 14:N:59:ALA:HB2   | 1.65                     | 0.78              |
| 5:E:105:VAL:HB    | 5:E:106:PRO:HD3   | 1.65                     | 0.78              |
| 15:O:36:ILE:O     | 15:O:40:SER:HB2   | 1.83                     | 0.78              |
| 26:A:1783:PAR:O52 | 26:A:1783:PAR:H11 | 1.81                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1509:U:H2'   | 1:A:1510:C:C5'   | 2.14                     | 0.78              |
| 1:A:923:A:H2'    | 1:A:924:G:C8     | 2.19                     | 0.78              |
| 3:C:70:VAL:O     | 3:C:106:VAL:HG23 | 1.84                     | 0.77              |
| 3:C:59:ARG:HG3   | 3:C:63:ASN:O     | 1.85                     | 0.77              |
| 23:X:36:U:C2'    | 23:X:37:12A:H5'' | 2.13                     | 0.77              |
| 19:S:33:THR:HG22 | 19:S:35:SER:N    | 1.99                     | 0.77              |
| 1:A:980:G:N1     | 1:A:981:G:C6     | 2.53                     | 0.77              |
| 1:A:1266:A:H4'   | 1:A:1267:A:O5'   | 1.83                     | 0.77              |
| 1:A:461:G:O2'    | 1:A:462:A:H5'    | 1.84                     | 0.77              |
| 1:A:982:A:C2'    | 1:A:983:A:OP1    | 2.31                     | 0.77              |
| 1:A:515:A:C4'    | 1:A:515:A:OP2    | 2.33                     | 0.77              |
| 1:A:1105:A:H2    | 10:J:39:PRO:HG3  | 1.48                     | 0.77              |
| 2:B:101:MET:HA   | 2:B:108:ILE:HG21 | 1.65                     | 0.77              |
| 18:R:55:ARG:HB3  | 18:R:55:ARG:NH1  | 2.00                     | 0.77              |
| 18:R:37:VAL:O    | 18:R:41:LYS:HG3  | 1.84                     | 0.77              |
| 1:A:936:A:H3'    | 1:A:937:U:C5'    | 2.15                     | 0.77              |
| 1:A:1286:G:N2    | 1:A:1312:G:O2'   | 2.18                     | 0.77              |
| 10:J:78:ASN:HB2  | 10:J:81:THR:OG1  | 1.85                     | 0.77              |
| 9:I:97:LYS:HB3   | 9:I:98:PRO:HD3   | 1.67                     | 0.76              |
| 7:G:41:ARG:O     | 7:G:45:ASP:HB2   | 1.85                     | 0.76              |
| 1:A:1042:C:C5    | 3:C:2:GLY:HA2    | 2.20                     | 0.76              |
| 16:P:28:ARG:HG2  | 16:P:29:ASP:OD2  | 1.85                     | 0.76              |
| 9:I:48:GLU:N     | 9:I:49:PRO:HD2   | 2.01                     | 0.76              |
| 13:M:15:VAL:HG23 | 13:M:43:THR:O    | 1.85                     | 0.76              |
| 20:T:58:LYS:O    | 20:T:62:LEU:HD12 | 1.85                     | 0.76              |
| 1:A:513:G:N3     | 1:A:513:G:H5''   | 2.00                     | 0.76              |
| 12:L:26:ALA:O    | 12:L:27:LEU:O    | 2.03                     | 0.76              |
| 13:M:121:LYS:HA  | 13:M:125:ARG:HD3 | 1.67                     | 0.76              |
| 19:S:30:LEU:O    | 19:S:31:ILE:HD13 | 1.86                     | 0.76              |
| 20:T:39:LYS:HD2  | 20:T:55:ILE:HD13 | 1.66                     | 0.76              |
| 1:A:102:A:H2'    | 1:A:321:G:H21    | 1.47                     | 0.76              |
| 1:A:899:G:H5'    | 5:E:20:GLN:NE2   | 2.01                     | 0.76              |
| 23:X:34:70U:H2'  | 23:X:35:U:C6     | 2.21                     | 0.76              |
| 7:G:12:LEU:H     | 7:G:12:LEU:HD12  | 1.51                     | 0.76              |
| 1:A:501:C:H4'    | 1:A:502:C:H5''   | 1.66                     | 0.75              |
| 12:L:91:LYS:HE3  | 12:L:91:LYS:HA   | 1.66                     | 0.75              |
| 5:E:51:VAL:HB    | 5:E:52:PRO:HD3   | 1.67                     | 0.75              |
| 1:A:1351:C:H2'   | 1:A:1352:G:C8    | 2.22                     | 0.75              |
| 1:A:433:G:H4'    | 1:A:434:A:OP1    | 1.87                     | 0.75              |
| 1:A:1302:C:H5''  | 1:A:1303:C:H2'   | 1.69                     | 0.75              |
| 7:G:147:ALA:C    | 7:G:148:ASN:HD22 | 1.90                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:G:15:ASP:HB3   | 7:G:19:GLY:N     | 2.00                     | 0.75              |
| 1:A:392:A:N7     | 1:A:530:A:O2'    | 2.19                     | 0.75              |
| 3:C:32:LEU:HD22  | 3:C:59:ARG:HH11  | 1.51                     | 0.75              |
| 4:D:35:ARG:N     | 4:D:35:ARG:HD2   | 2.01                     | 0.75              |
| 1:A:1134:A:H5''  | 10:J:13:HIS:CD2  | 2.21                     | 0.75              |
| 15:O:16:ALA:HB1  | 15:O:21:ASP:HB3  | 1.69                     | 0.75              |
| 1:A:513:G:C2'    | 1:A:514:U:OP2    | 2.33                     | 0.75              |
| 1:A:366:G:O2'    | 1:A:367:C:H5'    | 1.87                     | 0.75              |
| 3:C:191:THR:HG21 | 3:C:193:TYR:CZ   | 2.21                     | 0.74              |
| 1:A:982:A:H2'    | 1:A:983:A:OP1    | 1.87                     | 0.74              |
| 1:A:102:A:H4'    | 1:A:103:C:OP2    | 1.86                     | 0.74              |
| 2:B:230:VAL:HG12 | 2:B:231:GLU:H    | 1.51                     | 0.74              |
| 1:A:689:A:C1'    | 11:K:29:ILE:HD11 | 2.16                     | 0.74              |
| 4:D:34:GLU:O     | 4:D:35:ARG:HB2   | 1.87                     | 0.74              |
| 1:A:15:G:H4'     | 5:E:24:ARG:HH12  | 1.52                     | 0.74              |
| 1:A:1022:U:H2'   | 1:A:1023:A:H8    | 1.53                     | 0.74              |
| 1:A:1042:C:H2'   | 1:A:1043:G:H8    | 1.52                     | 0.74              |
| 1:A:203:A:H4'    | 1:A:204:G:O5'    | 1.84                     | 0.74              |
| 1:A:198:U:H1'    | 20:T:103:GLY:HA2 | 1.69                     | 0.74              |
| 12:L:41:ARG:HG2  | 12:L:42:THR:N    | 2.02                     | 0.74              |
| 13:M:10:PRO:HB2  | 13:M:18:ALA:HB1  | 1.70                     | 0.74              |
| 8:H:91:ARG:HG3   | 12:L:7:ILE:HG13  | 1.69                     | 0.74              |
| 1:A:297:G:H5''   | 12:L:17:LYS:HE2  | 1.69                     | 0.74              |
| 1:A:952:A:H4'    | 1:A:953:G:H5'    | 1.68                     | 0.74              |
| 1:A:1147:C:H2'   | 1:A:1148:G:H5'   | 1.68                     | 0.74              |
| 1:A:238:A:H4'    | 1:A:239:U:H5'    | 1.67                     | 0.74              |
| 5:E:78:HIS:ND1   | 8:H:104:ARG:HD2  | 2.03                     | 0.74              |
| 1:A:980:G:H1     | 1:A:1020:C:H42   | 1.36                     | 0.74              |
| 23:X:36:U:H2'    | 23:X:37:12A:C5'  | 2.18                     | 0.74              |
| 6:F:2:ARG:NE     | 6:F:69:GLU:HG2   | 2.01                     | 0.74              |
| 1:A:123:G:N3     | 1:A:189:U:H5'    | 2.01                     | 0.74              |
| 9:I:4:TYR:CE2    | 9:I:88:TYR:HA    | 2.22                     | 0.73              |
| 2:B:162:ILE:HD12 | 2:B:177:ALA:HB2  | 1.70                     | 0.73              |
| 1:A:1098:C:C2'   | 1:A:1099:G:H5''  | 2.18                     | 0.73              |
| 4:D:70:ILE:HD11  | 4:D:100:ARG:CD   | 2.18                     | 0.73              |
| 9:I:19:LEU:HD23  | 9:I:61:ALA:HB2   | 1.69                     | 0.73              |
| 1:A:1036:C:C4    | 23:X:34:70U:H4'  | 2.23                     | 0.73              |
| 1:A:1267:A:C8    | 1:A:1268:A:H4'   | 2.23                     | 0.73              |
| 3:C:52:LEU:HD12  | 3:C:52:LEU:O     | 1.88                     | 0.73              |
| 4:D:62:GLN:HE22  | 4:D:65:ARG:NH1   | 1.86                     | 0.73              |
| 12:L:36:VAL:HG22 | 12:L:82:VAL:HG12 | 1.71                     | 0.73              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1136:G:H2'   | 1:A:1137:G:H8     | 1.52                     | 0.73              |
| 1:A:923:A:H2'    | 1:A:924:G:H8      | 1.52                     | 0.73              |
| 4:D:199:ASN:HD21 | 4:D:201:GLN:HB3   | 1.53                     | 0.73              |
| 1:A:514:U:O2'    | 1:A:515:A:P       | 2.46                     | 0.73              |
| 1:A:1479:A:H5''  | 1:A:1480:A:OP2    | 1.88                     | 0.73              |
| 1:A:264:C:H2'    | 1:A:265:A:C8      | 2.23                     | 0.73              |
| 1:A:714:G:OP1    | 1:A:749:A:H1'     | 1.88                     | 0.73              |
| 19:S:64:GLU:O    | 19:S:67:VAL:HG23  | 1.88                     | 0.73              |
| 20:T:103:GLY:O   | 20:T:104:LEU:HD23 | 1.89                     | 0.73              |
| 1:A:1227:C:C2'   | 1:A:1228:U:H5'    | 2.17                     | 0.73              |
| 12:L:27:LEU:C    | 12:L:29:GLY:H     | 1.91                     | 0.73              |
| 12:L:28:LYS:O    | 12:L:30:ALA:N     | 2.22                     | 0.73              |
| 16:P:74:LEU:O    | 16:P:79:VAL:HG23  | 1.88                     | 0.73              |
| 1:A:31:G:O2'     | 1:A:32:A:OP1      | 2.07                     | 0.73              |
| 1:A:916:G:H5''   | 7:G:102:ARG:NH2   | 2.04                     | 0.73              |
| 1:A:1261:A:O2'   | 1:A:1262:U:OP1    | 2.05                     | 0.73              |
| 1:A:803:U:H4'    | 1:A:804:G:OP2     | 1.87                     | 0.73              |
| 1:A:1197:G:O2'   | 1:A:1198:C:H5'    | 1.88                     | 0.73              |
| 1:A:949:C:O5'    | 10:J:57:LYS:HD3   | 1.89                     | 0.73              |
| 1:A:733:G:N3     | 15:O:23:GLY:HA3   | 2.03                     | 0.72              |
| 4:D:140:VAL:HG11 | 4:D:146:ILE:HD11  | 1.70                     | 0.72              |
| 1:A:821:G:H2'    | 1:A:822:U:H5''    | 1.71                     | 0.72              |
| 1:A:513:G:H2'    | 1:A:514:U:OP2     | 1.89                     | 0.72              |
| 1:A:35:G:H2'     | 1:A:36:C:H6       | 1.54                     | 0.72              |
| 17:Q:59:ILE:HG22 | 17:Q:71:PHE:CD1   | 2.25                     | 0.72              |
| 4:D:3:ARG:HD3    | 4:D:118:ARG:HH11  | 1.55                     | 0.72              |
| 1:A:1082:C:H3'   | 1:A:1082:C:C6     | 2.24                     | 0.72              |
| 16:P:51:VAL:O    | 16:P:52:ASP:HB3   | 1.89                     | 0.72              |
| 1:A:1349:C:H5'   | 10:J:60:ARG:HH12  | 1.54                     | 0.72              |
| 1:A:982:A:C3'    | 1:A:983:A:H4'     | 2.19                     | 0.72              |
| 23:X:31:A:N3     | 23:X:31:A:H2'     | 2.04                     | 0.72              |
| 23:X:37:12A:C8   | 23:X:37:12A:H5'   | 2.17                     | 0.72              |
| 19:S:47:HIS:O    | 19:S:62:ILE:HG22  | 1.89                     | 0.72              |
| 4:D:127:THR:HG22 | 4:D:147:ALA:HB3   | 1.70                     | 0.72              |
| 13:M:79:LYS:HG2  | 13:M:83:ASP:OD2   | 1.89                     | 0.72              |
| 1:A:1004:G:H2'   | 1:A:1005:C:H5'    | 1.71                     | 0.72              |
| 8:H:85:ARG:NE    | 8:H:87:SER:O      | 2.22                     | 0.72              |
| 18:R:25:THR:HG22 | 18:R:42:ARG:HH11  | 1.54                     | 0.72              |
| 1:A:269:A:O2'    | 1:A:270:G:H8      | 1.72                     | 0.72              |
| 10:J:47:PHE:CE2  | 14:N:37:PHE:HE1   | 2.07                     | 0.72              |
| 16:P:34:GLU:OE2  | 16:P:55:ARG:HD3   | 1.89                     | 0.71              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:D:151:LYS:N    | 4:D:151:LYS:HD2   | 2.04                     | 0.71              |
| 3:C:157:ILE:HD13 | 3:C:166:GLU:HB2   | 1.72                     | 0.71              |
| 1:A:994:A:H2'    | 1:A:995:G:O4'     | 1.90                     | 0.71              |
| 20:T:57:ARG:HH21 | 20:T:100:ILE:HG22 | 1.54                     | 0.71              |
| 1:A:366:G:C2'    | 1:A:367:C:H5'     | 2.20                     | 0.71              |
| 10:J:39:PRO:HA   | 10:J:70:ARG:HH21  | 1.55                     | 0.71              |
| 1:A:170:C:H2'    | 1:A:171:C:H6      | 1.54                     | 0.71              |
| 1:A:337:C:H2'    | 1:A:338:U:H5'     | 1.73                     | 0.71              |
| 10:J:50:ILE:HA   | 10:J:60:ARG:HD2   | 1.71                     | 0.71              |
| 16:P:20:VAL:HG21 | 16:P:32:TYR:CG    | 2.26                     | 0.71              |
| 1:A:1449:U:H2'   | 1:A:1450:A:H8     | 1.54                     | 0.71              |
| 1:A:763:A:O2'    | 1:A:764:A:H5''    | 1.90                     | 0.71              |
| 3:C:91:LEU:HB3   | 3:C:99:VAL:HG21   | 1.72                     | 0.71              |
| 1:A:513:G:H8     | 23:X:35:U:O2'     | 1.68                     | 0.71              |
| 1:A:1254:G:H2'   | 1:A:1255:G:O4'    | 1.89                     | 0.71              |
| 9:I:16:ARG:HE    | 9:I:64:THR:CG2    | 2.02                     | 0.71              |
| 1:A:774:G:H2'    | 1:A:775:A:H5'     | 1.72                     | 0.71              |
| 1:A:984:C:C6     | 1:A:985:C:C5      | 2.79                     | 0.71              |
| 9:I:70:LYS:O     | 9:I:74:ILE:HG13   | 1.91                     | 0.71              |
| 10:J:10:GLY:N    | 10:J:16:LEU:HD11  | 2.06                     | 0.71              |
| 1:A:1124:G:C2'   | 1:A:1125:G:H5'    | 2.21                     | 0.71              |
| 2:B:69:LEU:HD12  | 2:B:155:LEU:HD11  | 1.72                     | 0.71              |
| 5:E:137:GLU:O    | 5:E:141:GLN:HG3   | 1.91                     | 0.71              |
| 1:A:1035:G:C5'   | 1:A:1036:C:H5'    | 2.20                     | 0.70              |
| 21:V:6:ARG:HD2   | 21:V:15:ARG:HH12  | 1.55                     | 0.70              |
| 23:X:39:PSU:O2'  | 23:X:40:C:H5'     | 1.90                     | 0.70              |
| 4:D:104:VAL:HG11 | 4:D:146:ILE:CD1   | 2.20                     | 0.70              |
| 1:A:1348:C:H2'   | 1:A:1349:C:C6     | 2.25                     | 0.70              |
| 14:N:37:PHE:CE2  | 14:N:53:LEU:HD13  | 2.25                     | 0.70              |
| 4:D:76:ARG:HG2   | 4:D:76:ARG:HH11   | 1.55                     | 0.70              |
| 10:J:90:LEU:N    | 10:J:91:PRO:HD2   | 2.04                     | 0.70              |
| 5:E:12:LEU:CD1   | 5:E:31:LEU:HB2    | 2.20                     | 0.70              |
| 1:A:1279:C:C5    | 7:G:114:ARG:HD3   | 2.26                     | 0.70              |
| 4:D:62:GLN:O     | 4:D:66:ARG:HB2    | 1.91                     | 0.70              |
| 17:Q:21:VAL:HG21 | 17:Q:59:ILE:HD11  | 1.73                     | 0.70              |
| 3:C:108:ASN:HD21 | 3:C:110:ASN:ND2   | 1.90                     | 0.70              |
| 2:B:47:THR:HA    | 2:B:202:PRO:HG2   | 1.74                     | 0.70              |
| 9:I:16:ARG:HH11  | 9:I:16:ARG:HG2    | 1.57                     | 0.70              |
| 6:F:14:LEU:HA    | 6:F:18:GLN:NE2    | 2.07                     | 0.69              |
| 13:M:49:THR:HG22 | 13:M:51:ALA:N     | 2.07                     | 0.69              |
| 15:O:26:GLU:HG3  | 15:O:81:LEU:HG    | 1.72                     | 0.69              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:238:A:C5'    | 1:A:239:U:H5'     | 2.22                     | 0.69              |
| 6:F:14:LEU:HB3   | 6:F:18:GLN:HB3    | 1.74                     | 0.69              |
| 2:B:107:THR:C    | 2:B:109:SER:H     | 1.95                     | 0.69              |
| 3:C:108:ASN:HD21 | 3:C:110:ASN:HD22  | 1.39                     | 0.69              |
| 1:A:1281:G:O2'   | 1:A:1282:U:H6     | 1.75                     | 0.69              |
| 16:P:67:THR:HG22 | 16:P:68:ASP:N     | 2.06                     | 0.69              |
| 12:L:6:THR:OG1   | 12:L:9:GLN:HG3    | 1.92                     | 0.69              |
| 14:N:9:LYS:HG3   | 14:N:21:TYR:O     | 1.92                     | 0.69              |
| 11:K:80:VAL:HG13 | 11:K:103:LEU:HD22 | 1.73                     | 0.69              |
| 8:H:86:ILE:O     | 8:H:88:LYS:HG2    | 1.93                     | 0.69              |
| 1:A:238:A:H5''   | 1:A:239:U:H5'     | 1.74                     | 0.69              |
| 2:B:102:LEU:HD21 | 2:B:162:ILE:HD11  | 1.74                     | 0.69              |
| 3:C:119:ARG:NE   | 3:C:140:ARG:HH12  | 1.90                     | 0.69              |
| 4:D:35:ARG:O     | 4:D:36:ARG:HG3    | 1.92                     | 0.69              |
| 4:D:189:PRO:HB2  | 4:D:194:LEU:CD2   | 2.20                     | 0.69              |
| 1:A:242:G:N7     | 17:Q:96:GLN:NE2   | 2.40                     | 0.69              |
| 19:S:29:ARG:N    | 19:S:29:ARG:HD2   | 2.08                     | 0.69              |
| 18:R:54:ARG:HD3  | 18:R:55:ARG:HG2   | 1.73                     | 0.69              |
| 1:A:1449:U:H2'   | 1:A:1450:A:C8     | 2.27                     | 0.69              |
| 1:A:238:A:H4'    | 1:A:239:U:C5'     | 2.22                     | 0.69              |
| 1:A:516:A:O5'    | 1:A:516:A:H8      | 1.75                     | 0.69              |
| 18:R:31:LEU:O    | 18:R:69:THR:HG21  | 1.92                     | 0.69              |
| 1:A:780:C:OP1    | 11:K:124:LYS:HE2  | 1.93                     | 0.69              |
| 10:J:12:ASP:HB3  | 10:J:15:THR:CG2   | 2.22                     | 0.69              |
| 2:B:136:VAL:HA   | 2:B:139:LYS:NZ    | 2.09                     | 0.69              |
| 2:B:213:LEU:O    | 2:B:217:ARG:HG2   | 1.93                     | 0.69              |
| 1:A:1228:U:H3'   | 1:A:1228:U:C6     | 2.29                     | 0.68              |
| 12:L:27:LEU:C    | 12:L:29:GLY:N     | 2.44                     | 0.68              |
| 1:A:269:A:HO2'   | 1:A:270:G:H8      | 1.39                     | 0.68              |
| 5:E:12:LEU:HD12  | 5:E:31:LEU:HB2    | 1.75                     | 0.68              |
| 13:M:17:VAL:O    | 13:M:20:THR:HB    | 1.93                     | 0.68              |
| 17:Q:3:LYS:HB2   | 17:Q:60:ILE:HD11  | 1.75                     | 0.68              |
| 1:A:1328:G:N2    | 1:A:1355:G:H2'    | 2.06                     | 0.68              |
| 1:A:930:G:H5'    | 1:A:942:A:H61     | 1.56                     | 0.68              |
| 1:A:1475:U:H2'   | 1:A:1520:C:OP1    | 1.94                     | 0.68              |
| 1:A:1082:C:H6    | 1:A:1082:C:H3'    | 1.56                     | 0.68              |
| 9:I:78:LYS:HE2   | 9:I:101:PHE:CD2   | 2.29                     | 0.68              |
| 1:A:635:U:H2'    | 1:A:735:G:H1      | 1.58                     | 0.68              |
| 1:A:748:G:H1     | 1:A:795:C:H2'     | 1.59                     | 0.68              |
| 1:A:980:G:C2     | 1:A:981:G:C6      | 2.82                     | 0.68              |
| 17:Q:67:LYS:HA   | 17:Q:70:ARG:NH1   | 2.08                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 10:J:3:LYS:N     | 10:J:75:ILE:HG22 | 2.09                     | 0.68              |
| 13:M:22:ILE:HD12 | 13:M:25:ILE:HD12 | 1.76                     | 0.68              |
| 1:A:458:G:H5''   | 16:P:81:ARG:NH1  | 2.09                     | 0.68              |
| 1:A:341:G:H2'    | 1:A:342:G:C5'    | 2.23                     | 0.68              |
| 1:A:1006:C:C6    | 1:A:1006:C:H3'   | 2.28                     | 0.68              |
| 2:B:7:VAL:HG23   | 2:B:8:LYS:N      | 2.07                     | 0.68              |
| 1:A:670:A:H4'    | 1:A:671:G:O5'    | 1.94                     | 0.67              |
| 17:Q:63:ARG:HG2  | 17:Q:64:PRO:HD2  | 1.76                     | 0.67              |
| 14:N:22:THR:HB   | 14:N:33:VAL:HG21 | 1.76                     | 0.67              |
| 3:C:111:LEU:HD21 | 3:C:144:SER:O    | 1.93                     | 0.67              |
| 21:V:3:LYS:H     | 21:V:3:LYS:HD2   | 1.60                     | 0.67              |
| 1:A:1221:U:OP1   | 7:G:116:ALA:HB2  | 1.94                     | 0.67              |
| 6:F:101:ALA:HB2  | 18:R:28:GLU:HG3  | 1.76                     | 0.67              |
| 2:B:86:GLU:C     | 2:B:88:ALA:H     | 1.97                     | 0.67              |
| 3:C:23:TYR:CD2   | 3:C:24:ALA:N     | 2.63                     | 0.67              |
| 1:A:1026:A:H8    | 1:A:1026:A:OP1   | 1.77                     | 0.67              |
| 1:A:1355:G:H5''  | 7:G:36:LYS:HB2   | 1.76                     | 0.67              |
| 1:A:60:A:H4'     | 1:A:61:G:O5'     | 1.94                     | 0.67              |
| 15:O:87:ILE:HG22 | 15:O:88:ARG:HG3  | 1.75                     | 0.67              |
| 1:A:525:G:P      | 4:D:10:ARG:HH22  | 2.18                     | 0.67              |
| 12:L:60:LEU:HD11 | 12:L:85:ILE:HD12 | 1.77                     | 0.67              |
| 3:C:188:LEU:O    | 3:C:189:ALA:HB2  | 1.94                     | 0.67              |
| 10:J:53:PRO:HA   | 14:N:41:ARG:HH21 | 1.59                     | 0.67              |
| 1:A:525:G:H2'    | 1:A:526:C:H6     | 1.59                     | 0.67              |
| 2:B:51:LEU:HD22  | 2:B:55:PHE:CE2   | 2.29                     | 0.67              |
| 11:K:57:THR:HG23 | 11:K:60:ALA:H    | 1.59                     | 0.67              |
| 14:N:16:PHE:HB2  | 14:N:18:VAL:HG22 | 1.77                     | 0.67              |
| 13:M:11:ARG:HG2  | 13:M:12:ASN:N    | 2.10                     | 0.67              |
| 1:A:361:C:O2'    | 1:A:389:G:N2     | 2.28                     | 0.67              |
| 1:A:1260:A:H5''  | 1:A:1261:A:OP1   | 1.94                     | 0.66              |
| 2:B:21:ARG:HG3   | 2:B:22:LYS:N     | 2.10                     | 0.66              |
| 12:L:25:PRO:C    | 12:L:27:LEU:H    | 1.98                     | 0.66              |
| 9:I:78:LYS:HE2   | 9:I:101:PHE:HD2  | 1.59                     | 0.66              |
| 7:G:145:ALA:C    | 7:G:147:ALA:H    | 1.98                     | 0.66              |
| 1:A:1379:C:H4'   | 1:A:1380:A:OP2   | 1.96                     | 0.66              |
| 1:A:1521:U:O3'   | 22:W:1:A:P       | 2.53                     | 0.66              |
| 1:A:960:A:H5'    | 1:A:961:C:OP2    | 1.96                     | 0.66              |
| 2:B:211:ILE:HG22 | 2:B:215:LEU:HD12 | 1.76                     | 0.66              |
| 1:A:774:G:C2'    | 1:A:775:A:H5'    | 2.25                     | 0.66              |
| 3:C:129:ALA:HB3  | 3:C:132:ARG:HE   | 1.60                     | 0.66              |
| 7:G:54:THR:HG22  | 7:G:56:GLN:H     | 1.60                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 12:L:75:HIS:CD2  | 12:L:77:LEU:H    | 2.07                     | 0.66              |
| 1:A:1231:A:H4'   | 9:I:68:GLY:N     | 2.10                     | 0.66              |
| 12:L:40:VAL:O    | 12:L:40:VAL:HG12 | 1.96                     | 0.66              |
| 2:B:104:ASN:ND2  | 2:B:107:THR:HB   | 2.10                     | 0.66              |
| 1:A:1130:U:H2'   | 1:A:1131:C:O4'   | 1.96                     | 0.66              |
| 3:C:20:SER:O     | 14:N:54:PRO:HB3  | 1.96                     | 0.66              |
| 1:A:670:A:N6     | 1:A:686:G:H1'    | 2.11                     | 0.66              |
| 3:C:188:LEU:HD13 | 3:C:189:ALA:H    | 1.60                     | 0.66              |
| 20:T:23:ARG:HH12 | 20:T:27:LYS:HZ1  | 1.43                     | 0.66              |
| 8:H:23:SER:HA    | 8:H:63:LEU:HD22  | 1.76                     | 0.66              |
| 1:A:208:U:H5''   | 1:A:209:U:OP2    | 1.95                     | 0.66              |
| 1:A:469:G:O2'    | 1:A:470:U:OP2    | 2.13                     | 0.66              |
| 16:P:18:ARG:HG3  | 16:P:35:LYS:HE3  | 1.76                     | 0.65              |
| 1:A:1337:G:H2'   | 1:A:1338:A:C8    | 2.31                     | 0.65              |
| 6:F:2:ARG:HE     | 6:F:69:GLU:CG    | 2.06                     | 0.65              |
| 1:A:392:A:H5'    | 1:A:393:C:OP1    | 1.95                     | 0.65              |
| 1:A:899:G:H4'    | 5:E:20:GLN:HA    | 1.77                     | 0.65              |
| 2:B:211:ILE:O    | 2:B:215:LEU:HB2  | 1.96                     | 0.65              |
| 4:D:3:ARG:CA     | 4:D:3:ARG:HE     | 2.09                     | 0.65              |
| 1:A:738:G:OP2    | 15:O:65:ARG:HD2  | 1.96                     | 0.65              |
| 1:A:424:U:H1'    | 1:A:425:A:H5''   | 1.78                     | 0.65              |
| 3:C:22:TRP:HB3   | 3:C:59:ARG:HB3   | 1.79                     | 0.65              |
| 1:A:930:G:C5'    | 1:A:942:A:H61    | 2.10                     | 0.65              |
| 3:C:131:ARG:O    | 3:C:135:LYS:HG3  | 1.97                     | 0.65              |
| 8:H:112:LEU:HD12 | 8:H:112:LEU:N    | 2.11                     | 0.65              |
| 23:X:39:PSU:C3'  | 23:X:40:C:C5'    | 2.73                     | 0.65              |
| 9:I:48:GLU:OE2   | 9:I:51:ARG:HD2   | 1.96                     | 0.65              |
| 1:A:578:G:H2'    | 1:A:624:U:O4     | 1.96                     | 0.65              |
| 17:Q:67:LYS:CA   | 17:Q:70:ARG:HH12 | 2.07                     | 0.65              |
| 1:A:1509:U:H2'   | 1:A:1510:C:H5'   | 1.78                     | 0.65              |
| 12:L:28:LYS:C    | 12:L:30:ALA:H    | 2.00                     | 0.65              |
| 11:K:87:THR:HG23 | 11:K:91:ARG:NH2  | 2.12                     | 0.65              |
| 1:A:1046:G:O2'   | 1:A:1171:G:N2    | 2.30                     | 0.65              |
| 1:A:371:G:OP2    | 16:P:67:THR:HG21 | 1.96                     | 0.65              |
| 1:A:1506:G:H5''  | 1:A:1507:G:OP2   | 1.97                     | 0.65              |
| 12:L:24:VAL:O    | 12:L:24:VAL:HG23 | 1.97                     | 0.65              |
| 3:C:139:GLN:HA   | 3:C:139:GLN:HE21 | 1.62                     | 0.65              |
| 1:A:513:G:N3     | 1:A:513:G:C5'    | 2.60                     | 0.65              |
| 11:K:58:PRO:HB2  | 11:K:93:GLN:HG3  | 1.79                     | 0.65              |
| 1:A:1205:G:O2'   | 1:A:1206:A:OP1   | 2.13                     | 0.65              |
| 15:O:4:THR:OG1   | 15:O:7:GLU:HG3   | 1.97                     | 0.65              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 12:L:68:ALA:HB1  | 12:L:100:ILE:HG13 | 1.79                     | 0.65              |
| 1:A:465:G:H2'    | 1:A:467:C:N4      | 2.12                     | 0.65              |
| 21:V:5:ASP:O     | 21:V:11:GLY:HA3   | 1.97                     | 0.65              |
| 1:A:704:G:H4'    | 1:A:705:A:O5'     | 1.96                     | 0.65              |
| 1:A:230:C:H5'    | 17:Q:70:ARG:HG2   | 1.78                     | 0.65              |
| 1:A:931:G:H21    | 1:A:1208:A:H62    | 1.43                     | 0.65              |
| 3:C:64:VAL:HG12  | 3:C:66:VAL:HG23   | 1.78                     | 0.65              |
| 13:M:84:ILE:O    | 13:M:86:CYS:N     | 2.30                     | 0.65              |
| 1:A:981:G:N2     | 1:A:1020:C:C2     | 2.64                     | 0.64              |
| 2:B:98:LEU:O     | 2:B:101:MET:HG3   | 1.96                     | 0.64              |
| 1:A:1461:C:H2'   | 1:A:1462:U:H5'    | 1.79                     | 0.64              |
| 1:A:1227:C:H2'   | 1:A:1228:U:C5'    | 2.27                     | 0.64              |
| 1:A:432:U:H5''   | 4:D:155:LEU:HD22  | 1.79                     | 0.64              |
| 1:A:1345:A:H1'   | 1:A:1347:G:N7     | 2.12                     | 0.64              |
| 1:A:400:U:H3'    | 1:A:401:G:H5'     | 1.78                     | 0.64              |
| 1:A:986:C:H42    | 1:A:1000:G:N2     | 1.96                     | 0.64              |
| 1:A:824:U:C6     | 1:A:825:C:H1'     | 2.32                     | 0.64              |
| 1:A:545:C:O2'    | 12:L:15:ARG:HB3   | 1.97                     | 0.64              |
| 19:S:53:ASN:N    | 19:S:53:ASN:HD22  | 1.94                     | 0.64              |
| 1:A:1243:C:H2'   | 1:A:1244:C:C5'    | 2.26                     | 0.64              |
| 21:V:6:ARG:HG2   | 21:V:15:ARG:NH1   | 2.12                     | 0.64              |
| 1:A:323:C:O2     | 1:A:323:C:H2'     | 1.96                     | 0.64              |
| 5:E:120:THR:HG22 | 5:E:121:LYS:N     | 2.11                     | 0.64              |
| 1:A:238:A:C4'    | 1:A:239:U:H5'     | 2.27                     | 0.64              |
| 3:C:139:GLN:HA   | 3:C:139:GLN:NE2   | 2.12                     | 0.64              |
| 2:B:117:GLU:O    | 2:B:120:ALA:HB3   | 1.97                     | 0.64              |
| 9:I:29:ASN:HD21  | 9:I:65:VAL:HG12   | 1.63                     | 0.64              |
| 1:A:1121:G:N2    | 1:A:1125:G:H21    | 1.95                     | 0.64              |
| 1:A:825:C:H3'    | 1:A:825:C:C6      | 2.32                     | 0.64              |
| 3:C:58:GLU:H     | 3:C:65:ALA:HB3    | 1.62                     | 0.64              |
| 2:B:118:LEU:HB2  | 2:B:142:LEU:HD12  | 1.78                     | 0.64              |
| 2:B:96:ARG:N     | 2:B:96:ARG:HD2    | 2.12                     | 0.64              |
| 12:L:55:VAL:CG1  | 12:L:67:THR:HG23  | 2.28                     | 0.64              |
| 1:A:866:A:H4'    | 1:A:867:G:O5'     | 1.97                     | 0.64              |
| 1:A:1333:C:H2'   | 1:A:1334:G:C8     | 2.33                     | 0.64              |
| 1:A:1433:G:H2'   | 1:A:1434:G:O4'    | 1.98                     | 0.64              |
| 1:A:1139:A:H5'   | 1:A:1140:C:C6     | 2.32                     | 0.64              |
| 1:A:1297:G:N2    | 1:A:1299:A:H3'    | 2.13                     | 0.64              |
| 1:A:934:U:H3     | 1:A:937:U:C5'     | 2.10                     | 0.64              |
| 1:A:1482:G:H4'   | 1:A:1483:U:O5'    | 1.97                     | 0.64              |
| 1:A:516:A:O2'    | 1:A:518:A:OP2     | 2.09                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:387:G:H2'    | 1:A:388:A:H8     | 1.63                     | 0.64              |
| 15:O:56:LEU:HA   | 15:O:59:MET:HE2  | 1.80                     | 0.64              |
| 3:C:156:ARG:H    | 3:C:163:ALA:HA   | 1.63                     | 0.64              |
| 1:A:795:C:HO2'   | 1:A:796:U:P      | 2.20                     | 0.64              |
| 3:C:148:GLY:HA3  | 3:C:172:ARG:O    | 1.98                     | 0.64              |
| 6:F:4:TYR:CZ     | 6:F:72:VAL:HG21  | 2.33                     | 0.64              |
| 1:A:1258:C:C6    | 1:A:1258:C:H3'   | 2.33                     | 0.64              |
| 20:T:82:SER:O    | 20:T:86:ARG:HB2  | 1.97                     | 0.63              |
| 1:A:1036:C:N3    | 23:X:34:70U:H4'  | 2.13                     | 0.63              |
| 1:A:1349:C:H5'   | 10:J:60:ARG:NH1  | 2.13                     | 0.63              |
| 13:M:106:ASN:O   | 13:M:107:ALA:HB2 | 1.99                     | 0.63              |
| 2:B:132:LYS:HG2  | 2:B:135:GLN:OE1  | 1.98                     | 0.63              |
| 4:D:117:ALA:O    | 4:D:121:VAL:HG23 | 1.98                     | 0.63              |
| 6:F:26:ILE:O     | 6:F:30:LEU:HG    | 1.99                     | 0.63              |
| 19:S:6:LYS:HG2   | 19:S:7:LYS:H     | 1.62                     | 0.63              |
| 1:A:1258:C:H6    | 1:A:1258:C:H3'   | 1.64                     | 0.63              |
| 2:B:189:ASP:O    | 2:B:191:ASP:N    | 2.30                     | 0.63              |
| 1:A:1301:C:N4    | 19:S:36:ARG:HG3  | 2.13                     | 0.63              |
| 15:O:17:ARG:HG3  | 15:O:17:ARG:NH1  | 2.07                     | 0.63              |
| 1:A:1022:U:H2'   | 1:A:1023:A:C8    | 2.33                     | 0.63              |
| 17:Q:65:ILE:N    | 17:Q:65:ILE:HD12 | 2.13                     | 0.63              |
| 1:A:1163:G:O2'   | 1:A:1164:A:OP2   | 2.16                     | 0.63              |
| 13:M:5:ALA:HB3   | 13:M:8:GLU:HB2   | 1.79                     | 0.63              |
| 3:C:204:LEU:HD23 | 3:C:204:LEU:N    | 2.14                     | 0.63              |
| 1:A:173:A:H2'    | 1:A:174:U:C6     | 2.34                     | 0.63              |
| 13:M:50:GLU:O    | 13:M:54:VAL:HG23 | 1.99                     | 0.63              |
| 8:H:56:LYS:N     | 8:H:56:LYS:HD2   | 2.14                     | 0.63              |
| 19:S:53:ASN:N    | 19:S:53:ASN:ND2  | 2.46                     | 0.63              |
| 10:J:8:LEU:HD12  | 10:J:20:ALA:HB2  | 1.81                     | 0.63              |
| 1:A:417:C:O2'    | 1:A:418:G:OP2    | 2.17                     | 0.63              |
| 1:A:669:U:O4     | 1:A:686:G:O2'    | 2.11                     | 0.62              |
| 1:A:981:G:H22    | 1:A:982:A:H1'    | 1.58                     | 0.62              |
| 4:D:70:ILE:HD11  | 4:D:100:ARG:NE   | 2.13                     | 0.62              |
| 8:H:64:LYS:CG    | 8:H:79:VAL:HG21  | 2.29                     | 0.62              |
| 8:H:4:ASP:OD2    | 8:H:85:ARG:NH1   | 2.32                     | 0.62              |
| 4:D:22:LYS:HB3   | 4:D:26:CYS:SG    | 2.38                     | 0.62              |
| 4:D:24:GLU:O     | 4:D:25:ARG:HB3   | 1.98                     | 0.62              |
| 19:S:16:LEU:O    | 19:S:19:VAL:HG12 | 1.98                     | 0.62              |
| 9:I:5:TYR:O      | 9:I:87:GLN:HG3   | 1.99                     | 0.62              |
| 6:F:11:ASN:O     | 6:F:14:LEU:HD11  | 1.99                     | 0.62              |
| 1:A:986:C:O5'    | 1:A:986:C:H6     | 1.81                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1035:G:N7     | 1:A:1181:C:H5''   | 2.15                     | 0.62              |
| 4:D:100:ARG:NH1   | 4:D:137:SER:HA    | 2.14                     | 0.62              |
| 1:A:275:C:H4'     | 1:A:276:G:OP2     | 1.97                     | 0.62              |
| 17:Q:67:LYS:O     | 17:Q:69:LYS:N     | 2.29                     | 0.62              |
| 5:E:99:GLY:O      | 5:E:117:ASP:HA    | 1.99                     | 0.62              |
| 5:E:145:LYS:HA    | 8:H:107:LEU:HD21  | 1.81                     | 0.62              |
| 2:B:178:ARG:NH1   | 2:B:178:ARG:HG3   | 2.13                     | 0.62              |
| 1:A:900:A:OP1     | 5:E:21:ALA:HB2    | 1.99                     | 0.62              |
| 1:A:446:A:O2'     | 1:A:447:A:O5'     | 2.15                     | 0.62              |
| 1:A:1121:G:H21    | 1:A:1125:G:H21    | 1.47                     | 0.62              |
| 1:A:1197:G:H5''   | 14:N:5:ALA:HB2    | 1.80                     | 0.62              |
| 1:A:1425:G:H5''   | 1:A:1426:A:H5'    | 1.82                     | 0.62              |
| 1:A:1425:G:H5''   | 1:A:1426:A:H4'    | 1.82                     | 0.62              |
| 10:J:49:VAL:O     | 10:J:60:ARG:HA    | 2.00                     | 0.62              |
| 1:A:1328:G:O2'    | 1:A:1329:U:OP2    | 2.18                     | 0.62              |
| 9:I:125:TYR:CE1   | 9:I:128:ARG:HB3   | 2.29                     | 0.62              |
| 5:E:79:GLU:HG3    | 5:E:93:PRO:HD2    | 1.81                     | 0.62              |
| 5:E:29:GLY:HA2    | 5:E:47:LYS:HG3    | 1.82                     | 0.62              |
| 20:T:37:SER:O     | 20:T:41:VAL:HG23  | 1.99                     | 0.62              |
| 1:A:8:A:H4'       | 1:A:9:G:OP1       | 1.97                     | 0.62              |
| 7:G:115:ARG:HB2   | 7:G:118:VAL:HG23  | 1.82                     | 0.62              |
| 2:B:9:GLU:HA      | 2:B:12:GLU:OE2    | 1.99                     | 0.62              |
| 3:C:14:ILE:HG22   | 3:C:15:THR:N      | 2.15                     | 0.62              |
| 12:L:28:LYS:C     | 12:L:30:ALA:N     | 2.54                     | 0.62              |
| 9:I:16:ARG:HE     | 9:I:64:THR:HG21   | 1.65                     | 0.62              |
| 1:A:423:G:H4'     | 1:A:424:U:O5'     | 1.99                     | 0.62              |
| 6:F:19:LEU:HD23   | 6:F:20:ALA:N      | 2.15                     | 0.62              |
| 1:A:937:U:O2'     | 1:A:1204:C:H4'    | 1.99                     | 0.61              |
| 26:A:1783:PAR:O62 | 26:A:1783:PAR:H13 | 1.99                     | 0.61              |
| 4:D:199:ASN:ND2   | 4:D:201:GLN:HB3   | 2.13                     | 0.61              |
| 20:T:10:LEU:O     | 20:T:13:LEU:HG    | 2.00                     | 0.61              |
