



## Full wwPDB X-ray Structure Validation Report ⓘ

Jun 21, 2026 – 10:03 am BST

PDB ID : 2UUA / pdb\_00002uua  
Title : Structure of the *Thermus thermophilus* 30S ribosomal subunit complexed with a Valine-ASL with cmo5U in position 34 bound to an mRNA with a GUC-codon in the A-site and paromomycin.  
Authors : Weixlbaumer, A.; Murphy, F.V.; Dziergowska, A.; Malkiewicz, A.; Vendeix, F.A.P.; Agris, P.F.; Ramakrishnan, V.  
Deposited on : 2007-03-01  
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

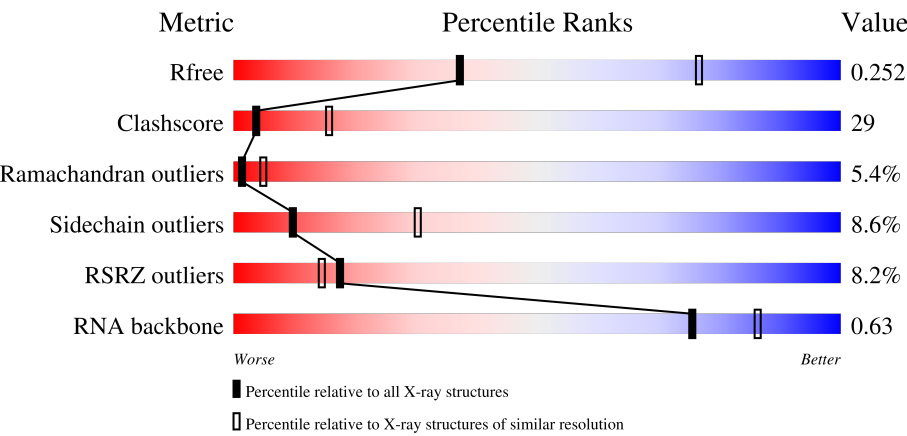
|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 1.8.4, CSD as541be (2020)                                        |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

# 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 2.90 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| R <sub>free</sub>     | 180053                      | 2481 (2.90-2.90)                                      |
| Clashscore            | 190562                      | 2690 (2.90-2.90)                                      |
| Ramachandran outliers | 187476                      | 2623 (2.90-2.90)                                      |
| Sidechain outliers    | 187428                      | 2625 (2.90-2.90)                                      |
| RSRZ outliers         | 180081                      | 2481 (2.90-2.90)                                      |
| RNA backbone          | 3983                        | 1120 (3.10-2.70)                                      |

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

| Mol | Chain | Length | Quality of chain                                                                             |
|-----|-------|--------|----------------------------------------------------------------------------------------------|
| 1   | A     | 1522   | <div><div>6%</div><div>41%</div><div>47%</div><div>9%</div><div>••</div></div>               |
| 2   | B     | 256    | <div><div>15%</div><div>23%</div><div>53%</div><div>14%</div><div>•</div><div>8%</div></div> |
| 3   | C     | 239    | <div><div>8%</div><div>26%</div><div>51%</div><div>9%</div><div>•</div><div>13%</div></div>  |
| 4   | D     | 209    | <div><div>8%</div><div>44%</div><div>48%</div><div>6%</div><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     | 135    |                  |
| 13  | M     | 126    |                  |
| 14  | N     | 61     |                  |
| 15  | O     | 89     |                  |
| 16  | P     | 88     |                  |
| 17  | Q     | 105    |                  |
| 18  | R     | 88     |                  |
| 19  | S     | 93     |                  |
| 20  | T     | 106    |                  |
| 21  | U     | 27     |                  |
| 22  | X     | 6      |                  |
| 23  | Y     | 17     |                  |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 25  | MG   | A     | 1604 | -         | -        | -       | X                |
| 25  | MG   | A     | 1610 | -         | -        | -       | X                |
| 25  | MG   | A     | 1642 | -         | -        | -       | X                |
| 25  | MG   | A     | 1653 | -         | -        | -       | X                |
| 25  | MG   | A     | 1665 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 25  | MG   | A     | 1688 | -         | -        | -       | X                |
| 25  | MG   | A     | 1699 | -         | -        | -       | X                |
| 25  | MG   | A     | 1755 | -         | -        | -       | X                |
| 25  | MG   | A     | 1758 | -         | -        | -       | X                |
| 27  | ZN   | N     | 101  | -         | -        | X       | -                |

## 2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 52344 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     | 1512     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32489 | 14462 | 6011 | 10505 | 1511 |         |         |       |

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | J     | 99       | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 793   | 498 | 157 | 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     | 125      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 971   | 611 | 196 | 163 | 1 |         |         |       |

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17  | Q     | 104      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 857   | 547 | 160 | 148 | 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     |
|     |       |          | 598   | 381 | 118 | 99 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | S     | 81       | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 648   | 414 | 120 | 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     |
|     |       |          | 763   | 470 | 162 | 129 | 2 |         |         |       |

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

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

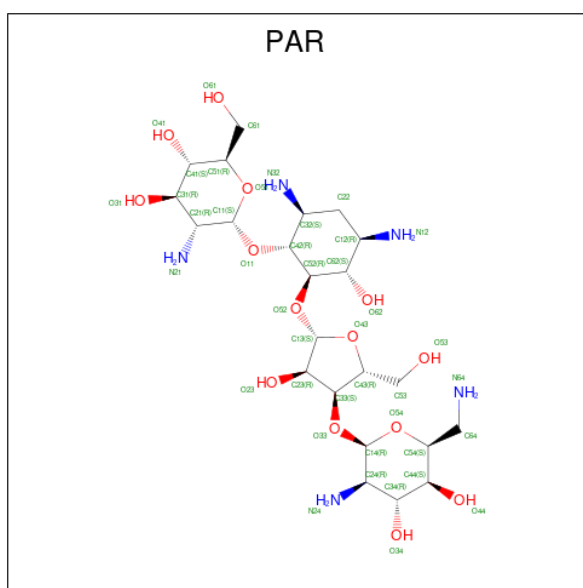
- Molecule 22 is a RNA chain called 5'-R(\*GP\*UP\*CP\*AP\*AP\*AP)-3'.

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 22  | X     | 5        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 104   | 48 | 20 | 32 | 4 |         |         |       |

- Molecule 23 is a RNA chain called 5'-R(\*CP\*CP\*UP\*CP\*CP\*CP\*UP\*CM0P\*AP\*CP\*6MZP\*AP\*GP\*GP\*AP\*GP\*G)-3'.

| Mol | Chain | Residues | Atoms |     |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 23  | Y     | 13       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 277   | 126 | 48 | 91 | 12 |         |         |       |

- Molecule 24 is PAROMOMYCIN (CCD ID: PAR) (formula: C<sub>23</sub>H<sub>45</sub>N<sub>5</sub>O<sub>14</sub>).



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

- Molecule 25 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 25  | A     | 161      | Total | Mg  | 0       | 0       |
|     |       |          | 161   | 161 |         |         |

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| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 25  | B     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 25  | D     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 25  | E     | 2        | Total Mg<br>2 2 | 0       | 0       |
| 25  | F     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 25  | G     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 25  | H     | 2        | Total Mg<br>2 2 | 0       | 0       |
| 25  | Q     | 1        | Total Mg<br>1 1 | 0       | 0       |

- Molecule 26 is POTASSIUM ION (CCD ID: K) (formula: K).

| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 26  | A     | 21       | Total K<br>21 21 | 0       | 0       |
| 26  | E     | 1        | Total K<br>1 1   | 0       | 0       |

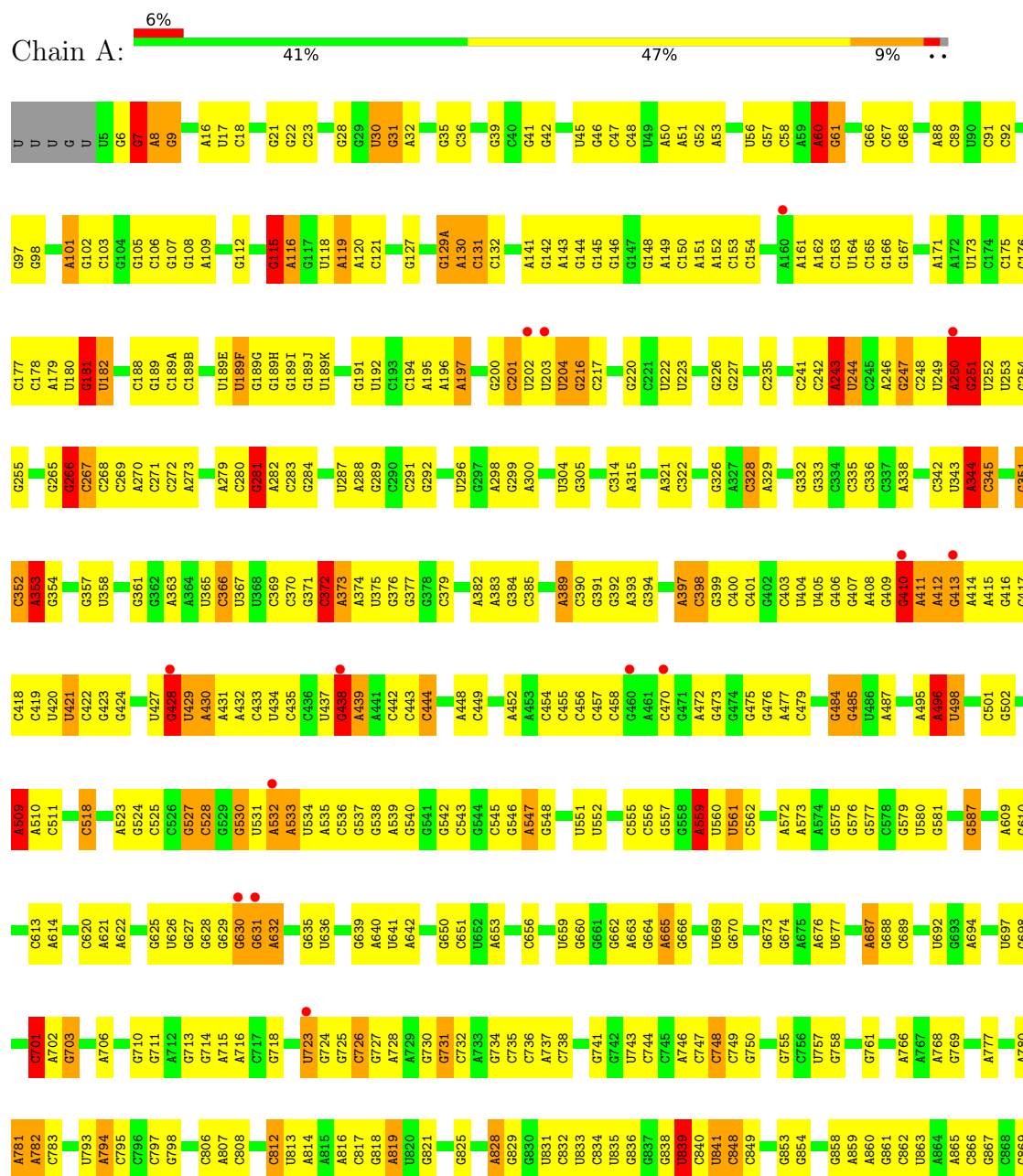
- Molecule 27 is ZINC ION (CCD ID: ZN) (formula: Zn).

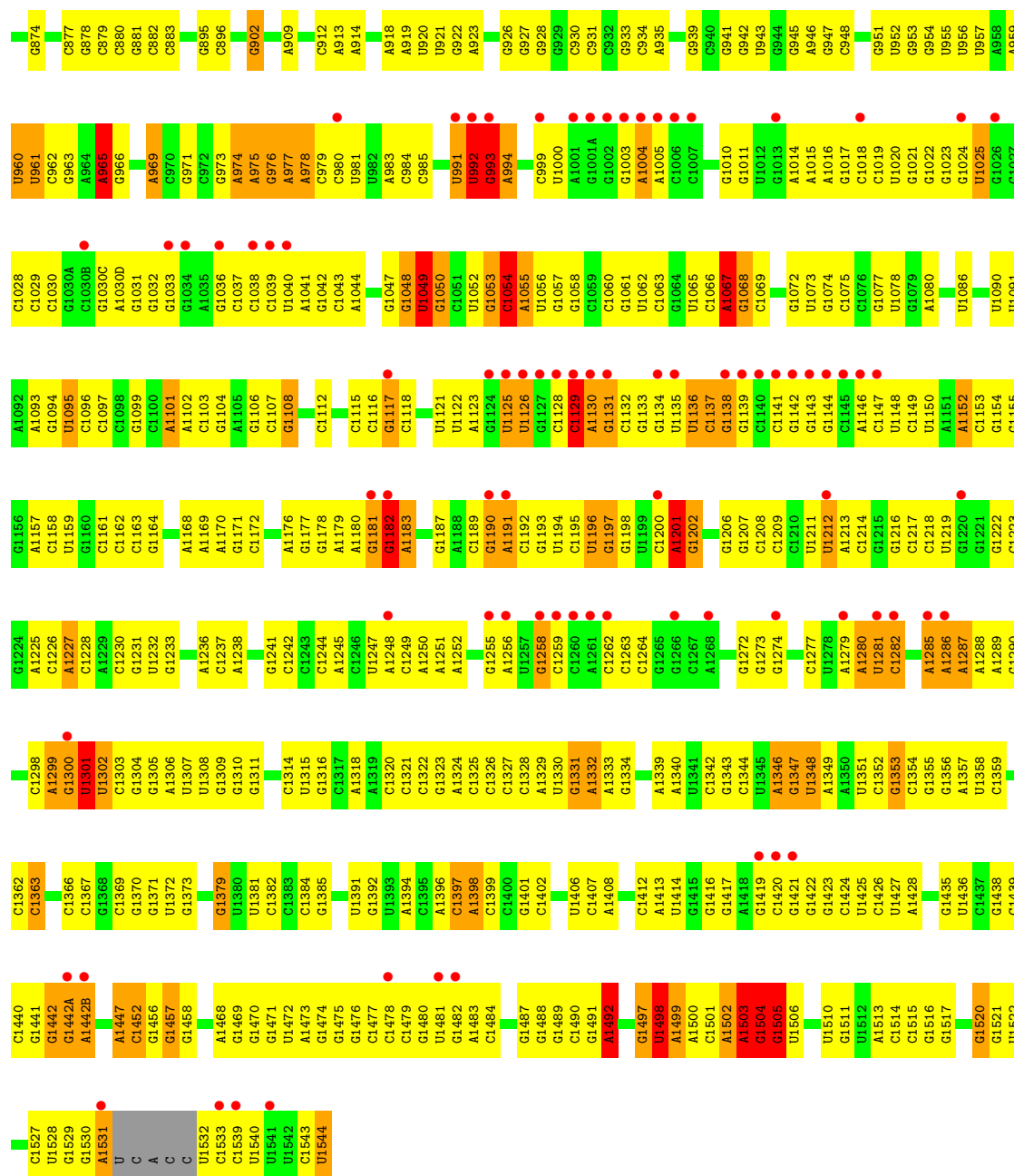
| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 27  | D     | 1        | Total Zn<br>1 1 | 0       | 0       |
| 27  | N     | 1        | Total Zn<br>1 1 | 0       | 0       |

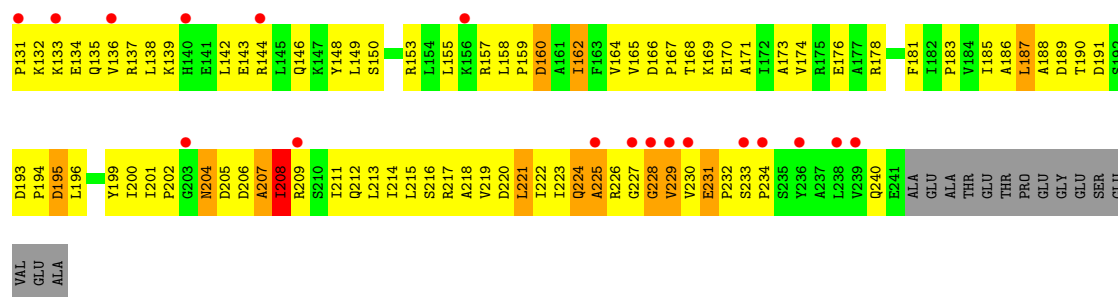
### 3 Residue-property plots

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

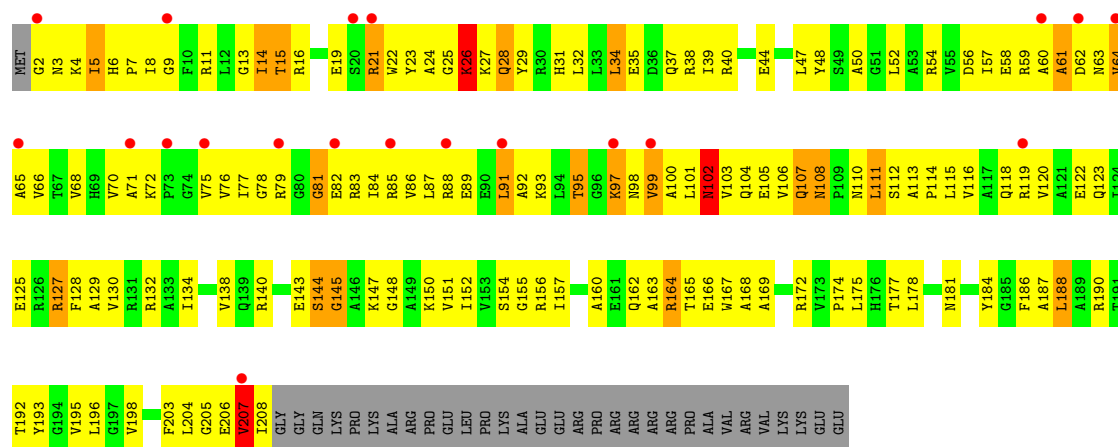
#### • Molecule 1: 16S rRNA



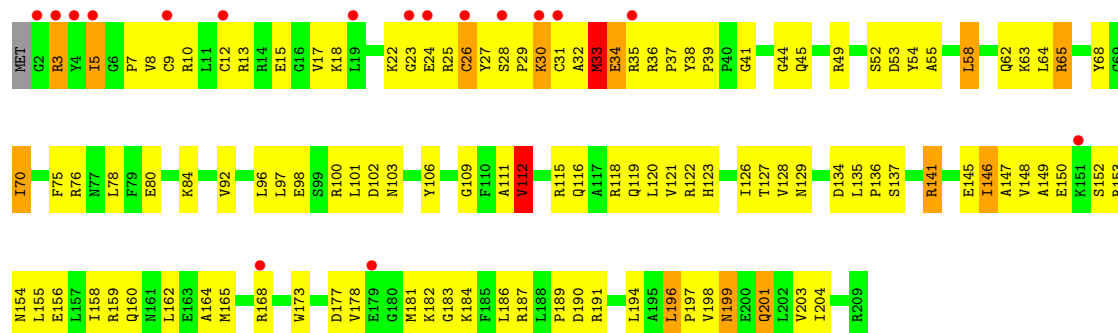
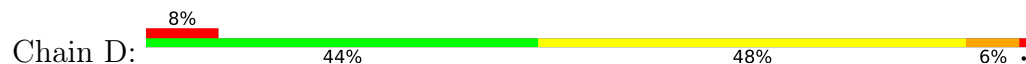




• Molecule 3: 30S RIBOSOMAL PROTEIN S3

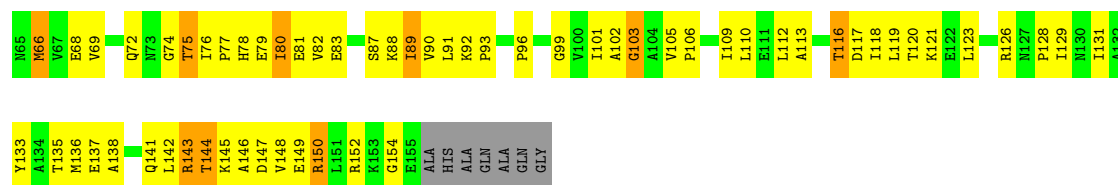


• Molecule 4: 30S RIBOSOMAL PROTEIN S4

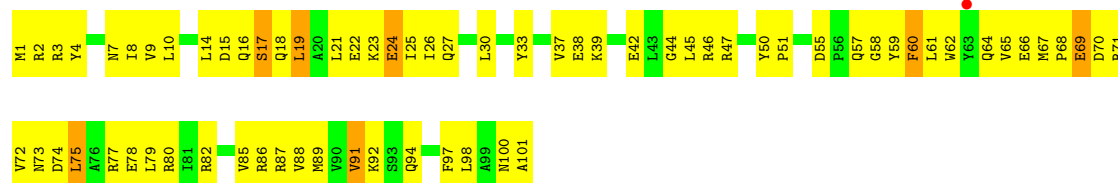


• Molecule 5: 30S RIBOSOMAL PROTEIN S5

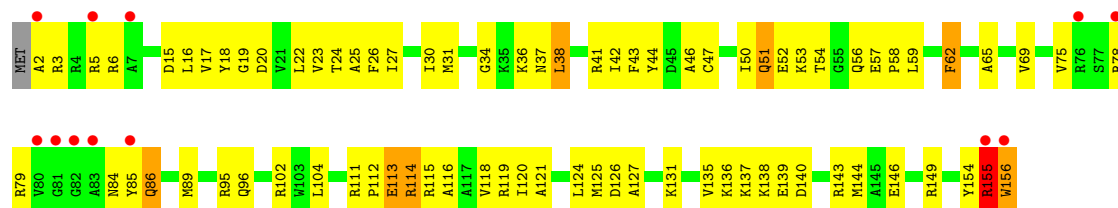




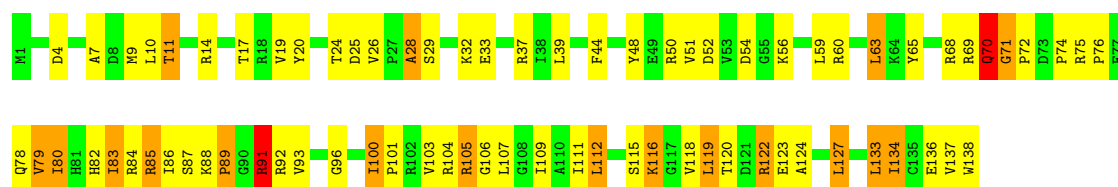
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



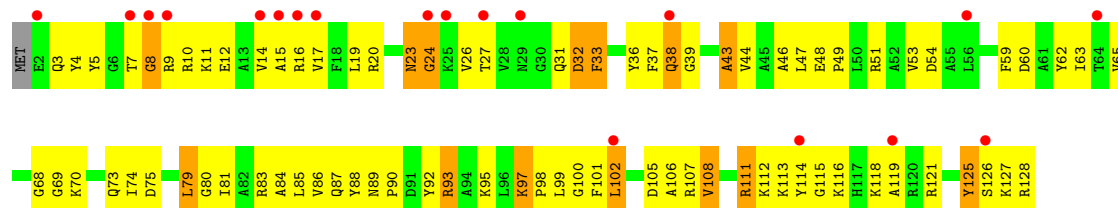
• Molecule 7: 30S RIBOSOMAL PROTEIN S7



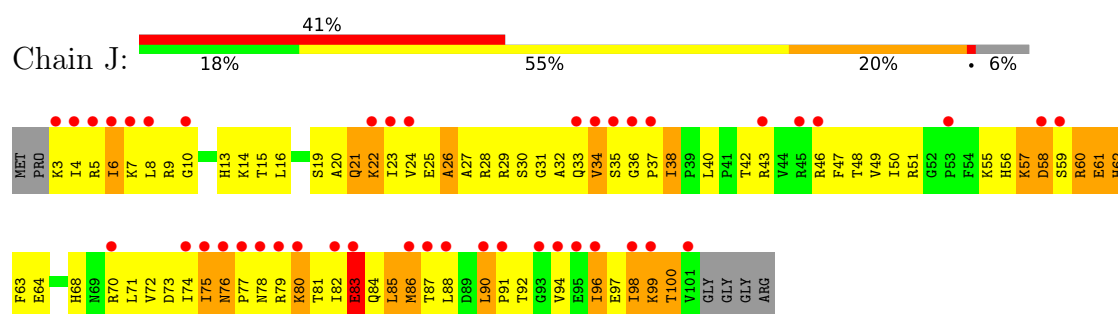
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



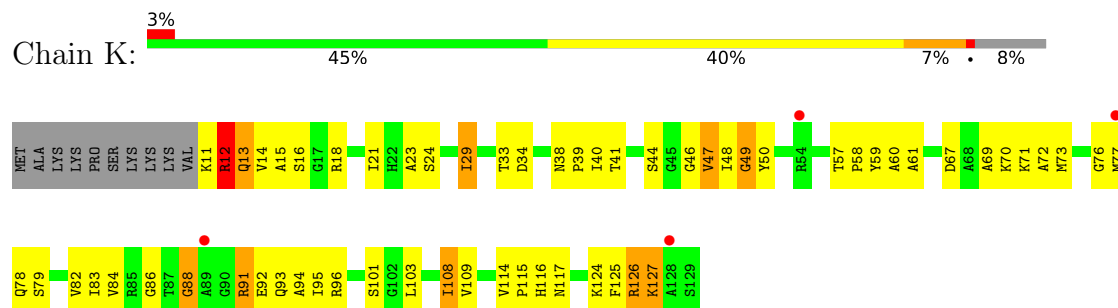
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



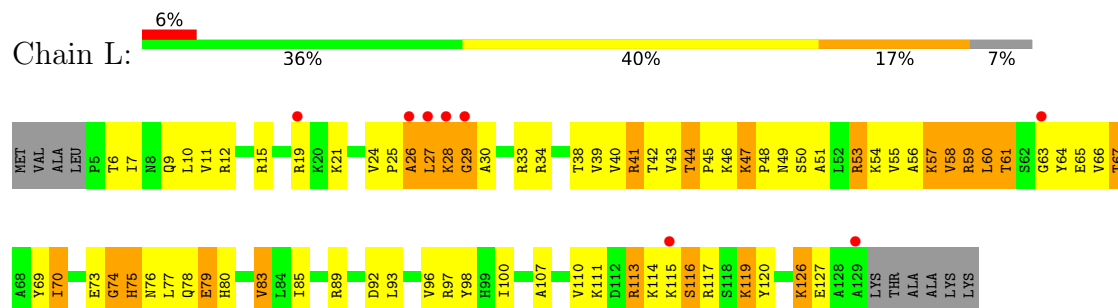
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



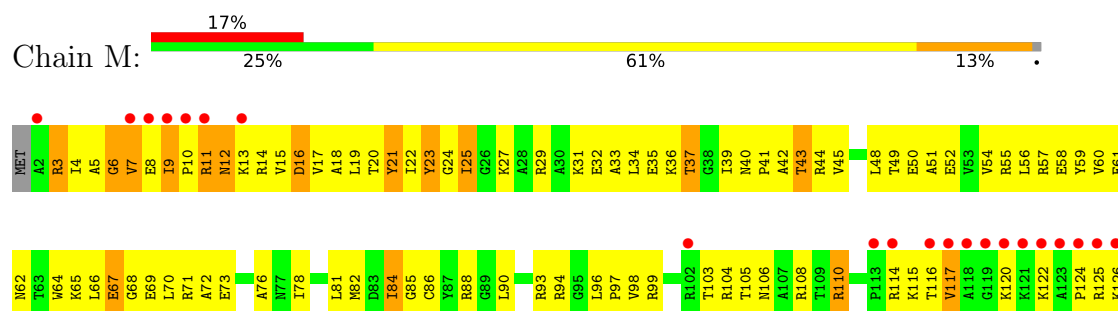
- Molecule 11: 30S RIBOSOMAL PROTEIN S11



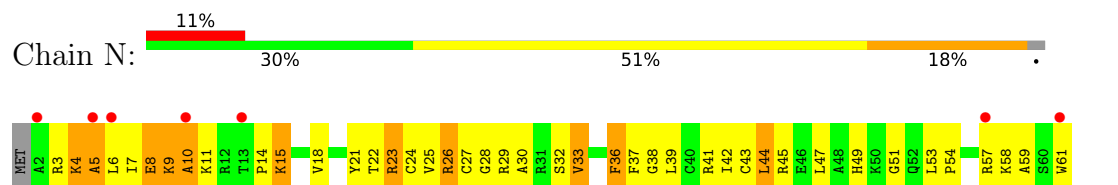
● Molecule 12: 30S RIBOSOMAL PROTEIN S12



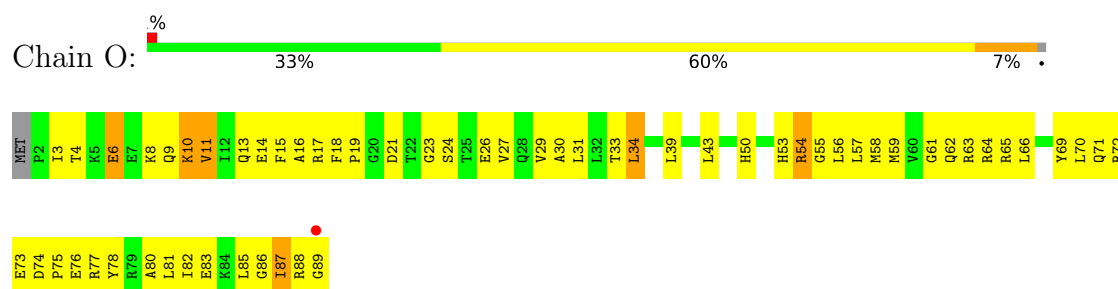
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



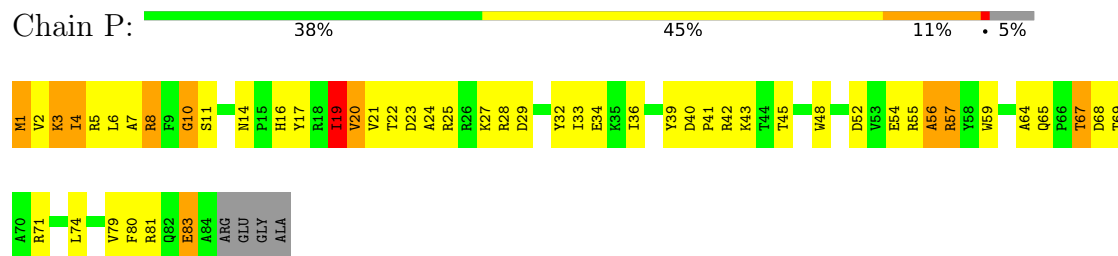
● Molecule 14: 30S RIBOSOMAL PROTEIN S14



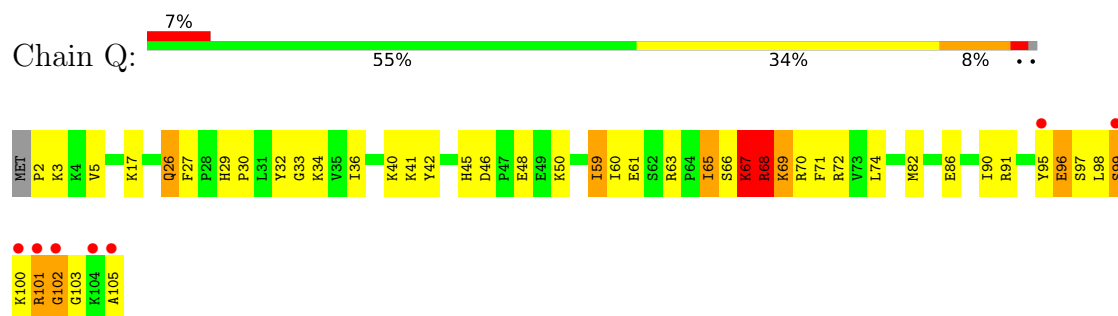
● Molecule 15: 30S RIBOSOMAL PROTEIN S15



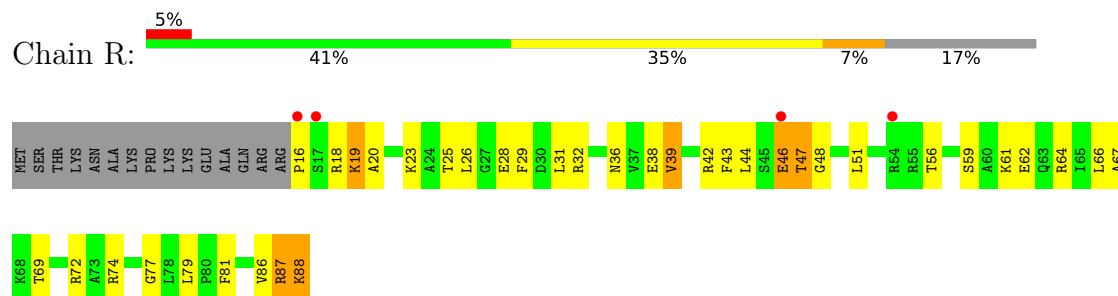
- Molecule 16: 30S RIBOSOMAL PROTEIN S16



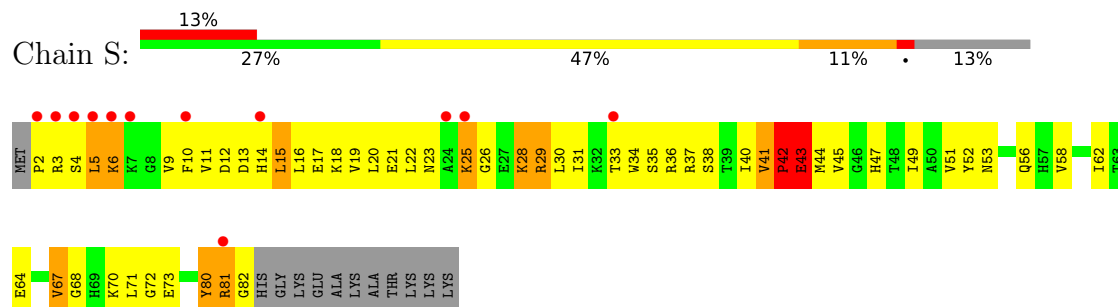
● Molecule 17: 30S RIBOSOMAL PROTEIN S17



- Molecule 18: 30S RIBOSOMAL PROTEIN S18

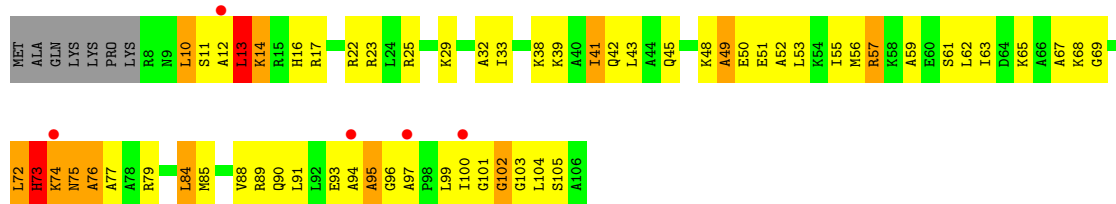


● Molecule 19: 30S RIBOSOMAL PROTEIN S19



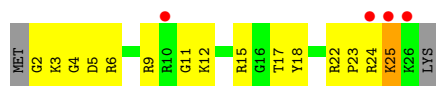
- Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain T: 

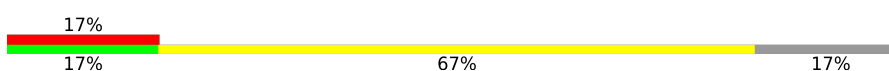


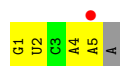
- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain U: 

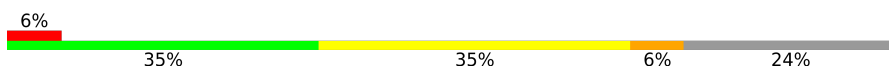


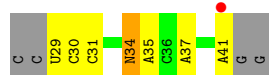
- Molecule 22: 5'-R(\*GP\*UP\*CP\*AP\*AP\*AP)-3'

Chain X: 



- Molecule 23: 5'-R(\*CP\*CP\*UP\*CP\*CP\*CP\*UP\*CM0P\*AP\*CP\*6MZP\*AP \*GP\*GP\*AP\*GP\*G)-3'

Chain Y: 



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 41 21 2                                                   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 401.92Å 401.92Å 174.59Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 29.88 – 2.90<br>29.88 – 2.90                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.3 (29.88-2.90)<br>99.3 (29.88-2.90)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.17                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.85 (at 2.91Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.2                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.223 , 0.254<br>0.222 , 0.252                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 15908 reflections (5.08%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 63.7                                                        | Xtriage          |
| Anisotropy                                                              | 0.212                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 87.6                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.92                                                        | EDS              |
| Total number of atoms                                                   | 52344                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 70.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CM0, MG, PAR, ZN, K, 6MZ

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

| Mol | Chain | Bond lengths |                | Bond angles |                  |
|-----|-------|--------------|----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5          |
| 1   | A     | 0.49         | 1/36365 (0.0%) | 0.66        | 55/56754 (0.1%)  |
| 2   | B     | 0.47         | 1/1936 (0.1%)  | 1.06        | 14/2611 (0.5%)   |
| 3   | C     | 0.51         | 1/1637 (0.1%)  | 0.98        | 4/2207 (0.2%)    |
| 4   | D     | 0.54         | 0/1733         | 1.04        | 11/2318 (0.5%)   |
| 5   | E     | 0.64         | 1/1163 (0.1%)  | 1.13        | 7/1566 (0.4%)    |
| 6   | F     | 0.45         | 0/856          | 0.97        | 2/1154 (0.2%)    |
| 7   | G     | 0.48         | 0/1276         | 0.94        | 3/1709 (0.2%)    |
| 8   | H     | 0.62         | 0/1136         | 1.26        | 13/1527 (0.9%)   |
| 9   | I     | 0.47         | 0/1029         | 1.05        | 4/1379 (0.3%)    |
| 10  | J     | 0.52         | 1/806 (0.1%)   | 1.02        | 7/1084 (0.6%)    |
| 11  | K     | 0.52         | 0/900          | 1.08        | 5/1213 (0.4%)    |
| 12  | L     | 0.60         | 0/987          | 1.22        | 7/1322 (0.5%)    |
| 13  | M     | 0.51         | 0/1008         | 1.03        | 4/1347 (0.3%)    |
| 14  | N     | 0.51         | 0/501          | 1.03        | 1/664 (0.2%)     |
| 15  | O     | 0.48         | 0/745          | 0.85        | 0/992            |
| 16  | P     | 0.60         | 1/717 (0.1%)   | 1.12        | 6/965 (0.6%)     |
| 17  | Q     | 0.60         | 0/870          | 1.12        | 2/1159 (0.2%)    |
| 18  | R     | 0.47         | 0/604          | 1.01        | 3/801 (0.4%)     |
| 19  | S     | 0.53         | 0/662          | 1.10        | 5/892 (0.6%)     |
| 20  | T     | 0.60         | 0/765          | 1.21        | 7/1007 (0.7%)    |
| 21  | U     | 0.65         | 1/213 (0.5%)   | 1.00        | 0/279            |
| 22  | X     | 0.50         | 0/116          | 0.80        | 0/179            |
| 23  | Y     | 0.44         | 0/253          | 0.65        | 0/387            |
| All | All   | 0.50         | 7/56278 (0.0%) | 0.81        | 160/83516 (0.2%) |

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     | 2                   | 17                  |
| 12  | L     | 0                   | 1                   |
| All | All   | 2                   | 18                  |

All (7) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | A     | 1531 | A    | O3'-P | 19.58 | 1.90        | 1.61     |
| 2   | B     | 240  | GLN  | C-N   | -5.72 | 1.25        | 1.33     |
| 10  | J     | 100  | THR  | C-N   | -5.57 | 1.25        | 1.33     |
| 3   | C     | 207  | VAL  | C-N   | -5.52 | 1.25        | 1.33     |
| 5   | E     | 154  | GLY  | C-N   | -5.13 | 1.26        | 1.33     |
| 16  | P     | 83   | GLU  | C-N   | -5.04 | 1.26        | 1.33     |
| 21  | U     | 25   | LYS  | C-N   | -5.02 | 1.26        | 1.33     |

All (160) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 1   | A     | 1498 | U    | C2'-C3'-O3' | 13.72  | 130.08      | 109.50   |
| 1   | A     | 281  | G    | C2'-C3'-O3' | 13.67  | 130.01      | 109.50   |
| 1   | A     | 243  | A    | C2'-C3'-O3' | 13.47  | 129.71      | 109.50   |
| 1   | A     | 366  | C    | C2'-C3'-O3' | 12.70  | 128.54      | 109.50   |
| 1   | A     | 812  | C    | C2'-C3'-O3' | 12.20  | 127.80      | 109.50   |
| 1   | A     | 559  | A    | C2'-C3'-O3' | 11.89  | 127.33      | 109.50   |
| 1   | A     | 687  | A    | C2'-C3'-O3' | 11.69  | 127.04      | 109.50   |
| 1   | A     | 965  | A    | C2'-C3'-O3' | 11.08  | 126.11      | 109.50   |
| 1   | A     | 1503 | A    | C2'-C3'-O3' | 11.01  | 126.02      | 109.50   |
| 5   | E     | 26   | PHE  | N-CA-C      | 10.64  | 124.26      | 110.53   |
| 12  | L     | 26   | ALA  | N-CA-C      | -10.60 | 98.30       | 112.72   |
| 9   | I     | 39   | GLY  | N-CA-C      | -10.47 | 100.72      | 114.85   |
| 1   | A     | 181  | G    | C2'-C3'-O3' | 10.40  | 125.10      | 109.50   |
| 18  | R     | 46   | GLU  | N-CA-C      | -10.27 | 100.08      | 111.28   |
| 4   | D     | 26   | CYS  | N-CA-C      | -10.17 | 101.05      | 113.15   |
| 8   | H     | 79   | VAL  | N-CA-C      | -10.09 | 101.04      | 110.82   |
| 1   | A     | 496  | A    | C2'-C3'-O3' | 10.08  | 124.61      | 109.50   |
| 8   | H     | 134  | ILE  | N-CA-C      | 9.99   | 120.01      | 110.42   |
| 1   | A     | 60   | A    | C2'-C3'-O3' | 9.99   | 124.48      | 109.50   |
| 20  | T     | 13   | LEU  | N-CA-C      | -9.62  | 99.37       | 112.94   |
| 1   | A     | 484  | G    | C2'-C3'-O3' | 9.28   | 123.42      | 109.50   |
| 1   | A     | 533  | A    | C2'-C3'-O3' | 9.26   | 123.40      | 109.50   |
| 1   | A     | 281  | G    | C4'-C3'-O3' | 9.21   | 123.21      | 109.40   |
| 9   | I     | 60   | ASP  | N-CA-C      | -9.00  | 95.33       | 109.72   |
| 8   | H     | 44   | PHE  | N-CA-C      | -8.93  | 102.97      | 114.04   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 1   | A     | 115    | G    | C2'-C3'-O3' | 8.92  | 122.88      | 109.50   |
| 20  | T     | 14     | LYS  | N-CA-C      | -8.87 | 101.53      | 111.82   |
| 11  | K     | 49     | GLY  | N-CA-C      | 8.80  | 123.29      | 112.64   |
| 1   | A     | 243    | A    | C4'-C3'-O3' | 8.76  | 122.54      | 109.40   |
| 1   | A     | 366    | C    | C4'-C3'-O3' | 8.75  | 122.53      | 109.40   |
| 20  | T     | 75     | ASN  | N-CA-C      | -8.71 | 102.64      | 113.18   |
| 3   | C     | 145    | GLY  | N-CA-C      | 8.69  | 126.92      | 115.36   |
| 1   | A     | 1505   | G    | C2'-C3'-O3' | 8.65  | 126.67      | 113.70   |
| 1   | A     | 428    | G    | C2'-C3'-O3' | 8.58  | 122.37      | 109.50   |
| 1   | A     | 372    | C    | C2'-C3'-O3' | 8.58  | 122.37      | 109.50   |
| 1   | A     | 1301   | U    | C2'-C3'-O3' | 8.39  | 122.08      | 109.50   |
| 1   | A     | 748    | C    | C2'-C3'-O3' | 8.30  | 121.94      | 109.50   |
| 11  | K     | 116    | HIS  | N-CA-C      | -8.25 | 101.03      | 112.25   |
| 12  | L     | 119    | LYS  | N-CA-C      | -8.19 | 98.36       | 110.48   |
| 1   | A     | 1067   | A    | C2'-C3'-O3' | 8.07  | 121.61      | 109.50   |
| 1   | A     | 129(A) | G    | C2'-C3'-O3' | 7.93  | 121.40      | 109.50   |
| 2   | B     | 64     | ARG  | N-CA-C      | -7.89 | 102.95      | 114.39   |
| 1   | A     | 687    | A    | C4'-C3'-O3' | 7.71  | 120.96      | 109.40   |
| 12  | L     | 58     | VAL  | N-CA-C      | 7.65  | 118.83      | 108.11   |
| 1   | A     | 1285   | A    | C2'-C3'-O3' | 7.60  | 120.91      | 109.50   |
| 19  | S     | 80     | TYR  | N-CA-C      | 7.55  | 121.80      | 109.72   |
| 4   | D     | 33     | MET  | N-CA-C      | -7.43 | 103.96      | 112.87   |
| 2   | B     | 133    | LYS  | N-CA-C      | -7.36 | 104.39      | 113.15   |
| 8   | H     | 89     | PRO  | N-CA-C      | -7.33 | 99.69       | 111.19   |
| 3   | C     | 111    | LEU  | N-CA-C      | -7.31 | 102.76      | 114.09   |
| 1   | A     | 7      | G    | C2'-C3'-O3' | 7.26  | 120.39      | 109.50   |
| 4   | D     | 12     | CYS  | N-CA-C      | -7.11 | 102.58      | 111.11   |
| 1   | A     | 559    | A    | C4'-C3'-O3' | 7.08  | 120.02      | 109.40   |
| 1   | A     | 266    | G    | C2'-C3'-O3' | 6.97  | 124.16      | 113.70   |
| 5   | E     | 48     | ALA  | N-CA-C      | 6.96  | 114.26      | 108.07   |
| 1   | A     | 812    | C    | C4'-C3'-O3' | 6.94  | 119.81      | 109.40   |
| 8   | H     | 100    | ILE  | N-CA-C      | -6.93 | 102.16      | 108.95   |
| 7   | G     | 85     | TYR  | N-CA-C      | 6.92  | 119.69      | 108.41   |
| 10  | J     | 60     | ARG  | N-CA-C      | 6.84  | 125.36      | 110.80   |
| 12  | L     | 61     | THR  | N-CA-C      | -6.81 | 104.23      | 112.54   |
| 1   | A     | 509    | A    | C2'-C3'-O3' | 6.80  | 123.90      | 113.70   |
| 16  | P     | 20     | VAL  | N-CA-C      | 6.73  | 119.72      | 108.81   |
| 2   | B     | 90     | MET  | N-CA-C      | 6.71  | 119.34      | 110.08   |
| 11  | K     | 126    | ARG  | N-CA-C      | 6.69  | 119.81      | 108.90   |
| 1   | A     | 1201   | A    | C2'-C3'-O3' | 6.68  | 119.52      | 109.50   |
| 2   | B     | 14     | GLY  | N-CA-C      | -6.65 | 106.61      | 115.32   |
| 8   | H     | 69     | ARG  | N-CA-C      | 6.58  | 119.17      | 109.69   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 2   | B     | 47     | THR  | N-CA-C      | -6.54 | 104.15      | 111.28   |
| 1   | A     | 129(A) | G    | C4'-C3'-O3' | 6.53  | 119.19      | 109.40   |
| 13  | M     | 25     | ILE  | N-CA-C      | 6.52  | 117.24      | 108.11   |
| 1   | A     | 1504   | G    | C4'-C3'-O3' | 6.50  | 119.15      | 109.40   |
| 1   | A     | 1544   | U    | C2'-C3'-O3' | -6.47 | 99.80       | 109.50   |
| 6   | F     | 91     | VAL  | N-CA-C      | 6.37  | 117.20      | 107.77   |
| 14  | N     | 51     | GLY  | N-CA-C      | -6.37 | 106.64      | 114.92   |
| 4   | D     | 178    | VAL  | N-CA-C      | 6.36  | 117.11      | 110.62   |
| 1   | A     | 701    | C    | C2'-C3'-O3' | 6.29  | 118.94      | 109.50   |
| 1   | A     | 1504   | G    | C2'-C3'-O3' | 6.29  | 118.93      | 109.50   |
| 2   | B     | 160    | ASP  | N-CA-C      | -6.27 | 105.79      | 113.50   |
| 1   | A     | 250    | A    | C2'-C3'-O3' | 6.27  | 118.90      | 109.50   |
| 5   | E     | 102    | ALA  | N-CA-C      | 6.24  | 118.33      | 108.79   |
| 3   | C     | 99     | VAL  | N-CA-C      | 6.22  | 119.23      | 108.90   |
| 1   | A     | 1299   | A    | N9-C1'-C2'  | 6.22  | 121.32      | 112.00   |
| 2   | B     | 76     | GLN  | N-CA-C      | -6.15 | 105.93      | 113.50   |
| 13  | M     | 106    | ASN  | CB-CA-C     | -6.13 | 108.49      | 115.79   |
| 2   | B     | 88     | ALA  | N-CA-C      | -6.11 | 99.76       | 109.23   |
| 6   | F     | 60     | PHE  | N-CA-C      | 6.11  | 119.48      | 109.76   |
| 8   | H     | 28     | ALA  | N-CA-C      | 6.11  | 119.52      | 110.48   |
| 4   | D     | 29     | PRO  | N-CA-C      | -6.09 | 102.99      | 113.70   |
| 18  | R     | 81     | PHE  | N-CA-C      | -6.09 | 105.98      | 113.41   |
| 11  | K     | 50     | TYR  | N-CA-C      | 6.07  | 118.85      | 110.35   |
| 17  | Q     | 65     | ILE  | N-CA-C      | -6.01 | 106.39      | 113.42   |
| 10  | J     | 62     | HIS  | N-CA-C      | 6.00  | 119.60      | 109.76   |
| 4   | D     | 8      | VAL  | N-CA-C      | 5.94  | 116.97      | 111.45   |
| 1   | A     | 438    | G    | C4'-C3'-O3' | 5.93  | 118.29      | 109.40   |
| 7   | G     | 154    | TYR  | N-CA-C      | -5.88 | 105.76      | 113.17   |
| 4   | D     | 112    | VAL  | N-CA-C      | 5.86  | 116.04      | 110.53   |
| 2   | B     | 186    | ALA  | N-CA-C      | 5.86  | 117.42      | 108.52   |
| 4   | D     | 30     | LYS  | N-CA-C      | 5.85  | 123.26      | 110.80   |
| 8   | H     | 70     | GLN  | N-CA-C      | 5.83  | 123.21      | 110.80   |
| 19  | S     | 10     | PHE  | N-CA-C      | 5.77  | 118.70      | 110.10   |
| 1   | A     | 1049   | U    | C2'-C3'-O3' | 5.74  | 118.10      | 109.50   |
| 1   | A     | 344    | A    | C2'-C3'-O3' | 5.73  | 118.09      | 109.50   |
| 13  | M     | 11     | ARG  | N-CA-C      | 5.70  | 116.80      | 108.14   |
| 1   | A     | 839    | U    | N1-C1'-C2'  | 5.68  | 120.52      | 112.00   |
| 2   | B     | 17     | PHE  | N-CA-C      | 5.66  | 122.86      | 110.80   |
| 16  | P     | 4      | ILE  | N-CA-C      | -5.64 | 99.51       | 107.75   |
| 2   | B     | 77     | ALA  | N-CA-C      | -5.64 | 107.03      | 114.31   |
| 19  | S     | 68     | GLY  | N-CA-C      | 5.61  | 119.46      | 112.73   |
| 8   | H     | 80     | ILE  | CB-CA-C     | -5.58 | 106.97      | 113.22   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 533  | A    | C4'-C3'-O3' | 5.56  | 117.73      | 109.40   |
| 16  | P     | 27   | LYS  | N-CA-C      | -5.55 | 103.16      | 110.43   |
| 1   | A     | 119  | A    | C2'-C3'-O3' | 5.54  | 117.82      | 109.50   |
| 1   | A     | 992  | U    | C2'-C3'-O3' | 5.54  | 117.81      | 109.50   |
| 1   | A     | 1108 | G    | C5'-C4'-C3' | 5.53  | 124.30      | 116.00   |
| 5   | E     | 23   | GLY  | N-CA-C      | 5.53  | 118.32      | 110.74   |
| 8   | H     | 116  | LYS  | N-CA-C      | -5.53 | 106.42      | 112.72   |
| 10  | J     | 38   | ILE  | CA-C-N      | 5.52  | 126.74      | 119.84   |
| 10  | J     | 38   | ILE  | C-N-CA      | 5.52  | 126.74      | 119.84   |
| 1   | A     | 1200 | C    | C2'-C3'-O3' | -5.49 | 105.46      | 113.70   |
| 10  | J     | 79   | ARG  | N-CA-C      | -5.48 | 106.59      | 113.28   |
| 20  | T     | 96   | GLY  | N-CA-C      | 5.48  | 123.11      | 112.04   |
| 18  | R     | 47   | THR  | N-CA-C      | -5.47 | 102.81      | 110.35   |
| 19  | S     | 41   | VAL  | CA-C-N      | 5.45  | 126.66      | 119.84   |
| 19  | S     | 41   | VAL  | C-N-CA      | 5.45  | 126.66      | 119.84   |
| 7   | G     | 114  | ARG  | N-CA-C      | 5.45  | 119.64      | 112.89   |
| 13  | M     | 84   | ILE  | N-CA-C      | -5.39 | 100.56      | 108.54   |
| 1   | A     | 1200 | C    | N1-C1'-C2'  | 5.34  | 120.01      | 112.00   |
| 2   | B     | 114  | ARG  | N-CA-C      | -5.33 | 106.91      | 113.41   |
| 5   | E     | 103  | GLY  | N-CA-C      | -5.31 | 105.29      | 112.14   |
| 17  | Q     | 67   | LYS  | N-CA-C      | -5.30 | 102.06      | 109.96   |
| 16  | P     | 3    | LYS  | N-CA-C      | 5.30  | 117.46      | 109.41   |
| 12  | L     | 44   | THR  | CA-C-N      | 5.29  | 126.03      | 120.11   |
| 12  | L     | 44   | THR  | C-N-CA      | 5.29  | 126.03      | 120.11   |
| 3   | C     | 130  | VAL  | N-CA-C      | 5.28  | 115.73      | 110.23   |
| 8   | H     | 137  | VAL  | CB-CA-C     | -5.28 | 103.67      | 111.80   |
| 8   | H     | 96   | GLY  | N-CA-C      | -5.24 | 105.59      | 112.82   |
| 1   | A     | 1182 | G    | C2'-C3'-O3' | 5.23  | 117.35      | 109.50   |
| 8   | H     | 19   | VAL  | N-CA-C      | -5.22 | 106.34      | 111.77   |
| 1   | A     | 389  | A    | C5'-C4'-C3' | 5.22  | 123.83      | 116.00   |
| 10  | J     | 58   | ASP  | N-CA-C      | 5.22  | 120.30      | 112.94   |
| 2   | B     | 168  | THR  | N-CA-C      | -5.20 | 105.50      | 111.07   |
| 9   | I     | 15   | ALA  | N-CA-C      | 5.19  | 116.88      | 108.26   |
| 1   | A     | 532  | A    | N9-C1'-C2'  | 5.18  | 119.77      | 112.00   |
| 20  | T     | 97   | ALA  | CA-C-N      | 5.18  | 126.32      | 119.84   |
| 20  | T     | 97   | ALA  | C-N-CA      | 5.18  | 126.32      | 119.84   |
| 2   | B     | 225  | ALA  | N-CA-C      | -5.18 | 106.99      | 113.72   |
| 12  | L     | 57   | LYS  | N-CA-C      | -5.16 | 100.76      | 108.96   |
| 16  | P     | 19   | ILE  | N-CA-C      | -5.15 | 101.98      | 108.93   |
| 11  | K     | 91   | ARG  | N-CA-C      | -5.14 | 105.59      | 111.14   |
| 4   | D     | 196  | LEU  | CA-C-N      | 5.12  | 126.24      | 119.84   |
| 4   | D     | 196  | LEU  | C-N-CA      | 5.12  | 126.24      | 119.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 353  | A    | C5'-C4'-O4' | -5.07 | 102.19      | 109.80   |
| 5   | E     | 66   | MET  | N-CA-C      | 5.07  | 118.07      | 109.76   |
| 9   | I     | 93   | ARG  | N-CA-C      | -5.04 | 105.69      | 111.14   |
| 16  | P     | 56   | ALA  | N-CA-C      | -5.04 | 104.87      | 111.02   |
| 10  | J     | 96   | ILE  | N-CA-C      | 5.04  | 115.97      | 108.46   |
| 1   | A     | 1129 | C    | C2'-C3'-O3' | 5.03  | 117.04      | 109.50   |
| 4   | D     | 22   | LYS  | N-CA-C      | -5.02 | 107.19      | 113.72   |
| 5   | E     | 13   | ILE  | N-CA-C      | -5.01 | 100.99      | 108.46   |
| 20  | T     | 76   | ALA  | N-CA-C      | -5.01 | 105.82      | 111.28   |

All (2) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1   | A     | 243 | A    | C3'  |
| 1   | A     | 281 | G    | C3'  |

All (18) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | A     | 1054 | C    | Sidechain |
| 1   | A     | 1067 | A    | Sidechain |
| 1   | A     | 1077 | G    | Sidechain |
| 1   | A     | 1414 | U    | Sidechain |
| 1   | A     | 1457 | G    | Sidechain |
| 1   | A     | 1492 | A    | Sidechain |
| 1   | A     | 250  | A    | Sidechain |
| 1   | A     | 251  | G    | Sidechain |
| 1   | A     | 410  | G    | Sidechain |
| 1   | A     | 528  | C    | Sidechain |
| 1   | A     | 530  | G    | Sidechain |
| 1   | A     | 561  | U    | Sidechain |
| 1   | A     | 587  | G    | Sidechain |
| 1   | A     | 724  | G    | Sidechain |
| 1   | A     | 727  | G    | Sidechain |
| 1   | A     | 902  | G    | Sidechain |
| 1   | A     | 993  | G    | Sidechain |
| 12  | L     | 127  | GLU  | Peptide   |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 32489 | 0        | 16401    | 846     | 0            |
| 2   | B     | 1901  | 0        | 1951     | 245     | 0            |
| 3   | C     | 1613  | 0        | 1677     | 187     | 0            |
| 4   | D     | 1703  | 0        | 1765     | 144     | 0            |
| 5   | E     | 1147  | 0        | 1207     | 124     | 0            |
| 6   | F     | 843   | 0        | 857      | 80      | 0            |
| 7   | G     | 1257  | 0        | 1296     | 83      | 0            |
| 8   | H     | 1116  | 0        | 1177     | 85      | 0            |
| 9   | I     | 1010  | 0        | 1037     | 92      | 0            |
| 10  | J     | 793   | 0        | 835      | 142     | 0            |
| 11  | K     | 885   | 0        | 904      | 66      | 0            |
| 12  | L     | 971   | 0        | 1057     | 96      | 0            |
| 13  | M     | 997   | 0        | 1072     | 107     | 0            |
| 14  | N     | 492   | 0        | 530      | 64      | 0            |
| 15  | O     | 734   | 0        | 771      | 76      | 0            |
| 16  | P     | 701   | 0        | 720      | 70      | 0            |
| 17  | Q     | 857   | 0        | 928      | 62      | 0            |
| 18  | R     | 598   | 0        | 670      | 48      | 0            |
| 19  | S     | 648   | 0        | 673      | 64      | 0            |
| 20  | T     | 763   | 0        | 861      | 78      | 0            |
| 21  | U     | 209   | 0        | 221      | 23      | 0            |
| 22  | X     | 104   | 0        | 55       | 3       | 0            |
| 23  | Y     | 277   | 0        | 146      | 6       | 0            |
| 24  | A     | 42    | 0        | 45       | 1       | 0            |
| 25  | A     | 161   | 0        | 0        | 0       | 0            |
| 25  | B     | 1     | 0        | 0        | 0       | 0            |
| 25  | D     | 1     | 0        | 0        | 0       | 0            |
| 25  | E     | 2     | 0        | 0        | 0       | 0            |
| 25  | F     | 1     | 0        | 0        | 0       | 0            |
| 25  | G     | 1     | 0        | 0        | 0       | 0            |
| 25  | H     | 2     | 0        | 0        | 0       | 0            |
| 25  | Q     | 1     | 0        | 0        | 0       | 0            |
| 26  | A     | 21    | 0        | 0        | 0       | 0            |
| 26  | E     | 1     | 0        | 0        | 0       | 0            |
| 27  | D     | 1     | 0        | 0        | 1       | 0            |
| 27  | N     | 1     | 0        | 0        | 2       | 0            |
| All | All   | 52344 | 0        | 36856    | 2578    | 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 (2578) 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) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:14:ILE:HG22  | 3:C:15:THR:H      | 1.09                     | 1.13              |
| 1:A:243:A:H4'    | 1:A:244:U:H5'     | 1.34                     | 1.09              |
| 3:C:50:ALA:HB1   | 3:C:70:VAL:HG11   | 1.32                     | 1.09              |
| 1:A:975:A:H4'    | 1:A:976:G:H5''    | 1.38                     | 1.05              |
| 10:J:32:ALA:HB1  | 10:J:75:ILE:HG13  | 1.37                     | 1.04              |
| 4:D:7:PRO:HB2    | 4:D:10:ARG:HD2    | 1.38                     | 1.03              |
| 3:C:64:VAL:HG23  | 3:C:99:VAL:HG11   | 1.40                     | 1.02              |
| 15:O:87:ILE:HG22 | 15:O:88:ARG:H     | 1.21                     | 1.01              |
| 10:J:38:ILE:HD11 | 10:J:71:LEU:HD12  | 1.38                     | 1.01              |
| 20:T:73:HIS:O    | 20:T:74:LYS:HB2   | 1.59                     | 1.00              |
| 2:B:118:LEU:HD22 | 2:B:142:LEU:HD13  | 1.44                     | 1.00              |
| 1:A:1277:C:HO2'  | 1:A:1279:A:H8     | 0.99                     | 0.98              |
| 5:E:150:ARG:HG3  | 5:E:150:ARG:HH11  | 1.26                     | 0.98              |
| 2:B:17:PHE:HB3   | 2:B:44:LEU:HD21   | 1.48                     | 0.96              |
| 13:M:10:PRO:HB2  | 13:M:18:ALA:HB1   | 1.47                     | 0.96              |
| 5:E:80:ILE:CD1   | 5:E:91:LEU:HB2    | 1.95                     | 0.95              |
| 17:Q:68:ARG:H    | 17:Q:70:ARG:NH1   | 1.63                     | 0.95              |
| 5:E:53:LEU:HD23  | 5:E:53:LEU:H      | 1.32                     | 0.94              |
| 2:B:84:GLU:HB3   | 2:B:219:VAL:HG21  | 1.47                     | 0.94              |
| 3:C:91:LEU:HD21  | 3:C:99:VAL:HG22   | 1.47                     | 0.94              |
| 1:A:1060:C:C5    | 3:C:2:GLY:HA3     | 2.03                     | 0.94              |
| 10:J:49:VAL:HG23 | 14:N:41:ARG:HB2   | 1.50                     | 0.94              |
| 5:E:51:VAL:HB    | 5:E:52:PRO:HD3    | 1.50                     | 0.93              |
| 1:A:1502:A:H2    | 1:A:1505:G:H1     | 1.13                     | 0.93              |
| 20:T:57:ARG:HE   | 20:T:102:GLY:HA2  | 1.33                     | 0.92              |
| 2:B:178:ARG:HH22 | 8:H:68:ARG:NH2    | 1.67                     | 0.92              |
| 10:J:5:ARG:HA    | 10:J:73:ASP:OD1   | 1.70                     | 0.92              |
| 1:A:246:A:O2'    | 17:Q:99:SER:HB3   | 1.68                     | 0.92              |
| 2:B:142:LEU:HG   | 2:B:146:GLN:HE21  | 1.34                     | 0.92              |
| 20:T:50:GLU:HA   | 20:T:100:ILE:HG22 | 1.52                     | 0.91              |
| 6:F:2:ARG:NE     | 6:F:69:GLU:HG2    | 1.85                     | 0.91              |
| 9:I:128:ARG:O    | 13:M:126:LYS:HD2  | 1.71                     | 0.91              |
| 19:S:64:GLU:O    | 19:S:67:VAL:HG23  | 1.71                     | 0.91              |
| 1:A:1060:C:H5    | 3:C:2:GLY:HA3     | 1.35                     | 0.91              |
| 2:B:60:ASP:HB3   | 2:B:64:ARG:HH12   | 1.33                     | 0.91              |
| 2:B:87:ARG:HH11  | 2:B:233:SER:HB2   | 1.35                     | 0.90              |
| 10:J:8:LEU:HB2   | 10:J:70:ARG:HB2   | 1.54                     | 0.90              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 13:M:11:ARG:HG3  | 13:M:12:ASN:N    | 1.85                     | 0.89              |
| 1:A:726:C:H6     | 1:A:726:C:H5'    | 1.36                     | 0.89              |
| 2:B:178:ARG:HH22 | 8:H:68:ARG:HH22  | 0.91                     | 0.89              |
| 19:S:36:ARG:HH21 | 19:S:53:ASN:HA   | 1.38                     | 0.89              |
| 20:T:57:ARG:NE   | 20:T:102:GLY:HA2 | 1.88                     | 0.89              |
| 2:B:178:ARG:NH2  | 8:H:68:ARG:HH22  | 1.70                     | 0.89              |
| 8:H:29:SER:OG    | 8:H:32:LYS:HB2   | 1.72                     | 0.89              |
| 17:Q:68:ARG:H    | 17:Q:70:ARG:HH11 | 1.21                     | 0.88              |
| 18:R:19:LYS:HG3  | 18:R:20:ALA:H    | 1.37                     | 0.88              |
| 10:J:90:LEU:H    | 10:J:91:PRO:HD2  | 1.36                     | 0.88              |
| 2:B:16:HIS:NE2   | 2:B:214:ILE:HD11 | 1.89                     | 0.88              |
| 18:R:87:ARG:O    | 18:R:88:LYS:HB2  | 1.74                     | 0.88              |
| 6:F:33:TYR:HA    | 6:F:71:ARG:HH21  | 1.37                     | 0.87              |
| 3:C:91:LEU:HD11  | 3:C:99:VAL:HG23  | 1.56                     | 0.87              |
| 3:C:110:ASN:ND2  | 3:C:140:ARG:HB3  | 1.89                     | 0.86              |
| 10:J:4:ILE:HA    | 10:J:100:THR:HA  | 1.58                     | 0.86              |
| 10:J:99:LYS:HD3  | 10:J:100:THR:H   | 1.39                     | 0.86              |
| 11:K:48:ILE:HG22 | 11:K:49:GLY:H    | 1.41                     | 0.86              |
| 10:J:46:ARG:HG2  | 10:J:46:ARG:HH11 | 1.39                     | 0.86              |
| 13:M:124:PRO:HB3 | 13:M:126:LYS:HE2 | 1.57                     | 0.86              |
| 3:C:70:VAL:HG12  | 3:C:72:LYS:H     | 1.38                     | 0.86              |
| 15:O:56:LEU:HA   | 15:O:59:MET:HE2  | 1.57                     | 0.85              |
| 7:G:146:GLU:HG2  | 7:G:149:ARG:HH21 | 1.41                     | 0.85              |
| 16:P:57:ARG:HG2  | 16:P:57:ARG:HH11 | 1.41                     | 0.85              |
| 4:D:18:LYS:NZ    | 4:D:31:CYS:HB3   | 1.92                     | 0.85              |
| 10:J:6:ILE:HG22  | 10:J:98:ILE:HA   | 1.59                     | 0.84              |
| 7:G:69:VAL:HG21  | 7:G:104:LEU:HD21 | 1.59                     | 0.84              |
| 3:C:188:LEU:HD11 | 3:C:195:VAL:HG13 | 1.59                     | 0.84              |
| 2:B:77:ALA:HB2   | 2:B:211:ILE:HD13 | 1.57                     | 0.84              |
| 21:U:9:ARG:NH1   | 21:U:22:ARG:HA   | 1.92                     | 0.84              |
| 2:B:95:GLN:C     | 2:B:96:ARG:HD2   | 2.02                     | 0.84              |
| 8:H:112:LEU:N    | 8:H:112:LEU:HD23 | 1.92                     | 0.84              |
| 19:S:5:LEU:O     | 19:S:6:LYS:HB2   | 1.77                     | 0.84              |
| 2:B:23:ARG:HD2   | 2:B:23:ARG:O     | 1.76                     | 0.84              |
| 1:A:1366:C:H2'   | 1:A:1367:C:H6    | 1.43                     | 0.84              |
| 14:N:14:PRO:O    | 14:N:15:LYS:HB2  | 1.76                     | 0.84              |
| 2:B:84:GLU:OE1   | 2:B:216:SER:HA   | 1.76                     | 0.83              |
| 7:G:75:VAL:HG21  | 7:G:86:GLN:HB3   | 1.59                     | 0.83              |
| 2:B:219:VAL:HA   | 2:B:222:ILE:HD12 | 1.59                     | 0.83              |
| 2:B:218:ALA:O    | 2:B:222:ILE:HG13 | 1.79                     | 0.83              |
| 12:L:41:ARG:HG2  | 12:L:42:THR:H    | 1.41                     | 0.83              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:H:122:ARG:HB3  | 8:H:122:ARG:NH1  | 1.93                     | 0.83              |
| 1:A:579:G:H5'    | 1:A:728:A:H1'    | 1.59                     | 0.83              |
| 11:K:124:LYS:HD2 | 11:K:125:PHE:CE1 | 2.12                     | 0.83              |
| 13:M:120:LYS:NZ  | 13:M:122:LYS:HB3 | 1.94                     | 0.83              |
| 1:A:1250:A:H4'   | 9:I:68:GLY:H     | 1.42                     | 0.82              |
| 1:A:1152:A:H5''  | 10:J:13:HIS:CD2  | 2.14                     | 0.82              |
| 10:J:27:ALA:HA   | 10:J:81:THR:HG23 | 1.61                     | 0.82              |
| 15:O:17:ARG:HG3  | 15:O:17:ARG:HH11 | 1.44                     | 0.82              |
| 1:A:1531:A:H2'   | 1:A:1532:U:H5'   | 1.61                     | 0.82              |
| 15:O:78:TYR:CZ   | 15:O:82:ILE:HD11 | 2.14                     | 0.82              |
| 10:J:38:ILE:HG13 | 10:J:71:LEU:HB3  | 1.59                     | 0.82              |
| 13:M:49:THR:HG22 | 13:M:51:ALA:H    | 1.44                     | 0.82              |
| 12:L:60:LEU:HD11 | 12:L:85:ILE:HD12 | 1.59                     | 0.82              |
| 6:F:15:ASP:H     | 6:F:18:GLN:NE2   | 1.78                     | 0.82              |
| 6:F:67:MET:HB2   | 6:F:68:PRO:HD2   | 1.62                     | 0.82              |
| 20:T:89:ARG:O    | 20:T:93:GLU:HG3  | 1.80                     | 0.82              |
| 14:N:43:CYS:HG   | 27:N:101:ZN:ZN   | 0.93                     | 0.81              |
| 15:O:3:ILE:HD13  | 15:O:34:LEU:HD13 | 1.61                     | 0.81              |
| 15:O:16:ALA:HB1  | 15:O:21:ASP:HB3  | 1.62                     | 0.81              |
| 1:A:1054:C:O2    | 1:A:1054:C:H3'   | 1.80                     | 0.81              |
| 18:R:19:LYS:CG   | 18:R:20:ALA:H    | 1.94                     | 0.81              |
| 13:M:3:ARG:HD3   | 13:M:9:ILE:HG23  | 1.63                     | 0.81              |
| 1:A:351:G:H4'    | 1:A:352:C:OP1    | 1.79                     | 0.80              |
| 9:I:97:LYS:HA    | 9:I:102:LEU:HD21 | 1.61                     | 0.80              |
| 5:E:50:GLU:HG3   | 5:E:52:PRO:HD2   | 1.62                     | 0.80              |
| 1:A:35:G:H2'     | 1:A:36:C:C6      | 2.16                     | 0.80              |
| 5:E:129:ILE:H    | 5:E:129:ILE:HD12 | 1.47                     | 0.80              |
| 1:A:677:U:H3     | 1:A:713:G:H22    | 1.29                     | 0.80              |
| 2:B:223:ILE:HD12 | 2:B:224:GLN:N    | 1.96                     | 0.80              |
| 15:O:65:ARG:HH11 | 15:O:65:ARG:HG2  | 1.45                     | 0.80              |
| 17:Q:66:SER:OG   | 17:Q:69:LYS:HB2  | 1.81                     | 0.80              |
| 2:B:165:VAL:HG23 | 2:B:166:ASP:H    | 1.45                     | 0.80              |
| 3:C:123:GLN:O    | 3:C:128:PHE:HB2  | 1.81                     | 0.80              |
| 2:B:124:SER:O    | 2:B:127:ILE:HG13 | 1.82                     | 0.79              |
| 9:I:65:VAL:HG11  | 9:I:73:GLN:HB3   | 1.63                     | 0.79              |
| 1:A:1250:A:H4'   | 9:I:68:GLY:N     | 1.97                     | 0.79              |
| 2:B:87:ARG:NH1   | 2:B:233:SER:HB2  | 1.96                     | 0.79              |
| 3:C:14:ILE:HG22  | 3:C:15:THR:N     | 1.92                     | 0.79              |
| 13:M:3:ARG:HA    | 13:M:8:GLU:O     | 1.83                     | 0.79              |
| 1:A:192:U:H4'    | 20:T:102:GLY:O   | 1.83                     | 0.79              |
| 2:B:204:ASN:C    | 2:B:204:ASN:HD22 | 1.88                     | 0.79              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:H:60:ARG:HH11   | 8:H:60:ARG:HG3    | 1.46                     | 0.79              |
| 2:B:105:PHE:HE1   | 2:B:155:LEU:HD23  | 1.47                     | 0.79              |
| 12:L:47:LYS:HB3   | 12:L:48:PRO:CD    | 2.13                     | 0.79              |
| 21:U:6:ARG:NH2    | 21:U:15:ARG:HH21  | 1.80                     | 0.79              |
| 11:K:84:VAL:HG11  | 11:K:91:ARG:HD3   | 1.62                     | 0.79              |
| 1:A:1228:C:H4'    | 13:M:116:THR:HA   | 1.63                     | 0.78              |
| 1:A:243:A:C4'     | 1:A:244:U:H5'     | 2.11                     | 0.78              |
| 1:A:975:A:H5'     | 1:A:975:A:H8      | 1.47                     | 0.78              |
| 1:A:1181:G:H4'    | 1:A:1182:G:OP1    | 1.83                     | 0.78              |
| 4:D:189:PRO:HB2   | 4:D:194:LEU:HD21  | 1.66                     | 0.78              |
| 1:A:371:G:O2'     | 1:A:372:C:H5'     | 1.83                     | 0.78              |
| 1:A:664:G:H22     | 1:A:741:G:H1      | 1.26                     | 0.78              |
| 2:B:111:ARG:HB3   | 2:B:149:LEU:HD11  | 1.63                     | 0.78              |
| 13:M:57:ARG:HG2   | 13:M:61:GLU:HG3   | 1.65                     | 0.78              |
| 1:A:250:A:H4'     | 1:A:251:G:O5'     | 1.82                     | 0.78              |
| 4:D:100:ARG:HH12  | 4:D:137:SER:HB3   | 1.48                     | 0.78              |
| 16:P:43:LYS:HG3   | 16:P:48:TRP:CD2   | 2.19                     | 0.78              |
| 1:A:1132:C:H2'    | 1:A:1133:G:H8     | 1.49                     | 0.78              |
| 15:O:10:LYS:HD3   | 15:O:10:LYS:C     | 2.08                     | 0.78              |
| 2:B:204:ASN:ND2   | 2:B:206:ASP:H     | 1.80                     | 0.78              |
| 3:C:14:ILE:CG2    | 3:C:15:THR:H      | 1.91                     | 0.78              |
| 3:C:64:VAL:CG2    | 3:C:99:VAL:HG11   | 2.14                     | 0.78              |
| 1:A:1442(A):G:H4' | 1:A:1442(B):A:H5' | 1.64                     | 0.78              |
| 8:H:51:VAL:HG11   | 8:H:60:ARG:HH11   | 1.49                     | 0.77              |
| 1:A:1054:C:H2'    | 1:A:1055:A:H5''   | 1.66                     | 0.77              |
| 12:L:60:LEU:HD21  | 12:L:66:VAL:HG22  | 1.67                     | 0.77              |
| 2:B:19:HIS:HD2    | 2:B:189:ASP:OD1   | 1.66                     | 0.77              |
| 3:C:119:ARG:HG3   | 3:C:119:ARG:HH11  | 1.50                     | 0.77              |
| 18:R:26:LEU:HD23  | 18:R:29:PHE:CE2   | 2.18                     | 0.77              |
| 2:B:7:VAL:HG12    | 2:B:221:LEU:HD23  | 1.66                     | 0.77              |
| 12:L:27:LEU:O     | 12:L:29:GLY:N     | 2.18                     | 0.77              |
| 1:A:954:G:H4'     | 13:M:120:LYS:HB3  | 1.65                     | 0.77              |
| 2:B:18:GLY:O      | 2:B:19:HIS:HB2    | 1.85                     | 0.77              |
| 17:Q:67:LYS:HA    | 17:Q:70:ARG:HH12  | 1.48                     | 0.77              |
| 12:L:55:VAL:HG12  | 12:L:56:ALA:H     | 1.49                     | 0.77              |
| 1:A:421:U:H5'     | 1:A:422:C:C5      | 2.20                     | 0.76              |
| 3:C:207:VAL:HG12  | 3:C:208:ILE:N     | 2.00                     | 0.76              |
| 10:J:7:LYS:HG3    | 10:J:71:LEU:HD23  | 1.65                     | 0.76              |
| 6:F:3:ARG:HH11    | 6:F:3:ARG:HG3     | 1.50                     | 0.76              |
| 10:J:49:VAL:HG23  | 14:N:41:ARG:HD2   | 1.67                     | 0.76              |
| 13:M:37:THR:HG23  | 13:M:55:ARG:HD2   | 1.66                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 14:N:9:LYS:HE3   | 14:N:21:TYR:O    | 1.86                     | 0.76              |
| 1:A:443:C:C2'    | 1:A:444:C:H5''   | 2.15                     | 0.76              |
| 11:K:11:LYS:HD2  | 11:K:11:LYS:O    | 1.84                     | 0.76              |
| 19:S:20:LEU:HD12 | 19:S:21:GLU:N    | 2.01                     | 0.76              |
| 21:U:6:ARG:HH21  | 21:U:15:ARG:NH2  | 1.84                     | 0.76              |
| 1:A:1425:U:H3    | 1:A:1475:G:H1    | 1.30                     | 0.76              |
| 5:E:80:ILE:HD11  | 5:E:91:LEU:HB2   | 1.66                     | 0.76              |
| 1:A:266:G:H5''   | 1:A:268:C:H41    | 1.49                     | 0.76              |
| 4:D:18:LYS:HZ2   | 4:D:31:CYS:HB3   | 1.49                     | 0.76              |
| 1:A:438:G:H4'    | 1:A:439:A:OP1    | 1.86                     | 0.75              |
| 4:D:36:ARG:HG2   | 4:D:38:TYR:CZ    | 2.21                     | 0.75              |
| 9:I:70:LYS:O     | 9:I:74:ILE:HG13  | 1.86                     | 0.75              |
| 1:A:946:A:H2'    | 1:A:947:G:C8     | 2.21                     | 0.75              |
| 3:C:156:ARG:HD2  | 3:C:160:ALA:O    | 1.87                     | 0.75              |
| 1:A:243:A:H4'    | 1:A:244:U:C5'    | 2.14                     | 0.75              |
| 1:A:909:A:OP1    | 12:L:21:LYS:HE2  | 1.86                     | 0.75              |
| 16:P:19:ILE:HG22 | 16:P:36:ILE:HG13 | 1.68                     | 0.75              |
| 1:A:112:G:H4'    | 1:A:389:A:H5''   | 1.68                     | 0.75              |
| 5:E:79:GLU:HG3   | 5:E:93:PRO:HD2   | 1.67                     | 0.75              |
| 10:J:37:PRO:HA   | 10:J:72:VAL:HG22 | 1.69                     | 0.75              |
| 5:E:8:GLU:HB3    | 5:E:34:VAL:HG23  | 1.69                     | 0.75              |
| 3:C:14:ILE:O     | 3:C:16:ARG:N     | 2.20                     | 0.75              |
| 10:J:29:ARG:HG3  | 10:J:84:GLN:HE22 | 1.52                     | 0.75              |
| 10:J:34:VAL:HG12 | 10:J:36:GLY:H    | 1.50                     | 0.75              |
| 10:J:90:LEU:H    | 10:J:91:PRO:CD   | 2.00                     | 0.74              |
| 1:A:1435:G:H2'   | 1:A:1436:U:C6    | 2.22                     | 0.74              |
| 3:C:6:HIS:CD2    | 3:C:8:ILE:HB     | 2.23                     | 0.74              |
| 3:C:91:LEU:HD11  | 3:C:99:VAL:CG2   | 2.17                     | 0.74              |
| 1:A:203:U:H5''   | 1:A:204:U:OP1    | 1.86                     | 0.74              |
| 1:A:718:G:H5'    | 11:K:117:ASN:ND2 | 2.02                     | 0.74              |
| 10:J:8:LEU:HB3   | 10:J:16:LEU:HD22 | 1.70                     | 0.74              |
| 10:J:32:ALA:H    | 10:J:78:ASN:ND2  | 1.84                     | 0.74              |
| 21:U:6:ARG:HH21  | 21:U:15:ARG:HH21 | 1.32                     | 0.74              |
| 12:L:53:ARG:HG2  | 12:L:69:TYR:HE1  | 1.53                     | 0.74              |
| 10:J:32:ALA:HB2  | 10:J:76:ASN:HB2  | 1.70                     | 0.74              |
| 11:K:47:VAL:HG12 | 11:K:48:ILE:HD13 | 1.69                     | 0.74              |
| 8:H:4:ASP:OD2    | 8:H:7:ALA:HB2    | 1.87                     | 0.74              |
| 2:B:60:ASP:HB3   | 2:B:64:ARG:NH1   | 2.03                     | 0.74              |
| 11:K:69:ALA:O    | 11:K:73:MET:HG2  | 1.88                     | 0.74              |
| 17:Q:101:ARG:HA  | 17:Q:101:ARG:HE  | 1.52                     | 0.74              |
| 10:J:82:ILE:O    | 10:J:86:MET:HB2  | 1.87                     | 0.73              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 11:K:126:ARG:O    | 11:K:127:LYS:HB2 | 1.86                     | 0.73              |
| 12:L:25:PRO:C     | 12:L:27:LEU:H    | 1.96                     | 0.73              |
| 4:D:111:ALA:HB2   | 4:D:120:LEU:HD12 | 1.69                     | 0.73              |
| 2:B:15:VAL:HG11   | 2:B:209:ARG:HB2  | 1.69                     | 0.73              |
| 5:E:150:ARG:HG3   | 5:E:150:ARG:NH1  | 2.01                     | 0.73              |
| 7:G:140:ASP:HA    | 7:G:143:ARG:NH1  | 2.03                     | 0.73              |
| 18:R:46:GLU:H     | 18:R:46:GLU:CD   | 1.96                     | 0.73              |
| 2:B:107:THR:HA    | 2:B:110:GLN:OE1  | 1.88                     | 0.73              |
| 1:A:523:A:H61     | 12:L:92:ASP:HB2  | 1.52                     | 0.73              |
| 4:D:36:ARG:HG2    | 4:D:38:TYR:OH    | 1.88                     | 0.73              |
| 20:T:53:LEU:HB2   | 20:T:100:ILE:CG2 | 2.19                     | 0.73              |
| 1:A:407:G:O2'     | 4:D:116:GLN:HG3  | 1.88                     | 0.73              |
| 1:A:991:U:C4      | 1:A:1212:U:H1'   | 2.23                     | 0.73              |
| 5:E:110:LEU:HD13  | 5:E:118:ILE:HG21 | 1.71                     | 0.73              |
| 10:J:4:ILE:HD11   | 10:J:74:ILE:HD12 | 1.69                     | 0.73              |
| 18:R:16:PRO:HB2   | 18:R:18:ARG:HE   | 1.53                     | 0.73              |
| 3:C:58:GLU:HB2    | 3:C:65:ALA:HB3   | 1.71                     | 0.73              |
| 9:I:93:ARG:NH1    | 9:I:93:ARG:HB3   | 2.03                     | 0.73              |
| 1:A:1132:C:H2'    | 1:A:1133:G:C8    | 2.24                     | 0.72              |
| 9:I:10:ARG:HD3    | 9:I:105:ASP:HB3  | 1.69                     | 0.72              |
| 1:A:939:G:H5''    | 7:G:102:ARG:NH2  | 2.04                     | 0.72              |
| 3:C:6:HIS:HD2     | 3:C:8:ILE:H      | 1.37                     | 0.72              |
| 4:D:62:GLN:HE22   | 4:D:65:ARG:HH12  | 1.36                     | 0.72              |
| 10:J:32:ALA:CB    | 10:J:75:ILE:HG13 | 2.16                     | 0.72              |
| 1:A:35:G:H2'      | 1:A:36:C:H6      | 1.54                     | 0.72              |
| 9:I:31:GLN:O      | 9:I:32:ASP:HB3   | 1.89                     | 0.72              |
| 1:A:984:C:H2'     | 1:A:985:C:H6     | 1.54                     | 0.72              |
| 1:A:1080:A:H5''   | 5:E:16:THR:HG21  | 1.70                     | 0.72              |
| 19:S:22:LEU:HD13  | 19:S:28:LYS:HB3  | 1.72                     | 0.72              |
| 13:M:67:GLU:O     | 13:M:69:GLU:N    | 2.23                     | 0.72              |
| 9:I:53:VAL:HG21   | 9:I:85:LEU:HD21  | 1.71                     | 0.72              |
| 6:F:14:LEU:HA     | 6:F:18:GLN:NE2   | 2.05                     | 0.72              |
| 20:T:50:GLU:HG3   | 20:T:100:ILE:HB  | 1.72                     | 0.72              |
| 1:A:1047:G:H2'    | 1:A:1048:G:C5'   | 2.19                     | 0.72              |
| 17:Q:63:ARG:O     | 17:Q:65:ILE:HD12 | 1.90                     | 0.72              |
| 4:D:24:GLU:OE1    | 4:D:25:ARG:N     | 2.23                     | 0.71              |
| 8:H:120:THR:OG1   | 8:H:123:GLU:HG3  | 1.90                     | 0.71              |
| 13:M:49:THR:HG22  | 13:M:51:ALA:N    | 2.04                     | 0.71              |
| 2:B:114:ARG:NH1   | 2:B:118:LEU:HD12 | 2.05                     | 0.71              |
| 15:O:6:GLU:H      | 15:O:6:GLU:CD    | 1.96                     | 0.71              |
| 1:A:1030(C):G:H2' | 1:A:1030(D):A:C8 | 2.24                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 16:P:57:ARG:NH1  | 16:P:79:VAL:O    | 2.23                     | 0.71              |
| 3:C:64:VAL:H     | 3:C:99:VAL:CG1   | 2.02                     | 0.71              |
| 7:G:111:ARG:HB3  | 7:G:113:GLU:OE2  | 1.89                     | 0.71              |
| 10:J:49:VAL:CG2  | 14:N:41:ARG:HB2  | 2.19                     | 0.71              |
| 14:N:43:CYS:SG   | 27:N:101:ZN:ZN   | 1.79                     | 0.71              |
| 1:A:1047:G:C2'   | 1:A:1048:G:H5''  | 2.21                     | 0.71              |
| 13:M:90:LEU:HD22 | 13:M:94:ARG:HH11 | 1.54                     | 0.71              |
| 14:N:57:ARG:HG2  | 14:N:58:LYS:H    | 1.55                     | 0.71              |
| 1:A:1502:A:H2    | 1:A:1505:G:N1    | 1.88                     | 0.71              |
| 1:A:673:G:H2'    | 1:A:674:G:C8     | 2.26                     | 0.70              |
| 1:A:706:A:O4'    | 11:K:29:ILE:HD11 | 1.91                     | 0.70              |
| 5:E:92:LYS:HB3   | 5:E:119:LEU:HB2  | 1.73                     | 0.70              |
| 14:N:3:ARG:O     | 14:N:5:ALA:N     | 2.23                     | 0.70              |
| 17:Q:67:LYS:HA   | 17:Q:70:ARG:NH1  | 2.06                     | 0.70              |
| 1:A:1281:U:H5'   | 1:A:1282:C:H5    | 1.56                     | 0.70              |
| 9:I:118:LYS:O    | 9:I:119:ALA:HB3  | 1.90                     | 0.70              |
| 16:P:34:GLU:OE2  | 16:P:55:ARG:HD3  | 1.91                     | 0.70              |
| 17:Q:68:ARG:N    | 17:Q:70:ARG:NH1  | 2.39                     | 0.70              |
| 17:Q:97:SER:HA   | 17:Q:102:GLY:HA2 | 1.74                     | 0.70              |
| 1:A:969:A:H61    | 13:M:126:LYS:HB2 | 1.56                     | 0.70              |
| 3:C:110:ASN:O    | 3:C:111:LEU:HD23 | 1.91                     | 0.70              |
| 15:O:87:ILE:HG22 | 15:O:88:ARG:N    | 1.99                     | 0.70              |
| 12:L:47:LYS:HB3  | 12:L:48:PRO:HD3  | 1.74                     | 0.70              |
| 13:M:8:GLU:HA    | 13:M:8:GLU:OE2   | 1.90                     | 0.70              |
| 2:B:12:GLU:C     | 2:B:14:GLY:H     | 1.99                     | 0.70              |
| 7:G:140:ASP:HA   | 7:G:143:ARG:HH11 | 1.57                     | 0.70              |
| 10:J:74:ILE:HD13 | 10:J:81:THR:HG21 | 1.73                     | 0.70              |
| 1:A:853:G:O2'    | 1:A:854:G:H5'    | 1.91                     | 0.70              |
| 2:B:215:LEU:O    | 2:B:219:VAL:HG23 | 1.90                     | 0.70              |
| 1:A:1499:A:H1'   | 1:A:1520:G:H5'   | 1.72                     | 0.70              |
| 4:D:146:ILE:N    | 4:D:146:ILE:HD12 | 2.07                     | 0.70              |
| 5:E:80:ILE:HD12  | 5:E:80:ILE:H     | 1.56                     | 0.70              |
| 5:E:144:THR:HB   | 5:E:147:ASP:OD2  | 1.91                     | 0.70              |
| 2:B:61:LEU:HD21  | 2:B:160:ASP:CB   | 2.21                     | 0.69              |
| 2:B:134:GLU:HG2  | 2:B:137:ARG:HH21 | 1.56                     | 0.69              |
| 4:D:35:ARG:O     | 4:D:36:ARG:HB2   | 1.90                     | 0.69              |
| 4:D:80:GLU:O     | 4:D:84:LYS:HG3   | 1.92                     | 0.69              |
| 10:J:49:VAL:O    | 10:J:60:ARG:HA   | 1.91                     | 0.69              |
| 12:L:55:VAL:HG12 | 12:L:56:ALA:N    | 2.07                     | 0.69              |
| 15:O:39:LEU:HD12 | 15:O:56:LEU:HD13 | 1.73                     | 0.69              |
| 1:A:725:G:H2'    | 1:A:726:C:C5'    | 2.22                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1047:G:H2'   | 1:A:1048:G:H5''  | 1.74                     | 0.69              |
| 8:H:91:ARG:HG3   | 12:L:7:ILE:HG13  | 1.73                     | 0.69              |
| 17:Q:67:LYS:O    | 17:Q:68:ARG:CB   | 2.39                     | 0.69              |
| 1:A:266:G:H5'    | 1:A:266:G:C8     | 2.28                     | 0.69              |
| 1:A:839:U:O2     | 1:A:839:U:H2'    | 1.91                     | 0.69              |
| 4:D:26:CYS:HA    | 4:D:31:CYS:HB2   | 1.74                     | 0.69              |
| 4:D:30:LYS:C     | 4:D:32:ALA:H     | 1.98                     | 0.69              |
| 4:D:64:LEU:HD12  | 4:D:75:PHE:CZ    | 2.27                     | 0.69              |
| 14:N:27:CYS:SG   | 14:N:29:ARG:HB2  | 2.32                     | 0.69              |
| 8:H:103:VAL:HG21 | 8:H:109:ILE:O    | 1.92                     | 0.69              |
| 11:K:126:ARG:O   | 11:K:127:LYS:HE2 | 1.93                     | 0.69              |
| 1:A:1189:C:P     | 10:J:51:ARG:HH22 | 2.15                     | 0.69              |
| 18:R:18:ARG:O    | 18:R:19:LYS:HB3  | 1.91                     | 0.69              |
| 18:R:19:LYS:HG3  | 18:R:20:ALA:N    | 2.07                     | 0.69              |
| 1:A:1038:C:H2'   | 1:A:1039:C:C6    | 2.27                     | 0.69              |
| 2:B:60:ASP:CB    | 2:B:64:ARG:HH12  | 2.05                     | 0.69              |
| 3:C:172:ARG:HB3  | 3:C:172:ARG:HH11 | 1.58                     | 0.69              |
| 18:R:32:ARG:HA   | 18:R:69:THR:HG21 | 1.74                     | 0.69              |
| 1:A:1133:G:H2'   | 1:A:1134:G:H8    | 1.56                     | 0.69              |
| 2:B:97:TRP:HZ2   | 2:B:102:LEU:HD13 | 1.55                     | 0.69              |
| 5:E:89:ILE:HD13  | 5:E:90:VAL:H     | 1.58                     | 0.69              |
| 8:H:122:ARG:HB3  | 8:H:122:ARG:HH11 | 1.56                     | 0.69              |
| 10:J:80:LYS:HA   | 10:J:83:GLU:OE2  | 1.93                     | 0.69              |
| 13:M:40:ASN:O    | 13:M:43:THR:HG23 | 1.93                     | 0.69              |
| 1:A:1144:G:H21   | 1:A:1146:A:N6    | 1.92                     | 0.68              |
| 18:R:25:THR:HG22 | 18:R:42:ARG:HH12 | 1.58                     | 0.68              |
| 1:A:1095:U:H2'   | 1:A:1096:C:C6    | 2.27                     | 0.68              |
| 1:A:1492:A:OP1   | 12:L:47:LYS:N    | 2.26                     | 0.68              |
| 8:H:51:VAL:HG11  | 8:H:60:ARG:NH1   | 2.08                     | 0.68              |
| 3:C:188:LEU:CD1  | 3:C:195:VAL:HG13 | 2.23                     | 0.68              |
| 12:L:45:PRO:HD3  | 12:L:51:ALA:O    | 1.92                     | 0.68              |
| 14:N:26:ARG:O    | 14:N:26:ARG:HG3  | 1.93                     | 0.68              |
| 6:F:47:ARG:N     | 6:F:47:ARG:HD3   | 2.08                     | 0.68              |
| 1:A:629:G:H2'    | 1:A:630:G:O4'    | 1.93                     | 0.68              |
| 1:A:1356:G:H2'   | 1:A:1357:A:C8    | 2.28                     | 0.68              |
| 1:A:1369:C:H2'   | 1:A:1370:G:C8    | 2.28                     | 0.68              |
| 7:G:46:ALA:O     | 7:G:50:ILE:HG12  | 1.94                     | 0.68              |
| 1:A:353:A:H5'    | 1:A:353:A:H8     | 1.59                     | 0.68              |
| 1:A:706:A:C1'    | 11:K:29:ILE:HD11 | 2.24                     | 0.68              |
| 1:A:1137:C:H4'   | 1:A:1138:G:C2    | 2.28                     | 0.68              |
| 3:C:70:VAL:HG12  | 3:C:71:ALA:N     | 2.08                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:I:106:ALA:O    | 9:I:108:VAL:HG23 | 1.93                     | 0.68              |
| 4:D:127:THR:CG2  | 4:D:147:ALA:HB3  | 2.24                     | 0.68              |
| 6:F:101:ALA:HB2  | 18:R:28:GLU:HG3  | 1.76                     | 0.68              |
| 8:H:28:ALA:HB2   | 8:H:59:LEU:HG    | 1.76                     | 0.68              |
| 9:I:48:GLU:HA    | 9:I:51:ARG:HH11  | 1.58                     | 0.68              |
| 1:A:247:G:OP2    | 17:Q:99:SER:HB2  | 1.94                     | 0.68              |
| 10:J:3:LYS:HA    | 10:J:76:ASN:H    | 1.57                     | 0.68              |
| 1:A:437:U:H5''   | 4:D:155:LEU:HD22 | 1.75                     | 0.68              |
| 3:C:29:TYR:OH    | 14:N:54:PRO:HD2  | 1.95                     | 0.68              |
| 20:T:56:MET:HE2  | 20:T:88:VAL:HG11 | 1.75                     | 0.68              |
| 5:E:50:GLU:HB3   | 5:E:53:LEU:HD21  | 1.76                     | 0.67              |
| 1:A:1241:G:H2'   | 1:A:1242:C:C6    | 2.29                     | 0.67              |
| 4:D:127:THR:HG23 | 4:D:147:ALA:HB3  | 1.76                     | 0.67              |
| 7:G:23:VAL:O     | 7:G:27:ILE:HG12  | 1.95                     | 0.67              |
| 6:F:80:ARG:NH1   | 6:F:88:VAL:HB    | 2.09                     | 0.67              |
| 10:J:26:ALA:HB1  | 10:J:84:GLN:HB2  | 1.76                     | 0.67              |
| 1:A:1125:U:H3    | 10:J:5:ARG:HH21  | 1.41                     | 0.67              |
| 2:B:98:LEU:HG    | 2:B:101:MET:HE3  | 1.76                     | 0.67              |
| 1:A:393:A:O2'    | 1:A:394:G:H5'    | 1.93                     | 0.67              |
| 3:C:77:ILE:C     | 3:C:83:ARG:HB3   | 2.19                     | 0.67              |
| 6:F:8:ILE:HD11   | 6:F:79:LEU:HD13  | 1.76                     | 0.67              |
| 3:C:147:LYS:HE2  | 3:C:205:GLY:N    | 2.10                     | 0.67              |
| 13:M:40:ASN:HD22 | 13:M:41:PRO:CD   | 2.07                     | 0.67              |
| 1:A:112:G:H5'    | 1:A:389:A:H4'    | 1.76                     | 0.67              |
| 1:A:1053:G:C4'   | 1:A:1054:C:H5'   | 2.25                     | 0.67              |
| 3:C:23:TYR:CD2   | 3:C:24:ALA:N     | 2.62                     | 0.67              |
| 4:D:128:VAL:HG12 | 4:D:129:ASN:ND2  | 2.10                     | 0.67              |
| 10:J:3:LYS:HA    | 10:J:74:ILE:O    | 1.94                     | 0.67              |
| 10:J:4:ILE:O     | 10:J:73:ASP:HA   | 1.94                     | 0.67              |
| 1:A:1497:G:H2'   | 1:A:1498:U:H5'   | 1.76                     | 0.67              |
| 2:B:98:LEU:HD23  | 2:B:98:LEU:N     | 2.10                     | 0.67              |
| 4:D:31:CYS:C     | 4:D:33:MET:H     | 2.02                     | 0.67              |
| 5:E:43:LEU:HB2   | 5:E:136:MET:HE2  | 1.77                     | 0.67              |
| 6:F:4:TYR:HE1    | 6:F:92:LYS:HG2   | 1.60                     | 0.67              |
| 12:L:28:LYS:O    | 12:L:29:GLY:C    | 2.38                     | 0.67              |
| 2:B:181:PHE:CD2  | 8:H:70:GLN:HB3   | 2.30                     | 0.67              |
| 7:G:18:TYR:HD2   | 7:G:59:LEU:HD22  | 1.59                     | 0.67              |
| 1:A:725:G:H2'    | 1:A:726:C:H5'    | 1.76                     | 0.66              |
| 1:A:1054:C:H5    | 1:A:1196:U:C5    | 2.14                     | 0.66              |
| 3:C:28:GLN:HA    | 3:C:31:HIS:HD2   | 1.60                     | 0.66              |
| 12:L:24:VAL:O    | 12:L:24:VAL:HG12 | 1.94                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1182:G:O2'   | 1:A:1183:A:OP2   | 2.08                     | 0.66              |
| 8:H:100:ILE:HG23 | 8:H:112:LEU:HD11 | 1.77                     | 0.66              |
| 1:A:818:G:C3'    | 1:A:819:A:H5''   | 2.25                     | 0.66              |
| 4:D:189:PRO:HB2  | 4:D:194:LEU:CD2  | 2.25                     | 0.66              |
| 9:I:48:GLU:N     | 9:I:49:PRO:HD2   | 2.11                     | 0.66              |
| 1:A:1366:C:H2'   | 1:A:1367:C:C6    | 2.28                     | 0.66              |
| 1:A:1412:C:H2'   | 1:A:1413:A:C8    | 2.30                     | 0.66              |
| 2:B:15:VAL:CG1   | 2:B:209:ARG:HB2  | 2.25                     | 0.66              |
| 3:C:34:LEU:HD13  | 3:C:34:LEU:C     | 2.21                     | 0.66              |
| 6:F:22:GLU:OE2   | 6:F:82:ARG:HD3   | 1.96                     | 0.66              |
| 4:D:3:ARG:NH1    | 4:D:115:ARG:HB3  | 2.09                     | 0.66              |
| 4:D:31:CYS:SG    | 27:D:301:ZN:ZN   | 1.85                     | 0.66              |
| 16:P:4:ILE:HG13  | 16:P:64:ALA:HB1  | 1.78                     | 0.66              |
| 2:B:178:ARG:HH21 | 2:B:196:LEU:C    | 2.04                     | 0.66              |
| 19:S:5:LEU:O     | 19:S:6:LYS:CB    | 2.43                     | 0.66              |
| 20:T:76:ALA:HA   | 20:T:79:ARG:NH1  | 2.11                     | 0.66              |
| 1:A:1116:C:C2'   | 1:A:1117:G:H5''  | 2.26                     | 0.66              |
| 1:A:1194:U:H2'   | 1:A:1195:C:H6    | 1.61                     | 0.66              |
| 8:H:54:ASP:O     | 8:H:56:LYS:HD3   | 1.96                     | 0.66              |
| 9:I:93:ARG:HB3   | 9:I:93:ARG:HH11  | 1.59                     | 0.66              |
| 1:A:344:A:H4'    | 1:A:345:C:OP2    | 1.95                     | 0.66              |
| 1:A:444:C:C6     | 1:A:444:C:H5'    | 2.31                     | 0.66              |
| 2:B:98:LEU:O     | 2:B:101:MET:HG3  | 1.96                     | 0.66              |
| 2:B:139:LYS:C    | 2:B:139:LYS:HD3  | 2.21                     | 0.66              |
| 3:C:102:ASN:N    | 3:C:102:ASN:HD22 | 1.94                     | 0.66              |
| 4:D:25:ARG:C     | 4:D:27:TYR:H     | 2.03                     | 0.66              |
| 7:G:113:GLU:HG2  | 7:G:119:ARG:HG2  | 1.77                     | 0.66              |
| 12:L:74:GLY:O    | 12:L:75:HIS:HB2  | 1.96                     | 0.66              |
| 10:J:61:GLU:OE1  | 14:N:45:ARG:NH1  | 2.28                     | 0.66              |
| 1:A:443:C:H2'    | 1:A:444:C:C5'    | 2.26                     | 0.65              |
| 2:B:51:LEU:HD22  | 2:B:55:PHE:CE1   | 2.31                     | 0.65              |
| 3:C:44:GLU:HG2   | 3:C:52:LEU:HD11  | 1.78                     | 0.65              |
| 4:D:25:ARG:HG2   | 4:D:25:ARG:HH11  | 1.62                     | 0.65              |
| 8:H:116:LYS:HD3  | 8:H:127:LEU:HD22 | 1.78                     | 0.65              |
| 10:J:20:ALA:O    | 10:J:24:VAL:HG23 | 1.96                     | 0.65              |
| 17:Q:59:ILE:HG23 | 17:Q:71:PHE:HB3  | 1.78                     | 0.65              |
| 19:S:13:ASP:HA   | 19:S:16:LEU:HB3  | 1.77                     | 0.65              |
| 2:B:61:LEU:HD21  | 2:B:160:ASP:HB3  | 1.78                     | 0.65              |
| 1:A:501:C:H2'    | 1:A:502:G:H8     | 1.59                     | 0.65              |
| 1:A:509:A:H5'    | 1:A:509:A:H8     | 1.60                     | 0.65              |
| 2:B:105:PHE:CE1  | 2:B:155:LEU:HD23 | 2.31                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 20:T:73:HIS:O    | 20:T:74:LYS:CB   | 2.40                     | 0.65              |
| 1:A:384:G:H2'    | 1:A:385:C:C6     | 2.30                     | 0.65              |
| 1:A:666:G:H5'    | 1:A:726:C:H1'    | 1.79                     | 0.65              |
| 1:A:725:G:C2'    | 1:A:726:C:H5''   | 2.26                     | 0.65              |
| 2:B:139:LYS:HD3  | 2:B:139:LYS:O    | 1.96                     | 0.65              |
| 1:A:1323:G:H2'   | 1:A:1324:A:C8    | 2.32                     | 0.65              |
| 1:A:1497:G:C2'   | 1:A:1498:U:H5'   | 2.27                     | 0.65              |
| 7:G:18:TYR:CE2   | 7:G:59:LEU:HB2   | 2.32                     | 0.65              |
| 13:M:37:THR:HG22 | 13:M:39:ILE:HG13 | 1.78                     | 0.65              |
| 15:O:54:ARG:HG2  | 15:O:54:ARG:HH11 | 1.61                     | 0.65              |
| 2:B:75:LYS:HA    | 2:B:78:GLN:HB2   | 1.77                     | 0.65              |
| 8:H:9:MET:SD     | 8:H:32:LYS:HG2   | 2.37                     | 0.65              |
| 15:O:55:GLY:HA2  | 15:O:58:MET:CE   | 2.25                     | 0.65              |
| 1:A:443:C:H2'    | 1:A:444:C:H5''   | 1.78                     | 0.65              |
| 1:A:1014:A:C2    | 1:A:1219:U:H1'   | 2.32                     | 0.65              |
| 3:C:157:ILE:CD1  | 3:C:166:GLU:HG3  | 2.27                     | 0.65              |
| 12:L:85:ILE:HG23 | 12:L:98:TYR:HB3  | 1.78                     | 0.65              |
| 3:C:64:VAL:N     | 3:C:99:VAL:HG11  | 2.12                     | 0.65              |
| 9:I:111:ARG:HD3  | 9:I:112:LYS:N    | 2.12                     | 0.65              |
| 4:D:30:LYS:HB3   | 4:D:35:ARG:HH21  | 1.61                     | 0.65              |
| 9:I:115:GLY:HA2  | 10:J:58:ASP:OD1  | 1.96                     | 0.65              |
| 13:M:15:VAL:HG23 | 13:M:43:THR:O    | 1.96                     | 0.65              |
| 3:C:147:LYS:HE2  | 3:C:205:GLY:CA   | 2.28                     | 0.64              |
| 3:C:172:ARG:HB3  | 3:C:172:ARG:NH1  | 2.13                     | 0.64              |
| 5:E:74:GLY:HA3   | 5:E:116:THR:HG22 | 1.77                     | 0.64              |
| 1:A:444:C:H5'    | 1:A:444:C:H6     | 1.63                     | 0.64              |
| 1:A:975:A:H5'    | 1:A:975:A:C8     | 2.33                     | 0.64              |
| 2:B:8:LYS:O      | 2:B:9:GLU:HB2    | 1.96                     | 0.64              |
| 2:B:97:TRP:CZ2   | 2:B:102:LEU:HD13 | 2.31                     | 0.64              |
| 7:G:120:ILE:HG22 | 7:G:124:LEU:HD12 | 1.79                     | 0.64              |
| 8:H:85:ARG:HD3   | 8:H:86:ILE:N     | 2.11                     | 0.64              |
| 15:O:65:ARG:HG2  | 15:O:65:ARG:NH1  | 2.10                     | 0.64              |
| 16:P:57:ARG:HH11 | 16:P:57:ARG:CG   | 2.09                     | 0.64              |
| 17:Q:27:PHE:CZ   | 17:Q:36:ILE:HD11 | 2.32                     | 0.64              |
| 1:A:1392:G:H21   | 1:A:1502:A:H8    | 1.43                     | 0.64              |
| 2:B:14:GLY:C     | 2:B:15:VAL:HG22  | 2.21                     | 0.64              |
| 19:S:16:LEU:O    | 19:S:19:VAL:HG12 | 1.98                     | 0.64              |
| 1:A:973:G:H3'    | 1:A:974:A:H5''   | 1.79                     | 0.64              |
| 17:Q:69:LYS:C    | 17:Q:70:ARG:HD2  | 2.23                     | 0.64              |
| 2:B:165:VAL:HG23 | 2:B:166:ASP:N    | 2.13                     | 0.64              |
| 5:E:76:ILE:HG13  | 5:E:142:LEU:CD1  | 2.28                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:76:ILE:HG22  | 5:E:78:HIS:O     | 1.97                     | 0.64              |
| 6:F:37:VAL:HA    | 6:F:65:VAL:HG12  | 1.79                     | 0.64              |
| 7:G:50:ILE:HD11  | 7:G:121:ALA:HA   | 1.78                     | 0.64              |
| 18:R:88:LYS:HB3  | 18:R:88:LYS:NZ   | 2.12                     | 0.64              |
| 1:A:1479:C:H2'   | 1:A:1480:G:C8    | 2.32                     | 0.64              |
| 10:J:49:VAL:O    | 10:J:60:ARG:O    | 2.15                     | 0.64              |
| 1:A:1208:C:H2'   | 1:A:1209:C:H6    | 1.63                     | 0.64              |
| 1:A:1330:U:OP1   | 13:M:23:TYR:O    | 2.15                     | 0.64              |
| 1:A:1479:C:H2'   | 1:A:1480:G:H8    | 1.63                     | 0.64              |
| 3:C:148:GLY:HA3  | 3:C:172:ARG:O    | 1.98                     | 0.64              |
| 5:E:79:GLU:HG3   | 5:E:93:PRO:CD    | 2.28                     | 0.64              |
| 6:F:75:LEU:C     | 6:F:75:LEU:HD23  | 2.23                     | 0.64              |
| 1:A:580:U:H2'    | 1:A:581:G:O4'    | 1.98                     | 0.64              |
| 10:J:90:LEU:N    | 10:J:91:PRO:HD2  | 2.09                     | 0.64              |
| 1:A:656:C:H4'    | 15:O:62:GLN:NE2  | 2.13                     | 0.63              |
| 1:A:1441:G:H4'   | 1:A:1442:G:C5    | 2.33                     | 0.63              |
| 9:I:111:ARG:HD3  | 9:I:112:LYS:C    | 2.23                     | 0.63              |
| 15:O:4:THR:HB    | 15:O:6:GLU:OE2   | 1.97                     | 0.63              |
| 19:S:43:GLU:H    | 19:S:43:GLU:CD   | 2.05                     | 0.63              |
| 3:C:119:ARG:HE   | 3:C:140:ARG:NE   | 1.96                     | 0.63              |
| 16:P:81:ARG:HG2  | 16:P:83:GLU:OE2  | 1.98                     | 0.63              |
| 5:E:76:ILE:HG13  | 5:E:142:LEU:HD11 | 1.81                     | 0.63              |
| 8:H:119:LEU:HD12 | 8:H:124:ALA:HA   | 1.79                     | 0.63              |
| 11:K:82:VAL:C    | 11:K:83:ILE:HD12 | 2.23                     | 0.63              |
| 16:P:67:THR:HG22 | 16:P:69:THR:N    | 2.12                     | 0.63              |
| 1:A:421:U:H5'    | 1:A:422:C:C6     | 2.33                     | 0.63              |
| 3:C:64:VAL:HB    | 3:C:99:VAL:HG21  | 1.80                     | 0.63              |
| 8:H:24:THR:HG22  | 8:H:63:LEU:HD21  | 1.80                     | 0.63              |
| 12:L:56:ALA:O    | 12:L:67:THR:HA   | 1.98                     | 0.63              |
| 13:M:17:VAL:O    | 13:M:20:THR:HB   | 1.98                     | 0.63              |
| 1:A:1032:G:H2'   | 1:A:1033:G:H8    | 1.62                     | 0.63              |
| 4:D:92:VAL:O     | 4:D:96:LEU:HD13  | 1.99                     | 0.63              |
| 7:G:52:GLU:HG2   | 7:G:52:GLU:O     | 1.98                     | 0.63              |
| 7:G:75:VAL:CG2   | 7:G:86:GLN:HB3   | 2.29                     | 0.63              |
| 9:I:69:GLY:O     | 9:I:73:GLN:HG3   | 1.98                     | 0.63              |
| 10:J:42:THR:HG22 | 10:J:43:ARG:N    | 2.13                     | 0.63              |
| 18:R:47:THR:HG22 | 18:R:48:GLY:H    | 1.64                     | 0.63              |
| 1:A:370:C:O2'    | 1:A:371:G:H5'    | 1.98                     | 0.63              |
| 1:A:377:G:OP1    | 16:P:3:LYS:HD3   | 1.99                     | 0.63              |
| 1:A:1305:G:N2    | 1:A:1331:G:O2'   | 2.32                     | 0.63              |
| 1:A:1347:G:N2    | 1:A:1373:G:H2'   | 2.14                     | 0.63              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:F:2:ARG:HE     | 6:F:69:GLU:HG2    | 1.61                     | 0.63              |
| 17:Q:67:LYS:O    | 17:Q:68:ARG:HB2   | 1.99                     | 0.63              |
| 23:Y:34:CM0:C8   | 23:Y:34:CM0:O4    | 2.47                     | 0.63              |
| 2:B:213:LEU:HD22 | 2:B:214:ILE:HD13  | 1.81                     | 0.63              |
| 17:Q:95:TYR:C    | 17:Q:97:SER:H     | 2.07                     | 0.63              |
| 1:A:1052:U:H2'   | 1:A:1055:A:OP1    | 1.99                     | 0.63              |
| 9:I:97:LYS:HB3   | 9:I:98:PRO:HD3    | 1.81                     | 0.63              |
| 2:B:189:ASP:HB2  | 2:B:205:ASP:OD2   | 1.99                     | 0.62              |
| 3:C:47:LEU:CD2   | 3:C:68:VAL:HG11   | 2.29                     | 0.62              |
| 3:C:147:LYS:HE2  | 3:C:205:GLY:HA2   | 1.80                     | 0.62              |
| 6:F:4:TYR:CE1    | 6:F:92:LYS:HG2    | 2.33                     | 0.62              |
| 11:K:108:ILE:N   | 11:K:108:ILE:HD12 | 2.14                     | 0.62              |
| 17:Q:27:PHE:CE1  | 17:Q:36:ILE:HD11  | 2.34                     | 0.62              |
| 17:Q:86:GLU:O    | 17:Q:90:ILE:HG13  | 1.99                     | 0.62              |
| 1:A:410:G:H4'    | 1:A:411:A:OP1     | 1.99                     | 0.62              |
| 1:A:1086:U:H3    | 1:A:1099:G:H22    | 1.47                     | 0.62              |
| 1:A:1101:A:H4'   | 1:A:1102:A:O5'    | 1.96                     | 0.62              |
| 1:A:1142:G:H2'   | 1:A:1143:G:O4'    | 2.00                     | 0.62              |
| 4:D:156:GLU:HG2  | 4:D:160:GLN:HE21  | 1.63                     | 0.62              |
| 1:A:392:G:H2'    | 1:A:393:A:H8      | 1.63                     | 0.62              |
| 1:A:1306:A:N6    | 1:A:1331:G:H1'    | 2.14                     | 0.62              |
| 5:E:80:ILE:HD12  | 5:E:91:LEU:HB2    | 1.81                     | 0.62              |
| 6:F:21:LEU:O     | 6:F:25:ILE:HG13   | 1.99                     | 0.62              |
| 11:K:93:GLN:NE2  | 11:K:96:ARG:HH21  | 1.98                     | 0.62              |
| 20:T:53:LEU:HD12 | 20:T:100:ILE:HG23 | 1.81                     | 0.62              |
| 2:B:74:LYS:NZ    | 2:B:206:ASP:HB2   | 2.14                     | 0.62              |
| 1:A:1075:C:H5'   | 2:B:103:THR:HG21  | 1.81                     | 0.62              |
| 2:B:62:ALA:C     | 2:B:64:ARG:H      | 2.06                     | 0.62              |
| 8:H:60:ARG:HG3   | 8:H:60:ARG:NH1    | 2.10                     | 0.62              |
| 10:J:76:ASN:C    | 10:J:78:ASN:H     | 2.07                     | 0.62              |
| 17:Q:40:LYS:HD2  | 17:Q:42:TYR:CZ    | 2.34                     | 0.62              |
| 1:A:1427:U:H2'   | 1:A:1428:A:C8     | 2.34                     | 0.62              |
| 4:D:32:ALA:C     | 4:D:34:GLU:H      | 2.06                     | 0.62              |
| 5:E:36:ASP:OD2   | 5:E:40:ARG:HB2    | 2.00                     | 0.62              |
| 9:I:8:GLY:HA2    | 9:I:79:LEU:HB3    | 1.81                     | 0.62              |
| 19:S:30:LEU:O    | 19:S:31:ILE:HD13  | 1.99                     | 0.62              |
| 1:A:838:G:H2'    | 1:A:839:U:H5''    | 1.82                     | 0.62              |
| 2:B:86:GLU:C     | 2:B:88:ALA:H      | 2.07                     | 0.62              |
| 6:F:23:LYS:NZ    | 6:F:42:GLU:OE2    | 2.33                     | 0.62              |
| 10:J:33:GLN:CB   | 10:J:75:ILE:HD11  | 2.30                     | 0.62              |
| 1:A:107:G:C2'    | 1:A:108:G:H5'     | 2.30                     | 0.62              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:254:G:OP1    | 17:Q:68:ARG:HB3   | 1.99                     | 0.62              |
| 1:A:363:A:H62    | 12:L:28:LYS:HE3   | 1.64                     | 0.62              |
| 1:A:392:G:H2'    | 1:A:393:A:C8      | 2.35                     | 0.62              |
| 1:A:538:G:H2'    | 1:A:539:A:C8      | 2.34                     | 0.62              |
| 15:O:39:LEU:CD1  | 15:O:56:LEU:HB2   | 2.29                     | 0.62              |
| 21:U:12:LYS:HB3  | 21:U:22:ARG:HD2   | 1.81                     | 0.62              |
| 1:A:1314:C:OP2   | 19:S:6:LYS:HD3    | 2.00                     | 0.62              |
| 1:A:1531:A:C2'   | 1:A:1532:U:H5'    | 2.27                     | 0.62              |
| 3:C:8:ILE:HG23   | 3:C:16:ARG:HG2    | 1.82                     | 0.62              |
| 5:E:24:ARG:HG2   | 5:E:24:ARG:HH11   | 1.64                     | 0.62              |
| 13:M:54:VAL:O    | 13:M:58:GLU:HG2   | 1.98                     | 0.62              |
| 20:T:10:LEU:HD12 | 20:T:12:ALA:H     | 1.64                     | 0.62              |
| 20:T:53:LEU:HB2  | 20:T:100:ILE:HG23 | 1.80                     | 0.62              |
| 20:T:72:LEU:O    | 20:T:72:LEU:HG    | 2.00                     | 0.62              |
| 1:A:457:C:H2'    | 1:A:458:C:H6      | 1.65                     | 0.62              |
| 1:A:750:G:N3     | 15:O:23:GLY:HA3   | 2.15                     | 0.62              |
| 11:K:14:VAL:HG21 | 11:K:40:ILE:HD11  | 1.81                     | 0.62              |
| 12:L:27:LEU:C    | 12:L:29:GLY:N     | 2.57                     | 0.62              |
| 20:T:94:ALA:O    | 20:T:95:ALA:HB2   | 1.98                     | 0.62              |
| 1:A:279:A:H5'    | 1:A:281:G:O4'     | 2.00                     | 0.61              |
| 1:A:1148:U:H2'   | 1:A:1149:C:O4'    | 1.99                     | 0.61              |
| 3:C:111:LEU:HD21 | 3:C:144:SER:HB2   | 1.82                     | 0.61              |
| 3:C:172:ARG:HH12 | 3:C:174:PRO:HG3   | 1.64                     | 0.61              |
| 5:E:12:LEU:HD13  | 5:E:31:LEU:HB2    | 1.82                     | 0.61              |
| 1:A:382:A:H2'    | 1:A:383:A:C8      | 2.35                     | 0.61              |
| 2:B:181:PHE:CE2  | 8:H:70:GLN:HB3    | 2.36                     | 0.61              |
| 3:C:60:ALA:O     | 3:C:61:ALA:HB2    | 2.00                     | 0.61              |
| 1:A:746:A:O2'    | 1:A:747:C:H5'     | 1.99                     | 0.61              |
| 1:A:1396:A:H4'   | 1:A:1397:C:H5''   | 1.82                     | 0.61              |
| 3:C:19:GLU:HG2   | 3:C:54:ARG:HE     | 1.64                     | 0.61              |
| 9:I:125:TYR:CD2  | 9:I:125:TYR:N     | 2.67                     | 0.61              |
| 1:A:659:U:O2'    | 1:A:660:G:H5'     | 2.01                     | 0.61              |
| 1:A:1510:U:H2'   | 1:A:1511:G:C8     | 2.36                     | 0.61              |
| 1:A:192:U:O4'    | 20:T:103:GLY:HA2  | 2.00                     | 0.61              |
| 1:A:1054:C:C2'   | 1:A:1055:A:H5''   | 2.30                     | 0.61              |
| 2:B:204:ASN:HD22 | 2:B:206:ASP:H     | 1.48                     | 0.61              |
| 1:A:421:U:O4     | 3:C:127:ARG:HD3   | 1.99                     | 0.61              |
| 3:C:13:GLY:HA3   | 14:N:57:ARG:HH21  | 1.66                     | 0.61              |
| 1:A:328:C:O2     | 1:A:328:C:H2'     | 1.99                     | 0.61              |
| 1:A:1048:G:H5'   | 1:A:1048:G:H8     | 1.65                     | 0.61              |
| 1:A:1096:C:H2'   | 1:A:1097:C:H6     | 1.66                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1425:U:H2'   | 1:A:1426:C:C6    | 2.36                     | 0.61              |
| 3:C:47:LEU:N     | 3:C:47:LEU:HD12  | 2.15                     | 0.61              |
| 5:E:93:PRO:HG2   | 8:H:105:ARG:NH2  | 2.15                     | 0.61              |
| 6:F:21:LEU:O     | 6:F:24:GLU:HG3   | 2.00                     | 0.61              |
| 6:F:97:PHE:HB2   | 18:R:32:ARG:NH2  | 2.14                     | 0.61              |
| 13:M:66:LEU:O    | 13:M:67:GLU:O    | 2.19                     | 0.61              |
| 14:N:22:THR:HG23 | 14:N:33:VAL:CG2  | 2.30                     | 0.61              |
| 1:A:1121:U:H2'   | 1:A:1122:U:H6    | 1.66                     | 0.61              |
| 1:A:1201:A:H4'   | 1:A:1202:G:O5'   | 2.01                     | 0.61              |
| 1:A:1307:U:H2'   | 1:A:1308:U:C6    | 2.36                     | 0.61              |
| 2:B:189:ASP:HB3  | 2:B:191:ASP:OD1  | 2.01                     | 0.61              |
| 3:C:64:VAL:N     | 3:C:99:VAL:CG1   | 2.63                     | 0.61              |
| 18:R:36:ASN:HD22 | 18:R:36:ASN:C    | 2.09                     | 0.61              |
| 19:S:44:MET:HE2  | 19:S:49:ILE:HD11 | 1.83                     | 0.61              |
| 20:T:65:LYS:HA   | 20:T:68:LYS:HG3  | 1.83                     | 0.61              |
| 1:A:1116:C:H2'   | 1:A:1117:G:H5''  | 1.82                     | 0.61              |
| 2:B:55:PHE:HD2   | 2:B:58:ILE:HD12  | 1.66                     | 0.61              |
| 10:J:6:ILE:HD12  | 10:J:6:ILE:O     | 2.00                     | 0.61              |
| 15:O:33:THR:HG23 | 15:O:63:ARG:HH12 | 1.64                     | 0.61              |
| 1:A:413:G:H1'    | 1:A:428:G:N2     | 2.16                     | 0.61              |
| 8:H:112:LEU:N    | 8:H:112:LEU:CD2  | 2.64                     | 0.61              |
| 10:J:9:ARG:HB3   | 10:J:9:ARG:NH1   | 2.15                     | 0.60              |
| 20:T:43:LEU:HB2  | 20:T:52:ALA:HB2  | 1.83                     | 0.60              |
| 1:A:1090:U:H2'   | 1:A:1091:U:H6    | 1.67                     | 0.60              |
| 1:A:1249:C:O2'   | 9:I:73:GLN:NE2   | 2.35                     | 0.60              |
| 15:O:29:VAL:HG12 | 15:O:85:LEU:CD1  | 2.31                     | 0.60              |
| 16:P:67:THR:HG22 | 16:P:69:THR:H    | 1.63                     | 0.60              |
| 1:A:1054:C:O2    | 1:A:1054:C:C3'   | 2.49                     | 0.60              |
| 1:A:1367:C:H5'   | 10:J:60:ARG:HH12 | 1.66                     | 0.60              |
| 1:A:701:C:H5''   | 1:A:703:G:O4'    | 2.01                     | 0.60              |
| 2:B:80:ILE:HD11  | 2:B:208:ILE:HG22 | 1.81                     | 0.60              |
| 20:T:56:MET:HE1  | 20:T:104:LEU:HG  | 1.83                     | 0.60              |
| 20:T:59:ALA:O    | 20:T:63:ILE:HG13 | 2.00                     | 0.60              |
| 1:A:1123:A:H4'   | 10:J:37:PRO:HD2  | 1.84                     | 0.60              |
| 1:A:1128:C:O2'   | 1:A:1130:A:N7    | 2.32                     | 0.60              |
| 3:C:155:GLY:HA3  | 3:C:196:LEU:HD13 | 1.83                     | 0.60              |
| 7:G:51:GLN:HG2   | 7:G:58:PRO:HD3   | 1.82                     | 0.60              |
| 10:J:49:VAL:CG2  | 14:N:41:ARG:HD2  | 2.31                     | 0.60              |
| 13:M:50:GLU:O    | 13:M:54:VAL:HG23 | 2.02                     | 0.60              |
| 1:A:107:G:H2'    | 1:A:108:G:H5'    | 1.84                     | 0.60              |
| 1:A:992:U:H4'    | 1:A:993:G:O5'    | 2.00                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1391:U:H2'   | 1:A:1392:G:C8    | 2.37                     | 0.60              |
| 2:B:142:LEU:O    | 2:B:146:GLN:HG3  | 2.00                     | 0.60              |
| 2:B:204:ASN:C    | 2:B:204:ASN:ND2  | 2.58                     | 0.60              |
| 2:B:223:ILE:C    | 2:B:225:ALA:H    | 2.08                     | 0.60              |
| 4:D:100:ARG:HH12 | 4:D:137:SER:CB   | 2.13                     | 0.60              |
| 12:L:7:ILE:O     | 12:L:11:VAL:HG23 | 2.02                     | 0.60              |
| 14:N:9:LYS:C     | 14:N:11:LYS:H    | 2.09                     | 0.60              |
| 16:P:28:ARG:HG3  | 16:P:29:ASP:OD2  | 2.01                     | 0.60              |
| 2:B:45:GLN:O     | 2:B:48:MET:HB2   | 2.02                     | 0.60              |
| 4:D:18:LYS:HZ2   | 4:D:31:CYS:CB    | 2.14                     | 0.60              |
| 4:D:32:ALA:C     | 4:D:34:GLU:N     | 2.59                     | 0.60              |
| 9:I:5:TYR:O      | 9:I:84:ALA:HA    | 2.01                     | 0.60              |
| 13:M:90:LEU:HD22 | 13:M:94:ARG:NH1  | 2.15                     | 0.60              |
| 14:N:29:ARG:HG2  | 14:N:29:ARG:HH11 | 1.66                     | 0.60              |
| 1:A:1117:G:H5'   | 1:A:1117:G:H8    | 1.65                     | 0.60              |
| 2:B:231:GLU:HB3  | 2:B:232:PRO:HD2  | 1.83                     | 0.60              |
| 6:F:22:GLU:HA    | 6:F:25:ILE:HD12  | 1.84                     | 0.60              |
| 6:F:68:PRO:HG2   | 6:F:71:ARG:HG3   | 1.83                     | 0.60              |
| 8:H:111:ILE:O    | 8:H:134:ILE:HB   | 2.01                     | 0.60              |
| 9:I:26:VAL:O     | 9:I:32:ASP:HA    | 2.01                     | 0.60              |
| 12:L:74:GLY:O    | 12:L:75:HIS:CB   | 2.50                     | 0.60              |
| 21:U:5:ASP:O     | 21:U:11:GLY:HA3  | 2.01                     | 0.60              |
| 1:A:254:G:O2'    | 1:A:255:G:H5'    | 2.01                     | 0.60              |
| 5:E:51:VAL:O     | 5:E:55:VAL:HG23  | 2.01                     | 0.60              |
| 12:L:26:ALA:O    | 12:L:27:LEU:O    | 2.20                     | 0.60              |
| 12:L:40:VAL:O    | 12:L:40:VAL:HG12 | 2.02                     | 0.60              |
| 20:T:53:LEU:O    | 20:T:57:ARG:HD2  | 2.01                     | 0.60              |
| 1:A:974:A:OP2    | 14:N:41:ARG:NH1  | 2.35                     | 0.60              |
| 4:D:122:ARG:HA   | 4:D:122:ARG:HE   | 1.67                     | 0.60              |
| 8:H:17:THR:HB    | 8:H:78:GLN:OE1   | 2.01                     | 0.60              |
| 11:K:93:GLN:HE21 | 11:K:96:ARG:HH21 | 1.50                     | 0.60              |
| 20:T:38:LYS:O    | 20:T:41:ILE:HG12 | 2.01                     | 0.60              |
| 1:A:975:A:H4'    | 1:A:976:G:C5'    | 2.24                     | 0.59              |
| 1:A:1392:G:N2    | 1:A:1502:A:H8    | 2.00                     | 0.59              |
| 2:B:95:GLN:O     | 2:B:96:ARG:HD2   | 2.01                     | 0.59              |
| 7:G:31:MET:SD    | 7:G:34:GLY:HA2   | 2.42                     | 0.59              |
| 10:J:25:GLU:C    | 10:J:27:ALA:H    | 2.10                     | 0.59              |
| 1:A:56:U:H2'     | 1:A:57:G:C8      | 2.37                     | 0.59              |
| 1:A:299:G:H2'    | 1:A:300:A:C8     | 2.37                     | 0.59              |
| 5:E:11:ILE:HD11  | 5:E:33:VAL:CG2   | 2.32                     | 0.59              |
| 5:E:11:ILE:HD11  | 5:E:33:VAL:HG21  | 1.83                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 13:M:88:ARG:HD2  | 19:S:3:ARG:HH21  | 1.67                     | 0.59              |
| 2:B:231:GLU:CB   | 2:B:232:PRO:HD2  | 2.32                     | 0.59              |
| 3:C:22:TRP:CE3   | 3:C:22:TRP:O     | 2.55                     | 0.59              |
| 8:H:91:ARG:NH1   | 17:Q:33:GLY:HA3  | 2.16                     | 0.59              |
| 2:B:55:PHE:CE2   | 2:B:218:ALA:HA   | 2.37                     | 0.59              |
| 9:I:79:LEU:HD22  | 9:I:83:ARG:HG3   | 1.85                     | 0.59              |
| 18:R:87:ARG:HG2  | 18:R:88:LYS:H    | 1.67                     | 0.59              |
| 1:A:1187:G:OP1   | 9:I:113:LYS:HE2  | 2.03                     | 0.59              |
| 3:C:19:GLU:HB3   | 3:C:40:ARG:NH2   | 2.17                     | 0.59              |
| 3:C:119:ARG:HE   | 3:C:140:ARG:HE   | 1.51                     | 0.59              |
| 4:D:70:ILE:HD11  | 4:D:100:ARG:NE   | 2.17                     | 0.59              |
| 11:K:21:ILE:HD12 | 11:K:95:ILE:HD13 | 1.85                     | 0.59              |
| 15:O:17:ARG:HG3  | 15:O:17:ARG:NH1  | 2.14                     | 0.59              |
| 1:A:509:A:H5'    | 4:D:54:TYR:HD2   | 1.67                     | 0.59              |
| 1:A:1208:C:H2'   | 1:A:1209:C:C6    | 2.38                     | 0.59              |
| 1:A:1352:C:H2'   | 1:A:1353:G:C8    | 2.37                     | 0.59              |
| 2:B:35:GLU:HA    | 2:B:39:ILE:O     | 2.03                     | 0.59              |
| 20:T:23:ARG:HG2  | 20:T:23:ARG:HH11 | 1.67                     | 0.59              |
| 1:A:357:G:O2'    | 1:A:358:U:H5'    | 2.03                     | 0.59              |
| 5:E:53:LEU:H     | 5:E:53:LEU:CD2   | 2.13                     | 0.59              |
| 5:E:89:ILE:HD13  | 5:E:90:VAL:N     | 2.18                     | 0.59              |
| 16:P:43:LYS:HA   | 16:P:48:TRP:HB3  | 1.84                     | 0.59              |
| 1:A:163:C:O2'    | 1:A:164:U:H5'    | 2.03                     | 0.59              |
| 1:A:353:A:H5'    | 1:A:353:A:C8     | 2.38                     | 0.59              |
| 1:A:620:C:N1     | 4:D:135:LEU:HD13 | 2.17                     | 0.59              |
| 1:A:979:C:H2'    | 1:A:980:C:H5'    | 1.85                     | 0.59              |
| 2:B:132:LYS:C    | 2:B:134:GLU:H    | 2.10                     | 0.59              |
| 8:H:25:ASP:OD1   | 8:H:60:ARG:HG2   | 2.03                     | 0.59              |
| 10:J:21:GLN:O    | 10:J:25:GLU:HG2  | 2.03                     | 0.59              |
| 10:J:99:LYS:HD3  | 10:J:100:THR:N   | 2.15                     | 0.59              |
| 15:O:70:LEU:HD12 | 15:O:78:TYR:HB2  | 1.85                     | 0.59              |
| 20:T:13:LEU:H    | 20:T:13:LEU:HD12 | 1.68                     | 0.59              |
| 1:A:448:A:OP2    | 1:A:485:G:N2     | 2.33                     | 0.59              |
| 1:A:501:C:H2'    | 1:A:502:G:C8     | 2.37                     | 0.59              |
| 1:A:1190:G:P     | 3:C:5:ILE:HG13   | 2.43                     | 0.59              |
| 3:C:119:ARG:HG3  | 3:C:119:ARG:NH1  | 2.13                     | 0.59              |
| 8:H:4:ASP:OD2    | 8:H:7:ALA:CB     | 2.50                     | 0.59              |
| 12:L:53:ARG:HD2  | 12:L:93:LEU:HD21 | 1.85                     | 0.59              |
| 1:A:631:G:H5'    | 1:A:632:A:OP1    | 2.03                     | 0.58              |
| 1:A:743:U:H2'    | 1:A:744:C:C6     | 2.38                     | 0.58              |
| 1:A:148:G:H2'    | 1:A:149:A:H8     | 1.68                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:991:U:O4     | 1:A:1212:U:H1'   | 2.02                     | 0.58              |
| 1:A:1032:G:H2'   | 1:A:1033:G:C8    | 2.38                     | 0.58              |
| 2:B:78:GLN:HG3   | 2:B:94:ASN:OD1   | 2.03                     | 0.58              |
| 3:C:50:ALA:CB    | 3:C:70:VAL:HG11  | 2.19                     | 0.58              |
| 3:C:107:GLN:NE2  | 3:C:107:GLN:H    | 2.00                     | 0.58              |
| 12:L:24:VAL:HG13 | 12:L:98:TYR:HE2  | 1.68                     | 0.58              |
| 1:A:1131:G:H2'   | 1:A:1132:C:C6    | 2.38                     | 0.58              |
| 1:A:1300:G:O2'   | 1:A:1301:U:H6    | 1.86                     | 0.58              |
| 2:B:60:ASP:C     | 2:B:64:ARG:HH12  | 2.11                     | 0.58              |
| 5:E:11:ILE:HB    | 5:E:31:LEU:HB3   | 1.85                     | 0.58              |
| 7:G:120:ILE:H    | 7:G:120:ILE:HD12 | 1.68                     | 0.58              |
| 9:I:113:LYS:H    | 9:I:119:ALA:HA   | 1.67                     | 0.58              |
| 14:N:8:GLU:OE1   | 14:N:8:GLU:C     | 2.45                     | 0.58              |
| 1:A:1392:G:O2'   | 1:A:1502:A:H5''  | 2.01                     | 0.58              |
| 3:C:11:ARG:NH1   | 3:C:177:THR:O    | 2.36                     | 0.58              |
| 4:D:98:GLU:HG2   | 4:D:189:PRO:HG3  | 1.84                     | 0.58              |
| 5:E:29:GLY:HA2   | 5:E:47:LYS:HG3   | 1.86                     | 0.58              |
| 13:M:23:TYR:O    | 13:M:25:ILE:N    | 2.36                     | 0.58              |
| 17:Q:45:HIS:HB3  | 17:Q:72:ARG:HG2  | 1.84                     | 0.58              |
| 1:A:1423:G:O2'   | 1:A:1424:C:H5'   | 2.02                     | 0.58              |
| 11:K:48:ILE:HG22 | 11:K:49:GLY:N    | 2.14                     | 0.58              |
| 2:B:101:MET:O    | 2:B:105:PHE:HA   | 2.03                     | 0.58              |
| 4:D:162:LEU:HD13 | 4:D:181:MET:HE2  | 1.84                     | 0.58              |
| 5:E:83:GLU:HG2   | 5:E:88:LYS:HG3   | 1.85                     | 0.58              |
| 15:O:74:ASP:CG   | 15:O:77:ARG:HG3  | 2.29                     | 0.58              |
| 1:A:269:C:H2'    | 1:A:270:A:C8     | 2.38                     | 0.58              |
| 1:A:1121:U:H2'   | 1:A:1122:U:C6    | 2.38                     | 0.58              |
| 2:B:14:GLY:O     | 2:B:15:VAL:HG22  | 2.03                     | 0.58              |
| 5:E:150:ARG:HH11 | 5:E:150:ARG:CG   | 2.09                     | 0.58              |
| 9:I:9:ARG:HG3    | 9:I:14:VAL:HG12  | 1.86                     | 0.58              |
| 1:A:781:A:H2'    | 1:A:782:A:H5'    | 1.85                     | 0.58              |
| 1:A:959:A:H3'    | 1:A:960:U:H5''   | 1.85                     | 0.58              |
| 1:A:1047:G:H2'   | 1:A:1048:G:H5'   | 1.85                     | 0.58              |
| 6:F:101:ALA:HB1  | 18:R:28:GLU:OE1  | 2.03                     | 0.58              |
| 10:J:48:THR:OG1  | 10:J:62:HIS:CD2  | 2.57                     | 0.58              |
| 1:A:669:U:H2'    | 1:A:670:G:C8     | 2.38                     | 0.58              |
| 1:A:1130:A:H3'   | 1:A:1130:A:OP2   | 2.03                     | 0.58              |
| 7:G:79:ARG:HB3   | 7:G:84:ASN:OD1   | 2.04                     | 0.58              |
| 1:A:539:A:H2'    | 1:A:540:G:C8     | 2.39                     | 0.58              |
| 2:B:7:VAL:C      | 2:B:8:LYS:HG3    | 2.29                     | 0.58              |
| 4:D:65:ARG:HB2   | 4:D:75:PHE:CD1   | 2.39                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 11:K:57:THR:HG22 | 11:K:59:TYR:H    | 1.68                     | 0.58              |
| 1:A:946:A:H2'    | 1:A:947:G:H8     | 1.69                     | 0.57              |
| 1:A:1016:A:H2'   | 1:A:1017:G:O4'   | 2.04                     | 0.57              |
| 2:B:132:LYS:HB3  | 2:B:136:VAL:HG23 | 1.86                     | 0.57              |
| 2:B:206:ASP:O    | 2:B:207:ALA:HB2  | 2.04                     | 0.57              |
| 10:J:16:LEU:HD13 | 10:J:70:ARG:HG2  | 1.86                     | 0.57              |
| 12:L:27:LEU:HG   | 12:L:28:LYS:H    | 1.68                     | 0.57              |
| 12:L:60:LEU:HD23 | 12:L:64:TYR:HB3  | 1.86                     | 0.57              |
| 1:A:664:G:OP1    | 18:R:64:ARG:HD2  | 2.04                     | 0.57              |
| 1:A:818:G:H3'    | 1:A:819:A:H5''   | 1.86                     | 0.57              |
| 1:A:1216:G:H5''  | 14:N:5:ALA:CB    | 2.34                     | 0.57              |
| 2:B:47:THR:HG23  | 2:B:202:PRO:O    | 2.03                     | 0.57              |
| 2:B:80:ILE:HD13  | 2:B:212:GLN:HB2  | 1.85                     | 0.57              |
| 4:D:162:LEU:HD13 | 4:D:181:MET:CG   | 2.34                     | 0.57              |
| 5:E:36:ASP:OD1   | 5:E:38:GLN:N     | 2.37                     | 0.57              |
| 13:M:124:PRO:CB  | 13:M:126:LYS:HE2 | 2.31                     | 0.57              |
| 6:F:46:ARG:HG2   | 6:F:47:ARG:N     | 2.17                     | 0.57              |
| 9:I:17:VAL:HG21  | 9:I:80:GLY:HA3   | 1.86                     | 0.57              |
| 15:O:39:LEU:HD12 | 15:O:56:LEU:HB2  | 1.85                     | 0.57              |
| 7:G:115:ARG:HB2  | 7:G:118:VAL:HG23 | 1.86                     | 0.57              |
| 1:A:495:A:H4'    | 1:A:496:A:O5'    | 2.04                     | 0.57              |
| 2:B:115:LEU:HD21 | 2:B:153:ARG:NH2  | 2.20                     | 0.57              |
| 13:M:3:ARG:HD3   | 13:M:9:ILE:CG2   | 2.34                     | 0.57              |
| 1:A:969:A:H61    | 13:M:126:LYS:CB  | 2.17                     | 0.57              |
| 1:A:1106:G:H5''  | 3:C:172:ARG:HG2  | 1.86                     | 0.57              |
| 4:D:28:SER:C     | 4:D:30:LYS:H     | 2.12                     | 0.57              |
| 4:D:58:LEU:CD2   | 4:D:62:GLN:HG2   | 2.35                     | 0.57              |
| 10:J:32:ALA:N    | 10:J:78:ASN:ND2  | 2.53                     | 0.57              |
| 15:O:54:ARG:HG2  | 15:O:54:ARG:NH1  | 2.20                     | 0.57              |
| 1:A:1280:A:H5'   | 10:J:40:LEU:HD22 | 1.86                     | 0.57              |
| 2:B:28:PHE:CD2   | 2:B:190:THR:HA   | 2.39                     | 0.57              |
| 2:B:118:LEU:HD23 | 2:B:118:LEU:C    | 2.30                     | 0.57              |
| 4:D:100:ARG:NH1  | 4:D:137:SER:HA   | 2.20                     | 0.57              |
| 4:D:100:ARG:O    | 4:D:103:ASN:HB3  | 2.05                     | 0.57              |
| 5:E:12:LEU:CD1   | 5:E:31:LEU:HB2   | 2.34                     | 0.57              |
| 9:I:3:GLN:HB3    | 9:I:20:ARG:HG2   | 1.85                     | 0.57              |
| 20:T:50:GLU:HA   | 20:T:100:ILE:CG2 | 2.32                     | 0.57              |
| 1:A:180:U:H2'    | 1:A:181:G:H5'    | 1.86                     | 0.57              |
| 1:A:412:A:C6     | 4:D:35:ARG:HB3   | 2.40                     | 0.57              |
| 1:A:923:A:OP1    | 5:E:21:ALA:HB2   | 2.04                     | 0.57              |
| 1:A:954:G:H4'    | 13:M:120:LYS:CB  | 2.33                     | 0.57              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1154:G:H2'   | 1:A:1155:G:H8     | 1.70                     | 0.57              |
| 3:C:82:GLU:O     | 3:C:86:VAL:HG23   | 2.03                     | 0.57              |
| 1:A:405:U:H3'    | 1:A:406:G:H5'     | 1.87                     | 0.57              |
| 1:A:639:G:O2'    | 1:A:640:A:H5'     | 2.05                     | 0.57              |
| 1:A:1053:G:C3'   | 1:A:1054:C:H5'    | 2.35                     | 0.57              |
| 1:A:1118:C:H1'   | 1:A:1179:A:C4     | 2.40                     | 0.57              |
| 3:C:172:ARG:NH1  | 3:C:174:PRO:HD3   | 2.19                     | 0.57              |
| 9:I:93:ARG:HH11  | 9:I:93:ARG:CB     | 2.17                     | 0.57              |
| 1:A:1347:G:O2'   | 1:A:1348:U:P      | 2.63                     | 0.57              |
| 4:D:162:LEU:HD13 | 4:D:181:MET:HG2   | 1.86                     | 0.57              |
| 5:E:5:ASP:CG     | 5:E:6:PHE:H       | 2.13                     | 0.57              |
| 8:H:20:TYR:HE2   | 8:H:75:ARG:HD2    | 1.70                     | 0.57              |
| 2:B:134:GLU:HG2  | 2:B:137:ARG:NH2   | 2.20                     | 0.56              |
| 2:B:231:GLU:H    | 2:B:231:GLU:CD    | 2.13                     | 0.56              |
| 3:C:89:GLU:OE2   | 3:C:93:LYS:HE2    | 2.05                     | 0.56              |
| 3:C:110:ASN:HD22 | 3:C:140:ARG:HB3   | 1.68                     | 0.56              |
| 13:M:36:LYS:HD2  | 13:M:59:TYR:OH    | 2.05                     | 0.56              |
| 13:M:84:ILE:O    | 13:M:84:ILE:HG13  | 2.04                     | 0.56              |
| 13:M:115:LYS:H   | 13:M:115:LYS:HD3  | 1.70                     | 0.56              |
| 16:P:43:LYS:HG3  | 16:P:48:TRP:CE3   | 2.39                     | 0.56              |
| 19:S:40:ILE:O    | 19:S:67:VAL:O     | 2.23                     | 0.56              |
| 20:T:85:MET:HE2  | 20:T:104:LEU:HD23 | 1.86                     | 0.56              |
| 1:A:127:G:HO2'   | 17:Q:2:PRO:N      | 2.02                     | 0.56              |
| 1:A:235:C:H5'    | 17:Q:70:ARG:HG2   | 1.87                     | 0.56              |
| 1:A:410:G:H2'    | 1:A:429:U:C5      | 2.40                     | 0.56              |
| 1:A:420:U:H2'    | 1:A:422:C:C5      | 2.40                     | 0.56              |
| 1:A:713:G:H2'    | 1:A:714:G:C8      | 2.41                     | 0.56              |
| 1:A:757:U:H2'    | 1:A:758:G:O4'     | 2.04                     | 0.56              |
| 2:B:61:LEU:HD21  | 2:B:160:ASP:HB2   | 1.87                     | 0.56              |
| 3:C:77:ILE:O     | 3:C:83:ARG:HB3    | 2.05                     | 0.56              |
| 6:F:14:LEU:HA    | 6:F:18:GLN:HE21   | 1.70                     | 0.56              |
| 20:T:53:LEU:HD12 | 20:T:100:ILE:CG2  | 2.35                     | 0.56              |
| 1:A:226:G:O2'    | 1:A:227:G:H5'     | 2.06                     | 0.56              |
| 1:A:390:C:H2'    | 1:A:391:G:C8      | 2.41                     | 0.56              |
| 1:A:1015:A:H2'   | 1:A:1016:A:C8     | 2.40                     | 0.56              |
| 1:A:1161:C:H2'   | 1:A:1162:C:C6     | 2.40                     | 0.56              |
| 1:A:1325:C:OP2   | 21:U:6:ARG:NH2    | 2.38                     | 0.56              |
| 2:B:20:GLU:OE2   | 2:B:189:ASP:OD1   | 2.24                     | 0.56              |
| 2:B:144:ARG:NH1  | 2:B:148:TYR:HD1   | 2.03                     | 0.56              |
| 4:D:68:TYR:CE2   | 4:D:97:LEU:HB3    | 2.41                     | 0.56              |
| 4:D:149:ALA:HB3  | 4:D:152:SER:OG    | 2.05                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:D:184:LYS:HG2  | 4:D:186:LEU:HD23  | 1.87                     | 0.56              |
| 6:F:3:ARG:HH11   | 6:F:3:ARG:CG      | 2.17                     | 0.56              |
| 6:F:51:PRO:HA    | 6:F:55:ASP:O      | 2.05                     | 0.56              |
| 7:G:54:THR:HG22  | 7:G:56:GLN:H      | 1.69                     | 0.56              |
| 9:I:23:ASN:HD22  | 9:I:23:ASN:C      | 2.13                     | 0.56              |
| 10:J:30:SER:HB2  | 10:J:80:LYS:O     | 2.06                     | 0.56              |
| 13:M:40:ASN:HD22 | 13:M:41:PRO:HD2   | 1.70                     | 0.56              |
| 19:S:15:LEU:O    | 19:S:19:VAL:N     | 2.39                     | 0.56              |
| 1:A:242:C:H2'    | 1:A:243:A:H5'     | 1.87                     | 0.56              |
| 1:A:287:U:O2'    | 1:A:288:A:H5'     | 2.04                     | 0.56              |
| 1:A:476:G:H2'    | 1:A:477:A:H8      | 1.70                     | 0.56              |
| 1:A:1250:A:H2'   | 1:A:1251:A:C8     | 2.40                     | 0.56              |
| 15:O:55:GLY:HA2  | 15:O:58:MET:HE2   | 1.88                     | 0.56              |
| 17:Q:96:GLU:O    | 17:Q:102:GLY:HA2  | 2.05                     | 0.56              |
| 1:A:403:C:O3'    | 4:D:122:ARG:HD2   | 2.06                     | 0.56              |
| 4:D:78:LEU:HD22  | 4:D:96:LEU:HB3    | 1.87                     | 0.56              |
| 5:E:40:ARG:NH1   | 5:E:68:GLU:OE1    | 2.34                     | 0.56              |
| 5:E:51:VAL:HB    | 5:E:52:PRO:CD     | 2.30                     | 0.56              |
| 10:J:15:THR:HG22 | 10:J:94:VAL:CG2   | 2.36                     | 0.56              |
| 13:M:15:VAL:HG21 | 13:M:48:LEU:HD21  | 1.87                     | 0.56              |
| 15:O:81:LEU:O    | 15:O:81:LEU:HD23  | 2.05                     | 0.56              |
| 22:X:1:G:O2'     | 22:X:2:U:H5'      | 2.05                     | 0.56              |
| 1:A:1191:A:P     | 3:C:3:ASN:ND2     | 2.78                     | 0.56              |
| 2:B:13:ALA:HA    | 2:B:17:PHE:HE2    | 1.71                     | 0.56              |
| 2:B:75:LYS:HE2   | 2:B:96:ARG:HH22   | 1.70                     | 0.56              |
| 2:B:223:ILE:HD13 | 2:B:229:VAL:HA    | 1.88                     | 0.56              |
| 7:G:65:ALA:HB1   | 7:G:127:ALA:HB3   | 1.86                     | 0.56              |
| 8:H:11:THR:HA    | 8:H:14:ARG:NH1    | 2.21                     | 0.56              |
| 10:J:99:LYS:CD   | 10:J:100:THR:H    | 2.15                     | 0.56              |
| 15:O:39:LEU:O    | 15:O:43:LEU:HG    | 2.06                     | 0.56              |
| 19:S:33:THR:HG22 | 19:S:35:SER:H     | 1.71                     | 0.56              |
| 6:F:44:GLY:O     | 6:F:60:PHE:N      | 2.35                     | 0.56              |
| 12:L:113:ARG:NH1 | 12:L:116:SER:H    | 2.02                     | 0.56              |
| 13:M:20:THR:C    | 13:M:22:ILE:H     | 2.12                     | 0.56              |
| 21:U:2:GLY:C     | 21:U:4:GLY:H      | 2.14                     | 0.56              |
| 1:A:1477:C:H2'   | 1:A:1478:C:H6     | 1.71                     | 0.56              |
| 3:C:91:LEU:HD23  | 3:C:92:ALA:N      | 2.20                     | 0.56              |
| 12:L:83:VAL:HG11 | 12:L:100:ILE:HD13 | 1.87                     | 0.56              |
| 16:P:19:ILE:CG2  | 16:P:36:ILE:HG13  | 2.35                     | 0.56              |
| 1:A:476:G:H2'    | 1:A:477:A:C8      | 2.41                     | 0.56              |
| 1:A:509:A:H5''   | 4:D:54:TYR:CD2    | 2.40                     | 0.56              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:A:725:G:C2'      | 1:A:726:C:C5'     | 2.83                     | 0.56              |
| 1:A:725:G:O2'      | 1:A:726:C:H5''    | 2.05                     | 0.56              |
| 1:A:1176:A:H2'     | 1:A:1177:G:C8     | 2.40                     | 0.56              |
| 2:B:188:ALA:HB3    | 2:B:200:ILE:HD11  | 1.88                     | 0.56              |
| 4:D:64:LEU:HD12    | 4:D:75:PHE:HZ     | 1.68                     | 0.56              |
| 5:E:55:VAL:O       | 5:E:58:ALA:HB3    | 2.05                     | 0.56              |
| 14:N:22:THR:HG23   | 14:N:33:VAL:HG21  | 1.88                     | 0.56              |
| 20:T:23:ARG:HG2    | 20:T:23:ARG:NH1   | 2.21                     | 0.56              |
| 1:A:524:G:H2'      | 1:A:525:C:C6      | 2.41                     | 0.56              |
| 3:C:64:VAL:HG23    | 3:C:99:VAL:CG1    | 2.27                     | 0.56              |
| 4:D:23:GLY:O       | 4:D:26:CYS:HB2    | 2.06                     | 0.56              |
| 7:G:16:LEU:HD22    | 7:G:16:LEU:N      | 2.20                     | 0.56              |
| 1:A:390:C:H2'      | 1:A:391:G:H8      | 1.70                     | 0.55              |
| 1:A:706:A:H1'      | 11:K:29:ILE:HD11  | 1.87                     | 0.55              |
| 24:A:1601:PAR:H642 | 24:A:1601:PAR:H43 | 1.88                     | 0.55              |
| 4:D:24:GLU:O       | 4:D:25:ARG:HB3    | 2.06                     | 0.55              |
| 5:E:60:TYR:CE1     | 5:E:64:ARG:CZ     | 2.89                     | 0.55              |
| 14:N:3:ARG:O       | 14:N:4:LYS:C      | 2.48                     | 0.55              |
| 17:Q:82:MET:O      | 17:Q:86:GLU:HG2   | 2.07                     | 0.55              |
| 19:S:80:TYR:O      | 19:S:82:GLY:N     | 2.39                     | 0.55              |
| 2:B:25:ASN:HD22    | 2:B:25:ASN:C      | 2.14                     | 0.55              |
| 3:C:172:ARG:HH12   | 3:C:174:PRO:CG    | 2.19                     | 0.55              |
| 4:D:126:ILE:HG22   | 4:D:127:THR:N     | 2.21                     | 0.55              |
| 10:J:7:LYS:HG3     | 10:J:71:LEU:CD2   | 2.36                     | 0.55              |
| 10:J:75:ILE:O      | 10:J:76:ASN:CG    | 2.49                     | 0.55              |
| 14:N:57:ARG:HG2    | 14:N:58:LYS:N     | 2.21                     | 0.55              |
| 1:A:1152:A:H5''    | 10:J:13:HIS:CG    | 2.41                     | 0.55              |
| 12:L:27:LEU:C      | 12:L:29:GLY:H     | 2.15                     | 0.55              |
| 20:T:57:ARG:HG2    | 20:T:57:ARG:NH1   | 2.21                     | 0.55              |
| 1:A:818:G:H3'      | 1:A:819:A:C5'     | 2.35                     | 0.55              |
| 2:B:114:ARG:HH11   | 2:B:118:LEU:HD12  | 1.71                     | 0.55              |
| 2:B:165:VAL:O      | 2:B:187:LEU:O     | 2.25                     | 0.55              |
| 5:E:78:HIS:HE1     | 5:E:80:ILE:HG23   | 1.71                     | 0.55              |
| 9:I:89:ASN:O       | 9:I:92:TYR:HB2    | 2.06                     | 0.55              |
| 11:K:21:ILE:HD13   | 11:K:94:ALA:CB    | 2.36                     | 0.55              |
| 13:M:40:ASN:ND2    | 13:M:42:ALA:H     | 2.03                     | 0.55              |
| 19:S:52:TYR:HA     | 19:S:56:GLN:O     | 2.06                     | 0.55              |
| 1:A:399:G:H2'      | 1:A:400:C:C6      | 2.42                     | 0.55              |
| 1:A:421:U:H5'      | 1:A:422:C:H5      | 1.69                     | 0.55              |
| 1:A:551:U:H2'      | 1:A:552:U:C6      | 2.41                     | 0.55              |
| 1:A:961:U:C2'      | 1:A:962:C:H5'     | 2.37                     | 0.55              |