| 1:A:501:C:N4      | 1:A:513:G:N2      | 2.48                     | 0.61              |
| 9:I:9:ARG:HA      | 9:I:13:ALA:O      | 1.99                     | 0.61              |
| 4:D:11:LEU:O      | 4:D:15:GLU:HB2    | 2.00                     | 0.61              |
| 1:A:775:A:H4'     | 1:A:776:U:C5'     | 2.30                     | 0.61              |
| 2:B:51:LEU:HD22   | 2:B:55:PHE:HE2    | 1.64                     | 0.61              |
| 19:S:51:VAL:O     | 19:S:58:VAL:HG22  | 1.99                     | 0.61              |
| 1:A:570:G:H4'     | 1:A:571:G:OP1     | 1.98                     | 0.61              |
| 1:A:1521:U:O2'    | 22:W:1:A:OP1      | 2.07                     | 0.61              |
| 16:P:36:ILE:O     | 16:P:51:VAL:O     | 2.18                     | 0.61              |
| 7:G:15:ASP:HB3    | 7:G:20:ASP:H      | 1.65                     | 0.61              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 2:B:230:VAL:HG12 | 2:B:231:GLU:N      | 2.15                     | 0.61              |
| 13:M:25:ILE:HD11 | 13:M:60:VAL:CG1    | 2.30                     | 0.61              |
| 12:L:39:VAL:HG12 | 12:L:41:ARG:H      | 1.64                     | 0.61              |
| 10:J:32:ALA:CB   | 10:J:75:ILE:HG13   | 2.30                     | 0.61              |
| 1:A:407:A:N1     | 4:D:35:ARG:HG3     | 2.15                     | 0.61              |
| 9:I:86:VAL:HG13  | 9:I:90:PRO:HA      | 1.83                     | 0.61              |
| 7:G:26:PHE:CE2   | 7:G:30:ILE:HD11    | 2.35                     | 0.61              |
| 11:K:126:ARG:O   | 11:K:127:LYS:HB2   | 1.99                     | 0.61              |
| 1:A:1031:U:H2'   | 14:N:3:ARG:HH11    | 1.66                     | 0.61              |
| 20:T:57:ARG:NH2  | 20:T:100:ILE:HG22  | 2.16                     | 0.61              |
| 1:A:1222:G:H2'   | 1:A:1223:C:C6      | 2.36                     | 0.61              |
| 13:M:25:ILE:HD11 | 13:M:60:VAL:HG11   | 1.81                     | 0.61              |
| 11:K:48:ILE:HD11 | 11:K:64:ALA:HA     | 1.82                     | 0.61              |
| 12:L:115:LYS:O   | 12:L:117:ARG:N     | 2.30                     | 0.61              |
| 2:B:76:GLN:HG3   | 2:B:206:ASP:OD1    | 2.00                     | 0.61              |
| 4:D:3:ARG:NH2    | 4:D:71:SER:HB3     | 2.15                     | 0.61              |
| 15:O:61:GLY:O    | 15:O:64:ARG:HG2    | 2.01                     | 0.61              |
| 3:C:155:GLY:HA3  | 3:C:163:ALA:HB1    | 1.83                     | 0.61              |
| 7:G:15:ASP:CB    | 7:G:20:ASP:H       | 2.12                     | 0.61              |
| 3:C:132:ARG:O    | 3:C:136:GLN:HG3    | 1.99                     | 0.61              |
| 3:C:58:GLU:HB2   | 3:C:65:ALA:CB      | 2.31                     | 0.61              |
| 6:F:8:ILE:HD11   | 6:F:79:LEU:HD13    | 1.81                     | 0.61              |
| 2:B:88:ALA:C     | 2:B:90:MET:H       | 2.04                     | 0.61              |
| 10:J:8:LEU:HB3   | 10:J:16:LEU:HD22   | 1.82                     | 0.61              |
| 1:A:1082:C:C3'   | 1:A:1082:C:C6      | 2.83                     | 0.61              |
| 17:Q:24:GLU:HG2  | 17:Q:39:SER:HB3    | 1.83                     | 0.61              |
| 3:C:40:ARG:O     | 3:C:44:GLU:HB3     | 2.01                     | 0.61              |
| 1:A:830:G:O2'    | 1:A:831:G:H5'      | 2.01                     | 0.61              |
| 12:L:91:LYS:CE   | 12:L:91:LYS:HA     | 2.31                     | 0.61              |
| 1:A:1373:U:H2'   | 1:A:1374:G:C8      | 2.36                     | 0.61              |
| 1:A:1387:G:P     | 26:A:1783:PAR:HO34 | 2.24                     | 0.61              |
| 11:K:14:VAL:HG21 | 11:K:40:ILE:HD11   | 1.83                     | 0.61              |
| 2:B:161:ALA:HB1  | 2:B:185:ILE:HD11   | 1.83                     | 0.61              |
| 4:D:15:GLU:HG3   | 4:D:63:LYS:HG3     | 1.83                     | 0.60              |
| 19:S:29:ARG:H    | 19:S:29:ARG:CD     | 2.12                     | 0.60              |
| 1:A:944:C:O2'    | 9:I:128:ARG:HD3    | 2.00                     | 0.60              |
| 1:A:341:G:C2'    | 1:A:342:G:H5'      | 2.31                     | 0.60              |
| 4:D:36:ARG:N     | 4:D:37:PRO:HD3     | 2.16                     | 0.60              |
| 1:A:966:C:H42    | 1:A:1197:G:H1      | 1.48                     | 0.60              |
| 2:B:47:THR:HG23  | 2:B:202:PRO:O      | 2.00                     | 0.60              |
| 17:Q:76:LEU:HD23 | 17:Q:77:VAL:N      | 2.16                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:36:ARG:HD2   | 2:B:41:ILE:HD13  | 1.82                     | 0.60              |
| 1:A:1008:C:N4    | 1:A:1014:G:N1    | 2.49                     | 0.60              |
| 1:A:1003:U:H3'   | 1:A:1003:U:H6    | 1.65                     | 0.60              |
| 1:A:983:A:OP2    | 1:A:984:C:C5     | 2.54                     | 0.60              |
| 1:A:952:A:H8     | 1:A:952:A:H5'    | 1.65                     | 0.60              |
| 7:G:38:LEU:HA    | 7:G:41:ARG:HD3   | 1.83                     | 0.60              |
| 15:O:25:THR:HG21 | 15:O:70:LEU:HB2  | 1.83                     | 0.60              |
| 1:A:1120:G:H3'   | 1:A:1120:G:N3    | 2.16                     | 0.60              |
| 3:C:82:GLU:HG3   | 3:C:83:ARG:H     | 1.67                     | 0.60              |
| 3:C:14:ILE:HG22  | 3:C:15:THR:HG23  | 1.83                     | 0.60              |
| 10:J:4:ILE:N     | 10:J:4:ILE:HD12  | 2.16                     | 0.60              |
| 18:R:25:THR:HG21 | 18:R:42:ARG:HD3  | 1.83                     | 0.60              |
| 4:D:31:CYS:C     | 4:D:33:MET:H     | 2.03                     | 0.60              |
| 1:A:472:C:H6     | 1:A:472:C:O5'    | 1.83                     | 0.60              |
| 23:X:33:U:H5'    | 23:X:34:70U:OP2  | 2.02                     | 0.60              |
| 2:B:80:ILE:CD1   | 2:B:208:ILE:HG23 | 2.19                     | 0.60              |
| 10:J:61:GLU:OE1  | 14:N:45:ARG:NH1  | 2.34                     | 0.60              |
| 1:A:635:U:H2'    | 1:A:735:G:N1     | 2.16                     | 0.60              |
| 9:I:48:GLU:HA    | 9:I:51:ARG:NH1   | 2.14                     | 0.60              |
| 2:B:33:TYR:HB3   | 2:B:41:ILE:HG13  | 1.82                     | 0.60              |
| 1:A:1131:C:H2'   | 1:A:1132:U:C6    | 2.36                     | 0.60              |
| 12:L:41:ARG:HB3  | 12:L:41:ARG:CZ   | 2.31                     | 0.60              |
| 6:F:33:TYR:CD1   | 6:F:75:LEU:HD23  | 2.37                     | 0.60              |
| 1:A:1109:G:H21   | 1:A:1128:A:H62   | 1.50                     | 0.60              |
| 1:A:448:C:H41    | 1:A:462:A:H2     | 1.50                     | 0.60              |
| 14:N:13:THR:HG22 | 14:N:13:THR:O    | 2.01                     | 0.60              |
| 1:A:1080:C:H2'   | 1:A:1081:G:C8    | 2.36                     | 0.60              |
| 23:X:39:PSU:C6   | 23:X:39:PSU:H5'  | 2.35                     | 0.60              |
| 2:B:142:LEU:HD21 | 2:B:146:GLN:OE1  | 2.01                     | 0.60              |
| 5:E:116:THR:HG23 | 5:E:117:ASP:OD2  | 2.02                     | 0.60              |
| 1:A:171:C:OP1    | 20:T:65:LYS:NZ   | 2.28                     | 0.60              |
| 8:H:83:ILE:O     | 8:H:83:ILE:HG23  | 2.01                     | 0.60              |
| 10:J:12:ASP:HB3  | 10:J:15:THR:HG22 | 1.82                     | 0.60              |
| 1:A:959:U:OP1    | 1:A:959:U:H6     | 1.84                     | 0.60              |
| 9:I:13:ALA:HA    | 9:I:67:GLY:O     | 2.02                     | 0.60              |
| 4:D:189:PRO:CB   | 4:D:194:LEU:HD21 | 2.27                     | 0.60              |
| 2:B:132:LYS:O    | 2:B:136:VAL:HG23 | 2.00                     | 0.60              |
| 1:A:1509:U:C2'   | 1:A:1510:C:H5'   | 2.31                     | 0.60              |
| 18:R:38:GLU:HA   | 18:R:41:LYS:HE2  | 1.82                     | 0.60              |
| 1:A:916:G:H5''   | 7:G:102:ARG:HH22 | 1.67                     | 0.60              |
| 1:A:84:C:O5'     | 1:A:84:C:H6      | 1.85                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:515:A:H5''   | 3:C:161:GLU:CD   | 2.20                     | 0.59              |
| 9:I:19:LEU:CD2   | 9:I:61:ALA:HB2   | 2.32                     | 0.59              |
| 4:D:127:THR:CG2  | 4:D:147:ALA:HB3  | 2.31                     | 0.59              |
| 1:A:795:C:H4'    | 1:A:796:U:H5'    | 1.82                     | 0.59              |
| 1:A:1193:U:O2'   | 1:A:1194:A:C8    | 2.49                     | 0.59              |
| 16:P:26:ARG:HD2  | 16:P:31:LYS:O    | 2.02                     | 0.59              |
| 1:A:1406:C:O2'   | 1:A:1407:U:H5'   | 2.01                     | 0.59              |
| 10:J:8:LEU:CD1   | 10:J:20:ALA:HB2  | 2.31                     | 0.59              |
| 3:C:58:GLU:HB2   | 3:C:65:ALA:HB2   | 1.83                     | 0.59              |
| 1:A:17:U:H2'     | 1:A:18:C:C6      | 2.37                     | 0.59              |
| 14:N:8:GLU:HB2   | 14:N:11:LYS:HB2  | 1.83                     | 0.59              |
| 2:B:28:PHE:CD2   | 2:B:190:THR:HA   | 2.37                     | 0.59              |
| 17:Q:27:PHE:HB2  | 17:Q:28:PRO:HD2  | 1.84                     | 0.59              |
| 1:A:954:A:H2'    | 1:A:955:A:H5''   | 1.84                     | 0.59              |
| 6:F:11:ASN:ND2   | 6:F:13:ASN:H     | 1.96                     | 0.59              |
| 13:M:40:ASN:ND2  | 13:M:41:PRO:HD2  | 2.17                     | 0.59              |
| 2:B:21:ARG:O     | 2:B:22:LYS:HD2   | 2.01                     | 0.59              |
| 14:N:32:SER:HB3  | 14:N:41:ARG:HB3  | 1.84                     | 0.59              |
| 3:C:139:GLN:CA   | 3:C:139:GLN:HE21 | 2.14                     | 0.59              |
| 1:A:1035:G:H5'   | 1:A:1036:C:C5'   | 2.29                     | 0.59              |
| 5:E:76:ILE:HG23  | 5:E:142:LEU:HD13 | 1.84                     | 0.59              |
| 3:C:175:LEU:HD21 | 3:C:201:TYR:HE2  | 1.66                     | 0.59              |
| 20:T:59:ALA:O    | 20:T:63:ILE:HG13 | 2.02                     | 0.59              |
| 1:A:1006:C:H2'   | 1:A:1007:C:O4'   | 2.02                     | 0.59              |
| 18:R:55:ARG:HB3  | 18:R:55:ARG:CZ   | 2.33                     | 0.59              |
| 5:E:120:THR:CG2  | 5:E:121:LYS:N    | 2.64                     | 0.59              |
| 8:H:89:PRO:HA    | 8:H:92:ARG:NH1   | 2.17                     | 0.59              |
| 1:A:969:U:O2'    | 1:A:970:G:OP2    | 2.20                     | 0.59              |
| 1:A:984:C:C6     | 1:A:985:C:H5     | 2.21                     | 0.59              |
| 1:A:625:A:C8     | 8:H:115:SER:HA   | 2.38                     | 0.59              |
| 12:L:124:LYS:HD2 | 12:L:125:PRO:HD2 | 1.85                     | 0.59              |
| 1:A:1394:C:H2'   | 1:A:1395:A:C8    | 2.37                     | 0.59              |
| 1:A:1005:C:H2'   | 1:A:1006:C:C5    | 2.37                     | 0.59              |
| 23:X:39:PSU:H2'  | 23:X:40:C:O4'    | 2.03                     | 0.59              |
| 9:I:111:ARG:HD2  | 14:N:61:TRP:OXT  | 2.03                     | 0.59              |
| 14:N:8:GLU:O     | 14:N:11:LYS:HB2  | 2.02                     | 0.59              |
| 1:A:276:G:O2'    | 1:A:277:A:OP2    | 2.18                     | 0.59              |
| 1:A:1082:C:N4    | 1:A:1085:C:OP1   | 2.35                     | 0.59              |
| 16:P:8:ARG:HB2   | 16:P:28:ARG:NH1  | 2.17                     | 0.59              |
| 15:O:21:ASP:OD1  | 15:O:24:SER:HB3  | 2.02                     | 0.59              |
| 9:I:16:ARG:NH1   | 9:I:16:ARG:HG2   | 2.18                     | 0.59              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1461:C:C2'   | 1:A:1462:U:H5'    | 2.32                     | 0.59              |
| 10:J:71:LEU:CD1  | 10:J:73:ASP:HB2   | 2.33                     | 0.59              |
| 18:R:86:VAL:O    | 18:R:87:ARG:HB2   | 2.02                     | 0.59              |
| 1:A:981:G:H21    | 1:A:982:A:C1'     | 2.08                     | 0.59              |
| 14:N:3:ARG:HH21  | 14:N:6:LEU:HD11   | 1.65                     | 0.59              |
| 5:E:81:GLU:CD    | 5:E:88:LYS:HE2    | 2.24                     | 0.59              |
| 1:A:408:G:H22    | 1:A:424:U:H5''    | 1.68                     | 0.59              |
| 1:A:396:C:H1'    | 1:A:605:A:H1'     | 1.84                     | 0.59              |
| 1:A:328:G:H4'    | 20:T:16:HIS:CE1   | 2.38                     | 0.59              |
| 1:A:999:G:O2'    | 1:A:1000:G:H5'    | 2.03                     | 0.58              |
| 13:M:94:ARG:NH1  | 19:S:81:ARG:HD3   | 2.09                     | 0.58              |
| 10:J:4:ILE:HD13  | 10:J:74:ILE:O     | 2.03                     | 0.58              |
| 8:H:68:ARG:NH1   | 8:H:68:ARG:HB3    | 2.14                     | 0.58              |
| 16:P:52:ASP:OD1  | 16:P:52:ASP:O     | 2.21                     | 0.58              |
| 9:I:16:ARG:NE    | 9:I:64:THR:CG2    | 2.66                     | 0.58              |
| 6:F:101:ALA:HB2  | 18:R:28:GLU:CG    | 2.33                     | 0.58              |
| 18:R:26:LEU:N    | 18:R:26:LEU:HD23  | 2.18                     | 0.58              |
| 11:K:69:ALA:O    | 11:K:73:MET:HG2   | 2.03                     | 0.58              |
| 1:A:1253:G:O2'   | 1:A:1254:G:H5'    | 2.03                     | 0.58              |
| 2:B:12:GLU:N     | 2:B:12:GLU:OE1    | 2.35                     | 0.58              |
| 1:A:1231:A:C4'   | 9:I:68:GLY:H      | 2.14                     | 0.58              |
| 1:A:1387:G:P     | 26:A:1783:PAR:O34 | 2.61                     | 0.58              |
| 19:S:44:MET:O    | 19:S:47:HIS:HB2   | 2.03                     | 0.58              |
| 1:A:1324:G:H2'   | 1:A:1325:C:C6     | 2.37                     | 0.58              |
| 13:M:37:THR:CG2  | 13:M:55:ARG:HD2   | 2.33                     | 0.58              |
| 1:A:1288:U:H5'   | 13:M:109:THR:HG21 | 1.85                     | 0.58              |
| 3:C:155:GLY:O    | 3:C:196:LEU:HD22  | 2.03                     | 0.58              |
| 3:C:22:TRP:CH2   | 3:C:32:LEU:HB2    | 2.37                     | 0.58              |
| 11:K:77:MET:HE1  | 11:K:80:VAL:HG12  | 1.86                     | 0.58              |
| 4:D:196:LEU:HB3  | 4:D:198:VAL:HG22  | 1.84                     | 0.58              |
| 4:D:64:LEU:HD21  | 4:D:97:LEU:CD1    | 2.33                     | 0.58              |
| 6:F:37:VAL:HA    | 6:F:65:VAL:HG12   | 1.84                     | 0.58              |
| 1:A:929:U:O4     | 13:M:104:ARG:HD3  | 2.03                     | 0.58              |
| 11:K:57:THR:OG1  | 11:K:58:PRO:HD2   | 2.04                     | 0.58              |
| 15:O:17:ARG:HH11 | 15:O:17:ARG:CG    | 2.12                     | 0.58              |
| 4:D:151:LYS:H    | 4:D:151:LYS:CD    | 2.10                     | 0.58              |
| 1:A:685:A:H4'    | 1:A:686:G:OP2     | 2.04                     | 0.58              |
| 10:J:61:GLU:OE2  | 14:N:58:LYS:NZ    | 2.36                     | 0.58              |
| 5:E:76:ILE:HG22  | 5:E:78:HIS:H      | 1.69                     | 0.58              |
| 13:M:40:ASN:HD22 | 13:M:41:PRO:N     | 2.00                     | 0.58              |
| 1:A:446:A:HO2'   | 1:A:447:A:C5'     | 2.16                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 12:L:47:LYS:HB2  | 12:L:47:LYS:NZ   | 2.17                     | 0.58              |
| 2:B:61:LEU:HD21  | 2:B:160:ASP:CB   | 2.32                     | 0.58              |
| 1:A:980:G:C2     | 1:A:981:G:C5     | 2.91                     | 0.58              |
| 2:B:118:LEU:CB   | 2:B:142:LEU:HD12 | 2.33                     | 0.58              |
| 1:A:1006:C:H6    | 1:A:1006:C:O5'   | 1.87                     | 0.58              |
| 1:A:1295:C:C5    | 19:S:6:LYS:HE2   | 2.39                     | 0.58              |
| 1:A:1062:A:O3'   | 5:E:16:THR:OG1   | 2.21                     | 0.58              |
| 7:G:66:VAL:O     | 7:G:70:LYS:HG3   | 2.03                     | 0.58              |
| 1:A:1286:G:N2    | 1:A:1312:G:HO2'  | 2.02                     | 0.58              |
| 18:R:22:VAL:HB   | 18:R:56:THR:HA   | 1.85                     | 0.58              |
| 10:J:49:VAL:HG13 | 14:N:41:ARG:HB2  | 1.85                     | 0.58              |
| 3:C:175:LEU:HD21 | 3:C:201:TYR:CE2  | 2.39                     | 0.58              |
| 4:D:64:LEU:HD21  | 4:D:97:LEU:HD13  | 1.84                     | 0.58              |
| 4:D:15:GLU:CG    | 4:D:63:LYS:HG3   | 2.34                     | 0.58              |
| 1:A:1354:U:O2'   | 1:A:1355:G:H5'   | 2.04                     | 0.58              |
| 1:A:1301:C:C2'   | 1:A:1302:C:O5'   | 2.51                     | 0.58              |
| 1:A:1301:C:H2'   | 1:A:1302:C:O5'   | 2.03                     | 0.58              |
| 9:I:9:ARG:HD3    | 9:I:14:VAL:CG1   | 2.34                     | 0.58              |
| 4:D:62:GLN:HE22  | 4:D:65:ARG:HH12  | 1.51                     | 0.58              |
| 1:A:824:U:C5     | 1:A:825:C:H1'    | 2.39                     | 0.58              |
| 16:P:20:VAL:HG23 | 16:P:34:GLU:O    | 2.03                     | 0.58              |
| 1:A:713:G:N2     | 1:A:748:G:H5''   | 2.19                     | 0.58              |
| 1:A:1505:U:O2'   | 1:A:1506:G:H3'   | 2.04                     | 0.58              |
| 1:A:120:G:HO2'   | 17:Q:2:PRO:N     | 2.02                     | 0.58              |
| 5:E:82:VAL:HG21  | 5:E:138:ALA:HA   | 1.85                     | 0.58              |
| 10:J:29:ARG:NH1  | 10:J:29:ARG:HG2  | 2.17                     | 0.58              |
| 23:X:34:70U:H2'  | 23:X:35:U:H6     | 1.69                     | 0.58              |
| 3:C:11:ARG:O     | 3:C:14:ILE:O     | 2.20                     | 0.58              |
| 1:A:1206:A:H3'   | 1:A:1207:C:C5    | 2.39                     | 0.58              |
| 1:A:406:A:C4     | 1:A:408:G:H1'    | 2.39                     | 0.58              |
| 1:A:705:A:H4'    | 1:A:706:U:OP1    | 2.04                     | 0.58              |
| 1:A:1299:A:OP2   | 1:A:1299:A:H8    | 1.87                     | 0.58              |
| 1:A:603:C:H2'    | 1:A:604:A:O4'    | 2.03                     | 0.58              |
| 1:A:1157:A:H2'   | 1:A:1158:G:C8    | 2.39                     | 0.58              |
| 1:A:629:U:H2'    | 1:A:630:C:C6     | 2.39                     | 0.58              |
| 1:A:726:U:H2'    | 1:A:727:C:C6     | 2.39                     | 0.58              |
| 8:H:49:GLU:HG2   | 8:H:62:TYR:HE2   | 1.68                     | 0.58              |
| 1:A:670:A:H62    | 1:A:686:G:H1'    | 1.69                     | 0.57              |
| 7:G:38:LEU:HD12  | 7:G:38:LEU:O     | 2.04                     | 0.57              |
| 1:A:823:C:H4'    | 1:A:824:U:OP1    | 2.04                     | 0.57              |
| 7:G:23:VAL:O     | 7:G:27:ILE:HG13  | 2.03                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:157:LEU:O    | 4:D:157:LEU:HD23 | 2.04                     | 0.57              |
| 4:D:3:ARG:HE     | 4:D:3:ARG:HA     | 1.68                     | 0.57              |
| 10:J:75:ILE:O    | 10:J:76:ASN:HB2  | 2.04                     | 0.57              |
| 2:B:7:VAL:HB     | 2:B:8:LYS:NZ     | 2.18                     | 0.57              |
| 3:C:193:TYR:HE1  | 3:C:196:LEU:HD21 | 1.69                     | 0.57              |
| 4:D:196:LEU:CD2  | 4:D:197:PRO:HD2  | 2.34                     | 0.57              |
| 1:A:1458:U:H2'   | 1:A:1459:G:H5'   | 1.86                     | 0.57              |
| 1:A:656:G:H2'    | 1:A:657:G:C8     | 2.40                     | 0.57              |
| 9:I:121:ARG:HH11 | 9:I:121:ARG:HG2  | 1.69                     | 0.57              |
| 1:A:1287:A:C2    | 1:A:1288:U:H1'   | 2.39                     | 0.57              |
| 10:J:60:ARG:HH11 | 10:J:60:ARG:HG2  | 1.69                     | 0.57              |
| 1:A:52:G:O2'     | 1:A:53:A:H5'     | 2.04                     | 0.57              |
| 10:J:3:LYS:N     | 10:J:75:ILE:HA   | 2.19                     | 0.57              |
| 2:B:7:VAL:CG2    | 2:B:8:LYS:HZ3    | 2.16                     | 0.57              |
| 5:E:24:ARG:HH11  | 5:E:24:ARG:HG2   | 1.70                     | 0.57              |
| 3:C:129:ALA:CB   | 3:C:132:ARG:HE   | 2.17                     | 0.57              |
| 13:M:3:ARG:HA    | 13:M:8:GLU:O     | 2.04                     | 0.57              |
| 15:O:71:GLN:HB2  | 15:O:78:TYR:CD1  | 2.40                     | 0.57              |
| 9:I:79:LEU:HD22  | 9:I:83:ARG:HG3   | 1.85                     | 0.57              |
| 3:C:126:ARG:HH11 | 3:C:126:ARG:HG3  | 1.69                     | 0.57              |
| 1:A:984:C:C2'    | 1:A:985:C:C5     | 2.86                     | 0.57              |
| 16:P:28:ARG:HG2  | 16:P:28:ARG:NH1  | 2.16                     | 0.57              |
| 2:B:101:MET:HG2  | 2:B:108:ILE:HD13 | 1.85                     | 0.57              |
| 7:G:38:LEU:O     | 7:G:42:ILE:HG13  | 2.04                     | 0.57              |
| 7:G:18:TYR:CD1   | 7:G:59:LEU:HB2   | 2.40                     | 0.57              |
| 7:G:121:ALA:O    | 7:G:125:MET:HG3  | 2.04                     | 0.57              |
| 1:A:1183:G:H2'   | 1:A:1184:C:C5'   | 2.34                     | 0.57              |
| 1:A:1131:C:O2'   | 1:A:1261:A:N1    | 2.37                     | 0.57              |
| 1:A:109:A:H2'    | 1:A:110:G:O4'    | 2.04                     | 0.57              |
| 4:D:8:VAL:HG11   | 4:D:115:ARG:NH1  | 2.19                     | 0.57              |
| 8:H:2:LEU:HD12   | 8:H:2:LEU:H      | 1.70                     | 0.57              |
| 17:Q:68:ARG:HH11 | 17:Q:68:ARG:HG3  | 1.69                     | 0.57              |
| 12:L:60:LEU:HB2  | 12:L:64:TYR:O    | 2.05                     | 0.57              |
| 20:T:23:ARG:HH12 | 20:T:27:LYS:NZ   | 2.03                     | 0.57              |
| 1:A:432:U:O2'    | 4:D:123:HIS:HD2  | 1.87                     | 0.57              |
| 1:A:520:G:OP1    | 12:L:113:ARG:NH2 | 2.37                     | 0.57              |
| 10:J:29:ARG:HH11 | 10:J:29:ARG:HG2  | 1.68                     | 0.57              |
| 6:F:99:ALA:O     | 6:F:100:ASN:HB2  | 2.04                     | 0.57              |
| 1:A:170:C:H2'    | 1:A:171:C:C6     | 2.37                     | 0.57              |
| 21:V:14:TRP:C    | 21:V:16:GLY:H    | 2.08                     | 0.57              |
| 20:T:23:ARG:HH11 | 20:T:23:ARG:HG2  | 1.69                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:10:PHE:CE2   | 3:C:178:LEU:HD13 | 2.40                     | 0.57              |
| 1:A:909:C:H5'    | 7:G:4:ARG:HG2    | 1.87                     | 0.57              |
| 1:A:980:G:N1     | 1:A:981:G:O6     | 2.37                     | 0.57              |
| 1:A:241:A:C4'    | 1:A:242:G:OP1    | 2.44                     | 0.57              |
| 9:I:97:LYS:HG2   | 9:I:102:LEU:HD12 | 1.87                     | 0.57              |
| 1:A:796:U:OP1    | 1:A:881:C:H5'    | 2.05                     | 0.57              |
| 10:J:80:LYS:O    | 10:J:83:GLU:HB3  | 2.04                     | 0.57              |
| 6:F:47:ARG:N     | 6:F:47:ARG:HD3   | 2.20                     | 0.57              |
| 14:N:44:LEU:O    | 14:N:44:LEU:HD12 | 2.05                     | 0.57              |
| 1:A:1031:U:H1'   | 1:A:1182:A:C8    | 2.40                     | 0.57              |
| 10:J:24:VAL:O    | 10:J:28:ARG:HG2  | 2.05                     | 0.57              |
| 14:N:57:ARG:HG2  | 14:N:58:LYS:N    | 2.14                     | 0.57              |
| 13:M:33:ALA:HA   | 13:M:59:TYR:HE2  | 1.70                     | 0.57              |
| 1:A:242:G:OP1    | 1:A:242:G:H4'    | 2.05                     | 0.56              |
| 19:S:16:LEU:HA   | 19:S:19:VAL:HG12 | 1.87                     | 0.56              |
| 2:B:87:ARG:NE    | 2:B:233:SER:HB3  | 2.20                     | 0.56              |
| 1:A:500:G:H5'    | 1:A:502:C:C2     | 2.40                     | 0.56              |
| 1:A:1303:C:C4'   | 1:A:1304:G:OP1   | 2.40                     | 0.56              |
| 1:A:953:G:O2'    | 1:A:954:A:H5'    | 2.03                     | 0.56              |
| 1:A:1126:G:H3'   | 1:A:1126:G:H8    | 1.71                     | 0.56              |
| 8:H:68:ARG:CB    | 8:H:68:ARG:HH11  | 2.17                     | 0.56              |
| 5:E:144:THR:O    | 5:E:148:VAL:HG23 | 2.04                     | 0.56              |
| 21:V:6:ARG:CD    | 21:V:15:ARG:HH12 | 2.17                     | 0.56              |
| 1:A:1220:A:H4'   | 1:A:1221:U:O5'   | 2.05                     | 0.56              |
| 14:N:12:ARG:C    | 14:N:14:PRO:HD3  | 2.26                     | 0.56              |
| 1:A:501:C:H5     | 1:A:513:G:C5'    | 2.18                     | 0.56              |
| 1:A:1521:U:HO3'  | 22:W:1:A:P       | 2.27                     | 0.56              |
| 10:J:90:LEU:H    | 10:J:91:PRO:CD   | 2.09                     | 0.56              |
| 1:A:1311:U:H2'   | 1:A:1312:G:H5'   | 1.87                     | 0.56              |
| 2:B:136:VAL:HA   | 2:B:139:LYS:HZ3  | 1.71                     | 0.56              |
| 13:M:65:LYS:O    | 13:M:66:LEU:HD23 | 2.05                     | 0.56              |
| 13:M:5:ALA:HB3   | 13:M:8:GLU:HG3   | 1.87                     | 0.56              |
| 1:A:996:C:O5'    | 1:A:996:C:H6     | 1.87                     | 0.56              |
| 23:X:37:12A:C5'  | 23:X:37:12A:H8   | 2.22                     | 0.56              |
| 4:D:194:LEU:HD22 | 4:D:194:LEU:N    | 2.20                     | 0.56              |
| 1:A:818:U:OP1    | 18:R:64:ARG:NH2  | 2.35                     | 0.56              |
| 1:A:1042:C:H5    | 3:C:2:GLY:HA2    | 1.69                     | 0.56              |
| 3:C:155:GLY:HA2  | 3:C:164:ARG:O    | 2.06                     | 0.56              |
| 3:C:191:THR:HG21 | 3:C:193:TYR:CE2  | 2.40                     | 0.56              |
| 6:F:8:ILE:HG22   | 6:F:10:LEU:HD23  | 1.88                     | 0.56              |
| 1:A:66:G:OP1     | 1:A:66:G:H8      | 1.88                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1006:C:N4    | 1:A:1016:G:N2    | 2.52                     | 0.56              |
| 2:B:79:ASP:O     | 2:B:82:ARG:HB3   | 2.06                     | 0.56              |
| 1:A:1301:C:N3    | 19:S:36:ARG:NE   | 2.52                     | 0.56              |
| 2:B:98:LEU:HB2   | 2:B:108:ILE:HD11 | 1.87                     | 0.56              |
| 2:B:218:ALA:O    | 2:B:222:ILE:HG13 | 2.05                     | 0.56              |
| 17:Q:90:ILE:HA   | 17:Q:93:GLN:HB2  | 1.87                     | 0.56              |
| 4:D:175:SER:HB3  | 4:D:184:LYS:HB2  | 1.87                     | 0.56              |
| 5:E:48:ALA:HB1   | 5:E:49:PRO:HD2   | 1.87                     | 0.56              |
| 16:P:3:LYS:O     | 16:P:21:VAL:HA   | 2.06                     | 0.56              |
| 4:D:209:ARG:HH11 | 4:D:209:ARG:HG2  | 1.71                     | 0.56              |
| 1:A:1006:C:C3'   | 1:A:1006:C:C6    | 2.87                     | 0.56              |
| 1:A:1286:G:H22   | 1:A:1312:G:C2'   | 2.18                     | 0.56              |
| 10:J:49:VAL:HG11 | 14:N:41:ARG:O    | 2.06                     | 0.56              |
| 21:V:6:ARG:CG    | 21:V:15:ARG:NH1  | 2.69                     | 0.56              |
| 5:E:11:ILE:HB    | 5:E:31:LEU:HB3   | 1.86                     | 0.56              |
| 1:A:713:G:H21    | 1:A:748:G:H5''   | 1.71                     | 0.56              |
| 10:J:5:ARG:HD2   | 10:J:99:LYS:HB2  | 1.87                     | 0.56              |
| 1:A:79:U:H3'     | 1:A:79:U:C6      | 2.41                     | 0.56              |
| 1:A:1262:U:H4'   | 1:A:1263:C:OP2   | 2.06                     | 0.56              |
| 1:A:1123:C:H2'   | 1:A:1124:G:C5'   | 2.35                     | 0.56              |
| 3:C:79:ARG:HG2   | 3:C:82:GLU:OE1   | 2.06                     | 0.56              |
| 1:A:1136:G:H2'   | 1:A:1137:G:C8    | 2.39                     | 0.56              |
| 14:N:14:PRO:C    | 14:N:16:PHE:H    | 2.08                     | 0.56              |
| 20:T:23:ARG:NH1  | 20:T:23:ARG:HG2  | 2.20                     | 0.56              |
| 1:A:401:G:H5''   | 4:D:5:ILE:HG23   | 1.87                     | 0.56              |
| 1:A:66:G:C8      | 1:A:66:G:OP1     | 2.59                     | 0.56              |
| 1:A:686:G:O2'    | 1:A:687:A:OP2    | 2.23                     | 0.56              |
| 14:N:29:ARG:HH22 | 14:N:41:ARG:HH12 | 1.52                     | 0.56              |
| 15:O:64:ARG:HH11 | 15:O:64:ARG:HG3  | 1.71                     | 0.56              |
| 12:L:53:ARG:HH11 | 12:L:53:ARG:HG2  | 1.71                     | 0.56              |
| 1:A:916:G:H2'    | 1:A:917:C:C6     | 2.41                     | 0.56              |
| 3:C:107:GLN:O    | 3:C:108:ASN:HB3  | 2.06                     | 0.56              |
| 17:Q:60:ILE:HD13 | 17:Q:61:GLU:N    | 2.21                     | 0.56              |
| 10:J:48:THR:OG1  | 10:J:62:HIS:CD2  | 2.58                     | 0.56              |
| 1:A:224:U:H5''   | 16:P:33:ILE:HD13 | 1.88                     | 0.56              |
| 1:A:1039:G:H5''  | 3:C:154:SER:HB2  | 1.88                     | 0.56              |
| 1:A:985:C:C2     | 1:A:986:C:C4     | 2.94                     | 0.56              |
| 10:J:94:VAL:HG12 | 10:J:95:GLU:N    | 2.21                     | 0.56              |
| 13:M:9:ILE:N     | 13:M:9:ILE:HD12  | 2.21                     | 0.56              |
| 2:B:46:LYS:HA    | 2:B:49:GLU:HB2   | 1.88                     | 0.56              |
| 9:I:55:ALA:C     | 9:I:57:GLY:H     | 2.09                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 10:J:24:VAL:HG21 | 10:J:37:PRO:HD3   | 1.87                     | 0.55              |
| 1:A:123:G:O2'    | 1:A:189:U:H5''    | 2.06                     | 0.55              |
| 1:A:949:C:P      | 10:J:57:LYS:HD3   | 2.47                     | 0.55              |
| 1:A:387:G:H2'    | 1:A:388:A:C8      | 2.41                     | 0.55              |
| 13:M:59:TYR:O    | 13:M:63:THR:HG22  | 2.06                     | 0.55              |
| 21:V:7:ARG:HB2   | 21:V:21:TYR:CE1   | 2.40                     | 0.55              |
| 19:S:52:TYR:HA   | 19:S:56:GLN:O     | 2.06                     | 0.55              |
| 12:L:110:VAL:O   | 12:L:122:THR:HG21 | 2.06                     | 0.55              |
| 8:H:80:ILE:O     | 8:H:80:ILE:HG22   | 2.05                     | 0.55              |
| 1:A:1105:A:C2    | 10:J:39:PRO:HG3   | 2.37                     | 0.55              |
| 4:D:3:ARG:HH21   | 4:D:71:SER:HB3    | 1.69                     | 0.55              |
| 1:A:1125:G:H2'   | 1:A:1126:G:C4     | 2.41                     | 0.55              |
| 2:B:162:ILE:HG22 | 2:B:164:VAL:HG23  | 1.88                     | 0.55              |
| 9:I:47:LEU:C     | 9:I:49:PRO:HD2    | 2.26                     | 0.55              |
| 1:A:79:U:H2'     | 1:A:81:U:OP2      | 2.06                     | 0.55              |
| 1:A:1516:C:N4    | 7:G:82:GLY:HA2    | 2.22                     | 0.55              |
| 1:A:1006:C:H6    | 1:A:1006:C:H3'    | 1.71                     | 0.55              |
| 2:B:88:ALA:HB1   | 2:B:90:MET:HG2    | 1.87                     | 0.55              |
| 9:I:48:GLU:N     | 9:I:49:PRO:CD     | 2.69                     | 0.55              |
| 20:T:54:LYS:HB2  | 20:T:100:ILE:CD1  | 2.36                     | 0.55              |
| 8:H:10:LEU:CD2   | 8:H:83:ILE:HD11   | 2.37                     | 0.55              |
| 1:A:816:U:H2'    | 1:A:817:C:C6      | 2.42                     | 0.55              |
| 1:A:1382:C:H4'   | 1:A:1383:G:OP2    | 2.06                     | 0.55              |
| 1:A:379:G:H2'    | 1:A:380:C:C6      | 2.41                     | 0.55              |
| 12:L:42:THR:HG21 | 12:L:52:LEU:HB3   | 1.89                     | 0.55              |
| 1:A:188:U:H4'    | 1:A:189:U:OP1     | 2.06                     | 0.55              |
| 3:C:65:ALA:O     | 3:C:66:VAL:HB     | 2.05                     | 0.55              |
| 1:A:482:A:O2'    | 1:A:483:G:C8      | 2.60                     | 0.55              |
| 5:E:78:HIS:HD1   | 8:H:104:ARG:HD2   | 1.71                     | 0.55              |
| 19:S:78:ARG:HH11 | 19:S:78:ARG:HG2   | 1.71                     | 0.55              |
| 1:A:500:G:O2'    | 1:A:501:C:OP2     | 2.21                     | 0.55              |
| 19:S:9:VAL:HG12  | 19:S:10:PHE:N     | 2.20                     | 0.55              |
| 14:N:11:LYS:HG2  | 14:N:11:LYS:O     | 2.06                     | 0.55              |
| 4:D:196:LEU:HD22 | 4:D:197:PRO:HD2   | 1.89                     | 0.55              |
| 1:A:1320:A:H2'   | 1:A:1321:A:O4'    | 2.06                     | 0.55              |
| 3:C:134:ILE:HG23 | 3:C:151:VAL:HB    | 1.89                     | 0.55              |
| 1:A:247:U:H6     | 1:A:247:U:H5'     | 1.72                     | 0.55              |
| 2:B:71:VAL:CG2   | 2:B:164:VAL:HG22  | 2.37                     | 0.55              |
| 17:Q:13:ASP:C    | 17:Q:15:MET:H     | 2.10                     | 0.55              |
| 1:A:652:U:H2'    | 1:A:653:G:C8      | 2.42                     | 0.55              |
| 6:F:80:ARG:NH1   | 6:F:88:VAL:HB     | 2.22                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1243:C:N4    | 1:A:1254:G:H1    | 1.96                     | 0.55              |
| 2:B:139:LYS:HB3  | 2:B:139:LYS:NZ   | 2.22                     | 0.55              |
| 1:A:1479:A:H2    | 1:A:1482:G:N1    | 1.99                     | 0.55              |
| 5:E:51:VAL:O     | 5:E:55:VAL:HG23  | 2.07                     | 0.55              |
| 5:E:12:LEU:O     | 5:E:12:LEU:HD13  | 2.07                     | 0.55              |
| 19:S:50:ALA:HA   | 19:S:58:VAL:O    | 2.06                     | 0.55              |
| 16:P:26:ARG:CD   | 16:P:31:LYS:O    | 2.55                     | 0.55              |
| 1:A:1039:G:H2'   | 1:A:1040:G:O4'   | 2.06                     | 0.55              |
| 20:T:49:ALA:HB1  | 20:T:99:LEU:HG   | 1.88                     | 0.55              |
| 1:A:300:G:O2'    | 1:A:301:G:OP2    | 2.13                     | 0.55              |
| 1:A:963:A:H1'    | 19:S:54:GLY:O    | 2.06                     | 0.55              |
| 1:A:1181:C:O2'   | 1:A:1182:A:OP2   | 2.18                     | 0.55              |
| 2:B:215:LEU:O    | 2:B:219:VAL:HG23 | 2.06                     | 0.55              |
| 10:J:16:LEU:HB3  | 10:J:70:ARG:HG3  | 1.89                     | 0.55              |
| 4:D:31:CYS:SG    | 4:D:31:CYS:O     | 2.65                     | 0.55              |
| 7:G:50:ILE:HG23  | 7:G:125:MET:SD   | 2.46                     | 0.55              |
| 2:B:115:LEU:HD23 | 2:B:153:ARG:HD3  | 1.88                     | 0.55              |
| 3:C:22:TRP:CB    | 3:C:59:ARG:HB3   | 2.37                     | 0.55              |
| 16:P:20:VAL:HG21 | 16:P:32:TYR:CB   | 2.38                     | 0.55              |
| 13:M:22:ILE:CD1  | 13:M:25:ILE:HD12 | 2.36                     | 0.55              |
| 17:Q:92:ARG:O    | 17:Q:95:TYR:HB2  | 2.06                     | 0.55              |
| 1:A:838:G:O2'    | 1:A:839:C:H5'    | 2.07                     | 0.55              |
| 2:B:7:VAL:HG13   | 2:B:221:LEU:HD11 | 1.89                     | 0.54              |
| 2:B:97:TRP:HZ2   | 2:B:102:LEU:HD13 | 1.73                     | 0.54              |
| 9:I:28:VAL:HA    | 9:I:63:ILE:O     | 2.08                     | 0.54              |
| 11:K:32:ILE:CG2  | 11:K:77:MET:HE2  | 2.36                     | 0.54              |