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| Atom-1          | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-------------------|--------------------------|-------------------|
| 8:H:29:SER:OG   | 8:H:32:LYS:HE3    | 2.06                     | 0.55              |
| 19:S:15:LEU:HA  | 19:S:18:LYS:HB3   | 1.87                     | 0.55              |
| 1:A:153:C:O2'   | 1:A:154:C:H5'     | 2.07                     | 0.55              |
| 1:A:443:C:O2'   | 1:A:444:C:H5''    | 2.06                     | 0.55              |
| 1:A:1090:U:H2'  | 1:A:1091:U:C6     | 2.41                     | 0.55              |
| 2:B:25:ASN:HD22 | 2:B:27:LYS:H      | 1.55                     | 0.55              |
| 2:B:55:PHE:CD2  | 2:B:58:ILE:HD12   | 2.41                     | 0.55              |
| 9:I:118:LYS:O   | 9:I:119:ALA:CB    | 2.54                     | 0.55              |
| 9:I:128:ARG:CZ  | 9:I:128:ARG:HB2   | 2.37                     | 0.55              |
| 17:Q:17:LYS:HA  | 17:Q:46:ASP:O     | 2.07                     | 0.55              |
| 1:A:265:G:H2'   | 1:A:267:C:H5      | 1.71                     | 0.55              |
| 1:A:731:G:OP1   | 1:A:766:A:H1'     | 2.07                     | 0.55              |
| 1:A:960:U:H1'   | 1:A:1223:C:H5'    | 1.88                     | 0.55              |
| 1:A:1343:G:H2'  | 1:A:1344:C:C6     | 2.42                     | 0.55              |
| 1:A:1355:G:O2'  | 1:A:1356:G:H5'    | 2.06                     | 0.55              |
| 4:D:36:ARG:HB2  | 4:D:36:ARG:HH11   | 1.71                     | 0.55              |
| 10:J:7:LYS:HD3  | 10:J:9:ARG:HH22   | 1.72                     | 0.55              |
| 11:K:15:ALA:HA  | 11:K:77:MET:HA    | 1.89                     | 0.55              |
| 13:M:78:ILE:O   | 13:M:82:MET:HG3   | 2.05                     | 0.55              |
| 20:T:100:ILE:O  | 20:T:100:ILE:HG12 | 2.07                     | 0.55              |
| 1:A:984:C:H2'   | 1:A:985:C:C6      | 2.40                     | 0.55              |
| 2:B:69:LEU:C    | 2:B:69:LEU:HD23   | 2.32                     | 0.55              |
| 4:D:62:GLN:NE2  | 4:D:65:ARG:HH12   | 2.05                     | 0.55              |
| 6:F:19:LEU:C    | 6:F:19:LEU:HD23   | 2.32                     | 0.55              |
| 1:A:52:G:O2'    | 1:A:53:A:H5'      | 2.06                     | 0.55              |
| 1:A:421:U:H4'   | 1:A:422:C:OP2     | 2.05                     | 0.55              |
| 1:A:556:C:O2'   | 1:A:557:G:H5'     | 2.06                     | 0.55              |
| 1:A:735:C:O2'   | 1:A:736:C:H5'     | 2.07                     | 0.55              |
| 1:A:1250:A:H5'  | 9:I:68:GLY:O      | 2.06                     | 0.55              |
| 1:A:1424:C:O2'  | 1:A:1425:U:H5'    | 2.07                     | 0.55              |
| 2:B:10:LEU:HG   | 2:B:48:MET:HE2    | 1.87                     | 0.55              |
| 2:B:142:LEU:CG  | 2:B:146:GLN:HE21  | 2.14                     | 0.55              |
| 2:B:169:LYS:O   | 2:B:169:LYS:HD3   | 2.06                     | 0.55              |
| 12:L:34:ARG:O   | 12:L:61:THR:HG23  | 2.07                     | 0.55              |
| 1:A:404:U:H2'   | 1:A:405:U:C6      | 2.42                     | 0.55              |
| 1:A:528:C:H41   | 12:L:49:ASN:ND2   | 2.04                     | 0.55              |
| 2:B:42:ILE:N    | 2:B:42:ILE:HD12   | 2.22                     | 0.55              |
| 3:C:32:LEU:HD22 | 3:C:59:ARG:HH11   | 1.72                     | 0.55              |
| 4:D:64:LEU:HD11 | 4:D:97:LEU:CD1    | 2.37                     | 0.55              |
| 6:F:10:LEU:HB2  | 6:F:59:TYR:HB3    | 1.89                     | 0.55              |
| 6:F:94:GLN:NE2  | 18:R:32:ARG:HD3   | 2.22                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:I:11:LYS:O     | 9:I:11:LYS:HG2   | 2.07                     | 0.55              |
| 9:I:36:TYR:HD2   | 9:I:37:PHE:CE2   | 2.25                     | 0.55              |
| 1:A:109:A:H2'    | 1:A:326:G:N2     | 2.22                     | 0.54              |
| 1:A:818:G:C2'    | 1:A:819:A:H5''   | 2.37                     | 0.54              |
| 1:A:1191:A:P     | 3:C:3:ASN:HD21   | 2.29                     | 0.54              |
| 1:A:1438:G:H2'   | 1:A:1439:C:C6    | 2.42                     | 0.54              |
| 3:C:154:SER:HB3  | 3:C:165:THR:HG23 | 1.89                     | 0.54              |
| 5:E:90:VAL:O     | 5:E:120:THR:HA   | 2.06                     | 0.54              |
| 18:R:88:LYS:HB3  | 18:R:88:LYS:HZ3  | 1.71                     | 0.54              |
| 1:A:1106:G:OP1   | 3:C:172:ARG:HD3  | 2.07                     | 0.54              |
| 1:A:1178:G:N2    | 1:A:1180:A:H3'   | 2.22                     | 0.54              |
| 2:B:189:ASP:HB2  | 2:B:205:ASP:CG   | 2.33                     | 0.54              |
| 6:F:4:TYR:HD1    | 6:F:92:LYS:HA    | 1.72                     | 0.54              |
| 7:G:15:ASP:HB3   | 7:G:20:ASP:H     | 1.71                     | 0.54              |
| 1:A:1054:C:H42   | 23:Y:34:CM0:C1'  | 2.20                     | 0.54              |
| 3:C:57:ILE:HA    | 3:C:65:ALA:O     | 2.06                     | 0.54              |
| 4:D:111:ALA:HB2  | 4:D:120:LEU:CD1  | 2.35                     | 0.54              |
| 5:E:51:VAL:O     | 5:E:54:ALA:HB3   | 2.07                     | 0.54              |
| 11:K:12:ARG:H    | 11:K:13:GLN:HE21 | 1.55                     | 0.54              |
| 1:A:1300:G:HO2'  | 1:A:1301:U:H6    | 1.55                     | 0.54              |
| 8:H:20:TYR:CE2   | 8:H:75:ARG:HD2   | 2.42                     | 0.54              |
| 17:Q:99:SER:C    | 17:Q:101:ARG:H   | 2.15                     | 0.54              |
| 1:A:457:C:H2'    | 1:A:458:C:C6     | 2.42                     | 0.54              |
| 2:B:64:ARG:HB2   | 2:B:64:ARG:HH11  | 1.72                     | 0.54              |
| 3:C:110:ASN:HD21 | 3:C:140:ARG:HB3  | 1.71                     | 0.54              |
| 6:F:45:LEU:HA    | 6:F:58:GLY:O     | 2.08                     | 0.54              |
| 6:F:75:LEU:O     | 6:F:78:GLU:HB3   | 2.08                     | 0.54              |
| 10:J:76:ASN:O    | 10:J:78:ASN:N    | 2.34                     | 0.54              |
| 1:A:248:C:O2'    | 1:A:249:U:H5'    | 2.08                     | 0.54              |
| 1:A:1072:G:H2'   | 1:A:1073:U:C6    | 2.42                     | 0.54              |
| 1:A:1196:U:O4    | 22:X:5:A:H1'     | 2.08                     | 0.54              |
| 1:A:1499:A:C1'   | 1:A:1520:G:H5'   | 2.37                     | 0.54              |
| 3:C:112:SER:HB3  | 3:C:115:LEU:HD12 | 1.89                     | 0.54              |
| 4:D:141:ARG:HB2  | 4:D:141:ARG:HH11 | 1.72                     | 0.54              |
| 10:J:46:ARG:HG2  | 10:J:46:ARG:NH1  | 2.12                     | 0.54              |
| 12:L:115:LYS:C   | 12:L:117:ARG:H   | 2.16                     | 0.54              |
| 15:O:18:PHE:HB2  | 15:O:19:PRO:HD2  | 1.89                     | 0.54              |
| 19:S:12:ASP:O    | 19:S:15:LEU:HD12 | 2.08                     | 0.54              |
| 19:S:51:VAL:O    | 19:S:58:VAL:HG22 | 2.07                     | 0.54              |
| 1:A:1149:C:H2'   | 1:A:1150:U:C6    | 2.43                     | 0.54              |
| 5:E:45:PHE:CE2   | 5:E:47:LYS:HD2   | 2.43                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:H:20:TYR:CE1   | 8:H:76:PRO:HG2   | 2.43                     | 0.54              |
| 9:I:19:LEU:HB3   | 9:I:59:PHE:CD2   | 2.43                     | 0.54              |
| 9:I:97:LYS:CA    | 9:I:102:LEU:HD21 | 2.34                     | 0.54              |
| 13:M:99:ARG:HG2  | 13:M:99:ARG:HH11 | 1.72                     | 0.54              |
| 16:P:22:THR:HA   | 16:P:33:ILE:HG13 | 1.89                     | 0.54              |
| 18:R:46:GLU:CD   | 18:R:46:GLU:N    | 2.66                     | 0.54              |
| 1:A:1157:A:H4'   | 1:A:1158:C:O5'   | 2.08                     | 0.54              |
| 2:B:120:ALA:C    | 2:B:122:PHE:H    | 2.16                     | 0.54              |
| 3:C:32:LEU:HD22  | 3:C:59:ARG:NH1   | 2.22                     | 0.54              |
| 10:J:49:VAL:HG21 | 14:N:41:ARG:O    | 2.08                     | 0.54              |
| 18:R:47:THR:HG22 | 18:R:48:GLY:N    | 2.22                     | 0.54              |
| 1:A:1280:A:C5'   | 10:J:40:LEU:HD22 | 2.37                     | 0.54              |
| 2:B:23:ARG:O     | 2:B:23:ARG:CD    | 2.55                     | 0.54              |
| 5:E:81:GLU:HG3   | 5:E:90:VAL:HG22  | 1.90                     | 0.54              |
| 6:F:91:VAL:HG13  | 18:R:72:ARG:NH2  | 2.22                     | 0.54              |
| 8:H:54:ASP:O     | 8:H:54:ASP:CG    | 2.51                     | 0.54              |
| 13:M:120:LYS:HZ1 | 13:M:122:LYS:HB3 | 1.69                     | 0.54              |
| 15:O:33:THR:HG23 | 15:O:63:ARG:NH1  | 2.23                     | 0.54              |
| 18:R:43:PHE:C    | 18:R:51:LEU:HD12 | 2.32                     | 0.54              |
| 20:T:100:ILE:C   | 20:T:102:GLY:N   | 2.66                     | 0.54              |
| 1:A:539:A:H2'    | 1:A:540:G:H8     | 1.72                     | 0.54              |
| 1:A:662:G:H2'    | 1:A:663:A:C8     | 2.43                     | 0.54              |
| 1:A:1367:C:H5'   | 10:J:60:ARG:NH1  | 2.23                     | 0.54              |
| 4:D:162:LEU:CD1  | 4:D:181:MET:HE2  | 2.37                     | 0.54              |
| 10:J:57:LYS:HE2  | 10:J:60:ARG:NH2  | 2.23                     | 0.54              |
| 16:P:21:VAL:HG21 | 16:P:59:TRP:CD1  | 2.43                     | 0.54              |
| 20:T:50:GLU:HB2  | 20:T:99:LEU:HD12 | 1.89                     | 0.54              |
| 1:A:960:U:O2     | 1:A:960:U:H2'    | 2.08                     | 0.53              |
| 7:G:116:ALA:O    | 7:G:120:ILE:HD12 | 2.09                     | 0.53              |
| 10:J:24:VAL:O    | 10:J:28:ARG:HG3  | 2.09                     | 0.53              |
| 12:L:58:VAL:O    | 12:L:65:GLU:HA   | 2.07                     | 0.53              |
| 16:P:20:VAL:HG11 | 16:P:32:TYR:HB3  | 1.90                     | 0.53              |
| 17:Q:59:ILE:HG22 | 17:Q:71:PHE:CD1  | 2.42                     | 0.53              |
| 2:B:230:VAL:HG12 | 2:B:231:GLU:N    | 2.23                     | 0.53              |
| 3:C:70:VAL:O     | 3:C:105:GLU:HA   | 2.08                     | 0.53              |
| 4:D:3:ARG:HG2    | 4:D:118:ARG:NE   | 2.24                     | 0.53              |
| 5:E:69:VAL:HG21  | 5:E:113:ALA:HB1  | 1.89                     | 0.53              |
| 10:J:84:GLN:O    | 10:J:88:LEU:HD12 | 2.07                     | 0.53              |
| 15:O:87:ILE:CG2  | 15:O:88:ARG:H    | 2.01                     | 0.53              |
| 17:Q:97:SER:HA   | 17:Q:102:GLY:CA  | 2.38                     | 0.53              |
| 1:A:246:A:HO2'   | 17:Q:99:SER:HB3  | 1.70                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:625:G:H2'    | 1:A:626:U:C6     | 2.43                     | 0.53              |
| 1:A:865:A:H5'    | 1:A:1078:U:O4    | 2.09                     | 0.53              |
| 1:A:1480:G:H2'   | 1:A:1481:U:C6    | 2.44                     | 0.53              |
| 2:B:111:ARG:CB   | 2:B:149:LEU:HD11 | 2.34                     | 0.53              |
| 7:G:23:VAL:HG13  | 7:G:43:PHE:CE2   | 2.43                     | 0.53              |
| 9:I:7:THR:O      | 9:I:8:GLY:O      | 2.27                     | 0.53              |
| 13:M:11:ARG:CG   | 13:M:12:ASN:N    | 2.64                     | 0.53              |
| 13:M:36:LYS:HB2  | 13:M:59:TYR:CE2  | 2.43                     | 0.53              |
| 1:A:130:A:C8     | 17:Q:63:ARG:HG3  | 2.44                     | 0.53              |
| 1:A:833:U:H2'    | 1:A:834:C:C6     | 2.43                     | 0.53              |
| 2:B:72:GLY:HA3   | 2:B:81:VAL:HG21  | 1.91                     | 0.53              |
| 2:B:74:LYS:C     | 2:B:76:GLN:H     | 2.15                     | 0.53              |
| 5:E:88:LYS:HB3   | 5:E:123:LEU:HB2  | 1.89                     | 0.53              |
| 8:H:112:LEU:HD23 | 8:H:112:LEU:H    | 1.71                     | 0.53              |
| 15:O:62:GLN:HA   | 15:O:65:ARG:HD2  | 1.90                     | 0.53              |
| 1:A:384:G:H2'    | 1:A:385:C:H6     | 1.71                     | 0.53              |
| 1:A:1347:G:H2'   | 1:A:1373:G:H1    | 1.72                     | 0.53              |
| 13:M:27:LYS:HB2  | 13:M:27:LYS:NZ   | 2.23                     | 0.53              |
| 15:O:55:GLY:HA2  | 15:O:58:MET:HE3  | 1.89                     | 0.53              |
| 16:P:20:VAL:HG11 | 16:P:32:TYR:CB   | 2.39                     | 0.53              |
| 1:A:89:C:O5'     | 1:A:89:C:H6      | 1.92                     | 0.53              |
| 1:A:1298:C:H4'   | 1:A:1299:A:O4'   | 2.09                     | 0.53              |
| 2:B:137:ARG:HB3  | 2:B:137:ARG:HH11 | 1.74                     | 0.53              |
| 3:C:86:VAL:O     | 3:C:89:GLU:HB3   | 2.09                     | 0.53              |
| 7:G:69:VAL:HG12  | 7:G:69:VAL:O     | 2.09                     | 0.53              |
| 13:M:25:ILE:HD11 | 13:M:60:VAL:HG13 | 1.89                     | 0.53              |
| 16:P:10:GLY:HA3  | 16:P:14:ASN:O    | 2.08                     | 0.53              |
| 19:S:20:LEU:HD12 | 19:S:21:GLU:H    | 1.73                     | 0.53              |
| 1:A:254:G:OP1    | 17:Q:67:LYS:O    | 2.25                     | 0.53              |
| 1:A:1062:U:H2'   | 1:A:1063:C:C6    | 2.44                     | 0.53              |
| 1:A:1527:C:O2'   | 1:A:1528:U:H5'   | 2.09                     | 0.53              |
| 12:L:119:LYS:O   | 12:L:120:TYR:HB2 | 2.08                     | 0.53              |
| 20:T:10:LEU:HD12 | 20:T:10:LEU:C    | 2.34                     | 0.53              |
| 1:A:1038:C:H2'   | 1:A:1039:C:C5    | 2.44                     | 0.53              |
| 1:A:1066:C:C2'   | 1:A:1067:A:H5'   | 2.39                     | 0.53              |
| 2:B:132:LYS:HA   | 2:B:135:GLN:HB2  | 1.90                     | 0.53              |
| 3:C:188:LEU:HD11 | 3:C:195:VAL:CG1  | 2.35                     | 0.53              |
| 5:E:116:THR:HG23 | 5:E:117:ASP:OD2  | 2.08                     | 0.53              |
| 7:G:15:ASP:HB3   | 7:G:19:GLY:N     | 2.24                     | 0.53              |
| 7:G:135:VAL:O    | 7:G:139:GLU:HG3  | 2.08                     | 0.53              |
| 9:I:84:ALA:O     | 9:I:87:GLN:HB2   | 2.09                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 19:S:4:SER:O     | 19:S:5:LEU:HG    | 2.08                     | 0.53              |
| 1:A:539:A:OP1    | 12:L:114:LYS:HE2 | 2.09                     | 0.53              |
| 2:B:17:PHE:HB3   | 2:B:44:LEU:CD2   | 2.31                     | 0.53              |
| 2:B:20:GLU:HB2   | 2:B:190:THR:OG1  | 2.09                     | 0.53              |
| 3:C:70:VAL:HG12  | 3:C:71:ALA:H     | 1.73                     | 0.53              |
| 3:C:108:ASN:HD21 | 3:C:144:SER:HB3  | 1.72                     | 0.53              |
| 13:M:6:GLY:O     | 13:M:7:VAL:HG22  | 2.09                     | 0.53              |
| 15:O:64:ARG:CB   | 15:O:64:ARG:HH11 | 2.21                     | 0.53              |
| 1:A:443:C:C2'    | 1:A:444:C:C5'    | 2.86                     | 0.53              |
| 1:A:1054:C:N3    | 23:Y:34:CM0:O4'  | 2.41                     | 0.53              |
| 1:A:1539:C:O5'   | 1:A:1539:C:H6    | 1.92                     | 0.53              |
| 10:J:6:ILE:HG22  | 10:J:97:GLU:O    | 2.09                     | 0.53              |
| 10:J:31:GLY:HA3  | 10:J:81:THR:OG1  | 2.08                     | 0.53              |
| 11:K:46:GLY:O    | 11:K:48:ILE:O    | 2.27                     | 0.53              |
| 12:L:59:ARG:NH1  | 12:L:65:GLU:OE2  | 2.43                     | 0.53              |
| 1:A:1258:G:O2'   | 1:A:1259:C:H5'   | 2.09                     | 0.52              |
| 2:B:88:ALA:HB2   | 2:B:219:VAL:HG13 | 1.90                     | 0.52              |
| 3:C:64:VAL:CB    | 3:C:99:VAL:HG11  | 2.39                     | 0.52              |
| 9:I:115:GLY:O    | 9:I:116:LYS:HD3  | 2.09                     | 0.52              |
| 11:K:12:ARG:O    | 11:K:12:ARG:HD2  | 2.09                     | 0.52              |
| 13:M:81:LEU:CD1  | 13:M:88:ARG:HD3  | 2.39                     | 0.52              |
| 14:N:23:ARG:NH1  | 14:N:30:ALA:HB2  | 2.25                     | 0.52              |
| 20:T:57:ARG:HG2  | 20:T:57:ARG:HH11 | 1.74                     | 0.52              |
| 20:T:76:ALA:HA   | 20:T:79:ARG:HH12 | 1.71                     | 0.52              |
| 1:A:1116:C:H2'   | 1:A:1117:G:C5'   | 2.39                     | 0.52              |
| 10:J:7:LYS:HD3   | 10:J:9:ARG:NH2   | 2.24                     | 0.52              |
| 12:L:10:LEU:HD21 | 12:L:15:ARG:HE   | 1.74                     | 0.52              |
| 13:M:84:ILE:O    | 13:M:86:CYS:N    | 2.38                     | 0.52              |
| 14:N:26:ARG:HE   | 14:N:47:LEU:HD11 | 1.72                     | 0.52              |
| 1:A:882:C:O2'    | 1:A:883:C:H5'    | 2.09                     | 0.52              |
| 1:A:1022:G:H2'   | 1:A:1023:G:H8    | 1.74                     | 0.52              |
| 2:B:130:ARG:O    | 2:B:135:GLN:HG3  | 2.09                     | 0.52              |
| 9:I:37:PHE:O     | 9:I:38:GLN:O     | 2.28                     | 0.52              |
| 16:P:52:ASP:CG   | 16:P:55:ARG:HG3  | 2.34                     | 0.52              |
| 23:Y:30:C:O2'    | 23:Y:31:C:H5'    | 2.10                     | 0.52              |
| 1:A:192:U:C4'    | 20:T:102:GLY:O   | 2.54                     | 0.52              |
| 1:A:1020:U:H2'   | 1:A:1021:G:C8    | 2.44                     | 0.52              |
| 2:B:118:LEU:CD2  | 2:B:142:LEU:HB2  | 2.39                     | 0.52              |
| 3:C:47:LEU:HD23  | 3:C:68:VAL:HG11  | 1.90                     | 0.52              |
| 4:D:76:ARG:HG2   | 4:D:76:ARG:HH11  | 1.74                     | 0.52              |
| 5:E:145:LYS:O    | 5:E:149:GLU:HG2  | 2.08                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 13:M:81:LEU:HD13 | 13:M:88:ARG:HD3  | 1.90                     | 0.52              |
| 15:O:81:LEU:HD23 | 15:O:81:LEU:C    | 2.35                     | 0.52              |
| 20:T:29:LYS:O    | 20:T:33:ILE:HG13 | 2.09                     | 0.52              |
| 20:T:101:GLY:O   | 20:T:102:GLY:C   | 2.50                     | 0.52              |
| 1:A:291:C:O2'    | 1:A:292:G:H5'    | 2.09                     | 0.52              |
| 1:A:434:U:H2'    | 1:A:435:C:C6     | 2.44                     | 0.52              |
| 1:A:1053:G:H4'   | 1:A:1054:C:H5'   | 1.91                     | 0.52              |
| 1:A:1181:G:H2'   | 1:A:1182:G:C5    | 2.44                     | 0.52              |
| 1:A:1372:U:O2'   | 1:A:1373:G:H5'   | 2.10                     | 0.52              |
| 2:B:42:ILE:HD12  | 2:B:42:ILE:H     | 1.75                     | 0.52              |
| 2:B:60:ASP:C     | 2:B:64:ARG:NH1   | 2.67                     | 0.52              |
| 2:B:122:PHE:O    | 2:B:127:ILE:HG12 | 2.09                     | 0.52              |
| 2:B:221:LEU:O    | 2:B:221:LEU:HD13 | 2.09                     | 0.52              |
| 4:D:25:ARG:HH11  | 4:D:25:ARG:CG    | 2.22                     | 0.52              |
| 4:D:30:LYS:HB3   | 4:D:35:ARG:NH2   | 2.23                     | 0.52              |
| 12:L:93:LEU:HB2  | 12:L:96:VAL:CG2  | 2.40                     | 0.52              |
| 16:P:8:ARG:HB2   | 16:P:28:ARG:NH1  | 2.24                     | 0.52              |
| 1:A:1069:C:O2'   | 1:A:1192:C:H1'   | 2.09                     | 0.52              |
| 1:A:1125:U:H5'   | 1:A:1126:U:H5    | 1.75                     | 0.52              |
| 2:B:130:ARG:O    | 2:B:135:GLN:NE2  | 2.39                     | 0.52              |
| 9:I:8:GLY:CA     | 9:I:79:LEU:HB3   | 2.39                     | 0.52              |
| 20:T:93:GLU:C    | 20:T:95:ALA:H    | 2.17                     | 0.52              |
| 1:A:536:C:H2'    | 1:A:537:G:C8     | 2.45                     | 0.52              |
| 1:A:953:G:H5'    | 1:A:965:A:H61    | 1.73                     | 0.52              |
| 1:A:1456:G:H2'   | 1:A:1457:G:O4'   | 2.09                     | 0.52              |
| 2:B:82:ARG:O     | 2:B:86:GLU:HG3   | 2.09                     | 0.52              |
| 2:B:204:ASN:HD22 | 2:B:205:ASP:N    | 2.08                     | 0.52              |
| 10:J:64:GLU:HG2  | 14:N:59:ALA:HB2  | 1.92                     | 0.52              |
| 15:O:21:ASP:OD1  | 15:O:24:SER:HB3  | 2.10                     | 0.52              |
| 15:O:70:LEU:HD12 | 15:O:78:TYR:CA   | 2.40                     | 0.52              |
| 21:U:24:ARG:O    | 21:U:25:LYS:HB2  | 2.09                     | 0.52              |
| 1:A:1068:G:OP2   | 1:A:1068:G:H8    | 1.93                     | 0.52              |
| 2:B:64:ARG:NH1   | 2:B:64:ARG:HB2   | 2.25                     | 0.52              |
| 3:C:27:LYS:HB2   | 3:C:28:GLN:HE21  | 1.73                     | 0.52              |
| 8:H:84:ARG:HD3   | 8:H:136:GLU:OE1  | 2.09                     | 0.52              |
| 8:H:86:ILE:HD12  | 8:H:133:LEU:HD22 | 1.91                     | 0.52              |
| 10:J:30:SER:HB3  | 10:J:84:GLN:HE21 | 1.74                     | 0.52              |
| 11:K:76:GLY:O    | 11:K:78:GLN:HG3  | 2.10                     | 0.52              |
| 15:O:81:LEU:HD21 | 15:O:85:LEU:HD12 | 1.92                     | 0.52              |
| 1:A:9:G:OP2      | 5:E:121:LYS:NZ   | 2.38                     | 0.52              |
| 1:A:1004:A:OP1   | 1:A:1025:U:N3    | 2.43                     | 0.52              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:1250:A:H4'    | 9:I:68:GLY:CA    | 2.40                     | 0.52              |
| 4:D:173:TRP:HB2   | 4:D:187:ARG:O    | 2.09                     | 0.52              |
| 5:E:6:PHE:HB3     | 5:E:34:VAL:HG22  | 1.91                     | 0.52              |
| 7:G:54:THR:C      | 7:G:56:GLN:N     | 2.67                     | 0.52              |
| 9:I:97:LYS:HG2    | 9:I:102:LEU:HD21 | 1.92                     | 0.52              |
| 10:J:55:LYS:HG3   | 10:J:56:HIS:N    | 2.25                     | 0.52              |
| 11:K:11:LYS:O     | 11:K:12:ARG:HB2  | 2.10                     | 0.52              |
| 16:P:42:ARG:O     | 16:P:43:LYS:C    | 2.52                     | 0.52              |
| 16:P:48:TRP:CD1   | 16:P:48:TRP:H    | 2.27                     | 0.52              |
| 1:A:166:G:O2'     | 1:A:167:G:H5'    | 2.10                     | 0.52              |
| 1:A:1305:G:H5'    | 21:U:4:GLY:HA3   | 1.92                     | 0.52              |
| 1:A:1351:U:O2'    | 1:A:1352:C:H5'   | 2.10                     | 0.52              |
| 2:B:87:ARG:HD3    | 2:B:233:SER:OG   | 2.10                     | 0.52              |
| 3:C:147:LYS:HZ1   | 3:C:206:GLU:HG2  | 1.74                     | 0.52              |
| 5:E:79:GLU:CG     | 5:E:93:PRO:HD2   | 2.38                     | 0.52              |
| 5:E:129:ILE:HD12  | 5:E:129:ILE:N    | 2.22                     | 0.52              |
| 7:G:120:ILE:HD12  | 7:G:120:ILE:N    | 2.25                     | 0.52              |
| 12:L:75:HIS:C     | 12:L:75:HIS:CD2  | 2.88                     | 0.52              |
| 17:Q:5:VAL:HA     | 17:Q:59:ILE:O    | 2.10                     | 0.52              |
| 18:R:31:LEU:O     | 18:R:69:THR:HG21 | 2.10                     | 0.52              |
| 1:A:542:G:OP1     | 4:D:10:ARG:NH2   | 2.42                     | 0.51              |
| 5:E:75:THR:HG23   | 5:E:76:ILE:N     | 2.25                     | 0.51              |
| 9:I:37:PHE:O      | 9:I:38:GLN:C     | 2.53                     | 0.51              |
| 1:A:182:U:O4      | 1:A:223:U:H1'    | 2.09                     | 0.51              |
| 1:A:407:G:H2'     | 1:A:408:A:H8     | 1.75                     | 0.51              |
| 1:A:1040:U:H2'    | 1:A:1041:A:C8    | 2.45                     | 0.51              |
| 13:M:116:THR:HG22 | 13:M:117:VAL:N   | 2.24                     | 0.51              |
| 15:O:82:ILE:O     | 15:O:86:GLY:N    | 2.32                     | 0.51              |
| 17:Q:40:LYS:HG2   | 17:Q:41:LYS:N    | 2.25                     | 0.51              |
| 1:A:21:G:H2'      | 1:A:22:G:C8      | 2.45                     | 0.51              |
| 1:A:1057:G:O2'    | 1:A:1058:G:H5'   | 2.10                     | 0.51              |
| 1:A:1144:G:H21    | 1:A:1146:A:H62   | 1.58                     | 0.51              |
| 3:C:72:LYS:O      | 3:C:75:VAL:HG23  | 2.10                     | 0.51              |
| 5:E:13:ILE:C      | 5:E:13:ILE:HD12  | 2.35                     | 0.51              |
| 9:I:31:GLN:O      | 9:I:32:ASP:CB    | 2.56                     | 0.51              |
| 12:L:24:VAL:HG13  | 12:L:98:TYR:CE2  | 2.45                     | 0.51              |
| 14:N:26:ARG:HH21  | 14:N:47:LEU:HG   | 1.76                     | 0.51              |
| 16:P:5:ARG:HH21   | 16:P:28:ARG:HA   | 1.75                     | 0.51              |
| 1:A:1310:G:N7     | 19:S:2:PRO:HD3   | 2.25                     | 0.51              |
| 3:C:108:ASN:ND2   | 3:C:144:SER:HB3  | 2.26                     | 0.51              |
| 10:J:16:LEU:HB3   | 10:J:70:ARG:HG3  | 1.92                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 15:O:26:GLU:HG3  | 15:O:81:LEU:HD12 | 1.91                     | 0.51              |
| 19:S:13:ASP:O    | 19:S:14:HIS:C    | 2.54                     | 0.51              |
| 21:U:15:ARG:HG2  | 21:U:15:ARG:HH11 | 1.76                     | 0.51              |
| 1:A:115:G:H1'    | 1:A:116:A:N7     | 2.25                     | 0.51              |
| 1:A:241:C:H4'    | 12:L:19:ARG:HH22 | 1.76                     | 0.51              |
| 1:A:383:A:H2'    | 1:A:384:G:H5'    | 1.93                     | 0.51              |
| 1:A:407:G:H2'    | 1:A:408:A:C8     | 2.44                     | 0.51              |
| 1:A:431:A:O2'    | 1:A:432:A:H5'    | 2.10                     | 0.51              |
| 1:A:669:U:H2'    | 1:A:670:G:H8     | 1.76                     | 0.51              |
| 1:A:976:G:H5'    | 1:A:1358:U:O2'   | 2.11                     | 0.51              |
| 1:A:1481:U:O2'   | 1:A:1482:G:H5'   | 2.10                     | 0.51              |
| 4:D:36:ARG:HB2   | 4:D:36:ARG:NH1   | 2.25                     | 0.51              |
| 6:F:46:ARG:HG2   | 6:F:47:ARG:H     | 1.76                     | 0.51              |
| 9:I:24:GLY:HA2   | 9:I:59:PHE:O     | 2.11                     | 0.51              |
| 10:J:7:LYS:HZ2   | 10:J:40:LEU:HD11 | 1.74                     | 0.51              |
| 10:J:47:PHE:HB2  | 10:J:63:PHE:HB2  | 1.92                     | 0.51              |
| 19:S:44:MET:HA   | 19:S:47:HIS:HD2  | 1.75                     | 0.51              |
| 20:T:100:ILE:C   | 20:T:102:GLY:H   | 2.19                     | 0.51              |
| 1:A:1303:C:H2'   | 1:A:1304:G:H5'   | 1.91                     | 0.51              |
| 3:C:56:ASP:N     | 3:C:56:ASP:OD1   | 2.43                     | 0.51              |
| 11:K:21:ILE:HD13 | 11:K:94:ALA:HB3  | 1.93                     | 0.51              |
| 1:A:328:C:O2     | 1:A:328:C:C2'    | 2.58                     | 0.51              |
| 1:A:613:C:O2'    | 1:A:614:A:H5'    | 2.11                     | 0.51              |
| 6:F:4:TYR:CZ     | 6:F:72:VAL:HG21  | 2.46                     | 0.51              |
| 6:F:75:LEU:C     | 6:F:75:LEU:CD2   | 2.83                     | 0.51              |
| 9:I:99:LEU:HB3   | 9:I:101:PHE:CE1  | 2.45                     | 0.51              |
| 14:N:25:VAL:HG12 | 14:N:38:GLY:O    | 2.10                     | 0.51              |
| 14:N:37:PHE:C    | 14:N:39:LEU:H    | 2.17                     | 0.51              |
| 19:S:15:LEU:HD12 | 19:S:16:LEU:H    | 1.76                     | 0.51              |
| 1:A:472:A:H4'    | 16:P:80:PHE:O    | 2.11                     | 0.51              |
| 1:A:537:G:OP1    | 12:L:113:ARG:NH2 | 2.44                     | 0.51              |
| 1:A:1457:G:H2'   | 1:A:1458:G:H8    | 1.76                     | 0.51              |
| 2:B:71:VAL:HB    | 2:B:164:VAL:HG22 | 1.92                     | 0.51              |
| 3:C:138:VAL:HG22 | 3:C:151:VAL:HG23 | 1.93                     | 0.51              |
| 6:F:69:GLU:O     | 6:F:72:VAL:HG23  | 2.11                     | 0.51              |
| 6:F:86:ARG:O     | 6:F:87:ARG:HG2   | 2.10                     | 0.51              |
| 13:M:33:ALA:O    | 13:M:37:THR:HB   | 2.10                     | 0.51              |
| 3:C:70:VAL:CG1   | 3:C:71:ALA:N     | 2.74                     | 0.51              |
| 3:C:147:LYS:HE3  | 3:C:203:PHE:CZ   | 2.46                     | 0.51              |
| 3:C:157:ILE:HD13 | 3:C:166:GLU:HG3  | 1.93                     | 0.51              |
| 5:E:96:PRO:HA    | 5:E:117:ASP:OD2  | 2.09                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:38:GLU:HB2   | 6:F:64:GLN:O     | 2.11                     | 0.51              |
| 8:H:103:VAL:HG21 | 8:H:109:ILE:C    | 2.36                     | 0.51              |
| 10:J:7:LYS:NZ    | 10:J:40:LEU:HD11 | 2.26                     | 0.51              |
| 1:A:403:C:O2'    | 1:A:404:U:H5'    | 2.10                     | 0.51              |
| 1:A:1042:G:O2'   | 1:A:1043:C:H5'   | 2.11                     | 0.51              |
| 1:A:1359:C:OP1   | 14:N:22:THR:HG22 | 2.11                     | 0.51              |
| 2:B:12:GLU:C     | 2:B:14:GLY:N     | 2.65                     | 0.51              |
| 5:E:11:ILE:CG2   | 5:E:105:VAL:HG22 | 2.41                     | 0.51              |
| 13:M:13:LYS:O    | 13:M:45:VAL:HG23 | 2.10                     | 0.51              |
| 18:R:19:LYS:CD   | 18:R:20:ALA:H    | 2.24                     | 0.51              |
| 19:S:20:LEU:O    | 19:S:23:ASN:HB2  | 2.10                     | 0.51              |
| 1:A:17:U:H2'     | 1:A:18:C:C6      | 2.45                     | 0.50              |
| 1:A:45:U:H2'     | 1:A:46:G:C8      | 2.46                     | 0.50              |
| 1:A:60:A:H4'     | 1:A:61:G:O5'     | 2.11                     | 0.50              |
| 1:A:620:C:H2'    | 1:A:621:A:O4'    | 2.11                     | 0.50              |
| 1:A:945:G:H2'    | 1:A:945:G:N3     | 2.26                     | 0.50              |
| 2:B:63:MET:O     | 2:B:63:MET:HE3   | 2.11                     | 0.50              |
| 6:F:26:ILE:O     | 6:F:30:LEU:HG    | 2.11                     | 0.50              |
| 10:J:85:LEU:O    | 10:J:87:THR:N    | 2.44                     | 0.50              |
| 14:N:5:ALA:O     | 14:N:8:GLU:HG2   | 2.11                     | 0.50              |
| 18:R:36:ASN:C    | 18:R:36:ASN:ND2  | 2.68                     | 0.50              |
| 20:T:57:ARG:HH11 | 20:T:57:ARG:CG   | 2.24                     | 0.50              |
| 1:A:1251:A:H2'   | 1:A:1252:A:C8    | 2.45                     | 0.50              |
| 4:D:64:LEU:HD12  | 4:D:75:PHE:CE1   | 2.45                     | 0.50              |
| 10:J:80:LYS:HB2  | 10:J:80:LYS:NZ   | 2.26                     | 0.50              |
| 16:P:21:VAL:HG12 | 16:P:33:ILE:HD12 | 1.93                     | 0.50              |
| 17:Q:101:ARG:HE  | 17:Q:101:ARG:CA  | 2.22                     | 0.50              |
| 8:H:85:ARG:HD3   | 8:H:85:ARG:C     | 2.36                     | 0.50              |
| 12:L:10:LEU:HD21 | 12:L:15:ARG:NE   | 2.26                     | 0.50              |
| 17:Q:29:HIS:CG   | 17:Q:30:PRO:HD2  | 2.46                     | 0.50              |
| 1:A:959:A:C2     | 1:A:1222:G:O4'   | 2.65                     | 0.50              |
| 1:A:1031:G:H2'   | 1:A:1032:G:C8    | 2.47                     | 0.50              |
| 1:A:1305:G:H22   | 1:A:1331:G:C2'   | 2.25                     | 0.50              |
| 2:B:13:ALA:HA    | 2:B:17:PHE:CE2   | 2.45                     | 0.50              |
| 5:E:13:ILE:HD12  | 5:E:13:ILE:O     | 2.12                     | 0.50              |
| 10:J:8:LEU:CD2   | 10:J:96:ILE:HG12 | 2.41                     | 0.50              |
| 19:S:44:MET:HE2  | 19:S:49:ILE:CD1  | 2.40                     | 0.50              |
| 21:U:23:PRO:C    | 21:U:25:LYS:H    | 2.19                     | 0.50              |
| 1:A:189(G):G:H4' | 1:A:189(H):G:OP2 | 2.12                     | 0.50              |
| 4:D:68:TYR:O     | 4:D:70:ILE:HD13  | 2.12                     | 0.50              |
| 16:P:23:ASP:OD1  | 16:P:25:ARG:N    | 2.43                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 20:T:67:ALA:HB2  | 20:T:77:ALA:HB2  | 1.93                     | 0.50              |
| 21:U:2:GLY:C     | 21:U:4:GLY:N     | 2.69                     | 0.50              |
| 1:A:179:A:H2'    | 1:A:180:U:C6     | 2.47                     | 0.50              |
| 1:A:726:C:H5'    | 1:A:726:C:C6     | 2.28                     | 0.50              |
| 1:A:1379:G:O6    | 7:G:2:ALA:HB3    | 2.11                     | 0.50              |
| 2:B:97:TRP:CZ3   | 2:B:176:GLU:OE2  | 2.65                     | 0.50              |
| 2:B:142:LEU:HG   | 2:B:146:GLN:NE2  | 2.16                     | 0.50              |
| 4:D:25:ARG:C     | 4:D:27:TYR:N     | 2.69                     | 0.50              |
| 4:D:119:GLN:HG3  | 4:D:123:HIS:CD2  | 2.47                     | 0.50              |
| 7:G:20:ASP:OD1   | 7:G:22:LEU:HB3   | 2.10                     | 0.50              |
| 13:M:108:ARG:HD3 | 13:M:114:ARG:NH1 | 2.27                     | 0.50              |
| 1:A:718:G:C5'    | 11:K:117:ASN:ND2 | 2.73                     | 0.50              |
| 1:A:761:G:H21    | 17:Q:105:ALA:HB1 | 1.75                     | 0.50              |
| 1:A:977:A:H2'    | 1:A:978:A:H5'    | 1.93                     | 0.50              |
| 1:A:1314:C:C5    | 19:S:6:LYS:HE2   | 2.47                     | 0.50              |
| 2:B:111:ARG:HB3  | 2:B:149:LEU:CD1  | 2.38                     | 0.50              |
| 7:G:149:ARG:HD2  | 11:K:59:TYR:CE1  | 2.47                     | 0.50              |
| 10:J:51:ARG:HG3  | 10:J:59:SER:HB2  | 1.93                     | 0.50              |
| 19:S:19:VAL:HG13 | 19:S:20:LEU:N    | 2.27                     | 0.50              |
| 20:T:67:ALA:O    | 20:T:73:HIS:CE1  | 2.64                     | 0.50              |
| 2:B:19:HIS:NE2   | 2:B:206:ASP:HB3  | 2.27                     | 0.50              |
| 2:B:102:LEU:N    | 2:B:102:LEU:HD12 | 2.26                     | 0.50              |
| 6:F:44:GLY:HA2   | 6:F:59:TYR:CE1   | 2.47                     | 0.50              |
| 6:F:62:TRP:CH2   | 6:F:64:GLN:HB2   | 2.47                     | 0.50              |
| 8:H:101:PRO:HG3  | 8:H:133:LEU:HD11 | 1.93                     | 0.50              |
| 12:L:61:THR:C    | 12:L:63:GLY:H    | 2.19                     | 0.50              |
| 18:R:19:LYS:CG   | 18:R:20:ALA:N    | 2.62                     | 0.50              |
| 1:A:509:A:H5'    | 1:A:509:A:C8     | 2.45                     | 0.50              |
| 1:A:930:C:O2'    | 1:A:931:C:H5'    | 2.12                     | 0.50              |
| 1:A:1521:G:H2'   | 1:A:1522:U:C6    | 2.47                     | 0.50              |
| 5:E:76:ILE:HG23  | 5:E:142:LEU:HD22 | 1.94                     | 0.50              |
| 6:F:45:LEU:HD12  | 6:F:45:LEU:O     | 2.12                     | 0.50              |
| 13:M:73:GLU:O    | 13:M:76:ALA:HB3  | 2.12                     | 0.50              |
| 1:A:404:U:H2'    | 1:A:405:U:H6     | 1.76                     | 0.49              |
| 1:A:443:C:H2'    | 1:A:444:C:H5'    | 1.94                     | 0.49              |
| 1:A:537:G:H2'    | 1:A:538:G:C8     | 2.47                     | 0.49              |
| 1:A:738:C:H5''   | 6:F:69:GLU:HB3   | 1.93                     | 0.49              |
| 1:A:1169:A:H2'   | 1:A:1170:A:C8    | 2.47                     | 0.49              |
| 1:A:1194:U:H2'   | 1:A:1195:C:C6    | 2.44                     | 0.49              |
| 3:C:79:ARG:C     | 3:C:81:GLY:H     | 2.19                     | 0.49              |
| 3:C:150:LYS:HD3  | 3:C:152:ILE:HD11 | 1.93                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 18:R:44:LEU:CD1  | 18:R:79:LEU:HD22 | 2.42                     | 0.49              |
| 1:A:780:A:O2'    | 1:A:781:A:H5''   | 2.12                     | 0.49              |
| 1:A:1010:G:H2'   | 1:A:1011:G:H8    | 1.77                     | 0.49              |
| 1:A:1136:U:H5''  | 1:A:1137:C:OP2   | 2.12                     | 0.49              |
| 4:D:65:ARG:HB2   | 4:D:75:PHE:CE1   | 2.47                     | 0.49              |
| 7:G:126:ASP:CG   | 7:G:131:LYS:HE3  | 2.38                     | 0.49              |
| 9:I:48:GLU:HA    | 9:I:51:ARG:NH1   | 2.25                     | 0.49              |
| 13:M:14:ARG:NH1  | 13:M:16:ASP:OD2  | 2.39                     | 0.49              |
| 16:P:1:MET:HE3   | 16:P:3:LYS:HG2   | 1.94                     | 0.49              |
| 16:P:43:LYS:HD2  | 16:P:43:LYS:N    | 2.27                     | 0.49              |
| 1:A:189(I):G:O2' | 1:A:189(J):G:H5' | 2.13                     | 0.49              |
| 8:H:87:SER:HB2   | 8:H:93:VAL:H     | 1.78                     | 0.49              |
| 16:P:11:SER:OG   | 16:P:14:ASN:HB3  | 2.12                     | 0.49              |
| 17:Q:68:ARG:HG2  | 17:Q:68:ARG:HH11 | 1.77                     | 0.49              |
| 1:A:1125:U:H6    | 1:A:1125:U:H5''  | 1.77                     | 0.49              |
| 2:B:61:LEU:HD13  | 2:B:61:LEU:O     | 2.13                     | 0.49              |
| 3:C:23:TYR:CD2   | 3:C:23:TYR:C     | 2.89                     | 0.49              |
| 3:C:107:GLN:O    | 3:C:108:ASN:CB   | 2.60                     | 0.49              |
| 6:F:75:LEU:HD23  | 6:F:75:LEU:O     | 2.13                     | 0.49              |
| 21:U:9:ARG:HH12  | 21:U:23:PRO:CD   | 2.26                     | 0.49              |
| 5:E:39:GLY:HA2   | 5:E:69:VAL:HB    | 1.95                     | 0.49              |
| 11:K:34:ASP:C    | 11:K:34:ASP:OD1  | 2.56                     | 0.49              |
| 11:K:41:THR:HG21 | 11:K:71:LYS:HB3  | 1.95                     | 0.49              |
| 1:A:620:C:C2     | 4:D:135:LEU:HD13 | 2.48                     | 0.49              |
| 1:A:818:G:C3'    | 1:A:819:A:C5'    | 2.91                     | 0.49              |
| 5:E:36:ASP:O     | 5:E:38:GLN:HG3   | 2.12                     | 0.49              |
| 5:E:129:ILE:H    | 5:E:129:ILE:CD1  | 2.21                     | 0.49              |
| 8:H:82:HIS:HB3   | 8:H:138:TRP:CD2  | 2.48                     | 0.49              |
| 1:A:30:U:O2'     | 1:A:31:G:OP1     | 2.28                     | 0.49              |
| 2:B:53:ARG:NH1   | 2:B:199:TYR:HD2  | 2.09                     | 0.49              |
| 2:B:55:PHE:HA    | 2:B:58:ILE:HD12  | 1.94                     | 0.49              |
| 10:J:35:SER:CB   | 10:J:73:ASP:HB2  | 2.43                     | 0.49              |
| 20:T:72:LEU:O    | 20:T:73:HIS:C    | 2.55                     | 0.49              |
| 1:A:537:G:H2'    | 1:A:538:G:H8     | 1.78                     | 0.49              |
| 1:A:697:U:H2'    | 1:A:698:G:H5'    | 1.95                     | 0.49              |
| 1:A:951:G:O2'    | 1:A:952:U:H5'    | 2.12                     | 0.49              |
| 1:A:977:A:C2'    | 1:A:978:A:H5'    | 2.42                     | 0.49              |
| 1:A:1024:G:H2'   | 1:A:1025:U:O4'   | 2.12                     | 0.49              |
| 1:A:1057:G:H2'   | 1:A:1058:G:O4'   | 2.12                     | 0.49              |
| 1:A:1251:A:H1'   | 1:A:1369:C:O2'   | 2.13                     | 0.49              |
| 1:A:1327:C:O2'   | 1:A:1328:C:H5'   | 2.13                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:36:ARG:HB2   | 2:B:41:ILE:HD11  | 1.94                     | 0.49              |
| 4:D:164:ALA:O    | 4:D:168:ARG:HD2  | 2.12                     | 0.49              |
| 6:F:91:VAL:CG1   | 18:R:72:ARG:NH2  | 2.76                     | 0.49              |
| 13:M:86:CYS:HA   | 19:S:73:GLU:O    | 2.13                     | 0.49              |
| 14:N:9:LYS:C     | 14:N:11:LYS:N    | 2.71                     | 0.49              |
| 15:O:29:VAL:HG12 | 15:O:85:LEU:HD12 | 1.95                     | 0.49              |
| 18:R:74:ARG:HA   | 18:R:79:LEU:O    | 2.12                     | 0.49              |
| 1:A:620:C:C1'    | 4:D:135:LEU:HD13 | 2.43                     | 0.49              |
| 4:D:121:VAL:HG12 | 4:D:134:ASP:HA   | 1.94                     | 0.49              |
| 6:F:97:PHE:HB2   | 18:R:32:ARG:HH21 | 1.77                     | 0.49              |
| 7:G:17:VAL:HG12  | 7:G:18:TYR:CE1   | 2.48                     | 0.49              |
| 10:J:47:PHE:CZ   | 14:N:37:PHE:HE1  | 2.30                     | 0.49              |
| 12:L:41:ARG:HG2  | 12:L:42:THR:N    | 2.18                     | 0.49              |
| 19:S:44:MET:HB2  | 19:S:62:ILE:CD1  | 2.42                     | 0.49              |
| 1:A:737:A:H2'    | 1:A:738:C:C6     | 2.47                     | 0.49              |
| 1:A:737:A:H1'    | 6:F:73:ASN:OD1   | 2.12                     | 0.49              |
| 1:A:1080:A:C5'   | 5:E:16:THR:HG21  | 2.41                     | 0.49              |
| 2:B:53:ARG:HH12  | 2:B:199:TYR:HA   | 1.78                     | 0.49              |
| 2:B:96:ARG:HD2   | 2:B:96:ARG:N     | 2.22                     | 0.49              |
| 7:G:50:ILE:HD11  | 7:G:121:ALA:CA   | 2.41                     | 0.49              |
| 11:K:33:THR:HG22 | 11:K:39:PRO:HA   | 1.94                     | 0.49              |
| 13:M:20:THR:C    | 13:M:22:ILE:N    | 2.71                     | 0.49              |
| 1:A:269:C:H2'    | 1:A:270:A:H8     | 1.77                     | 0.48              |
| 2:B:118:LEU:HD22 | 2:B:142:LEU:HB2  | 1.95                     | 0.48              |
| 3:C:56:ASP:O     | 3:C:57:ILE:HG13  | 2.12                     | 0.48              |
| 4:D:3:ARG:HH11   | 4:D:115:ARG:HB3  | 1.77                     | 0.48              |
| 4:D:30:LYS:CB    | 4:D:35:ARG:HH21  | 2.25                     | 0.48              |
| 8:H:85:ARG:NE    | 8:H:87:SER:O     | 2.46                     | 0.48              |
| 12:L:54:LYS:HB3  | 12:L:70:ILE:HG13 | 1.95                     | 0.48              |
| 14:N:6:LEU:C     | 14:N:8:GLU:H     | 2.20                     | 0.48              |
| 16:P:20:VAL:CG1  | 16:P:21:VAL:N    | 2.76                     | 0.48              |
| 22:X:5:A:H8      | 22:X:5:A:O5'     | 1.95                     | 0.48              |
| 1:A:189(A):C:H2' | 1:A:189(B):C:H6  | 1.77                     | 0.48              |
| 1:A:1206:G:H1'   | 3:C:193:TYR:O    | 2.12                     | 0.48              |
| 1:A:1474:G:H2'   | 1:A:1475:G:H8    | 1.78                     | 0.48              |
| 2:B:61:LEU:HD13  | 2:B:61:LEU:C     | 2.39                     | 0.48              |
| 3:C:87:LEU:C     | 3:C:89:GLU:N     | 2.69                     | 0.48              |
| 3:C:100:ALA:HB1  | 3:C:102:ASN:HD21 | 1.77                     | 0.48              |
| 4:D:31:CYS:SG    | 4:D:31:CYS:O     | 2.71                     | 0.48              |
| 6:F:100:ASN:HB2  | 18:R:23:LYS:HE3  | 1.96                     | 0.48              |
| 7:G:54:THR:C     | 7:G:56:GLN:H     | 2.21                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 9:I:48:GLU:OE2   | 9:I:51:ARG:HD2    | 2.13                     | 0.48              |
| 19:S:16:LEU:C    | 19:S:19:VAL:HG12  | 2.38                     | 0.48              |
| 19:S:33:THR:CG2  | 19:S:35:SER:H     | 2.26                     | 0.48              |
| 1:A:642:A:N7     | 8:H:115:SER:HA    | 2.28                     | 0.48              |
| 1:A:807:A:H2'    | 1:A:808:C:C6      | 2.49                     | 0.48              |
| 1:A:1014:A:H2    | 1:A:1219:U:H1'    | 1.78                     | 0.48              |
| 1:A:1096:C:H2'   | 1:A:1097:C:C6     | 2.47                     | 0.48              |
| 1:A:1171:G:H2'   | 1:A:1172:C:C6     | 2.48                     | 0.48              |
| 1:A:1237:C:H4'   | 1:A:1334:G:N2     | 2.28                     | 0.48              |
| 1:A:1540:U:O5'   | 1:A:1540:U:H6     | 1.96                     | 0.48              |
| 2:B:217:ARG:HA   | 2:B:220:ASP:OD2   | 2.13                     | 0.48              |
| 9:I:8:GLY:HA2    | 9:I:79:LEU:HD13   | 1.95                     | 0.48              |
| 10:J:46:ARG:NH1  | 10:J:64:GLU:HB3   | 2.27                     | 0.48              |
| 14:N:24:CYS:HB2  | 14:N:29:ARG:HB3   | 1.96                     | 0.48              |
| 16:P:57:ARG:HH12 | 16:P:79:VAL:C     | 2.20                     | 0.48              |
| 1:A:148:G:H2'    | 1:A:149:A:C8      | 2.47                     | 0.48              |
| 1:A:1470:G:O2'   | 1:A:1471:G:H5'    | 2.14                     | 0.48              |
| 2:B:100:GLY:O    | 2:B:104:ASN:N     | 2.43                     | 0.48              |
| 2:B:137:ARG:NH1  | 2:B:137:ARG:CB    | 2.76                     | 0.48              |
| 2:B:181:PHE:HD2  | 8:H:70:GLN:HB3    | 1.76                     | 0.48              |
| 4:D:76:ARG:HG2   | 4:D:76:ARG:NH1    | 2.28                     | 0.48              |
| 7:G:5:ARG:HD2    | 7:G:5:ARG:C       | 2.39                     | 0.48              |
| 17:Q:48:GLU:C    | 17:Q:50:LYS:H     | 2.21                     | 0.48              |
| 19:S:5:LEU:HD11  | 19:S:70:LYS:NZ    | 2.29                     | 0.48              |
| 1:A:768:A:H2'    | 1:A:769:G:O4'     | 2.13                     | 0.48              |
| 4:D:62:GLN:NE2   | 4:D:62:GLN:HA     | 2.28                     | 0.48              |
| 8:H:63:LEU:HD22  | 8:H:63:LEU:H      | 1.78                     | 0.48              |
| 8:H:68:ARG:HG2   | 8:H:68:ARG:HH11   | 1.78                     | 0.48              |
| 8:H:88:LYS:O     | 8:H:92:ARG:HD2    | 2.12                     | 0.48              |
| 20:T:50:GLU:O    | 20:T:100:ILE:HG21 | 2.13                     | 0.48              |
| 1:A:477:A:O2'    | 1:A:479:C:H5'     | 2.13                     | 0.48              |
| 1:A:954:G:H2'    | 1:A:955:U:C6      | 2.48                     | 0.48              |
| 1:A:1543:C:O2'   | 1:A:1544:U:H5'    | 2.14                     | 0.48              |
| 2:B:86:GLU:C     | 2:B:88:ALA:N      | 2.71                     | 0.48              |
| 4:D:24:GLU:C     | 4:D:26:CYS:H      | 2.22                     | 0.48              |
| 5:E:101:ILE:HG22 | 5:E:101:ILE:O     | 2.13                     | 0.48              |
| 1:A:528:C:H5'    | 1:A:535:A:N6      | 2.28                     | 0.48              |
| 1:A:1370:G:O2'   | 1:A:1371:G:H5'    | 2.14                     | 0.48              |
| 3:C:107:GLN:O    | 3:C:108:ASN:HB3   | 2.14                     | 0.48              |
| 3:C:181:ASN:ND2  | 3:C:204:LEU:CD1   | 2.76                     | 0.48              |
| 4:D:146:ILE:N    | 4:D:146:ILE:CD1   | 2.76                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:10:MET:HG3   | 5:E:10:MET:O     | 2.13                     | 0.48              |
| 5:E:87:SER:HB3   | 5:E:131:ILE:HD13 | 1.95                     | 0.48              |
| 8:H:9:MET:O      | 8:H:10:LEU:C     | 2.55                     | 0.48              |
| 12:L:7:ILE:HG21  | 17:Q:34:LYS:HB2  | 1.95                     | 0.48              |
| 12:L:38:THR:HB   | 12:L:57:LYS:HB3  | 1.95                     | 0.48              |
| 13:M:20:THR:O    | 13:M:22:ILE:N    | 2.45                     | 0.48              |
| 13:M:40:ASN:HD22 | 13:M:41:PRO:N    | 2.12                     | 0.48              |
| 1:A:782:A:H2'    | 1:A:783:C:O4'    | 2.14                     | 0.48              |
| 1:A:794:A:H2'    | 1:A:795:C:C6     | 2.48                     | 0.48              |
| 1:A:1218:C:H2'   | 1:A:1219:U:C6    | 2.49                     | 0.48              |
| 1:A:1342:C:O2'   | 1:A:1343:G:H5'   | 2.14                     | 0.48              |
| 2:B:118:LEU:HD22 | 2:B:142:LEU:CD1  | 2.28                     | 0.48              |
| 8:H:87:SER:CB    | 8:H:93:VAL:H     | 2.26                     | 0.48              |
| 1:A:253:U:H2'    | 1:A:254:G:H8     | 1.77                     | 0.48              |
| 1:A:397:A:H5'    | 1:A:398:C:OP1    | 2.12                     | 0.48              |
| 1:A:818:G:O2'    | 1:A:819:A:H5''   | 2.14                     | 0.48              |
| 1:A:1513:A:H2'   | 1:A:1514:C:C6    | 2.48                     | 0.48              |
| 2:B:47:THR:HA    | 2:B:202:PRO:HG2  | 1.95                     | 0.48              |
| 2:B:206:ASP:O    | 2:B:207:ALA:CB   | 2.61                     | 0.48              |
| 4:D:52:SER:O     | 4:D:53:ASP:C     | 2.57                     | 0.48              |
| 5:E:91:LEU:CD2   | 5:E:120:THR:HG22 | 2.44                     | 0.48              |
| 5:E:99:GLY:O     | 5:E:117:ASP:HA   | 2.13                     | 0.48              |
| 10:J:3:LYS:N     | 10:J:3:LYS:HD3   | 2.29                     | 0.48              |
| 10:J:9:ARG:HB3   | 10:J:9:ARG:HH11  | 1.79                     | 0.48              |
| 12:L:25:PRO:C    | 12:L:27:LEU:N    | 2.66                     | 0.48              |
| 14:N:8:GLU:C     | 14:N:10:ALA:N    | 2.69                     | 0.48              |
| 16:P:57:ARG:HG2  | 16:P:57:ARG:NH1  | 2.20                     | 0.48              |
| 17:Q:33:GLY:O    | 17:Q:34:LYS:C    | 2.57                     | 0.48              |
| 1:A:457:C:O2'    | 1:A:458:C:H5'    | 2.14                     | 0.48              |
| 1:A:1019:C:C2'   | 1:A:1020:U:H5'   | 2.43                     | 0.48              |
| 1:A:1152:A:OP1   | 10:J:68:HIS:ND1  | 2.47                     | 0.48              |
| 1:A:1474:G:H2'   | 1:A:1475:G:C8    | 2.48                     | 0.48              |
| 3:C:125:GLU:HG2  | 3:C:190:ARG:O    | 2.14                     | 0.48              |
| 5:E:103:GLY:O    | 5:E:106:PRO:HD2  | 2.14                     | 0.48              |
| 6:F:15:ASP:N     | 6:F:18:GLN:NE2   | 2.55                     | 0.48              |
| 8:H:4:ASP:OD2    | 8:H:85:ARG:NH1   | 2.47                     | 0.48              |
| 8:H:10:LEU:HD12  | 8:H:85:ARG:HG2   | 1.94                     | 0.48              |
| 10:J:32:ALA:H    | 10:J:78:ASN:HD21 | 1.57                     | 0.48              |
| 10:J:33:GLN:HB3  | 10:J:75:ILE:HD11 | 1.95                     | 0.48              |
| 12:L:83:VAL:HG23 | 12:L:107:ALA:HB2 | 1.96                     | 0.48              |
| 13:M:120:LYS:HZ2 | 13:M:122:LYS:HB3 | 1.72                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 15:O:30:ALA:HA   | 15:O:85:LEU:HD11 | 1.95                     | 0.48              |
| 20:T:53:LEU:HB3  | 20:T:102:GLY:HA3 | 1.95                     | 0.48              |
| 1:A:22:G:H2'     | 1:A:23:C:C6      | 2.49                     | 0.47              |
| 1:A:961:U:H2'    | 1:A:962:C:H5'    | 1.96                     | 0.47              |
| 1:A:1244:C:O2'   | 1:A:1245:A:H5'   | 2.13                     | 0.47              |
| 1:A:1255:G:OP2   | 10:J:43:ARG:NH2  | 2.47                     | 0.47              |
| 1:A:1286:A:C8    | 1:A:1287:A:H4'   | 2.49                     | 0.47              |
| 3:C:115:LEU:HD23 | 3:C:118:GLN:OE1  | 2.13                     | 0.47              |
| 6:F:19:LEU:C     | 6:F:19:LEU:CD2   | 2.87                     | 0.47              |
| 8:H:60:ARG:NH1   | 8:H:60:ARG:CG    | 2.76                     | 0.47              |
| 10:J:46:ARG:NH1  | 10:J:46:ARG:CG   | 2.76                     | 0.47              |
| 13:M:96:LEU:O    | 13:M:110:ARG:NH1 | 2.47                     | 0.47              |
| 15:O:72:ARG:HD2  | 15:O:73:GLU:OE2  | 2.14                     | 0.47              |
| 21:U:6:ARG:CZ    | 21:U:15:ARG:HH21 | 2.25                     | 0.47              |
| 1:A:175:C:H2'    | 1:A:176:C:H6     | 1.78                     | 0.47              |
| 1:A:723:U:O2     | 1:A:723:U:H2'    | 2.14                     | 0.47              |
| 1:A:825:G:N2     | 8:H:11:THR:HG21  | 2.29                     | 0.47              |
| 1:A:1422:G:O2'   | 1:A:1423:G:H5'   | 2.14                     | 0.47              |
| 1:A:1483:A:H2'   | 1:A:1484:C:O4'   | 2.14                     | 0.47              |
| 3:C:40:ARG:O     | 3:C:44:GLU:HG3   | 2.14                     | 0.47              |
| 4:D:190:ASP:O    | 4:D:191:ARG:C    | 2.57                     | 0.47              |
| 9:I:86:VAL:HG13  | 9:I:90:PRO:HA    | 1.96                     | 0.47              |
| 13:M:65:LYS:O    | 13:M:66:LEU:HD23 | 2.13                     | 0.47              |
| 14:N:29:ARG:HG2  | 14:N:29:ARG:NH1  | 2.28                     | 0.47              |
| 16:P:4:ILE:HA    | 16:P:20:VAL:O    | 2.14                     | 0.47              |
| 20:T:39:LYS:HD3  | 20:T:55:ILE:HD13 | 1.96                     | 0.47              |
| 1:A:105:G:H2'    | 1:A:106:C:C6     | 2.49                     | 0.47              |
| 1:A:692:U:H2'    | 1:A:694:A:OP2    | 2.13                     | 0.47              |
| 1:A:716:A:N3     | 11:K:117:ASN:O   | 2.47                     | 0.47              |
| 1:A:834:C:H2'    | 1:A:835:U:C6     | 2.49                     | 0.47              |
| 1:A:1056:U:H5'   | 3:C:163:ALA:CB   | 2.44                     | 0.47              |
| 1:A:1112:C:C4    | 3:C:178:LEU:HD23 | 2.49                     | 0.47              |
| 1:A:1190:G:HO2'  | 1:A:1191:A:P     | 2.37                     | 0.47              |
| 1:A:1347:G:C2'   | 1:A:1348:U:OP2   | 2.63                     | 0.47              |
| 1:A:1362:C:H2'   | 1:A:1363:C:H5''  | 1.96                     | 0.47              |
| 1:A:1419:G:O2'   | 1:A:1420:C:H5'   | 2.14                     | 0.47              |
| 7:G:115:ARG:HB2  | 7:G:118:VAL:CG2  | 2.43                     | 0.47              |
| 10:J:35:SER:HB3  | 10:J:73:ASP:HB2  | 1.96                     | 0.47              |
| 10:J:59:SER:O    | 10:J:60:ARG:HB2  | 2.14                     | 0.47              |
| 11:K:93:GLN:HE21 | 11:K:96:ARG:NH2  | 2.10                     | 0.47              |
| 19:S:28:LYS:O    | 19:S:29:ARG:O    | 2.32                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:253:U:H2'    | 1:A:254:G:C8     | 2.49                     | 0.47              |
| 1:A:399:G:H2'    | 1:A:400:C:H6     | 1.80                     | 0.47              |
| 5:E:92:LYS:N     | 5:E:119:LEU:O    | 2.46                     | 0.47              |
| 8:H:63:LEU:HD22  | 8:H:63:LEU:N     | 2.29                     | 0.47              |
| 8:H:119:LEU:CD1  | 8:H:124:ALA:HA   | 2.44                     | 0.47              |
| 10:J:9:ARG:HH11  | 10:J:9:ARG:CB    | 2.28                     | 0.47              |
| 12:L:43:VAL:HG12 | 12:L:44:THR:N    | 2.28                     | 0.47              |
| 16:P:74:LEU:O    | 16:P:79:VAL:HG23 | 2.15                     | 0.47              |
| 1:A:67:C:O2'     | 1:A:171:A:H1'    | 2.14                     | 0.47              |
| 1:A:242:C:C2'    | 1:A:243:A:H5'    | 2.44                     | 0.47              |
| 1:A:371:G:C2'    | 1:A:372:C:H5'    | 2.44                     | 0.47              |
| 1:A:587:G:OP1    | 8:H:89:PRO:HB3   | 2.13                     | 0.47              |
| 1:A:881:G:P      | 12:L:12:ARG:HH22 | 2.37                     | 0.47              |
| 1:A:1152:A:H2'   | 1:A:1153:C:C6    | 2.49                     | 0.47              |
| 1:A:1331:G:HO2'  | 1:A:1332:A:P     | 2.36                     | 0.47              |
| 1:A:1447:A:O2'   | 1:A:1452:C:OP1   | 2.33                     | 0.47              |
| 1:A:1505:G:C8    | 1:A:1505:G:H3'   | 2.50                     | 0.47              |
| 2:B:120:ALA:C    | 2:B:122:PHE:N    | 2.72                     | 0.47              |
| 5:E:74:GLY:CA    | 5:E:116:THR:HG22 | 2.43                     | 0.47              |
| 10:J:19:SER:HA   | 10:J:22:LYS:NZ   | 2.29                     | 0.47              |
| 18:R:69:THR:O    | 18:R:72:ARG:HB2  | 2.15                     | 0.47              |
| 1:A:730:G:C5     | 1:A:731:G:H1'    | 2.49                     | 0.47              |
| 1:A:1305:G:H22   | 1:A:1331:G:H2'   | 1.80                     | 0.47              |
| 1:A:1438:G:H2'   | 1:A:1439:C:H6    | 1.78                     | 0.47              |
| 2:B:77:ALA:CB    | 2:B:211:ILE:HD13 | 2.38                     | 0.47              |
| 3:C:35:GLU:CD    | 3:C:59:ARG:HH22  | 2.23                     | 0.47              |
| 5:E:36:ASP:CG    | 5:E:40:ARG:HB2   | 2.40                     | 0.47              |
| 11:K:67:ASP:OD1  | 11:K:71:LYS:HE3  | 2.15                     | 0.47              |
| 20:T:94:ALA:O    | 20:T:95:ALA:CB   | 2.63                     | 0.47              |
| 1:A:279:A:H5''   | 1:A:280:C:H3'    | 1.96                     | 0.47              |
| 1:A:518:C:H2'    | 1:A:530:G:N3     | 2.29                     | 0.47              |
| 1:A:825:G:H21    | 8:H:11:THR:HG21  | 1.79                     | 0.47              |
| 1:A:861:G:O2'    | 1:A:862:C:H5'    | 2.15                     | 0.47              |
| 1:A:956:U:O2'    | 1:A:957:U:H5'    | 2.14                     | 0.47              |
| 1:A:1468:A:H2'   | 1:A:1469:G:O4'   | 2.14                     | 0.47              |
| 1:A:1481:U:C2'   | 1:A:1482:G:H5'   | 2.45                     | 0.47              |
| 2:B:14:GLY:C     | 2:B:15:VAL:CG2   | 2.87                     | 0.47              |
| 3:C:62:ASP:HA    | 3:C:97:LYS:HB3   | 1.97                     | 0.47              |
| 3:C:181:ASN:ND2  | 3:C:204:LEU:HD11 | 2.30                     | 0.47              |
| 4:D:64:LEU:C     | 4:D:64:LEU:HD13  | 2.39                     | 0.47              |
| 4:D:109:GLY:C    | 4:D:111:ALA:N    | 2.71                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:150:ARG:NH1  | 5:E:150:ARG:CG   | 2.69                     | 0.47              |
| 6:F:42:GLU:HG3   | 6:F:61:LEU:CD2   | 2.44                     | 0.47              |
| 6:F:50:TYR:CE1   | 18:R:77:GLY:HA2  | 2.50                     | 0.47              |
| 9:I:53:VAL:O     | 9:I:54:ASP:HB2   | 2.13                     | 0.47              |
| 11:K:115:PRO:C   | 11:K:117:ASN:H   | 2.23                     | 0.47              |
| 12:L:53:ARG:CG   | 12:L:69:TYR:HE1  | 2.24                     | 0.47              |
| 12:L:75:HIS:CD2  | 12:L:77:LEU:H    | 2.32                     | 0.47              |
| 13:M:125:ARG:O   | 13:M:126:LYS:C   | 2.57                     | 0.47              |
| 15:O:66:LEU:O    | 15:O:69:TYR:HB3  | 2.14                     | 0.47              |
| 19:S:44:MET:HB2  | 19:S:62:ILE:HD13 | 1.95                     | 0.47              |
| 21:U:15:ARG:HG2  | 21:U:15:ARG:NH1  | 2.29                     | 0.47              |
| 1:A:112:G:C4'    | 1:A:389:A:H5''   | 2.42                     | 0.47              |
| 1:A:523:A:N6     | 12:L:92:ASP:HB2  | 2.27                     | 0.47              |
| 1:A:895:G:H2'    | 1:A:896:C:C6     | 2.50                     | 0.47              |
| 1:A:1129:C:O2'   | 1:A:1130:A:P     | 2.73                     | 0.47              |
| 1:A:1300:G:O2'   | 1:A:1301:U:P     | 2.72                     | 0.47              |
| 5:E:144:THR:CG2  | 5:E:146:ALA:H    | 2.28                     | 0.47              |
| 10:J:6:ILE:CD1   | 10:J:72:VAL:HB   | 2.45                     | 0.47              |
| 13:M:125:ARG:HD2 | 13:M:125:ARG:C   | 2.39                     | 0.47              |
| 16:P:1:MET:CE    | 16:P:3:LYS:HG2   | 2.45                     | 0.47              |
| 16:P:54:GLU:CD   | 16:P:54:GLU:C    | 2.82                     | 0.47              |
| 1:A:438:G:C4'    | 1:A:439:A:OP1    | 2.61                     | 0.47              |
| 1:A:961:U:O2'    | 1:A:962:C:H5'    | 2.14                     | 0.47              |
| 1:A:983:A:H5'    | 1:A:984:C:OP2    | 2.14                     | 0.47              |
| 1:A:1241:G:H2'   | 1:A:1242:C:H6    | 1.79                     | 0.47              |
| 1:A:1381:U:O2'   | 1:A:1382:C:H5'   | 2.14                     | 0.47              |
| 2:B:102:LEU:N    | 2:B:102:LEU:CD1  | 2.77                     | 0.47              |
| 2:B:118:LEU:C    | 2:B:120:ALA:N    | 2.71                     | 0.47              |
| 3:C:34:LEU:HD23  | 14:N:25:VAL:CG2  | 2.44                     | 0.47              |
| 3:C:129:ALA:HB3  | 3:C:132:ARG:CZ   | 2.45                     | 0.47              |
| 9:I:17:VAL:CG2   | 9:I:80:GLY:HA3   | 2.45                     | 0.47              |
| 9:I:48:GLU:N     | 9:I:49:PRO:CD    | 2.78                     | 0.47              |
| 12:L:27:LEU:O    | 12:L:28:LYS:C    | 2.57                     | 0.47              |
| 12:L:28:LYS:O    | 12:L:30:ALA:N    | 2.48                     | 0.47              |
| 14:N:44:LEU:HD12 | 14:N:44:LEU:O    | 2.15                     | 0.47              |
| 21:U:9:ARG:HH12  | 21:U:23:PRO:HD2  | 1.79                     | 0.47              |
| 1:A:28:G:O2'     | 1:A:296:U:OP1    | 2.32                     | 0.47              |
| 1:A:321:A:O2'    | 1:A:322:C:H5'    | 2.15                     | 0.47              |
| 1:A:333:G:H4'    | 20:T:16:HIS:CD2  | 2.50                     | 0.47              |
| 2:B:43:ASP:OD1   | 2:B:46:LYS:HG3   | 2.15                     | 0.47              |
| 3:C:111:LEU:CD2  | 3:C:144:SER:HB2  | 2.44                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:80:ILE:HD12  | 5:E:80:ILE:N     | 2.27                     | 0.47              |
| 8:H:70:GLN:NE2   | 8:H:70:GLN:HA    | 2.30                     | 0.47              |
| 8:H:86:ILE:HD12  | 8:H:133:LEU:CD2  | 2.45                     | 0.47              |
| 10:J:81:THR:HG22 | 10:J:85:LEU:HD12 | 1.97                     | 0.47              |
| 16:P:19:ILE:HG22 | 16:P:36:ILE:CG1  | 2.42                     | 0.47              |
| 1:A:838:G:C2'    | 1:A:839:U:H5''   | 2.44                     | 0.46              |
| 1:A:1039:C:H2'   | 1:A:1040:U:H6    | 1.80                     | 0.46              |
| 1:A:1108:G:H4'   | 1:A:1191:A:O4'   | 2.14                     | 0.46              |
| 1:A:1116:C:O2'   | 1:A:1117:G:H5''  | 2.16                     | 0.46              |
| 1:A:1353:G:H2'   | 1:A:1354:C:H6    | 1.80                     | 0.46              |
| 2:B:115:LEU:HD21 | 2:B:153:ARG:CZ   | 2.45                     | 0.46              |
| 3:C:122:GLU:O    | 3:C:123:GLN:C    | 2.58                     | 0.46              |
| 7:G:146:GLU:HG2  | 7:G:149:ARG:NH2  | 2.21                     | 0.46              |
| 10:J:21:GLN:CA   | 10:J:21:GLN:HE21 | 2.27                     | 0.46              |
| 16:P:20:VAL:CG1  | 16:P:32:TYR:HB2  | 2.45                     | 0.46              |
| 1:A:1047:G:C2'   | 1:A:1048:G:C5'   | 2.85                     | 0.46              |
| 1:A:1201:A:O2'   | 1:A:1202:G:OP2   | 2.31                     | 0.46              |
| 2:B:12:GLU:HB3   | 2:B:16:HIS:ND1   | 2.30                     | 0.46              |
| 2:B:213:LEU:HD23 | 2:B:213:LEU:C    | 2.40                     | 0.46              |
| 3:C:19:GLU:HB3   | 3:C:40:ARG:HH21  | 1.79                     | 0.46              |
| 3:C:89:GLU:O     | 3:C:93:LYS:HG2   | 2.16                     | 0.46              |
| 3:C:113:ALA:N    | 3:C:114:PRO:CD   | 2.78                     | 0.46              |
| 4:D:165:MET:SD   | 4:D:168:ARG:HD3  | 2.55                     | 0.46              |
| 7:G:113:GLU:CD   | 7:G:113:GLU:H    | 2.24                     | 0.46              |
| 11:K:101:SER:C   | 11:K:103:LEU:H   | 2.24                     | 0.46              |
| 1:A:189(E):U:O2' | 1:A:189(F):U:H5' | 2.15                     | 0.46              |
| 1:A:189(J):G:O2' | 1:A:189(K):U:H5' | 2.15                     | 0.46              |
| 1:A:834:C:H2'    | 1:A:835:U:H6     | 1.79                     | 0.46              |
| 1:A:991:U:O2     | 1:A:993:G:H8     | 1.98                     | 0.46              |
| 1:A:1226:C:N4    | 13:M:104:ARG:HG3 | 2.31                     | 0.46              |
| 2:B:55:PHE:HE2   | 2:B:218:ALA:HA   | 1.79                     | 0.46              |
| 2:B:187:LEU:HD23 | 2:B:201:ILE:O    | 2.14                     | 0.46              |
| 4:D:31:CYS:C     | 4:D:33:MET:N     | 2.71                     | 0.46              |
| 4:D:156:GLU:HG2  | 4:D:160:GLN:NE2  | 2.28                     | 0.46              |
| 14:N:6:LEU:C     | 14:N:8:GLU:N     | 2.73                     | 0.46              |
| 19:S:28:LYS:O    | 19:S:29:ARG:C    | 2.57                     | 0.46              |
| 1:A:67:C:H2'     | 1:A:68:G:C8      | 2.50                     | 0.46              |
| 1:A:993:G:O2'    | 1:A:994:A:P      | 2.74                     | 0.46              |
| 1:A:1031:G:H2'   | 1:A:1032:G:H8    | 1.81                     | 0.46              |
| 1:A:1236:A:O2'   | 1:A:1304:G:H4'   | 2.15                     | 0.46              |
| 1:A:1326:C:OP1   | 21:U:12:LYS:NZ   | 2.44                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:21:ARG:HH11  | 2:B:21:ARG:HG3    | 1.81                     | 0.46              |
| 6:F:27:GLN:HA    | 6:F:27:GLN:HE21   | 1.79                     | 0.46              |
| 6:F:69:GLU:C     | 6:F:71:ARG:H      | 2.24                     | 0.46              |
| 6:F:74:ASP:OD1   | 6:F:77:ARG:NH2    | 2.49                     | 0.46              |
| 6:F:77:ARG:HD2   | 6:F:77:ARG:C      | 2.41                     | 0.46              |
| 9:I:16:ARG:O     | 9:I:63:ILE:HG23   | 2.16                     | 0.46              |
| 12:L:78:GLN:O    | 12:L:80:HIS:N     | 2.48                     | 0.46              |
| 17:Q:26:GLN:O    | 17:Q:27:PHE:HB3   | 2.15                     | 0.46              |
| 3:C:23:TYR:CD1   | 10:J:10:GLY:HA2   | 2.50                     | 0.46              |
| 3:C:60:ALA:O     | 3:C:61:ALA:CB     | 2.61                     | 0.46              |
| 5:E:43:LEU:N     | 5:E:136:MET:HE2   | 2.31                     | 0.46              |
| 7:G:54:THR:O     | 7:G:56:GLN:N      | 2.48                     | 0.46              |
| 7:G:120:ILE:HG22 | 7:G:124:LEU:CD1   | 2.46                     | 0.46              |
| 12:L:33:ARG:HD2  | 12:L:33:ARG:HA    | 1.78                     | 0.46              |
| 12:L:93:LEU:O    | 12:L:96:VAL:HG23  | 2.15                     | 0.46              |
| 1:A:287:U:C2'    | 1:A:288:A:H5'     | 2.46                     | 0.46              |
| 1:A:1202:G:C2    | 14:N:42:ILE:HG21  | 2.51                     | 0.46              |
| 1:A:1318:A:O2'   | 19:S:37:ARG:HB2   | 2.16                     | 0.46              |
| 1:A:1339:A:H2'   | 1:A:1340:A:O4'    | 2.16                     | 0.46              |
| 1:A:1477:C:H2'   | 1:A:1478:C:C6     | 2.49                     | 0.46              |
| 3:C:26:LYS:HB3   | 3:C:26:LYS:NZ     | 2.30                     | 0.46              |
| 5:E:91:LEU:HD23  | 5:E:120:THR:HG22  | 1.98                     | 0.46              |
| 6:F:3:ARG:CG     | 6:F:3:ARG:NH1     | 2.78                     | 0.46              |
| 13:M:31:LYS:O    | 13:M:35:GLU:HB2   | 2.16                     | 0.46              |
| 23:Y:29:U:H3     | 23:Y:41:A:H61     | 1.62                     | 0.46              |
| 1:A:382:A:H2'    | 1:A:383:A:H8      | 1.78                     | 0.46              |
| 1:A:475:G:O2'    | 1:A:476:G:H5'     | 2.16                     | 0.46              |
| 1:A:627:G:H2'    | 1:A:628:G:H8      | 1.80                     | 0.46              |
| 1:A:951:G:O6     | 13:M:105:THR:HG21 | 2.14                     | 0.46              |
| 1:A:1020:U:H2'   | 1:A:1021:G:H8     | 1.80                     | 0.46              |
| 2:B:159:PRO:HG3  | 2:B:162:ILE:CD1   | 2.46                     | 0.46              |
| 2:B:185:ILE:HA   | 2:B:199:TYR:O     | 2.15                     | 0.46              |
| 4:D:28:SER:C     | 4:D:30:LYS:N      | 2.72                     | 0.46              |
| 4:D:196:LEU:HD23 | 4:D:197:PRO:HD2   | 1.98                     | 0.46              |
| 7:G:17:VAL:HG12  | 7:G:18:TYR:CD1    | 2.50                     | 0.46              |
| 12:L:55:VAL:CG1  | 12:L:56:ALA:H     | 2.25                     | 0.46              |
| 12:L:55:VAL:CG1  | 12:L:56:ALA:N     | 2.78                     | 0.46              |
| 12:L:93:LEU:HB2  | 12:L:96:VAL:HG21  | 1.97                     | 0.46              |
| 13:M:120:LYS:CE  | 13:M:122:LYS:HB3  | 2.45                     | 0.46              |
| 20:T:50:GLU:H    | 20:T:99:LEU:HD12  | 1.80                     | 0.46              |
| 20:T:69:GLY:C    | 20:T:73:HIS:CD2   | 2.94                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:194:C:OP1    | 20:T:61:SER:OG    | 2.33                     | 0.46              |
| 1:A:267:C:P      | 17:Q:67:LYS:HB2   | 2.56                     | 0.46              |
| 1:A:1288:A:H2'   | 1:A:1289:A:C8     | 2.51                     | 0.46              |
| 3:C:23:TYR:CG    | 3:C:24:ALA:N      | 2.84                     | 0.46              |
| 3:C:60:ALA:HB3   | 3:C:63:ASN:HD22   | 1.80                     | 0.46              |
| 6:F:3:ARG:HD3    | 6:F:64:GLN:NE2    | 2.30                     | 0.46              |
| 9:I:23:ASN:C     | 9:I:23:ASN:ND2    | 2.73                     | 0.46              |
| 12:L:53:ARG:HG2  | 12:L:93:LEU:HD11  | 1.98                     | 0.46              |
| 12:L:83:VAL:HG22 | 12:L:100:ILE:HG23 | 1.98                     | 0.46              |
| 13:M:34:LEU:HD13 | 13:M:41:PRO:HA    | 1.98                     | 0.46              |
| 14:N:23:ARG:NH1  | 14:N:28:GLY:O     | 2.48                     | 0.46              |
| 15:O:39:LEU:HD11 | 15:O:56:LEU:HB2   | 1.96                     | 0.46              |
| 1:A:222:U:H2'    | 1:A:223:U:C6      | 2.50                     | 0.46              |
| 1:A:376:G:OP2    | 16:P:67:THR:HG21  | 2.16                     | 0.46              |
| 1:A:382:A:C2     | 1:A:383:A:C4      | 3.04                     | 0.46              |
| 1:A:528:C:H5'    | 1:A:535:A:C6      | 2.51                     | 0.46              |
| 1:A:1472:U:H2'   | 1:A:1473:A:H8     | 1.81                     | 0.46              |
| 2:B:223:ILE:C    | 2:B:225:ALA:N     | 2.74                     | 0.46              |
| 4:D:63:LYS:HD2   | 4:D:198:VAL:HG22  | 1.98                     | 0.46              |
| 4:D:119:GLN:NE2  | 4:D:123:HIS:NE2   | 2.60                     | 0.46              |
| 6:F:1:MET:HE3    | 6:F:66:GLU:HG2    | 1.97                     | 0.46              |
| 9:I:10:ARG:HG2   | 9:I:75:ASP:HB2    | 1.96                     | 0.46              |
| 10:J:32:ALA:N    | 10:J:78:ASN:HD21  | 2.11                     | 0.46              |
| 15:O:64:ARG:NH1  | 15:O:64:ARG:HB3   | 2.30                     | 0.46              |
| 1:A:66:G:H4'     | 1:A:173:U:C5      | 2.51                     | 0.46              |
| 2:B:50:GLU:HB3   | 2:B:200:ILE:O     | 2.16                     | 0.46              |
| 3:C:91:LEU:CD2   | 3:C:99:VAL:HG22   | 2.33                     | 0.46              |
| 3:C:155:GLY:CA   | 3:C:196:LEU:HD13  | 2.45                     | 0.46              |
| 5:E:20:GLN:NE2   | 5:E:21:ALA:O      | 2.49                     | 0.46              |
| 9:I:43:ALA:O     | 9:I:44:VAL:C      | 2.59                     | 0.46              |
| 10:J:9:ARG:HG3   | 10:J:9:ARG:O      | 2.16                     | 0.46              |
| 13:M:23:TYR:C    | 13:M:25:ILE:H     | 2.24                     | 0.46              |
| 14:N:7:ILE:O     | 14:N:7:ILE:HG22   | 2.15                     | 0.46              |
| 16:P:43:LYS:HA   | 16:P:48:TRP:CB    | 2.45                     | 0.46              |
| 17:Q:98:LEU:O    | 17:Q:99:SER:O     | 2.33                     | 0.46              |
| 19:S:15:LEU:O    | 19:S:16:LEU:C     | 2.59                     | 0.46              |
| 1:A:41:G:H2'     | 1:A:42:G:C8       | 2.51                     | 0.45              |
| 1:A:46:G:O2'     | 1:A:365:U:H1'     | 2.15                     | 0.45              |
| 1:A:630:G:H5'    | 1:A:631:G:OP2     | 2.16                     | 0.45              |
| 1:A:1010:G:O2'   | 1:A:1011:G:H5'    | 2.16                     | 0.45              |
| 1:A:1055:A:O2'   | 3:C:156:ARG:HD3   | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1399:C:C2    | 1:A:1502:A:N6    | 2.84                     | 0.45              |
| 2:B:188:ALA:CB   | 2:B:200:ILE:HD11 | 2.46                     | 0.45              |
| 3:C:7:PRO:HG2    | 3:C:184:TYR:HB2  | 1.98                     | 0.45              |
| 8:H:10:LEU:HD22  | 8:H:83:ILE:HD11  | 1.97                     | 0.45              |
| 10:J:16:LEU:CD2  | 10:J:94:VAL:HG13 | 2.46                     | 0.45              |
| 10:J:64:GLU:CG   | 14:N:59:ALA:HB2  | 2.46                     | 0.45              |
| 13:M:49:THR:HB   | 13:M:52:GLU:HG3  | 1.97                     | 0.45              |
| 15:O:8:LYS:O     | 15:O:11:VAL:HG13 | 2.15                     | 0.45              |
| 20:T:69:GLY:O    | 20:T:73:HIS:CD2  | 2.69                     | 0.45              |
| 1:A:509:A:C8     | 1:A:509:A:H3'    | 2.51                     | 0.45              |
| 1:A:1038:C:H2'   | 1:A:1039:C:H6    | 1.81                     | 0.45              |
| 1:A:1349:A:OP2   | 9:I:118:LYS:NZ   | 2.48                     | 0.45              |
| 2:B:74:LYS:HZ2   | 2:B:206:ASP:HB2  | 1.80                     | 0.45              |
| 2:B:193:ASP:HB3  | 2:B:196:LEU:HD13 | 1.98                     | 0.45              |
| 3:C:8:ILE:O      | 3:C:9:GLY:C      | 2.59                     | 0.45              |
| 3:C:47:LEU:N     | 3:C:47:LEU:CD1   | 2.78                     | 0.45              |
| 3:C:48:TYR:HE1   | 3:C:118:GLN:HE21 | 1.61                     | 0.45              |
| 3:C:143:GLU:C    | 3:C:145:GLY:H    | 2.24                     | 0.45              |
| 7:G:89:MET:HE3   | 7:G:155:ARG:O    | 2.16                     | 0.45              |
| 10:J:16:LEU:HB3  | 10:J:70:ARG:CG   | 2.46                     | 0.45              |
| 16:P:40:ASP:HB3  | 16:P:48:TRP:CB   | 2.45                     | 0.45              |
| 17:Q:3:LYS:HB3   | 17:Q:61:GLU:HB3  | 1.98                     | 0.45              |
| 18:R:16:PRO:HB2  | 18:R:18:ARG:NE   | 2.26                     | 0.45              |
| 18:R:44:LEU:HD11 | 18:R:79:LEU:HD22 | 1.97                     | 0.45              |
| 19:S:80:TYR:CG   | 19:S:81:ARG:N    | 2.84                     | 0.45              |
| 1:A:204:U:O2     | 1:A:204:U:H2'    | 2.16                     | 0.45              |
| 1:A:216:G:H1'    | 1:A:217:C:C6     | 2.51                     | 0.45              |
| 1:A:542:G:H5'    | 4:D:41:GLY:HA3   | 1.99                     | 0.45              |
| 1:A:920:U:H2'    | 1:A:921:U:C6     | 2.51                     | 0.45              |
| 1:A:1054:C:C5    | 1:A:1196:U:C5    | 3.01                     | 0.45              |
| 1:A:1315:U:H2'   | 1:A:1316:G:O4'   | 2.15                     | 0.45              |
| 2:B:24:TRP:CD1   | 2:B:24:TRP:H     | 2.34                     | 0.45              |
| 3:C:102:ASN:N    | 3:C:102:ASN:ND2  | 2.63                     | 0.45              |
| 4:D:68:TYR:N     | 4:D:68:TYR:CD1   | 2.84                     | 0.45              |
| 10:J:57:LYS:CE   | 10:J:60:ARG:NH2  | 2.79                     | 0.45              |
| 11:K:33:THR:HB   | 11:K:38:ASN:C    | 2.42                     | 0.45              |
| 13:M:19:LEU:HD11 | 13:M:34:LEU:HD21 | 1.97                     | 0.45              |
| 13:M:96:LEU:C    | 13:M:110:ARG:HG2 | 2.41                     | 0.45              |
| 16:P:43:LYS:CG   | 16:P:48:TRP:CD2  | 2.95                     | 0.45              |
| 16:P:56:ALA:O    | 16:P:57:ARG:C    | 2.59                     | 0.45              |
| 16:P:67:THR:CG2  | 16:P:68:ASP:N    | 2.78                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 20:T:67:ALA:O    | 20:T:73:HIS:ND1  | 2.49                     | 0.45              |
| 1:A:103:C:P      | 20:T:17:ARG:NH1  | 2.90                     | 0.45              |
| 1:A:448:A:H2'    | 1:A:449:C:C6     | 2.52                     | 0.45              |
| 1:A:947:G:H2'    | 1:A:948:C:O4'    | 2.17                     | 0.45              |
| 1:A:1247:U:O2'   | 1:A:1248:A:H5'   | 2.17                     | 0.45              |
| 1:A:1407:C:O2'   | 1:A:1408:A:H5'   | 2.16                     | 0.45              |
| 3:C:147:LYS:HE3  | 3:C:203:PHE:CE2  | 2.51                     | 0.45              |
| 4:D:101:LEU:O    | 4:D:102:ASP:C    | 2.59                     | 0.45              |
| 4:D:194:LEU:HD22 | 4:D:194:LEU:N    | 2.32                     | 0.45              |
| 9:I:4:TYR:CE1    | 9:I:88:TYR:HA    | 2.51                     | 0.45              |
| 11:K:34:ASP:OD2  | 11:K:38:ASN:HB2  | 2.17                     | 0.45              |
| 12:L:126:LYS:HD2 | 12:L:126:LYS:O   | 2.17                     | 0.45              |
| 15:O:14:GLU:HG3  | 15:O:15:PHE:CD1  | 2.51                     | 0.45              |
| 1:A:149:A:H2'    | 1:A:150:C:C6     | 2.52                     | 0.45              |
| 1:A:165:C:H2'    | 1:A:166:G:H8     | 1.82                     | 0.45              |
| 1:A:642:A:C5     | 8:H:115:SER:HA   | 2.52                     | 0.45              |
| 2:B:84:GLU:HB3   | 2:B:219:VAL:CG2  | 2.34                     | 0.45              |
| 2:B:167:PRO:O    | 2:B:171:ALA:N    | 2.50                     | 0.45              |
| 4:D:5:ILE:O      | 4:D:5:ILE:HG22   | 2.15                     | 0.45              |
| 5:E:13:ILE:HA    | 5:E:29:GLY:O     | 2.17                     | 0.45              |
| 9:I:126:SER:O    | 9:I:128:ARG:N    | 2.50                     | 0.45              |
| 10:J:19:SER:HA   | 10:J:22:LYS:HZ3  | 1.82                     | 0.45              |
| 10:J:23:ILE:O    | 10:J:23:ILE:HG22 | 2.17                     | 0.45              |
| 10:J:42:THR:CG2  | 10:J:43:ARG:N    | 2.79                     | 0.45              |
| 11:K:40:ILE:HG22 | 11:K:41:THR:HG23 | 1.97                     | 0.45              |
| 11:K:78:GLN:O    | 11:K:103:LEU:HA  | 2.16                     | 0.45              |
| 15:O:39:LEU:HD12 | 15:O:56:LEU:CD1  | 2.46                     | 0.45              |
| 16:P:14:ASN:OD1  | 16:P:16:HIS:HE1  | 2.00                     | 0.45              |
| 19:S:17:GLU:O    | 19:S:21:GLU:HG3  | 2.17                     | 0.45              |
| 20:T:22:ARG:HG2  | 20:T:22:ARG:NH1  | 2.32                     | 0.45              |
| 21:U:6:ARG:HE    | 21:U:15:ARG:NH2  | 2.15                     | 0.45              |
| 1:A:200:G:H2'    | 1:A:201:C:O4'    | 2.17                     | 0.45              |
| 1:A:390:C:O3'    | 16:P:28:ARG:NH2  | 2.48                     | 0.45              |
| 1:A:650:G:O2'    | 1:A:651:C:H5'    | 2.17                     | 0.45              |
| 1:A:1019:C:O2'   | 1:A:1020:U:H5'   | 2.16                     | 0.45              |
| 1:A:1091:U:O2    | 1:A:1093:A:C8    | 2.69                     | 0.45              |
| 1:A:1279:A:O2'   | 1:A:1282:C:N4    | 2.50                     | 0.45              |
| 1:A:1289:A:H2'   | 1:A:1290:G:H5'   | 1.99                     | 0.45              |
| 1:A:1301:U:O2'   | 1:A:1302:U:OP1   | 2.34                     | 0.45              |
| 1:A:1372:U:H2'   | 1:A:1373:G:O4'   | 2.16                     | 0.45              |
| 2:B:42:ILE:H     | 2:B:42:ILE:CD1   | 2.30                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:132:LYS:C    | 2:B:134:GLU:N    | 2.74                     | 0.45              |
| 3:C:76:VAL:O     | 3:C:83:ARG:HG3   | 2.17                     | 0.45              |
| 4:D:26:CYS:HA    | 4:D:31:CYS:CB    | 2.45                     | 0.45              |
| 7:G:6:ARG:HB3    | 7:G:6:ARG:HH11   | 1.82                     | 0.45              |
| 12:L:119:LYS:O   | 12:L:120:TYR:CB  | 2.63                     | 0.45              |
| 15:O:70:LEU:HD12 | 15:O:78:TYR:CB   | 2.46                     | 0.45              |
| 1:A:270:A:H2'    | 1:A:271:C:C6     | 2.52                     | 0.45              |
| 1:A:1036:G:O2'   | 1:A:1037:C:H5'   | 2.16                     | 0.45              |
| 1:A:1287:A:H2'   | 1:A:1288:A:C8    | 2.52                     | 0.45              |
| 2:B:73:THR:O     | 2:B:75:LYS:N     | 2.50                     | 0.45              |
| 3:C:8:ILE:O      | 3:C:11:ARG:N     | 2.43                     | 0.45              |
| 3:C:193:TYR:HE1  | 3:C:196:LEU:HD21 | 1.81                     | 0.45              |
| 4:D:199:ASN:HD22 | 4:D:199:ASN:C    | 2.23                     | 0.45              |
| 7:G:136:LYS:O    | 7:G:137:LYS:C    | 2.60                     | 0.45              |
| 7:G:138:LYS:HD3  | 7:G:138:LYS:C    | 2.42                     | 0.45              |
| 8:H:122:ARG:HH11 | 8:H:122:ARG:CB   | 2.26                     | 0.45              |
| 9:I:114:TYR:CE1  | 10:J:59:SER:O    | 2.69                     | 0.45              |
| 10:J:16:LEU:HD23 | 10:J:94:VAL:HG22 | 1.99                     | 0.45              |
| 10:J:81:THR:HG22 | 10:J:85:LEU:CD1  | 2.47                     | 0.45              |
| 12:L:78:GLN:HE21 | 12:L:78:GLN:HB2  | 1.57                     | 0.45              |
| 12:L:113:ARG:NH1 | 12:L:116:SER:N   | 2.64                     | 0.45              |
| 15:O:3:ILE:HD13  | 15:O:34:LEU:CD1  | 2.42                     | 0.45              |
| 15:O:24:SER:OG   | 15:O:27:VAL:HG23 | 2.16                     | 0.45              |
| 16:P:59:TRP:HB3  | 16:P:64:ALA:HB2  | 1.98                     | 0.45              |
| 1:A:375:U:O3'    | 16:P:6:LEU:HB2   | 2.16                     | 0.45              |
| 1:A:429:U:H1'    | 1:A:430:A:H5''   | 1.99                     | 0.45              |
| 1:A:928:G:O2'    | 1:A:1533:C:OP1   | 2.32                     | 0.45              |
| 1:A:1320:C:O2    | 19:S:36:ARG:NH1  | 2.50                     | 0.45              |
| 4:D:121:VAL:HG12 | 4:D:134:ASP:C    | 2.42                     | 0.45              |
| 5:E:78:HIS:O     | 5:E:93:PRO:HD3   | 2.16                     | 0.45              |
| 7:G:115:ARG:O    | 7:G:116:ALA:C    | 2.59                     | 0.45              |
| 8:H:100:ILE:CG2  | 8:H:112:LEU:HD11 | 2.45                     | 0.45              |
| 11:K:58:PRO:O    | 11:K:61:ALA:HB3  | 2.17                     | 0.45              |
| 15:O:88:ARG:HB3  | 15:O:89:GLY:H    | 1.56                     | 0.45              |
| 16:P:40:ASP:O    | 16:P:48:TRP:HB2  | 2.17                     | 0.45              |
| 1:A:189(A):C:H2' | 1:A:189(B):C:C6  | 2.52                     | 0.45              |
| 1:A:806:C:O2'    | 1:A:807:A:H5'    | 2.16                     | 0.45              |
| 1:A:1135:U:H4'   | 1:A:1136:U:C5    | 2.52                     | 0.45              |
| 2:B:27:LYS:C     | 2:B:29:ALA:H     | 2.25                     | 0.45              |
| 2:B:124:SER:HB2  | 2:B:125:PRO:HD2  | 1.98                     | 0.45              |
| 9:I:27:THR:HG23  | 9:I:62:TYR:HA    | 1.99                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 9:I:111:ARG:HG3  | 9:I:111:ARG:NH1   | 2.31                     | 0.45              |
| 11:K:40:ILE:HD12 | 11:K:77:MET:CE    | 2.47                     | 0.45              |
| 13:M:5:ALA:O     | 13:M:6:GLY:C      | 2.59                     | 0.45              |
| 14:N:8:GLU:O     | 14:N:10:ALA:N     | 2.50                     | 0.45              |
| 19:S:42:PRO:C    | 19:S:44:MET:H     | 2.25                     | 0.45              |
| 1:A:97:G:O2'     | 1:A:98:G:H5'      | 2.17                     | 0.45              |
| 1:A:188:C:O2'    | 1:A:189:G:H5'     | 2.17                     | 0.45              |
| 1:A:547:A:H4'    | 1:A:548:G:O5'     | 2.17                     | 0.45              |
| 1:A:1226:C:H6    | 13:M:103:THR:OG1  | 1.99                     | 0.45              |
| 4:D:203:VAL:O    | 4:D:204:ILE:C     | 2.58                     | 0.45              |
| 5:E:72:GLN:NE2   | 5:E:77:PRO:HB3    | 2.31                     | 0.45              |
| 15:O:56:LEU:HA   | 15:O:59:MET:CE    | 2.38                     | 0.45              |
| 19:S:36:ARG:NH1  | 19:S:72:GLY:CA    | 2.80                     | 0.45              |
| 20:T:53:LEU:HB2  | 20:T:100:ILE:HG21 | 1.96                     | 0.45              |
| 21:U:2:GLY:O     | 21:U:4:GLY:N      | 2.50                     | 0.45              |
| 1:A:88:A:H2'     | 1:A:89:C:O4'      | 2.17                     | 0.44              |
| 1:A:131:C:H2'    | 1:A:132:C:C6      | 2.52                     | 0.44              |
| 1:A:343:U:H2'    | 1:A:345:C:N4      | 2.32                     | 0.44              |
| 1:A:527:G:O2'    | 1:A:535:A:N1      | 2.49                     | 0.44              |
| 1:A:559:A:P      | 5:E:126:ARG:HH22  | 2.40                     | 0.44              |
| 1:A:1181:G:O2'   | 1:A:1182:G:O5'    | 2.33                     | 0.44              |
| 1:A:1211:U:H5'   | 1:A:1212:U:P      | 2.57                     | 0.44              |
| 3:C:134:ILE:HG23 | 3:C:151:VAL:HB    | 1.99                     | 0.44              |
| 3:C:150:LYS:HG3  | 3:C:169:ALA:HB2   | 1.99                     | 0.44              |
| 4:D:122:ARG:HA   | 4:D:122:ARG:NE    | 2.30                     | 0.44              |
| 6:F:67:MET:HB2   | 6:F:68:PRO:CD     | 2.40                     | 0.44              |
| 6:F:101:ALA:HB2  | 18:R:28:GLU:CG    | 2.44                     | 0.44              |
| 7:G:18:TYR:CD2   | 7:G:59:LEU:HB2    | 2.52                     | 0.44              |
| 7:G:26:PHE:CE2   | 7:G:30:ILE:HD11   | 2.52                     | 0.44              |
| 14:N:22:THR:HG23 | 14:N:33:VAL:HG23  | 1.99                     | 0.44              |
| 1:A:6:G:H4'      | 1:A:298:A:H4'     | 1.99                     | 0.44              |
| 1:A:279:A:H4'    | 1:A:281:G:C8      | 2.52                     | 0.44              |
| 1:A:1043:C:O2'   | 1:A:1044:A:H5'    | 2.16                     | 0.44              |
| 1:A:1053:G:C5'   | 1:A:1054:C:H5'    | 2.47                     | 0.44              |
| 2:B:72:GLY:HA2   | 2:B:165:VAL:CG2   | 2.47                     | 0.44              |
| 2:B:107:THR:O    | 2:B:108:ILE:C     | 2.57                     | 0.44              |
| 3:C:68:VAL:HG12  | 3:C:70:VAL:HG23   | 1.99                     | 0.44              |
| 5:E:135:THR:O    | 5:E:138:ALA:HB3   | 2.17                     | 0.44              |
| 1:A:243:A:C2     | 1:A:246:A:C8      | 3.05                     | 0.44              |
| 1:A:427:U:OP1    | 4:D:13:ARG:NH2    | 2.50                     | 0.44              |
| 1:A:1047:G:O2'   | 1:A:1048:G:H5''   | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1347:G:O2'   | 1:A:1348:U:OP2   | 2.34                     | 0.44              |
| 2:B:233:SER:OG   | 2:B:234:PRO:HD2  | 2.16                     | 0.44              |
| 4:D:199:ASN:C    | 4:D:199:ASN:ND2  | 2.74                     | 0.44              |
| 8:H:33:GLU:HG3   | 8:H:48:TYR:CE1   | 2.52                     | 0.44              |
| 10:J:76:ASN:C    | 10:J:78:ASN:N    | 2.73                     | 0.44              |
| 12:L:89:ARG:CB   | 12:L:97:ARG:HA   | 2.48                     | 0.44              |
| 12:L:115:LYS:O   | 12:L:117:ARG:N   | 2.50                     | 0.44              |
| 15:O:87:ILE:CG2  | 15:O:88:ARG:N    | 2.70                     | 0.44              |
| 17:Q:95:TYR:C    | 17:Q:97:SER:N    | 2.73                     | 0.44              |
| 20:T:10:LEU:HD11 | 20:T:12:ALA:HB3  | 1.99                     | 0.44              |
| 1:A:418:C:H2'    | 1:A:419:C:C6     | 2.52                     | 0.44              |
| 1:A:1053:G:C3'   | 1:A:1054:C:C5'   | 2.95                     | 0.44              |
| 1:A:1154:G:O2'   | 1:A:1155:G:H5'   | 2.18                     | 0.44              |
| 1:A:1333:A:H2'   | 1:A:1334:G:O4'   | 2.17                     | 0.44              |
| 1:A:1359:C:OP1   | 14:N:22:THR:CG2  | 2.65                     | 0.44              |
| 2:B:117:GLU:C    | 2:B:117:GLU:CD   | 2.85                     | 0.44              |
| 3:C:78:GLY:HA3   | 3:C:83:ARG:CB    | 2.48                     | 0.44              |
| 4:D:49:ARG:HH11  | 4:D:49:ARG:HG3   | 1.82                     | 0.44              |
| 6:F:15:ASP:O     | 6:F:17:SER:N     | 2.51                     | 0.44              |
| 7:G:15:ASP:HB2   | 7:G:20:ASP:O     | 2.17                     | 0.44              |
| 12:L:54:LYS:N    | 12:L:54:LYS:CD   | 2.79                     | 0.44              |
| 14:N:36:PHE:O    | 14:N:36:PHE:CD1  | 2.70                     | 0.44              |
| 1:A:50:A:N6      | 1:A:361:G:H4'    | 2.32                     | 0.44              |
| 1:A:106:C:O2     | 1:A:379:C:H4'    | 2.18                     | 0.44              |
| 1:A:268:C:H2'    | 1:A:269:C:C6     | 2.53                     | 0.44              |
| 1:A:342:C:C2'    | 1:A:343:U:H5'    | 2.48                     | 0.44              |
| 1:A:417:C:H2'    | 1:A:418:C:C6     | 2.53                     | 0.44              |
| 1:A:454:C:H2'    | 1:A:455:C:H5'    | 1.99                     | 0.44              |
| 1:A:545:C:O2'    | 1:A:546:G:H5'    | 2.17                     | 0.44              |
| 1:A:1163:C:O2'   | 1:A:1164:G:H5'   | 2.18                     | 0.44              |
| 1:A:1190:G:C2'   | 1:A:1191:A:OP2   | 2.66                     | 0.44              |
| 1:A:1373:G:H5''  | 7:G:36:LYS:HB2   | 2.00                     | 0.44              |
| 1:A:1475:G:H2'   | 1:A:1476:G:H8    | 1.81                     | 0.44              |
| 1:A:1503:A:HO2'  | 1:A:1504:G:P     | 2.40                     | 0.44              |
| 2:B:7:VAL:O      | 2:B:8:LYS:HG3    | 2.18                     | 0.44              |
| 2:B:90:MET:HA    | 2:B:91:PRO:HD3   | 1.77                     | 0.44              |
| 3:C:35:GLU:OE2   | 3:C:59:ARG:NH2   | 2.49                     | 0.44              |
| 5:E:36:ASP:OD2   | 5:E:40:ARG:HD3   | 2.18                     | 0.44              |
| 5:E:76:ILE:HG13  | 5:E:142:LEU:HD13 | 1.98                     | 0.44              |
| 7:G:15:ASP:O     | 7:G:19:GLY:HA2   | 2.18                     | 0.44              |
| 7:G:58:PRO:HG2   | 7:G:59:LEU:H     | 1.83                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:I:100:GLY:C    | 9:I:102:LEU:N    | 2.75                     | 0.44              |
| 11:K:24:SER:O    | 11:K:88:GLY:HA3  | 2.18                     | 0.44              |
| 16:P:57:ARG:NH1  | 16:P:57:ARG:CG   | 2.71                     | 0.44              |
| 1:A:103:C:P      | 20:T:17:ARG:HH11 | 2.41                     | 0.44              |
| 1:A:191:G:H1'    | 20:T:105:SER:HA  | 1.99                     | 0.44              |
| 1:A:725:G:H2'    | 1:A:726:C:H5''   | 1.88                     | 0.44              |
| 1:A:1161:C:H2'   | 1:A:1162:C:H6    | 1.81                     | 0.44              |
| 1:A:1416:G:C2'   | 1:A:1417:G:H5'   | 2.47                     | 0.44              |
| 2:B:213:LEU:O    | 2:B:217:ARG:HG2  | 2.18                     | 0.44              |
| 2:B:225:ALA:O    | 2:B:226:ARG:HG3  | 2.17                     | 0.44              |
| 3:C:187:ALA:HB3  | 3:C:198:VAL:HB   | 1.99                     | 0.44              |
| 5:E:51:VAL:CB    | 5:E:52:PRO:HD3   | 2.35                     | 0.44              |
| 7:G:17:VAL:HG12  | 7:G:17:VAL:O     | 2.17                     | 0.44              |
| 8:H:118:VAL:O    | 8:H:119:LEU:HD23 | 2.18                     | 0.44              |
| 10:J:75:ILE:O    | 10:J:76:ASN:ND2  | 2.51                     | 0.44              |
| 13:M:88:ARG:HG2  | 13:M:98:VAL:CG1  | 2.47                     | 0.44              |
| 15:O:72:ARG:HG2  | 15:O:72:ARG:O    | 2.18                     | 0.44              |
| 1:A:314:C:O2'    | 1:A:315:A:H5'    | 2.17                     | 0.44              |
| 1:A:433:C:O2'    | 1:A:434:U:H5'    | 2.18                     | 0.44              |
| 1:A:941:G:C2'    | 1:A:942:G:O5'    | 2.66                     | 0.44              |
| 1:A:1191:A:OP1   | 3:C:4:LYS:HE2    | 2.18                     | 0.44              |
| 1:A:1286:A:H2'   | 1:A:1287:A:H4'   | 1.99                     | 0.44              |
| 1:A:1329:A:C2'   | 1:A:1330:U:H5'   | 2.46                     | 0.44              |
| 2:B:10:LEU:HG    | 2:B:48:MET:CE    | 2.48                     | 0.44              |
| 5:E:26:PHE:CD1   | 5:E:26:PHE:N     | 2.86                     | 0.44              |
| 6:F:19:LEU:HD23  | 6:F:19:LEU:O     | 2.18                     | 0.44              |
| 8:H:104:ARG:O    | 8:H:106:GLY:N    | 2.51                     | 0.44              |
| 8:H:118:VAL:C    | 8:H:119:LEU:HD23 | 2.43                     | 0.44              |
| 14:N:26:ARG:HH21 | 14:N:47:LEU:CD2  | 2.30                     | 0.44              |
| 15:O:4:THR:OG1   | 15:O:6:GLU:HG2   | 2.16                     | 0.44              |
| 17:Q:99:SER:C    | 17:Q:101:ARG:N   | 2.76                     | 0.44              |
| 19:S:11:VAL:HG13 | 19:S:38:SER:HB2  | 1.99                     | 0.44              |
| 20:T:10:LEU:O    | 20:T:12:ALA:N    | 2.50                     | 0.44              |
| 1:A:197:A:N1     | 1:A:220:G:O2'    | 2.49                     | 0.44              |
| 1:A:714:G:H2'    | 1:A:715:A:C8     | 2.53                     | 0.44              |
| 1:A:877:C:O2'    | 1:A:878:G:H5'    | 2.17                     | 0.44              |
| 1:A:978:A:O2'    | 1:A:1322:C:N3    | 2.48                     | 0.44              |
| 1:A:1251:A:H5'   | 9:I:12:GLU:CG    | 2.47                     | 0.44              |
| 1:A:1401:G:C2    | 1:A:1402:C:H1'   | 2.53                     | 0.44              |
| 2:B:124:SER:C    | 2:B:126:GLU:H    | 2.25                     | 0.44              |
| 2:B:224:GLN:HG3  | 2:B:229:VAL:HG22 | 1.99                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:193:TYR:CE1  | 3:C:196:LEU:HD21 | 2.53                     | 0.44              |
| 10:J:81:THR:C    | 10:J:83:GLU:N    | 2.75                     | 0.44              |
| 11:K:24:SER:C    | 11:K:88:GLY:HA3  | 2.42                     | 0.44              |
| 12:L:50:SER:O    | 12:L:51:ALA:HB2  | 2.18                     | 0.44              |
| 13:M:21:TYR:HD1  | 13:M:21:TYR:H    | 1.66                     | 0.44              |
| 13:M:22:ILE:HB   | 13:M:25:ILE:HB   | 1.99                     | 0.44              |
| 13:M:35:GLU:C    | 13:M:37:THR:H    | 2.24                     | 0.44              |
| 1:A:1299:A:C8    | 1:A:1301:U:H1'   | 2.52                     | 0.44              |
| 1:A:1373:G:H5''  | 7:G:36:LYS:CB    | 2.48                     | 0.44              |
| 3:C:76:VAL:O     | 3:C:83:ARG:CG    | 2.66                     | 0.44              |
| 7:G:44:TYR:O     | 7:G:47:CYS:HB2   | 2.17                     | 0.44              |
| 7:G:79:ARG:HA    | 7:G:84:ASN:HA    | 1.99                     | 0.44              |
| 9:I:111:ARG:HD3  | 9:I:112:LYS:O    | 2.18                     | 0.44              |
| 12:L:60:LEU:HD23 | 12:L:64:TYR:CB   | 2.48                     | 0.44              |
| 15:O:76:GLU:O    | 15:O:77:ARG:C    | 2.61                     | 0.44              |
| 19:S:44:MET:CB   | 19:S:62:ILE:HD13 | 2.48                     | 0.44              |
| 1:A:1054:C:H5    | 1:A:1196:U:C4    | 2.35                     | 0.43              |
| 1:A:1182:G:HO2'  | 1:A:1183:A:P     | 2.36                     | 0.43              |
| 2:B:68:ILE:HB    | 2:B:90:MET:HE3   | 2.00                     | 0.43              |
| 5:E:144:THR:HG22 | 5:E:146:ALA:HB3  | 2.00                     | 0.43              |
| 6:F:1:MET:HE1    | 6:F:67:MET:HA    | 2.00                     | 0.43              |
| 6:F:82:ARG:HB2   | 6:F:85:VAL:CG2   | 2.48                     | 0.43              |
| 7:G:65:ALA:O     | 7:G:69:VAL:HG23  | 2.17                     | 0.43              |
| 7:G:95:ARG:O     | 7:G:96:GLN:C     | 2.61                     | 0.43              |
| 10:J:7:LYS:HZ2   | 10:J:71:LEU:HD23 | 1.83                     | 0.43              |
| 15:O:65:ARG:NH1  | 15:O:65:ARG:CG   | 2.76                     | 0.43              |
| 1:A:57:G:H2'     | 1:A:58:C:C6      | 2.53                     | 0.43              |
| 1:A:251:G:H4'    | 1:A:252:U:O5'    | 2.17                     | 0.43              |
| 1:A:265:G:H2'    | 1:A:267:C:C5     | 2.53                     | 0.43              |
| 1:A:999:C:H2'    | 1:A:1000:U:C6    | 2.54                     | 0.43              |
| 1:A:1384:C:H2'   | 1:A:1385:G:C8    | 2.53                     | 0.43              |
| 1:A:1480:G:H2'   | 1:A:1481:U:H6    | 1.82                     | 0.43              |
| 2:B:24:TRP:CD1   | 2:B:24:TRP:N     | 2.85                     | 0.43              |
| 2:B:75:LYS:HD3   | 2:B:78:GLN:OE1   | 2.17                     | 0.43              |
| 3:C:134:ILE:O    | 3:C:138:VAL:HG23 | 2.17                     | 0.43              |
| 4:D:64:LEU:HD11  | 4:D:97:LEU:HD11  | 1.99                     | 0.43              |
| 8:H:65:TYR:HA    | 8:H:79:VAL:HG23  | 1.99                     | 0.43              |
| 8:H:104:ARG:O    | 8:H:107:LEU:N    | 2.49                     | 0.43              |
| 11:K:76:GLY:O    | 11:K:77:MET:C    | 2.61                     | 0.43              |
| 12:L:40:VAL:HG11 | 12:L:77:LEU:O    | 2.18                     | 0.43              |
| 13:M:57:ARG:HG2  | 13:M:61:GLU:CG   | 2.44                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 13:M:81:LEU:HA   | 13:M:81:LEU:HD23 | 1.79                     | 0.43              |
| 13:M:81:LEU:HD22 | 13:M:86:CYS:SG   | 2.58                     | 0.43              |
| 18:R:86:VAL:HG12 | 18:R:87:ARG:N    | 2.33                     | 0.43              |
| 20:T:10:LEU:O    | 20:T:13:LEU:HG   | 2.18                     | 0.43              |
| 1:A:161:A:H2'    | 1:A:162:A:C8     | 2.53                     | 0.43              |
| 1:A:828:A:H5''   | 1:A:859:A:C2     | 2.53                     | 0.43              |
| 1:A:833:U:H2'    | 1:A:834:C:H6     | 1.84                     | 0.43              |
| 1:A:954:G:H2'    | 1:A:955:U:H6     | 1.82                     | 0.43              |
| 1:A:1197:G:O2'   | 1:A:1198:G:H5'   | 2.18                     | 0.43              |
| 1:A:1226:C:C4    | 13:M:104:ARG:HG3 | 2.53                     | 0.43              |
| 1:A:1475:G:H2'   | 1:A:1476:G:C8    | 2.53                     | 0.43              |
| 2:B:21:ARG:HG3   | 2:B:21:ARG:H     | 1.50                     | 0.43              |
| 2:B:178:ARG:HH21 | 2:B:196:LEU:CA   | 2.30                     | 0.43              |
| 3:C:64:VAL:O     | 3:C:99:VAL:HB    | 2.18                     | 0.43              |
| 3:C:150:LYS:HG2  | 3:C:151:VAL:N    | 2.33                     | 0.43              |
| 4:D:54:TYR:O     | 4:D:55:ALA:C     | 2.60                     | 0.43              |
| 11:K:57:THR:HG23 | 11:K:58:PRO:HD2  | 2.01                     | 0.43              |
| 13:M:3:ARG:NH1   | 13:M:7:VAL:HA    | 2.33                     | 0.43              |
| 17:Q:68:ARG:HH11 | 17:Q:68:ARG:CG   | 2.29                     | 0.43              |
| 18:R:18:ARG:HA   | 18:R:18:ARG:HD3  | 1.91                     | 0.43              |
| 18:R:59:SER:OG   | 18:R:62:GLU:HG3  | 2.18                     | 0.43              |
| 19:S:41:VAL:HB   | 19:S:42:PRO:HD2  | 1.99                     | 0.43              |
| 1:A:151:A:H2'    | 1:A:152:A:O4'    | 2.18                     | 0.43              |
| 1:A:343:U:H2'    | 1:A:345:C:C4     | 2.53                     | 0.43              |
| 1:A:1115:C:H1'   | 14:N:61:TRP:O    | 2.19                     | 0.43              |
| 2:B:21:ARG:HB2   | 2:B:22:LYS:H     | 1.61                     | 0.43              |
| 2:B:173:ALA:O    | 2:B:174:VAL:C    | 2.61                     | 0.43              |
| 3:C:157:ILE:HG21 | 3:C:164:ARG:NH2  | 2.33                     | 0.43              |
| 6:F:27:GLN:HA    | 6:F:27:GLN:NE2   | 2.33                     | 0.43              |
| 7:G:62:PHE:HA    | 7:G:124:LEU:HD22 | 2.01                     | 0.43              |
| 10:J:25:GLU:O    | 10:J:27:ALA:N    | 2.49                     | 0.43              |
| 10:J:26:ALA:HB3  | 10:J:85:LEU:HD23 | 1.99                     | 0.43              |
| 11:K:40:ILE:HD12 | 11:K:77:MET:HE1  | 1.99                     | 0.43              |
| 13:M:66:LEU:O    | 13:M:67:GLU:C    | 2.61                     | 0.43              |
| 1:A:743:U:H2'    | 1:A:744:C:H6     | 1.84                     | 0.43              |
| 1:A:860:A:H2'    | 1:A:861:G:O4'    | 2.18                     | 0.43              |
| 1:A:895:G:H2'    | 1:A:896:C:H6     | 1.83                     | 0.43              |
| 1:A:1230:C:O2'   | 1:A:1231:G:H5'   | 2.18                     | 0.43              |
| 1:A:1320:C:H2'   | 1:A:1321:C:O4'   | 2.18                     | 0.43              |
| 2:B:21:ARG:NH1   | 2:B:23:ARG:HG2   | 2.33                     | 0.43              |
| 2:B:60:ASP:CA    | 2:B:64:ARG:HH12  | 2.31                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:200:ILE:HG23 | 2:B:202:PRO:HD3   | 1.99                     | 0.43              |
| 3:C:207:VAL:CG1  | 3:C:208:ILE:N     | 2.69                     | 0.43              |
| 4:D:145:GLU:HG3  | 4:D:183:GLY:O     | 2.18                     | 0.43              |
| 5:E:131:ILE:HD13 | 5:E:131:ILE:HA    | 1.85                     | 0.43              |
| 6:F:7:ASN:HB2    | 6:F:89:MET:HB3    | 2.00                     | 0.43              |
| 12:L:38:THR:HG22 | 12:L:39:VAL:HG23  | 2.00                     | 0.43              |
| 13:M:120:LYS:HE3 | 13:M:122:LYS:C    | 2.43                     | 0.43              |
| 19:S:38:SER:OG   | 19:S:71:LEU:HD12  | 2.18                     | 0.43              |
| 1:A:369:C:O2'    | 1:A:370:C:H5'     | 2.18                     | 0.43              |
| 1:A:374:A:C6     | 1:A:375:U:C4      | 3.07                     | 0.43              |
| 1:A:710:G:O2'    | 1:A:711:G:H5'     | 2.18                     | 0.43              |
| 1:A:750:G:H1'    | 15:O:23:GLY:H     | 1.84                     | 0.43              |
| 1:A:922:G:H4'    | 5:E:20:GLN:HA     | 2.00                     | 0.43              |
| 1:A:1039:C:H2'   | 1:A:1040:U:C6     | 2.54                     | 0.43              |
| 1:A:1074:G:O3'   | 2:B:103:THR:CG2   | 2.67                     | 0.43              |
| 1:A:1137:C:H4'   | 1:A:1138:G:N1     | 2.33                     | 0.43              |
| 2:B:77:ALA:CB    | 2:B:211:ILE:HG21  | 2.49                     | 0.43              |
| 2:B:137:ARG:HH11 | 2:B:137:ARG:CB    | 2.31                     | 0.43              |
| 3:C:21:ARG:H     | 3:C:21:ARG:HG2    | 1.51                     | 0.43              |
| 4:D:15:GLU:C     | 4:D:17:VAL:H      | 2.27                     | 0.43              |
| 7:G:38:LEU:O     | 7:G:41:ARG:HB3    | 2.19                     | 0.43              |
| 12:L:55:VAL:O    | 12:L:70:ILE:HD11  | 2.19                     | 0.43              |
| 12:L:83:VAL:HG21 | 12:L:100:ILE:HD13 | 2.00                     | 0.43              |
| 17:Q:67:LYS:CA   | 17:Q:70:ARG:HH12  | 2.24                     | 0.43              |
| 17:Q:67:LYS:CA   | 17:Q:70:ARG:NH1   | 2.78                     | 0.43              |
| 1:A:91:C:H2'     | 1:A:92:C:H6       | 1.84                     | 0.43              |
| 1:A:538:G:H2'    | 1:A:539:A:H8      | 1.82                     | 0.43              |
| 1:A:848:C:O2'    | 1:A:849:C:H5'     | 2.19                     | 0.43              |
| 1:A:1066:C:O2'   | 1:A:1067:A:H5'    | 2.18                     | 0.43              |
| 1:A:1169:A:C6    | 1:A:1170:A:C6     | 3.07                     | 0.43              |
| 1:A:1230:C:H2'   | 1:A:1231:G:H8     | 1.84                     | 0.43              |
| 2:B:119:GLU:HG2  | 2:B:142:LEU:HD11  | 2.01                     | 0.43              |
| 2:B:178:ARG:HH21 | 2:B:196:LEU:HA    | 1.82                     | 0.43              |
| 3:C:25:GLY:O     | 3:C:27:LYS:N      | 2.52                     | 0.43              |
| 3:C:206:GLU:HB3  | 3:C:207:VAL:H     | 1.68                     | 0.43              |
| 5:E:143:ARG:HA   | 5:E:143:ARG:HD3   | 1.69                     | 0.43              |
| 7:G:58:PRO:O     | 7:G:59:LEU:C      | 2.61                     | 0.43              |
| 9:I:93:ARG:O     | 9:I:97:LYS:HB2    | 2.19                     | 0.43              |
| 10:J:25:GLU:C    | 10:J:27:ALA:N     | 2.76                     | 0.43              |
| 10:J:34:VAL:HG22 | 10:J:74:ILE:HG23  | 1.99                     | 0.43              |
| 14:N:7:ILE:C     | 14:N:9:LYS:H      | 2.26                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 15:O:8:LYS:O     | 15:O:11:VAL:CG1  | 2.67                     | 0.43              |
| 16:P:20:VAL:CG1  | 16:P:32:TYR:CB   | 2.96                     | 0.43              |
| 1:A:103:C:OP2    | 20:T:17:ARG:NH1  | 2.51                     | 0.43              |
| 1:A:141:A:H1'    | 1:A:182:U:O2     | 2.19                     | 0.43              |
| 1:A:411:A:H1'    | 1:A:413:G:O4'    | 2.19                     | 0.43              |
| 1:A:1029:C:O2'   | 1:A:1030:C:H5'   | 2.18                     | 0.43              |
| 1:A:1300:G:C2'   | 1:A:1301:U:OP2   | 2.66                     | 0.43              |
| 1:A:1347:G:C6    | 9:I:107:ARG:NH2  | 2.87                     | 0.43              |
| 1:A:1441:G:H4'   | 1:A:1442:G:C6    | 2.54                     | 0.43              |
| 1:A:1539:C:O5'   | 1:A:1539:C:C6    | 2.71                     | 0.43              |
| 3:C:112:SER:O    | 3:C:116:VAL:HG23 | 2.19                     | 0.43              |
| 9:I:32:ASP:O     | 9:I:33:PHE:C     | 2.62                     | 0.43              |
| 9:I:100:GLY:C    | 9:I:102:LEU:H    | 2.27                     | 0.43              |
| 10:J:42:THR:HG22 | 10:J:43:ARG:H    | 1.81                     | 0.43              |
| 17:Q:65:ILE:HD12 | 17:Q:65:ILE:N    | 2.34                     | 0.43              |
| 19:S:44:MET:O    | 19:S:45:VAL:C    | 2.62                     | 0.43              |
| 1:A:143:A:H2     | 1:A:220:G:H22    | 1.67                     | 0.43              |
| 1:A:180:U:C2'    | 1:A:181:G:H5'    | 2.49                     | 0.43              |
| 1:A:609:A:H2'    | 1:A:610:G:H5'    | 2.00                     | 0.43              |
| 1:A:939:G:H5''   | 7:G:102:ARG:HH22 | 1.82                     | 0.43              |
| 3:C:29:TYR:C     | 3:C:29:TYR:CD2   | 2.97                     | 0.43              |
| 4:D:38:TYR:CE1   | 4:D:45:GLN:HG2   | 2.54                     | 0.43              |
| 4:D:63:LYS:HD2   | 4:D:198:VAL:CG2  | 2.49                     | 0.43              |
| 5:E:144:THR:HG22 | 5:E:146:ALA:N    | 2.34                     | 0.43              |
| 11:K:33:THR:HB   | 11:K:38:ASN:O    | 2.18                     | 0.43              |
| 16:P:1:MET:O     | 16:P:24:ALA:HB2  | 2.18                     | 0.43              |
| 17:Q:3:LYS:HD3   | 17:Q:61:GLU:O    | 2.19                     | 0.43              |
| 17:Q:48:GLU:C    | 17:Q:50:LYS:N    | 2.77                     | 0.43              |
| 1:A:7:G:H21      | 5:E:121:LYS:HG2  | 1.84                     | 0.43              |
| 1:A:689:C:P      | 11:K:46:GLY:HA3  | 2.59                     | 0.43              |
| 1:A:1107:C:H2'   | 1:A:1108:G:H5'   | 2.01                     | 0.43              |
| 1:A:1190:G:OP1   | 3:C:5:ILE:HG13   | 2.19                     | 0.43              |
| 1:A:1251:A:H5''  | 9:I:12:GLU:OE2   | 2.19                     | 0.43              |
| 1:A:1272:G:O2'   | 1:A:1273:G:H5'   | 2.19                     | 0.43              |
| 1:A:1399:C:C2    | 1:A:1401:G:C5    | 3.06                     | 0.43              |
| 1:A:1497:G:O2'   | 1:A:1498:U:H5'   | 2.18                     | 0.43              |
| 1:A:1515:C:O2'   | 1:A:1516:G:H5'   | 2.18                     | 0.43              |
| 2:B:9:GLU:HG2    | 2:B:217:ARG:HH12 | 1.83                     | 0.43              |
| 3:C:34:LEU:HD13  | 3:C:34:LEU:O     | 2.19                     | 0.43              |
| 3:C:87:LEU:C     | 3:C:89:GLU:H     | 2.26                     | 0.43              |
| 3:C:116:VAL:O    | 3:C:120:VAL:HG23 | 2.19                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:25:ARG:CG    | 4:D:25:ARG:NH1   | 2.81                     | 0.43              |
| 4:D:30:LYS:C     | 4:D:32:ALA:N     | 2.66                     | 0.43              |
| 4:D:100:ARG:HB3  | 4:D:102:ASP:OD1  | 2.18                     | 0.43              |
| 7:G:50:ILE:HD12  | 7:G:125:MET:HG3  | 2.00                     | 0.43              |
| 12:L:55:VAL:C    | 12:L:70:ILE:HD11 | 2.44                     | 0.43              |
| 14:N:3:ARG:NH1   | 14:N:6:LEU:HD11  | 2.34                     | 0.43              |
| 14:N:45:ARG:O    | 14:N:49:HIS:CD2  | 2.72                     | 0.43              |
| 1:A:145:G:O2'    | 1:A:146:G:H5'    | 2.18                     | 0.42              |
| 1:A:338:A:H2     | 1:A:351:G:H22    | 1.66                     | 0.42              |
| 1:A:389:A:H2'    | 1:A:390:C:O4'    | 2.19                     | 0.42              |
| 1:A:930:C:C2'    | 1:A:931:C:H5'    | 2.49                     | 0.42              |
| 1:A:1125:U:H5'   | 1:A:1126:U:C5    | 2.52                     | 0.42              |
| 1:A:1347:G:H2'   | 1:A:1373:G:N1    | 2.34                     | 0.42              |
| 1:A:1490:C:O2'   | 1:A:1491:G:H5'   | 2.19                     | 0.42              |
| 2:B:139:LYS:HE3  | 2:B:143:GLU:OE2  | 2.19                     | 0.42              |
| 4:D:121:VAL:O    | 4:D:134:ASP:HA   | 2.19                     | 0.42              |
| 5:E:5:ASP:CG     | 5:E:6:PHE:N      | 2.77                     | 0.42              |
| 5:E:144:THR:HG23 | 5:E:146:ALA:H    | 1.84                     | 0.42              |
| 7:G:112:PRO:O    | 7:G:113:GLU:C    | 2.60                     | 0.42              |
| 9:I:81:ILE:O     | 9:I:85:LEU:HB2   | 2.19                     | 0.42              |
| 10:J:6:ILE:HD11  | 10:J:72:VAL:HB   | 2.00                     | 0.42              |
| 10:J:33:GLN:HB2  | 10:J:75:ILE:HD11 | 2.01                     | 0.42              |
| 10:J:48:THR:HG1  | 10:J:62:HIS:CD2  | 2.36                     | 0.42              |
| 14:N:4:LYS:O     | 14:N:7:ILE:N     | 2.47                     | 0.42              |
| 18:R:43:PHE:HA   | 18:R:51:LEU:HD12 | 2.01                     | 0.42              |
| 20:T:49:ALA:HB3  | 20:T:99:LEU:HG   | 2.01                     | 0.42              |
| 1:A:176:C:H2'    | 1:A:177:C:H6     | 1.84                     | 0.42              |
| 1:A:448:A:C4     | 1:A:487:A:C2     | 3.07                     | 0.42              |
| 1:A:992:U:O2'    | 1:A:993:G:OP2    | 2.32                     | 0.42              |
| 1:A:1179:A:O2'   | 1:A:1180:A:H5'   | 2.19                     | 0.42              |
| 2:B:80:ILE:HD11  | 2:B:208:ILE:CG2  | 2.49                     | 0.42              |
| 2:B:204:ASN:ND2  | 2:B:206:ASP:N    | 2.57                     | 0.42              |
| 2:B:227:GLY:O    | 2:B:229:VAL:N    | 2.52                     | 0.42              |
| 3:C:84:ILE:O     | 3:C:88:ARG:HG3   | 2.20                     | 0.42              |
| 5:E:50:GLU:O     | 5:E:51:VAL:C     | 2.61                     | 0.42              |
| 8:H:80:ILE:O     | 8:H:80:ILE:HG22  | 2.19                     | 0.42              |
| 11:K:16:SER:HA   | 11:K:79:SER:O    | 2.18                     | 0.42              |
| 11:K:58:PRO:HB2  | 11:K:93:GLN:HG3  | 2.01                     | 0.42              |
| 12:L:54:LYS:N    | 12:L:54:LYS:HD2  | 2.33                     | 0.42              |
| 12:L:113:ARG:NH1 | 12:L:116:SER:HB2 | 2.35                     | 0.42              |
| 12:L:126:LYS:NZ  | 12:L:126:LYS:H   | 2.16                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 13:M:21:TYR:N    | 13:M:21:TYR:CD1   | 2.87                     | 0.42              |
| 13:M:71:ARG:O    | 13:M:72:ALA:C     | 2.62                     | 0.42              |
| 15:O:76:GLU:C    | 15:O:78:TYR:N     | 2.77                     | 0.42              |
| 16:P:7:ALA:O     | 16:P:17:TYR:HA    | 2.19                     | 0.42              |
| 19:S:18:LYS:O    | 19:S:22:LEU:HG    | 2.18                     | 0.42              |
| 20:T:53:LEU:CD1  | 20:T:100:ILE:HG23 | 2.49                     | 0.42              |
| 1:A:142:G:N3     | 1:A:196:A:H2      | 2.18                     | 0.42              |
| 1:A:272:C:O2'    | 1:A:273:A:H5'     | 2.20                     | 0.42              |
| 1:A:456:C:H2'    | 1:A:457:C:C6      | 2.54                     | 0.42              |
| 1:A:629:G:H2'    | 1:A:630:G:C1'     | 2.49                     | 0.42              |
| 1:A:1074:G:O2'   | 2:B:103:THR:HG22  | 2.18                     | 0.42              |
| 1:A:1305:G:N2    | 1:A:1331:G:C2'    | 2.82                     | 0.42              |
| 1:A:1353:G:H2'   | 1:A:1354:C:C6     | 2.54                     | 0.42              |
| 1:A:1487:G:O2'   | 1:A:1488:G:H5'    | 2.18                     | 0.42              |
| 2:B:74:LYS:O     | 2:B:75:LYS:HB2    | 2.19                     | 0.42              |
| 12:L:28:LYS:C    | 12:L:30:ALA:N     | 2.76                     | 0.42              |
| 15:O:6:GLU:CD    | 15:O:6:GLU:N      | 2.73                     | 0.42              |
| 20:T:45:GLN:HA   | 20:T:91:LEU:HB3   | 2.00                     | 0.42              |
| 1:A:509:A:C8     | 1:A:509:A:C3'     | 3.02                     | 0.42              |
| 1:A:831:U:H2'    | 1:A:832:C:C6      | 2.55                     | 0.42              |
| 1:A:921:U:O2'    | 5:E:19:MET:O      | 2.26                     | 0.42              |
| 1:A:1141:C:H2'   | 1:A:1142:G:H8     | 1.85                     | 0.42              |
| 1:A:1305:G:H5''  | 21:U:4:GLY:C      | 2.45                     | 0.42              |
| 2:B:28:PHE:HD1   | 2:B:194:PRO:HG3   | 1.85                     | 0.42              |
| 2:B:157:ARG:O    | 2:B:158:LEU:C     | 2.63                     | 0.42              |
| 2:B:189:ASP:OD1  | 2:B:205:ASP:OD1   | 2.36                     | 0.42              |
| 3:C:66:VAL:O     | 3:C:66:VAL:HG12   | 2.18                     | 0.42              |
| 5:E:31:LEU:HD23  | 5:E:31:LEU:HA     | 1.78                     | 0.42              |
| 5:E:129:ILE:CG2  | 5:E:133:TYR:HE1   | 2.32                     | 0.42              |
| 6:F:69:GLU:HA    | 6:F:72:VAL:HG23   | 2.02                     | 0.42              |
| 7:G:156:TRP:CD1  | 7:G:156:TRP:C     | 2.97                     | 0.42              |
| 8:H:11:THR:HA    | 8:H:14:ARG:HH12   | 1.84                     | 0.42              |
| 9:I:9:ARG:CD     | 9:I:14:VAL:HG12   | 2.50                     | 0.42              |
| 10:J:5:ARG:N     | 10:J:99:LYS:O     | 2.51                     | 0.42              |
| 10:J:21:GLN:CA   | 10:J:21:GLN:NE2   | 2.82                     | 0.42              |
| 13:M:32:GLU:OE1  | 13:M:64:TRP:HZ2   | 2.01                     | 0.42              |
| 15:O:10:LYS:HE2  | 15:O:14:GLU:HB2   | 2.00                     | 0.42              |
| 15:O:50:HIS:O    | 15:O:53:HIS:HB3   | 2.19                     | 0.42              |
| 20:T:39:LYS:O    | 20:T:43:LEU:HG    | 2.19                     | 0.42              |
| 1:A:189(A):C:O2' | 1:A:189(B):C:H5'  | 2.20                     | 0.42              |
| 1:A:858:G:O6     | 1:A:869:G:C8      | 2.72                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:994:A:OP1    | 1:A:994:A:C8     | 2.72                     | 0.42              |
| 1:A:1262:C:H2'   | 1:A:1263:C:C6    | 2.54                     | 0.42              |
| 1:A:1397:C:H4'   | 1:A:1398:A:OP2   | 2.19                     | 0.42              |
| 2:B:88:ALA:C     | 2:B:90:MET:H     | 2.28                     | 0.42              |
| 4:D:154:ASN:HA   | 4:D:159:ARG:CZ   | 2.48                     | 0.42              |
| 5:E:76:ILE:CG2   | 5:E:78:HIS:O     | 2.64                     | 0.42              |
| 7:G:41:ARG:O     | 7:G:42:ILE:C     | 2.63                     | 0.42              |
| 7:G:53:LYS:HE3   | 7:G:53:LYS:HB2   | 1.79                     | 0.42              |
| 12:L:10:LEU:HB3  | 17:Q:32:TYR:CE1  | 2.54                     | 0.42              |
| 13:M:90:LEU:HD23 | 13:M:90:LEU:HA   | 1.87                     | 0.42              |
| 15:O:64:ARG:HH11 | 15:O:64:ARG:HB2  | 1.84                     | 0.42              |
| 17:Q:68:ARG:CG   | 17:Q:68:ARG:NH1  | 2.81                     | 0.42              |
| 21:U:15:ARG:C    | 21:U:17:THR:H    | 2.27                     | 0.42              |
| 1:A:179:A:O2'    | 1:A:180:U:H5'    | 2.19                     | 0.42              |
| 1:A:413:G:H1'    | 1:A:428:G:H21    | 1.80                     | 0.42              |
| 1:A:415:A:H2'    | 1:A:416:G:C8     | 2.54                     | 0.42              |
| 1:A:528:C:H41    | 12:L:49:ASN:CG   | 2.27                     | 0.42              |
| 1:A:918:A:H2'    | 1:A:919:A:O4'    | 2.19                     | 0.42              |
| 1:A:933:G:OP2    | 7:G:3:ARG:HB3    | 2.19                     | 0.42              |
| 1:A:946:A:C2     | 1:A:1236:A:C2    | 3.07                     | 0.42              |
| 1:A:1226:C:H4'   | 19:S:80:TYR:CZ   | 2.54                     | 0.42              |
| 1:A:1302:U:OP2   | 13:M:17:VAL:HG13 | 2.19                     | 0.42              |
| 1:A:1304:G:C6    | 1:A:1305:G:N1    | 2.88                     | 0.42              |
| 3:C:64:VAL:H     | 3:C:99:VAL:HG12  | 1.80                     | 0.42              |
| 3:C:70:VAL:CG1   | 3:C:71:ALA:H     | 2.32                     | 0.42              |
| 4:D:33:MET:O     | 4:D:37:PRO:HB3   | 2.19                     | 0.42              |
| 4:D:38:TYR:CZ    | 4:D:45:GLN:HG2   | 2.55                     | 0.42              |
| 6:F:4:TYR:CE2    | 6:F:72:VAL:CG2   | 3.02                     | 0.42              |
| 7:G:15:ASP:OD2   | 7:G:44:TYR:OH    | 2.37                     | 0.42              |
| 9:I:111:ARG:HG3  | 9:I:111:ARG:HH11 | 1.85                     | 0.42              |
| 12:L:76:ASN:O    | 12:L:76:ASN:CG   | 2.60                     | 0.42              |
| 14:N:37:PHE:C    | 14:N:39:LEU:N    | 2.77                     | 0.42              |
| 1:A:941:G:H2'    | 1:A:942:G:O5'    | 2.19                     | 0.42              |
| 1:A:1060:C:H2'   | 1:A:1061:G:H8    | 1.85                     | 0.42              |
| 1:A:1104:G:OP1   | 2:B:111:ARG:HD2  | 2.20                     | 0.42              |
| 1:A:1406:U:O2'   | 1:A:1407:C:H5'   | 2.19                     | 0.42              |
| 2:B:196:LEU:HD12 | 2:B:196:LEU:N    | 2.34                     | 0.42              |
| 3:C:39:ILE:HG22  | 3:C:40:ARG:N     | 2.33                     | 0.42              |
| 5:E:33:VAL:HG11  | 5:E:109:ILE:HA   | 2.01                     | 0.42              |
| 9:I:33:PHE:CE1   | 9:I:47:LEU:HD21  | 2.55                     | 0.42              |
| 13:M:8:GLU:OE2   | 13:M:8:GLU:CA    | 2.63                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 13:M:49:THR:CG2  | 13:M:51:ALA:HB3  | 2.50                     | 0.42              |
| 16:P:39:TYR:CZ   | 16:P:41:PRO:HA   | 2.55                     | 0.42              |
| 1:A:335:C:H2'    | 1:A:336:C:C6     | 2.55                     | 0.42              |
| 1:A:542:G:O2'    | 1:A:543:C:H5'    | 2.19                     | 0.42              |
| 1:A:609:A:C2'    | 1:A:610:G:H5'    | 2.50                     | 0.42              |
| 1:A:628:G:H2'    | 1:A:629:G:C8     | 2.55                     | 0.42              |
| 1:A:1018:C:O5'   | 1:A:1018:C:H6    | 2.02                     | 0.42              |
| 1:A:1320:C:OP1   | 19:S:70:LYS:HE2  | 2.20                     | 0.42              |
| 2:B:166:ASP:CG   | 2:B:169:LYS:HB2  | 2.45                     | 0.42              |
| 5:E:152:ARG:NH2  | 8:H:107:LEU:O    | 2.52                     | 0.42              |
| 13:M:96:LEU:O    | 13:M:97:PRO:C    | 2.60                     | 0.42              |
| 15:O:74:ASP:O    | 15:O:76:GLU:N    | 2.52                     | 0.42              |
| 20:T:43:LEU:HD13 | 20:T:51:GLU:CG   | 2.49                     | 0.42              |
| 1:A:101:A:O2'    | 1:A:102:G:H5'    | 2.19                     | 0.42              |
| 1:A:175:C:H4'    | 20:T:25:ARG:HD3  | 2.02                     | 0.42              |
| 1:A:200:G:H2'    | 1:A:201:C:C6     | 2.55                     | 0.42              |
| 1:A:455:C:O2'    | 1:A:456:C:H5'    | 2.20                     | 0.42              |
| 1:A:665:A:N3     | 1:A:732:C:H2'    | 2.35                     | 0.42              |
| 1:A:1179:A:H2'   | 1:A:1180:A:O4'   | 2.20                     | 0.42              |
| 1:A:1286:A:C2    | 21:U:18:TYR:OH   | 2.73                     | 0.42              |
| 1:A:1457:G:O2'   | 1:A:1458:G:H5'   | 2.19                     | 0.42              |
| 1:A:1476:G:O2'   | 1:A:1477:C:H5'   | 2.20                     | 0.42              |
| 1:A:1505:G:H3'   | 1:A:1505:G:H8    | 1.85                     | 0.42              |
| 3:C:79:ARG:HG3   | 3:C:79:ARG:HH11  | 1.84                     | 0.42              |
| 4:D:24:GLU:O     | 4:D:25:ARG:CB    | 2.67                     | 0.42              |
| 6:F:80:ARG:CZ    | 6:F:88:VAL:HB    | 2.49                     | 0.42              |
| 7:G:27:ILE:HD11  | 7:G:43:PHE:CD2   | 2.55                     | 0.42              |
| 8:H:71:GLY:HA3   | 8:H:72:PRO:HD2   | 1.93                     | 0.42              |
| 8:H:83:ILE:HG23  | 8:H:83:ILE:O     | 2.19                     | 0.42              |
| 10:J:15:THR:HG22 | 10:J:94:VAL:HG23 | 2.00                     | 0.42              |
| 13:M:14:ARG:CZ   | 13:M:42:ALA:HA   | 2.49                     | 0.42              |
| 16:P:22:THR:HA   | 16:P:33:ILE:CD1  | 2.49                     | 0.42              |
| 16:P:79:VAL:O    | 16:P:79:VAL:HG12 | 2.20                     | 0.42              |
| 20:T:45:GLN:NE2  | 20:T:45:GLN:O    | 2.52                     | 0.42              |
| 1:A:178:C:O2'    | 1:A:179:A:H5'    | 2.20                     | 0.42              |
| 1:A:342:C:H2'    | 1:A:343:U:H5'    | 2.02                     | 0.42              |
| 1:A:555:C:H2'    | 1:A:556:C:C6     | 2.55                     | 0.42              |
| 1:A:942:G:H2'    | 1:A:943:U:H6     | 1.85                     | 0.42              |
| 1:A:1346:A:O4'   | 1:A:1348:U:C6    | 2.73                     | 0.42              |
| 4:D:196:LEU:C    | 4:D:198:VAL:H    | 2.28                     | 0.42              |
| 5:E:53:LEU:HD23  | 5:E:53:LEU:N     | 2.16                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:I:9:ARG:HD3    | 9:I:14:VAL:HG12  | 2.01                     | 0.42              |
| 9:I:112:LYS:C    | 9:I:112:LYS:HD3  | 2.45                     | 0.42              |
| 15:O:61:GLY:O    | 15:O:62:GLN:C    | 2.63                     | 0.42              |
| 16:P:54:GLU:O    | 16:P:57:ARG:HB2  | 2.19                     | 0.42              |
| 17:Q:99:SER:O    | 17:Q:101:ARG:N   | 2.52                     | 0.42              |
| 1:A:344:A:O2'    | 1:A:345:C:OP1    | 2.37                     | 0.41              |
| 1:A:496:A:H1'    | 1:A:498:U:OP1    | 2.19                     | 0.41              |
| 1:A:866:C:H2'    | 1:A:867:G:O4'    | 2.20                     | 0.41              |
| 2:B:139:LYS:O    | 2:B:143:GLU:HG3  | 2.20                     | 0.41              |
| 3:C:111:LEU:HD21 | 3:C:144:SER:O    | 2.19                     | 0.41              |
| 5:E:15:ARG:CZ    | 5:E:26:PHE:CE2   | 3.04                     | 0.41              |
| 5:E:28:PHE:O     | 5:E:47:LYS:HA    | 2.20                     | 0.41              |
| 5:E:144:THR:O    | 5:E:145:LYS:C    | 2.63                     | 0.41              |
| 11:K:70:LYS:C    | 11:K:72:ALA:N    | 2.75                     | 0.41              |
| 11:K:108:ILE:N   | 11:K:108:ILE:CD1 | 2.81                     | 0.41              |
| 13:M:57:ARG:CG   | 13:M:61:GLU:HG3  | 2.44                     | 0.41              |
| 17:Q:66:SER:HG   | 17:Q:69:LYS:HB2  | 1.84                     | 0.41              |
| 23:Y:34:CM0:H2'  | 23:Y:35:A:C8     | 2.55                     | 0.41              |
| 1:A:118:U:H3'    | 1:A:288:A:H61    | 1.84                     | 0.41              |
| 1:A:376:G:P      | 16:P:67:THR:HG21 | 2.60                     | 0.41              |
| 1:A:769:G:H4'    | 1:A:1513:A:H4'   | 2.02                     | 0.41              |
| 1:A:1028:C:H2'   | 1:A:1029:C:C6    | 2.55                     | 0.41              |
| 1:A:1168:A:C6    | 1:A:1169:A:C6    | 3.09                     | 0.41              |
| 1:A:1206:G:C6    | 1:A:1207:G:C5    | 3.07                     | 0.41              |
| 1:A:1352:C:H2'   | 1:A:1353:G:H8    | 1.82                     | 0.41              |
| 2:B:216:SER:O    | 2:B:219:VAL:N    | 2.53                     | 0.41              |
| 3:C:98:ASN:C     | 3:C:99:VAL:HG13  | 2.45                     | 0.41              |
| 5:E:81:GLU:CD    | 5:E:88:LYS:HE2   | 2.46                     | 0.41              |
| 5:E:137:GLU:OE1  | 5:E:141:GLN:NE2  | 2.42                     | 0.41              |
| 6:F:47:ARG:HA    | 6:F:57:GLN:HG2   | 2.01                     | 0.41              |
| 10:J:50:ILE:HA   | 10:J:60:ARG:HD3  | 2.02                     | 0.41              |
| 11:K:23:ALA:O    | 11:K:86:GLY:HA3  | 2.20                     | 0.41              |
| 12:L:44:THR:HA   | 12:L:45:PRO:HD3  | 1.82                     | 0.41              |
| 13:M:22:ILE:CD1  | 13:M:25:ILE:HD12 | 2.49                     | 0.41              |
| 13:M:32:GLU:O    | 13:M:35:GLU:HB3  | 2.20                     | 0.41              |
| 18:R:66:LEU:O    | 18:R:67:ALA:C    | 2.63                     | 0.41              |
| 1:A:115:G:O2'    | 1:A:116:A:OP2    | 2.37                     | 0.41              |
| 1:A:304:U:H2'    | 1:A:305:G:C8     | 2.55                     | 0.41              |
| 1:A:627:G:H2'    | 1:A:628:G:C8     | 2.55                     | 0.41              |
| 1:A:1003:G:N2    | 1:A:1038:C:C2    | 2.88                     | 0.41              |
| 1:A:1066:C:H2'   | 1:A:1067:A:H5'   | 2.01                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1402:C:O2    | 1:A:1500:A:N1     | 2.53                     | 0.41              |
| 2:B:25:ASN:ND2   | 2:B:27:LYS:H      | 2.16                     | 0.41              |
| 3:C:6:HIS:CD2    | 3:C:8:ILE:H       | 2.27                     | 0.41              |
| 4:D:64:LEU:HB2   | 4:D:198:VAL:HG11  | 2.02                     | 0.41              |
| 4:D:150:GLU:O    | 4:D:153:ARG:HG3   | 2.20                     | 0.41              |
| 7:G:50:ILE:O     | 7:G:54:THR:HB     | 2.19                     | 0.41              |
| 16:P:52:ASP:OD2  | 16:P:55:ARG:HG3   | 2.21                     | 0.41              |
| 17:Q:95:TYR:O    | 17:Q:97:SER:N     | 2.53                     | 0.41              |
| 19:S:33:THR:HG22 | 19:S:35:SER:N     | 2.34                     | 0.41              |
| 19:S:33:THR:HG22 | 19:S:34:TRP:N     | 2.35                     | 0.41              |
| 20:T:84:LEU:CD2  | 20:T:88:VAL:HG23  | 2.50                     | 0.41              |
| 1:A:1010:G:H2'   | 1:A:1011:G:C8     | 2.55                     | 0.41              |
| 1:A:1237:C:C4'   | 1:A:1334:G:N2     | 2.84                     | 0.41              |
| 1:A:1311:G:N7    | 19:S:2:PRO:HA     | 2.35                     | 0.41              |
| 2:B:212:GLN:NE2  | 2:B:216:SER:HB3   | 2.35                     | 0.41              |
| 3:C:35:GLU:O     | 3:C:38:ARG:N      | 2.53                     | 0.41              |
| 3:C:156:ARG:O    | 3:C:157:ILE:C     | 2.61                     | 0.41              |
| 5:E:43:LEU:HD22  | 5:E:44:GLY:N      | 2.34                     | 0.41              |
| 5:E:144:THR:HG22 | 5:E:147:ASP:H     | 1.85                     | 0.41              |
| 7:G:24:THR:O     | 7:G:25:ALA:C      | 2.63                     | 0.41              |
| 10:J:47:PHE:CZ   | 14:N:37:PHE:CE1   | 3.07                     | 0.41              |
| 11:K:77:MET:HG3  | 11:K:103:LEU:HD21 | 2.01                     | 0.41              |
| 14:N:9:LYS:O     | 14:N:11:LYS:N     | 2.53                     | 0.41              |
| 15:O:9:GLN:O     | 15:O:13:GLN:HG3   | 2.20                     | 0.41              |
| 18:R:36:ASN:ND2  | 18:R:39:VAL:H     | 2.17                     | 0.41              |
| 20:T:57:ARG:NH1  | 20:T:57:ARG:CG    | 2.82                     | 0.41              |
| 1:A:103:C:OP2    | 20:T:14:LYS:HE3   | 2.19                     | 0.41              |
| 1:A:112:G:C5'    | 1:A:389:A:H4'     | 2.46                     | 0.41              |
| 1:A:372:C:O2'    | 1:A:373:A:OP2     | 2.36                     | 0.41              |
| 1:A:991:U:C5     | 1:A:1212:U:H1'    | 2.55                     | 0.41              |
| 1:A:1060:C:OP1   | 14:N:45:ARG:NH2   | 2.53                     | 0.41              |
| 1:A:1112:C:N4    | 3:C:178:LEU:HD23  | 2.36                     | 0.41              |
| 1:A:1232:U:H2'   | 1:A:1233:G:O4'    | 2.21                     | 0.41              |
| 1:A:1305:G:O2'   | 1:A:1331:G:N2     | 2.53                     | 0.41              |
| 1:A:1321:C:H2'   | 1:A:1322:C:C5     | 2.55                     | 0.41              |
| 1:A:1329:A:O2'   | 1:A:1330:U:H5'    | 2.21                     | 0.41              |
| 1:A:1366:C:C2    | 1:A:1367:C:C5     | 3.09                     | 0.41              |
| 2:B:223:ILE:HD12 | 2:B:224:GLN:H     | 1.81                     | 0.41              |
| 4:D:111:ALA:HB1  | 4:D:116:GLN:OE1   | 2.19                     | 0.41              |
| 9:I:4:TYR:HB3    | 9:I:87:GLN:HB2    | 2.02                     | 0.41              |
| 9:I:36:TYR:CD2   | 9:I:37:PHE:CE2    | 3.06                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 10:J:51:ARG:CZ   | 10:J:61:GLU:HB2   | 2.50                     | 0.41              |
| 11:K:60:ALA:O    | 11:K:61:ALA:C     | 2.62                     | 0.41              |
| 11:K:108:ILE:O   | 11:K:109:VAL:HG23 | 2.20                     | 0.41              |
| 13:M:29:ARG:HB3  | 13:M:64:TRP:CH2   | 2.55                     | 0.41              |
| 13:M:93:ARG:NH1  | 13:M:93:ARG:HB2   | 2.35                     | 0.41              |
| 14:N:58:LYS:HE3  | 14:N:58:LYS:HB3   | 1.85                     | 0.41              |
| 1:A:16:A:C2'     | 1:A:17:U:H5'      | 2.49                     | 0.41              |
| 1:A:397:A:H3'    | 1:A:397:A:N3      | 2.34                     | 0.41              |
| 1:A:663:A:H5''   | 18:R:61:LYS:HE3   | 2.02                     | 0.41              |
| 1:A:841:U:H3'    | 1:A:848:C:O4'     | 2.20                     | 0.41              |
| 1:A:955:U:O2'    | 1:A:956:U:H5'     | 2.21                     | 0.41              |
| 1:A:1048:G:H5'   | 1:A:1048:G:C8     | 2.49                     | 0.41              |
| 1:A:1147:C:O2'   | 9:I:5:TYR:OH      | 2.34                     | 0.41              |
| 1:A:1488:G:H2'   | 1:A:1489:G:C8     | 2.55                     | 0.41              |
| 2:B:58:ILE:O     | 2:B:59:GLU:C      | 2.64                     | 0.41              |
| 3:C:35:GLU:CG    | 3:C:59:ARG:HH22   | 2.33                     | 0.41              |
| 7:G:54:THR:HG22  | 7:G:56:GLN:HB2    | 2.02                     | 0.41              |
| 8:H:82:HIS:HD2   | 8:H:138:TRP:NE1   | 2.18                     | 0.41              |
| 11:K:57:THR:HG22 | 11:K:59:TYR:N     | 2.33                     | 0.41              |
| 12:L:60:LEU:CD2  | 12:L:66:VAL:HG22  | 2.46                     | 0.41              |
| 15:O:64:ARG:CB   | 15:O:64:ARG:NH1   | 2.83                     | 0.41              |
| 19:S:33:THR:CG2  | 19:S:34:TRP:N     | 2.84                     | 0.41              |
| 20:T:57:ARG:HH21 | 20:T:100:ILE:HG12 | 1.85                     | 0.41              |
| 20:T:89:ARG:HB2  | 20:T:104:LEU:HD13 | 2.02                     | 0.41              |
| 1:A:423:G:H2'    | 1:A:424:G:H5'     | 2.03                     | 0.41              |
| 1:A:640:A:O2'    | 1:A:641:U:H5'     | 2.21                     | 0.41              |
| 1:A:828:A:H2'    | 1:A:829:G:O4'     | 2.20                     | 0.41              |
| 1:A:942:G:H2'    | 1:A:943:U:C6      | 2.56                     | 0.41              |
| 1:A:976:G:C8     | 1:A:1358:U:C2     | 3.08                     | 0.41              |
| 1:A:1192:C:C5    | 1:A:1193:G:C8     | 3.09                     | 0.41              |
| 1:A:1277:C:O2'   | 1:A:1279:A:C8     | 2.63                     | 0.41              |
| 1:A:1499:A:O2'   | 1:A:1500:A:H5'    | 2.21                     | 0.41              |
| 2:B:120:ALA:O    | 2:B:122:PHE:N     | 2.54                     | 0.41              |
| 2:B:134:GLU:O    | 2:B:138:LEU:HG    | 2.21                     | 0.41              |
| 2:B:195:ASP:O    | 8:H:74:PRO:HG3    | 2.20                     | 0.41              |
| 4:D:36:ARG:C     | 4:D:38:TYR:H      | 2.28                     | 0.41              |
| 4:D:102:ASP:HB3  | 4:D:136:PRO:HA    | 2.02                     | 0.41              |
| 5:E:15:ARG:HD2   | 5:E:26:PHE:CD2    | 2.55                     | 0.41              |
| 5:E:144:THR:O    | 5:E:148:VAL:HG23  | 2.21                     | 0.41              |
| 8:H:122:ARG:HB3  | 8:H:122:ARG:CZ    | 2.49                     | 0.41              |
| 10:J:15:THR:HG22 | 10:J:94:VAL:HG21  | 2.00                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 10:J:26:ALA:HB1  | 10:J:84:GLN:CB   | 2.49                     | 0.41              |
| 13:M:23:TYR:N    | 13:M:67:GLU:OE2  | 2.44                     | 0.41              |
| 14:N:37:PHE:CE2  | 14:N:53:LEU:HD13 | 2.56                     | 0.41              |
| 15:O:74:ASP:C    | 15:O:76:GLU:H    | 2.28                     | 0.41              |
| 1:A:429:U:H4'    | 1:A:430:A:O5'    | 2.19                     | 0.41              |
| 1:A:841:U:C5     | 1:A:848:C:H1'    | 2.55                     | 0.41              |
| 1:A:1217:C:H2'   | 1:A:1218:C:O4'   | 2.21                     | 0.41              |
| 1:A:1320:C:O2'   | 1:A:1321:C:H5'   | 2.21                     | 0.41              |
| 2:B:21:ARG:HG3   | 2:B:21:ARG:NH1   | 2.35                     | 0.41              |
| 4:D:39:PRO:O     | 4:D:44:GLY:HA3   | 2.20                     | 0.41              |
| 5:E:112:LEU:HD23 | 5:E:112:LEU:HA   | 1.87                     | 0.41              |
| 7:G:51:GLN:C     | 7:G:53:LYS:H     | 2.29                     | 0.41              |
| 9:I:95:LYS:HD3   | 9:I:95:LYS:HA    | 1.91                     | 0.41              |
| 12:L:7:ILE:O     | 12:L:11:VAL:N    | 2.48                     | 0.41              |
| 12:L:47:LYS:CB   | 12:L:48:PRO:CD   | 2.86                     | 0.41              |
| 15:O:82:ILE:O    | 15:O:83:GLU:C    | 2.63                     | 0.41              |
| 16:P:52:ASP:CG   | 16:P:55:ARG:CG   | 2.94                     | 0.41              |
| 16:P:54:GLU:O    | 16:P:54:GLU:OE2  | 2.38                     | 0.41              |
| 19:S:5:LEU:HD11  | 19:S:70:LYS:HZ2  | 1.85                     | 0.41              |
| 20:T:32:ALA:O    | 20:T:33:ILE:C    | 2.64                     | 0.41              |
| 1:A:8:A:H5'      | 5:E:101:ILE:HG22 | 2.03                     | 0.41              |
| 1:A:268:C:H2'    | 1:A:269:C:H6     | 1.85                     | 0.41              |
| 1:A:401:C:H1'    | 1:A:622:A:H1'    | 2.02                     | 0.41              |
| 1:A:635:G:O2'    | 1:A:636:U:H5'    | 2.21                     | 0.41              |
| 1:A:862:C:O2'    | 1:A:863:U:H5'    | 2.21                     | 0.41              |
| 1:A:954:G:H2'    | 1:A:955:U:O4'    | 2.20                     | 0.41              |
| 1:A:975:A:C4'    | 1:A:976:G:H5''   | 2.28                     | 0.41              |
| 1:A:1225:A:H2'   | 1:A:1226:C:C5    | 2.55                     | 0.41              |
| 1:A:1263:C:H2'   | 1:A:1264:C:C6    | 2.55                     | 0.41              |
| 1:A:1425:U:H2'   | 1:A:1426:C:H6    | 1.85                     | 0.41              |
| 2:B:12:GLU:CD    | 2:B:213:LEU:HD11 | 2.46                     | 0.41              |
| 2:B:76:GLN:OE1   | 2:B:76:GLN:HA    | 2.20                     | 0.41              |
| 2:B:132:LYS:N    | 2:B:132:LYS:HD2  | 2.35                     | 0.41              |
| 3:C:58:GLU:HB3   | 10:J:92:THR:HG21 | 2.03                     | 0.41              |
| 3:C:70:VAL:O     | 3:C:106:VAL:N    | 2.51                     | 0.41              |
| 3:C:152:ILE:HG12 | 3:C:167:TRP:CB   | 2.51                     | 0.41              |
| 3:C:162:GLN:O    | 3:C:164:ARG:HG2  | 2.21                     | 0.41              |
| 3:C:186:PHE:CZ   | 3:C:188:LEU:HD23 | 2.56                     | 0.41              |
| 4:D:33:MET:HE3   | 4:D:37:PRO:CA    | 2.51                     | 0.41              |
| 4:D:96:LEU:N     | 4:D:96:LEU:HD12  | 2.35                     | 0.41              |
| 4:D:100:ARG:NH1  | 4:D:137:SER:CB   | 2.81                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:D:100:ARG:NH1  | 4:D:137:SER:CA    | 2.84                     | 0.41              |
| 4:D:199:ASN:HD21 | 4:D:201:GLN:HB2   | 1.86                     | 0.41              |
| 5:E:75:THR:HG23  | 5:E:76:ILE:O      | 2.21                     | 0.41              |
| 6:F:3:ARG:NH1    | 6:F:38:GLU:OE1    | 2.54                     | 0.41              |
| 7:G:146:GLU:CD   | 7:G:146:GLU:C     | 2.88                     | 0.41              |
| 8:H:50:ARG:C     | 8:H:51:VAL:HG13   | 2.46                     | 0.41              |
| 9:I:33:PHE:CE2   | 9:I:47:LEU:HD11   | 2.56                     | 0.41              |
| 10:J:32:ALA:O    | 10:J:34:VAL:HG23  | 2.21                     | 0.41              |
| 13:M:40:ASN:HA   | 13:M:41:PRO:HD3   | 1.92                     | 0.41              |
| 14:N:42:ILE:O    | 14:N:45:ARG:HB3   | 2.20                     | 0.41              |
| 15:O:18:PHE:C    | 15:O:18:PHE:CD1   | 2.98                     | 0.41              |
| 16:P:1:MET:HE3   | 16:P:65:GLN:HB2   | 2.02                     | 0.41              |
| 16:P:6:LEU:CD1   | 16:P:6:LEU:N      | 2.83                     | 0.41              |
| 18:R:43:PHE:HD2  | 18:R:56:THR:HG22  | 1.86                     | 0.41              |
| 20:T:38:LYS:HA   | 20:T:41:ILE:HD11  | 2.03                     | 0.41              |
| 1:A:718:G:H5'    | 11:K:117:ASN:HD22 | 1.82                     | 0.41              |
| 1:A:1061:G:H1'   | 10:J:56:HIS:CE1   | 2.56                     | 0.41              |
| 1:A:1144:G:N2    | 1:A:1146:A:N6     | 2.63                     | 0.41              |
| 1:A:1227:A:C4    | 19:S:81:ARG:NH1   | 2.87                     | 0.41              |
| 1:A:1308:U:O2'   | 1:A:1309:G:H5'    | 2.20                     | 0.41              |
| 3:C:83:ARG:C     | 3:C:85:ARG:H      | 2.29                     | 0.41              |
| 4:D:148:VAL:HG11 | 4:D:158:ILE:HD13  | 2.03                     | 0.41              |
| 5:E:6:PHE:CZ     | 5:E:66:MET:HE2    | 2.56                     | 0.41              |
| 6:F:27:GLN:HE21  | 6:F:27:GLN:CA     | 2.34                     | 0.41              |
| 10:J:4:ILE:HG13  | 10:J:74:ILE:H     | 1.86                     | 0.41              |
| 10:J:34:VAL:C    | 10:J:36:GLY:H     | 2.29                     | 0.41              |
| 11:K:21:ILE:HD13 | 11:K:94:ALA:HB1   | 2.03                     | 0.41              |
| 15:O:74:ASP:C    | 15:O:76:GLU:N     | 2.78                     | 0.41              |
| 19:S:17:GLU:HG3  | 19:S:18:LYS:N     | 2.36                     | 0.41              |
| 1:A:473:G:H5''   | 16:P:81:ARG:NH1   | 2.36                     | 0.40              |
| 1:A:559:A:OP1    | 5:E:126:ARG:NH2   | 2.50                     | 0.40              |
| 1:A:662:G:O2'    | 1:A:836:G:H5'     | 2.21                     | 0.40              |
| 1:A:797:C:O2'    | 1:A:798:G:H5'     | 2.21                     | 0.40              |
| 1:A:912:C:O2'    | 1:A:913:A:H5'     | 2.21                     | 0.40              |
| 1:A:1004:A:H2'   | 1:A:1005:A:O4'    | 2.21                     | 0.40              |
| 1:A:1222:G:O2'   | 1:A:1223:C:H5'    | 2.21                     | 0.40              |
| 1:A:1273:G:H2'   | 1:A:1274:G:O4'    | 2.21                     | 0.40              |
| 2:B:54:THR:O     | 2:B:57:PHE:HB3    | 2.21                     | 0.40              |
| 2:B:73:THR:HB    | 2:B:170:GLU:OE1   | 2.21                     | 0.40              |
| 2:B:160:ASP:O    | 2:B:183:PRO:HD2   | 2.21                     | 0.40              |
| 2:B:164:VAL:HG11 | 2:B:167:PRO:HA    | 2.03                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:228:GLY:O    | 2:B:229:VAL:C    | 2.63                     | 0.40              |
| 3:C:60:ALA:HB3   | 3:C:63:ASN:HB2   | 2.03                     | 0.40              |
| 3:C:134:ILE:HG22 | 3:C:168:ALA:HB3  | 2.03                     | 0.40              |
| 7:G:37:ASN:O     | 7:G:38:LEU:C     | 2.64                     | 0.40              |
| 9:I:9:ARG:HE     | 9:I:9:ARG:HB2    | 1.65                     | 0.40              |
| 13:M:40:ASN:HD22 | 13:M:40:ASN:C    | 2.28                     | 0.40              |
| 18:R:36:ASN:HD21 | 18:R:38:GLU:HB2  | 1.86                     | 0.40              |
| 1:A:267:C:OP1    | 17:Q:67:LYS:HB2  | 2.21                     | 0.40              |
| 1:A:283:C:C2     | 1:A:284:G:C8     | 3.08                     | 0.40              |
| 1:A:757:U:O2'    | 1:A:879:C:H1'    | 2.21                     | 0.40              |
| 1:A:839:U:O2     | 1:A:839:U:C2'    | 2.63                     | 0.40              |
| 1:A:879:C:O2'    | 1:A:880:C:H5'    | 2.22                     | 0.40              |
| 1:A:962:C:H2'    | 1:A:963:G:O4'    | 2.21                     | 0.40              |
| 1:A:1288:A:H2'   | 1:A:1289:A:H8    | 1.86                     | 0.40              |
| 2:B:78:GLN:CG    | 2:B:94:ASN:OD1   | 2.69                     | 0.40              |
| 2:B:84:GLU:CD    | 2:B:216:SER:HA   | 2.46                     | 0.40              |
| 2:B:212:GLN:O    | 2:B:213:LEU:C    | 2.63                     | 0.40              |
| 3:C:34:LEU:O     | 3:C:34:LEU:HD22  | 2.20                     | 0.40              |
| 4:D:58:LEU:CD2   | 4:D:58:LEU:C     | 2.94                     | 0.40              |
| 4:D:106:TYR:CE1  | 4:D:112:VAL:O    | 2.74                     | 0.40              |
| 5:E:20:GLN:O     | 5:E:21:ALA:C     | 2.63                     | 0.40              |
| 6:F:38:GLU:O     | 6:F:39:LYS:HB3   | 2.21                     | 0.40              |
| 10:J:26:ALA:HB3  | 10:J:85:LEU:CD2  | 2.51                     | 0.40              |
| 12:L:6:THR:OG1   | 12:L:9:GLN:HG3   | 2.22                     | 0.40              |
| 12:L:38:THR:O    | 12:L:79:GLU:HG3  | 2.21                     | 0.40              |
| 18:R:25:THR:HG22 | 18:R:42:ARG:NH1  | 2.29                     | 0.40              |
| 19:S:15:LEU:HD12 | 19:S:16:LEU:N    | 2.35                     | 0.40              |
| 1:A:409:G:OP1    | 4:D:24:GLU:O     | 2.39                     | 0.40              |
| 1:A:1049:U:O2'   | 1:A:1050:G:OP2   | 2.37                     | 0.40              |
| 1:A:1102:A:H2'   | 1:A:1103:C:C6    | 2.57                     | 0.40              |
| 1:A:1143:G:H2'   | 1:A:1144:G:C8    | 2.56                     | 0.40              |
| 1:A:1503:A:H5'   | 1:A:1531:A:O4'   | 2.21                     | 0.40              |
| 2:B:127:ILE:HG13 | 2:B:127:ILE:H    | 1.58                     | 0.40              |
| 3:C:35:GLU:HG3   | 3:C:95:THR:HG22  | 2.02                     | 0.40              |
| 4:D:38:TYR:HB2   | 4:D:39:PRO:HD2   | 2.04                     | 0.40              |
| 6:F:9:VAL:HB     | 6:F:87:ARG:HB2   | 2.03                     | 0.40              |
| 8:H:82:HIS:CD2   | 8:H:138:TRP:NE1  | 2.90                     | 0.40              |
| 9:I:16:ARG:HG3   | 9:I:16:ARG:HH11  | 1.86                     | 0.40              |
| 9:I:46:ALA:HB2   | 9:I:74:ILE:HG23  | 2.03                     | 0.40              |
| 11:K:44:SER:H    | 11:K:47:VAL:HB   | 1.84                     | 0.40              |
| 11:K:82:VAL:O    | 11:K:83:ILE:HD12 | 2.22                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 13:M:39:ILE:O    | 13:M:40:ASN:C    | 2.64                     | 0.40              |
| 13:M:62:ASN:HD22 | 13:M:62:ASN:HA   | 1.67                     | 0.40              |
| 15:O:81:LEU:C    | 15:O:81:LEU:CD2  | 2.95                     | 0.40              |
| 1:A:676:A:H1'    | 11:K:115:PRO:HB3 | 2.04                     | 0.40              |
| 1:A:814:A:H2'    | 1:A:816:A:H5''   | 2.04                     | 0.40              |
| 1:A:828:A:OP1    | 1:A:828:A:H4'    | 2.22                     | 0.40              |
| 1:A:952:U:O2'    | 1:A:953:G:H5'    | 2.22                     | 0.40              |
| 1:A:980:C:H2'    | 1:A:981:U:O4'    | 2.22                     | 0.40              |
| 1:A:1176:A:H2'   | 1:A:1177:G:O4'   | 2.22                     | 0.40              |
| 1:A:1416:G:O2'   | 1:A:1417:G:H5'   | 2.20                     | 0.40              |
| 1:A:1440:C:C2'   | 1:A:1441:G:H5'   | 2.51                     | 0.40              |
| 3:C:44:GLU:HA    | 3:C:52:LEU:HD11  | 2.02                     | 0.40              |
| 4:D:182:LYS:HE2  | 4:D:182:LYS:HB3  | 1.94                     | 0.40              |
| 7:G:65:ALA:HB1   | 7:G:127:ALA:CB   | 2.52                     | 0.40              |
| 7:G:136:LYS:O    | 7:G:139:GLU:N    | 2.54                     | 0.40              |
| 10:J:3:LYS:HA    | 10:J:76:ASN:N    | 2.31                     | 0.40              |
| 10:J:81:THR:C    | 10:J:83:GLU:H    | 2.29                     | 0.40              |
| 15:O:77:ARG:O    | 15:O:80:ALA:HB3  | 2.22                     | 0.40              |
| 16:P:28:ARG:HH11 | 16:P:29:ASP:CG   | 2.30                     | 0.40              |
| 16:P:71:ARG:HH11 | 16:P:71:ARG:HD2  | 1.76                     | 0.40              |
| 17:Q:60:ILE:C    | 17:Q:71:PHE:HD1  | 2.29                     | 0.40              |
| 19:S:25:LYS:HB2  | 19:S:26:GLY:H    | 1.68                     | 0.40              |
| 1:A:437:U:C5'    | 4:D:155:LEU:HD22 | 2.49                     | 0.40              |
| 1:A:542:G:H2'    | 1:A:543:C:H6     | 1.87                     | 0.40              |
| 1:A:974:A:P      | 14:N:41:ARG:HH12 | 2.44                     | 0.40              |
| 1:A:1103:C:H5''  | 2:B:98:LEU:HD13  | 2.02                     | 0.40              |
| 1:A:1394:A:C5    | 1:A:1501:C:H4'   | 2.57                     | 0.40              |
| 1:A:1413:A:H2    | 1:A:1487:G:H22   | 1.67                     | 0.40              |
| 1:A:1427:U:H2'   | 1:A:1428:A:H8    | 1.81                     | 0.40              |
| 2:B:101:MET:O    | 2:B:105:PHE:CA   | 2.70                     | 0.40              |
| 3:C:25:GLY:C     | 3:C:27:LYS:H     | 2.30                     | 0.40              |
| 5:E:106:PRO:O    | 5:E:110:LEU:HG   | 2.22                     | 0.40              |
| 6:F:14:LEU:CA    | 6:F:18:GLN:HE21  | 2.33                     | 0.40              |
| 6:F:21:LEU:HG    | 6:F:25:ILE:HD11  | 2.04                     | 0.40              |
| 8:H:104:ARG:O    | 8:H:105:ARG:C    | 2.64                     | 0.40              |
| 9:I:16:ARG:HG3   | 9:I:16:ARG:NH1   | 2.37                     | 0.40              |
| 11:K:101:SER:C   | 11:K:103:LEU:N   | 2.80                     | 0.40              |
| 16:P:20:VAL:HG13 | 16:P:32:TYR:HB2  | 2.04                     | 0.40              |
| 16:P:34:GLU:OE1  | 16:P:55:ARG:NH1  | 2.54                     | 0.40              |
| 19:S:12:ASP:HB3  | 19:S:14:HIS:CD2  | 2.57                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 2   | B     | 233/256 (91%)   | 157 (67%)  | 55 (24%)  | 21 (9%)  | 0           | 1  |
| 3   | C     | 205/239 (86%)   | 151 (74%)  | 41 (20%)  | 13 (6%)  | 1           | 3  |
| 4   | D     | 206/209 (99%)   | 170 (82%)  | 34 (16%)  | 2 (1%)   | 12          | 39 |
| 5   | E     | 149/162 (92%)   | 134 (90%)  | 14 (9%)   | 1 (1%)   | 18          | 48 |
| 6   | F     | 99/101 (98%)    | 84 (85%)   | 12 (12%)  | 3 (3%)   | 3           | 14 |
| 7   | G     | 153/156 (98%)   | 121 (79%)  | 29 (19%)  | 3 (2%)   | 6           | 22 |
| 8   | H     | 136/138 (99%)   | 119 (88%)  | 12 (9%)   | 5 (4%)   | 2           | 11 |
| 9   | I     | 125/128 (98%)   | 97 (78%)   | 19 (15%)  | 9 (7%)   | 1           | 2  |
| 10  | J     | 97/105 (92%)    | 73 (75%)   | 13 (13%)  | 11 (11%) | 0           | 1  |
| 11  | K     | 117/129 (91%)   | 95 (81%)   | 18 (15%)  | 4 (3%)   | 3           | 12 |
| 12  | L     | 123/135 (91%)   | 96 (78%)   | 17 (14%)  | 10 (8%)  | 1           | 1  |
| 13  | M     | 123/126 (98%)   | 88 (72%)   | 23 (19%)  | 12 (10%) | 0           | 1  |
| 14  | N     | 58/61 (95%)     | 47 (81%)   | 5 (9%)    | 6 (10%)  | 0           | 1  |
| 15  | O     | 86/89 (97%)     | 67 (78%)   | 17 (20%)  | 2 (2%)   | 5           | 19 |
| 16  | P     | 82/88 (93%)     | 73 (89%)   | 8 (10%)   | 1 (1%)   | 10          | 34 |
| 17  | Q     | 102/105 (97%)   | 88 (86%)   | 8 (8%)    | 6 (6%)   | 1           | 4  |
| 18  | R     | 71/88 (81%)     | 63 (89%)   | 6 (8%)    | 2 (3%)   | 4           | 15 |
| 19  | S     | 79/93 (85%)     | 58 (73%)   | 11 (14%)  | 10 (13%) | 0           | 0  |
| 20  | T     | 97/106 (92%)    | 76 (78%)   | 15 (16%)  | 6 (6%)   | 1           | 3  |
| 21  | U     | 23/27 (85%)     | 14 (61%)   | 8 (35%)   | 1 (4%)   | 2           | 8  |
| All | All   | 2364/2541 (93%) | 1871 (79%) | 365 (15%) | 128 (5%) | 1           | 5  |