| 9:I:95:LYS:O     | 9:I:99:LEU:HD23  | 2.07                     | 0.54              |
| 1:A:75:G:O2'     | 1:A:76:G:H5'     | 2.07                     | 0.54              |
| 20:T:96:GLY:O    | 20:T:97:ALA:HB3  | 2.06                     | 0.54              |
| 1:A:1247:G:N2    | 1:A:1250:A:OP2   | 2.40                     | 0.54              |
| 13:M:88:ARG:NH1  | 19:S:3:ARG:HH21  | 2.05                     | 0.54              |
| 16:P:11:SER:OG   | 16:P:14:ASN:HB3  | 2.07                     | 0.54              |
| 1:A:1118:U:H6    | 1:A:1118:U:O5'   | 1.89                     | 0.54              |
| 1:A:1316:C:O2'   | 1:A:1317:C:OP2   | 2.15                     | 0.54              |
| 19:S:40:ILE:HG21 | 19:S:62:ILE:HD11 | 1.89                     | 0.54              |
| 1:A:484:C:H2'    | 1:A:485:G:H8     | 1.70                     | 0.54              |
| 1:A:209:U:H4'    | 1:A:210:U:OP1    | 2.07                     | 0.54              |
| 1:A:1129:C:HO2'  | 9:I:5:TYR:HH     | 1.54                     | 0.54              |
| 1:A:601:C:H3'    | 1:A:602:U:C5'    | 2.37                     | 0.54              |
| 18:R:46:GLU:H    | 18:R:46:GLU:CD   | 2.11                     | 0.54              |
| 1:A:332:C:H2'    | 1:A:333:A:C8     | 2.42                     | 0.54              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:825:C:C6      | 1:A:825:C:C3'    | 2.89                     | 0.54              |
| 1:A:525:G:H2'     | 1:A:526:C:C6     | 2.42                     | 0.54              |
| 1:A:1193:U:O2     | 1:A:1193:U:H2'   | 2.07                     | 0.54              |
| 1:A:969:U:H4'     | 1:A:970:G:O5'    | 2.08                     | 0.54              |
| 1:A:1225:C:OP2    | 21:V:9:ARG:HB2   | 2.07                     | 0.54              |
| 4:D:170:VAL:HG12  | 4:D:171:GLY:N    | 2.22                     | 0.54              |
| 1:A:985:C:O2      | 1:A:986:C:C4     | 2.60                     | 0.54              |
| 1:A:1286:G:C5'    | 21:V:4:GLY:HA3   | 2.30                     | 0.54              |
| 1:A:1111:C:N4     | 1:A:1117:U:H3    | 2.04                     | 0.54              |
| 13:M:65:LYS:HE2   | 13:M:69:GLU:OE2  | 2.07                     | 0.54              |
| 15:O:7:GLU:O      | 15:O:11:VAL:HG23 | 2.08                     | 0.54              |
| 1:A:51:A:OP2      | 1:A:52:G:H8      | 1.91                     | 0.54              |
| 1:A:997:C:H2'     | 1:A:998:U:O4'    | 2.07                     | 0.54              |
| 1:A:453:G:H3'     | 1:A:454:A:C5'    | 2.38                     | 0.54              |
| 12:L:65:GLU:CD    | 12:L:65:GLU:N    | 2.61                     | 0.54              |
| 12:L:113:ARG:HH12 | 12:L:116:SER:HB2 | 1.72                     | 0.54              |
| 4:D:190:ASP:HB2   | 4:D:193:ASP:OD2  | 2.07                     | 0.54              |
| 5:E:143:ARG:NH1   | 8:H:77:GLU:OE2   | 2.40                     | 0.54              |
| 1:A:1035:G:C4'    | 1:A:1036:C:H5'   | 2.38                     | 0.54              |
| 2:B:81:VAL:HG12   | 2:B:81:VAL:O     | 2.06                     | 0.54              |
| 1:A:647:G:N2      | 1:A:724:G:H1     | 1.96                     | 0.54              |
| 1:A:1329:U:H4'    | 9:I:120:ARG:HD2  | 1.89                     | 0.54              |
| 1:A:1143:C:O2'    | 1:A:1144:C:H5'   | 2.07                     | 0.54              |
| 7:G:13:GLN:HE21   | 7:G:14:PRO:HD2   | 1.73                     | 0.54              |
| 22:W:1:A:H62      | 23:X:37:12A:HG22 | 1.73                     | 0.54              |
| 1:A:903:G:H3'     | 1:A:1482:G:H21   | 1.73                     | 0.54              |
| 9:I:16:ARG:NE     | 9:I:64:THR:HG21  | 2.23                     | 0.54              |
| 17:Q:83:ASP:O     | 17:Q:86:GLU:HB2  | 2.08                     | 0.54              |
| 1:A:1194:A:H4'    | 1:A:1195:C:OP1   | 2.08                     | 0.54              |
| 1:A:601:C:H3'     | 1:A:602:U:H5'    | 1.89                     | 0.54              |
| 6:F:98:LEU:H      | 6:F:98:LEU:HD12  | 1.72                     | 0.54              |
| 1:A:622:G:O2'     | 1:A:623:A:H5'    | 2.08                     | 0.54              |
| 1:A:1004:G:N2     | 1:A:1018:G:H22   | 2.06                     | 0.54              |
| 5:E:80:ILE:HG22   | 8:H:104:ARG:NH2  | 2.23                     | 0.54              |
| 3:C:16:ARG:HH11   | 3:C:16:ARG:CG    | 2.18                     | 0.54              |
| 1:A:578:G:N1      | 1:A:624:U:H2'    | 2.23                     | 0.54              |
| 1:A:264:C:H2'     | 1:A:265:A:H8     | 1.67                     | 0.54              |
| 7:G:73:MET:HA     | 7:G:91:VAL:HG23  | 1.88                     | 0.54              |
| 21:V:2:GLY:C      | 21:V:4:GLY:H     | 2.11                     | 0.54              |
| 9:I:125:TYR:CE1   | 9:I:128:ARG:NE   | 2.76                     | 0.54              |
| 3:C:51:GLY:O      | 3:C:70:VAL:HG12  | 2.08                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:L:91:LYS:HE3   | 12:L:91:LYS:CA    | 2.37                     | 0.54              |
| 1:A:1350:G:O2'    | 1:A:1351:C:H5'    | 2.08                     | 0.54              |
| 18:R:25:THR:HG22  | 18:R:42:ARG:NH1   | 2.20                     | 0.54              |
| 1:A:424:U:H4'     | 1:A:425:A:O5'     | 2.08                     | 0.54              |
| 1:A:1164:A:O2'    | 1:A:1165:G:OP1    | 2.19                     | 0.54              |
| 8:H:10:LEU:HD23   | 8:H:83:ILE:HD11   | 1.90                     | 0.54              |
| 1:A:145:A:H2'     | 1:A:146:A:O4'     | 2.08                     | 0.54              |
| 1:A:1447:G:O2'    | 1:A:1448:G:H5'    | 2.08                     | 0.54              |
| 9:I:118:LYS:HB2   | 9:I:118:LYS:HZ2   | 1.73                     | 0.54              |
| 2:B:208:ILE:C     | 2:B:210:SER:H     | 2.11                     | 0.54              |
| 1:A:1289:U:C5'    | 13:M:110:ARG:HH21 | 2.20                     | 0.54              |
| 21:V:2:GLY:O      | 21:V:4:GLY:N      | 2.41                     | 0.54              |
| 1:A:123:G:O2'     | 1:A:189:U:H3'     | 2.07                     | 0.54              |
| 6:F:10:LEU:HD11   | 6:F:59:TYR:HD2    | 1.71                     | 0.54              |
| 10:J:38:ILE:HD12  | 10:J:71:LEU:HD12  | 1.89                     | 0.54              |
| 7:G:9:VAL:O       | 7:G:10:ARG:C      | 2.45                     | 0.54              |
| 1:A:980:G:C6      | 1:A:981:G:C6      | 2.95                     | 0.53              |
| 1:A:986:C:H42     | 1:A:1000:G:H22    | 1.56                     | 0.53              |
| 1:A:635:U:H4'     | 1:A:636:A:OP1     | 2.08                     | 0.53              |
| 20:T:53:LEU:HD21  | 20:T:104:LEU:HD12 | 1.90                     | 0.53              |
| 1:A:188:U:O2'     | 1:A:189:U:O5'     | 2.20                     | 0.53              |
| 1:A:1348:C:H2'    | 1:A:1349:C:H6     | 1.72                     | 0.53              |
| 3:C:23:TYR:O      | 3:C:24:ALA:HB2    | 2.08                     | 0.53              |
| 1:A:1469:A:OP1    | 12:L:47:LYS:N     | 2.41                     | 0.53              |
| 9:I:106:ALA:O     | 9:I:108:VAL:HG23  | 2.07                     | 0.53              |
| 1:A:455:C:O2'     | 1:A:456:G:OP1     | 2.23                     | 0.53              |
| 1:A:1170:C:OP1    | 10:J:51:ARG:NH2   | 2.40                     | 0.53              |
| 1:A:385:C:H2'     | 1:A:386:G:C8      | 2.43                     | 0.53              |
| 1:A:824:U:H3'     | 1:A:825:C:O4'     | 2.09                     | 0.53              |
| 11:K:109:VAL:HG22 | 18:R:86:VAL:HG13  | 1.89                     | 0.53              |
| 1:A:108:G:H1'     | 1:A:109:A:N7      | 2.23                     | 0.53              |
| 1:A:1272:G:OP1    | 7:G:37:ASN:ND2    | 2.41                     | 0.53              |
| 1:A:383:G:O2'     | 1:A:384:A:P       | 2.67                     | 0.53              |
| 1:A:515:A:H5'     | 3:C:161:GLU:OE1   | 2.02                     | 0.53              |
| 16:P:28:ARG:NH1   | 16:P:29:ASP:OD2   | 2.41                     | 0.53              |
| 1:A:578:G:C6      | 1:A:624:U:H2'     | 2.43                     | 0.53              |
| 7:G:18:TYR:CD1    | 7:G:59:LEU:HD22   | 2.44                     | 0.53              |
| 1:A:125:C:OP1     | 1:A:190:G:N2      | 2.42                     | 0.53              |
| 10:J:60:ARG:NH1   | 10:J:60:ARG:HG2   | 2.23                     | 0.53              |
| 14:N:14:PRO:O     | 14:N:15:LYS:HB2   | 2.07                     | 0.53              |
| 1:A:1215:C:H5'    | 1:A:1347:G:OP1    | 2.08                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:G:50:ILE:HG21  | 7:G:61:VAL:HG21  | 1.90                     | 0.53              |
| 1:A:1241:C:OP1   | 1:A:1265:C:H4'   | 2.08                     | 0.53              |
| 1:A:1431:A:H4'   | 1:A:1432:C:OP2   | 2.05                     | 0.53              |
| 11:K:79:SER:CB   | 11:K:104:GLN:HB3 | 2.38                     | 0.53              |
| 12:L:119:LYS:O   | 12:L:120:TYR:HB2 | 2.08                     | 0.53              |
| 7:G:87:VAL:HG11  | 7:G:154:TYR:O    | 2.09                     | 0.53              |
| 10:J:14:LYS:O    | 10:J:18:ALA:HB3  | 2.07                     | 0.53              |
| 10:J:46:ARG:HG3  | 10:J:46:ARG:NH1  | 2.24                     | 0.53              |
| 5:E:126:ARG:HG3  | 5:E:126:ARG:NH1  | 2.22                     | 0.53              |
| 9:I:16:ARG:HE    | 9:I:64:THR:HG23  | 1.71                     | 0.53              |
| 2:B:95:GLN:C     | 2:B:96:ARG:HD2   | 2.29                     | 0.53              |
| 14:N:8:GLU:O     | 14:N:11:LYS:CB   | 2.56                     | 0.53              |
| 1:A:886:A:H2'    | 1:A:887:C:O4'    | 2.08                     | 0.53              |
| 1:A:648:A:N3     | 1:A:715:C:H2'    | 2.24                     | 0.53              |
| 15:O:39:LEU:O    | 15:O:39:LEU:HD23 | 2.09                     | 0.53              |
| 1:A:1126:G:H3'   | 1:A:1126:G:C8    | 2.44                     | 0.53              |
| 2:B:71:VAL:HG21  | 2:B:164:VAL:HG22 | 1.89                     | 0.53              |
| 6:F:14:LEU:N     | 6:F:14:LEU:HD12  | 2.24                     | 0.53              |
| 1:A:1206:A:H3'   | 1:A:1207:C:H6    | 1.71                     | 0.53              |
| 1:A:49:U:O2'     | 1:A:50:A:OP1     | 2.25                     | 0.53              |
| 1:A:268:A:H1'    | 17:Q:16:GLN:NE2  | 2.23                     | 0.53              |
| 21:V:3:LYS:HB3   | 21:V:14:TRP:CG   | 2.43                     | 0.53              |
| 3:C:29:TYR:CZ    | 14:N:54:PRO:HG2  | 2.44                     | 0.53              |
| 1:A:1381:C:H4'   | 1:A:1382:C:O5'   | 2.09                     | 0.53              |
| 1:A:1150:A:H2'   | 1:A:1151:A:C8    | 2.43                     | 0.53              |
| 7:G:6:ARG:O      | 7:G:7:ALA:O      | 2.25                     | 0.53              |
| 1:A:1036:C:C3'   | 1:A:1036:C:H6    | 2.09                     | 0.53              |
| 1:A:1184:C:O5'   | 1:A:1184:C:H6    | 1.91                     | 0.53              |
| 1:A:821:G:C2'    | 1:A:822:U:H5''   | 2.39                     | 0.53              |
| 1:A:22:G:H2'     | 1:A:23:C:C6      | 2.44                     | 0.53              |
| 20:T:56:MET:HE3  | 20:T:88:VAL:HG11 | 1.90                     | 0.53              |
| 11:K:93:GLN:OE1  | 11:K:93:GLN:HA   | 2.08                     | 0.53              |
| 10:J:24:VAL:HG13 | 10:J:28:ARG:NH1  | 2.23                     | 0.53              |
| 4:D:19:LEU:HD21  | 4:D:67:ILE:CG1   | 2.33                     | 0.53              |
| 1:A:1098:C:H2'   | 1:A:1099:G:H5'   | 1.90                     | 0.53              |
| 3:C:130:VAL:HG11 | 3:C:157:ILE:HG23 | 1.90                     | 0.53              |
| 1:A:1024:G:H2'   | 1:A:1025:C:H6    | 1.73                     | 0.53              |
| 1:A:1460:A:H2'   | 1:A:1461:C:O5'   | 2.09                     | 0.53              |
| 11:K:14:VAL:O    | 11:K:15:ALA:HB3  | 2.09                     | 0.53              |
| 1:A:603:C:C2     | 4:D:135:LEU:HD13 | 2.42                     | 0.53              |
| 1:A:160:G:O2'    | 1:A:161:G:H5'    | 2.08                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:50:TYR:CE1   | 18:R:77:GLY:HA2  | 2.44                     | 0.53              |
| 2:B:97:TRP:CZ2   | 2:B:102:LEU:HD13 | 2.43                     | 0.53              |
| 8:H:92:ARG:HH11  | 8:H:92:ARG:HG2   | 1.74                     | 0.53              |
| 1:A:1077:U:H2'   | 1:A:1078:C:O4'   | 2.09                     | 0.53              |
| 9:I:36:TYR:CD2   | 9:I:37:PHE:CE2   | 2.97                     | 0.53              |
| 1:A:465:G:H2'    | 1:A:467:C:H41    | 1.72                     | 0.53              |
| 1:A:338:U:H2'    | 1:A:340:C:C4     | 2.43                     | 0.53              |
| 13:M:35:GLU:C    | 13:M:37:THR:H    | 2.12                     | 0.53              |
| 2:B:87:ARG:HD2   | 2:B:234:PRO:HD2  | 1.91                     | 0.53              |
| 1:A:453:G:H3'    | 1:A:454:A:H5''   | 1.91                     | 0.53              |
| 9:I:12:GLU:O     | 9:I:12:GLU:HG2   | 2.09                     | 0.53              |
| 1:A:980:G:C4     | 1:A:981:G:N7     | 2.76                     | 0.53              |
| 9:I:111:ARG:HG2  | 9:I:112:LYS:N    | 2.24                     | 0.53              |
| 16:P:1:MET:O     | 16:P:24:ALA:HB2  | 2.09                     | 0.53              |
| 1:A:1300:A:H4'   | 19:S:37:ARG:NH1  | 2.24                     | 0.53              |
| 15:O:3:ILE:HD12  | 15:O:3:ILE:N     | 2.23                     | 0.53              |
| 1:A:953:G:N7     | 1:A:1339:U:C2    | 2.77                     | 0.52              |
| 1:A:1286:G:O2'   | 1:A:1287:A:C8    | 2.45                     | 0.52              |
| 1:A:1287:A:N6    | 1:A:1312:G:H1'   | 2.25                     | 0.52              |
| 1:A:516:A:C4'    | 1:A:517:U:OP1    | 2.53                     | 0.52              |
| 2:B:107:THR:C    | 2:B:109:SER:N    | 2.62                     | 0.52              |
| 1:A:1113:G:C8    | 1:A:1113:G:H3'   | 2.44                     | 0.52              |
| 10:J:49:VAL:CG1  | 14:N:41:ARG:HD2  | 2.39                     | 0.52              |
| 12:L:43:VAL:HG12 | 12:L:44:THR:N    | 2.24                     | 0.52              |
| 5:E:71:LEU:HD11  | 5:E:114:GLY:HA3  | 1.90                     | 0.52              |
| 1:A:927:U:H5     | 13:M:102:ARG:NE  | 2.07                     | 0.52              |
| 7:G:137:LYS:O    | 7:G:141:VAL:HG23 | 2.09                     | 0.52              |
| 1:A:501:C:O2'    | 1:A:502:C:OP2    | 2.23                     | 0.52              |
| 1:A:1521:U:O3'   | 22:W:1:A:OP1     | 2.28                     | 0.52              |
| 1:A:1134:A:H2'   | 1:A:1135:C:C6    | 2.44                     | 0.52              |
| 19:S:19:VAL:HG13 | 19:S:20:LEU:N    | 2.24                     | 0.52              |
| 5:E:39:GLY:O     | 5:E:68:GLU:HA    | 2.09                     | 0.52              |
| 1:A:1362:U:O2'   | 1:A:1363:U:OP2   | 2.24                     | 0.52              |
| 5:E:147:ASP:O    | 5:E:151:LEU:HD13 | 2.09                     | 0.52              |
| 1:A:952:A:C8     | 1:A:952:A:H5'    | 2.44                     | 0.52              |
| 10:J:39:PRO:HA   | 10:J:70:ARG:NH2  | 2.24                     | 0.52              |
| 5:E:13:ILE:HD12  | 5:E:13:ILE:C     | 2.29                     | 0.52              |
| 18:R:22:VAL:HG23 | 18:R:55:ARG:O    | 2.09                     | 0.52              |
| 16:P:18:ARG:CG   | 16:P:35:LYS:HE3  | 2.40                     | 0.52              |
| 5:E:45:PHE:CE2   | 5:E:47:LYS:HD2   | 2.44                     | 0.52              |
| 1:A:1031:U:O2'   | 1:A:1032:G:OP2   | 2.25                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:74:LYS:HG2   | 2:B:76:GLN:H     | 1.74                     | 0.52              |
| 6:F:30:LEU:HA    | 6:F:75:LEU:HD21  | 1.91                     | 0.52              |
| 2:B:14:GLY:C     | 2:B:15:VAL:HG22  | 2.30                     | 0.52              |
| 13:M:45:VAL:HA   | 13:M:48:LEU:HG   | 1.90                     | 0.52              |
| 3:C:188:LEU:CD1  | 3:C:189:ALA:H    | 2.21                     | 0.52              |
| 3:C:188:LEU:O    | 3:C:189:ALA:CB   | 2.57                     | 0.52              |
| 1:A:611:G:O2'    | 1:A:612:G:H5'    | 2.09                     | 0.52              |
| 1:A:1172:A:OP2   | 3:C:3:ASN:ND2    | 2.42                     | 0.52              |
| 10:J:64:GLU:CG   | 14:N:59:ALA:HB2  | 2.38                     | 0.52              |
| 7:G:18:TYR:CE1   | 7:G:59:LEU:HB2   | 2.45                     | 0.52              |
| 11:K:33:THR:HG22 | 11:K:39:PRO:HA   | 1.91                     | 0.52              |
| 1:A:335:U:H2'    | 1:A:336:C:C6     | 2.44                     | 0.52              |
| 2:B:166:ASP:O    | 2:B:170:GLU:HB2  | 2.10                     | 0.52              |
| 2:B:206:ASP:O    | 2:B:207:ALA:HB3  | 2.09                     | 0.52              |
| 2:B:7:VAL:CG2    | 2:B:8:LYS:H      | 2.16                     | 0.52              |
| 4:D:104:VAL:HG21 | 4:D:140:VAL:HG21 | 1.90                     | 0.52              |
| 1:A:102:A:C4'    | 1:A:103:C:OP2    | 2.57                     | 0.52              |
| 16:P:67:THR:CG2  | 16:P:68:ASP:N    | 2.72                     | 0.52              |
| 3:C:23:TYR:OH    | 10:J:9:ARG:HD3   | 2.10                     | 0.52              |
| 2:B:189:ASP:OD2  | 2:B:205:ASP:OD2  | 2.27                     | 0.52              |
| 6:F:100:ASN:ND2  | 18:R:23:LYS:NZ   | 2.57                     | 0.52              |
| 6:F:43:LEU:N     | 6:F:43:LEU:HD22  | 2.25                     | 0.52              |
| 2:B:77:ALA:HB2   | 2:B:211:ILE:HG21 | 1.91                     | 0.52              |
| 10:J:15:THR:O    | 10:J:94:VAL:HG21 | 2.10                     | 0.52              |
| 12:L:60:LEU:HD23 | 12:L:66:VAL:HG22 | 1.92                     | 0.52              |
| 11:K:15:ALA:HA   | 11:K:76:GLY:O    | 2.10                     | 0.52              |
| 17:Q:89:LEU:O    | 17:Q:92:ARG:HB2  | 2.10                     | 0.52              |
| 1:A:94:A:O2'     | 1:A:95:G:H5'     | 2.09                     | 0.52              |
| 18:R:53:ARG:HD3  | 18:R:58:LEU:O    | 2.10                     | 0.52              |
| 1:A:114:C:H4'    | 1:A:115:G:OP1    | 2.10                     | 0.52              |
| 3:C:55:VAL:HG12  | 3:C:55:VAL:O     | 2.10                     | 0.52              |
| 19:S:80:TYR:CG   | 19:S:81:ARG:N    | 2.78                     | 0.52              |
| 7:G:115:ARG:HB2  | 7:G:118:VAL:CG2  | 2.39                     | 0.52              |
| 6:F:20:ALA:O     | 6:F:24:GLU:HB2   | 2.09                     | 0.52              |
| 15:O:17:ARG:NH1  | 15:O:17:ARG:CG   | 2.73                     | 0.52              |
| 1:A:1171:G:OP1   | 3:C:4:LYS:HA     | 2.10                     | 0.52              |
| 3:C:87:LEU:O     | 3:C:91:LEU:HB2   | 2.10                     | 0.52              |
| 10:J:46:ARG:HG3  | 10:J:46:ARG:HH11 | 1.75                     | 0.52              |
| 11:K:52:GLY:H    | 11:K:55:LYS:HE2  | 1.75                     | 0.52              |
| 14:N:57:ARG:CG   | 14:N:58:LYS:H    | 2.17                     | 0.52              |
| 3:C:196:LEU:N    | 3:C:196:LEU:HD23 | 2.24                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 12:L:27:LEU:O    | 12:L:29:GLY:N    | 2.43                     | 0.52              |
| 1:A:1094:C:O2    | 3:C:179:ARG:HB3  | 2.10                     | 0.52              |
| 9:I:118:LYS:NZ   | 9:I:118:LYS:CB   | 2.72                     | 0.52              |
| 7:G:85:TYR:O     | 7:G:87:VAL:HG23  | 2.10                     | 0.52              |
| 1:A:21:G:H2'     | 1:A:22:G:C8      | 2.45                     | 0.52              |
| 1:A:522:A:H2'    | 1:A:523:G:C8     | 2.45                     | 0.52              |
| 3:C:43:LEU:O     | 3:C:47:LEU:HD13  | 2.10                     | 0.52              |
| 12:L:89:ARG:H    | 12:L:89:ARG:CD   | 2.22                     | 0.52              |
| 2:B:208:ILE:HA   | 2:B:211:ILE:HD12 | 1.91                     | 0.51              |
| 10:J:16:LEU:HD21 | 10:J:94:VAL:HG13 | 1.90                     | 0.51              |
| 4:D:15:GLU:C     | 4:D:17:VAL:H     | 2.14                     | 0.51              |
| 3:C:91:LEU:HD23  | 3:C:99:VAL:HG21  | 1.92                     | 0.51              |
| 1:A:1008:C:N4    | 1:A:1014:G:H1    | 2.09                     | 0.51              |
| 2:B:187:LEU:HD23 | 2:B:201:ILE:O    | 2.10                     | 0.51              |
| 2:B:95:GLN:OE1   | 2:B:95:GLN:HA    | 2.10                     | 0.51              |
| 1:A:364:C:H2'    | 1:A:365:C:C6     | 2.45                     | 0.51              |
| 6:F:19:LEU:HD23  | 6:F:19:LEU:C     | 2.31                     | 0.51              |
| 7:G:58:PRO:O     | 7:G:61:VAL:HG22  | 2.10                     | 0.51              |
| 19:S:55:LYS:HG2  | 19:S:56:GLN:HG3  | 1.90                     | 0.51              |
| 1:A:1100:C:H1'   | 1:A:1160:A:C4    | 2.46                     | 0.51              |
| 18:R:59:SER:C    | 18:R:61:LYS:N    | 2.63                     | 0.51              |
| 2:B:58:ILE:HG23  | 2:B:68:ILE:CD1   | 2.41                     | 0.51              |
| 11:K:12:ARG:O    | 11:K:12:ARG:HG2  | 2.09                     | 0.51              |
| 1:A:1286:G:O2'   | 1:A:1287:A:P     | 2.68                     | 0.51              |
| 5:E:79:GLU:CG    | 5:E:93:PRO:HD2   | 2.41                     | 0.51              |
| 1:A:1186:U:O2'   | 3:C:195:VAL:HG23 | 2.10                     | 0.51              |
| 1:A:506:A:H61    | 12:L:92:ASP:HB2  | 1.74                     | 0.51              |
| 3:C:33:LEU:HD21  | 14:N:53:LEU:CD2  | 2.40                     | 0.51              |
| 1:A:854:C:OP1    | 8:H:88:LYS:HE2   | 2.10                     | 0.51              |
| 13:M:5:ALA:HB3   | 13:M:8:GLU:CB    | 2.40                     | 0.51              |
| 13:M:4:ILE:CD1   | 13:M:56:LEU:HD13 | 2.40                     | 0.51              |
| 1:A:1286:G:N2    | 1:A:1312:G:C2'   | 2.72                     | 0.51              |
| 14:N:29:ARG:HH11 | 14:N:29:ARG:HG2  | 1.75                     | 0.51              |
| 20:T:24:LEU:HD12 | 20:T:27:LYS:CE   | 2.41                     | 0.51              |
| 1:A:1461:C:H3'   | 1:A:1461:C:C6    | 2.45                     | 0.51              |
| 13:M:3:ARG:HG2   | 13:M:9:ILE:HG23  | 1.93                     | 0.51              |
| 1:A:701:G:H4'    | 11:K:117:ASN:ND2 | 2.26                     | 0.51              |
| 10:J:79:ARG:O    | 10:J:83:GLU:HB2  | 2.09                     | 0.51              |
| 13:M:88:ARG:HH11 | 19:S:3:ARG:HH21  | 1.57                     | 0.51              |
| 4:D:98:GLU:HG2   | 4:D:189:PRO:HG3  | 1.92                     | 0.51              |
| 5:E:148:VAL:CG2  | 8:H:107:LEU:HD22 | 2.34                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:191:THR:HG22 | 3:C:193:TYR:H    | 1.76                     | 0.51              |
| 2:B:107:THR:O    | 2:B:109:SER:N    | 2.43                     | 0.51              |
| 1:A:801:G:O2'    | 1:A:803:U:C5     | 2.63                     | 0.51              |
| 16:P:51:VAL:O    | 16:P:52:ASP:CB   | 2.56                     | 0.51              |
| 1:A:1213:U:H5''  | 9:I:124:GLN:O    | 2.10                     | 0.51              |
| 15:O:78:TYR:CZ   | 15:O:82:ILE:HD11 | 2.46                     | 0.51              |
| 7:G:125:MET:O    | 7:G:129:GLU:HG2  | 2.10                     | 0.51              |
| 1:A:1300:A:C4'   | 19:S:37:ARG:HH12 | 2.22                     | 0.51              |
| 1:A:798:A:O2'    | 1:A:799:A:P      | 2.68                     | 0.51              |
| 1:A:1153:C:H2'   | 1:A:1154:G:C8    | 2.45                     | 0.51              |
| 1:A:1328:G:H22   | 1:A:1355:G:H2'   | 1.76                     | 0.51              |
| 1:A:377:A:H2'    | 1:A:378:A:C8     | 2.45                     | 0.51              |
| 1:A:983:A:OP1    | 1:A:984:C:P      | 2.69                     | 0.51              |
| 1:A:245:A:C4'    | 1:A:246:G:O5'    | 2.49                     | 0.51              |
| 1:A:1302:C:H5''  | 1:A:1303:C:C2'   | 2.39                     | 0.51              |
| 15:O:39:LEU:C    | 15:O:39:LEU:HD23 | 2.31                     | 0.51              |
| 9:I:33:PHE:CE2   | 9:I:47:LEU:HD11  | 2.45                     | 0.51              |
| 1:A:1172:A:OP1   | 3:C:4:LYS:NZ     | 2.42                     | 0.51              |
| 7:G:15:ASP:HB3   | 7:G:19:GLY:CA    | 2.41                     | 0.51              |
| 1:A:966:C:HO2'   | 1:A:995:G:HO2'   | 1.59                     | 0.51              |
| 4:D:126:ILE:HG22 | 4:D:127:THR:N    | 2.26                     | 0.51              |
| 13:M:11:ARG:HG2  | 13:M:12:ASN:H    | 1.74                     | 0.51              |
| 9:I:17:VAL:HG11  | 9:I:81:ILE:HG12  | 1.93                     | 0.51              |
| 1:A:934:U:H3     | 1:A:937:U:H5'    | 1.76                     | 0.51              |
| 1:A:1261:A:O4'   | 10:J:41:PRO:HG3  | 2.10                     | 0.51              |
| 2:B:104:ASN:HD21 | 2:B:107:THR:HB   | 1.75                     | 0.51              |
| 1:A:1133:A:O2'   | 1:A:1134:A:O5'   | 2.29                     | 0.51              |
| 1:A:364:C:H2'    | 1:A:365:C:H6     | 1.75                     | 0.51              |
| 11:K:14:VAL:HG21 | 11:K:40:ILE:CD1  | 2.41                     | 0.51              |
| 12:L:8:ASN:O     | 12:L:12:ARG:HB2  | 2.11                     | 0.51              |
| 1:A:1054:G:H2'   | 1:A:1055:U:C6    | 2.45                     | 0.51              |
| 1:A:911:C:H5'    | 1:A:912:A:OP1    | 2.10                     | 0.51              |
| 12:L:34:ARG:O    | 12:L:61:THR:HG23 | 2.10                     | 0.51              |
| 1:A:41:G:H2'     | 1:A:42:G:C8      | 2.46                     | 0.51              |
| 20:T:34:LYS:O    | 20:T:38:LYS:HG3  | 2.10                     | 0.51              |
| 15:O:37:ASN:O    | 15:O:41:GLU:HB2  | 2.11                     | 0.51              |
| 10:J:16:LEU:O    | 10:J:19:SER:N    | 2.44                     | 0.51              |
| 4:D:107:ARG:C    | 4:D:109:GLY:H    | 2.14                     | 0.51              |
| 1:A:735:G:O2'    | 1:A:736:A:P      | 2.69                     | 0.51              |
| 1:A:1408:C:O2'   | 1:A:1409:U:H5'   | 2.10                     | 0.51              |
| 13:M:84:ILE:C    | 13:M:86:CYS:H    | 2.15                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1057:C:H5'   | 2:B:103:THR:HG21 | 1.93                     | 0.51              |
| 1:A:1210:A:C2    | 1:A:1211:C:C4    | 2.99                     | 0.51              |
| 2:B:143:GLU:O    | 2:B:147:LYS:HG3  | 2.11                     | 0.51              |
| 1:A:402:G:O2'    | 4:D:116:GLN:HG3  | 2.11                     | 0.51              |
| 12:L:111:LYS:HG2 | 12:L:112:ASP:N   | 2.26                     | 0.51              |
| 1:A:1228:U:C6    | 1:A:1228:U:C3'   | 2.92                     | 0.51              |
| 1:A:1187:G:H1'   | 3:C:193:TYR:O    | 2.11                     | 0.51              |
| 1:A:82:U:C6      | 1:A:82:U:H3'     | 2.46                     | 0.51              |
| 1:A:700:C:O2'    | 1:A:701:G:OP2    | 2.22                     | 0.51              |
| 11:K:27:ASN:OD1  | 11:K:28:THR:N    | 2.42                     | 0.51              |
| 1:A:1051:C:O2'   | 1:A:1173:C:H1'   | 2.11                     | 0.51              |
| 4:D:58:LEU:HD22  | 4:D:58:LEU:O     | 2.11                     | 0.51              |
| 1:A:981:G:N2     | 1:A:1020:C:N3    | 2.59                     | 0.50              |
| 7:G:28:ASN:HD21  | 7:G:36:LYS:CE    | 2.23                     | 0.50              |
| 1:A:1434:G:O2'   | 1:A:1435:G:H5'   | 2.10                     | 0.50              |
| 1:A:402:G:H2'    | 1:A:403:A:C8     | 2.46                     | 0.50              |
| 1:A:352:G:O2'    | 1:A:353:U:H5'    | 2.10                     | 0.50              |
| 7:G:86:GLN:OE1   | 7:G:144:MET:HE1  | 2.11                     | 0.50              |
| 6:F:1:MET:HA     | 6:F:1:MET:HE2    | 1.92                     | 0.50              |
| 1:A:823:C:H5''   | 1:A:824:U:OP2    | 2.11                     | 0.50              |
| 12:L:60:LEU:N    | 12:L:64:TYR:O    | 2.41                     | 0.50              |
| 13:M:54:VAL:HG12 | 13:M:58:GLU:HG2  | 1.92                     | 0.50              |
| 1:A:1269:A:H2'   | 1:A:1270:A:C8    | 2.46                     | 0.50              |
| 1:A:1307:C:OP1   | 21:V:12:LYS:NZ   | 2.44                     | 0.50              |
| 2:B:42:ILE:HG22  | 2:B:43:ASP:N     | 2.25                     | 0.50              |
| 12:L:86:ARG:HG3  | 12:L:86:ARG:HH11 | 1.77                     | 0.50              |
| 1:A:1029:G:O2'   | 1:A:1030:G:H5'   | 2.12                     | 0.50              |
| 1:A:245:A:H5'    | 1:A:247:U:O4'    | 2.11                     | 0.50              |
| 1:A:1202:G:OP1   | 1:A:1301:C:N4    | 2.44                     | 0.50              |
| 1:A:332:C:H2'    | 1:A:333:A:H8     | 1.76                     | 0.50              |
| 1:A:1286:G:H22   | 1:A:1312:G:H2'   | 1.76                     | 0.50              |
| 6:F:54:LYS:HE2   | 6:F:54:LYS:CA    | 2.41                     | 0.50              |
| 3:C:73:PRO:C     | 3:C:75:VAL:H     | 2.15                     | 0.50              |
| 4:D:34:GLU:C     | 4:D:35:ARG:HD2   | 2.32                     | 0.50              |
| 19:S:44:MET:O    | 19:S:62:ILE:HG21 | 2.11                     | 0.50              |
| 1:A:763:A:HO2'   | 1:A:764:A:H5''   | 1.74                     | 0.50              |
| 8:H:77:GLU:HG2   | 8:H:78:GLN:N     | 2.26                     | 0.50              |
| 6:F:97:PHE:O     | 6:F:98:LEU:O     | 2.30                     | 0.50              |
| 11:K:45:GLY:HA3  | 11:K:55:LYS:HG2  | 1.94                     | 0.50              |
| 5:E:64:ARG:O     | 5:E:65:ASN:HB3   | 2.12                     | 0.50              |
| 8:H:26:VAL:HG23  | 8:H:27:PRO:O     | 2.11                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:H:36:LEU:HD12  | 8:H:59:LEU:HD13  | 1.93                     | 0.50              |
| 1:A:1388:U:O2'   | 1:A:1389:C:H5'   | 2.11                     | 0.50              |
| 10:J:49:VAL:CG1  | 14:N:41:ARG:HB2  | 2.41                     | 0.50              |
| 1:A:1279:C:C6    | 7:G:114:ARG:NH1  | 2.79                     | 0.50              |
| 1:A:795:C:O2'    | 1:A:796:U:P      | 2.68                     | 0.50              |
| 3:C:46:GLU:C     | 3:C:47:LEU:HD12  | 2.31                     | 0.50              |
| 1:A:985:C:O2     | 1:A:986:C:N3     | 2.45                     | 0.50              |
| 1:A:516:A:O2'    | 1:A:517:U:OP1    | 2.29                     | 0.50              |
| 1:A:1127:C:H1'   | 1:A:1128:A:C8    | 2.46                     | 0.50              |
| 3:C:58:GLU:N     | 3:C:65:ALA:HB3   | 2.26                     | 0.50              |
| 2:B:142:LEU:HD23 | 2:B:142:LEU:O    | 2.11                     | 0.50              |
| 1:A:1163:G:H4'   | 1:A:1164:A:H5''  | 1.94                     | 0.50              |
| 20:T:90:GLN:O    | 20:T:93:GLU:HB2  | 2.11                     | 0.50              |
| 16:P:1:MET:HE3   | 16:P:3:LYS:HE3   | 1.93                     | 0.50              |
| 3:C:134:ILE:CG2  | 3:C:168:ALA:HB3  | 2.42                     | 0.50              |
| 1:A:1384:C:O2    | 1:A:1477:A:N1    | 2.45                     | 0.50              |
| 1:A:983:A:OP1    | 1:A:983:A:O3'    | 2.30                     | 0.50              |
| 1:A:937:U:O2'    | 1:A:1204:C:C5'   | 2.60                     | 0.50              |
| 1:A:516:A:O2'    | 1:A:517:U:P      | 2.69                     | 0.50              |
| 20:T:57:ARG:CD   | 20:T:102:GLY:HA3 | 2.41                     | 0.50              |
| 1:A:1111:C:O2'   | 1:A:1112:A:P     | 2.70                     | 0.50              |
| 9:I:16:ARG:NE    | 9:I:64:THR:HG23  | 2.25                     | 0.50              |
| 16:P:67:THR:HG22 | 16:P:68:ASP:H    | 1.75                     | 0.50              |
| 1:A:603:C:N1     | 4:D:135:LEU:HD13 | 2.26                     | 0.50              |
| 2:B:229:VAL:O    | 2:B:229:VAL:HG12 | 2.12                     | 0.50              |
| 1:A:1124:G:H2'   | 1:A:1125:G:C5'   | 2.34                     | 0.50              |
| 13:M:19:LEU:HD11 | 13:M:34:LEU:HD21 | 1.93                     | 0.50              |
| 20:T:65:LYS:O    | 20:T:68:LYS:HB2  | 2.12                     | 0.50              |
| 1:A:385:C:H2'    | 1:A:386:G:H8     | 1.75                     | 0.50              |
| 16:P:8:ARG:HG2   | 16:P:17:TYR:CE2  | 2.47                     | 0.50              |
| 3:C:35:GLU:OE1   | 3:C:95:THR:HG23  | 2.12                     | 0.50              |
| 1:A:123:G:HO2'   | 1:A:189:U:H3'    | 1.77                     | 0.50              |
| 1:A:1279:C:H2'   | 7:G:114:ARG:HH12 | 1.77                     | 0.50              |
| 17:Q:78:GLU:OE2  | 17:Q:81:ARG:HD2  | 2.11                     | 0.50              |
| 4:D:52:SER:O     | 4:D:53:ASP:C     | 2.50                     | 0.50              |
| 1:A:1311:U:OP1   | 13:M:23:TYR:O    | 2.29                     | 0.50              |
| 10:J:34:VAL:HG22 | 10:J:74:ILE:HG22 | 1.93                     | 0.50              |
| 4:D:62:GLN:NE2   | 4:D:65:ARG:NH1   | 2.58                     | 0.50              |
| 17:Q:3:LYS:CB    | 17:Q:60:ILE:HD11 | 2.41                     | 0.50              |
| 11:K:126:ARG:O   | 11:K:127:LYS:CB  | 2.59                     | 0.50              |
| 9:I:10:ARG:HD2   | 9:I:75:ASP:HB3   | 1.94                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 12:L:89:ARG:H    | 12:L:89:ARG:NE    | 2.09                     | 0.50              |
| 6:F:91:VAL:HG11  | 18:R:72:ARG:NH1   | 2.27                     | 0.50              |
| 1:A:450:C:H2'    | 1:A:451:C:C6      | 2.46                     | 0.50              |
| 4:D:150:GLU:O    | 4:D:153:ARG:HG3   | 2.11                     | 0.50              |
| 11:K:54:ARG:O    | 11:K:57:THR:CG2   | 2.49                     | 0.50              |
| 2:B:158:LEU:HD21 | 2:B:180:LEU:HD13  | 1.94                     | 0.50              |
| 8:H:104:ARG:NH2  | 8:H:138:TRP:CH2   | 2.80                     | 0.50              |
| 1:A:1186:U:H2'   | 1:A:1187:G:C8     | 2.47                     | 0.50              |
| 1:A:1349:C:C5'   | 10:J:60:ARG:HH12  | 2.21                     | 0.50              |
| 1:A:268:A:H1'    | 17:Q:16:GLN:HE21  | 1.76                     | 0.50              |
| 1:A:726:U:H2'    | 1:A:727:C:H6      | 1.76                     | 0.50              |
| 1:A:1073:U:O2    | 1:A:1075:A:C8     | 2.64                     | 0.50              |
| 8:H:29:SER:OG    | 8:H:32:LYS:HG3    | 2.12                     | 0.50              |
| 1:A:294:G:H2'    | 1:A:295:A:C8      | 2.47                     | 0.50              |
| 1:A:1289:U:H5'   | 13:M:110:ARG:HH21 | 1.77                     | 0.49              |
| 1:A:670:A:HO2'   | 1:A:671:G:P       | 2.35                     | 0.49              |
| 3:C:22:TRP:O     | 3:C:22:TRP:CE3    | 2.65                     | 0.49              |
| 1:A:1133:A:H2'   | 1:A:1134:A:C8     | 2.47                     | 0.49              |
| 1:A:48:C:O2'     | 1:A:49:U:OP1      | 2.29                     | 0.49              |
| 1:A:371:G:P      | 16:P:67:THR:HG21  | 2.52                     | 0.49              |
| 1:A:1003:U:C6    | 1:A:1003:U:H3'    | 2.47                     | 0.49              |