All (128) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 15  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 17  | PHE  |
| 2   | B     | 74  | LYS  |
| 2   | B     | 207 | ALA  |
| 3   | C     | 15  | THR  |
| 3   | C     | 61  | ALA  |
| 3   | C     | 207 | VAL  |
| 8   | H     | 70  | GLN  |
| 8   | H     | 91  | ARG  |
| 8   | H     | 105 | ARG  |
| 9   | I     | 8   | GLY  |
| 9   | I     | 23  | ASN  |
| 9   | I     | 38  | GLN  |
| 9   | I     | 43  | ALA  |
| 10  | J     | 76  | ASN  |
| 10  | J     | 83  | GLU  |
| 10  | J     | 85  | LEU  |
| 10  | J     | 86  | MET  |
| 11  | K     | 12  | ARG  |
| 11  | K     | 127 | LYS  |
| 12  | L     | 27  | LEU  |
| 12  | L     | 28  | LYS  |
| 12  | L     | 41  | ARG  |
| 12  | L     | 47  | LYS  |
| 12  | L     | 75  | HIS  |
| 12  | L     | 79  | GLU  |
| 13  | M     | 23  | TYR  |
| 13  | M     | 67  | GLU  |
| 13  | M     | 68  | GLY  |
| 14  | N     | 4   | LYS  |
| 17  | Q     | 99  | SER  |
| 19  | S     | 6   | LYS  |
| 19  | S     | 9   | VAL  |
| 19  | S     | 29  | ARG  |
| 19  | S     | 43  | GLU  |
| 19  | S     | 81  | ARG  |
| 20  | T     | 74  | LYS  |
| 20  | T     | 95  | ALA  |
| 20  | T     | 102 | GLY  |
| 2   | B     | 19  | HIS  |
| 2   | B     | 95  | GLN  |
| 2   | B     | 195 | ASP  |
| 2   | B     | 208 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 95  | THR  |
| 6   | F     | 70  | ASP  |
| 8   | H     | 71  | GLY  |
| 8   | H     | 83  | ILE  |
| 9   | I     | 33  | PHE  |
| 10  | J     | 26  | ALA  |
| 10  | J     | 34  | VAL  |
| 10  | J     | 57  | LYS  |
| 10  | J     | 61  | GLU  |
| 10  | J     | 90  | LEU  |
| 11  | K     | 13  | GLN  |
| 11  | K     | 88  | GLY  |
| 13  | M     | 6   | GLY  |
| 13  | M     | 21  | TYR  |
| 13  | M     | 24  | GLY  |
| 13  | M     | 85  | GLY  |
| 13  | M     | 117 | VAL  |
| 14  | N     | 9   | LYS  |
| 14  | N     | 10  | ALA  |
| 14  | N     | 15  | LYS  |
| 17  | Q     | 68  | ARG  |
| 17  | Q     | 96  | GLU  |
| 17  | Q     | 100 | LYS  |
| 18  | R     | 87  | ARG  |
| 19  | S     | 28  | LYS  |
| 20  | T     | 11  | SER  |
| 20  | T     | 73  | HIS  |
| 2   | B     | 16  | HIS  |
| 3   | C     | 26  | LYS  |
| 6   | F     | 16  | GLN  |
| 7   | G     | 86  | GLN  |
| 7   | G     | 155 | ARG  |
| 10  | J     | 75  | ILE  |
| 12  | L     | 116 | SER  |
| 14  | N     | 5   | ALA  |
| 14  | N     | 36  | PHE  |
| 18  | R     | 19  | LYS  |
| 19  | S     | 5   | LEU  |
| 19  | S     | 25  | LYS  |
| 19  | S     | 67  | VAL  |
| 2   | B     | 9   | GLU  |
| 2   | B     | 63  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 121 | LEU  |
| 3   | C     | 102 | ASN  |
| 3   | C     | 108 | ASN  |
| 7   | G     | 62  | PHE  |
| 9   | I     | 24  | GLY  |
| 9   | I     | 32  | ASP  |
| 9   | I     | 121 | ARG  |
| 9   | I     | 127 | LYS  |
| 13  | M     | 12  | ASN  |
| 21  | U     | 3   | LYS  |
| 2   | B     | 13  | ALA  |
| 2   | B     | 20  | GLU  |
| 2   | B     | 150 | SER  |
| 2   | B     | 224 | GLN  |
| 2   | B     | 228 | GLY  |
| 3   | C     | 81  | GLY  |
| 3   | C     | 91  | LEU  |
| 3   | C     | 144 | SER  |
| 4   | D     | 3   | ARG  |
| 6   | F     | 98  | LEU  |
| 13  | M     | 3   | ARG  |
| 13  | M     | 37  | THR  |
| 16  | P     | 10  | GLY  |
| 2   | B     | 83  | MET  |
| 3   | C     | 127 | ARG  |
| 17  | Q     | 102 | GLY  |
| 20  | T     | 49  | ALA  |
| 2   | B     | 127 | ILE  |
| 2   | B     | 131 | PRO  |
| 3   | C     | 14  | ILE  |
| 3   | C     | 103 | VAL  |
| 12  | L     | 29  | GLY  |
| 13  | M     | 7   | VAL  |
| 17  | Q     | 103 | GLY  |
| 2   | B     | 229 | VAL  |
| 5   | E     | 128 | PRO  |
| 19  | S     | 42  | PRO  |
| 4   | D     | 5   | ILE  |
| 12  | L     | 110 | VAL  |
| 15  | O     | 75  | PRO  |
| 12  | L     | 74  | GLY  |
| 15  | O     | 87  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | J     | 77  | 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%)   | 187 (93%)  | 15 (7%)  | 13          | 38  |
| 3   | C     | 160/188 (85%)   | 144 (90%)  | 16 (10%) | 7           | 24  |
| 4   | D     | 180/181 (99%)   | 168 (93%)  | 12 (7%)  | 15          | 43  |
| 5   | E     | 115/123 (94%)   | 100 (87%)  | 15 (13%) | 4           | 13  |
| 6   | F     | 90/90 (100%)    | 85 (94%)   | 5 (6%)   | 19          | 50  |
| 7   | G     | 126/127 (99%)   | 117 (93%)  | 9 (7%)   | 13          | 40  |
| 8   | H     | 119/119 (100%)  | 106 (89%)  | 13 (11%) | 6           | 20  |
| 9   | I     | 98/99 (99%)     | 92 (94%)   | 6 (6%)   | 17          | 46  |
| 10  | J     | 87/92 (95%)     | 79 (91%)   | 8 (9%)   | 8           | 27  |
| 11  | K     | 90/99 (91%)     | 83 (92%)   | 7 (8%)   | 11          | 35  |
| 12  | L     | 104/111 (94%)   | 93 (89%)   | 11 (11%) | 6           | 22  |
| 13  | M     | 100/101 (99%)   | 92 (92%)   | 8 (8%)   | 11          | 34  |
| 14  | N     | 49/50 (98%)     | 42 (86%)   | 7 (14%)  | 3           | 11  |
| 15  | O     | 79/80 (99%)     | 71 (90%)   | 8 (10%)  | 7           | 24  |
| 16  | P     | 72/74 (97%)     | 65 (90%)   | 7 (10%)  | 8           | 25  |
| 17  | Q     | 96/97 (99%)     | 88 (92%)   | 8 (8%)   | 10          | 32  |
| 18  | R     | 64/77 (83%)     | 62 (97%)   | 2 (3%)   | 35          | 69  |
| 19  | S     | 71/80 (89%)     | 68 (96%)   | 3 (4%)   | 26          | 60  |
| 20  | T     | 76/82 (93%)     | 64 (84%)   | 12 (16%) | 2           | 8   |
| 21  | U     | 19/22 (86%)     | 19 (100%)  | 0        | 100         | 100 |
| All | All   | 1997/2112 (95%) | 1825 (91%) | 172 (9%) | 10          | 30  |

All (172) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 12  | GLU  |
| 2   | B     | 15  | VAL  |
| 2   | B     | 21  | ARG  |
| 2   | B     | 23  | ARG  |
| 2   | B     | 25  | ASN  |
| 2   | B     | 82  | ARG  |
| 2   | B     | 98  | LEU  |
| 2   | B     | 117 | GLU  |
| 2   | B     | 121 | LEU  |
| 2   | B     | 162 | ILE  |
| 2   | B     | 187 | LEU  |
| 2   | B     | 204 | ASN  |
| 2   | B     | 208 | ILE  |
| 2   | B     | 221 | LEU  |
| 2   | B     | 231 | GLU  |
| 3   | C     | 5   | ILE  |
| 3   | C     | 21  | ARG  |
| 3   | C     | 26  | LYS  |
| 3   | C     | 28  | GLN  |
| 3   | C     | 34  | LEU  |
| 3   | C     | 37  | GLN  |
| 3   | C     | 64  | VAL  |
| 3   | C     | 97  | LYS  |
| 3   | C     | 101 | LEU  |
| 3   | C     | 102 | ASN  |
| 3   | C     | 104 | GLN  |
| 3   | C     | 107 | GLN  |
| 3   | C     | 164 | ARG  |
| 3   | C     | 175 | LEU  |
| 3   | C     | 188 | LEU  |
| 3   | C     | 192 | THR  |
| 4   | D     | 9   | CYS  |
| 4   | D     | 33  | MET  |
| 4   | D     | 34  | GLU  |
| 4   | D     | 58  | LEU  |
| 4   | D     | 65  | ARG  |
| 4   | D     | 70  | ILE  |
| 4   | D     | 112 | VAL  |
| 4   | D     | 141 | ARG  |
| 4   | D     | 146 | ILE  |
| 4   | D     | 177 | ASP  |
| 4   | D     | 199 | ASN  |
| 4   | D     | 201 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | E     | 12  | LEU  |
| 5   | E     | 20  | GLN  |
| 5   | E     | 31  | LEU  |
| 5   | E     | 41  | VAL  |
| 5   | E     | 43  | LEU  |
| 5   | E     | 53  | LEU  |
| 5   | E     | 64  | ARG  |
| 5   | E     | 75  | THR  |
| 5   | E     | 80  | ILE  |
| 5   | E     | 82  | VAL  |
| 5   | E     | 89  | ILE  |
| 5   | E     | 116 | THR  |
| 5   | E     | 143 | ARG  |
| 5   | E     | 144 | THR  |
| 5   | E     | 150 | ARG  |
| 6   | F     | 17  | SER  |
| 6   | F     | 19  | LEU  |
| 6   | F     | 24  | GLU  |
| 6   | F     | 69  | GLU  |
| 6   | F     | 75  | LEU  |
| 7   | G     | 38  | LEU  |
| 7   | G     | 51  | GLN  |
| 7   | G     | 57  | GLU  |
| 7   | G     | 78  | ARG  |
| 7   | G     | 113 | GLU  |
| 7   | G     | 114 | ARG  |
| 7   | G     | 144 | MET  |
| 7   | G     | 155 | ARG  |
| 7   | G     | 156 | TRP  |
| 8   | H     | 11  | THR  |
| 8   | H     | 26  | VAL  |
| 8   | H     | 37  | ARG  |
| 8   | H     | 39  | LEU  |
| 8   | H     | 52  | ASP  |
| 8   | H     | 63  | LEU  |
| 8   | H     | 85  | ARG  |
| 8   | H     | 91  | ARG  |
| 8   | H     | 112 | LEU  |
| 8   | H     | 119 | LEU  |
| 8   | H     | 122 | ARG  |
| 8   | H     | 127 | LEU  |
| 8   | H     | 133 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | I     | 79  | LEU  |
| 9   | I     | 97  | LYS  |
| 9   | I     | 102 | LEU  |
| 9   | I     | 108 | VAL  |
| 9   | I     | 111 | ARG  |
| 9   | I     | 125 | TYR  |
| 10  | J     | 6   | ILE  |
| 10  | J     | 14  | LYS  |
| 10  | J     | 21  | GLN  |
| 10  | J     | 22  | LYS  |
| 10  | J     | 80  | LYS  |
| 10  | J     | 83  | GLU  |
| 10  | J     | 98  | ILE  |
| 10  | J     | 99  | LYS  |
| 11  | K     | 12  | ARG  |
| 11  | K     | 18  | ARG  |
| 11  | K     | 29  | ILE  |
| 11  | K     | 47  | VAL  |
| 11  | K     | 92  | GLU  |
| 11  | K     | 108 | ILE  |
| 11  | K     | 114 | VAL  |
| 12  | L     | 46  | LYS  |
| 12  | L     | 53  | ARG  |
| 12  | L     | 59  | ARG  |
| 12  | L     | 60  | LEU  |
| 12  | L     | 67  | THR  |
| 12  | L     | 70  | ILE  |
| 12  | L     | 73  | GLU  |
| 12  | L     | 83  | VAL  |
| 12  | L     | 111 | LYS  |
| 12  | L     | 113 | ARG  |
| 12  | L     | 126 | LYS  |
| 13  | M     | 4   | ILE  |
| 13  | M     | 9   | ILE  |
| 13  | M     | 16  | ASP  |
| 13  | M     | 43  | THR  |
| 13  | M     | 44  | ARG  |
| 13  | M     | 56  | LEU  |
| 13  | M     | 70  | LEU  |
| 13  | M     | 110 | ARG  |
| 14  | N     | 8   | GLU  |
| 14  | N     | 18  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | N     | 23  | ARG  |
| 14  | N     | 26  | ARG  |
| 14  | N     | 32  | SER  |
| 14  | N     | 33  | VAL  |
| 14  | N     | 44  | LEU  |
| 15  | O     | 6   | GLU  |
| 15  | O     | 10  | LYS  |
| 15  | O     | 11  | VAL  |
| 15  | O     | 31  | LEU  |
| 15  | O     | 34  | LEU  |
| 15  | O     | 54  | ARG  |
| 15  | O     | 57  | LEU  |
| 15  | O     | 71  | GLN  |
| 16  | P     | 1   | MET  |
| 16  | P     | 2   | VAL  |
| 16  | P     | 8   | ARG  |
| 16  | P     | 19  | ILE  |
| 16  | P     | 45  | THR  |
| 16  | P     | 57  | ARG  |
| 16  | P     | 67  | THR  |
| 17  | Q     | 26  | GLN  |
| 17  | Q     | 59  | ILE  |
| 17  | Q     | 67  | LYS  |
| 17  | Q     | 68  | ARG  |
| 17  | Q     | 69  | LYS  |
| 17  | Q     | 74  | LEU  |
| 17  | Q     | 91  | ARG  |
| 17  | Q     | 101 | ARG  |
| 18  | R     | 39  | VAL  |
| 18  | R     | 88  | LYS  |
| 19  | S     | 15  | LEU  |
| 19  | S     | 42  | PRO  |
| 19  | S     | 43  | GLU  |
| 20  | T     | 10  | LEU  |
| 20  | T     | 13  | LEU  |
| 20  | T     | 41  | ILE  |
| 20  | T     | 42  | GLN  |
| 20  | T     | 48  | LYS  |
| 20  | T     | 57  | ARG  |
| 20  | T     | 62  | LEU  |
| 20  | T     | 72  | LEU  |
| 20  | T     | 73  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | T     | 75  | ASN  |
| 20  | T     | 84  | LEU  |
| 20  | T     | 90  | GLN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 19  | HIS  |
| 2   | B     | 25  | ASN  |
| 2   | B     | 146 | GLN  |
| 2   | B     | 204 | ASN  |
| 2   | B     | 212 | GLN  |
| 2   | B     | 240 | GLN  |
| 3   | C     | 6   | HIS  |
| 3   | C     | 28  | GLN  |
| 3   | C     | 31  | HIS  |
| 3   | C     | 37  | GLN  |
| 3   | C     | 63  | ASN  |
| 3   | C     | 102 | ASN  |
| 3   | C     | 104 | GLN  |
| 3   | C     | 107 | GLN  |
| 3   | C     | 110 | ASN  |
| 3   | C     | 136 | GLN  |
| 3   | C     | 162 | GLN  |
| 3   | C     | 176 | HIS  |
| 3   | C     | 181 | ASN  |
| 4   | D     | 42  | GLN  |
| 4   | D     | 43  | HIS  |
| 4   | D     | 62  | GLN  |
| 4   | D     | 160 | GLN  |
| 4   | D     | 199 | ASN  |
| 5   | E     | 20  | GLN  |
| 5   | E     | 73  | ASN  |
| 6   | F     | 7   | ASN  |
| 6   | F     | 18  | GLN  |
| 6   | F     | 27  | GLN  |
| 6   | F     | 32  | ASN  |
| 6   | F     | 57  | GLN  |
| 6   | F     | 64  | GLN  |
| 6   | F     | 94  | GLN  |
| 7   | G     | 37  | ASN  |
| 7   | G     | 56  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | G     | 64  | GLN  |
| 7   | G     | 96  | GLN  |
| 7   | G     | 106 | GLN  |
| 8   | H     | 70  | GLN  |
| 9   | I     | 3   | GLN  |
| 9   | I     | 23  | ASN  |
| 9   | I     | 31  | GLN  |
| 9   | I     | 73  | GLN  |
| 9   | I     | 87  | GLN  |
| 10  | J     | 21  | GLN  |
| 10  | J     | 78  | ASN  |
| 10  | J     | 84  | GLN  |
| 11  | K     | 13  | GLN  |
| 11  | K     | 22  | HIS  |
| 11  | K     | 38  | ASN  |
| 11  | K     | 62  | GLN  |
| 11  | K     | 93  | GLN  |
| 11  | K     | 117 | ASN  |
| 12  | L     | 49  | ASN  |
| 12  | L     | 75  | HIS  |
| 12  | L     | 78  | GLN  |
| 13  | M     | 40  | ASN  |
| 13  | M     | 62  | ASN  |
| 14  | N     | 49  | HIS  |
| 15  | O     | 13  | GLN  |
| 15  | O     | 37  | ASN  |
| 15  | O     | 71  | GLN  |
| 16  | P     | 16  | HIS  |
| 16  | P     | 65  | GLN  |
| 16  | P     | 76  | GLN  |
| 17  | Q     | 16  | GLN  |
| 17  | Q     | 26  | GLN  |
| 18  | R     | 36  | ASN  |
| 19  | S     | 14  | HIS  |
| 19  | S     | 23  | ASN  |
| 19  | S     | 47  | HIS  |
| 19  | S     | 56  | GLN  |
| 20  | T     | 42  | GLN  |
| 20  | T     | 73  | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | A     | 1510/1522 (99%) | 202 (13%)         | 58 (3%)         |
| 22  | X     | 4/6 (66%)       | 1 (25%)           | 0               |
| 23  | Y     | 12/17 (70%)     | 0                 | 0               |
| All | All   | 1526/1545 (98%) | 203 (13%)         | 58 (3%)         |