| 13:M:36:LYS:HD2  | 13:M:59:TYR:OH    | 2.12                     | 0.49              |
| 21:V:7:ARG:O     | 21:V:7:ARG:HG3    | 2.12                     | 0.49              |
| 1:A:1159:G:N2    | 1:A:1161:A:H3'    | 2.27                     | 0.49              |
| 1:A:1182:A:H4'   | 1:A:1183:G:O5'    | 2.13                     | 0.49              |
| 1:A:955:A:C1'    | 1:A:1303:C:O2     | 2.57                     | 0.49              |
| 1:A:154:A:C2     | 1:A:338:U:H4'     | 2.48                     | 0.49              |
| 1:A:114:C:H5'    | 1:A:115:G:OP1     | 2.11                     | 0.49              |
| 1:A:695:A:H2'    | 1:A:696:G:O4'     | 2.12                     | 0.49              |
| 1:A:276:G:HO2'   | 1:A:277:A:P       | 2.32                     | 0.49              |
| 1:A:1042:C:O2    | 1:A:1179:G:C2     | 2.66                     | 0.49              |
| 2:B:69:LEU:HD12  | 2:B:155:LEU:CD1   | 2.41                     | 0.49              |
| 1:A:339:A:H5''   | 1:A:340:C:OP2     | 2.13                     | 0.49              |
| 1:A:675:U:OP1    | 11:K:124:LYS:HE3  | 2.12                     | 0.49              |
| 21:V:5:ASP:HB3   | 21:V:8:THR:OG1    | 2.13                     | 0.49              |
| 1:A:323:C:OP1    | 1:A:324:A:H5'     | 2.11                     | 0.49              |
| 19:S:13:ASP:HA   | 19:S:16:LEU:HB3   | 1.95                     | 0.49              |
| 3:C:40:ARG:O     | 3:C:44:GLU:CB     | 2.60                     | 0.49              |
| 9:I:10:ARG:NH1   | 9:I:11:LYS:HB2    | 2.27                     | 0.49              |
| 7:G:136:LYS:O    | 7:G:140:ASP:HB2   | 2.12                     | 0.49              |
| 1:A:310:A:O2'    | 1:A:311:G:OP2     | 2.24                     | 0.49              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:124:A:O2'     | 1:A:125:C:O5'    | 2.25                     | 0.49              |
| 15:O:65:ARG:HH11  | 15:O:65:ARG:HG3  | 1.77                     | 0.49              |
| 1:A:1258:C:C3'    | 1:A:1258:C:C6    | 2.92                     | 0.49              |
| 16:P:21:VAL:HG21  | 16:P:59:TRP:CD1  | 2.47                     | 0.49              |
| 12:L:89:ARG:HA    | 12:L:97:ARG:HA   | 1.94                     | 0.49              |
| 1:A:154:A:H2'     | 1:A:155:A:O4'    | 2.13                     | 0.49              |
| 3:C:32:LEU:O      | 3:C:36:ASP:HB2   | 2.13                     | 0.49              |
| 1:A:854:C:O2'     | 1:A:855:G:H5'    | 2.12                     | 0.49              |
| 1:A:1461:C:H2'    | 1:A:1462:U:C5'   | 2.43                     | 0.49              |
| 12:L:55:VAL:HG13  | 12:L:67:THR:HG23 | 1.94                     | 0.49              |
| 20:T:90:GLN:HA    | 20:T:93:GLU:HG2  | 1.95                     | 0.49              |
| 5:E:82:VAL:HG11   | 5:E:134:ALA:O    | 2.11                     | 0.49              |
| 1:A:79:U:C3'      | 1:A:79:U:C6      | 2.96                     | 0.49              |
| 5:E:39:GLY:O      | 5:E:69:VAL:N     | 2.43                     | 0.49              |
| 10:J:42:THR:HG23  | 10:J:67:THR:C    | 2.32                     | 0.49              |
| 1:A:981:G:N1      | 1:A:982:A:N3     | 2.61                     | 0.49              |
| 13:M:49:THR:HB    | 13:M:52:GLU:CG   | 2.41                     | 0.49              |
| 1:A:1098:C:O2'    | 1:A:1099:G:H5''  | 2.12                     | 0.49              |
| 3:C:13:GLY:O      | 3:C:14:ILE:HD13  | 2.13                     | 0.49              |
| 19:S:46:GLY:N     | 19:S:62:ILE:HG23 | 2.27                     | 0.49              |
| 3:C:119:ARG:HE    | 3:C:140:ARG:HH12 | 1.60                     | 0.49              |
| 12:L:33:ARG:HE    | 12:L:62:SER:HB3  | 1.77                     | 0.49              |
| 3:C:134:ILE:HG21  | 3:C:168:ALA:HB3  | 1.94                     | 0.49              |
| 6:F:91:VAL:HG12   | 6:F:92:LYS:O     | 2.12                     | 0.49              |
| 2:B:129:GLU:O     | 2:B:130:ARG:HB2  | 2.11                     | 0.49              |
| 11:K:13:GLN:HA    | 11:K:75:TYR:O    | 2.12                     | 0.49              |
| 1:A:959:U:H4'     | 1:A:960:A:O5'    | 2.13                     | 0.49              |
| 1:A:1301:C:H2'    | 1:A:1302:C:O4'   | 2.13                     | 0.49              |
| 1:A:1485:G:O2'    | 1:A:1486:C:H5'   | 2.13                     | 0.49              |
| 1:A:530:A:OP2     | 4:D:2:GLY:HA3    | 2.13                     | 0.49              |
| 13:M:117:VAL:HG12 | 13:M:118:ALA:N   | 2.22                     | 0.49              |
| 1:A:775:A:H4'     | 1:A:776:U:H5''   | 1.95                     | 0.49              |
| 4:D:5:ILE:HG22    | 4:D:5:ILE:O      | 2.11                     | 0.49              |
| 2:B:114:ARG:HE    | 2:B:118:LEU:HD11 | 1.78                     | 0.49              |
| 11:K:79:SER:HB2   | 11:K:104:GLN:HB3 | 1.93                     | 0.49              |
| 6:F:23:LYS:HD2    | 6:F:42:GLU:OE1   | 2.13                     | 0.49              |
| 1:A:175:G:H4'     | 1:A:176:U:C5'    | 2.43                     | 0.49              |
| 6:F:40:VAL:HG22   | 6:F:41:GLU:N     | 2.26                     | 0.49              |
| 23:X:39:PSU:H2'   | 23:X:40:C:C5'    | 2.38                     | 0.49              |
| 1:A:1261:A:H5'    | 10:J:40:LEU:HD22 | 1.94                     | 0.49              |
| 17:Q:67:LYS:CA    | 17:Q:70:ARG:NH1  | 2.71                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:635:U:O2'    | 1:A:636:A:O5'     | 2.30                     | 0.49              |
| 3:C:14:ILE:O     | 3:C:16:ARG:N      | 2.45                     | 0.49              |
| 1:A:562:G:C5'    | 1:A:711:A:H1'     | 2.37                     | 0.49              |
| 3:C:22:TRP:CZ3   | 3:C:32:LEU:HB2    | 2.48                     | 0.49              |
| 12:L:60:LEU:HD21 | 12:L:85:ILE:HD12  | 1.93                     | 0.49              |
| 10:J:48:THR:HG1  | 10:J:62:HIS:CD2   | 2.30                     | 0.49              |
| 9:I:36:TYR:HD2   | 9:I:37:PHE:CE2    | 2.31                     | 0.49              |
| 1:A:1436:C:O2'   | 1:A:1437:A:H5'    | 2.13                     | 0.49              |
| 1:A:919:G:C2     | 1:A:920:U:C6      | 3.01                     | 0.49              |
| 10:J:12:ASP:O    | 10:J:15:THR:HG22  | 2.13                     | 0.49              |
| 7:G:15:ASP:OD2   | 7:G:18:TYR:N      | 2.34                     | 0.49              |
| 4:D:76:ARG:NH1   | 4:D:76:ARG:HG2    | 2.26                     | 0.49              |
| 2:B:223:ILE:HG13 | 2:B:224:GLN:N     | 2.28                     | 0.49              |
| 13:M:5:ALA:HB3   | 13:M:8:GLU:CG     | 2.41                     | 0.49              |
| 13:M:37:THR:HG22 | 13:M:55:ARG:HD2   | 1.95                     | 0.49              |
| 13:M:37:THR:HG23 | 13:M:55:ARG:HD2   | 1.95                     | 0.49              |
| 1:A:1458:U:H2'   | 1:A:1459:G:C5'    | 2.43                     | 0.49              |
| 15:O:33:THR:O    | 15:O:37:ASN:OD1   | 2.29                     | 0.49              |
| 6:F:21:LEU:O     | 6:F:25:ILE:HG13   | 2.13                     | 0.49              |
| 1:A:457:A:C4'    | 16:P:82:GLN:HE21  | 2.26                     | 0.49              |
| 7:G:138:LYS:C    | 7:G:138:LYS:HD3   | 2.33                     | 0.49              |
| 13:M:23:TYR:HB2  | 13:M:67:GLU:OE2   | 2.12                     | 0.49              |
| 1:A:1253:G:C2'   | 1:A:1254:G:H5'    | 2.43                     | 0.49              |
| 1:A:1042:C:H2'   | 1:A:1043:G:C8     | 2.41                     | 0.49              |
| 13:M:34:LEU:CD1  | 13:M:41:PRO:HA    | 2.42                     | 0.49              |
| 3:C:91:LEU:HD23  | 3:C:99:VAL:CG2    | 2.43                     | 0.49              |
| 1:A:525:G:H5''   | 4:D:40:PRO:O      | 2.13                     | 0.49              |
| 1:A:485:G:H4'    | 1:A:533:G:H4'     | 1.95                     | 0.49              |
| 12:L:83:VAL:CG2  | 12:L:100:ILE:HG23 | 2.43                     | 0.49              |
| 19:S:32:LYS:HA   | 19:S:50:ALA:O     | 2.12                     | 0.49              |
| 4:D:175:SER:HB3  | 4:D:184:LYS:CB    | 2.43                     | 0.49              |
| 1:A:79:U:H3'     | 1:A:80:U:H5''     | 1.95                     | 0.49              |
| 3:C:167:TRP:O    | 3:C:168:ALA:HB3   | 2.12                     | 0.49              |
| 1:A:1191:C:H2'   | 1:A:1192:U:O4'    | 2.13                     | 0.49              |
| 1:A:1005:C:H2'   | 1:A:1006:C:C4     | 2.48                     | 0.48              |
| 1:A:1121:G:H21   | 1:A:1125:G:N2     | 2.11                     | 0.48              |
| 9:I:3:GLN:OE1    | 9:I:20:ARG:NE     | 2.46                     | 0.48              |
| 1:A:795:C:H4'    | 1:A:796:U:C5'     | 2.41                     | 0.48              |
| 1:A:469:G:O2'    | 1:A:470:U:P       | 2.71                     | 0.48              |
| 13:M:9:ILE:H     | 13:M:9:ILE:HD12   | 1.78                     | 0.48              |
| 9:I:5:TYR:CG     | 9:I:6:GLY:N       | 2.80                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:31:CYS:O     | 4:D:32:ALA:HB3   | 2.13                     | 0.48              |
| 9:I:17:VAL:HB    | 9:I:80:GLY:O     | 2.13                     | 0.48              |
| 5:E:36:ASP:CG    | 5:E:40:ARG:HB2   | 2.33                     | 0.48              |
| 1:A:1184:C:H2'   | 1:A:1185:A:O4'   | 2.14                     | 0.48              |
| 10:J:32:ALA:HB3  | 10:J:75:ILE:HG13 | 1.94                     | 0.48              |
| 19:S:28:LYS:HB3  | 19:S:31:ILE:HD11 | 1.95                     | 0.48              |
| 5:E:122:GLU:O    | 5:E:123:LEU:HD23 | 2.13                     | 0.48              |
| 1:A:1509:U:O2'   | 1:A:1510:C:H5'   | 2.13                     | 0.48              |
| 18:R:41:LYS:O    | 18:R:43:PHE:N    | 2.46                     | 0.48              |
| 8:H:2:LEU:HD12   | 8:H:2:LEU:N      | 2.28                     | 0.48              |
| 2:B:170:GLU:O    | 2:B:173:ALA:HB3  | 2.13                     | 0.48              |
| 11:K:24:SER:C    | 11:K:26:ASN:H    | 2.16                     | 0.48              |
| 5:E:8:GLU:HB3    | 5:E:34:VAL:HG22  | 1.95                     | 0.48              |
| 1:A:192:G:O2'    | 1:A:193:G:H5'    | 2.13                     | 0.48              |
| 15:O:54:ARG:O    | 15:O:58:MET:HG3  | 2.13                     | 0.48              |
| 1:A:513:G:O2'    | 1:A:514:U:OP2    | 2.30                     | 0.48              |
| 20:T:53:LEU:O    | 20:T:54:LYS:C    | 2.52                     | 0.48              |
| 10:J:6:ILE:O     | 10:J:71:LEU:O    | 2.30                     | 0.48              |
| 7:G:73:MET:HG2   | 7:G:90:GLU:HA    | 1.94                     | 0.48              |
| 1:A:1300:A:C4'   | 19:S:37:ARG:NH1  | 2.77                     | 0.48              |
| 1:A:156:A:N7     | 1:A:157:C:H1'    | 2.28                     | 0.48              |
| 1:A:1472:U:H2'   | 1:A:1473:C:H6    | 1.78                     | 0.48              |
| 2:B:27:LYS:O     | 2:B:194:PRO:HG3  | 2.13                     | 0.48              |
| 23:X:31:A:C2'    | 23:X:31:A:N3     | 2.74                     | 0.48              |
| 10:J:37:PRO:HA   | 10:J:72:VAL:H    | 1.78                     | 0.48              |
| 2:B:100:GLY:O    | 2:B:104:ASN:N    | 2.43                     | 0.48              |
| 1:A:323:C:O2     | 1:A:323:C:C2'    | 2.61                     | 0.48              |
| 6:F:9:VAL:HB     | 6:F:87:ARG:HB2   | 1.94                     | 0.48              |
| 17:Q:26:GLN:O    | 17:Q:27:PHE:HB3  | 2.14                     | 0.48              |
| 1:A:667:A:N6     | 1:A:668:G:C6     | 2.81                     | 0.48              |
| 1:A:1027:C:H2'   | 1:A:1028:A:O5'   | 2.14                     | 0.48              |
| 1:A:1217:A:OP1   | 21:V:2:GLY:HA3   | 2.13                     | 0.48              |
| 5:E:10:MET:SD    | 5:E:13:ILE:HG23  | 2.53                     | 0.48              |
| 5:E:30:ALA:O     | 5:E:45:PHE:HA    | 2.14                     | 0.48              |
| 3:C:107:GLN:O    | 3:C:108:ASN:CB   | 2.61                     | 0.48              |
| 2:B:213:LEU:HD23 | 2:B:217:ARG:CG   | 2.43                     | 0.48              |
| 2:B:55:PHE:HE1   | 2:B:218:ALA:HA   | 1.77                     | 0.48              |
| 5:E:143:ARG:HH12 | 8:H:77:GLU:CD    | 2.16                     | 0.48              |
| 1:A:982:A:O2'    | 1:A:983:A:OP1    | 2.30                     | 0.48              |
| 9:I:50:LEU:O     | 9:I:53:VAL:HG22  | 2.13                     | 0.48              |
| 1:A:1236:G:H2'   | 1:A:1239:G:H21   | 1.77                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 17:Q:97:SER:HB2  | 17:Q:105:ALA:HB2 | 1.94                     | 0.48              |
| 5:E:76:ILE:HG23  | 5:E:142:LEU:CD1  | 2.43                     | 0.48              |
| 3:C:14:ILE:O     | 3:C:15:THR:C     | 2.52                     | 0.48              |
| 9:I:3:GLN:HG3    | 9:I:4:TYR:N      | 2.28                     | 0.48              |
| 1:A:416:U:H4'    | 1:A:417:C:OP2    | 2.14                     | 0.48              |
| 20:T:91:LEU:C    | 20:T:93:GLU:H    | 2.17                     | 0.48              |
| 1:A:602:U:O2     | 4:D:133:VAL:HA   | 2.14                     | 0.48              |
| 1:A:647:G:OP1    | 18:R:64:ARG:HD2  | 2.13                     | 0.48              |
| 20:T:39:LYS:HD2  | 20:T:55:ILE:HD12 | 1.93                     | 0.48              |
| 3:C:16:ARG:NH1   | 3:C:16:ARG:HG3   | 2.19                     | 0.48              |
| 1:A:626:C:H4'    | 8:H:31:PHE:CE2   | 2.49                     | 0.48              |
| 18:R:37:VAL:HG22 | 18:R:78:LEU:HB3  | 1.96                     | 0.48              |
| 17:Q:3:LYS:HG2   | 17:Q:3:LYS:H     | 1.51                     | 0.48              |
| 4:D:60:GLU:HG2   | 4:D:202:LEU:HD12 | 1.94                     | 0.48              |
| 1:A:1516:C:H41   | 7:G:82:GLY:HA2   | 1.78                     | 0.48              |
| 1:A:1437:A:H2'   | 1:A:1438:G:O4'   | 2.13                     | 0.48              |
| 1:A:649:G:H5'    | 1:A:709:C:H1'    | 1.96                     | 0.48              |
| 3:C:5:ILE:O      | 3:C:5:ILE:HD12   | 2.14                     | 0.48              |
| 1:A:1114:C:O5'   | 1:A:1114:C:H6    | 1.97                     | 0.48              |
| 1:A:238:A:H4'    | 1:A:239:U:O5'    | 2.13                     | 0.48              |
| 3:C:8:ILE:O      | 3:C:11:ARG:N     | 2.34                     | 0.48              |
| 3:C:35:GLU:O     | 3:C:38:ARG:N     | 2.46                     | 0.48              |
| 1:A:948:G:H4'    | 1:A:949:C:OP2    | 2.14                     | 0.48              |
| 1:A:1282:U:O2'   | 1:A:1283:U:OP1   | 2.28                     | 0.48              |
| 2:B:185:ILE:HG23 | 2:B:199:TYR:HB2  | 1.95                     | 0.48              |
| 15:O:74:ASP:O    | 15:O:76:GLU:N    | 2.47                     | 0.48              |
| 9:I:113:LYS:N    | 9:I:113:LYS:HD2  | 2.29                     | 0.48              |
| 8:H:97:VAL:HG13  | 8:H:98:LYS:N     | 2.27                     | 0.48              |
| 4:D:81:GLU:O     | 4:D:85:LYS:HG3   | 2.13                     | 0.48              |
| 2:B:52:GLU:O     | 2:B:56:ARG:HG3   | 2.14                     | 0.48              |
| 4:D:14:ARG:HA    | 4:D:39:PRO:HB3   | 1.95                     | 0.48              |
| 1:A:986:C:N4     | 1:A:1000:G:H22   | 2.11                     | 0.48              |
| 20:T:8:ARG:CB    | 20:T:8:ARG:HH11  | 2.05                     | 0.48              |
| 4:D:98:GLU:OE2   | 4:D:103:ASN:ND2  | 2.39                     | 0.48              |
| 1:A:275:C:H6     | 1:A:275:C:O5'    | 1.97                     | 0.48              |
| 20:T:45:GLN:HA   | 20:T:91:LEU:HD22 | 1.96                     | 0.48              |
| 1:A:507:G:H2'    | 1:A:508:C:C6     | 2.48                     | 0.48              |
| 1:A:1423:G:H4'   | 1:A:1424:G:C5    | 2.48                     | 0.48              |
| 1:A:945:A:H4'    | 1:A:946:A:OP2    | 2.13                     | 0.48              |
| 16:P:42:ARG:H    | 16:P:42:ARG:HG2  | 1.36                     | 0.48              |
| 10:J:40:LEU:HD22 | 10:J:41:PRO:HD2  | 1.96                     | 0.48              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 10:J:94:VAL:CG1 | 10:J:95:GLU:N    | 2.77                     | 0.48              |
| 4:D:3:ARG:O     | 4:D:4:TYR:HB3    | 2.12                     | 0.48              |
| 1:A:685:A:O2'   | 1:A:686:G:OP1    | 2.32                     | 0.48              |
| 1:A:1098:C:C2'  | 1:A:1099:G:C5'   | 2.84                     | 0.48              |
| 7:G:145:ALA:O   | 7:G:147:ALA:N    | 2.46                     | 0.48              |
| 1:A:15:G:C4'    | 5:E:24:ARG:HH12  | 2.26                     | 0.48              |
| 1:A:949:C:OP1   | 10:J:57:LYS:HD3  | 2.13                     | 0.48              |
| 12:L:47:LYS:CB  | 12:L:47:LYS:NZ   | 2.77                     | 0.48              |
| 9:I:121:ARG:NH1 | 9:I:121:ARG:HG2  | 2.29                     | 0.48              |
| 4:D:8:VAL:CG1   | 4:D:115:ARG:NH1  | 2.77                     | 0.48              |
| 1:A:450:C:H2'   | 1:A:451:C:H6     | 1.78                     | 0.48              |
| 1:A:558:G:H4'   | 1:A:559:G:O5'    | 2.14                     | 0.48              |
| 7:G:80:VAL:HG12 | 7:G:81:GLY:N     | 2.29                     | 0.48              |
| 1:A:45:U:H2'    | 1:A:46:G:C8      | 2.49                     | 0.48              |
| 19:S:5:LEU:HD12 | 19:S:6:LYS:N     | 2.28                     | 0.47              |
| 8:H:119:LEU:HB3 | 8:H:123:GLU:HB2  | 1.95                     | 0.47              |
| 1:A:407:A:C2    | 4:D:35:ARG:CG    | 2.97                     | 0.47              |
| 9:I:4:TYR:CZ    | 9:I:88:TYR:HA    | 2.48                     | 0.47              |
| 1:A:966:C:O2'   | 1:A:967:C:H5'    | 2.14                     | 0.47              |
| 2:B:41:ILE:HG13 | 2:B:41:ILE:O     | 2.13                     | 0.47              |
| 4:D:13:ARG:NH1  | 4:D:38:TYR:O     | 2.47                     | 0.47              |
| 17:Q:99:SER:OG  | 17:Q:100:LYS:N   | 2.44                     | 0.47              |
| 1:A:1374:G:N2   | 1:A:1479:A:H8    | 2.12                     | 0.47              |
| 2:B:19:HIS:O    | 2:B:20:GLU:C     | 2.52                     | 0.47              |
| 1:A:748:G:N2    | 1:A:795:C:O2'    | 2.47                     | 0.47              |
| 1:A:1378:A:H4'  | 1:A:1379:C:H5'   | 1.95                     | 0.47              |
| 1:A:1345:A:H1'  | 1:A:1347:G:C8    | 2.49                     | 0.47              |
| 1:A:1193:U:HO2' | 1:A:1194:A:H8    | 1.53                     | 0.47              |
| 1:A:1476:A:O2'  | 1:A:1477:A:H5'   | 2.13                     | 0.47              |
| 10:J:84:GLN:C   | 10:J:86:MET:H    | 2.17                     | 0.47              |
| 1:A:67:C:O2'    | 1:A:165:A:H1'    | 2.14                     | 0.47              |
| 1:A:876:C:O5'   | 1:A:876:C:H6     | 1.98                     | 0.47              |
| 2:B:7:VAL:HB    | 2:B:8:LYS:HZ2    | 1.78                     | 0.47              |
| 14:N:45:ARG:O   | 14:N:49:HIS:CD2  | 2.67                     | 0.47              |
| 2:B:71:VAL:O    | 2:B:165:VAL:HG22 | 2.14                     | 0.47              |
| 9:I:127:LYS:O   | 9:I:128:ARG:HB2  | 2.15                     | 0.47              |
| 1:A:563:U:H2'   | 1:A:564:G:O4'    | 2.14                     | 0.47              |
| 7:G:143:ARG:O   | 7:G:147:ALA:HB2  | 2.14                     | 0.47              |
| 2:B:87:ARG:HE   | 2:B:233:SER:HA   | 1.79                     | 0.47              |
| 1:A:1107:U:H3   | 10:J:5:ARG:NH2   | 2.12                     | 0.47              |
| 3:C:147:LYS:HE2 | 3:C:205:GLY:H    | 1.79                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 20:T:29:LYS:O    | 20:T:33:ILE:HG13 | 2.15                     | 0.47              |
| 1:A:986:C:N4     | 1:A:1000:G:N2    | 2.62                     | 0.47              |
| 4:D:100:ARG:NH2  | 4:D:102:ASP:OD2  | 2.48                     | 0.47              |
| 4:D:70:ILE:HG22  | 4:D:71:SER:O     | 2.15                     | 0.47              |
| 17:Q:69:LYS:C    | 17:Q:70:ARG:HD2  | 2.35                     | 0.47              |
| 1:A:636:A:O2'    | 1:A:637:G:OP1    | 2.24                     | 0.47              |
| 1:A:1047:U:O2'   | 1:A:1048:C:OP2   | 2.32                     | 0.47              |
| 1:A:433:G:C4'    | 1:A:434:A:OP1    | 2.61                     | 0.47              |
| 1:A:124:A:C8     | 17:Q:63:ARG:HG3  | 2.49                     | 0.47              |
| 17:Q:64:PRO:C    | 17:Q:65:ILE:HD12 | 2.34                     | 0.47              |
| 1:A:50:A:H3'     | 1:A:50:A:P       | 2.54                     | 0.47              |
| 1:A:822:U:H5'    | 1:A:823:C:H5     | 1.79                     | 0.47              |
| 13:M:58:GLU:OE2  | 13:M:58:GLU:HA   | 2.14                     | 0.47              |
| 6:F:22:GLU:OE2   | 6:F:82:ARG:NE    | 2.40                     | 0.47              |
| 1:A:1487:U:H2'   | 1:A:1488:G:C8    | 2.49                     | 0.47              |
| 2:B:158:LEU:CD2  | 2:B:180:LEU:HD13 | 2.45                     | 0.47              |
| 2:B:158:LEU:HD23 | 2:B:182:ILE:HD11 | 1.96                     | 0.47              |
| 1:A:1189:C:H2'   | 1:A:1190:C:H6    | 1.78                     | 0.47              |
| 1:A:423:G:O2'    | 1:A:424:U:OP2    | 2.31                     | 0.47              |
| 12:L:83:VAL:HG22 | 12:L:84:LEU:N    | 2.29                     | 0.47              |
| 2:B:120:ALA:C    | 2:B:122:PHE:H    | 2.18                     | 0.47              |
| 1:A:26:A:N6      | 1:A:541:G:H1'    | 2.29                     | 0.47              |
| 1:A:1211:C:H2'   | 1:A:1212:G:H8    | 1.80                     | 0.47              |
| 1:A:660:U:H3     | 1:A:696:G:H22    | 1.62                     | 0.47              |
| 7:G:15:ASP:HB2   | 7:G:20:ASP:O     | 2.14                     | 0.47              |
| 1:A:1197:G:H5''  | 14:N:5:ALA:CB    | 2.44                     | 0.47              |
| 3:C:108:ASN:HD21 | 3:C:110:ASN:HB2  | 1.79                     | 0.47              |
| 1:A:446:A:H4'    | 16:P:72:ARG:HE   | 1.80                     | 0.47              |
| 1:A:176:U:H2'    | 1:A:177:G:O5'    | 2.15                     | 0.47              |
| 1:A:96:C:P       | 20:T:17:ARG:HH11 | 2.37                     | 0.47              |
| 1:A:1174:G:O2'   | 1:A:1175:U:H5'   | 2.15                     | 0.47              |
| 1:A:1502:G:O2'   | 1:A:1503:G:H5'   | 2.14                     | 0.47              |
| 1:A:597:A:H2'    | 1:A:598:C:O4'    | 2.14                     | 0.47              |
| 1:A:982:A:O2'    | 1:A:983:A:P      | 2.73                     | 0.47              |
| 1:A:1035:G:O6    | 1:A:1180:U:H2'   | 2.15                     | 0.47              |
| 13:M:109:THR:CG2 | 13:M:110:ARG:N   | 2.78                     | 0.47              |
| 4:D:140:VAL:CG1  | 4:D:146:ILE:HD11 | 2.43                     | 0.47              |
| 1:A:1171:G:HO2'  | 1:A:1172:A:P     | 2.38                     | 0.47              |
| 1:A:563:U:O2'    | 15:O:57:LEU:HG   | 2.15                     | 0.47              |
| 6:F:60:PHE:CZ    | 18:R:78:LEU:HD21 | 2.50                     | 0.47              |
| 1:A:480:A:O2'    | 1:A:481:U:OP1    | 2.26                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:G:15:ASP:HB3   | 7:G:20:ASP:N     | 2.30                     | 0.47              |
| 1:A:823:C:H3'    | 1:A:823:C:OP2    | 2.15                     | 0.47              |
| 1:A:1354:U:H2'   | 1:A:1355:G:O4'   | 2.14                     | 0.47              |
| 2:B:114:ARG:O    | 2:B:117:GLU:HB3  | 2.15                     | 0.47              |
| 20:T:60:GLU:O    | 20:T:63:ILE:HB   | 2.13                     | 0.47              |
| 1:A:639:C:O2'    | 15:O:28:GLN:OE1  | 2.20                     | 0.47              |
| 14:N:36:PHE:O    | 14:N:36:PHE:CD1  | 2.68                     | 0.47              |
| 2:B:181:PHE:HD2  | 8:H:70:GLN:HG2   | 1.79                     | 0.47              |
| 1:A:539:C:O2'    | 1:A:540:G:H5'    | 2.15                     | 0.47              |
| 1:A:720:A:H1'    | 6:F:73:ASN:HD21  | 1.79                     | 0.47              |
| 1:A:953:G:H4'    | 1:A:954:A:OP1    | 2.14                     | 0.47              |
| 6:F:33:TYR:HA    | 6:F:71:ARG:HH21  | 1.80                     | 0.47              |
| 20:T:54:LYS:O    | 20:T:57:ARG:HB2  | 2.15                     | 0.47              |
| 1:A:31:G:H2'     | 1:A:48:C:N4      | 2.30                     | 0.47              |
| 1:A:173:A:H2'    | 1:A:174:U:H6     | 1.79                     | 0.47              |
| 1:A:1469:A:OP1   | 12:L:47:LYS:HA   | 2.15                     | 0.47              |
| 18:R:47:THR:HG23 | 18:R:83:GLU:O    | 2.15                     | 0.47              |
| 1:A:56:U:H2'     | 1:A:57:G:C8      | 2.50                     | 0.47              |
| 1:A:1518:U:H3'   | 1:A:1518:U:C6    | 2.50                     | 0.47              |
| 2:B:77:ALA:HB1   | 2:B:81:VAL:HG23  | 1.97                     | 0.47              |
| 4:D:70:ILE:HD11  | 4:D:100:ARG:HD2  | 1.93                     | 0.47              |
| 1:A:241:A:N6     | 1:A:276:G:H1'    | 2.30                     | 0.47              |
| 1:A:485:G:OP1    | 12:L:118:SER:CB  | 2.63                     | 0.47              |
| 12:L:83:VAL:HG21 | 12:L:100:ILE:CG2 | 2.44                     | 0.47              |
| 1:A:7:G:H21      | 5:E:121:LYS:HG2  | 1.79                     | 0.47              |
| 13:M:106:ASN:O   | 13:M:107:ALA:CB  | 2.63                     | 0.47              |
| 15:O:74:ASP:C    | 15:O:76:GLU:H    | 2.17                     | 0.47              |
| 2:B:115:LEU:HD21 | 2:B:153:ARG:NH1  | 2.30                     | 0.47              |
| 5:E:50:GLU:HG3   | 5:E:53:LEU:HB2   | 1.97                     | 0.47              |
| 1:A:1183:G:H2'   | 1:A:1184:C:O5'   | 2.14                     | 0.47              |
| 1:A:1083:A:H8    | 2:B:172:ILE:HD13 | 1.79                     | 0.47              |
| 1:A:124:A:O2'    | 1:A:125:C:P      | 2.73                     | 0.47              |
| 1:A:409:A:OP2    | 1:A:423:G:N2     | 2.46                     | 0.47              |
| 5:E:102:ALA:HB2  | 5:E:120:THR:HB   | 1.96                     | 0.47              |
| 1:A:701:G:H1'    | 11:K:116:HIS:HA  | 1.95                     | 0.47              |
| 16:P:21:VAL:HG21 | 16:P:59:TRP:CG   | 2.50                     | 0.47              |
| 1:A:152:G:C6     | 1:A:158:U:O2     | 2.68                     | 0.47              |
| 11:K:34:ASP:OD2  | 11:K:38:ASN:HB2  | 2.15                     | 0.47              |
| 18:R:19:LYS:HG3  | 18:R:20:ALA:N    | 2.29                     | 0.47              |
| 1:A:645:G:H2'    | 1:A:646:A:C8     | 2.49                     | 0.47              |
| 1:A:985:C:H2'    | 1:A:986:C:C5     | 2.48                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 12:L:50:SER:O    | 12:L:51:ALA:HB2  | 2.15                     | 0.46              |
| 1:A:249:G:OP1    | 17:Q:67:LYS:O    | 2.33                     | 0.46              |
| 6:F:15:ASP:CG    | 6:F:18:GLN:HB2   | 2.35                     | 0.46              |
| 4:D:63:LYS:O     | 4:D:67:ILE:HG13  | 2.14                     | 0.46              |
| 1:A:1024:G:H2'   | 1:A:1025:C:C6    | 2.49                     | 0.46              |
| 1:A:705:A:N3     | 1:A:705:A:H3'    | 2.30                     | 0.46              |
| 5:E:135:THR:O    | 5:E:138:ALA:HB3  | 2.15                     | 0.46              |
| 4:D:52:SER:O     | 4:D:54:TYR:N     | 2.49                     | 0.46              |
| 16:P:4:ILE:HG13  | 16:P:64:ALA:HB1  | 1.97                     | 0.46              |
| 1:A:494:C:O2'    | 1:A:495:U:O5'    | 2.33                     | 0.46              |
| 2:B:80:ILE:C     | 2:B:82:ARG:H     | 2.17                     | 0.46              |
| 18:R:36:ASN:OD1  | 18:R:38:GLU:HG2  | 2.15                     | 0.46              |
| 19:S:40:ILE:HG21 | 19:S:62:ILE:CD1  | 2.45                     | 0.46              |
| 1:A:432:U:O2'    | 4:D:123:HIS:CD2  | 2.68                     | 0.46              |
| 12:L:55:VAL:HG11 | 12:L:67:THR:HG23 | 1.97                     | 0.46              |
| 7:G:70:LYS:HB3   | 7:G:96:GLN:HG2   | 1.98                     | 0.46              |
| 6:F:47:ARG:HA    | 6:F:57:GLN:HG2   | 1.97                     | 0.46              |
| 1:A:652:U:H2'    | 1:A:653:G:H8     | 1.80                     | 0.46              |
| 17:Q:4:LYS:HD2   | 17:Q:6:LEU:CD2   | 2.45                     | 0.46              |
| 14:N:25:VAL:HG13 | 14:N:26:ARG:N    | 2.30                     | 0.46              |
| 1:A:1288:U:H2'   | 1:A:1289:U:C6    | 2.51                     | 0.46              |
| 5:E:76:ILE:HG23  | 5:E:77:PRO:HD2   | 1.96                     | 0.46              |
| 9:I:3:GLN:HB2    | 9:I:19:LEU:O     | 2.15                     | 0.46              |
| 3:C:119:ARG:HG3  | 3:C:123:GLN:HE21 | 1.79                     | 0.46              |
| 9:I:126:SER:O    | 9:I:127:LYS:C    | 2.54                     | 0.46              |
| 4:D:199:ASN:HD21 | 4:D:201:GLN:CB   | 2.26                     | 0.46              |
| 1:A:31:G:N1      | 1:A:48:C:H5''    | 2.31                     | 0.46              |
| 1:A:801:G:O2'    | 1:A:802:A:H5''   | 2.15                     | 0.46              |
| 8:H:25:ASP:OD2   | 8:H:60:ARG:NH1   | 2.46                     | 0.46              |
| 7:G:64:GLN:HG2   | 7:G:128:ALA:HB1  | 1.97                     | 0.46              |
| 10:J:45:ARG:HG2  | 10:J:45:ARG:NH1  | 2.30                     | 0.46              |
| 2:B:82:ARG:O     | 2:B:86:GLU:HG3   | 2.15                     | 0.46              |
| 9:I:15:ALA:HB2   | 9:I:65:VAL:HG23  | 1.96                     | 0.46              |
| 1:A:238:A:N6     | 1:A:276:G:O2'    | 2.47                     | 0.46              |
| 15:O:39:LEU:HD23 | 15:O:43:LEU:HG   | 1.97                     | 0.46              |
| 5:E:79:GLU:O     | 8:H:104:ARG:CZ   | 2.63                     | 0.46              |
| 3:C:82:GLU:HG3   | 3:C:83:ARG:N     | 2.31                     | 0.46              |
| 1:A:1352:G:O2'   | 1:A:1353:G:H5'   | 2.15                     | 0.46              |
| 1:A:1162:G:O2'   | 1:A:1163:G:C5'   | 2.64                     | 0.46              |
| 17:Q:90:ILE:O    | 17:Q:93:GLN:N    | 2.48                     | 0.46              |
| 17:Q:45:HIS:NE2  | 17:Q:47:PRO:HG3  | 2.30                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 23:X:30:G:H2'    | 23:X:31:A:C8      | 2.51                     | 0.46              |
| 1:A:1231:A:H2'   | 1:A:1232:A:C8     | 2.51                     | 0.46              |
| 1:A:1328:G:HO2'  | 1:A:1355:G:H1     | 1.64                     | 0.46              |
| 7:G:28:ASN:HD21  | 7:G:36:LYS:HE3    | 1.79                     | 0.46              |
| 9:I:99:LEU:HB3   | 9:I:101:PHE:CE1   | 2.50                     | 0.46              |
| 13:M:54:VAL:O    | 13:M:58:GLU:HG2   | 2.15                     | 0.46              |
| 17:Q:81:ARG:HB2  | 17:Q:83:ASP:OD1   | 2.15                     | 0.46              |
| 1:A:1153:C:H2'   | 1:A:1154:G:H8     | 1.80                     | 0.46              |
| 1:A:537:C:H2'    | 1:A:538:C:C6      | 2.51                     | 0.46              |
| 1:A:906:G:H2'    | 1:A:907:C:O4'     | 2.16                     | 0.46              |
| 2:B:91:PRO:CG    | 2:B:154:LEU:HB3   | 2.36                     | 0.46              |
| 1:A:1108:U:H2'   | 1:A:1109:G:O5'    | 2.16                     | 0.46              |
| 10:J:9:ARG:NH1   | 10:J:9:ARG:HB3    | 2.30                     | 0.46              |
| 1:A:1378:A:O2'   | 1:A:1379:C:OP2    | 2.26                     | 0.46              |
| 20:T:23:ARG:HH22 | 20:T:27:LYS:HZ3   | 1.63                     | 0.46              |
| 1:A:453:G:C3'    | 1:A:454:A:H5''    | 2.45                     | 0.46              |
| 12:L:10:LEU:O    | 12:L:14:GLY:N     | 2.48                     | 0.46              |
| 15:O:42:HIS:O    | 15:O:45:VAL:O     | 2.34                     | 0.46              |
| 1:A:1338:A:N7    | 1:A:1339:U:C5     | 2.84                     | 0.46              |
| 15:O:69:TYR:O    | 15:O:73:GLU:HG2   | 2.15                     | 0.46              |
| 1:A:1099:G:H4'   | 9:I:104:ARG:NH1   | 2.31                     | 0.46              |
| 18:R:37:VAL:HG12 | 18:R:41:LYS:HD3   | 1.97                     | 0.46              |
| 7:G:145:ALA:C    | 7:G:147:ALA:N     | 2.64                     | 0.46              |
| 1:A:189:U:O2'    | 1:A:190:G:OP1     | 2.28                     | 0.46              |
| 8:H:6:ILE:HB     | 8:H:85:ARG:HH12   | 1.80                     | 0.46              |
| 8:H:36:LEU:CD1   | 8:H:59:LEU:HD13   | 2.46                     | 0.46              |
| 1:A:404:G:H2'    | 1:A:405:G:O5'     | 2.15                     | 0.46              |
| 2:B:80:ILE:C     | 2:B:82:ARG:N      | 2.70                     | 0.46              |
| 23:X:36:U:O2'    | 23:X:37:12A:H5''  | 2.16                     | 0.46              |
| 1:A:1217:A:O2'   | 1:A:1285:G:H4'    | 2.16                     | 0.46              |
| 1:A:669:U:H2'    | 1:A:670:A:O5'     | 2.16                     | 0.46              |
| 12:L:53:ARG:HH12 | 12:L:92:ASP:CB    | 2.29                     | 0.46              |
| 1:A:1023:A:N3    | 1:A:1023:A:H2'    | 2.31                     | 0.46              |
| 1:A:1406:C:C2'   | 1:A:1407:U:H5'    | 2.46                     | 0.46              |
| 12:L:110:VAL:O   | 12:L:122:THR:CG2  | 2.63                     | 0.46              |
| 10:J:8:LEU:HB2   | 10:J:70:ARG:CB    | 2.29                     | 0.46              |
| 1:A:1285:G:C6    | 1:A:1286:G:N1     | 2.83                     | 0.46              |
| 10:J:35:SER:HB3  | 10:J:72:VAL:O     | 2.16                     | 0.46              |
| 3:C:15:THR:HB    | 3:C:181:ASN:HB2   | 1.98                     | 0.46              |
| 20:T:54:LYS:H    | 20:T:100:ILE:HD12 | 1.79                     | 0.46              |
| 12:L:82:VAL:HG22 | 12:L:106:ASP:OD1  | 2.16                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:108:ASN:OD1   | 3:C:144:SER:HB2   | 2.15                     | 0.46              |
| 1:A:485:G:C2      | 1:A:486:C:C2      | 3.04                     | 0.46              |
| 12:L:33:ARG:HB3   | 12:L:60:LEU:HD12  | 1.97                     | 0.46              |
| 2:B:142:LEU:C     | 2:B:142:LEU:HD23  | 2.37                     | 0.46              |
| 1:A:1299:A:H4'    | 19:S:10:PHE:CD1   | 2.51                     | 0.46              |
| 1:A:926:A:C2      | 1:A:1214:G:N3     | 2.84                     | 0.46              |
| 20:T:41:VAL:O     | 20:T:45:GLN:HB2   | 2.16                     | 0.46              |
| 13:M:59:TYR:O     | 13:M:63:THR:CG2   | 2.63                     | 0.46              |
| 4:D:150:GLU:C     | 4:D:152:SER:H     | 2.19                     | 0.46              |
| 1:A:143:A:H2'     | 1:A:144:C:H6      | 1.81                     | 0.46              |
| 1:A:777:A:H2'     | 1:A:778:C:O4'     | 2.16                     | 0.46              |
| 1:A:1463:G:H2'    | 1:A:1464:G:O4'    | 2.15                     | 0.46              |
| 8:H:20:TYR:CE1    | 8:H:76:PRO:HD2    | 2.51                     | 0.46              |
| 1:A:238:A:C2      | 1:A:241:A:C8      | 3.04                     | 0.45              |
| 20:T:50:GLU:HG2   | 20:T:100:ILE:HG12 | 1.97                     | 0.45              |
| 3:C:108:ASN:ND2   | 3:C:110:ASN:HB2   | 2.31                     | 0.45              |
| 2:B:55:PHE:CE1    | 2:B:218:ALA:HA    | 2.50                     | 0.45              |
| 14:N:12:ARG:C     | 14:N:14:PRO:CD    | 2.85                     | 0.45              |
| 1:A:1461:C:H3'    | 1:A:1461:C:H6     | 1.80                     | 0.45              |
| 10:J:38:ILE:HB    | 10:J:71:LEU:CB    | 2.46                     | 0.45              |
| 1:A:919:G:O2'     | 1:A:920:U:H5'     | 2.16                     | 0.45              |
| 1:A:1294:U:H5     | 19:S:4:SER:HB2    | 1.81                     | 0.45              |
| 13:M:29:ARG:HB3   | 13:M:64:TRP:CH2   | 2.51                     | 0.45              |
| 3:C:34:LEU:O      | 3:C:34:LEU:HD23   | 2.14                     | 0.45              |
| 1:A:246:G:H5'     | 1:A:247:U:OP1     | 2.16                     | 0.45              |
| 1:A:1288:U:C5'    | 13:M:109:THR:HG21 | 2.47                     | 0.45              |
| 2:B:7:VAL:CG1     | 2:B:221:LEU:HD11  | 2.47                     | 0.45              |
| 1:A:1042:C:H4'    | 10:J:52:GLY:H     | 1.81                     | 0.45              |
| 2:B:50:GLU:HB3    | 2:B:200:ILE:O     | 2.16                     | 0.45              |
| 1:A:516:A:C2      | 1:A:519:C:C5      | 3.04                     | 0.45              |
| 21:V:3:LYS:H      | 21:V:3:LYS:CD     | 2.28                     | 0.45              |
| 4:D:24:GLU:OE1    | 4:D:25:ARG:N      | 2.45                     | 0.45              |
| 4:D:64:LEU:HD23   | 4:D:64:LEU:O      | 2.15                     | 0.45              |
| 6:F:12:PRO:HG3    | 6:F:55:ASP:CG     | 2.36                     | 0.45              |
| 1:A:438:C:H2'     | 1:A:439:G:H8      | 1.82                     | 0.45              |
| 3:C:19:GLU:OE1    | 14:N:52:GLN:HG3   | 2.16                     | 0.45              |
| 4:D:200:GLU:OE1   | 4:D:200:GLU:N     | 2.43                     | 0.45              |
| 13:M:114:ARG:HH11 | 13:M:114:ARG:HG2  | 1.81                     | 0.45              |
| 1:A:315:C:H2'     | 1:A:316:A:C8      | 2.51                     | 0.45              |
| 2:B:86:GLU:C      | 2:B:88:ALA:N      | 2.67                     | 0.45              |
| 1:A:1237:A:H2'    | 1:A:1238:U:C5'    | 2.45                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1217:A:H4'   | 1:A:1285:G:H4'   | 1.97                     | 0.45              |
| 1:A:1082:C:C3'   | 1:A:1082:C:H6    | 2.24                     | 0.45              |
| 12:L:53:ARG:HH12 | 12:L:92:ASP:HB2  | 1.81                     | 0.45              |
| 1:A:1049:A:C4'   | 1:A:1050:G:O5'   | 2.59                     | 0.45              |
| 8:H:91:ARG:CG    | 12:L:7:ILE:HG13  | 2.44                     | 0.45              |
| 4:D:201:GLN:OE1  | 4:D:201:GLN:HA   | 2.16                     | 0.45              |
| 1:A:1349:C:C5'   | 10:J:60:ARG:NH1  | 2.79                     | 0.45              |
| 1:A:424:U:HO2'   | 1:A:425:A:P      | 2.39                     | 0.45              |
| 1:A:1297:G:H22   | 1:A:1299:A:H3'   | 1.80                     | 0.45              |
| 1:A:41:G:H2'     | 1:A:42:G:H8      | 1.80                     | 0.45              |
| 11:K:21:ILE:HD13 | 11:K:94:ALA:HB3  | 1.99                     | 0.45              |
| 16:P:53:VAL:O    | 16:P:57:ARG:HG3  | 2.17                     | 0.45              |
| 2:B:25:ASN:O     | 2:B:26:PRO:C     | 2.55                     | 0.45              |
| 20:T:43:LEU:HB3  | 20:T:48:LYS:HB2  | 1.97                     | 0.45              |
| 1:A:689:A:O4'    | 11:K:29:ILE:HD11 | 2.16                     | 0.45              |
| 1:A:198:U:C1'    | 20:T:103:GLY:HA2 | 2.43                     | 0.45              |
| 12:L:7:ILE:O     | 12:L:11:VAL:HG23 | 2.16                     | 0.45              |
| 1:A:190:G:H4'    | 1:A:191:G:OP2    | 2.17                     | 0.45              |
| 9:I:4:TYR:CE1    | 9:I:88:TYR:HD1   | 2.35                     | 0.45              |
| 3:C:29:TYR:C     | 3:C:29:TYR:CD2   | 2.90                     | 0.45              |
| 1:A:408:G:H2'    | 1:A:423:G:N2     | 2.32                     | 0.45              |
| 7:G:23:VAL:HG13  | 7:G:43:PHE:CE2   | 2.52                     | 0.45              |
| 13:M:33:ALA:HA   | 13:M:59:TYR:CE2  | 2.50                     | 0.45              |
| 1:A:504:G:OP1    | 12:L:73:GLU:O    | 2.34                     | 0.45              |
| 5:E:92:LYS:HB3   | 5:E:119:LEU:HB2  | 1.99                     | 0.45              |
| 1:A:568:G:N3     | 1:A:856:C:H4'    | 2.31                     | 0.45              |
| 1:A:965:G:H22    | 1:A:1199:C:H1'   | 1.81                     | 0.45              |
| 1:A:743:G:O2'    | 17:Q:98:LEU:HD22 | 2.17                     | 0.45              |
| 2:B:8:LYS:HB2    | 2:B:9:GLU:H      | 1.46                     | 0.45              |
| 2:B:71:VAL:O     | 2:B:71:VAL:HG23  | 2.17                     | 0.45              |
| 2:B:19:HIS:HA    | 2:B:39:ILE:CG2   | 2.46                     | 0.45              |
| 1:A:297:G:H5''   | 12:L:17:LYS:CE   | 2.44                     | 0.45              |
| 1:A:1112:A:O2'   | 9:I:3:GLN:NE2    | 2.50                     | 0.45              |
| 1:A:824:U:H6     | 1:A:825:C:H1'    | 1.81                     | 0.45              |
| 3:C:33:LEU:HD21  | 14:N:53:LEU:HD22 | 1.99                     | 0.45              |
| 18:R:29:PHE:CE1  | 18:R:31:LEU:HG   | 2.51                     | 0.45              |
| 1:A:748:G:H22    | 1:A:795:C:HO2'   | 1.63                     | 0.45              |
| 15:O:56:LEU:O    | 15:O:60:VAL:HG23 | 2.16                     | 0.45              |
| 1:A:160:G:H2'    | 1:A:161:G:H8     | 1.82                     | 0.45              |
| 20:T:77:ALA:O    | 20:T:80:ARG:HB2  | 2.17                     | 0.45              |
| 1:A:1030:G:H5''  | 14:N:3:ARG:HG3   | 1.97                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:131:PRO:O    | 2:B:135:GLN:HB2  | 2.16                     | 0.45              |
| 1:A:903:G:H3'    | 1:A:1482:G:N2    | 2.31                     | 0.45              |
| 9:I:3:GLN:HB3    | 9:I:20:ARG:HB3   | 1.98                     | 0.45              |
| 10:J:53:PRO:HA   | 14:N:41:ARG:NH2  | 2.29                     | 0.45              |
| 10:J:50:ILE:HG12 | 10:J:60:ARG:HE   | 1.81                     | 0.45              |
| 3:C:203:PHE:C    | 3:C:204:LEU:HD23 | 2.36                     | 0.45              |
| 9:I:5:TYR:CD1    | 9:I:6:GLY:N      | 2.84                     | 0.45              |
| 6:F:23:LYS:NZ    | 6:F:42:GLU:OE2   | 2.40                     | 0.45              |
| 13:M:96:LEU:HB3  | 13:M:97:PRO:HD2  | 1.98                     | 0.45              |
| 5:E:5:ASP:CG     | 5:E:6:PHE:H      | 2.20                     | 0.45              |
| 1:A:1371:C:H2'   | 1:A:1372:U:O4'   | 2.17                     | 0.45              |
| 23:X:31:A:H3'    | 23:X:32:C:C6     | 2.51                     | 0.45              |
| 6:F:15:ASP:OD1   | 6:F:18:GLN:HB2   | 2.16                     | 0.45              |
| 1:A:1086:G:OP1   | 2:B:111:ARG:HD2  | 2.17                     | 0.45              |
| 1:A:1509:U:H2'   | 1:A:1510:C:C4'   | 2.47                     | 0.45              |
| 7:G:15:ASP:CB    | 7:G:20:ASP:N     | 2.80                     | 0.45              |
| 1:A:1133:A:H4'   | 1:A:1134:A:OP1   | 2.17                     | 0.45              |
| 1:A:268:A:N6     | 1:A:269:A:C6     | 2.85                     | 0.45              |
| 5:E:31:LEU:HD23  | 5:E:45:PHE:HB2   | 1.98                     | 0.45              |
| 1:A:431:C:H2'    | 1:A:432:U:C6     | 2.52                     | 0.45              |
| 3:C:19:GLU:OE2   | 3:C:54:ARG:HD2   | 2.17                     | 0.45              |
| 1:A:278:C:O2'    | 1:A:279:G:H5'    | 2.17                     | 0.45              |
| 1:A:501:C:C4     | 1:A:513:G:C2     | 3.04                     | 0.45              |
| 1:A:934:U:H3     | 1:A:937:U:H5''   | 1.80                     | 0.45              |
| 8:H:104:ARG:O    | 8:H:106:GLY:N    | 2.49                     | 0.45              |
| 1:A:337:C:H2'    | 1:A:338:U:C5'    | 2.45                     | 0.45              |
| 1:A:562:G:H2'    | 1:A:563:U:C6     | 2.51                     | 0.45              |
| 1:A:562:G:H1     | 1:A:745:C:H42    | 1.65                     | 0.45              |
| 1:A:1133:A:O2'   | 1:A:1134:A:C8    | 2.70                     | 0.45              |
| 19:S:40:ILE:O    | 19:S:67:VAL:O    | 2.35                     | 0.45              |
| 7:G:36:LYS:O     | 7:G:39:ALA:HB3   | 2.17                     | 0.45              |
| 20:T:24:LEU:HD12 | 20:T:27:LYS:HE3  | 1.97                     | 0.45              |
| 1:A:705:A:O2'    | 1:A:706:U:H3'    | 2.16                     | 0.45              |
| 6:F:9:VAL:HA     | 6:F:59:TYR:O     | 2.16                     | 0.45              |
| 17:Q:76:LEU:HD23 | 17:Q:76:LEU:C    | 2.37                     | 0.45              |
| 11:K:122:LYS:O   | 11:K:123:LYS:C   | 2.55                     | 0.45              |
| 17:Q:67:LYS:HG2  | 17:Q:68:ARG:N    | 2.32                     | 0.45              |
| 3:C:84:ILE:HG13  | 3:C:88:ARG:CZ    | 2.47                     | 0.45              |
| 1:A:123:G:C5     | 1:A:191:G:H1'    | 2.51                     | 0.45              |
| 19:S:42:PRO:O    | 19:S:44:MET:N    | 2.50                     | 0.45              |
| 1:A:801:G:O2'    | 1:A:803:U:H5     | 2.00                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:33:LEU:HD11  | 14:N:53:LEU:HD23 | 1.99                     | 0.45              |
| 9:I:43:ALA:N     | 9:I:74:ILE:HD13  | 2.32                     | 0.45              |
| 1:A:484:C:O3'    | 12:L:118:SER:HB2 | 2.16                     | 0.45              |
| 1:A:1297:G:C2    | 1:A:1299:A:H5''  | 2.52                     | 0.45              |
| 1:A:83:A:H2'     | 1:A:84:C:H5'     | 1.98                     | 0.45              |
| 4:D:64:LEU:HD23  | 4:D:64:LEU:C     | 2.37                     | 0.45              |
| 2:B:27:LYS:HD3   | 2:B:195:ASP:OD2  | 2.17                     | 0.45              |
| 1:A:707:G:O2'    | 1:A:708:G:H5'    | 2.16                     | 0.45              |
| 20:T:30:LYS:O    | 20:T:31:SER:C    | 2.55                     | 0.45              |
| 5:E:81:GLU:OE1   | 5:E:88:LYS:HE2   | 2.17                     | 0.45              |
| 20:T:50:GLU:HG2  | 20:T:100:ILE:CG1 | 2.47                     | 0.45              |
| 1:A:257:A:C6     | 1:A:258:A:C6     | 3.04                     | 0.45              |
| 9:I:59:PHE:HZ    | 9:I:88:TYR:CG    | 2.35                     | 0.45              |
| 16:P:19:ILE:HG22 | 16:P:36:ILE:CG1  | 2.47                     | 0.45              |
| 19:S:9:VAL:CG1   | 19:S:10:PHE:N    | 2.80                     | 0.45              |
| 4:D:31:CYS:O     | 4:D:33:MET:N     | 2.46                     | 0.45              |
| 7:G:62:PHE:HD1   | 7:G:124:LEU:HD21 | 1.82                     | 0.45              |
| 12:L:44:THR:HA   | 12:L:45:PRO:HD3  | 1.85                     | 0.45              |
| 1:A:731:C:H4'    | 1:A:732:C:O5'    | 2.17                     | 0.45              |
| 1:A:591:A:H2'    | 1:A:592:A:H5'    | 1.99                     | 0.45              |
| 1:A:5:U:O2'      | 1:A:6:G:OP2      | 2.30                     | 0.45              |
| 3:C:7:PRO:HG2    | 3:C:184:TYR:HB2  | 2.00                     | 0.45              |
| 1:A:982:A:N7     | 1:A:1019:C:C2    | 2.86                     | 0.44              |
| 1:A:1043:G:H1'   | 10:J:56:HIS:CE1  | 2.52                     | 0.44              |
| 2:B:39:ILE:HG22  | 2:B:40:HIS:N     | 2.32                     | 0.44              |
| 20:T:57:ARG:HD2  | 20:T:102:GLY:HA3 | 1.99                     | 0.44              |
| 17:Q:63:ARG:O    | 17:Q:65:ILE:HD12 | 2.17                     | 0.44              |
| 13:M:84:ILE:C    | 13:M:86:CYS:N    | 2.71                     | 0.44              |
| 1:A:64:G:O2'     | 1:A:65:U:OP2     | 2.29                     | 0.44              |
| 1:A:378:A:H2'    | 1:A:379:G:H5'    | 2.00                     | 0.44              |
| 1:A:261:G:H5'    | 1:A:262:C:OP1    | 2.17                     | 0.44              |
| 1:A:922:G:H21    | 1:A:1315:G:H4'   | 1.81                     | 0.44              |
| 1:A:740:U:H2'    | 1:A:741:G:O4'    | 2.16                     | 0.44              |
| 1:A:1006:C:N4    | 1:A:1007:C:C4    | 2.85                     | 0.44              |
| 1:A:984:C:C2'    | 1:A:985:C:C6     | 2.75                     | 0.44              |
| 1:A:1301:C:C2    | 19:S:72:GLY:HA3  | 2.52                     | 0.44              |
| 2:B:102:LEU:CD1  | 2:B:102:LEU:N    | 2.80                     | 0.44              |
| 5:E:145:LYS:HA   | 8:H:107:LEU:CD2  | 2.46                     | 0.44              |
| 2:B:101:MET:O    | 2:B:105:PHE:HA   | 2.17                     | 0.44              |
| 3:C:51:GLY:O     | 3:C:52:LEU:HB3   | 2.16                     | 0.44              |
| 13:M:11:ARG:CG   | 13:M:12:ASN:N    | 2.78                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:398:C:O2'    | 1:A:399:U:H5'    | 2.18                     | 0.44              |
| 9:I:55:ALA:O     | 9:I:56:LEU:HB2   | 2.17                     | 0.44              |
| 20:T:12:ALA:O    | 20:T:15:ARG:HB2  | 2.18                     | 0.44              |
| 4:D:28:SER:O     | 4:D:30:LYS:N     | 2.51                     | 0.44              |
| 1:A:565:U:C2     | 1:A:743:G:C6     | 3.05                     | 0.44              |
| 17:Q:66:SER:OG   | 17:Q:69:LYS:HB2  | 2.17                     | 0.44              |
| 2:B:7:VAL:HG21   | 2:B:8:LYS:HZ3    | 1.81                     | 0.44              |
| 1:A:1126:G:C8    | 1:A:1126:G:C3'   | 3.00                     | 0.44              |
| 5:E:75:THR:HG23  | 5:E:76:ILE:O     | 2.18                     | 0.44              |
| 1:A:1231:A:H5''  | 9:I:68:GLY:N     | 2.32                     | 0.44              |
| 3:C:191:THR:HG22 | 3:C:192:THR:N    | 2.32                     | 0.44              |
| 2:B:15:VAL:HG12  | 2:B:209:ARG:O    | 2.17                     | 0.44              |
| 1:A:1134:A:H2'   | 1:A:1135:C:H6    | 1.82                     | 0.44              |
| 12:L:60:LEU:CD2  | 12:L:66:VAL:HG22 | 2.47                     | 0.44              |
| 1:A:362:U:C6     | 1:A:389:G:N2     | 2.85                     | 0.44              |
| 1:A:630:C:H2'    | 1:A:631:A:H8     | 1.83                     | 0.44              |
| 7:G:61:VAL:HG23  | 7:G:62:PHE:N     | 2.33                     | 0.44              |
| 1:A:1218:C:H4'   | 1:A:1315:G:N2    | 2.31                     | 0.44              |
| 1:A:100:G:C3'    | 1:A:101:G:H5''   | 2.47                     | 0.44              |
| 1:A:501:C:OP2    | 1:A:513:G:H1'    | 2.17                     | 0.44              |
| 8:H:64:LYS:HG2   | 8:H:79:VAL:CG2   | 2.41                     | 0.44              |
| 1:A:167:U:H5''   | 1:A:203:A:O4'    | 2.18                     | 0.44              |
| 1:A:915:A:N6     | 1:A:916:G:C6     | 2.86                     | 0.44              |
| 5:E:137:GLU:HG2  | 5:E:140:ARG:HH12 | 1.82                     | 0.44              |
| 7:G:28:ASN:O     | 7:G:31:MET:HB3   | 2.18                     | 0.44              |
| 13:M:60:VAL:HG12 | 13:M:66:LEU:HD11 | 1.98                     | 0.44              |
| 11:K:87:THR:HG23 | 11:K:91:ARG:HH22 | 1.79                     | 0.44              |
| 3:C:64:VAL:HG12  | 3:C:66:VAL:CG2   | 2.44                     | 0.44              |
| 1:A:1163:G:C8    | 1:A:1163:G:O5'   | 2.70                     | 0.44              |
| 5:E:74:GLY:HA3   | 5:E:116:THR:HG22 | 2.00                     | 0.44              |
| 6:F:10:LEU:H     | 6:F:10:LEU:HG    | 1.65                     | 0.44              |
| 4:D:60:GLU:OE2   | 4:D:198:VAL:HA   | 2.17                     | 0.44              |
| 12:L:47:LYS:HB3  | 12:L:48:PRO:HD3  | 1.99                     | 0.44              |
| 1:A:1095:C:H1'   | 3:C:178:LEU:HD21 | 1.99                     | 0.44              |
| 1:A:1203:G:P     | 19:S:77:THR:HG21 | 2.57                     | 0.44              |
| 2:B:115:LEU:HD21 | 2:B:153:ARG:CZ   | 2.48                     | 0.44              |
| 18:R:59:SER:O    | 18:R:61:LYS:N    | 2.51                     | 0.44              |
| 1:A:1168:G:OP1   | 9:I:113:LYS:NZ   | 2.51                     | 0.44              |
| 19:S:12:ASP:HB3  | 19:S:14:HIS:CD2  | 2.52                     | 0.44              |
| 1:A:1238:U:O2'   | 1:A:1239:G:P     | 2.76                     | 0.44              |
| 10:J:24:VAL:HG13 | 10:J:28:ARG:HH12 | 1.83                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 10:J:34:VAL:HG13 | 10:J:74:ILE:HG22 | 1.99                     | 0.44              |
| 12:L:53:ARG:NH1  | 12:L:53:ARG:HG2  | 2.33                     | 0.44              |
| 7:G:18:TYR:HD1   | 7:G:59:LEU:HD22  | 1.80                     | 0.44              |
| 1:A:407:A:C2     | 4:D:35:ARG:HG3   | 2.52                     | 0.44              |
| 9:I:3:GLN:CB     | 9:I:20:ARG:HB3   | 2.48                     | 0.44              |
| 1:A:801:G:C3'    | 1:A:802:A:H5'    | 2.48                     | 0.44              |
| 1:A:408:G:N2     | 1:A:423:G:H1'    | 2.32                     | 0.44              |
| 1:A:364:C:O2     | 1:A:388:A:C2     | 2.70                     | 0.44              |
| 1:A:1068:U:H3    | 1:A:1081:G:H22   | 1.65                     | 0.44              |
| 2:B:61:LEU:CD2   | 2:B:66:GLY:HA3   | 2.47                     | 0.44              |
| 3:C:126:ARG:NH1  | 3:C:126:ARG:HG3  | 2.32                     | 0.44              |
| 5:E:143:ARG:NH1  | 8:H:77:GLU:CD    | 2.71                     | 0.44              |
| 1:A:175:G:H4'    | 1:A:176:U:H5'    | 1.97                     | 0.44              |
| 8:H:75:ARG:HA    | 8:H:76:PRO:HD3   | 1.78                     | 0.44              |
| 3:C:113:ALA:N    | 3:C:114:PRO:CD   | 2.81                     | 0.44              |
| 3:C:113:ALA:HB3  | 3:C:114:PRO:HD3  | 2.00                     | 0.44              |
| 6:F:61:LEU:O     | 6:F:62:TRP:HB2   | 2.16                     | 0.44              |
| 1:A:502:C:H2'    | 1:A:503:A:O4'    | 2.17                     | 0.44              |
| 2:B:145:LEU:O    | 2:B:149:LEU:HB2  | 2.18                     | 0.44              |
| 8:H:123:GLU:O    | 8:H:127:LEU:HD23 | 2.18                     | 0.44              |
| 9:I:19:LEU:HB3   | 9:I:59:PHE:CD2   | 2.53                     | 0.44              |
| 10:J:47:PHE:CE2  | 14:N:37:PHE:CE1  | 2.98                     | 0.44              |
| 1:A:470:U:O2'    | 1:A:471:A:H5'    | 2.17                     | 0.44              |
| 1:A:1426:A:O2'   | 1:A:1427:G:OP1   | 2.35                     | 0.44              |
| 5:E:82:VAL:HB    | 5:E:138:ALA:HB2  | 1.99                     | 0.44              |
| 3:C:178:LEU:O    | 3:C:179:ARG:HB2  | 2.18                     | 0.44              |
| 1:A:492:A:H5'    | 4:D:54:TYR:HD2   | 1.81                     | 0.44              |
| 1:A:731:C:H1'    | 1:A:732:C:H5     | 1.83                     | 0.44              |
| 7:G:21:VAL:HG23  | 7:G:22:LEU:N     | 2.32                     | 0.44              |
| 1:A:1037:A:H8    | 1:A:1037:A:H5'   | 1.83                     | 0.44              |
| 2:B:81:VAL:O     | 2:B:85:ALA:HB2   | 2.18                     | 0.44              |
| 4:D:98:GLU:CD    | 4:D:107:ARG:HH21 | 2.20                     | 0.44              |
| 4:D:3:ARG:O      | 4:D:4:TYR:CB     | 2.66                     | 0.44              |
| 1:A:1112:A:H3'   | 1:A:1113:G:C8    | 2.52                     | 0.44              |
| 1:A:350:C:O4'    | 1:A:383:G:O2'    | 2.31                     | 0.44              |
| 5:E:69:VAL:HG21  | 5:E:113:ALA:HB1  | 1.99                     | 0.44              |
| 1:A:1210:A:H2'   | 1:A:1211:C:C6    | 2.52                     | 0.44              |
| 1:A:55:A:O2'     | 1:A:56:U:H5'     | 2.18                     | 0.44              |
| 3:C:182:ILE:HA   | 3:C:202:ILE:O    | 2.17                     | 0.44              |
| 4:D:166:LYS:HG3  | 4:D:178:VAL:HG11 | 1.98                     | 0.44              |
| 16:P:6:LEU:N     | 16:P:6:LEU:HD12  | 2.33                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 23:X:36:U:C2'    | 23:X:37:12A:C5'   | 2.86                     | 0.44              |
| 1:A:565:U:OP1    | 15:O:64:ARG:NH1   | 2.51                     | 0.44              |
| 1:A:1083:A:C8    | 2:B:172:ILE:HD13  | 2.53                     | 0.44              |
| 14:N:27:CYS:SG   | 14:N:29:ARG:HB2   | 2.58                     | 0.44              |
| 14:N:23:ARG:C    | 14:N:33:VAL:HG11  | 2.37                     | 0.44              |
| 1:A:209:U:C4'    | 1:A:210:U:OP1     | 2.65                     | 0.44              |
| 12:L:83:VAL:HG22 | 12:L:84:LEU:H     | 1.82                     | 0.44              |
| 1:A:520:G:H5''   | 12:L:113:ARG:HH21 | 1.82                     | 0.44              |
| 1:A:82:U:H6      | 1:A:82:U:H3'      | 1.83                     | 0.44              |
| 3:C:10:PHE:CZ    | 3:C:178:LEU:HD13  | 2.53                     | 0.44              |
| 10:J:87:THR:O    | 10:J:88:LEU:HG    | 2.17                     | 0.44              |
| 13:M:108:ARG:O   | 13:M:112:GLY:N    | 2.51                     | 0.44              |
| 1:A:1091:C:OP2   | 3:C:176:HIS:CD2   | 2.71                     | 0.44              |
| 14:N:45:ARG:HG3  | 14:N:45:ARG:HH11  | 1.82                     | 0.44              |
| 2:B:91:PRO:HG2   | 2:B:155:LEU:HG    | 2.00                     | 0.44              |
| 1:A:635:U:HO2'   | 1:A:636:A:P       | 2.41                     | 0.44              |
| 14:N:61:TRP:N    | 14:N:61:TRP:CE3   | 2.85                     | 0.44              |
| 17:Q:65:ILE:N    | 17:Q:65:ILE:CD1   | 2.81                     | 0.44              |
| 9:I:20:ARG:O     | 9:I:21:PRO:C      | 2.56                     | 0.44              |
| 9:I:27:THR:HG22  | 9:I:28:VAL:N      | 2.32                     | 0.44              |
| 17:Q:76:LEU:HD21 | 17:Q:78:GLU:C     | 2.38                     | 0.44              |
| 1:A:1008:C:H2'   | 1:A:1009:G:C8     | 2.53                     | 0.44              |
| 1:A:457:A:O4'    | 16:P:82:GLN:NE2   | 2.38                     | 0.44              |
| 20:T:14:LYS:HE2  | 20:T:18:GLN:NE2   | 2.32                     | 0.44              |
| 9:I:58:ARG:HH11  | 9:I:58:ARG:HG3    | 1.83                     | 0.44              |
| 23:X:32:C:H2'    | 23:X:33:U:O4'     | 2.18                     | 0.43              |
| 1:A:953:G:H8     | 1:A:1339:U:O2'    | 2.01                     | 0.43              |
| 1:A:349:G:H2'    | 1:A:349:G:N3      | 2.33                     | 0.43              |
| 12:L:52:LEU:O    | 12:L:54:LYS:HD2   | 2.18                     | 0.43              |
| 2:B:69:LEU:HD23  | 2:B:69:LEU:C      | 2.39                     | 0.43              |
| 9:I:127:LYS:HB2  | 9:I:127:LYS:HE2   | 1.73                     | 0.43              |
| 9:I:33:PHE:CZ    | 9:I:47:LEU:HD21   | 2.53                     | 0.43              |
| 1:A:505:C:H41    | 12:L:53:ARG:HH22  | 1.61                     | 0.43              |
| 18:R:55:ARG:HB3  | 18:R:55:ARG:HH11  | 1.79                     | 0.43              |
| 14:N:37:PHE:CD2  | 14:N:53:LEU:HD13  | 2.53                     | 0.43              |
| 1:A:324:A:H4'    | 1:A:325:C:OP1     | 2.18                     | 0.43              |
| 1:A:1139:A:O2'   | 1:A:1140:C:OP2    | 2.28                     | 0.43              |
| 4:D:121:VAL:O    | 4:D:134:ASP:HA    | 2.18                     | 0.43              |
| 12:L:86:ARG:HG3  | 12:L:86:ARG:NH1   | 2.32                     | 0.43              |
| 6:F:12:PRO:HG3   | 6:F:55:ASP:OD1    | 2.18                     | 0.43              |
| 13:M:108:ARG:NE  | 13:M:108:ARG:HA   | 2.32                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:92:TYR:CD2   | 2:B:151:GLY:HA3  | 2.53                     | 0.43              |
| 1:A:290:C:H2'    | 1:A:291:U:O4'    | 2.17                     | 0.43              |
| 1:A:463:C:H2'    | 1:A:464:U:O4'    | 2.18                     | 0.43              |
| 1:A:117:G:C6     | 1:A:118:U:C4     | 3.06                     | 0.43              |
| 1:A:1259:U:H5''  | 1:A:1260:A:O4'   | 2.17                     | 0.43              |
| 15:O:17:ARG:NH2  | 15:O:77:ARG:HD3  | 2.33                     | 0.43              |
| 21:V:2:GLY:C     | 21:V:4:GLY:N     | 2.72                     | 0.43              |
| 19:S:22:LEU:HD21 | 19:S:28:LYS:HB2  | 2.00                     | 0.43              |
| 1:A:1046:G:H4'   | 1:A:1047:U:OP1   | 2.17                     | 0.43              |
| 1:A:1049:A:HO2'  | 1:A:1050:G:H8    | 1.63                     | 0.43              |
| 1:A:1049:A:O2'   | 1:A:1050:G:C8    | 2.68                     | 0.43              |
| 3:C:35:GLU:O     | 3:C:36:ASP:C     | 2.56                     | 0.43              |
| 1:A:259:U:O2'    | 17:Q:64:PRO:HB2  | 2.18                     | 0.43              |
| 1:A:1221:U:HO2'  | 1:A:1222:G:P     | 2.39                     | 0.43              |
| 6:F:101:ALA:CB   | 18:R:28:GLU:HG3  | 2.46                     | 0.43              |
| 1:A:1461:C:C6    | 1:A:1461:C:C3'   | 3.00                     | 0.43              |
| 5:E:121:LYS:HD2  | 5:E:121:LYS:HA   | 1.79                     | 0.43              |
| 1:A:831:G:C6     | 1:A:832:G:N7     | 2.86                     | 0.43              |
| 18:R:47:THR:HG22 | 18:R:48:GLY:H    | 1.83                     | 0.43              |
| 4:D:190:ASP:O    | 4:D:191:ARG:C    | 2.56                     | 0.43              |
| 4:D:187:ARG:HG3  | 4:D:188:LEU:N    | 2.34                     | 0.43              |
| 1:A:872:G:H2'    | 1:A:873:C:C6     | 2.52                     | 0.43              |
| 1:A:513:G:OP1    | 1:A:514:U:H5''   | 2.18                     | 0.43              |
| 1:A:1259:U:C5'   | 1:A:1260:A:O4'   | 2.66                     | 0.43              |
| 1:A:169:C:O2'    | 1:A:170:C:H5'    | 2.19                     | 0.43              |
| 1:A:1220:A:H2'   | 1:A:1279:C:H42   | 1.84                     | 0.43              |
| 3:C:65:ALA:O     | 3:C:66:VAL:CB    | 2.67                     | 0.43              |
| 9:I:113:LYS:H    | 9:I:119:ALA:HA   | 1.83                     | 0.43              |
| 11:K:49:GLY:O    | 11:K:50:TYR:C    | 2.57                     | 0.43              |
| 7:G:99:LEU:HA    | 7:G:99:LEU:HD23  | 1.90                     | 0.43              |
| 1:A:670:A:O2'    | 1:A:671:G:OP2    | 2.35                     | 0.43              |
| 9:I:45:ALA:O     | 9:I:48:GLU:N     | 2.38                     | 0.43              |
| 3:C:68:VAL:HG12  | 3:C:70:VAL:HG13  | 2.01                     | 0.43              |
| 14:N:29:ARG:HH22 | 14:N:41:ARG:NH1  | 2.15                     | 0.43              |
| 3:C:132:ARG:HA   | 3:C:135:LYS:HD3  | 1.99                     | 0.43              |
| 1:A:926:A:N7     | 13:M:106:ASN:ND2 | 2.66                     | 0.43              |
| 1:A:832:G:H2'    | 1:A:833:C:C6     | 2.54                     | 0.43              |
| 1:A:82:U:C6      | 1:A:82:U:C3'     | 3.00                     | 0.43              |
| 12:L:89:ARG:HD2  | 12:L:89:ARG:N    | 2.33                     | 0.43              |
| 9:I:40:LEU:O     | 9:I:42:ARG:N     | 2.51                     | 0.43              |
| 19:S:23:ASN:C    | 19:S:25:LYS:H    | 2.22                     | 0.43              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:859:C:O2'   | 1:A:860:C:H5'    | 2.19                     | 0.43              |
| 1:A:627:G:C5    | 1:A:628:C:C5     | 3.07                     | 0.43              |
| 1:A:936:A:HO2'  | 1:A:961:C:HO2'   | 1.67                     | 0.43              |
| 1:A:333:A:H2    | 1:A:346:G:H22    | 1.67                     | 0.43              |
| 10:J:75:ILE:O   | 10:J:76:ASN:CB   | 2.66                     | 0.43              |
| 1:A:1374:G:N2   | 1:A:1479:A:C8    | 2.86                     | 0.43              |
| 3:C:157:ILE:HB  | 3:C:164:ARG:NH2  | 2.32                     | 0.43              |
| 1:A:392:A:H3'   | 1:A:392:A:N3     | 2.34                     | 0.43              |
| 1:A:1109:G:H21  | 1:A:1128:A:N6    | 2.13                     | 0.43              |
| 1:A:1133:A:O2'  | 1:A:1134:A:P     | 2.77                     | 0.43              |
| 2:B:231:GLU:HB3 | 2:B:232:PRO:HD2  | 2.01                     | 0.43              |
| 12:L:113:ARG:O  | 12:L:117:ARG:HG2 | 2.18                     | 0.43              |
| 20:T:16:HIS:NE2 | 20:T:20:LEU:HD21 | 2.34                     | 0.43              |
| 7:G:58:PRO:HA   | 7:G:61:VAL:HG22  | 2.00                     | 0.43              |
| 1:A:114:C:C4'   | 1:A:115:G:OP1    | 2.65                     | 0.43              |
| 12:L:89:ARG:N   | 12:L:89:ARG:CD   | 2.81                     | 0.43              |
| 20:T:94:ALA:O   | 20:T:95:ALA:HB3  | 2.19                     | 0.43              |
| 13:M:6:GLY:O    | 13:M:7:VAL:HG22  | 2.18                     | 0.43              |
| 1:A:752:G:H4'   | 1:A:1490:A:H4'   | 1.99                     | 0.43              |
| 1:A:985:C:H6    | 1:A:985:C:O5'    | 2.00                     | 0.43              |
| 9:I:116:LYS:O   | 9:I:117:HIS:C    | 2.56                     | 0.43              |
| 1:A:1281:G:O2'  | 1:A:1282:U:P     | 2.75                     | 0.43              |
| 13:M:65:LYS:HD3 | 13:M:69:GLU:HG2  | 1.99                     | 0.43              |
| 1:A:484:C:H2'   | 1:A:485:G:C8     | 2.52                     | 0.43              |
| 4:D:31:CYS:C    | 4:D:33:MET:N     | 2.68                     | 0.43              |
| 1:A:53:A:N6     | 1:A:54:C:C4      | 2.85                     | 0.43              |
| 1:A:143:A:H2'   | 1:A:144:C:C6     | 2.53                     | 0.43              |
| 1:A:1216:U:H2'  | 1:A:1217:A:O4'   | 2.19                     | 0.43              |
| 1:A:723:U:O2'   | 1:A:724:G:H5'    | 2.18                     | 0.43              |
| 2:B:69:LEU:HD22 | 2:B:71:VAL:HG13  | 1.99                     | 0.43              |
| 1:A:736:A:C4'   | 1:A:737:C:O5'    | 2.58                     | 0.43              |
| 5:E:83:GLU:HG3  | 5:E:88:LYS:HG3   | 2.00                     | 0.43              |
| 16:P:74:LEU:CG  | 16:P:79:VAL:HG21 | 2.41                     | 0.43              |
| 4:D:34:GLU:O    | 4:D:35:ARG:CB    | 2.60                     | 0.43              |
| 1:A:270:G:H5'   | 17:Q:14:LYS:HB3  | 2.00                     | 0.43              |
| 1:A:780:C:OP1   | 11:K:124:LYS:CE  | 2.64                     | 0.43              |
| 1:A:1504:C:O2'  | 1:A:1505:U:H5'   | 2.19                     | 0.43              |
| 15:O:82:ILE:O   | 15:O:85:LEU:N    | 2.51                     | 0.43              |
| 2:B:61:LEU:O    | 2:B:61:LEU:HD22  | 2.18                     | 0.43              |
| 12:L:65:GLU:N   | 12:L:65:GLU:OE1  | 2.52                     | 0.43              |
| 1:A:1384:C:C5   | 1:A:1385:C:C5    | 3.07                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:35:GLY:HA2   | 5:E:40:ARG:O     | 2.19                     | 0.43              |
| 1:A:608:G:H2'    | 1:A:609:U:C6     | 2.54                     | 0.43              |
| 19:S:11:VAL:HG13 | 19:S:38:SER:HB2  | 1.99                     | 0.43              |
| 1:A:1029:G:C2'   | 1:A:1030:G:H5'   | 2.49                     | 0.43              |
| 1:A:501:C:O2'    | 12:L:50:SER:HB3  | 2.18                     | 0.43              |
| 1:A:636:A:OP1    | 8:H:56:LYS:NZ    | 2.49                     | 0.43              |
| 3:C:73:PRO:O     | 3:C:75:VAL:N     | 2.51                     | 0.43              |
| 19:S:40:ILE:HD13 | 19:S:62:ILE:HD13 | 2.00                     | 0.43              |
| 3:C:23:TYR:CG    | 3:C:24:ALA:N     | 2.86                     | 0.43              |
| 2:B:114:ARG:NE   | 2:B:118:LEU:HD11 | 2.34                     | 0.43              |
| 18:R:48:GLY:O    | 18:R:74:ARG:NH2  | 2.52                     | 0.43              |
| 15:O:33:THR:HG23 | 15:O:63:ARG:NH1  | 2.34                     | 0.43              |
| 4:D:149:ALA:HB3  | 4:D:152:SER:HB2  | 2.01                     | 0.43              |
| 5:E:36:ASP:OD2   | 5:E:40:ARG:HD3   | 2.18                     | 0.43              |
| 7:G:64:GLN:HG3   | 7:G:68:ASN:ND2   | 2.34                     | 0.43              |
| 1:A:888:U:H2'    | 1:A:889:C:C6     | 2.53                     | 0.43              |
| 19:S:43:GLU:O    | 19:S:43:GLU:HG2  | 2.18                     | 0.43              |
| 2:B:76:GLN:O     | 2:B:208:ILE:HG12 | 2.19                     | 0.43              |
| 2:B:81:VAL:O     | 2:B:81:VAL:CG1   | 2.66                     | 0.43              |
| 9:I:14:VAL:O     | 9:I:65:VAL:HG23  | 2.18                     | 0.43              |
| 2:B:111:ARG:HB3  | 2:B:149:LEU:HD11 | 2.00                     | 0.43              |
| 3:C:15:THR:O     | 3:C:16:ARG:CB    | 2.58                     | 0.43              |
| 1:A:385:C:O3'    | 16:P:28:ARG:NH2  | 2.52                     | 0.43              |
| 2:B:209:ARG:NH1  | 2:B:239:VAL:HG21 | 2.34                     | 0.43              |
| 1:A:562:G:H5'    | 1:A:711:A:C1'    | 2.42                     | 0.43              |
| 13:M:15:VAL:HG21 | 13:M:48:LEU:HD21 | 2.00                     | 0.43              |
| 7:G:148:ASN:N    | 7:G:148:ASN:HD22 | 2.08                     | 0.43              |
| 1:A:1133:A:C2'   | 1:A:1134:A:C8    | 3.02                     | 0.43              |
| 1:A:915:A:C6     | 1:A:916:G:C5     | 3.07                     | 0.43              |
| 5:E:28:PHE:O     | 5:E:47:LYS:HA    | 2.18                     | 0.43              |
| 1:A:399:U:H2'    | 1:A:400:U:C6     | 2.53                     | 0.43              |
| 15:O:76:GLU:C    | 15:O:78:TYR:N    | 2.72                     | 0.43              |
| 1:A:625:A:N7     | 8:H:115:SER:HA   | 2.34                     | 0.43              |
| 12:L:119:LYS:O   | 12:L:120:TYR:CB  | 2.67                     | 0.43              |
| 12:L:8:ASN:OD1   | 17:Q:34:LYS:HE2  | 2.19                     | 0.43              |
| 1:A:197:G:H22    | 20:T:85:MET:HE3  | 1.84                     | 0.43              |
| 20:T:67:ALA:O    | 20:T:73:HIS:CE1  | 2.72                     | 0.43              |
| 2:B:88:ALA:C     | 2:B:90:MET:N     | 2.70                     | 0.43              |
| 8:H:104:ARG:O    | 8:H:107:LEU:N    | 2.46                     | 0.43              |
| 1:A:1099:G:O3'   | 9:I:104:ARG:NH1  | 2.52                     | 0.43              |
| 1:A:340:C:H4'    | 1:A:341:G:O5'    | 2.18                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:407:A:C2      | 4:D:35:ARG:HB3   | 2.54                     | 0.43              |
| 1:A:198:U:H1'     | 20:T:103:GLY:CA  | 2.45                     | 0.43              |
| 4:D:199:ASN:C     | 4:D:199:ASN:ND2  | 2.71                     | 0.43              |
| 16:P:19:ILE:HG22  | 16:P:36:ILE:HG13 | 2.01                     | 0.43              |
| 14:N:24:CYS:SG    | 14:N:40:CYS:N    | 2.92                     | 0.43              |
| 1:A:867:G:O2'     | 1:A:868:U:OP2    | 2.23                     | 0.43              |
| 1:A:1298:C:H2'    | 1:A:1299:A:O4'   | 2.18                     | 0.43              |
| 1:A:328:G:O2'     | 1:A:329:C:H5'    | 2.19                     | 0.43              |
| 1:A:402:G:H2'     | 1:A:403:A:H8     | 1.83                     | 0.43              |
| 1:A:1293:G:O6     | 19:S:4:SER:HB3   | 2.18                     | 0.43              |
| 2:B:92:TYR:O      | 2:B:151:GLY:HA3  | 2.19                     | 0.43              |
| 9:I:89:ASN:O      | 9:I:92:TYR:HB2   | 2.18                     | 0.43              |
| 1:A:869:A:C2      | 1:A:884:A:C4     | 3.07                     | 0.43              |