All (203) RNA backbone outliers are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 8      | A    |
| 1   | A     | 9      | G    |
| 1   | A     | 31     | G    |
| 1   | A     | 32     | A    |
| 1   | A     | 39     | G    |
| 1   | A     | 47     | C    |
| 1   | A     | 48     | C    |
| 1   | A     | 51     | A    |
| 1   | A     | 60     | A    |
| 1   | A     | 61     | G    |
| 1   | A     | 101    | A    |
| 1   | A     | 116    | A    |
| 1   | A     | 120    | A    |
| 1   | A     | 121    | C    |
| 1   | A     | 129(A) | G    |
| 1   | A     | 130    | A    |
| 1   | A     | 131    | C    |
| 1   | A     | 144    | G    |
| 1   | A     | 181    | G    |
| 1   | A     | 182    | U    |
| 1   | A     | 189(F) | U    |
| 1   | A     | 195    | A    |
| 1   | A     | 197    | A    |
| 1   | A     | 201    | C    |
| 1   | A     | 202    | U    |
| 1   | A     | 204    | U    |
| 1   | A     | 216    | G    |
| 1   | A     | 244    | U    |
| 1   | A     | 247    | G    |
| 1   | A     | 251    | G    |
| 1   | A     | 266    | G    |
| 1   | A     | 267    | C    |
| 1   | A     | 282    | A    |
| 1   | A     | 289    | G    |
| 1   | A     | 328    | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 329 | A    |
| 1   | A     | 332 | G    |
| 1   | A     | 345 | C    |
| 1   | A     | 352 | C    |
| 1   | A     | 353 | A    |
| 1   | A     | 354 | G    |
| 1   | A     | 367 | U    |
| 1   | A     | 373 | A    |
| 1   | A     | 397 | A    |
| 1   | A     | 398 | C    |
| 1   | A     | 411 | A    |
| 1   | A     | 412 | A    |
| 1   | A     | 413 | G    |
| 1   | A     | 414 | A    |
| 1   | A     | 421 | U    |
| 1   | A     | 429 | U    |
| 1   | A     | 430 | A    |
| 1   | A     | 439 | A    |
| 1   | A     | 442 | C    |
| 1   | A     | 444 | C    |
| 1   | A     | 452 | A    |
| 1   | A     | 470 | C    |
| 1   | A     | 484 | G    |
| 1   | A     | 485 | G    |
| 1   | A     | 496 | A    |
| 1   | A     | 498 | U    |
| 1   | A     | 509 | A    |
| 1   | A     | 510 | A    |
| 1   | A     | 511 | C    |
| 1   | A     | 518 | C    |
| 1   | A     | 527 | G    |
| 1   | A     | 531 | U    |
| 1   | A     | 532 | A    |
| 1   | A     | 533 | A    |
| 1   | A     | 534 | U    |
| 1   | A     | 547 | A    |
| 1   | A     | 559 | A    |
| 1   | A     | 560 | U    |
| 1   | A     | 561 | U    |
| 1   | A     | 562 | C    |
| 1   | A     | 572 | A    |
| 1   | A     | 573 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 576 | G    |
| 1   | A     | 577 | G    |
| 1   | A     | 630 | G    |
| 1   | A     | 631 | G    |
| 1   | A     | 632 | A    |
| 1   | A     | 653 | A    |
| 1   | A     | 665 | A    |
| 1   | A     | 688 | G    |
| 1   | A     | 701 | C    |
| 1   | A     | 702 | A    |
| 1   | A     | 703 | G    |
| 1   | A     | 723 | U    |
| 1   | A     | 726 | C    |
| 1   | A     | 731 | G    |
| 1   | A     | 734 | G    |
| 1   | A     | 749 | C    |
| 1   | A     | 755 | G    |
| 1   | A     | 777 | A    |
| 1   | A     | 781 | A    |
| 1   | A     | 782 | A    |
| 1   | A     | 794 | A    |
| 1   | A     | 813 | U    |
| 1   | A     | 817 | C    |
| 1   | A     | 819 | A    |
| 1   | A     | 821 | G    |
| 1   | A     | 828 | A    |
| 1   | A     | 839 | U    |
| 1   | A     | 840 | C    |
| 1   | A     | 841 | U    |
| 1   | A     | 848 | C    |
| 1   | A     | 874 | G    |
| 1   | A     | 902 | G    |
| 1   | A     | 914 | A    |
| 1   | A     | 926 | G    |
| 1   | A     | 927 | G    |
| 1   | A     | 934 | C    |
| 1   | A     | 935 | A    |
| 1   | A     | 960 | U    |
| 1   | A     | 961 | U    |
| 1   | A     | 965 | A    |
| 1   | A     | 966 | G    |
| 1   | A     | 969 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 971  | G    |
| 1   | A     | 974  | A    |
| 1   | A     | 975  | A    |
| 1   | A     | 976  | G    |
| 1   | A     | 977  | A    |
| 1   | A     | 978  | A    |
| 1   | A     | 991  | U    |
| 1   | A     | 992  | U    |
| 1   | A     | 993  | G    |
| 1   | A     | 994  | A    |
| 1   | A     | 1004 | A    |
| 1   | A     | 1025 | U    |
| 1   | A     | 1048 | G    |
| 1   | A     | 1050 | G    |
| 1   | A     | 1053 | G    |
| 1   | A     | 1054 | C    |
| 1   | A     | 1055 | A    |
| 1   | A     | 1065 | U    |
| 1   | A     | 1068 | G    |
| 1   | A     | 1094 | G    |
| 1   | A     | 1095 | U    |
| 1   | A     | 1101 | A    |
| 1   | A     | 1117 | G    |
| 1   | A     | 1125 | U    |
| 1   | A     | 1126 | U    |
| 1   | A     | 1129 | C    |
| 1   | A     | 1130 | A    |
| 1   | A     | 1131 | G    |
| 1   | A     | 1136 | U    |
| 1   | A     | 1137 | C    |
| 1   | A     | 1138 | G    |
| 1   | A     | 1139 | G    |
| 1   | A     | 1152 | A    |
| 1   | A     | 1159 | U    |
| 1   | A     | 1182 | G    |
| 1   | A     | 1183 | A    |
| 1   | A     | 1191 | A    |
| 1   | A     | 1196 | U    |
| 1   | A     | 1197 | G    |
| 1   | A     | 1201 | A    |
| 1   | A     | 1202 | G    |
| 1   | A     | 1212 | U    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | A     | 1213    | A    |
| 1   | A     | 1214    | C    |
| 1   | A     | 1227    | A    |
| 1   | A     | 1238    | A    |
| 1   | A     | 1256    | A    |
| 1   | A     | 1258    | G    |
| 1   | A     | 1280    | A    |
| 1   | A     | 1281    | U    |
| 1   | A     | 1282    | C    |
| 1   | A     | 1285    | A    |
| 1   | A     | 1286    | A    |
| 1   | A     | 1287    | A    |
| 1   | A     | 1300    | G    |
| 1   | A     | 1301    | U    |
| 1   | A     | 1302    | U    |
| 1   | A     | 1332    | A    |
| 1   | A     | 1346    | A    |
| 1   | A     | 1347    | G    |
| 1   | A     | 1348    | U    |
| 1   | A     | 1353    | G    |
| 1   | A     | 1363    | C    |
| 1   | A     | 1379    | G    |
| 1   | A     | 1398    | A    |
| 1   | A     | 1421    | G    |
| 1   | A     | 1442    | G    |
| 1   | A     | 1442(A) | G    |
| 1   | A     | 1442(B) | A    |
| 1   | A     | 1452    | C    |
| 1   | A     | 1492    | A    |
| 1   | A     | 1497    | G    |
| 1   | A     | 1498    | U    |
| 1   | A     | 1499    | A    |
| 1   | A     | 1502    | A    |
| 1   | A     | 1503    | A    |
| 1   | A     | 1504    | G    |
| 1   | A     | 1505    | G    |
| 1   | A     | 1506    | U    |
| 1   | A     | 1517    | G    |
| 1   | A     | 1520    | G    |
| 1   | A     | 1529    | G    |
| 1   | A     | 1530    | G    |
| 22  | X     | 4       | A    |

All (58) RNA pucker outliers are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 7      | G    |
| 1   | A     | 30     | U    |
| 1   | A     | 60     | A    |
| 1   | A     | 115    | G    |
| 1   | A     | 119    | A    |
| 1   | A     | 129(A) | G    |
| 1   | A     | 181    | G    |
| 1   | A     | 243    | A    |
| 1   | A     | 250    | A    |
| 1   | A     | 266    | G    |
| 1   | A     | 281    | G    |
| 1   | A     | 344    | A    |
| 1   | A     | 351    | G    |
| 1   | A     | 353    | A    |
| 1   | A     | 366    | C    |
| 1   | A     | 372    | C    |
| 1   | A     | 410    | G    |
| 1   | A     | 428    | G    |
| 1   | A     | 429    | U    |
| 1   | A     | 438    | G    |
| 1   | A     | 484    | G    |
| 1   | A     | 496    | A    |
| 1   | A     | 509    | A    |
| 1   | A     | 532    | A    |
| 1   | A     | 533    | A    |
| 1   | A     | 559    | A    |
| 1   | A     | 560    | U    |
| 1   | A     | 575    | G    |
| 1   | A     | 687    | A    |
| 1   | A     | 701    | C    |
| 1   | A     | 748    | C    |
| 1   | A     | 793    | U    |
| 1   | A     | 812    | C    |
| 1   | A     | 960    | U    |
| 1   | A     | 965    | A    |
| 1   | A     | 991    | U    |
| 1   | A     | 992    | U    |
| 1   | A     | 993    | G    |
| 1   | A     | 1049   | U    |
| 1   | A     | 1067   | A    |
| 1   | A     | 1129   | C    |
| 1   | A     | 1181   | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1182 | G    |
| 1   | A     | 1190 | G    |
| 1   | A     | 1201 | A    |
| 1   | A     | 1212 | U    |
| 1   | A     | 1281 | U    |
| 1   | A     | 1285 | A    |
| 1   | A     | 1300 | G    |
| 1   | A     | 1301 | U    |
| 1   | A     | 1331 | G    |
| 1   | A     | 1347 | G    |
| 1   | A     | 1397 | C    |
| 1   | A     | 1447 | A    |
| 1   | A     | 1498 | U    |
| 1   | A     | 1503 | A    |
| 1   | A     | 1504 | G    |
| 1   | A     | 1505 | G    |

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

2 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  | CM0  | Y     | 34  | 23   | 22,26,27     | 1.07 | 2 (9%)   | 28,37,40    | 3.05 | 3 (10%)  |
| 23  | 6MZ  | Y     | 37  | 23   | 22,25,26     | 0.50 | 0        | 30,36,39    | 0.63 | 1 (3%)   |

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  | CM0  | Y     | 34  | 23   | -       | 5/12/30/31 | 0/2/2/2 |
| 23  | 6MZ  | Y     | 37  | 23   | -       | 0/9/27/28  | 0/3/3/3 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 23  | Y     | 34  | CM0  | O5-C7 | 3.68 | 1.53        | 1.44     |
| 23  | Y     | 34  | CM0  | O8-C8 | 2.08 | 1.37        | 1.30     |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 23  | Y     | 34  | CM0  | C7-O5-C5 | 14.64 | 136.75      | 117.58   |
| 23  | Y     | 34  | CM0  | O5-C7-C8 | 5.33  | 122.45      | 110.88   |
| 23  | Y     | 37  | 6MZ  | C9-N6-C6 | 2.43  | 124.97      | 122.87   |
| 23  | Y     | 34  | CM0  | O4-C4-N3 | -2.14 | 116.01      | 120.12   |

There are no chirality outliers.

All (5) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 23  | Y     | 34  | CM0  | C4-C5-O5-C7 |
| 23  | Y     | 34  | CM0  | C6-C5-O5-C7 |
| 23  | Y     | 34  | CM0  | C8-C7-O5-C5 |
| 23  | Y     | 34  | CM0  | O5-C7-C8-O8 |
| 23  | Y     | 34  | CM0  | O5-C7-C8-O9 |

There are no ring outliers.