| 17:Q:84:LEU:O     | 17:Q:85:VAL:C    | 2.57                     | 0.43              |
| 1:A:757:G:H2'     | 1:A:758:G:O4'    | 2.19                     | 0.43              |
| 1:A:985:C:N3      | 1:A:986:C:N4     | 2.66                     | 0.42              |
| 1:A:1339:U:H3'    | 1:A:1340:C:C6    | 2.54                     | 0.42              |
| 1:A:239:U:H4'     | 1:A:240:C:O5'    | 2.19                     | 0.42              |
| 19:S:5:LEU:O      | 19:S:6:LYS:CB    | 2.66                     | 0.42              |
| 10:J:55:LYS:O     | 10:J:56:HIS:HB2  | 2.18                     | 0.42              |
| 14:N:29:ARG:HB3   | 14:N:40:CYS:CB   | 2.49                     | 0.42              |
| 1:A:951:A:OP2     | 14:N:41:ARG:NH1  | 2.51                     | 0.42              |
| 2:B:217:ARG:HA    | 2:B:220:ASP:OD2  | 2.19                     | 0.42              |
| 11:K:109:VAL:HG22 | 18:R:86:VAL:HG22 | 2.00                     | 0.42              |
| 7:G:62:PHE:HA     | 7:G:124:LEU:HD23 | 2.01                     | 0.42              |
| 7:G:46:ALA:O      | 7:G:50:ILE:HG13  | 2.19                     | 0.42              |
| 13:M:61:GLU:C     | 13:M:62:ASN:HD22 | 2.23                     | 0.42              |
| 1:A:1076:G:O2'    | 1:A:1077:U:OP2   | 2.34                     | 0.42              |
| 9:I:10:ARG:HD2    | 9:I:75:ASP:CB    | 2.48                     | 0.42              |
| 1:A:295:A:H1'     | 1:A:548:U:O2     | 2.19                     | 0.42              |
| 1:A:156:A:C5      | 1:A:157:C:H1'    | 2.54                     | 0.42              |
| 10:J:45:ARG:HG2   | 10:J:45:ARG:HH11 | 1.83                     | 0.42              |
| 1:A:100:G:H3'     | 1:A:101:G:H5''   | 2.01                     | 0.42              |
| 1:A:197:G:N2      | 20:T:85:MET:HE3  | 2.33                     | 0.42              |
| 1:A:221:G:O2'     | 1:A:222:G:H5'    | 2.19                     | 0.42              |
| 13:M:94:ARG:HH12  | 19:S:81:ARG:CD   | 2.15                     | 0.42              |
| 17:Q:43:LEU:HD12  | 17:Q:68:ARG:HB3  | 2.01                     | 0.42              |
| 6:F:14:LEU:HB3    | 6:F:18:GLN:CB    | 2.46                     | 0.42              |
| 10:J:47:PHE:CZ    | 14:N:37:PHE:HE1  | 2.37                     | 0.42              |
| 3:C:29:TYR:CE1    | 14:N:54:PRO:HG2  | 2.54                     | 0.42              |
| 13:M:84:ILE:HG13  | 13:M:86:CYS:HB2  | 2.00                     | 0.42              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:415:U:H2'   | 1:A:417:C:C4     | 2.54                     | 0.42              |
| 17:Q:86:GLU:O   | 17:Q:90:ILE:HG13 | 2.19                     | 0.42              |
| 14:N:8:GLU:OE2  | 14:N:11:LYS:HD2  | 2.19                     | 0.42              |
| 1:A:1240:C:O2   | 1:A:1264:G:H1'   | 2.19                     | 0.42              |
| 1:A:1092:A:O5'  | 1:A:1092:A:H8    | 2.02                     | 0.42              |
| 1:A:936:A:C5'   | 1:A:937:U:OP2    | 2.55                     | 0.42              |
| 2:B:88:ALA:HB2  | 2:B:219:VAL:HG13 | 2.01                     | 0.42              |
| 1:A:952:A:H4'   | 1:A:953:G:OP2    | 2.18                     | 0.42              |
| 2:B:230:VAL:CG1 | 2:B:231:GLU:H    | 2.27                     | 0.42              |
| 1:A:124:A:HO2'  | 1:A:125:C:P      | 2.42                     | 0.42              |
| 1:A:269:A:O2'   | 1:A:270:G:C8     | 2.60                     | 0.42              |
| 1:A:1221:U:O2'  | 1:A:1222:G:OP1   | 2.28                     | 0.42              |
| 1:A:1282:U:O2'  | 1:A:1283:U:P     | 2.77                     | 0.42              |
| 1:A:401:G:C4    | 1:A:479:A:C5     | 3.08                     | 0.42              |
| 1:A:925:C:O2'   | 1:A:926:A:H5'    | 2.19                     | 0.42              |
| 1:A:1003:U:C6   | 1:A:1003:U:C3'   | 3.01                     | 0.42              |
| 1:A:1039:G:H5'' | 3:C:154:SER:CB   | 2.49                     | 0.42              |
| 20:T:67:ALA:HA  | 20:T:73:HIS:H    | 1.83                     | 0.42              |
| 16:P:41:PRO:O   | 16:P:43:LYS:HG3  | 2.19                     | 0.42              |
| 1:A:1335:C:O2'  | 1:A:1336:G:H5'   | 2.19                     | 0.42              |
| 6:F:36:ARG:NH1  | 6:F:38:GLU:HG2   | 2.34                     | 0.42              |
| 1:A:984:C:H6    | 1:A:984:C:H3'    | 1.85                     | 0.42              |
| 1:A:469:G:HO2'  | 1:A:470:U:P      | 2.35                     | 0.42              |
| 12:L:47:LYS:HB2 | 12:L:47:LYS:HZ2  | 1.81                     | 0.42              |
| 2:B:61:LEU:HD21 | 2:B:66:GLY:HA3   | 2.01                     | 0.42              |
| 1:A:630:C:H2'   | 1:A:631:A:C8     | 2.54                     | 0.42              |
| 6:F:100:ASN:ND2 | 18:R:23:LYS:HZ2  | 2.16                     | 0.42              |
| 1:A:1094:C:N3   | 3:C:178:LEU:N    | 2.61                     | 0.42              |
| 10:J:79:ARG:HG2 | 10:J:79:ARG:HH11 | 1.84                     | 0.42              |
| 5:E:36:ASP:OD1  | 5:E:40:ARG:HB2   | 2.19                     | 0.42              |
| 10:J:86:MET:CE  | 10:J:86:MET:HA   | 2.49                     | 0.42              |
| 1:A:878:A:C5    | 1:A:879:G:H1'    | 2.55                     | 0.42              |
| 1:A:412:C:H6    | 1:A:412:C:O5'    | 2.02                     | 0.42              |
| 1:A:936:A:C3'   | 1:A:937:U:C5'    | 2.92                     | 0.42              |
| 2:B:88:ALA:CB   | 2:B:90:MET:HG2   | 2.49                     | 0.42              |
| 1:A:724:G:H5''  | 15:O:39:LEU:HD12 | 2.00                     | 0.42              |
| 1:A:102:A:C6    | 1:A:321:G:C6     | 3.07                     | 0.42              |
| 1:A:578:G:H22   | 1:A:626:C:H41    | 1.66                     | 0.42              |
| 2:B:18:GLY:O    | 2:B:40:HIS:HB3   | 2.20                     | 0.42              |
| 1:A:1280:A:C5   | 1:A:1282:U:O2    | 2.72                     | 0.42              |
| 1:A:1296:U:H2'  | 1:A:1297:G:O4'   | 2.19                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 17:Q:81:ARG:HG3  | 17:Q:81:ARG:O     | 2.19                     | 0.42              |
| 3:C:149:ALA:HA   | 3:C:201:TYR:O     | 2.19                     | 0.42              |
| 3:C:122:GLU:HG2  | 3:C:126:ARG:HH21  | 1.85                     | 0.42              |
| 5:E:107:ARG:HG2  | 5:E:108:ALA:N     | 2.35                     | 0.42              |
| 1:A:242:G:P      | 17:Q:99:SER:OG    | 2.77                     | 0.42              |
| 3:C:76:VAL:O     | 3:C:83:ARG:O      | 2.38                     | 0.42              |
| 1:A:337:C:C2'    | 1:A:338:U:H5'     | 2.47                     | 0.42              |
| 18:R:41:LYS:C    | 18:R:43:PHE:H     | 2.23                     | 0.42              |
| 1:A:399:U:H5'    | 4:D:122:ARG:HD2   | 2.01                     | 0.42              |
| 1:A:85:U:H6      | 1:A:85:U:O5'      | 2.03                     | 0.42              |
| 13:M:62:ASN:O    | 13:M:63:THR:HB    | 2.19                     | 0.42              |
| 1:A:377:A:C2     | 1:A:378:A:C4      | 3.08                     | 0.42              |
| 16:P:45:THR:C    | 16:P:47:ASP:N     | 2.73                     | 0.42              |
| 1:A:959:U:C6     | 1:A:959:U:OP1     | 2.69                     | 0.42              |
| 1:A:465:G:C2'    | 1:A:467:C:N4      | 2.79                     | 0.42              |
| 16:P:29:ASP:OD2  | 16:P:29:ASP:N     | 2.53                     | 0.42              |
| 5:E:51:VAL:HB    | 5:E:52:PRO:CD     | 2.46                     | 0.42              |
| 7:G:15:ASP:HB2   | 7:G:20:ASP:H      | 1.82                     | 0.42              |
| 20:T:50:GLU:HA   | 20:T:100:ILE:HG13 | 2.01                     | 0.42              |
| 2:B:114:ARG:HG2  | 2:B:114:ARG:HH11  | 1.83                     | 0.42              |
| 1:A:1163:G:H4'   | 1:A:1164:A:C5'    | 2.50                     | 0.42              |
| 1:A:1213:U:H2'   | 1:A:1214:G:O4'    | 2.20                     | 0.42              |
| 6:F:10:LEU:CD1   | 6:F:59:TYR:HD2    | 2.33                     | 0.42              |
| 18:R:47:THR:HG22 | 18:R:48:GLY:N     | 2.35                     | 0.42              |
| 1:A:1077:U:H2'   | 1:A:1078:C:C6     | 2.55                     | 0.42              |
| 1:A:523:G:H2'    | 1:A:524:G:O4'     | 2.19                     | 0.42              |
| 12:L:61:THR:C    | 12:L:63:GLY:H     | 2.22                     | 0.42              |
| 1:A:1269:A:C2    | 1:A:1270:A:C4     | 3.08                     | 0.42              |
| 1:A:451:C:H2'    | 1:A:452:C:H6      | 1.83                     | 0.42              |
| 1:A:1501:C:OP1   | 11:K:120:ARG:NH1  | 2.52                     | 0.42              |
| 1:A:720:A:H2'    | 1:A:721:C:O4'     | 2.20                     | 0.42              |
| 3:C:116:VAL:HG21 | 3:C:202:ILE:HD11  | 2.02                     | 0.42              |
| 11:K:44:SER:H    | 11:K:47:VAL:HB    | 1.83                     | 0.42              |
| 4:D:105:VAL:HG13 | 4:D:110:PHE:HB2   | 2.02                     | 0.42              |
| 12:L:93:LEU:HB2  | 12:L:96:VAL:CG2   | 2.49                     | 0.42              |
| 1:A:1520:C:C2'   | 1:A:1521:U:H5'    | 2.50                     | 0.42              |
| 6:F:1:MET:O      | 6:F:2:ARG:HG3     | 2.19                     | 0.42              |
| 6:F:30:LEU:HD23  | 6:F:75:LEU:HD21   | 2.01                     | 0.42              |
| 1:A:1187:G:C6    | 1:A:1188:G:C5     | 3.08                     | 0.42              |
| 4:D:36:ARG:H     | 4:D:37:PRO:HD3    | 1.85                     | 0.42              |
| 19:S:16:LEU:CA   | 19:S:19:VAL:HG12  | 2.50                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1095:C:H1'    | 3:C:178:LEU:CD2   | 2.48                     | 0.42              |
| 16:P:14:ASN:N     | 16:P:15:PRO:CD    | 2.83                     | 0.42              |
| 5:E:143:ARG:HA    | 5:E:143:ARG:HD3   | 1.78                     | 0.42              |
| 1:A:494:C:HO2'    | 1:A:495:U:H6      | 1.67                     | 0.42              |
| 6:F:36:ARG:HH12   | 6:F:38:GLU:HG2    | 1.84                     | 0.42              |
| 1:A:813:G:H2'     | 1:A:814:U:O4'     | 2.20                     | 0.42              |
| 13:M:16:ASP:OD1   | 13:M:16:ASP:N     | 2.50                     | 0.42              |
| 20:T:65:LYS:O     | 20:T:68:LYS:CB    | 2.68                     | 0.42              |
| 5:E:24:ARG:HH11   | 5:E:24:ARG:CG     | 2.33                     | 0.42              |
| 1:A:1113:G:C3'    | 1:A:1113:G:C8     | 3.03                     | 0.42              |
| 1:A:970:G:O2'     | 1:A:971:A:OP1     | 2.30                     | 0.42              |
| 1:A:29:G:H5'      | 1:A:291:U:OP1     | 2.20                     | 0.42              |
| 1:A:1331:A:C2     | 1:A:1332:U:C2     | 3.08                     | 0.42              |
| 17:Q:17:LYS:HA    | 17:Q:46:ASP:O     | 2.19                     | 0.42              |
| 1:A:16:A:N1       | 1:A:896:A:H2      | 2.18                     | 0.42              |
| 1:A:246:G:C4'     | 1:A:247:U:H5'     | 2.42                     | 0.42              |
| 1:A:669:U:C2'     | 1:A:670:A:O5'     | 2.68                     | 0.42              |
| 2:B:177:ALA:O     | 2:B:180:LEU:N     | 2.45                     | 0.42              |
| 1:A:1207:C:C4'    | 1:A:1208:A:OP1    | 2.60                     | 0.42              |
| 1:A:849:A:C4'     | 1:A:850:A:OP1     | 2.60                     | 0.42              |
| 1:A:825:C:H6      | 1:A:825:C:H3'     | 1.80                     | 0.42              |
| 1:A:951:A:OP2     | 14:N:32:SER:OG    | 2.37                     | 0.42              |
| 9:I:71:SER:HA     | 9:I:74:ILE:HB     | 2.01                     | 0.42              |
| 18:R:29:PHE:HE1   | 18:R:31:LEU:HG    | 1.84                     | 0.42              |
| 19:S:77:THR:HG22  | 19:S:78:ARG:N     | 2.33                     | 0.42              |
| 1:A:837:A:H2'     | 1:A:838:G:O4'     | 2.20                     | 0.42              |
| 9:I:10:ARG:HH11   | 9:I:11:LYS:HB2    | 1.85                     | 0.42              |
| 1:A:157:C:C2'     | 1:A:158:U:H5'     | 2.50                     | 0.42              |
| 1:A:936:A:C3'     | 1:A:937:U:H5''    | 2.30                     | 0.41              |
| 1:A:961:C:H2'     | 1:A:962:C:C6      | 2.55                     | 0.41              |
| 2:B:76:GLN:HB3    | 2:B:211:ILE:HD11  | 2.01                     | 0.41              |
| 23:X:37:12A:N     | 23:X:37:12A:N1    | 2.51                     | 0.41              |
| 19:S:7:LYS:CD     | 19:S:7:LYS:O      | 2.53                     | 0.41              |
| 10:J:3:LYS:C      | 10:J:4:ILE:HD12   | 2.40                     | 0.41              |
| 26:A:1783:PAR:H43 | 26:A:1783:PAR:N64 | 2.35                     | 0.41              |
| 7:G:38:LEU:HA     | 7:G:41:ARG:CD     | 2.47                     | 0.41              |
| 14:N:22:THR:HB    | 14:N:33:VAL:CG2   | 2.47                     | 0.41              |
| 14:N:13:THR:N     | 14:N:14:PRO:CD    | 2.83                     | 0.41              |
| 1:A:1506:G:C4'    | 1:A:1507:G:OP2    | 2.68                     | 0.41              |
| 19:S:15:LEU:O     | 19:S:19:VAL:N     | 2.53                     | 0.41              |
| 1:A:218:U:H2'     | 1:A:219:C:O4'     | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 14:N:39:LEU:CD1  | 14:N:47:LEU:HD12 | 2.50                     | 0.41              |
| 1:A:576:G:O2'    | 1:A:577:G:H5'    | 2.20                     | 0.41              |
| 1:A:1131:C:OP1   | 9:I:14:VAL:HG11  | 2.20                     | 0.41              |
| 1:A:242:G:C8     | 17:Q:96:GLN:NE2  | 2.88                     | 0.41              |
| 1:A:1049:A:H1'   | 1:A:1050:G:O4'   | 2.21                     | 0.41              |
| 1:A:1509:U:H2'   | 1:A:1510:C:H4'   | 2.02                     | 0.41              |
| 1:A:714:G:H5'    | 1:A:749:A:H4'    | 2.02                     | 0.41              |
| 1:A:821:G:HO2'   | 1:A:822:U:H6     | 1.65                     | 0.41              |
| 1:A:854:C:O2     | 8:H:3:THR:OG1    | 2.33                     | 0.41              |
| 1:A:1323:C:O2'   | 9:I:124:GLN:HB2  | 2.20                     | 0.41              |
| 1:A:1193:U:H2'   | 1:A:1194:A:OP2   | 2.21                     | 0.41              |
| 1:A:699:A:O2'    | 1:A:700:C:H5'    | 2.20                     | 0.41              |
| 7:G:120:ILE:O    | 7:G:124:LEU:HD13 | 2.20                     | 0.41              |
| 1:A:1247:G:N2    | 1:A:1251:C:N3    | 2.67                     | 0.41              |
| 9:I:118:LYS:CB   | 9:I:118:LYS:HZ2  | 2.32                     | 0.41              |
| 5:E:126:ARG:CG   | 5:E:126:ARG:HH11 | 2.33                     | 0.41              |
| 11:K:45:GLY:C    | 11:K:55:LYS:HG2  | 2.41                     | 0.41              |
| 15:O:45:VAL:HG12 | 15:O:46:HIS:ND1  | 2.35                     | 0.41              |
| 1:A:1092:A:N6    | 1:A:1093:A:C6    | 2.88                     | 0.41              |
| 1:A:1420:G:H2'   | 1:A:1421:C:C6    | 2.55                     | 0.41              |
| 1:A:1341:A:H2'   | 1:A:1342:G:O4'   | 2.20                     | 0.41              |
| 13:M:73:GLU:O    | 13:M:77:ASN:HB2  | 2.20                     | 0.41              |
| 8:H:81:HIS:N     | 8:H:81:HIS:ND1   | 2.66                     | 0.41              |
| 1:A:986:C:C4     | 1:A:1000:G:N2    | 2.87                     | 0.41              |
| 1:A:954:A:N3     | 1:A:954:A:H2'    | 2.34                     | 0.41              |
| 10:J:4:ILE:N     | 10:J:4:ILE:CD1   | 2.83                     | 0.41              |
| 2:B:164:VAL:HB   | 2:B:186:ALA:HB2  | 2.01                     | 0.41              |
| 5:E:144:THR:O    | 5:E:145:LYS:C    | 2.58                     | 0.41              |
| 3:C:84:ILE:HG13  | 3:C:88:ARG:NH2   | 2.36                     | 0.41              |
| 4:D:120:LEU:O    | 4:D:126:ILE:HG12 | 2.20                     | 0.41              |
| 9:I:43:ALA:O     | 9:I:44:VAL:C     | 2.58                     | 0.41              |
| 7:G:31:MET:SD    | 7:G:34:GLY:HA2   | 2.61                     | 0.41              |
| 9:I:99:LEU:CB    | 9:I:101:PHE:CE1  | 3.03                     | 0.41              |
| 15:O:74:ASP:C    | 15:O:76:GLU:N    | 2.73                     | 0.41              |
| 1:A:84:C:H2'     | 1:A:85:U:O4'     | 2.21                     | 0.41              |
| 1:A:65:U:O2'     | 1:A:66:G:OP2     | 2.32                     | 0.41              |
| 1:A:816:U:H2'    | 1:A:817:C:H6     | 1.83                     | 0.41              |
| 1:A:1269:A:H2'   | 1:A:1270:A:H8    | 1.85                     | 0.41              |
| 1:A:591:A:C2'    | 1:A:592:A:H5'    | 2.50                     | 0.41              |
| 1:A:436:C:H2'    | 1:A:437:C:C6     | 2.55                     | 0.41              |
| 1:A:1202:G:OP1   | 1:A:1302:C:N3    | 2.53                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:669:U:O4      | 1:A:670:A:N6      | 2.53                     | 0.41              |
| 3:C:191:THR:HG21  | 3:C:193:TYR:CE1   | 2.55                     | 0.41              |
| 3:C:195:VAL:O     | 3:C:196:LEU:HD23  | 2.19                     | 0.41              |
| 7:G:15:ASP:HB3    | 7:G:19:GLY:H      | 1.79                     | 0.41              |
| 9:I:19:LEU:HB3    | 9:I:59:PHE:HD2    | 1.85                     | 0.41              |
| 4:D:111:ALA:HB2   | 4:D:120:LEU:HD12  | 2.02                     | 0.41              |
| 15:O:65:ARG:HG3   | 15:O:65:ARG:NH1   | 2.34                     | 0.41              |
| 8:H:112:LEU:HD12  | 8:H:112:LEU:H     | 1.81                     | 0.41              |
| 15:O:70:LEU:HD12  | 15:O:78:TYR:HA    | 2.02                     | 0.41              |
| 13:M:35:GLU:O     | 13:M:37:THR:N     | 2.53                     | 0.41              |
| 9:I:118:LYS:NZ    | 9:I:118:LYS:HB3   | 2.35                     | 0.41              |
| 5:E:118:ILE:HG12  | 5:E:119:LEU:N     | 2.35                     | 0.41              |
| 1:A:304:G:O2'     | 1:A:305:G:H5'     | 2.20                     | 0.41              |
| 1:A:249:G:OP1     | 17:Q:68:ARG:HB2   | 2.20                     | 0.41              |
| 1:A:735:G:H4'     | 15:O:69:TYR:OH    | 2.21                     | 0.41              |
| 11:K:95:ILE:CG2   | 11:K:108:ILE:HD13 | 2.51                     | 0.41              |
| 1:A:1231:A:H5'    | 9:I:68:GLY:O      | 2.19                     | 0.41              |
| 5:E:19:MET:O      | 5:E:20:GLN:NE2    | 2.46                     | 0.41              |
| 1:A:1134:A:H5'    | 10:J:13:HIS:HB2   | 2.02                     | 0.41              |
| 1:A:31:G:H1       | 1:A:48:C:H5"      | 1.86                     | 0.41              |
| 11:K:77:MET:CE    | 11:K:80:VAL:HG12  | 2.51                     | 0.41              |
| 1:A:1193:U:C2'    | 1:A:1194:A:OP2    | 2.69                     | 0.41              |
| 1:A:838:G:C2'     | 1:A:839:C:H5'     | 2.50                     | 0.41              |
| 1:A:1317:C:H4'    | 1:A:1318:G:OP2    | 2.20                     | 0.41              |
| 1:A:1077:U:P      | 1:A:1090:G:H1     | 2.44                     | 0.41              |
| 1:A:44:G:O2'      | 1:A:45:U:H5'      | 2.20                     | 0.41              |
| 7:G:113:GLU:CG    | 7:G:119:ARG:HG2   | 2.51                     | 0.41              |
| 1:A:588:U:H2'     | 1:A:589:G:O4'     | 2.20                     | 0.41              |
| 6:F:27:GLN:HE21   | 6:F:27:GLN:HB3    | 1.57                     | 0.41              |
| 17:Q:101:ARG:HH11 | 17:Q:101:ARG:HG2  | 1.86                     | 0.41              |
| 12:L:76:ASN:ND2   | 12:L:76:ASN:O     | 2.54                     | 0.41              |
| 1:A:982:A:HO2'    | 1:A:983:A:P       | 2.43                     | 0.41              |
| 1:A:1123:C:C2'    | 1:A:1124:G:H5'    | 2.43                     | 0.41              |
| 1:A:1189:C:H2'    | 1:A:1190:C:C6     | 2.55                     | 0.41              |
| 16:P:34:GLU:OE1   | 16:P:55:ARG:NH1   | 2.53                     | 0.41              |
| 4:D:76:ARG:NH1    | 4:D:80:GLU:OE1    | 2.53                     | 0.41              |
| 12:L:6:THR:HG1    | 12:L:9:GLN:HG3    | 1.84                     | 0.41              |
| 15:O:87:ILE:O     | 15:O:88:ARG:HB2   | 2.20                     | 0.41              |
| 1:A:1460:A:C2'    | 1:A:1461:C:O5'    | 2.69                     | 0.41              |
| 19:S:17:GLU:HA    | 19:S:20:LEU:HG    | 2.03                     | 0.41              |
| 1:A:750:A:H2'     | 1:A:751:A:O4'     | 2.20                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:D:131:ARG:HE   | 4:D:131:ARG:HB2   | 1.68                     | 0.41              |
| 2:B:30:ARG:HG2   | 2:B:30:ARG:H      | 1.57                     | 0.41              |
| 4:D:102:ASP:OD1  | 4:D:103:ASN:N     | 2.54                     | 0.41              |
| 11:K:58:PRO:O    | 11:K:61:ALA:HB3   | 2.21                     | 0.41              |
| 10:J:76:ASN:O    | 10:J:78:ASN:N     | 2.51                     | 0.41              |
| 2:B:72:GLY:HA2   | 2:B:165:VAL:CG2   | 2.50                     | 0.41              |
| 1:A:735:G:O2'    | 1:A:736:A:OP2     | 2.38                     | 0.41              |
| 5:E:75:THR:HG23  | 5:E:76:ILE:N      | 2.35                     | 0.41              |
| 2:B:18:GLY:O     | 2:B:19:HIS:C      | 2.59                     | 0.41              |
| 20:T:54:LYS:N    | 20:T:100:ILE:HD12 | 2.36                     | 0.41              |
| 1:A:1111:C:OP1   | 9:I:62:TYR:OH     | 2.38                     | 0.41              |
| 1:A:1113:G:O5'   | 1:A:1113:G:H8     | 2.04                     | 0.41              |
| 9:I:43:ALA:HA    | 9:I:74:ILE:HD13   | 2.03                     | 0.41              |
| 1:A:1382:C:C4'   | 1:A:1383:G:OP2    | 2.68                     | 0.41              |
| 1:A:1264:G:O2'   | 1:A:1265:C:H5'    | 2.21                     | 0.41              |
| 1:A:494:C:O2'    | 1:A:495:U:C5'     | 2.69                     | 0.41              |
| 20:T:69:GLY:O    | 20:T:73:HIS:CD2   | 2.73                     | 0.41              |
| 1:A:1357:A:H2'   | 1:A:1358:U:O4'    | 2.21                     | 0.41              |
| 1:A:959:U:H5''   | 14:N:3:ARG:HH22   | 1.86                     | 0.41              |
| 2:B:82:ARG:NH1   | 2:B:83:MET:CE     | 2.83                     | 0.41              |
| 23:X:36:U:H2'    | 23:X:37:12A:H5'   | 1.99                     | 0.41              |
| 10:J:8:LEU:CD2   | 10:J:96:ILE:HG12  | 2.50                     | 0.41              |
| 1:A:743:G:H2'    | 1:A:744:G:H5'     | 2.02                     | 0.41              |
| 19:S:22:LEU:HD22 | 19:S:26:GLY:O     | 2.20                     | 0.41              |
| 5:E:79:GLU:O     | 8:H:104:ARG:NH1   | 2.54                     | 0.41              |
| 3:C:85:ARG:HA    | 3:C:88:ARG:HH21   | 1.86                     | 0.41              |
| 2:B:20:GLU:O     | 2:B:21:ARG:C      | 2.59                     | 0.41              |
| 1:A:899:G:H5'    | 5:E:20:GLN:HE22   | 1.82                     | 0.41              |
| 3:C:139:GLN:CA   | 3:C:139:GLN:NE2   | 2.76                     | 0.41              |
| 1:A:705:A:O2'    | 1:A:706:U:O5'     | 2.38                     | 0.41              |
| 1:A:387:G:C4     | 1:A:388:A:C8      | 3.09                     | 0.41              |
| 1:A:1194:A:HO2'  | 1:A:1195:C:P      | 2.42                     | 0.41              |
| 11:K:70:LYS:HA   | 11:K:73:MET:HG3   | 2.02                     | 0.41              |
| 5:E:126:ARG:HG3  | 5:E:126:ARG:HH11  | 1.84                     | 0.41              |
| 1:A:1502:G:P     | 11:K:120:ARG:HH22 | 2.44                     | 0.41              |
| 1:A:278:C:C2'    | 1:A:279:G:H5'     | 2.50                     | 0.41              |
| 17:Q:74:LEU:O    | 17:Q:74:LEU:HD23  | 2.19                     | 0.41              |
| 1:A:981:G:O2'    | 1:A:982:A:OP1     | 2.30                     | 0.41              |
| 1:A:960:A:N3     | 1:A:960:A:H3'     | 2.36                     | 0.41              |
| 2:B:84:GLU:OE1   | 2:B:216:SER:HA    | 2.19                     | 0.41              |
| 1:A:1259:U:O2'   | 1:A:1260:A:OP2    | 2.26                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:635:U:O2'    | 1:A:636:A:C5'    | 2.69                     | 0.41              |
| 11:K:84:VAL:CG2  | 11:K:110:ASP:HA  | 2.42                     | 0.41              |
| 1:A:932:U:O2'    | 1:A:933:U:H5'    | 2.21                     | 0.41              |
| 1:A:505:C:H2'    | 1:A:506:A:O4'    | 2.21                     | 0.41              |
| 2:B:239:VAL:HG12 | 2:B:240:GLN:NE2  | 2.36                     | 0.41              |
| 1:A:1127:C:O2'   | 1:A:1128:A:P     | 2.79                     | 0.41              |
| 9:I:16:ARG:O     | 9:I:63:ILE:HG23  | 2.21                     | 0.41              |
| 2:B:220:ASP:O    | 2:B:224:GLN:HB2  | 2.20                     | 0.41              |
| 21:V:3:LYS:HG2   | 21:V:14:TRP:CD1  | 2.56                     | 0.41              |
| 13:M:8:GLU:C     | 13:M:9:ILE:HG13  | 2.40                     | 0.41              |
| 1:A:446:A:O2'    | 1:A:447:A:H8     | 2.03                     | 0.41              |
| 1:A:1426:A:O2'   | 1:A:1427:G:P     | 2.79                     | 0.41              |
| 20:T:93:GLU:OE2  | 20:T:93:GLU:HA   | 2.21                     | 0.41              |
| 1:A:1009:G:O5'   | 1:A:1009:G:H8    | 2.04                     | 0.41              |
| 2:B:28:PHE:HE1   | 2:B:188:ALA:HB1  | 1.85                     | 0.41              |
| 1:A:1395:A:H2'   | 1:A:1396:U:O4'   | 2.21                     | 0.41              |
| 4:D:196:LEU:HA   | 4:D:196:LEU:HD23 | 1.80                     | 0.41              |
| 1:A:658:A:H1'    | 11:K:116:HIS:CG  | 2.56                     | 0.41              |
| 1:A:657:G:H2'    | 1:A:658:A:C8     | 2.55                     | 0.41              |
| 3:C:122:GLU:HG2  | 3:C:126:ARG:NH2  | 2.36                     | 0.41              |
| 1:A:1203:G:OP1   | 19:S:77:THR:HG21 | 2.20                     | 0.41              |
| 1:A:334:C:H2'    | 1:A:335:U:C6     | 2.55                     | 0.41              |
| 1:A:492:A:H5'    | 4:D:54:TYR:CD2   | 2.56                     | 0.41              |
| 1:A:659:A:O2'    | 1:A:660:U:H5'    | 2.20                     | 0.41              |
| 1:A:919:G:N3     | 1:A:920:U:C6     | 2.89                     | 0.41              |
| 7:G:138:LYS:HE2  | 7:G:142:GLU:OE1  | 2.20                     | 0.41              |
| 1:A:157:C:H2'    | 1:A:158:U:H5'    | 2.03                     | 0.41              |
| 1:A:44:G:C2      | 1:A:45:U:H1'     | 2.56                     | 0.41              |
| 5:E:101:ILE:HD12 | 5:E:119:LEU:HD23 | 2.03                     | 0.41              |
| 1:A:739:C:C4     | 1:A:740:U:C4     | 3.09                     | 0.41              |
| 1:A:914:A:C2     | 1:A:1361:G:O6    | 2.74                     | 0.41              |
| 15:O:29:VAL:HG11 | 15:O:67:LEU:HD21 | 2.03                     | 0.41              |
| 10:J:34:VAL:HG12 | 10:J:35:SER:N    | 2.36                     | 0.41              |
| 10:J:54:PHE:O    | 10:J:55:LYS:HG2  | 2.21                     | 0.41              |
| 1:A:1085:C:H2'   | 1:A:1086:G:O4'   | 2.22                     | 0.41              |
| 1:A:1170:C:C5'   | 1:A:1171:G:OP2   | 2.60                     | 0.41              |
| 1:A:1171:G:C2'   | 1:A:1172:A:OP2   | 2.69                     | 0.41              |
| 1:A:1025:C:H2'   | 1:A:1026:A:OP2   | 2.20                     | 0.41              |
| 15:O:26:GLU:HA   | 15:O:81:LEU:HD11 | 2.04                     | 0.41              |
| 1:A:408:G:N2     | 1:A:423:G:O2'    | 2.54                     | 0.41              |
| 17:Q:86:GLU:O    | 17:Q:89:LEU:HB2  | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:68:GLU:O     | 5:E:70:PRO:HD3   | 2.21                     | 0.41              |
| 2:B:54:THR:O     | 2:B:58:ILE:HG13  | 2.21                     | 0.41              |
| 1:A:539:C:C2'    | 1:A:540:G:H5'    | 2.50                     | 0.41              |
| 1:A:404:G:C2'    | 1:A:405:G:O5'    | 2.68                     | 0.41              |
| 1:A:280:G:O2'    | 1:A:281:G:H5'    | 2.21                     | 0.41              |
| 13:M:98:VAL:C    | 13:M:100:GLY:H   | 2.25                     | 0.41              |
| 1:A:1237:A:O2'   | 1:A:1238:U:H4'   | 2.19                     | 0.40              |
| 10:J:8:LEU:HD23  | 10:J:96:ILE:HG12 | 2.02                     | 0.40              |
| 1:A:1286:G:O2'   | 1:A:1287:A:O5'   | 2.39                     | 0.40              |
| 1:A:669:U:O2     | 11:K:42:TRP:CZ2  | 2.73                     | 0.40              |
| 1:A:670:A:H2     | 1:A:683:G:N3     | 2.20                     | 0.40              |
| 1:A:1042:C:OP1   | 14:N:45:ARG:NH2  | 2.54                     | 0.40              |
| 10:J:63:PHE:HA   | 14:N:57:ARG:O    | 2.21                     | 0.40              |
| 1:A:1484:A:C2    | 1:A:1485:G:C4    | 3.09                     | 0.40              |
| 1:A:370:U:O2     | 16:P:28:ARG:NE   | 2.51                     | 0.40              |
| 1:A:1127:C:O2'   | 1:A:1128:A:O5'   | 2.32                     | 0.40              |
| 7:G:18:TYR:HB3   | 7:G:59:LEU:HD22  | 2.03                     | 0.40              |
| 16:P:18:ARG:O    | 16:P:20:VAL:HG12 | 2.20                     | 0.40              |
| 1:A:942:A:O2'    | 1:A:943:G:OP2    | 2.39                     | 0.40              |
| 1:A:1506:G:C5'   | 1:A:1507:G:OP2   | 2.67                     | 0.40              |
| 6:F:19:LEU:O     | 6:F:22:GLU:N     | 2.54                     | 0.40              |
| 1:A:110:G:O6     | 1:A:284:G:H1'    | 2.21                     | 0.40              |
| 17:Q:15:MET:HB2  | 17:Q:18:THR:O    | 2.22                     | 0.40              |
| 5:E:91:LEU:HD22  | 5:E:118:ILE:CD1  | 2.51                     | 0.40              |
| 1:A:1103:U:H2'   | 1:A:1104:U:C6    | 2.56                     | 0.40              |
| 1:A:245:A:O4'    | 1:A:247:U:C6     | 2.74                     | 0.40              |
| 1:A:1311:U:C2'   | 1:A:1312:G:H5'   | 2.51                     | 0.40              |
| 5:E:79:GLU:O     | 5:E:80:ILE:HG23  | 2.19                     | 0.40              |
| 1:A:1483:U:O2'   | 1:A:1484:A:OP1   | 2.38                     | 0.40              |
| 1:A:931:G:H2'    | 1:A:932:U:C6     | 2.56                     | 0.40              |
| 1:A:1023:A:C6    | 1:A:1024:G:N7    | 2.89                     | 0.40              |
| 13:M:25:ILE:HD11 | 13:M:60:VAL:HG13 | 2.02                     | 0.40              |
| 19:S:15:LEU:H    | 19:S:15:LEU:HD23 | 1.86                     | 0.40              |
| 13:M:37:THR:O    | 13:M:37:THR:HG22 | 2.21                     | 0.40              |
| 1:A:457:A:H4'    | 16:P:80:PHE:O    | 2.21                     | 0.40              |
| 1:A:1422:C:H2'   | 1:A:1423:G:H5'   | 2.02                     | 0.40              |
| 1:A:1424:G:N3    | 1:A:1424:G:H2'   | 2.37                     | 0.40              |
| 7:G:64:GLN:O     | 7:G:67:GLU:N     | 2.54                     | 0.40              |
| 4:D:49:ARG:O     | 4:D:51:PRO:HD3   | 2.20                     | 0.40              |
| 1:A:847:U:H4'    | 1:A:848:U:O5'    | 2.21                     | 0.40              |
| 1:A:1044:U:H2'   | 1:A:1045:C:C6    | 2.55                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 10:J:8:LEU:O     | 10:J:69:ASN:HA    | 2.21                     | 0.40              |
| 1:A:1123:C:O2    | 1:A:1123:C:H2'    | 2.21                     | 0.40              |
| 1:A:1084:A:H2'   | 1:A:1085:C:C6     | 2.57                     | 0.40              |
| 2:B:60:ASP:OD2   | 2:B:60:ASP:N      | 2.55                     | 0.40              |
| 1:A:1188:G:H2'   | 1:A:1189:C:H6     | 1.86                     | 0.40              |
| 8:H:31:PHE:CZ    | 8:H:134:ILE:HD13  | 2.57                     | 0.40              |
| 1:A:775:A:O2'    | 1:A:776:U:OP2     | 2.39                     | 0.40              |
| 14:N:23:ARG:NH1  | 14:N:30:ALA:HB2   | 2.36                     | 0.40              |
| 17:Q:81:ARG:HE   | 17:Q:81:ARG:HB2   | 1.75                     | 0.40              |
| 1:A:1008:C:H2'   | 1:A:1009:G:H8     | 1.85                     | 0.40              |
| 1:A:82:U:H2'     | 1:A:83:A:C8       | 2.56                     | 0.40              |
| 4:D:196:LEU:HD23 | 4:D:197:PRO:HD2   | 2.04                     | 0.40              |
| 1:A:701:G:O6     | 18:R:74:ARG:NH1   | 2.55                     | 0.40              |
| 17:Q:13:ASP:C    | 17:Q:15:MET:N     | 2.75                     | 0.40              |
| 5:E:126:ARG:CG   | 5:E:126:ARG:NH1   | 2.85                     | 0.40              |
| 9:I:11:LYS:O     | 9:I:12:GLU:HB3    | 2.21                     | 0.40              |
| 13:M:114:ARG:NH1 | 13:M:114:ARG:HG2  | 2.37                     | 0.40              |
| 1:A:808:G:N2     | 8:H:11:THR:HG21   | 2.36                     | 0.40              |
| 1:A:952:A:H4'    | 1:A:953:G:C5'     | 2.45                     | 0.40              |
| 6:F:69:GLU:C     | 6:F:71:ARG:H      | 2.25                     | 0.40              |
| 19:S:29:ARG:O    | 19:S:30:LEU:HB2   | 2.22                     | 0.40              |
| 3:C:11:ARG:HG3   | 3:C:11:ARG:HH11   | 1.86                     | 0.40              |
| 1:A:1509:U:C2'   | 1:A:1510:C:C5'    | 2.88                     | 0.40              |
| 1:A:434:A:C4     | 1:A:480:A:C2      | 3.09                     | 0.40              |
| 1:A:124:A:H1'    | 1:A:258:A:O2'     | 2.21                     | 0.40              |
| 21:V:6:ARG:HG2   | 21:V:15:ARG:HH11  | 1.84                     | 0.40              |
| 11:K:101:SER:C   | 11:K:103:LEU:H    | 2.24                     | 0.40              |
| 2:B:55:PHE:HE1   | 2:B:218:ALA:CA    | 2.33                     | 0.40              |
| 3:C:29:TYR:OH    | 14:N:54:PRO:CD    | 2.70                     | 0.40              |
| 15:O:11:VAL:HG21 | 15:O:34:LEU:HD22  | 2.03                     | 0.40              |
| 12:L:83:VAL:HG21 | 12:L:100:ILE:HG21 | 2.03                     | 0.40              |
| 21:V:5:ASP:HB3   | 21:V:8:THR:CG2    | 2.52                     | 0.40              |
| 1:A:9:G:N7       | 1:A:541:G:O2'     | 2.51                     | 0.40              |
| 17:Q:78:GLU:CD   | 17:Q:81:ARG:HD2   | 2.41                     | 0.40              |
| 14:N:44:LEU:C    | 14:N:44:LEU:HD12  | 2.42                     | 0.40              |
| 3:C:134:ILE:O    | 3:C:138:VAL:HG23  | 2.22                     | 0.40              |
| 1:A:592:A:C2'    | 1:A:593:G:H5'     | 2.51                     | 0.40              |
| 1:A:1326:U:O2'   | 1:A:1327:A:OP2    | 2.34                     | 0.40              |
| 12:L:98:TYR:N    | 12:L:98:TYR:CD1   | 2.89                     | 0.40              |
| 10:J:89:ASP:O    | 10:J:90:LEU:HD23  | 2.22                     | 0.40              |
| 18:R:41:LYS:C    | 18:R:43:PHE:N     | 2.74                     | 0.40              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 13:M:15:VAL:CG2 | 13:M:48:LEU:HD21 | 2.51                     | 0.40              |
| 20:T:57:ARG:NH2 | 20:T:100:ILE:CG2 | 2.84                     | 0.40              |
| 4:D:127:THR:OG1 | 4:D:130:GLY:O    | 2.35                     | 0.40              |
| 21:V:15:ARG:O   | 21:V:17:THR:HG23 | 2.20                     | 0.40              |
| 1:A:545:C:H4'   | 1:A:546:A:O5'    | 2.21                     | 0.40              |
| 1:A:1425:G:H5'' | 1:A:1426:A:C5'   | 2.48                     | 0.40              |
| 6:F:8:ILE:CD1   | 6:F:79:LEU:HD22  | 2.52                     | 0.40              |