1 monomer is involved in 4 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 23  | Y     | 34  | CM0  | 4       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 195 ligands modelled in this entry, 194 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 24  | PAR  | A     | 1601 | -    | 45,45,45     | 1.56 | 7 (15%)     | 64,67,67    | 1.27 | 8 (12%)     |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 24  | PAR  | A     | 1601 | -    | -       | 2/18/94/94 | 0/4/4/4 |

All (7) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 24  | A     | 1601 | PAR  | C64-C54 | 5.01 | 1.58        | 1.52     |
| 24  | A     | 1601 | PAR  | C52-C42 | 3.07 | 1.58        | 1.52     |
| 24  | A     | 1601 | PAR  | O54-C14 | 3.01 | 1.49        | 1.41     |
| 24  | A     | 1601 | PAR  | C31-C21 | 2.70 | 1.56        | 1.53     |
| 24  | A     | 1601 | PAR  | C11-C21 | 2.41 | 1.57        | 1.52     |
| 24  | A     | 1601 | PAR  | O54-C54 | 2.05 | 1.49        | 1.44     |
| 24  | A     | 1601 | PAR  | C14-C24 | 2.04 | 1.56        | 1.52     |

All (8) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | A     | 1601 | PAR  | O33-C14-C24 | 4.20  | 115.45      | 108.22   |
| 24  | A     | 1601 | PAR  | O54-C54-C64 | 4.05  | 113.55      | 106.01   |
| 24  | A     | 1601 | PAR  | C14-O54-C54 | 3.35  | 120.26      | 113.69   |
| 24  | A     | 1601 | PAR  | O52-C13-C23 | 2.85  | 113.87      | 107.96   |
| 24  | A     | 1601 | PAR  | O52-C13-O43 | -2.51 | 108.71      | 111.43   |
| 24  | A     | 1601 | PAR  | C22-C32-C42 | 2.24  | 115.20      | 109.53   |
| 24  | A     | 1601 | PAR  | O11-C11-C21 | 2.19  | 111.99      | 108.22   |
| 24  | A     | 1601 | PAR  | C11-O51-C51 | 2.10  | 117.82      | 113.69   |

There are no chirality outliers.

All (2) torsion outliers are listed below:

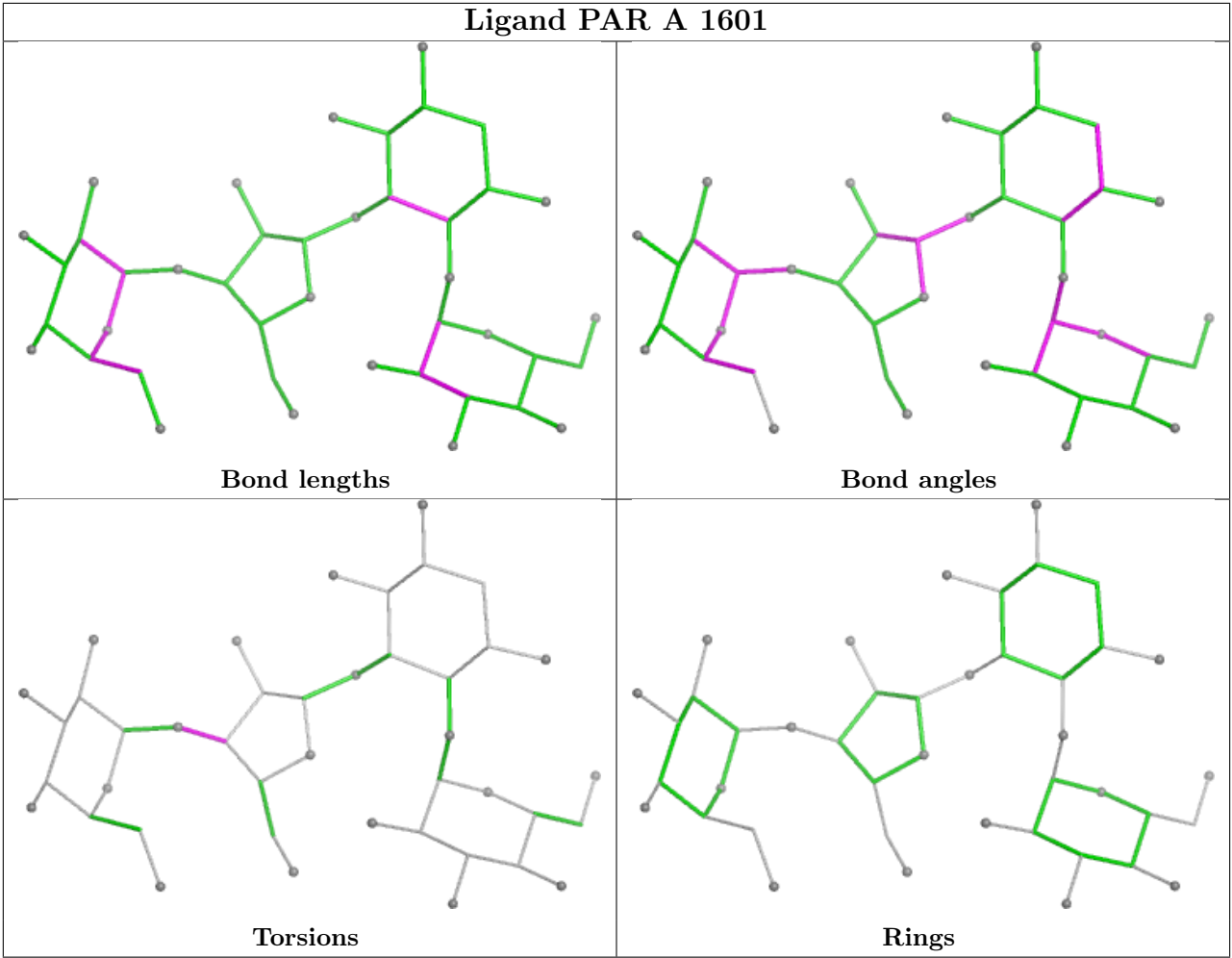
| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 24  | A     | 1601 | PAR  | C23-C33-O33-C14 |
| 24  | A     | 1601 | PAR  | C43-C33-O33-C14 |

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 24  | A     | 1601 | PAR  | 1       | 0            |

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1   | A     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | A     | 1533:C    | O3'    | 1539:C    | P      | 23.27        |

## 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     | 1512/1522 (99%) | 0.31   | 95 (6%) 26 20  | 30, 61, 130, 184      | 0     |
| 2   | B     | 235/256 (91%)   | 1.03   | 38 (16%) 4 4   | 51, 85, 127, 143      | 0     |
| 3   | C     | 207/239 (86%)   | 0.98   | 20 (9%) 13 11  | 53, 77, 110, 117      | 0     |
| 4   | D     | 208/209 (99%)   | 0.52   | 17 (8%) 17 14  | 49, 67, 88, 96        | 0     |
| 5   | E     | 151/162 (93%)   | 0.07   | 1 (0%) 84 79   | 35, 51, 70, 88        | 0     |
| 6   | F     | 101/101 (100%)  | 0.56   | 1 (0%) 79 73   | 60, 84, 92, 100       | 0     |
| 7   | G     | 155/156 (99%)   | 0.51   | 12 (7%) 19 16  | 52, 72, 104, 116      | 0     |
| 8   | H     | 138/138 (100%)  | -0.04  | 0 100 100      | 32, 51, 66, 74        | 0     |
| 9   | I     | 127/128 (99%)   | 1.09   | 19 (14%) 5 4   | 49, 83, 100, 106      | 0     |
| 10  | J     | 99/105 (94%)    | 1.94   | 43 (43%) 0 0   | 50, 104, 140, 145     | 0     |
| 11  | K     | 119/129 (92%)   | 0.30   | 4 (3%) 48 39   | 38, 59, 82, 100       | 0     |
| 12  | L     | 125/135 (92%)   | 0.52   | 8 (6%) 25 20   | 23, 60, 79, 100       | 0     |
| 13  | M     | 125/126 (99%)   | 1.09   | 21 (16%) 4 3   | 55, 73, 130, 159      | 0     |
| 14  | N     | 60/61 (98%)     | 0.97   | 7 (11%) 9 8    | 56, 70, 91, 102       | 0     |
| 15  | O     | 88/89 (98%)     | 0.08   | 1 (1%) 78 71   | 48, 66, 84, 103       | 0     |
| 16  | P     | 84/88 (95%)     | 0.06   | 0 100 100      | 41, 51, 65, 93        | 0     |
| 17  | Q     | 104/105 (99%)   | 0.33   | 7 (6%) 24 19   | 36, 55, 102, 132      | 0     |
| 18  | R     | 73/88 (82%)     | 0.41   | 4 (5%) 30 24   | 54, 69, 105, 134      | 0     |
| 19  | S     | 81/93 (87%)     | 1.29   | 12 (14%) 5 4   | 60, 87, 107, 116      | 0     |
| 20  | T     | 99/106 (93%)    | 0.43   | 5 (5%) 33 26   | 39, 57, 81, 87        | 0     |
| 21  | U     | 25/27 (92%)     | 1.11   | 4 (16%) 5 4    | 46, 64, 85, 88        | 0     |
| 22  | X     | 5/6 (83%)       | 0.61   | 1 (20%) 3 2    | 61, 64, 98, 105       | 0     |
| 23  | Y     | 11/17 (64%)     | 0.95   | 1 (9%) 15 12   | 69, 101, 135, 141     | 0     |
| All | All   | 3932/4086 (96%) | 0.52   | 321 (8%) 17 14 | 23, 66, 116, 184      | 0     |

All (321) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 17  | Q     | 105  | ALA  | 10.4 |
| 13  | M     | 125  | ARG  | 9.0  |
| 13  | M     | 119  | GLY  | 8.5  |
| 13  | M     | 126  | LYS  | 8.4  |
| 19  | S     | 3    | ARG  | 8.0  |
| 13  | M     | 124  | PRO  | 7.3  |
| 2   | B     | 16   | HIS  | 7.1  |
| 1   | A     | 1129 | C    | 6.8  |
| 4   | D     | 23   | GLY  | 5.7  |
| 13  | M     | 118  | ALA  | 5.4  |
| 21  | U     | 26   | LYS  | 5.3  |
| 13  | M     | 121  | LYS  | 5.2  |
| 1   | A     | 1003 | G    | 5.2  |
| 2   | B     | 19   | HIS  | 5.1  |
| 4   | D     | 26   | CYS  | 5.1  |
| 4   | D     | 31   | CYS  | 5.1  |
| 20  | T     | 100  | ILE  | 4.9  |
| 2   | B     | 10   | LEU  | 4.9  |
| 1   | A     | 1539 | C    | 4.9  |
| 17  | Q     | 100  | LYS  | 4.7  |
| 19  | S     | 5    | LEU  | 4.7  |
| 10  | J     | 88   | LEU  | 4.7  |
| 10  | J     | 90   | LEU  | 4.7  |
| 10  | J     | 82   | ILE  | 4.7  |
| 10  | J     | 75   | ILE  | 4.6  |
| 1   | A     | 1130 | A    | 4.6  |
| 13  | M     | 123  | ALA  | 4.5  |
| 13  | M     | 122  | LYS  | 4.5  |
| 11  | K     | 128  | ALA  | 4.5  |
| 10  | J     | 93   | GLY  | 4.5  |
| 1   | A     | 1124 | G    | 4.4  |
| 19  | S     | 2    | PRO  | 4.4  |
| 2   | B     | 230  | VAL  | 4.4  |
| 10  | J     | 43   | ARG  | 4.4  |
| 17  | Q     | 104  | LYS  | 4.3  |
| 10  | J     | 24   | VAL  | 4.2  |
| 1   | A     | 1533 | C    | 4.1  |
| 4   | D     | 9    | CYS  | 4.0  |
| 1   | A     | 1127 | G    | 4.0  |
| 10  | J     | 35   | SER  | 4.0  |
| 1   | A     | 1478 | C    | 3.9  |
| 2   | B     | 229  | VAL  | 3.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 10  | J     | 59   | SER  | 3.9  |
| 1   | A     | 1004 | A    | 3.9  |
| 1   | A     | 1126 | U    | 3.8  |
| 17  | Q     | 99   | SER  | 3.8  |
| 7   | G     | 156  | TRP  | 3.8  |
| 4   | D     | 24   | GLU  | 3.7  |
| 7   | G     | 5    | ARG  | 3.7  |
| 3   | C     | 60   | ALA  | 3.7  |
| 1   | A     | 1034 | G    | 3.7  |
| 1   | A     | 1144 | G    | 3.7  |
| 10  | J     | 79   | ARG  | 3.6  |
| 12  | L     | 26   | ALA  | 3.6  |
| 13  | M     | 120  | LYS  | 3.6  |
| 2   | B     | 14   | GLY  | 3.6  |
| 19  | S     | 4    | SER  | 3.5  |
| 3   | C     | 2    | GLY  | 3.5  |
| 2   | B     | 7    | VAL  | 3.5  |
| 1   | A     | 1125 | U    | 3.5  |
| 9   | I     | 102  | LEU  | 3.5  |
| 9   | I     | 8    | GLY  | 3.4  |
| 17  | Q     | 101  | ARG  | 3.4  |
| 10  | J     | 77   | PRO  | 3.4  |
| 13  | M     | 7    | VAL  | 3.4  |
| 1   | A     | 410  | G    | 3.4  |
| 1   | A     | 993  | G    | 3.4  |
| 1   | A     | 1531 | A    | 3.4  |
| 1   | A     | 1128 | C    | 3.4  |
| 2   | B     | 123  | ALA  | 3.4  |
| 2   | B     | 239  | VAL  | 3.4  |
| 10  | J     | 94   | VAL  | 3.4  |
| 15  | O     | 89   | GLY  | 3.4  |
| 1   | A     | 1256 | A    | 3.4  |
| 10  | J     | 87   | THR  | 3.4  |
| 1   | A     | 1259 | C    | 3.4  |
| 1   | A     | 1005 | A    | 3.4  |
| 4   | D     | 19   | LEU  | 3.3  |
| 1   | A     | 1258 | G    | 3.3  |
| 10  | J     | 101  | VAL  | 3.3  |
| 2   | B     | 122  | PHE  | 3.3  |
| 1   | A     | 1131 | G    | 3.3  |
| 19  | S     | 7    | LYS  | 3.3  |
| 1   | A     | 532  | A    | 3.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | B     | 234  | PRO  | 3.3  |
| 10  | J     | 37   | PRO  | 3.2  |
| 21  | U     | 25   | LYS  | 3.2  |
| 7   | G     | 85   | TYR  | 3.2  |
| 1   | A     | 1135 | U    | 3.2  |
| 3   | C     | 65   | ALA  | 3.2  |
| 14  | N     | 2    | ALA  | 3.2  |
| 1   | A     | 250  | A    | 3.2  |
| 1   | A     | 992  | U    | 3.2  |
| 1   | A     | 1281 | U    | 3.2  |
| 19  | S     | 14   | HIS  | 3.2  |
| 1   | A     | 631  | G    | 3.2  |
| 14  | N     | 13   | THR  | 3.2  |
| 19  | S     | 33   | THR  | 3.2  |
| 13  | M     | 10   | PRO  | 3.2  |
| 4   | D     | 151  | LYS  | 3.1  |
| 1   | A     | 1002 | G    | 3.1  |
| 2   | B     | 144  | ARG  | 3.1  |
| 9   | I     | 119  | ALA  | 3.1  |
| 13  | M     | 8    | GLU  | 3.1  |
| 4   | D     | 35   | ARG  | 3.1  |
| 10  | J     | 22   | LYS  | 3.1  |
| 10  | J     | 91   | PRO  | 3.1  |
| 19  | S     | 10   | PHE  | 3.1  |
| 10  | J     | 36   | GLY  | 3.1  |
| 1   | A     | 1541 | U    | 3.1  |
| 21  | U     | 24   | ARG  | 3.1  |
| 1   | A     | 1024 | G    | 3.0  |
| 1   | A     | 203  | U    | 3.0  |
| 2   | B     | 127  | ILE  | 3.0  |
| 18  | R     | 17   | SER  | 3.0  |
| 7   | G     | 80   | VAL  | 3.0  |
| 20  | T     | 74   | LYS  | 3.0  |
| 7   | G     | 83   | ALA  | 3.0  |
| 9   | I     | 64   | THR  | 3.0  |
| 4   | D     | 30   | LYS  | 2.9  |
| 7   | G     | 7    | ALA  | 2.9  |
| 12  | L     | 29   | GLY  | 2.9  |
| 3   | C     | 207  | VAL  | 2.9  |
| 12  | L     | 28   | LYS  | 2.9  |
| 1   | A     | 1134 | G    | 2.9  |
| 1   | A     | 1143 | G    | 2.9  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 4   | D     | 5       | ILE  | 2.9  |
| 1   | A     | 991     | U    | 2.9  |
| 9   | I     | 114     | TYR  | 2.9  |
| 7   | G     | 2       | ALA  | 2.9  |
| 9   | I     | 16      | ARG  | 2.9  |
| 13  | M     | 11      | ARG  | 2.9  |
| 3   | C     | 91      | LEU  | 2.9  |
| 1   | A     | 1140    | C    | 2.9  |
| 1   | A     | 1001(A) | G    | 2.9  |
| 18  | R     | 16      | PRO  | 2.9  |
| 10  | J     | 34      | VAL  | 2.9  |
| 10  | J     | 58      | ASP  | 2.9  |
| 2   | B     | 125     | PRO  | 2.8  |
| 13  | M     | 114     | ARG  | 2.8  |
| 1   | A     | 1146    | A    | 2.8  |
| 9   | I     | 17      | VAL  | 2.8  |
| 19  | S     | 81      | ARG  | 2.8  |
| 1   | A     | 1285    | A    | 2.8  |
| 12  | L     | 63      | GLY  | 2.8  |
| 19  | S     | 24      | ALA  | 2.8  |
| 1   | A     | 1039    | C    | 2.8  |
| 5   | E     | 20      | GLN  | 2.8  |
| 3   | C     | 64      | VAL  | 2.8  |
| 10  | J     | 74      | ILE  | 2.8  |
| 19  | S     | 6       | LYS  | 2.8  |
| 3   | C     | 82      | GLU  | 2.7  |
| 1   | A     | 460     | G    | 2.7  |
| 1   | A     | 1139    | G    | 2.7  |
| 2   | B     | 22      | LYS  | 2.7  |
| 1   | A     | 1001    | A    | 2.7  |
| 1   | A     | 1220    | G    | 2.7  |
| 3   | C     | 21      | ARG  | 2.7  |
| 10  | J     | 3       | LYS  | 2.7  |
| 7   | G     | 82      | GLY  | 2.7  |
| 1   | A     | 1421    | G    | 2.7  |
| 3   | C     | 71      | ALA  | 2.7  |
| 13  | M     | 9       | ILE  | 2.7  |
| 1   | A     | 1260    | C    | 2.7  |
| 2   | B     | 236     | TYR  | 2.7  |
| 10  | J     | 99      | LYS  | 2.6  |
| 2   | B     | 97      | TRP  | 2.6  |
| 1   | A     | 1141    | C    | 2.6  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 9   | I     | 14      | VAL  | 2.6  |
| 20  | T     | 12      | ALA  | 2.6  |
| 1   | A     | 1266    | G    | 2.6  |
| 2   | B     | 203     | GLY  | 2.6  |
| 2   | B     | 44      | LEU  | 2.6  |
| 2   | B     | 136     | VAL  | 2.6  |
| 4   | D     | 28      | SER  | 2.6  |
| 3   | C     | 85      | ARG  | 2.6  |
| 7   | G     | 155     | ARG  | 2.6  |
| 13  | M     | 2       | ALA  | 2.6  |
| 1   | A     | 1147    | C    | 2.6  |
| 1   | A     | 1200    | C    | 2.6  |
| 2   | B     | 238     | LEU  | 2.6  |
| 1   | A     | 1142    | G    | 2.5  |
| 10  | J     | 5       | ARG  | 2.5  |
| 7   | G     | 78      | ARG  | 2.5  |
| 3   | C     | 97      | LYS  | 2.5  |
| 1   | A     | 438     | G    | 2.5  |
| 1   | A     | 1181    | G    | 2.5  |
| 1   | A     | 1145    | C    | 2.5  |
| 18  | R     | 46      | GLU  | 2.5  |
| 10  | J     | 70      | ARG  | 2.5  |
| 10  | J     | 80      | LYS  | 2.5  |
| 10  | J     | 86      | MET  | 2.5  |
| 1   | A     | 1420    | C    | 2.5  |
| 1   | A     | 630     | G    | 2.5  |
| 4   | D     | 168     | ARG  | 2.5  |
| 2   | B     | 133     | LYS  | 2.5  |
| 3   | C     | 73      | PRO  | 2.5  |
| 2   | B     | 23      | ARG  | 2.5  |
| 1   | A     | 1006    | C    | 2.5  |
| 1   | A     | 1030(B) | C    | 2.5  |
| 2   | B     | 233     | SER  | 2.4  |
| 10  | J     | 46      | ARG  | 2.4  |
| 21  | U     | 10      | ARG  | 2.4  |
| 13  | M     | 13      | LYS  | 2.4  |
| 1   | A     | 1036    | G    | 2.4  |
| 4   | D     | 3       | ARG  | 2.4  |
| 1   | A     | 723     | U    | 2.4  |
| 10  | J     | 76      | ASN  | 2.4  |
| 2   | B     | 131     | PRO  | 2.4  |
| 9   | I     | 24      | GLY  | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 9   | I     | 9    | ARG  | 2.4  |
| 1   | A     | 1018 | C    | 2.4  |
| 2   | B     | 225  | ALA  | 2.4  |
| 2   | B     | 124  | SER  | 2.4  |
| 1   | A     | 1482 | G    | 2.4  |
| 9   | I     | 25   | LYS  | 2.3  |
| 13  | M     | 117  | VAL  | 2.3  |
| 1   | A     | 1038 | C    | 2.3  |
| 1   | A     | 1013 | G    | 2.3  |
| 4   | D     | 2    | GLY  | 2.3  |
| 9   | I     | 15   | ALA  | 2.3  |
| 2   | B     | 11   | LEU  | 2.3  |
| 9   | I     | 56   | LEU  | 2.3  |
| 10  | J     | 98   | ILE  | 2.3  |
| 7   | G     | 81   | GLY  | 2.3  |
| 10  | J     | 53   | PRO  | 2.3  |
| 1   | A     | 1261 | A    | 2.3  |
| 3   | C     | 9    | GLY  | 2.3  |
| 1   | A     | 413  | G    | 2.3  |
| 1   | A     | 428  | G    | 2.3  |
| 1   | A     | 1182 | G    | 2.3  |
| 9   | I     | 27   | THR  | 2.3  |
| 17  | Q     | 95   | TYR  | 2.3  |
| 1   | A     | 202  | U    | 2.3  |
| 1   | A     | 160  | A    | 2.2  |
| 23  | Y     | 41   | A    | 2.2  |
| 10  | J     | 7    | LYS  | 2.2  |
| 12  | L     | 115  | LYS  | 2.2  |
| 2   | B     | 140  | HIS  | 2.2  |
| 1   | A     | 1274 | G    | 2.2  |
| 11  | K     | 77   | MET  | 2.2  |
| 14  | N     | 10   | ALA  | 2.2  |
| 1   | A     | 1286 | A    | 2.2  |
| 3   | C     | 62   | ASP  | 2.2  |
| 7   | G     | 76   | ARG  | 2.2  |
| 2   | B     | 15   | VAL  | 2.2  |
| 3   | C     | 75   | VAL  | 2.2  |
| 9   | I     | 126  | SER  | 2.2  |
| 2   | B     | 18   | GLY  | 2.2  |
| 17  | Q     | 102  | GLY  | 2.2  |
| 1   | A     | 1026 | G    | 2.2  |
| 1   | A     | 1300 | G    | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 10  | J     | 83   | GLU  | 2.2  |
| 1   | A     | 1040 | U    | 2.2  |
| 3   | C     | 79   | ARG  | 2.2  |
| 10  | J     | 45   | ARG  | 2.2  |
| 13  | M     | 102  | ARG  | 2.2  |
| 1   | A     | 1279 | A    | 2.2  |
| 6   | F     | 63   | TYR  | 2.2  |
| 19  | S     | 25   | LYS  | 2.2  |
| 9   | I     | 29   | ASN  | 2.2  |
| 1   | A     | 1138 | G    | 2.2  |
| 1   | A     | 470  | C    | 2.2  |
| 2   | B     | 156  | LYS  | 2.2  |
| 2   | B     | 227  | GLY  | 2.2  |
| 10  | J     | 8    | LEU  | 2.2  |
| 3   | C     | 119  | ARG  | 2.1  |
| 10  | J     | 23   | ILE  | 2.1  |
| 18  | R     | 54   | ARG  | 2.1  |
| 1   | A     | 1212 | U    | 2.1  |
| 1   | A     | 1255 | G    | 2.1  |
| 1   | A     | 1419 | G    | 2.1  |
| 10  | J     | 10   | GLY  | 2.1  |
| 1   | A     | 1282 | C    | 2.1  |
| 20  | T     | 94   | ALA  | 2.1  |
| 2   | B     | 209  | ARG  | 2.1  |
| 2   | B     | 95   | GLN  | 2.1  |
| 10  | J     | 33   | GLN  | 2.1  |
| 3   | C     | 99   | VAL  | 2.1  |
| 2   | B     | 89   | GLY  | 2.1  |
| 1   | A     | 1191 | A    | 2.1  |
| 1   | A     | 1268 | A    | 2.1  |
| 12  | L     | 19   | ARG  | 2.1  |
| 20  | T     | 97   | ALA  | 2.1  |
| 22  | X     | 5    | A    | 2.1  |
| 9   | I     | 2    | GLU  | 2.1  |
| 1   | A     | 980  | C    | 2.1  |
| 1   | A     | 999  | C    | 2.1  |
| 1   | A     | 1262 | C    | 2.1  |
| 13  | M     | 113  | PRO  | 2.1  |
| 2   | B     | 13   | ALA  | 2.1  |
| 4   | D     | 179  | GLU  | 2.1  |
| 10  | J     | 4    | ILE  | 2.1  |
| 4   | D     | 12   | CYS  | 2.1  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 1   | A     | 1007    | C    | 2.1  |
| 1   | A     | 1190    | G    | 2.1  |
| 1   | A     | 1442(A) | G    | 2.1  |
| 12  | L     | 27      | LEU  | 2.1  |
| 2   | B     | 228     | GLY  | 2.1  |
| 3   | C     | 88      | ARG  | 2.1  |
| 14  | N     | 5       | ALA  | 2.1  |
| 10  | J     | 95      | GLU  | 2.1  |
| 1   | A     | 1248    | A    | 2.0  |
| 10  | J     | 78      | ASN  | 2.0  |
| 11  | K     | 54      | ARG  | 2.0  |
| 14  | N     | 57      | ARG  | 2.0  |
| 9   | I     | 7       | THR  | 2.0  |
| 10  | J     | 6       | ILE  | 2.0  |
| 11  | K     | 89      | ALA  | 2.0  |
| 4   | D     | 4       | TYR  | 2.0  |
| 3   | C     | 20      | SER  | 2.0  |
| 9   | I     | 38      | GLN  | 2.0  |
| 1   | A     | 1442(B) | A    | 2.0  |
| 14  | N     | 6       | LEU  | 2.0  |
| 10  | J     | 96      | ILE  | 2.0  |
| 12  | L     | 129     | ALA  | 2.0  |
| 13  | M     | 116     | THR  | 2.0  |
| 1   | A     | 1481    | U    | 2.0  |
| 1   | A     | 1033    | G    | 2.0  |
| 1   | A     | 1117    | G    | 2.0  |
| 14  | N     | 61      | TRP  | 2.0  |

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 23  | CM0  | Y     | 34  | 25/26 | 0.88 | 0.14 | 74,83,92,94                | 0     |
| 23  | 6MZ  | Y     | 37  | 23/24 | 0.94 | 0.11 | 70,72,74,76                | 0     |

### 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

### 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 25  | MG   | A     | 1653 | 1/1   | 0.31 | 0.62 | 114,114,114,114            | 0     |
| 26  | K    | A     | 1769 | 1/1   | 0.56 | 0.25 | 113,113,113,113            | 0     |
| 25  | MG   | A     | 1604 | 1/1   | 0.59 | 0.61 | 83,83,83,83                | 0     |
| 25  | MG   | A     | 1758 | 1/1   | 0.63 | 0.42 | 72,72,72,72                | 0     |
| 25  | MG   | A     | 1642 | 1/1   | 0.63 | 0.43 | 77,77,77,77                | 0     |
| 25  | MG   | A     | 1605 | 1/1   | 0.67 | 0.25 | 80,80,80,80                | 0     |
| 25  | MG   | A     | 1665 | 1/1   | 0.68 | 0.42 | 83,83,83,83                | 0     |
| 25  | MG   | A     | 1614 | 1/1   | 0.74 | 0.26 | 66,66,66,66                | 0     |
| 25  | MG   | A     | 1667 | 1/1   | 0.75 | 0.36 | 75,75,75,75                | 0     |
| 25  | MG   | A     | 1745 | 1/1   | 0.76 | 0.32 | 72,72,72,72                | 0     |
| 26  | K    | A     | 1776 | 1/1   | 0.77 | 0.15 | 98,98,98,98                | 0     |
| 25  | MG   | A     | 1610 | 1/1   | 0.78 | 0.41 | 76,76,76,76                | 0     |
| 26  | K    | A     | 1777 | 1/1   | 0.78 | 0.17 | 99,99,99,99                | 0     |
| 25  | MG   | A     | 1699 | 1/1   | 0.79 | 0.48 | 66,66,66,66                | 0     |
| 25  | MG   | G     | 201  | 1/1   | 0.79 | 0.20 | 77,77,77,77                | 0     |
| 25  | MG   | A     | 1730 | 1/1   | 0.79 | 0.13 | 38,38,38,38                | 0     |
| 25  | MG   | A     | 1688 | 1/1   | 0.79 | 0.43 | 70,70,70,70                | 0     |
| 25  | MG   | A     | 1755 | 1/1   | 0.79 | 0.42 | 68,68,68,68                | 0     |
| 25  | MG   | A     | 1747 | 1/1   | 0.80 | 0.23 | 57,57,57,57                | 0     |
| 25  | MG   | A     | 1749 | 1/1   | 0.80 | 0.30 | 60,60,60,60                | 0     |
| 26  | K    | A     | 1773 | 1/1   | 0.80 | 0.21 | 87,87,87,87                | 0     |
| 25  | MG   | A     | 1720 | 1/1   | 0.80 | 0.22 | 68,68,68,68                | 0     |
| 25  | MG   | A     | 1721 | 1/1   | 0.80 | 0.36 | 53,53,53,53                | 0     |
| 26  | K    | A     | 1778 | 1/1   | 0.81 | 0.18 | 105,105,105,105            | 0     |
| 25  | MG   | Q     | 201  | 1/1   | 0.82 | 0.24 | 71,71,71,71                | 0     |
| 25  | MG   | A     | 1687 | 1/1   | 0.82 | 0.48 | 77,77,77,77                | 0     |
| 25  | MG   | A     | 1686 | 1/1   | 0.82 | 0.48 | 85,85,85,85                | 0     |
| 25  | MG   | A     | 1741 | 1/1   | 0.83 | 0.18 | 46,46,46,46                | 0     |
| 25  | MG   | A     | 1673 | 1/1   | 0.83 | 0.31 | 58,58,58,58                | 0     |
| 26  | K    | A     | 1767 | 1/1   | 0.83 | 0.17 | 102,102,102,102            | 0     |
| 25  | MG   | A     | 1646 | 1/1   | 0.83 | 0.27 | 55,55,55,55                | 0     |
| 25  | MG   | A     | 1615 | 1/1   | 0.84 | 0.29 | 74,74,74,74                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 25  | MG   | A     | 1619 | 1/1   | 0.84 | 0.20 | 57,57,57,57                 | 0     |
| 25  | MG   | A     | 1714 | 1/1   | 0.84 | 0.18 | 43,43,43,43                 | 0     |
| 26  | K    | A     | 1765 | 1/1   | 0.84 | 0.14 | 97,97,97,97                 | 0     |
| 25  | MG   | A     | 1717 | 1/1   | 0.84 | 0.17 | 46,46,46,46                 | 0     |
| 26  | K    | A     | 1780 | 1/1   | 0.84 | 0.13 | 92,92,92,92                 | 0     |
| 25  | MG   | A     | 1636 | 1/1   | 0.85 | 0.17 | 52,52,52,52                 | 0     |
| 25  | MG   | A     | 1711 | 1/1   | 0.85 | 0.61 | 75,75,75,75                 | 0     |
| 25  | MG   | H     | 202  | 1/1   | 0.85 | 0.20 | 63,63,63,63                 | 0     |
| 25  | MG   | A     | 1634 | 1/1   | 0.85 | 0.27 | 50,50,50,50                 | 0     |
| 25  | MG   | A     | 1754 | 1/1   | 0.85 | 0.17 | 37,37,37,37                 | 0     |
| 25  | MG   | A     | 1662 | 1/1   | 0.85 | 0.50 | 94,94,94,94                 | 0     |
| 26  | K    | E     | 203  | 1/1   | 0.85 | 0.12 | 94,94,94,94                 | 0     |
| 25  | MG   | A     | 1658 | 1/1   | 0.86 | 0.27 | 73,73,73,73                 | 0     |
| 26  | K    | A     | 1771 | 1/1   | 0.86 | 0.31 | 108,108,108,108             | 0     |
| 25  | MG   | A     | 1638 | 1/1   | 0.86 | 0.32 | 67,67,67,67                 | 0     |
| 26  | K    | A     | 1775 | 1/1   | 0.86 | 0.12 | 97,97,97,97                 | 0     |
| 25  | MG   | A     | 1742 | 1/1   | 0.86 | 0.14 | 55,55,55,55                 | 0     |
| 25  | MG   | A     | 1620 | 1/1   | 0.86 | 0.27 | 72,72,72,72                 | 0     |
| 25  | MG   | A     | 1709 | 1/1   | 0.86 | 0.11 | 44,44,44,44                 | 0     |
| 25  | MG   | A     | 1710 | 1/1   | 0.86 | 0.25 | 66,66,66,66                 | 0     |
| 25  | MG   | A     | 1724 | 1/1   | 0.86 | 0.15 | 54,54,54,54                 | 0     |
| 25  | MG   | A     | 1641 | 1/1   | 0.87 | 0.33 | 64,64,64,64                 | 0     |
| 25  | MG   | A     | 1705 | 1/1   | 0.87 | 0.24 | 54,54,54,54                 | 0     |
| 25  | MG   | A     | 1612 | 1/1   | 0.87 | 0.13 | 57,57,57,57                 | 0     |
| 25  | MG   | A     | 1727 | 1/1   | 0.88 | 0.33 | 60,60,60,60                 | 0     |
| 25  | MG   | A     | 1748 | 1/1   | 0.88 | 0.25 | 56,56,56,56                 | 0     |
| 25  | MG   | A     | 1650 | 1/1   | 0.88 | 0.49 | 73,73,73,73                 | 0     |
| 25  | MG   | A     | 1738 | 1/1   | 0.88 | 0.46 | 73,73,73,73                 | 0     |
| 25  | MG   | A     | 1696 | 1/1   | 0.89 | 0.25 | 30,30,30,30                 | 0     |
| 25  | MG   | A     | 1681 | 1/1   | 0.89 | 0.16 | 41,41,41,41                 | 0     |
| 25  | MG   | A     | 1718 | 1/1   | 0.89 | 0.21 | 46,46,46,46                 | 0     |
| 25  | MG   | A     | 1782 | 1/1   | 0.89 | 0.10 | 45,45,45,45                 | 0     |
| 26  | K    | A     | 1779 | 1/1   | 0.89 | 0.18 | 102,102,102,102             | 0     |
| 25  | MG   | A     | 1750 | 1/1   | 0.89 | 0.21 | 55,55,55,55                 | 0     |
| 25  | MG   | A     | 1751 | 1/1   | 0.89 | 0.08 | 33,33,33,33                 | 0     |
| 25  | MG   | A     | 1740 | 1/1   | 0.90 | 0.09 | 49,49,49,49                 | 0     |
| 25  | MG   | A     | 1632 | 1/1   | 0.90 | 0.24 | 34,34,34,34                 | 0     |
| 25  | MG   | A     | 1603 | 1/1   | 0.90 | 0.50 | 73,73,73,73                 | 0     |
| 25  | MG   | A     | 1644 | 1/1   | 0.90 | 0.45 | 62,62,62,62                 | 0     |
| 25  | MG   | F     | 201  | 1/1   | 0.90 | 0.14 | 68,68,68,68                 | 0     |
| 25  | MG   | A     | 1609 | 1/1   | 0.90 | 0.22 | 60,60,60,60                 | 0     |
| 25  | MG   | A     | 1623 | 1/1   | 0.90 | 0.30 | 32,32,32,32                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 25  | MG   | A     | 1690 | 1/1   | 0.90 | 0.27 | 39,39,39,39                 | 0     |
| 25  | MG   | A     | 1732 | 1/1   | 0.90 | 0.38 | 66,66,66,66                 | 0     |
| 25  | MG   | A     | 1668 | 1/1   | 0.90 | 0.19 | 47,47,47,47                 | 0     |
| 24  | PAR  | A     | 1601 | 42/42 | 0.91 | 0.19 | 47,52,74,78                 | 0     |
| 25  | MG   | A     | 1680 | 1/1   | 0.91 | 0.24 | 35,35,35,35                 | 0     |
| 25  | MG   | A     | 1664 | 1/1   | 0.91 | 0.14 | 42,42,42,42                 | 0     |
| 25  | MG   | A     | 1706 | 1/1   | 0.91 | 0.22 | 48,48,48,48                 | 0     |
| 26  | K    | A     | 1768 | 1/1   | 0.91 | 0.20 | 88,88,88,88                 | 0     |
| 25  | MG   | A     | 1725 | 1/1   | 0.91 | 0.20 | 43,43,43,43                 | 0     |
| 25  | MG   | A     | 1708 | 1/1   | 0.91 | 0.07 | 33,33,33,33                 | 0     |
| 25  | MG   | A     | 1728 | 1/1   | 0.91 | 0.15 | 64,64,64,64                 | 0     |
| 26  | K    | A     | 1774 | 1/1   | 0.91 | 0.11 | 80,80,80,80                 | 0     |
| 25  | MG   | A     | 1654 | 1/1   | 0.91 | 0.63 | 73,73,73,73                 | 0     |
| 25  | MG   | A     | 1616 | 1/1   | 0.91 | 0.35 | 73,73,73,73                 | 0     |
| 25  | MG   | A     | 1757 | 1/1   | 0.91 | 0.20 | 74,74,74,74                 | 0     |
| 25  | MG   | A     | 1736 | 1/1   | 0.91 | 0.09 | 32,32,32,32                 | 0     |
| 25  | MG   | A     | 1659 | 1/1   | 0.91 | 0.13 | 31,31,31,31                 | 0     |
| 25  | MG   | A     | 1671 | 1/1   | 0.91 | 0.23 | 32,32,32,32                 | 0     |
| 25  | MG   | A     | 1693 | 1/1   | 0.91 | 0.23 | 31,31,31,31                 | 0     |
| 25  | MG   | A     | 1608 | 1/1   | 0.92 | 0.20 | 10,10,10,10                 | 0     |
| 25  | MG   | A     | 1744 | 1/1   | 0.92 | 0.10 | 39,39,39,39                 | 0     |
| 26  | K    | A     | 1762 | 1/1   | 0.92 | 0.06 | 74,74,74,74                 | 0     |
| 25  | MG   | A     | 1695 | 1/1   | 0.92 | 0.26 | 42,42,42,42                 | 0     |
| 25  | MG   | A     | 1660 | 1/1   | 0.92 | 0.10 | 46,46,46,46                 | 0     |
| 25  | MG   | A     | 1676 | 1/1   | 0.92 | 0.17 | 37,37,37,37                 | 0     |
| 25  | MG   | A     | 1703 | 1/1   | 0.92 | 0.15 | 45,45,45,45                 | 0     |
| 25  | MG   | A     | 1678 | 1/1   | 0.92 | 0.12 | 34,34,34,34                 | 0     |
| 26  | K    | A     | 1772 | 1/1   | 0.92 | 0.10 | 90,90,90,90                 | 0     |
| 25  | MG   | A     | 1652 | 1/1   | 0.92 | 0.40 | 57,57,57,57                 | 0     |
| 25  | MG   | A     | 1707 | 1/1   | 0.92 | 0.10 | 33,33,33,33                 | 0     |
| 25  | MG   | A     | 1602 | 1/1   | 0.92 | 0.54 | 69,69,69,69                 | 0     |
| 25  | MG   | A     | 1647 | 1/1   | 0.92 | 0.36 | 54,54,54,54                 | 0     |
| 25  | MG   | A     | 1666 | 1/1   | 0.92 | 0.18 | 59,59,59,59                 | 0     |
| 25  | MG   | A     | 1655 | 1/1   | 0.92 | 0.18 | 42,42,42,42                 | 0     |
| 25  | MG   | B     | 301  | 1/1   | 0.92 | 0.14 | 51,51,51,51                 | 0     |
| 25  | MG   | A     | 1649 | 1/1   | 0.92 | 0.25 | 32,32,32,32                 | 0     |
| 25  | MG   | A     | 1716 | 1/1   | 0.92 | 0.10 | 59,59,59,59                 | 0     |
| 25  | MG   | A     | 1629 | 1/1   | 0.93 | 0.22 | 33,33,33,33                 | 0     |
| 25  | MG   | A     | 1704 | 1/1   | 0.93 | 0.25 | 69,69,69,69                 | 0     |
| 25  | MG   | A     | 1734 | 1/1   | 0.93 | 0.21 | 29,29,29,29                 | 0     |
| 25  | MG   | A     | 1674 | 1/1   | 0.93 | 0.47 | 61,61,61,61                 | 0     |
| 25  | MG   | A     | 1613 | 1/1   | 0.93 | 0.14 | 33,33,33,33                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 25  | MG   | A     | 1611 | 1/1   | 0.93 | 0.07 | 45,45,45,45                 | 0     |
| 25  | MG   | A     | 1648 | 1/1   | 0.93 | 0.29 | 56,56,56,56                 | 0     |
| 25  | MG   | A     | 1663 | 1/1   | 0.93 | 0.14 | 38,38,38,38                 | 0     |
| 25  | MG   | A     | 1635 | 1/1   | 0.93 | 0.38 | 60,60,60,60                 | 0     |
| 25  | MG   | A     | 1621 | 1/1   | 0.93 | 0.45 | 70,70,70,70                 | 0     |
| 25  | MG   | A     | 1622 | 1/1   | 0.93 | 0.25 | 31,31,31,31                 | 0     |
| 25  | MG   | A     | 1640 | 1/1   | 0.93 | 0.33 | 46,46,46,46                 | 0     |
| 25  | MG   | A     | 1691 | 1/1   | 0.93 | 0.37 | 46,46,46,46                 | 0     |
| 25  | MG   | A     | 1617 | 1/1   | 0.93 | 0.43 | 56,56,56,56                 | 0     |
| 25  | MG   | A     | 1694 | 1/1   | 0.93 | 0.15 | 35,35,35,35                 | 0     |
| 25  | MG   | A     | 1753 | 1/1   | 0.93 | 0.18 | 51,51,51,51                 | 0     |
| 25  | MG   | A     | 1669 | 1/1   | 0.93 | 0.35 | 55,55,55,55                 | 0     |
| 25  | MG   | A     | 1625 | 1/1   | 0.93 | 0.50 | 70,70,70,70                 | 0     |
| 25  | MG   | A     | 1697 | 1/1   | 0.93 | 0.08 | 36,36,36,36                 | 0     |
| 25  | MG   | A     | 1672 | 1/1   | 0.93 | 0.15 | 37,37,37,37                 | 0     |
| 25  | MG   | A     | 1700 | 1/1   | 0.93 | 0.20 | 57,57,57,57                 | 0     |
| 25  | MG   | A     | 1729 | 1/1   | 0.94 | 0.20 | 33,33,33,33                 | 0     |
| 25  | MG   | A     | 1685 | 1/1   | 0.94 | 0.29 | 51,51,51,51                 | 0     |
| 25  | MG   | A     | 1631 | 1/1   | 0.94 | 0.15 | 39,39,39,39                 | 0     |
| 25  | MG   | A     | 1627 | 1/1   | 0.94 | 0.33 | 35,35,35,35                 | 0     |
| 25  | MG   | A     | 1633 | 1/1   | 0.94 | 0.37 | 42,42,42,42                 | 0     |
| 25  | MG   | A     | 1702 | 1/1   | 0.94 | 0.10 | 45,45,45,45                 | 0     |
| 25  | MG   | A     | 1689 | 1/1   | 0.94 | 0.36 | 64,64,64,64                 | 0     |
| 25  | MG   | A     | 1719 | 1/1   | 0.94 | 0.11 | 26,26,26,26                 | 0     |
| 25  | MG   | A     | 1630 | 1/1   | 0.94 | 0.25 | 52,52,52,52                 | 0     |
| 25  | MG   | A     | 1656 | 1/1   | 0.94 | 0.37 | 63,63,63,63                 | 0     |
| 25  | MG   | A     | 1692 | 1/1   | 0.94 | 0.11 | 31,31,31,31                 | 0     |
| 25  | MG   | A     | 1670 | 1/1   | 0.94 | 0.13 | 34,34,34,34                 | 0     |
| 25  | MG   | A     | 1657 | 1/1   | 0.94 | 0.16 | 29,29,29,29                 | 0     |
| 26  | K    | A     | 1761 | 1/1   | 0.94 | 0.08 | 83,83,83,83                 | 0     |
| 25  | MG   | A     | 1682 | 1/1   | 0.94 | 0.14 | 26,26,26,26                 | 0     |
| 26  | K    | A     | 1764 | 1/1   | 0.95 | 0.23 | 88,88,88,88                 | 0     |
| 25  | MG   | A     | 1743 | 1/1   | 0.95 | 0.24 | 55,55,55,55                 | 0     |
| 26  | K    | A     | 1766 | 1/1   | 0.95 | 0.12 | 88,88,88,88                 | 0     |
| 25  | MG   | A     | 1645 | 1/1   | 0.95 | 0.27 | 33,33,33,33                 | 0     |
| 25  | MG   | A     | 1723 | 1/1   | 0.95 | 0.23 | 48,48,48,48                 | 0     |
| 25  | MG   | A     | 1701 | 1/1   | 0.95 | 0.11 | 35,35,35,35                 | 0     |
| 25  | MG   | A     | 1735 | 1/1   | 0.95 | 0.12 | 23,23,23,23                 | 0     |
| 25  | MG   | D     | 302  | 1/1   | 0.95 | 0.12 | 42,42,42,42                 | 0     |
| 25  | MG   | E     | 202  | 1/1   | 0.95 | 0.14 | 62,62,62,62                 | 0     |
| 25  | MG   | A     | 1643 | 1/1   | 0.95 | 0.08 | 28,28,28,28                 | 0     |
| 25  | MG   | A     | 1726 | 1/1   | 0.95 | 0.07 | 35,35,35,35                 | 0     |

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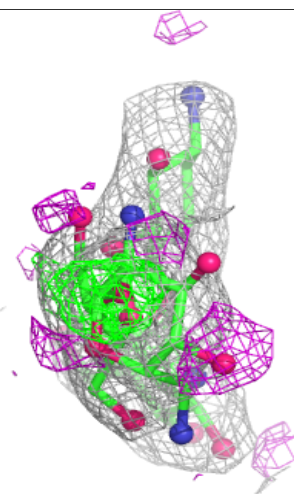
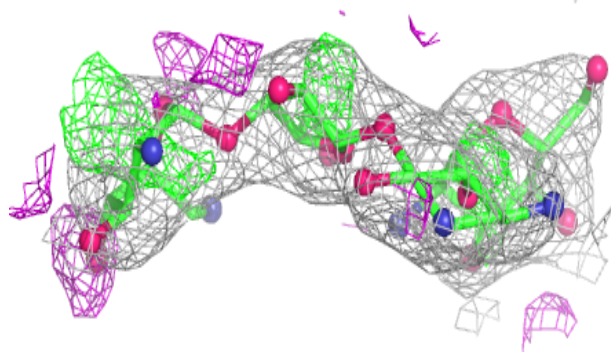
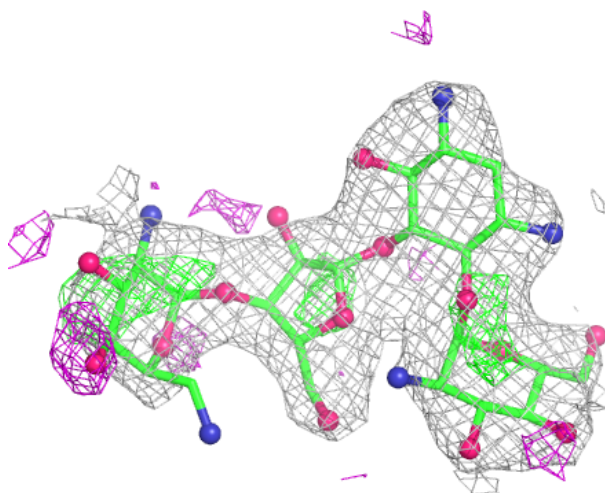
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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 25  | MG   | H     | 201  | 1/1   | 0.95 | 0.18 | 62,62,62,62                 | 0     |
| 25  | MG   | A     | 1618 | 1/1   | 0.95 | 0.34 | 45,45,45,45                 | 0     |
| 25  | MG   | A     | 1752 | 1/1   | 0.95 | 0.14 | 62,62,62,62                 | 0     |
| 26  | K    | A     | 1760 | 1/1   | 0.95 | 0.06 | 68,68,68,68                 | 0     |
| 25  | MG   | A     | 1698 | 1/1   | 0.95 | 0.21 | 36,36,36,36                 | 0     |
| 25  | MG   | A     | 1661 | 1/1   | 0.95 | 0.29 | 41,41,41,41                 | 0     |
| 27  | ZN   | D     | 301  | 1/1   | 0.95 | 0.19 | 70,70,70,70                 | 0     |
| 26  | K    | A     | 1770 | 1/1   | 0.96 | 0.05 | 98,98,98,98                 | 0     |
| 25  | MG   | A     | 1756 | 1/1   | 0.96 | 0.46 | 79,79,79,79                 | 0     |
| 25  | MG   | A     | 1624 | 1/1   | 0.96 | 0.39 | 37,37,37,37                 | 0     |
| 25  | MG   | A     | 1675 | 1/1   | 0.96 | 0.21 | 43,43,43,43                 | 0     |
| 25  | MG   | A     | 1759 | 1/1   | 0.96 | 0.08 | 44,44,44,44                 | 0     |
| 25  | MG   | A     | 1781 | 1/1   | 0.96 | 0.09 | 34,34,34,34                 | 0     |
| 25  | MG   | A     | 1637 | 1/1   | 0.96 | 0.10 | 35,35,35,35                 | 0     |
| 25  | MG   | A     | 1683 | 1/1   | 0.96 | 0.33 | 45,45,45,45                 | 0     |
| 25  | MG   | A     | 1684 | 1/1   | 0.96 | 0.08 | 16,16,16,16                 | 0     |
| 25  | MG   | E     | 201  | 1/1   | 0.96 | 0.24 | 41,41,41,41                 | 0     |
| 25  | MG   | A     | 1715 | 1/1   | 0.96 | 0.15 | 51,51,51,51                 | 0     |
| 25  | MG   | A     | 1626 | 1/1   | 0.96 | 0.34 | 52,52,52,52                 | 0     |
| 25  | MG   | A     | 1679 | 1/1   | 0.96 | 0.33 | 43,43,43,43                 | 0     |
| 26  | K    | A     | 1763 | 1/1   | 0.97 | 0.08 | 88,88,88,88                 | 0     |
| 25  | MG   | A     | 1737 | 1/1   | 0.97 | 0.07 | 28,28,28,28                 | 0     |
| 25  | MG   | A     | 1606 | 1/1   | 0.97 | 0.37 | 38,38,38,38                 | 0     |
| 25  | MG   | A     | 1739 | 1/1   | 0.97 | 0.07 | 37,37,37,37                 | 0     |
| 25  | MG   | A     | 1722 | 1/1   | 0.97 | 0.07 | 41,41,41,41                 | 0     |
| 25  | MG   | A     | 1607 | 1/1   | 0.97 | 0.19 | 36,36,36,36                 | 0     |
| 25  | MG   | A     | 1628 | 1/1   | 0.97 | 0.32 | 32,32,32,32                 | 0     |
| 25  | MG   | A     | 1712 | 1/1   | 0.97 | 0.06 | 27,27,27,27                 | 0     |
| 25  | MG   | A     | 1713 | 1/1   | 0.97 | 0.15 | 28,28,28,28                 | 0     |
| 25  | MG   | A     | 1651 | 1/1   | 0.97 | 0.40 | 57,57,57,57                 | 0     |
| 25  | MG   | A     | 1731 | 1/1   | 0.98 | 0.03 | 20,20,20,20                 | 0     |
| 25  | MG   | A     | 1733 | 1/1   | 0.98 | 0.05 | 23,23,23,23                 | 0     |
| 25  | MG   | A     | 1746 | 1/1   | 0.98 | 0.04 | 15,15,15,15                 | 0     |
| 25  | MG   | A     | 1783 | 1/1   | 0.98 | 0.07 | 58,58,58,58                 | 0     |
| 25  | MG   | A     | 1677 | 1/1   | 0.99 | 0.12 | 23,23,23,23                 | 0     |
| 25  | MG   | A     | 1639 | 1/1   | 0.99 | 0.17 | 2,2,2,2                     | 0     |
| 27  | ZN   | N     | 101  | 1/1   | 0.99 | 0.02 | 67,67,67,67                 | 0     |

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

**Electron density around PAR A 1601:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.