| 16:P:26:ARG:HG2 | 16:P:27:LYS:H    | 1.87                     | 0.40              |
| 10:J:38:ILE:CG1 | 10:J:71:LEU:HB3  | 2.51                     | 0.40              |
| 1:A:328:G:H2'   | 1:A:329:C:H6     | 1.87                     | 0.40              |
| 18:R:24:ALA:O   | 18:R:26:LEU:N    | 2.55                     | 0.40              |
| 1:A:109:A:H61   | 1:A:308:A:H1'    | 1.86                     | 0.40              |
| 1:A:1478:C:C5   | 1:A:1481:G:C4    | 3.09                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 2   | B     | 232/256 (91%) | 165 (71%) | 47 (20%) | 20 (9%)  | 1           | 5   |
| 3   | C     | 204/239 (85%) | 151 (74%) | 33 (16%) | 20 (10%) | 1           | 4   |
| 4   | D     | 206/209 (99%) | 171 (83%) | 29 (14%) | 6 (3%)   | 6           | 30  |
| 5   | E     | 148/162 (91%) | 135 (91%) | 13 (9%)  | 0        | 100         | 100 |
| 6   | F     | 99/101 (98%)  | 78 (79%)  | 16 (16%) | 5 (5%)   | 2           | 16  |
| 7   | G     | 153/156 (98%) | 120 (78%) | 27 (18%) | 6 (4%)   | 4           | 22  |
| 8   | H     | 136/138 (99%) | 121 (89%) | 12 (9%)  | 3 (2%)   | 8           | 37  |
| 9   | I     | 125/128 (98%) | 93 (74%)  | 24 (19%) | 8 (6%)   | 2           | 10  |
| 10  | J     | 96/105 (91%)  | 69 (72%)  | 18 (19%) | 9 (9%)   | 1           | 4   |
| 11  | K     | 117/129 (91%) | 94 (80%)  | 17 (14%) | 6 (5%)   | 2           | 16  |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 12  | L     | 122/132 (92%)   | 93 (76%)   | 22 (18%)  | 7 (6%)   | 2           | 13 |
| 13  | M     | 123/126 (98%)   | 90 (73%)   | 23 (19%)  | 10 (8%)  | 1           | 6  |
| 14  | N     | 58/61 (95%)     | 40 (69%)   | 12 (21%)  | 6 (10%)  | 1           | 3  |
| 15  | O     | 86/89 (97%)     | 68 (79%)   | 14 (16%)  | 4 (5%)   | 3           | 17 |
| 16  | P     | 81/88 (92%)     | 64 (79%)   | 14 (17%)  | 3 (4%)   | 4           | 23 |
| 17  | Q     | 102/105 (97%)   | 82 (80%)   | 16 (16%)  | 4 (4%)   | 4           | 22 |
| 18  | R     | 71/88 (81%)     | 57 (80%)   | 9 (13%)   | 5 (7%)   | 1           | 8  |
| 19  | S     | 78/93 (84%)     | 60 (77%)   | 10 (13%)  | 8 (10%)  | 1           | 3  |
| 20  | T     | 97/106 (92%)    | 70 (72%)   | 20 (21%)  | 7 (7%)   | 1           | 7  |
| 21  | V     | 22/27 (82%)     | 15 (68%)   | 5 (23%)   | 2 (9%)   | 1           | 5  |
| All | All   | 2356/2538 (93%) | 1836 (78%) | 381 (16%) | 139 (6%) | 2           | 12 |

All (139) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 15  | VAL  |
| 2   | B     | 20  | GLU  |
| 2   | B     | 190 | THR  |
| 3   | C     | 15  | THR  |
| 3   | C     | 16  | ARG  |
| 3   | C     | 20  | SER  |
| 3   | C     | 24  | ALA  |
| 3   | C     | 65  | ALA  |
| 3   | C     | 179 | ARG  |
| 3   | C     | 189 | ALA  |
| 4   | D     | 30  | LYS  |
| 6   | F     | 98  | LEU  |
| 7   | G     | 5   | ARG  |
| 7   | G     | 7   | ALA  |
| 9   | I     | 117 | HIS  |
| 10  | J     | 34  | VAL  |
| 10  | J     | 39  | PRO  |
| 10  | J     | 51  | ARG  |
| 10  | J     | 54  | PHE  |
| 11  | K     | 12  | ARG  |
| 11  | K     | 127 | LYS  |
| 12  | L     | 27  | LEU  |
| 12  | L     | 116 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | M     | 63  | THR  |
| 13  | M     | 67  | GLU  |
| 13  | M     | 107 | ALA  |
| 18  | R     | 87  | ARG  |
| 19  | S     | 5   | LEU  |
| 19  | S     | 9   | VAL  |
| 21  | V     | 3   | LYS  |
| 2   | B     | 19  | HIS  |
| 2   | B     | 108 | ILE  |
| 2   | B     | 209 | ARG  |
| 2   | B     | 230 | VAL  |
| 3   | C     | 61  | ALA  |
| 3   | C     | 74  | GLY  |
| 3   | C     | 167 | TRP  |
| 3   | C     | 168 | ALA  |
| 4   | D     | 4   | TYR  |
| 4   | D     | 29  | PRO  |
| 4   | D     | 31  | CYS  |
| 8   | H     | 105 | ARG  |
| 9   | I     | 41  | VAL  |
| 10  | J     | 90  | LEU  |
| 11  | K     | 50  | TYR  |
| 11  | K     | 128 | ALA  |
| 12  | L     | 29  | GLY  |
| 12  | L     | 115 | LYS  |
| 13  | M     | 36  | LYS  |
| 13  | M     | 85  | GLY  |
| 13  | M     | 106 | ASN  |
| 13  | M     | 120 | LYS  |
| 13  | M     | 124 | PRO  |
| 14  | N     | 8   | GLU  |
| 14  | N     | 23  | ARG  |
| 17  | Q     | 99  | SER  |
| 18  | R     | 25  | THR  |
| 19  | S     | 6   | LYS  |
| 2   | B     | 78  | GLN  |
| 2   | B     | 87  | ARG  |
| 3   | C     | 4   | LYS  |
| 3   | C     | 66  | VAL  |
| 3   | C     | 82  | GLU  |
| 3   | C     | 108 | ASN  |
| 3   | C     | 130 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 154 | SER  |
| 6   | F     | 70  | ASP  |
| 7   | G     | 4   | ARG  |
| 7   | G     | 9   | VAL  |
| 7   | G     | 90  | GLU  |
| 8   | H     | 91  | ARG  |
| 9   | I     | 119 | ALA  |
| 9   | I     | 127 | LYS  |
| 10  | J     | 40  | LEU  |
| 10  | J     | 73  | ASP  |
| 11  | K     | 25  | TYR  |
| 13  | M     | 23  | TYR  |
| 14  | N     | 29  | ARG  |
| 14  | N     | 32  | SER  |
| 15  | O     | 88  | ARG  |
| 17  | Q     | 68  | ARG  |
| 18  | R     | 42  | ARG  |
| 18  | R     | 45  | SER  |
| 19  | S     | 43  | GLU  |
| 19  | S     | 44  | MET  |
| 20  | T     | 54  | LYS  |
| 20  | T     | 73  | HIS  |
| 20  | T     | 94  | ALA  |
| 2   | B     | 64  | ARG  |
| 2   | B     | 95  | GLN  |
| 3   | C     | 188 | LEU  |
| 4   | D     | 53  | ASP  |
| 4   | D     | 88  | VAL  |
| 6   | F     | 62  | TRP  |
| 6   | F     | 99  | ALA  |
| 10  | J     | 60  | ARG  |
| 10  | J     | 72  | VAL  |
| 12  | L     | 41  | ARG  |
| 12  | L     | 51  | ALA  |
| 14  | N     | 13  | THR  |
| 14  | N     | 31  | ARG  |
| 16  | P     | 52  | ASP  |
| 19  | S     | 8   | GLY  |
| 19  | S     | 30  | LEU  |
| 20  | T     | 49  | ALA  |
| 20  | T     | 102 | GLY  |
| 2   | B     | 10  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 52  | GLU  |
| 2   | B     | 97  | TRP  |
| 2   | B     | 131 | PRO  |
| 3   | C     | 53  | ALA  |
| 9   | I     | 12  | GLU  |
| 11  | K     | 35  | PRO  |
| 13  | M     | 117 | VAL  |
| 15  | O     | 13  | GLN  |
| 15  | O     | 24  | SER  |
| 18  | R     | 28  | GLU  |
| 19  | S     | 69  | HIS  |
| 20  | T     | 9   | ASN  |
| 21  | V     | 15  | ARG  |
| 2   | B     | 45  | GLN  |
| 2   | B     | 121 | LEU  |
| 6   | F     | 37  | VAL  |
| 9   | I     | 24  | GLY  |
| 15  | O     | 75  | PRO  |
| 16  | P     | 10  | GLY  |
| 2   | B     | 130 | ARG  |
| 7   | G     | 80  | VAL  |
| 20  | T     | 96  | GLY  |
| 8   | H     | 83  | ILE  |
| 2   | B     | 202 | PRO  |
| 3   | C     | 84  | ILE  |
| 9   | I     | 21  | PRO  |
| 17  | Q     | 33  | GLY  |
| 2   | B     | 232 | PRO  |
| 9   | I     | 44  | VAL  |
| 12  | L     | 121 | GLY  |
| 16  | P     | 19  | ILE  |
| 17  | Q     | 64  | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 2   | B     | 202/220 (92%)   | 181 (90%)  | 21 (10%)  | 9           | 32 |
| 3   | C     | 160/188 (85%)   | 143 (89%)  | 17 (11%)  | 8           | 31 |
| 4   | D     | 180/181 (99%)   | 162 (90%)  | 18 (10%)  | 9           | 34 |
| 5   | E     | 115/123 (94%)   | 100 (87%)  | 15 (13%)  | 5           | 22 |
| 6   | F     | 90/90 (100%)    | 87 (97%)   | 3 (3%)    | 45          | 79 |
| 7   | G     | 126/127 (99%)   | 114 (90%)  | 12 (10%)  | 11          | 38 |
| 8   | H     | 119/119 (100%)  | 104 (87%)  | 15 (13%)  | 5           | 22 |
| 9   | I     | 98/99 (99%)     | 84 (86%)   | 14 (14%)  | 4           | 17 |
| 10  | J     | 87/92 (95%)     | 81 (93%)   | 6 (7%)    | 19          | 55 |
| 11  | K     | 90/99 (91%)     | 85 (94%)   | 5 (6%)    | 26          | 63 |
| 12  | L     | 104/109 (95%)   | 91 (88%)   | 13 (12%)  | 6           | 23 |
| 13  | M     | 100/101 (99%)   | 94 (94%)   | 6 (6%)    | 24          | 60 |
| 14  | N     | 49/50 (98%)     | 44 (90%)   | 5 (10%)   | 9           | 33 |
| 15  | O     | 79/80 (99%)     | 74 (94%)   | 5 (6%)    | 22          | 58 |
| 16  | P     | 72/74 (97%)     | 65 (90%)   | 7 (10%)   | 10          | 36 |
| 17  | Q     | 96/97 (99%)     | 92 (96%)   | 4 (4%)    | 36          | 73 |
| 18  | R     | 64/77 (83%)     | 57 (89%)   | 7 (11%)   | 8           | 31 |
| 19  | S     | 71/80 (89%)     | 65 (92%)   | 6 (8%)    | 13          | 45 |
| 20  | T     | 76/82 (93%)     | 66 (87%)   | 10 (13%)  | 5           | 21 |
| 21  | V     | 19/22 (86%)     | 18 (95%)   | 1 (5%)    | 28          | 65 |
| All | All   | 1997/2110 (95%) | 1807 (90%) | 190 (10%) | 11          | 38 |

All (190) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 8   | LYS  |
| 2   | B     | 12  | GLU  |
| 2   | B     | 15  | VAL  |
| 2   | B     | 16  | HIS  |
| 2   | B     | 17  | PHE  |
| 2   | B     | 24  | TRP  |
| 2   | B     | 37  | ASN  |
| 2   | B     | 40  | HIS  |
| 2   | B     | 67  | THR  |
| 2   | B     | 96  | ARG  |
| 2   | B     | 102 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 114 | ARG  |
| 2   | B     | 128 | GLU  |
| 2   | B     | 144 | ARG  |
| 2   | B     | 154 | LEU  |
| 2   | B     | 170 | GLU  |
| 2   | B     | 178 | ARG  |
| 2   | B     | 187 | LEU  |
| 2   | B     | 200 | ILE  |
| 2   | B     | 204 | ASN  |
| 2   | B     | 236 | TYR  |
| 3   | C     | 3   | ASN  |
| 3   | C     | 16  | ARG  |
| 3   | C     | 21  | ARG  |
| 3   | C     | 29  | TYR  |
| 3   | C     | 36  | ASP  |
| 3   | C     | 37  | GLN  |
| 3   | C     | 39  | ILE  |
| 3   | C     | 42  | LEU  |
| 3   | C     | 56  | ASP  |
| 3   | C     | 83  | ARG  |
| 3   | C     | 104 | GLN  |
| 3   | C     | 108 | ASN  |
| 3   | C     | 162 | GLN  |
| 3   | C     | 167 | TRP  |
| 3   | C     | 188 | LEU  |
| 3   | C     | 196 | LEU  |
| 3   | C     | 204 | LEU  |
| 4   | D     | 3   | ARG  |
| 4   | D     | 9   | CYS  |
| 4   | D     | 21  | LEU  |
| 4   | D     | 34  | GLU  |
| 4   | D     | 35  | ARG  |
| 4   | D     | 47  | ARG  |
| 4   | D     | 53  | ASP  |
| 4   | D     | 58  | LEU  |
| 4   | D     | 61  | LYS  |
| 4   | D     | 66  | ARG  |
| 4   | D     | 96  | LEU  |
| 4   | D     | 122 | ARG  |
| 4   | D     | 127 | THR  |
| 4   | D     | 131 | ARG  |
| 4   | D     | 134 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 141 | ARG  |
| 4   | D     | 153 | ARG  |
| 4   | D     | 199 | ASN  |
| 5   | E     | 6   | PHE  |
| 5   | E     | 12  | LEU  |
| 5   | E     | 15  | ARG  |
| 5   | E     | 16  | THR  |
| 5   | E     | 20  | GLN  |
| 5   | E     | 24  | ARG  |
| 5   | E     | 38  | GLN  |
| 5   | E     | 41  | VAL  |
| 5   | E     | 53  | LEU  |
| 5   | E     | 73  | ASN  |
| 5   | E     | 78  | HIS  |
| 5   | E     | 82  | VAL  |
| 5   | E     | 89  | ILE  |
| 5   | E     | 125 | SER  |
| 5   | E     | 126 | ARG  |
| 6   | F     | 10  | LEU  |
| 6   | F     | 47  | ARG  |
| 6   | F     | 98  | LEU  |
| 7   | G     | 4   | ARG  |
| 7   | G     | 11  | GLN  |
| 7   | G     | 12  | LEU  |
| 7   | G     | 16  | LEU  |
| 7   | G     | 22  | LEU  |
| 7   | G     | 45  | ASP  |
| 7   | G     | 76  | ARG  |
| 7   | G     | 85  | TYR  |
| 7   | G     | 96  | GLN  |
| 7   | G     | 113 | GLU  |
| 7   | G     | 126 | ASP  |
| 7   | G     | 140 | ASP  |
| 8   | H     | 22  | GLU  |
| 8   | H     | 26  | VAL  |
| 8   | H     | 39  | LEU  |
| 8   | H     | 63  | LEU  |
| 8   | H     | 68  | ARG  |
| 8   | H     | 69  | ARG  |
| 8   | H     | 81  | HIS  |
| 8   | H     | 84  | ARG  |
| 8   | H     | 85  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | H     | 88  | LYS  |
| 8   | H     | 91  | ARG  |
| 8   | H     | 92  | ARG  |
| 8   | H     | 102 | ARG  |
| 8   | H     | 127 | LEU  |
| 8   | H     | 133 | LEU  |
| 9   | I     | 10  | ARG  |
| 9   | I     | 14  | VAL  |
| 9   | I     | 16  | ARG  |
| 9   | I     | 20  | ARG  |
| 9   | I     | 23  | ASN  |
| 9   | I     | 35  | GLU  |
| 9   | I     | 47  | LEU  |
| 9   | I     | 56  | LEU  |
| 9   | I     | 64  | THR  |
| 9   | I     | 75  | ASP  |
| 9   | I     | 91  | ASP  |
| 9   | I     | 113 | LYS  |
| 9   | I     | 114 | TYR  |
| 9   | I     | 121 | ARG  |
| 10  | J     | 3   | LYS  |
| 10  | J     | 28  | ARG  |
| 10  | J     | 60  | ARG  |
| 10  | J     | 65  | LEU  |
| 10  | J     | 70  | ARG  |
| 10  | J     | 71  | LEU  |
| 11  | K     | 29  | ILE  |
| 11  | K     | 35  | PRO  |
| 11  | K     | 48  | ILE  |
| 11  | K     | 81  | ASP  |
| 11  | K     | 92  | GLU  |
| 12  | L     | 12  | ARG  |
| 12  | L     | 19  | ARG  |
| 12  | L     | 41  | ARG  |
| 12  | L     | 46  | LYS  |
| 12  | L     | 47  | LYS  |
| 12  | L     | 53  | ARG  |
| 12  | L     | 79  | GLU  |
| 12  | L     | 85  | ILE  |
| 12  | L     | 89  | ARG  |
| 12  | L     | 91  | LYS  |
| 12  | L     | 99  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | L     | 113 | ARG  |
| 12  | L     | 126 | LYS  |
| 13  | M     | 9   | ILE  |
| 13  | M     | 40  | ASN  |
| 13  | M     | 70  | LEU  |
| 13  | M     | 77  | ASN  |
| 13  | M     | 105 | THR  |
| 13  | M     | 121 | LYS  |
| 14  | N     | 8   | GLU  |
| 14  | N     | 16  | PHE  |
| 14  | N     | 22  | THR  |
| 14  | N     | 33  | VAL  |
| 14  | N     | 44  | LEU  |
| 15  | O     | 6   | GLU  |
| 15  | O     | 24  | SER  |
| 15  | O     | 31  | LEU  |
| 15  | O     | 40  | SER  |
| 15  | O     | 81  | LEU  |
| 16  | P     | 1   | MET  |
| 16  | P     | 2   | VAL  |
| 16  | P     | 8   | ARG  |
| 16  | P     | 42  | ARG  |
| 16  | P     | 45  | THR  |
| 16  | P     | 76  | GLN  |
| 16  | P     | 80  | PHE  |
| 17  | Q     | 38  | ARG  |
| 17  | Q     | 60  | ILE  |
| 17  | Q     | 74  | LEU  |
| 17  | Q     | 92  | ARG  |
| 18  | R     | 26  | LEU  |
| 18  | R     | 28  | GLU  |
| 18  | R     | 39  | VAL  |
| 18  | R     | 53  | ARG  |
| 18  | R     | 54  | ARG  |
| 18  | R     | 69  | THR  |
| 18  | R     | 87  | ARG  |
| 19  | S     | 5   | LEU  |
| 19  | S     | 7   | LYS  |
| 19  | S     | 13  | ASP  |
| 19  | S     | 22  | LEU  |
| 19  | S     | 53  | ASN  |
| 19  | S     | 78  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | T     | 8   | ARG  |
| 20  | T     | 9   | ASN  |
| 20  | T     | 10  | LEU  |
| 20  | T     | 42  | GLN  |
| 20  | T     | 57  | ARG  |
| 20  | T     | 68  | LYS  |
| 20  | T     | 73  | HIS  |
| 20  | T     | 75  | ASN  |
| 20  | T     | 83  | ARG  |
| 20  | T     | 84  | LEU  |
| 21  | V     | 3   | LYS  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 37  | ASN  |
| 2   | B     | 204 | ASN  |
| 3   | C     | 28  | GLN  |
| 3   | C     | 31  | HIS  |
| 3   | C     | 108 | ASN  |
| 3   | C     | 110 | ASN  |
| 3   | C     | 123 | GLN  |
| 3   | C     | 139 | GLN  |
| 3   | C     | 170 | GLN  |
| 3   | C     | 176 | HIS  |
| 4   | D     | 45  | GLN  |
| 4   | D     | 62  | GLN  |
| 4   | D     | 123 | HIS  |
| 4   | D     | 161 | ASN  |
| 4   | D     | 199 | ASN  |
| 5   | E     | 20  | GLN  |
| 5   | E     | 73  | ASN  |
| 6   | F     | 11  | ASN  |
| 6   | F     | 18  | GLN  |
| 6   | F     | 27  | GLN  |
| 6   | F     | 57  | GLN  |
| 6   | F     | 73  | ASN  |
| 6   | F     | 100 | ASN  |
| 7   | G     | 11  | GLN  |
| 7   | G     | 13  | GLN  |
| 7   | G     | 28  | ASN  |
| 7   | G     | 68  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | G     | 106 | GLN  |
| 7   | G     | 148 | ASN  |
| 9   | I     | 23  | ASN  |
| 9   | I     | 29  | ASN  |
| 9   | I     | 73  | GLN  |
| 10  | J     | 13  | HIS  |
| 10  | J     | 56  | HIS  |
| 10  | J     | 62  | HIS  |
| 10  | J     | 78  | ASN  |
| 11  | K     | 22  | HIS  |
| 11  | K     | 117 | ASN  |
| 12  | L     | 49  | ASN  |
| 12  | L     | 75  | HIS  |
| 13  | M     | 12  | ASN  |
| 13  | M     | 40  | ASN  |
| 13  | M     | 62  | ASN  |
| 14  | N     | 52  | GLN  |
| 15  | O     | 13  | GLN  |
| 15  | O     | 46  | HIS  |
| 17  | Q     | 16  | GLN  |
| 19  | S     | 14  | HIS  |
| 19  | S     | 23  | ASN  |
| 19  | S     | 53  | ASN  |
| 20  | T     | 9   | ASN  |
| 20  | T     | 90  | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed         | Backbone Outliers | Pucker Outliers |
|-----|-------|------------------|-------------------|-----------------|
| 1   | A     | 1513/1513 (100%) | 344 (22%)         | 188 (12%)       |
| 22  | W     | 2/3 (66%)        | 0                 | 0               |
| 23  | X     | 8/11 (72%)       | 3 (37%)           | 2 (25%)         |
| All | All   | 1523/1527 (99%)  | 347 (22%)         | 190 (12%)       |

All (347) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 6   | G    |
| 1   | A     | 8   | A    |
| 1   | A     | 9   | G    |
| 1   | A     | 13  | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 14  | U    |
| 1   | A     | 26  | A    |
| 1   | A     | 31  | G    |
| 1   | A     | 32  | A    |
| 1   | A     | 39  | G    |
| 1   | A     | 47  | C    |
| 1   | A     | 48  | C    |
| 1   | A     | 49  | U    |
| 1   | A     | 50  | A    |
| 1   | A     | 51  | A    |
| 1   | A     | 52  | G    |
| 1   | A     | 61  | G    |
| 1   | A     | 65  | U    |
| 1   | A     | 66  | G    |
| 1   | A     | 80  | U    |
| 1   | A     | 94  | A    |
| 1   | A     | 101 | G    |
| 1   | A     | 102 | A    |
| 1   | A     | 103 | C    |
| 1   | A     | 109 | A    |
| 1   | A     | 113 | A    |
| 1   | A     | 114 | C    |
| 1   | A     | 115 | G    |
| 1   | A     | 123 | G    |
| 1   | A     | 124 | A    |
| 1   | A     | 125 | C    |
| 1   | A     | 157 | C    |
| 1   | A     | 167 | U    |
| 1   | A     | 168 | C    |
| 1   | A     | 176 | U    |
| 1   | A     | 177 | G    |
| 1   | A     | 189 | U    |
| 1   | A     | 190 | G    |
| 1   | A     | 191 | G    |
| 1   | A     | 203 | A    |
| 1   | A     | 204 | G    |
| 1   | A     | 208 | U    |
| 1   | A     | 209 | U    |
| 1   | A     | 210 | U    |
| 1   | A     | 239 | U    |
| 1   | A     | 240 | C    |
| 1   | A     | 242 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 246 | G    |
| 1   | A     | 247 | U    |
| 1   | A     | 248 | U    |
| 1   | A     | 261 | G    |
| 1   | A     | 262 | C    |
| 1   | A     | 270 | G    |
| 1   | A     | 274 | A    |
| 1   | A     | 275 | C    |
| 1   | A     | 276 | G    |
| 1   | A     | 277 | A    |
| 1   | A     | 284 | G    |
| 1   | A     | 292 | G    |
| 1   | A     | 293 | A    |
| 1   | A     | 301 | G    |
| 1   | A     | 311 | G    |
| 1   | A     | 316 | A    |
| 1   | A     | 323 | C    |
| 1   | A     | 324 | A    |
| 1   | A     | 325 | C    |
| 1   | A     | 327 | G    |
| 1   | A     | 339 | A    |
| 1   | A     | 340 | C    |
| 1   | A     | 341 | G    |
| 1   | A     | 342 | G    |
| 1   | A     | 347 | C    |
| 1   | A     | 348 | A    |
| 1   | A     | 349 | G    |
| 1   | A     | 362 | U    |
| 1   | A     | 363 | U    |
| 1   | A     | 368 | A    |
| 1   | A     | 384 | A    |
| 1   | A     | 392 | A    |
| 1   | A     | 393 | C    |
| 1   | A     | 405 | G    |
| 1   | A     | 406 | A    |
| 1   | A     | 407 | A    |
| 1   | A     | 408 | G    |
| 1   | A     | 417 | C    |
| 1   | A     | 418 | G    |
| 1   | A     | 419 | G    |
| 1   | A     | 423 | G    |
| 1   | A     | 424 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 425 | A    |
| 1   | A     | 434 | A    |
| 1   | A     | 446 | A    |
| 1   | A     | 447 | A    |
| 1   | A     | 454 | A    |
| 1   | A     | 455 | C    |
| 1   | A     | 456 | G    |
| 1   | A     | 465 | G    |
| 1   | A     | 466 | A    |
| 1   | A     | 468 | G    |
| 1   | A     | 469 | G    |
| 1   | A     | 470 | U    |
| 1   | A     | 480 | A    |
| 1   | A     | 481 | U    |
| 1   | A     | 483 | G    |
| 1   | A     | 491 | C    |
| 1   | A     | 492 | A    |
| 1   | A     | 494 | C    |
| 1   | A     | 495 | U    |
| 1   | A     | 501 | C    |
| 1   | A     | 502 | C    |
| 1   | A     | 510 | G    |
| 1   | A     | 513 | G    |
| 1   | A     | 514 | U    |
| 1   | A     | 515 | A    |
| 1   | A     | 516 | A    |
| 1   | A     | 517 | U    |
| 1   | A     | 519 | C    |
| 1   | A     | 531 | G    |
| 1   | A     | 533 | G    |
| 1   | A     | 542 | A    |
| 1   | A     | 543 | U    |
| 1   | A     | 544 | U    |
| 1   | A     | 545 | C    |
| 1   | A     | 546 | A    |
| 1   | A     | 550 | G    |
| 1   | A     | 555 | A    |
| 1   | A     | 556 | A    |
| 1   | A     | 558 | G    |
| 1   | A     | 559 | G    |
| 1   | A     | 560 | G    |
| 1   | A     | 571 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 578 | G    |
| 1   | A     | 579 | C    |
| 1   | A     | 602 | U    |
| 1   | A     | 625 | A    |
| 1   | A     | 636 | A    |
| 1   | A     | 637 | G    |
| 1   | A     | 648 | A    |
| 1   | A     | 670 | A    |
| 1   | A     | 671 | G    |
| 1   | A     | 684 | C    |
| 1   | A     | 685 | A    |
| 1   | A     | 686 | G    |
| 1   | A     | 687 | A    |
| 1   | A     | 701 | G    |
| 1   | A     | 704 | G    |
| 1   | A     | 705 | A    |
| 1   | A     | 706 | U    |
| 1   | A     | 707 | G    |
| 1   | A     | 714 | G    |
| 1   | A     | 716 | A    |
| 1   | A     | 717 | G    |
| 1   | A     | 732 | C    |
| 1   | A     | 736 | A    |
| 1   | A     | 737 | C    |
| 1   | A     | 738 | G    |
| 1   | A     | 760 | A    |
| 1   | A     | 764 | A    |
| 1   | A     | 770 | A    |
| 1   | A     | 775 | A    |
| 1   | A     | 776 | U    |
| 1   | A     | 777 | A    |
| 1   | A     | 796 | U    |
| 1   | A     | 798 | A    |
| 1   | A     | 799 | A    |
| 1   | A     | 800 | C    |
| 1   | A     | 801 | G    |
| 1   | A     | 802 | A    |
| 1   | A     | 803 | U    |
| 1   | A     | 804 | G    |
| 1   | A     | 811 | A    |
| 1   | A     | 822 | U    |
| 1   | A     | 823 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 824 | U    |
| 1   | A     | 825 | C    |
| 1   | A     | 826 | C    |
| 1   | A     | 835 | G    |
| 1   | A     | 848 | U    |
| 1   | A     | 849 | A    |
| 1   | A     | 850 | A    |
| 1   | A     | 851 | G    |
| 1   | A     | 862 | G    |
| 1   | A     | 866 | A    |
| 1   | A     | 867 | G    |
| 1   | A     | 868 | U    |
| 1   | A     | 879 | G    |
| 1   | A     | 891 | A    |
| 1   | A     | 899 | G    |
| 1   | A     | 903 | G    |
| 1   | A     | 904 | G    |
| 1   | A     | 911 | C    |
| 1   | A     | 912 | A    |
| 1   | A     | 922 | G    |
| 1   | A     | 936 | A    |
| 1   | A     | 937 | U    |
| 1   | A     | 938 | U    |
| 1   | A     | 943 | G    |
| 1   | A     | 945 | A    |
| 1   | A     | 946 | A    |
| 1   | A     | 948 | G    |
| 1   | A     | 949 | C    |
| 1   | A     | 951 | A    |
| 1   | A     | 952 | A    |
| 1   | A     | 953 | G    |
| 1   | A     | 954 | A    |
| 1   | A     | 955 | A    |
| 1   | A     | 959 | U    |
| 1   | A     | 960 | A    |
| 1   | A     | 961 | C    |
| 1   | A     | 969 | U    |
| 1   | A     | 970 | G    |
| 1   | A     | 971 | A    |
| 1   | A     | 981 | G    |
| 1   | A     | 982 | A    |
| 1   | A     | 983 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 984  | C    |
| 1   | A     | 986  | C    |
| 1   | A     | 987  | G    |
| 1   | A     | 988  | G    |
| 1   | A     | 1002 | G    |
| 1   | A     | 1003 | U    |
| 1   | A     | 1004 | G    |
| 1   | A     | 1007 | C    |
| 1   | A     | 1010 | C    |
| 1   | A     | 1025 | C    |
| 1   | A     | 1026 | A    |
| 1   | A     | 1028 | A    |
| 1   | A     | 1032 | G    |
| 1   | A     | 1036 | C    |
| 1   | A     | 1037 | A    |
| 1   | A     | 1047 | U    |
| 1   | A     | 1048 | C    |
| 1   | A     | 1050 | G    |
| 1   | A     | 1067 | U    |
| 1   | A     | 1068 | U    |
| 1   | A     | 1076 | G    |
| 1   | A     | 1082 | C    |
| 1   | A     | 1083 | A    |
| 1   | A     | 1084 | A    |
| 1   | A     | 1099 | G    |
| 1   | A     | 1106 | G    |
| 1   | A     | 1107 | U    |
| 1   | A     | 1109 | G    |
| 1   | A     | 1111 | C    |
| 1   | A     | 1112 | A    |
| 1   | A     | 1115 | G    |
| 1   | A     | 1117 | U    |
| 1   | A     | 1118 | U    |
| 1   | A     | 1119 | C    |
| 1   | A     | 1120 | G    |
| 1   | A     | 1121 | G    |
| 1   | A     | 1122 | C    |
| 1   | A     | 1128 | A    |
| 1   | A     | 1134 | A    |
| 1   | A     | 1139 | A    |
| 1   | A     | 1140 | C    |
| 1   | A     | 1141 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1142 | G    |
| 1   | A     | 1164 | A    |
| 1   | A     | 1165 | G    |
| 1   | A     | 1172 | A    |
| 1   | A     | 1177 | U    |
| 1   | A     | 1178 | G    |
| 1   | A     | 1181 | C    |
| 1   | A     | 1182 | A    |
| 1   | A     | 1183 | G    |
| 1   | A     | 1184 | C    |
| 1   | A     | 1192 | U    |
| 1   | A     | 1193 | U    |
| 1   | A     | 1194 | A    |
| 1   | A     | 1195 | C    |
| 1   | A     | 1196 | G    |
| 1   | A     | 1206 | A    |
| 1   | A     | 1207 | C    |
| 1   | A     | 1208 | A    |
| 1   | A     | 1217 | A    |
| 1   | A     | 1219 | A    |
| 1   | A     | 1221 | U    |
| 1   | A     | 1222 | G    |
| 1   | A     | 1237 | A    |
| 1   | A     | 1238 | U    |
| 1   | A     | 1239 | G    |
| 1   | A     | 1241 | C    |
| 1   | A     | 1243 | C    |
| 1   | A     | 1260 | A    |
| 1   | A     | 1261 | A    |
| 1   | A     | 1262 | U    |
| 1   | A     | 1263 | C    |
| 1   | A     | 1266 | A    |
| 1   | A     | 1267 | A    |
| 1   | A     | 1268 | A    |
| 1   | A     | 1279 | C    |
| 1   | A     | 1280 | A    |
| 1   | A     | 1281 | G    |
| 1   | A     | 1282 | U    |
| 1   | A     | 1283 | U    |
| 1   | A     | 1284 | C    |
| 1   | A     | 1287 | A    |
| 1   | A     | 1300 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1301 | C    |
| 1   | A     | 1313 | A    |
| 1   | A     | 1317 | C    |
| 1   | A     | 1318 | G    |
| 1   | A     | 1327 | A    |
| 1   | A     | 1328 | G    |
| 1   | A     | 1329 | U    |
| 1   | A     | 1334 | G    |
| 1   | A     | 1344 | C    |
| 1   | A     | 1345 | A    |
| 1   | A     | 1346 | U    |
| 1   | A     | 1347 | G    |
| 1   | A     | 1361 | G    |
| 1   | A     | 1363 | U    |
| 1   | A     | 1376 | A    |
| 1   | A     | 1377 | C    |
| 1   | A     | 1379 | C    |
| 1   | A     | 1380 | A    |
| 1   | A     | 1382 | C    |
| 1   | A     | 1383 | G    |
| 1   | A     | 1424 | G    |
| 1   | A     | 1426 | A    |
| 1   | A     | 1427 | G    |
| 1   | A     | 1432 | C    |
| 1   | A     | 1433 | G    |
| 1   | A     | 1460 | A    |
| 1   | A     | 1461 | C    |
| 1   | A     | 1467 | C    |
| 1   | A     | 1469 | A    |
| 1   | A     | 1474 | G    |
| 1   | A     | 1475 | U    |
| 1   | A     | 1476 | A    |
| 1   | A     | 1479 | A    |
| 1   | A     | 1480 | A    |
| 1   | A     | 1481 | G    |
| 1   | A     | 1482 | G    |
| 1   | A     | 1483 | U    |
| 1   | A     | 1484 | A    |
| 1   | A     | 1494 | G    |
| 1   | A     | 1496 | A    |
| 1   | A     | 1497 | G    |
| 1   | A     | 1506 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1507 | G    |
| 1   | A     | 1510 | C    |
| 1   | A     | 1511 | A    |
| 1   | A     | 1516 | C    |
| 23  | X     | 32   | C    |
| 23  | X     | 39   | PSU  |
| 23  | X     | 40   | C    |

All (190) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 5   | U    |
| 1   | A     | 7   | G    |
| 1   | A     | 8   | A    |
| 1   | A     | 13  | U    |
| 1   | A     | 30  | U    |
| 1   | A     | 31  | G    |
| 1   | A     | 47  | C    |
| 1   | A     | 48  | C    |
| 1   | A     | 49  | U    |
| 1   | A     | 50  | A    |
| 1   | A     | 51  | A    |
| 1   | A     | 60  | A    |
| 1   | A     | 64  | G    |
| 1   | A     | 65  | U    |
| 1   | A     | 102 | A    |
| 1   | A     | 108 | G    |
| 1   | A     | 112 | A    |
| 1   | A     | 114 | C    |
| 1   | A     | 123 | G    |
| 1   | A     | 124 | A    |
| 1   | A     | 167 | U    |
| 1   | A     | 175 | G    |
| 1   | A     | 188 | U    |
| 1   | A     | 189 | U    |
| 1   | A     | 190 | G    |
| 1   | A     | 203 | A    |
| 1   | A     | 208 | U    |
| 1   | A     | 209 | U    |
| 1   | A     | 211 | G    |
| 1   | A     | 238 | A    |
| 1   | A     | 239 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 241 | A    |
| 1   | A     | 245 | A    |
| 1   | A     | 246 | G    |
| 1   | A     | 261 | G    |
| 1   | A     | 269 | A    |
| 1   | A     | 274 | A    |
| 1   | A     | 275 | C    |
| 1   | A     | 276 | G    |
| 1   | A     | 300 | G    |
| 1   | A     | 310 | A    |
| 1   | A     | 322 | A    |
| 1   | A     | 323 | C    |
| 1   | A     | 324 | A    |
| 1   | A     | 339 | A    |
| 1   | A     | 340 | C    |
| 1   | A     | 346 | G    |
| 1   | A     | 361 | C    |
| 1   | A     | 362 | U    |
| 1   | A     | 367 | C    |
| 1   | A     | 383 | G    |
| 1   | A     | 407 | A    |
| 1   | A     | 416 | U    |
| 1   | A     | 417 | C    |
| 1   | A     | 423 | G    |
| 1   | A     | 424 | U    |
| 1   | A     | 433 | G    |
| 1   | A     | 445 | A    |
| 1   | A     | 446 | A    |
| 1   | A     | 454 | A    |
| 1   | A     | 455 | C    |
| 1   | A     | 465 | G    |
| 1   | A     | 468 | G    |
| 1   | A     | 469 | G    |
| 1   | A     | 479 | A    |
| 1   | A     | 480 | A    |
| 1   | A     | 482 | A    |
| 1   | A     | 491 | C    |
| 1   | A     | 494 | C    |
| 1   | A     | 500 | G    |
| 1   | A     | 501 | C    |
| 1   | A     | 513 | G    |
| 1   | A     | 516 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 518 | A    |
| 1   | A     | 530 | A    |
| 1   | A     | 542 | A    |
| 1   | A     | 544 | U    |
| 1   | A     | 545 | C    |
| 1   | A     | 549 | G    |
| 1   | A     | 558 | G    |
| 1   | A     | 559 | G    |
| 1   | A     | 570 | G    |
| 1   | A     | 578 | G    |
| 1   | A     | 624 | U    |
| 1   | A     | 635 | U    |
| 1   | A     | 636 | A    |
| 1   | A     | 670 | A    |
| 1   | A     | 684 | C    |
| 1   | A     | 685 | A    |
| 1   | A     | 686 | G    |
| 1   | A     | 700 | C    |
| 1   | A     | 704 | G    |
| 1   | A     | 705 | A    |
| 1   | A     | 716 | A    |
| 1   | A     | 731 | C    |
| 1   | A     | 735 | G    |
| 1   | A     | 736 | A    |
| 1   | A     | 775 | A    |
| 1   | A     | 776 | U    |
| 1   | A     | 795 | C    |
| 1   | A     | 798 | A    |
| 1   | A     | 800 | C    |
| 1   | A     | 801 | G    |
| 1   | A     | 802 | A    |
| 1   | A     | 803 | U    |
| 1   | A     | 823 | C    |
| 1   | A     | 847 | U    |
| 1   | A     | 848 | U    |
| 1   | A     | 849 | A    |
| 1   | A     | 850 | A    |
| 1   | A     | 861 | U    |
| 1   | A     | 866 | A    |
| 1   | A     | 867 | G    |
| 1   | A     | 890 | A    |
| 1   | A     | 911 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 937  | U    |
| 1   | A     | 942  | A    |
| 1   | A     | 945  | A    |
| 1   | A     | 948  | G    |
| 1   | A     | 951  | A    |
| 1   | A     | 952  | A    |
| 1   | A     | 953  | G    |
| 1   | A     | 959  | U    |
| 1   | A     | 969  | U    |
| 1   | A     | 970  | G    |
| 1   | A     | 982  | A    |
| 1   | A     | 1031 | U    |
| 1   | A     | 1047 | U    |
| 1   | A     | 1049 | A    |
| 1   | A     | 1067 | U    |
| 1   | A     | 1083 | A    |
| 1   | A     | 1106 | G    |
| 1   | A     | 1111 | C    |
| 1   | A     | 1121 | G    |
| 1   | A     | 1127 | C    |
| 1   | A     | 1133 | A    |
| 1   | A     | 1139 | A    |
| 1   | A     | 1141 | U    |
| 1   | A     | 1163 | G    |
| 1   | A     | 1164 | A    |
| 1   | A     | 1171 | G    |
| 1   | A     | 1177 | U    |
| 1   | A     | 1181 | C    |
| 1   | A     | 1182 | A    |
| 1   | A     | 1194 | A    |
| 1   | A     | 1195 | C    |
| 1   | A     | 1205 | G    |
| 1   | A     | 1206 | A    |
| 1   | A     | 1207 | C    |
| 1   | A     | 1220 | A    |
| 1   | A     | 1221 | U    |
| 1   | A     | 1238 | U    |
| 1   | A     | 1259 | U    |
| 1   | A     | 1261 | A    |
| 1   | A     | 1262 | U    |
| 1   | A     | 1266 | A    |
| 1   | A     | 1278 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1279 | C    |
| 1   | A     | 1281 | G    |
| 1   | A     | 1282 | U    |
| 1   | A     | 1283 | U    |
| 1   | A     | 1286 | G    |
| 1   | A     | 1312 | G    |
| 1   | A     | 1316 | C    |
| 1   | A     | 1317 | C    |
| 1   | A     | 1326 | U    |
| 1   | A     | 1327 | A    |
| 1   | A     | 1328 | G    |
| 1   | A     | 1345 | A    |
| 1   | A     | 1346 | U    |
| 1   | A     | 1362 | U    |
| 1   | A     | 1376 | A    |
| 1   | A     | 1378 | A    |
| 1   | A     | 1379 | C    |
| 1   | A     | 1381 | C    |
| 1   | A     | 1382 | C    |
| 1   | A     | 1426 | A    |
| 1   | A     | 1431 | A    |
| 1   | A     | 1432 | C    |
| 1   | A     | 1475 | U    |
| 1   | A     | 1479 | A    |
| 1   | A     | 1480 | A    |
| 1   | A     | 1481 | G    |
| 1   | A     | 1482 | G    |
| 1   | A     | 1483 | U    |
| 1   | A     | 1505 | U    |
| 1   | A     | 1506 | G    |
| 1   | A     | 1510 | C    |
| 23  | X     | 31   | A    |
| 23  | X     | 39   | PSU  |

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

3 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 | $\# Z  > 2$ |
| 23  | 70U  | X     | 34  | 22,23 | 17,26,27     | 1.04 | 2 (11%)     | 20,37,40    | 3.20 | 3 (15%)     |
| 23  | 12A  | X     | 37  | 23    | 24,36,37     | 1.30 | 4 (16%)     | 28,52,55    | 1.95 | 8 (28%)     |
| 23  | PSU  | X     | 39  | 23    | 13,21,22     | 0.68 | 0           | 18,30,33    | 5.09 | 6 (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   |
|-----|------|-------|-----|-------|---------|------------|---------|
| 23  | 70U  | X     | 34  | 22,23 | -       | 0/9/31/32  | 0/2/2/2 |
| 23  | 12A  | X     | 37  | 23    | -       | 0/17/43/44 | 0/3/3/3 |
| 23  | PSU  | X     | 39  | 23    | -       | 0/7/25/26  | 0/2/2/2 |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 23  | X     | 34  | 70U  | C6-N1   | 2.03 | 1.38        | 1.35     |
| 23  | X     | 37  | 12A  | C6-N1   | 2.07 | 1.35        | 1.33     |
| 23  | X     | 37  | 12A  | O4'-C1' | 2.09 | 1.43        | 1.41     |
| 23  | X     | 37  | 12A  | CA-N    | 2.25 | 1.51        | 1.46     |
| 23  | X     | 34  | 70U  | C4-N3   | 3.22 | 1.39        | 1.33     |
| 23  | X     | 37  | 12A  | C6-N6   | 3.32 | 1.42        | 1.36     |

All (17) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 23  | X     | 39  | PSU  | N1-C2-N3    | -17.37 | 117.25      | 128.33   |
| 23  | X     | 34  | 70U  | C5-C4-N3    | -9.23  | 114.59      | 125.04   |
| 23  | X     | 37  | 12A  | C6-N6-CC    | -6.01  | 122.35      | 130.39   |
| 23  | X     | 37  | 12A  | OO-CC-N6    | -2.95  | 119.10      | 123.58   |
| 23  | X     | 37  | 12A  | C5-C6-N1    | -2.90  | 117.49      | 120.48   |
| 23  | X     | 37  | 12A  | C4-C5-N7    | -2.81  | 106.90      | 109.48   |
| 23  | X     | 39  | PSU  | C5-C1'-C2'  | -2.77  | 110.61      | 115.52   |
| 23  | X     | 37  | 12A  | N3-C2-N1    | -2.69  | 121.64      | 126.79   |
| 23  | X     | 34  | 70U  | C5M-C5-C4   | -2.48  | 116.92      | 120.93   |
| 23  | X     | 37  | 12A  | C1'-N9-C4   | -2.09  | 123.78      | 126.94   |
| 23  | X     | 39  | PSU  | C4'-O4'-C1' | 2.43   | 112.06      | 109.58   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23  | X     | 37  | 12A  | C2-N1-C6    | 3.14  | 122.57      | 113.35   |
| 23  | X     | 37  | 12A  | N6-CC-N     | 3.26  | 119.00      | 113.81   |
| 23  | X     | 39  | PSU  | C3'-C2'-C1' | 5.14  | 107.75      | 101.79   |
| 23  | X     | 39  | PSU  | C6-N1-C2    | 5.34  | 124.06      | 115.47   |
| 23  | X     | 39  | PSU  | C4-N3-C2    | 9.14  | 123.14      | 115.25   |
| 23  | X     | 34  | 70U  | C2-N3-C4    | 10.25 | 127.19      | 115.95   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 25 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 23  | X     | 34  | 70U  | 5       | 0            |
| 23  | X     | 37  | 12A  | 11      | 0            |
| 23  | X     | 39  | PSU  | 9       | 0            |

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 188 ligands modelled in this entry, 187 are monoatomic - leaving 1 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 26  | PAR  | A     | 1783 | -    | 45,45,45     | 0.64 | 0           | 59,67,67    | 1.32 | 7 (11%)     |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 26  | PAR  | A     | 1783 | -    | -       | 0/18/94/94 | 0/4/4/4 |

There are no bond length outliers.

All (7) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 26  | A     | 1783 | PAR  | C14-O33-C33 | -3.98 | 107.60      | 118.01   |
| 26  | A     | 1783 | PAR  | C64-C54-C44 | -3.09 | 107.33      | 113.17   |
| 26  | A     | 1783 | PAR  | C11-O11-C42 | -2.98 | 110.21      | 118.01   |
| 26  | A     | 1783 | PAR  | C13-O52-C52 | -2.65 | 111.08      | 118.01   |
| 26  | A     | 1783 | PAR  | C11-O51-C51 | -2.37 | 109.14      | 113.75   |
| 26  | A     | 1783 | PAR  | C23-C33-C43 | -2.18 | 99.20       | 103.29   |
| 26  | A     | 1783 | PAR  | O54-C54-C64 | 4.16  | 114.23      | 106.10   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 26  | A     | 1783 | PAR  | 5       | 0            |

## 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     | 1512/1513 (99%) | 0.95   | 80 (5%) 30 12  | 29, 58, 125, 178      | 0     |
| 2   | B     | 234/256 (91%)   | 0.61   | 18 (7%) 16 5   | 50, 92, 137, 145      | 0     |
| 3   | C     | 206/239 (86%)   | 0.45   | 8 (3%) 43 21   | 57, 83, 119, 125      | 0     |
| 4   | D     | 208/209 (99%)   | 0.42   | 14 (6%) 21 8   | 45, 66, 101, 106      | 0     |
| 5   | E     | 150/162 (92%)   | 0.30   | 3 (2%) 68 47   | 33, 51, 67, 82        | 0     |
| 6   | F     | 101/101 (100%)  | 0.23   | 3 (2%) 54 30   | 64, 85, 102, 106      | 0     |
| 7   | G     | 155/156 (99%)   | 0.30   | 4 (2%) 59 37   | 51, 75, 110, 123      | 0     |
| 8   | H     | 138/138 (100%)  | 0.25   | 2 (1%) 78 61   | 30, 47, 61, 70        | 0     |
| 9   | I     | 127/128 (99%)   | 0.59   | 13 (10%) 9 3   | 44, 85, 102, 108      | 0     |
| 10  | J     | 98/105 (93%)    | 1.03   | 16 (16%) 2 1   | 57, 116, 139, 143     | 0     |
| 11  | K     | 119/129 (92%)   | 0.41   | 4 (3%) 49 25   | 42, 58, 84, 97        | 0     |
| 12  | L     | 124/132 (93%)   | 0.43   | 7 (5%) 28 11   | 19, 57, 70, 97        | 0     |
| 13  | M     | 125/126 (99%)   | 0.77   | 16 (12%) 5 2   | 59, 71, 129, 157      | 0     |
| 14  | N     | 60/61 (98%)     | 0.80   | 6 (10%) 9 3    | 58, 74, 109, 114      | 0     |
| 15  | O     | 88/89 (98%)     | 0.16   | 2 (2%) 64 41   | 39, 61, 87, 104       | 0     |
| 16  | P     | 83/88 (94%)     | 0.32   | 0 100 100      | 38, 47, 59, 83        | 0     |
| 17  | Q     | 104/105 (99%)   | 0.37   | 4 (3%) 44 22   | 33, 50, 108, 131      | 0     |
| 18  | R     | 73/88 (82%)     | 0.29   | 1 (1%) 78 61   | 49, 70, 111, 129      | 0     |
| 19  | S     | 80/93 (86%)     | 0.40   | 5 (6%) 23 9    | 80, 93, 112, 115      | 0     |
| 20  | T     | 99/106 (93%)    | 0.28   | 2 (2%) 68 47   | 40, 55, 80, 86        | 0     |
| 21  | V     | 24/27 (88%)     | 1.07   | 3 (12%) 5 2    | 49, 63, 79, 89        | 0     |
| 22  | W     | 3/3 (100%)      | 0.96   | 0 100 100      | 57, 57, 62, 63        | 0     |
| 23  | X     | 8/11 (72%)      | 1.01   | 1 (12%) 5 2    | 67, 101, 127, 137     | 0     |
| All | All   | 3919/4065 (96%) | 0.64   | 212 (5%) 29 12 | 19, 64, 121, 178      | 0     |

All (212) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 13  | M     | 121  | LYS  | 9.1  |
| 1   | A     | 1516 | C    | 7.0  |
| 13  | M     | 120  | LYS  | 6.8  |
| 13  | M     | 124  | PRO  | 6.0  |
| 2   | B     | 10   | LEU  | 5.9  |
| 11  | K     | 128  | ALA  | 5.4  |
| 9   | I     | 128  | ARG  | 5.2  |
| 19  | S     | 37   | ARG  | 5.1  |
| 1   | A     | 1510 | C    | 5.1  |
| 2   | B     | 123  | ALA  | 4.9  |
| 13  | M     | 118  | ALA  | 4.9  |
| 13  | M     | 126  | LYS  | 4.8  |
| 4   | D     | 21   | LEU  | 4.7  |
| 13  | M     | 122  | LYS  | 4.6  |
| 13  | M     | 117  | VAL  | 4.5  |
| 1   | A     | 1518 | U    | 4.5  |
| 19  | S     | 3    | ARG  | 4.5  |
| 2   | B     | 133  | LYS  | 4.3  |
| 1   | A     | 983  | A    | 4.3  |
| 3   | C     | 21   | ARG  | 4.3  |
| 13  | M     | 7    | VAL  | 4.1  |
| 20  | T     | 103  | GLY  | 4.1  |
| 10  | J     | 24   | VAL  | 4.0  |
| 2   | B     | 11   | LEU  | 4.0  |
| 1   | A     | 1111 | C    | 4.0  |
| 3   | C     | 54   | ARG  | 3.9  |
| 6   | F     | 101  | ALA  | 3.9  |
| 13  | M     | 119  | GLY  | 3.9  |
| 2   | B     | 13   | ALA  | 3.8  |
| 9   | I     | 19   | LEU  | 3.8  |
| 1   | A     | 1004 | G    | 3.8  |
| 4   | D     | 23   | GLY  | 3.7  |
| 1   | A     | 1517 | U    | 3.7  |
| 4   | D     | 74   | GLN  | 3.7  |
| 9   | I     | 70   | LYS  | 3.7  |
| 14  | N     | 30   | ALA  | 3.6  |
| 1   | A     | 433  | G    | 3.6  |
| 21  | V     | 6    | ARG  | 3.6  |
| 1   | A     | 513  | G    | 3.5  |
| 11  | K     | 129  | SER  | 3.5  |
| 10  | J     | 74   | ILE  | 3.5  |
| 20  | T     | 68   | LYS  | 3.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 17  | Q     | 104  | LYS  | 3.4  |
| 1   | A     | 1003 | U    | 3.4  |
| 13  | M     | 123  | ALA  | 3.3  |
| 17  | Q     | 105  | ALA  | 3.3  |
| 7   | G     | 85   | TYR  | 3.3  |
| 10  | J     | 7    | LYS  | 3.2  |
| 2   | B     | 229  | VAL  | 3.2  |
| 4   | D     | 49   | ARG  | 3.2  |
| 2   | B     | 81   | VAL  | 3.1  |
| 4   | D     | 73   | ARG  | 3.1  |
| 2   | B     | 21   | ARG  | 3.1  |
| 10  | J     | 5    | ARG  | 3.1  |
| 6   | F     | 98   | LEU  | 3.1  |
| 15  | O     | 89   | GLY  | 3.1  |
| 15  | O     | 88   | ARG  | 3.1  |
| 18  | R     | 16   | PRO  | 3.1  |
| 12  | L     | 19   | ARG  | 3.0  |
| 13  | M     | 106  | ASN  | 3.0  |
| 10  | J     | 20   | ALA  | 3.0  |
| 4   | D     | 27   | TYR  | 3.0  |
| 21  | V     | 10   | ARG  | 3.0  |
| 1   | A     | 1018 | G    | 3.0  |
| 1   | A     | 1035 | G    | 3.0  |
| 7   | G     | 5    | ARG  | 3.0  |
| 23  | X     | 40   | C    | 3.0  |
| 1   | A     | 981  | G    | 3.0  |
| 1   | A     | 1185 | A    | 3.0  |
| 9   | I     | 18   | PHE  | 2.9  |
| 21  | V     | 24   | ARG  | 2.9  |
| 8   | H     | 2    | LEU  | 2.9  |
| 17  | Q     | 96   | GLN  | 2.9  |
| 2   | B     | 230  | VAL  | 2.9  |
| 14  | N     | 60   | SER  | 2.9  |
| 1   | A     | 1455 | C    | 2.9  |
| 11  | K     | 51   | LYS  | 2.8  |
| 1   | A     | 984  | C    | 2.8  |
| 1   | A     | 408  | G    | 2.8  |
| 1   | A     | 1039 | G    | 2.8  |
| 1   | A     | 1109 | G    | 2.8  |
| 1   | A     | 1123 | C    | 2.8  |
| 10  | J     | 54   | PHE  | 2.8  |
| 2   | B     | 26   | PRO  | 2.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 19  | S     | 2    | PRO  | 2.8  |
| 2   | B     | 240  | GLN  | 2.8  |
| 5   | E     | 20   | GLN  | 2.8  |
| 14  | N     | 18   | VAL  | 2.7  |
| 17  | Q     | 17   | LYS  | 2.7  |
| 2   | B     | 23   | ARG  | 2.7  |
| 2   | B     | 76   | GLN  | 2.7  |
| 7   | G     | 84   | ASN  | 2.7  |
| 3   | C     | 26   | LYS  | 2.6  |
| 9   | I     | 17   | VAL  | 2.6  |
| 2   | B     | 231  | GLU  | 2.6  |
| 4   | D     | 75   | PHE  | 2.6  |
| 10  | J     | 92   | THR  | 2.6  |
| 3   | C     | 58   | GLU  | 2.6  |
| 4   | D     | 77   | ASN  | 2.6  |
| 4   | D     | 26   | CYS  | 2.6  |
| 1   | A     | 47   | C    | 2.6  |
| 9   | I     | 114  | TYR  | 2.6  |
| 1   | A     | 1027 | C    | 2.6  |
| 1   | A     | 955  | A    | 2.5  |
| 12  | L     | 20   | LYS  | 2.5  |
| 1   | A     | 1303 | C    | 2.5  |
| 1   | A     | 1128 | A    | 2.5  |
| 9   | I     | 92   | TYR  | 2.5  |
| 1   | A     | 391  | G    | 2.5  |
| 1   | A     | 1076 | G    | 2.5  |
| 1   | A     | 1336 | G    | 2.5  |
| 4   | D     | 22   | LYS  | 2.5  |
| 4   | D     | 70   | ILE  | 2.4  |
| 10  | J     | 72   | VAL  | 2.4  |
| 5   | E     | 5    | ASP  | 2.4  |
| 1   | A     | 1079 | C    | 2.4  |
| 1   | A     | 1508 | A    | 2.4  |
| 10  | J     | 41   | PRO  | 2.4  |
| 2   | B     | 29   | ALA  | 2.4  |
| 1   | A     | 1490 | A    | 2.4  |
| 4   | D     | 71   | SER  | 2.4  |
| 11  | K     | 11   | LYS  | 2.4  |
| 1   | A     | 372  | G    | 2.4  |
| 1   | A     | 1029 | G    | 2.4  |
| 13  | M     | 94   | ARG  | 2.4  |
| 10  | J     | 34   | VAL  | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 432  | U    | 2.4  |
| 1   | A     | 1270 | A    | 2.4  |
| 9   | I     | 124  | GLN  | 2.4  |
| 14  | N     | 13   | THR  | 2.4  |
| 19  | S     | 81   | ARG  | 2.4  |
| 1   | A     | 1165 | G    | 2.3  |
| 1   | A     | 1315 | G    | 2.3  |
| 13  | M     | 103  | THR  | 2.3  |
| 1   | A     | 527  | G    | 2.3  |
| 13  | M     | 104  | ARG  | 2.3  |
| 10  | J     | 6    | ILE  | 2.3  |
| 10  | J     | 53   | PRO  | 2.3  |
| 14  | N     | 6    | LEU  | 2.3  |
| 1   | A     | 954  | A    | 2.3  |
| 9   | I     | 61   | ALA  | 2.3  |
| 1   | A     | 1181 | C    | 2.3  |
| 1   | A     | 1241 | C    | 2.3  |
| 12  | L     | 31   | PRO  | 2.3  |
| 9   | I     | 9    | ARG  | 2.3  |
| 1   | A     | 528  | C    | 2.3  |
| 1   | A     | 1050 | G    | 2.3  |
| 3   | C     | 76   | VAL  | 2.2  |
| 1   | A     | 1396 | U    | 2.2  |
| 1   | A     | 67   | C    | 2.2  |
| 1   | A     | 846  | G    | 2.2  |
| 1   | A     | 1281 | G    | 2.2  |
| 13  | M     | 116  | THR  | 2.2  |
| 1   | A     | 515  | A    | 2.2  |
| 12  | L     | 17   | LYS  | 2.2  |
| 2   | B     | 35   | GLU  | 2.2  |
| 1   | A     | 1186 | U    | 2.2  |
| 1   | A     | 1205 | G    | 2.2  |
| 3   | C     | 151  | VAL  | 2.2  |
| 1   | A     | 1229 | A    | 2.2  |
| 1   | A     | 1207 | C    | 2.2  |
| 4   | D     | 72   | GLU  | 2.2  |
| 1   | A     | 1323 | C    | 2.2  |
| 1   | A     | 1509 | U    | 2.1  |
| 10  | J     | 42   | THR  | 2.1  |
| 13  | M     | 105  | THR  | 2.1  |
| 1   | A     | 1500 | G    | 2.1  |
| 9   | I     | 15   | ALA  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 116  | C    | 2.1  |
| 1   | A     | 539  | C    | 2.1  |
| 1   | A     | 1348 | C    | 2.1  |
| 3   | C     | 57   | ILE  | 2.1  |
| 1   | A     | 405  | G    | 2.1  |
| 6   | F     | 36   | ARG  | 2.1  |
| 14  | N     | 21   | TYR  | 2.1  |
| 1   | A     | 1519 | U    | 2.1  |
| 2   | B     | 27   | LYS  | 2.1  |
| 1   | A     | 309  | C    | 2.1  |
| 1   | A     | 1036 | C    | 2.1  |
| 1   | A     | 1167 | G    | 2.1  |
| 3   | C     | 110  | ASN  | 2.1  |
| 9   | I     | 125  | TYR  | 2.1  |
| 1   | A     | 1051 | C    | 2.1  |
| 1   | A     | 525  | G    | 2.1  |
| 1   | A     | 1071 | G    | 2.1  |
| 1   | A     | 1116 | G    | 2.1  |
| 1   | A     | 1257 | G    | 2.1  |
| 1   | A     | 1304 | G    | 2.1  |
| 10  | J     | 85   | LEU  | 2.1  |
| 12  | L     | 32   | PHE  | 2.1  |
| 2   | B     | 77   | ALA  | 2.1  |
| 12  | L     | 18   | VAL  | 2.1  |
| 19  | S     | 34   | TRP  | 2.1  |
| 1   | A     | 949  | C    | 2.1  |
| 10  | J     | 17   | ASP  | 2.1  |
| 1   | A     | 649  | G    | 2.0  |
| 1   | A     | 1474 | G    | 2.0  |
| 4   | D     | 3    | ARG  | 2.0  |
| 1   | A     | 1049 | A    | 2.0  |
| 1   | A     | 1299 | A    | 2.0  |
| 9   | I     | 102  | LEU  | 2.0  |
| 1   | A     | 22   | G    | 2.0  |
| 1   | A     | 980  | G    | 2.0  |
| 5   | E     | 60   | TYR  | 2.0  |
| 12  | L     | 51   | ALA  | 2.0  |
| 1   | A     | 486  | C    | 2.0  |
| 1   | A     | 1230 | C    | 2.0  |
| 10  | J     | 99   | LYS  | 2.0  |
| 1   | A     | 21   | G    | 2.0  |
| 1   | A     | 1032 | G    | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 7   | G     | 150 | ALA  | 2.0  |
| 8   | H     | 3   | THR  | 2.0  |

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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 |
|-----|------|-------|-----|-------|------|------|------|----------------------------|-------|
| 23  | 12A  | X     | 37  | 34/35 | 0.94 | 0.23 | -    | 71,71,71,71                | 0     |
| 23  | 70U  | X     | 34  | 25/26 | 0.92 | 0.29 | -    | 68,81,93,97                | 0     |
| 23  | PSU  | X     | 39  | 20/21 | 0.85 | 0.21 | -    | 86,86,88,88                | 0     |

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 24  | MG   | A     | 1683 | 1/1   | 0.76 | 1.03 | 42.18 | 27,27,27,27                | 1     |
| 24  | MG   | A     | 1737 | 1/1   | 0.48 | 1.08 | 28.95 | 22,22,22,22                | 1     |
| 24  | MG   | A     | 1756 | 1/1   | 0.32 | 0.83 | 28.63 | 30,30,30,30                | 1     |
| 24  | MG   | A     | 1779 | 1/1   | 0.85 | 0.57 | 12.51 | 24,24,24,24                | 1     |
| 24  | MG   | A     | 1757 | 1/1   | 0.32 | 0.52 | 9.26  | 9,9,9,9                    | 1     |
| 24  | MG   | A     | 1680 | 1/1   | 0.90 | 0.34 | 8.55  | 15,15,15,15                | 1     |
| 24  | MG   | A     | 1650 | 1/1   | 0.98 | 0.37 | 8.48  | 18,18,18,18                | 1     |
| 24  | MG   | A     | 1707 | 1/1   | 0.59 | 0.41 | 7.68  | 47,47,47,47                | 1     |
| 24  | MG   | A     | 1762 | 1/1   | 0.89 | 0.41 | 6.53  | 18,18,18,18                | 1     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 24  | MG   | A     | 1637 | 1/1   | 0.77 | 0.32 | 3.90  | 21,21,21,21                 | 1     |
| 24  | MG   | A     | 1667 | 1/1   | 0.76 | 0.37 | 2.89  | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1749 | 1/1   | 0.67 | 0.35 | 2.75  | 17,17,17,17                 | 1     |
| 24  | MG   | A     | 1755 | 1/1   | 0.77 | 0.29 | 2.39  | 3,3,3,3                     | 1     |
| 24  | MG   | A     | 1603 | 1/1   | 0.56 | 0.32 | 2.30  | 58,58,58,58                 | 0     |
| 24  | MG   | A     | 1621 | 1/1   | 0.84 | 0.26 | 1.74  | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1654 | 1/1   | 0.98 | 0.29 | 1.46  | 13,13,13,13                 | 1     |
| 24  | MG   | A     | 1761 | 1/1   | 0.97 | 0.29 | 1.39  | 8,8,8,8                     | 1     |
| 26  | PAR  | A     | 1783 | 42/42 | 0.94 | 0.29 | 1.25  | 43,53,68,70                 | 0     |
| 24  | MG   | A     | 1670 | 1/1   | 0.98 | 0.38 | 1.15  | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1724 | 1/1   | 0.85 | 0.27 | 0.80  | 15,15,15,15                 | 1     |
| 25  | ZN   | D     | 301  | 1/1   | 0.94 | 0.43 | 0.74  | 97,97,97,97                 | 0     |
| 24  | MG   | A     | 1723 | 1/1   | 0.91 | 0.29 | 0.41  | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1679 | 1/1   | 0.96 | 0.28 | -0.05 | 9,9,9,9                     | 1     |
| 24  | MG   | A     | 1740 | 1/1   | 0.93 | 0.24 | -0.19 | 1,1,1,1                     | 1     |
| 25  | ZN   | N     | 101  | 1/1   | 0.99 | 0.21 | -0.65 | 69,69,69,69                 | 0     |
| 24  | MG   | A     | 1758 | 1/1   | 0.96 | 0.25 | -0.70 | 12,12,12,12                 | 1     |
| 24  | MG   | A     | 1778 | 1/1   | 0.95 | 0.24 | -0.76 | 4,4,4,4                     | 1     |
| 24  | MG   | A     | 1625 | 1/1   | 0.76 | 0.24 | -0.80 | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1618 | 1/1   | 0.87 | 0.24 | -1.09 | 41,41,41,41                 | 1     |
| 24  | MG   | A     | 1673 | 1/1   | 0.87 | 0.19 | -1.10 | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1726 | 1/1   | 0.96 | 0.25 | -1.25 | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1770 | 1/1   | 0.98 | 0.21 | -1.42 | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1731 | 1/1   | 0.99 | 0.24 | -1.59 | 9,9,9,9                     | 1     |
| 24  | MG   | A     | 1688 | 1/1   | 0.95 | 0.21 | -1.88 | 16,16,16,16                 | 1     |
| 24  | MG   | A     | 1663 | 1/1   | 0.95 | 0.19 | -2.16 | 21,21,21,21                 | 1     |
| 24  | MG   | A     | 1648 | 1/1   | 0.97 | 0.23 | -2.20 | 11,11,11,11                 | 0     |
| 24  | MG   | A     | 1664 | 1/1   | 0.98 | 0.15 | -2.97 | 3,3,3,3                     | 1     |
| 24  | MG   | A     | 1775 | 1/1   | 0.86 | 0.18 | -3.06 | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1660 | 1/1   | 0.89 | 0.17 | -3.83 | 14,14,14,14                 | 1     |
| 24  | MG   | A     | 1708 | 1/1   | 0.95 | 0.15 | -4.62 | 8,8,8,8                     | 1     |
| 24  | MG   | A     | 1727 | 1/1   | 0.97 | 0.09 | -4.81 | 14,14,14,14                 | 1     |
| 24  | MG   | A     | 1691 | 1/1   | 0.93 | 0.08 | -4.87 | 16,16,16,16                 | 1     |
| 24  | MG   | A     | 1759 | 1/1   | 0.97 | 0.18 | -4.92 | 7,7,7,7                     | 1     |
| 24  | MG   | A     | 1711 | 1/1   | 0.82 | 0.42 | -     | 5,5,5,5                     | 1     |
| 24  | MG   | A     | 1669 | 1/1   | 0.73 | 1.31 | -     | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1709 | 1/1   | 0.91 | 0.38 | -     | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1645 | 1/1   | 0.86 | 0.23 | -     | 7,7,7,7                     | 1     |
| 24  | MG   | A     | 1629 | 1/1   | 0.89 | 0.23 | -     | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1631 | 1/1   | 0.68 | 0.64 | -     | 45,45,45,45                 | 1     |
| 24  | MG   | A     | 1763 | 1/1   | 0.74 | 0.29 | -     | 11,11,11,11                 | 1     |
| 24  | MG   | A     | 1777 | 1/1   | 0.85 | 0.38 | -     | 41,41,41,41                 | 1     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 24  | MG   | A     | 1748 | 1/1   | 0.95 | 0.18 | -    | 3,3,3,3                     | 1     |
| 24  | MG   | A     | 1633 | 1/1   | 0.91 | 0.25 | -    | 36,36,36,36                 | 1     |
| 24  | MG   | A     | 1782 | 1/1   | 0.84 | 0.29 | -    | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1656 | 1/1   | 0.92 | 0.30 | -    | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1634 | 1/1   | 0.96 | 0.23 | -    | 23,23,23,23                 | 1     |
| 24  | MG   | A     | 1747 | 1/1   | 0.94 | 0.31 | -    | 26,26,26,26                 | 1     |
| 24  | MG   | A     | 1700 | 1/1   | 0.29 | 0.97 | -    | 44,44,44,44                 | 1     |
| 24  | MG   | A     | 1729 | 1/1   | 0.83 | 0.28 | -    | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1602 | 1/1   | 0.69 | 0.24 | -    | 118,118,118,118             | 0     |
| 24  | MG   | A     | 1684 | 1/1   | 0.57 | 1.30 | -    | 28,28,28,28                 | 1     |
| 24  | MG   | A     | 1751 | 1/1   | 0.92 | 0.31 | -    | 42,42,42,42                 | 1     |
| 24  | MG   | A     | 1642 | 1/1   | 0.88 | 0.32 | -    | 22,22,22,22                 | 1     |
| 24  | MG   | A     | 1612 | 1/1   | 0.99 | 0.18 | -    | 8,8,8,8                     | 1     |
| 24  | MG   | A     | 1694 | 1/1   | 0.46 | 0.25 | -    | 26,26,26,26                 | 1     |
| 24  | MG   | A     | 1705 | 1/1   | 0.23 | 0.70 | -    | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1719 | 1/1   | 0.88 | 0.42 | -    | 19,19,19,19                 | 1     |
| 24  | MG   | A     | 1622 | 1/1   | 0.82 | 0.21 | -    | 47,47,47,47                 | 1     |
| 24  | MG   | A     | 1773 | 1/1   | 0.78 | 0.43 | -    | 31,31,31,31                 | 1     |
| 24  | MG   | S     | 101  | 1/1   | 0.74 | 0.82 | -    | 67,67,67,67                 | 1     |
| 24  | MG   | A     | 1624 | 1/1   | 0.99 | 0.20 | -    | 39,39,39,39                 | 1     |
| 24  | MG   | A     | 1746 | 1/1   | 0.90 | 0.39 | -    | 22,22,22,22                 | 1     |
| 24  | MG   | A     | 1672 | 1/1   | 0.80 | 0.35 | -    | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1703 | 1/1   | 0.89 | 0.36 | -    | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1616 | 1/1   | 0.78 | 0.28 | -    | 23,23,23,23                 | 1     |
| 24  | MG   | A     | 1655 | 1/1   | 0.92 | 0.32 | -    | 6,6,6,6                     | 1     |
| 24  | MG   | A     | 1627 | 1/1   | 0.89 | 0.23 | -    | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1651 | 1/1   | 0.95 | 0.33 | -    | 2,2,2,2                     | 1     |
| 24  | MG   | A     | 1720 | 1/1   | 0.89 | 0.37 | -    | 16,16,16,16                 | 1     |
| 24  | MG   | A     | 1668 | 1/1   | 0.97 | 0.32 | -    | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1697 | 1/1   | 0.92 | 0.23 | -    | 10,10,10,10                 | 1     |
| 24  | MG   | A     | 1732 | 1/1   | 0.76 | 0.26 | -    | 4,4,4,4                     | 1     |
| 24  | MG   | A     | 1772 | 1/1   | 0.89 | 0.31 | -    | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1676 | 1/1   | 0.77 | 0.16 | -    | 20,20,20,20                 | 1     |
| 24  | MG   | A     | 1649 | 1/1   | 0.97 | 0.24 | -    | 3,3,3,3                     | 1     |
| 24  | MG   | A     | 1687 | 1/1   | 0.92 | 0.45 | -    | 11,11,11,11                 | 1     |
| 24  | MG   | L     | 201  | 1/1   | 0.86 | 0.22 | -    | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1685 | 1/1   | 0.85 | 0.35 | -    | 25,25,25,25                 | 1     |
| 24  | MG   | A     | 1712 | 1/1   | 0.96 | 0.12 | -    | 23,23,23,23                 | 1     |
| 24  | MG   | A     | 1639 | 1/1   | 0.73 | 0.54 | -    | 59,59,59,59                 | 1     |
| 24  | MG   | A     | 1662 | 1/1   | 0.77 | 0.26 | -    | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1689 | 1/1   | 0.94 | 0.23 | -    | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1661 | 1/1   | 0.93 | 0.32 | -    | 4,4,4,4                     | 1     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 24  | MG   | A     | 1738 | 1/1   | 0.78 | 0.30 | -    | 15,15,15,15                 | 1     |
| 24  | MG   | A     | 1710 | 1/1   | 0.61 | 0.35 | -    | 47,47,47,47                 | 1     |
| 24  | MG   | A     | 1613 | 1/1   | 0.94 | 0.27 | -    | 30,30,30,30                 | 1     |
| 24  | MG   | A     | 1640 | 1/1   | 0.97 | 0.26 | -    | 66,66,66,66                 | 1     |
| 24  | MG   | A     | 1765 | 1/1   | 0.89 | 0.31 | -    | 8,8,8,8                     | 1     |
| 24  | MG   | A     | 1717 | 1/1   | 0.72 | 0.55 | -    | 7,7,7,7                     | 1     |
| 24  | MG   | A     | 1769 | 1/1   | 0.68 | 0.32 | -    | 15,15,15,15                 | 1     |
| 24  | MG   | A     | 1609 | 1/1   | 0.90 | 0.35 | -    | 35,35,35,35                 | 1     |
| 24  | MG   | A     | 1753 | 1/1   | 0.94 | 0.28 | -    | 5,5,5,5                     | 1     |
| 24  | MG   | A     | 1728 | 1/1   | 0.96 | 0.20 | -    | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1611 | 1/1   | 0.95 | 0.31 | -    | 18,18,18,18                 | 0     |
| 24  | MG   | B     | 301  | 1/1   | 0.73 | 0.19 | -    | 9,9,9,9                     | 1     |
| 24  | MG   | A     | 1666 | 1/1   | 0.48 | 0.32 | -    | 14,14,14,14                 | 1     |
| 24  | MG   | A     | 1628 | 1/1   | 0.75 | 0.37 | -    | 37,37,37,37                 | 1     |
| 24  | MG   | A     | 1739 | 1/1   | 0.79 | 0.35 | -    | 14,14,14,14                 | 1     |
| 24  | MG   | A     | 1733 | 1/1   | 0.94 | 0.28 | -    | 13,13,13,13                 | 1     |
| 24  | MG   | A     | 1608 | 1/1   | 0.57 | 0.19 | -    | 40,40,40,40                 | 1     |
| 24  | MG   | A     | 1665 | 1/1   | 0.92 | 0.16 | -    | 7,7,7,7                     | 1     |
| 24  | MG   | A     | 1735 | 1/1   | 0.92 | 0.44 | -    | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1695 | 1/1   | 0.65 | 0.36 | -    | 2,2,2,2                     | 1     |
| 24  | MG   | A     | 1644 | 1/1   | 0.34 | 0.33 | -    | 23,23,23,23                 | 1     |
| 24  | MG   | A     | 1659 | 1/1   | 0.91 | 0.23 | -    | 7,7,7,7                     | 1     |
| 24  | MG   | A     | 1715 | 1/1   | 0.94 | 0.32 | -    | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1657 | 1/1   | 0.86 | 0.33 | -    | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1647 | 1/1   | 0.73 | 0.35 | -    | 39,39,39,39                 | 1     |
| 24  | MG   | A     | 1678 | 1/1   | 0.88 | 0.19 | -    | 6,6,6,6                     | 1     |
| 24  | MG   | A     | 1698 | 1/1   | 0.66 | 0.29 | -    | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1681 | 1/1   | 0.97 | 0.18 | -    | 11,11,11,11                 | 1     |
| 24  | MG   | A     | 1750 | 1/1   | 0.65 | 0.36 | -    | 10,10,10,10                 | 1     |
| 24  | MG   | A     | 1604 | 1/1   | 0.65 | 0.66 | -    | 122,122,122,122             | 0     |
| 24  | MG   | A     | 1638 | 1/1   | 0.83 | 0.18 | -    | 11,11,11,11                 | 1     |
| 24  | MG   | A     | 1752 | 1/1   | 0.98 | 0.27 | -    | 19,19,19,19                 | 1     |
| 24  | MG   | A     | 1641 | 1/1   | 0.84 | 0.25 | -    | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1677 | 1/1   | 0.94 | 0.30 | -    | 2,2,2,2                     | 1     |
| 24  | MG   | A     | 1630 | 1/1   | 0.88 | 1.68 | -    | 87,87,87,87                 | 1     |
| 24  | MG   | A     | 1686 | 1/1   | 0.97 | 0.16 | -    | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1730 | 1/1   | 0.93 | 0.41 | -    | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1721 | 1/1   | 0.91 | 0.29 | -    | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1653 | 1/1   | 0.95 | 0.29 | -    | 5,5,5,5                     | 1     |
| 24  | MG   | A     | 1674 | 1/1   | 0.94 | 0.17 | -    | 24,24,24,24                 | 1     |
| 24  | MG   | A     | 1718 | 1/1   | 0.88 | 0.21 | -    | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1619 | 1/1   | 0.79 | 0.46 | -    | 46,46,46,46                 | 1     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 24  | MG   | A     | 1742 | 1/1   | 0.95 | 0.34 | -    | 22,22,22,22                 | 1     |
| 24  | MG   | A     | 1646 | 1/1   | 0.57 | 0.83 | -    | 24,24,24,24                 | 1     |
| 24  | MG   | A     | 1745 | 1/1   | 0.90 | 0.40 | -    | 11,11,11,11                 | 1     |
| 24  | MG   | A     | 1635 | 1/1   | 0.54 | 0.37 | -    | 14,14,14,14                 | 1     |
| 24  | MG   | A     | 1774 | 1/1   | 0.47 | 0.71 | -    | 35,35,35,35                 | 1     |
| 24  | MG   | A     | 1682 | 1/1   | 0.97 | 0.28 | -    | 16,16,16,16                 | 1     |
| 24  | MG   | A     | 1643 | 1/1   | 0.74 | 0.62 | -    | 37,37,37,37                 | 1     |
| 24  | MG   | A     | 1767 | 1/1   | 0.59 | 0.42 | -    | 26,26,26,26                 | 1     |
| 24  | MG   | A     | 1744 | 1/1   | 0.97 | 0.19 | -    | 8,8,8,8                     | 1     |
| 24  | MG   | A     | 1632 | 1/1   | 0.49 | 0.48 | -    | 28,28,28,28                 | 1     |
| 24  | MG   | A     | 1764 | 1/1   | 0.94 | 0.54 | -    | 40,40,40,40                 | 1     |
| 24  | MG   | A     | 1768 | 1/1   | 0.77 | 0.37 | -    | 9,9,9,9                     | 1     |
| 24  | MG   | A     | 1776 | 1/1   | 0.97 | 0.30 | -    | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1734 | 1/1   | 0.73 | 0.28 | -    | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1696 | 1/1   | 0.86 | 0.25 | -    | 28,28,28,28                 | 1     |
| 24  | MG   | A     | 1743 | 1/1   | 0.73 | 0.40 | -    | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1781 | 1/1   | 0.87 | 0.30 | -    | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1771 | 1/1   | 0.96 | 0.31 | -    | 19,19,19,19                 | 1     |
| 24  | MG   | A     | 1706 | 1/1   | 0.83 | 0.27 | -    | 2,2,2,2                     | 1     |
| 24  | MG   | A     | 1610 | 1/1   | 0.81 | 0.21 | -    | 56,56,56,56                 | 0     |
| 24  | MG   | A     | 1623 | 1/1   | 0.94 | 0.22 | -    | 46,46,46,46                 | 1     |
| 24  | MG   | A     | 1736 | 1/1   | 0.95 | 0.17 | -    | 5,5,5,5                     | 1     |
| 24  | MG   | A     | 1766 | 1/1   | 0.67 | 0.29 | -    | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1725 | 1/1   | 0.84 | 0.22 | -    | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1760 | 1/1   | 0.84 | 0.23 | -    | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1690 | 1/1   | 0.95 | 0.18 | -    | 14,14,14,14                 | 1     |
| 24  | MG   | A     | 1780 | 1/1   | 0.95 | 0.56 | -    | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1722 | 1/1   | 0.47 | 0.52 | -    | 24,24,24,24                 | 1     |
| 24  | MG   | A     | 1658 | 1/1   | 0.95 | 0.23 | -    | 31,31,31,31                 | 1     |
| 24  | MG   | A     | 1617 | 1/1   | 0.73 | 0.64 | -    | 56,56,56,56                 | 1     |
| 24  | MG   | A     | 1626 | 1/1   | 0.73 | 0.27 | -    | 36,36,36,36                 | 1     |
| 24  | MG   | A     | 1614 | 1/1   | 0.67 | 0.71 | -    | 55,55,55,55                 | 1     |
| 24  | MG   | A     | 1701 | 1/1   | 0.42 | 0.78 | -    | 76,76,76,76                 | 1     |
| 24  | MG   | A     | 1636 | 1/1   | 0.88 | 0.38 | -    | 26,26,26,26                 | 1     |
| 24  | MG   | A     | 1671 | 1/1   | 0.90 | 0.29 | -    | 20,20,20,20                 | 1     |
| 24  | MG   | A     | 1652 | 1/1   | 0.77 | 0.33 | -    | 49,49,49,49                 | 1     |
| 24  | MG   | A     | 1702 | 1/1   | 0.96 | 0.26 | -    | 9,9,9,9                     | 1     |
| 24  | MG   | A     | 1692 | 1/1   | 0.85 | 0.38 | -    | 28,28,28,28                 | 1     |
| 24  | MG   | A     | 1620 | 1/1   | 0.79 | 1.42 | -    | 52,52,52,52                 | 1     |
| 24  | MG   | A     | 1699 | 1/1   | 0.59 | 1.36 | -    | 30,30,30,30                 | 1     |
| 24  | MG   | A     | 1704 | 1/1   | 0.82 | 0.53 | -    | 1,1,1,1                     | 1     |
| 24  | MG   | A     | 1754 | 1/1   | 0.92 | 0.12 | -    | 1,1,1,1                     | 1     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 24  | MG   | A     | 1607 | 1/1   | 0.88 | 0.40 | -    | 62,62,62,62                 | 1     |
| 24  | MG   | A     | 1713 | 1/1   | 0.51 | 0.31 | -    | 42,42,42,42                 | 1     |
| 24  | MG   | A     | 1606 | 1/1   | 0.98 | 0.23 | -    | 29,29,29,29                 | 1     |
| 24  | MG   | A     | 1675 | 1/1   | 0.94 | 0.21 | -    | 8,8,8,8                     | 1     |
| 24  | MG   | A     | 1601 | 1/1   | 0.76 | 0.16 | -    | 34,34,34,34                 | 0     |
| 24  | MG   | A     | 1615 | 1/1   | 0.95 | 0.30 | -    | 1,1,1,1                     | 0     |
| 24  | MG   | A     | 1693 | 1/1   | 0.43 | 0.65 | -    | 34,34,34,34                 | 1     |
| 24  | MG   | A     | 1605 | 1/1   | 0.61 | 0.37 | -    | 36,36,36,36                 | 1     |
| 24  | MG   | A     | 1714 | 1/1   | 0.75 | 0.24 | -    | 2,2,2,2                     | 1     |
| 24  | MG   | A     | 1741 | 1/1   | 0.92 | 0.39 | -    | 5,5,5,5                     | 1     |
| 24  | MG   | A     | 1716 | 1/1   | 0.88 | 0.42 | -    | 6,6,6,6                     | 1     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.