



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2018 – 02:46 PM EST

PDB ID : 2VQE  
Title : Modified uridines with C5-methylene substituents at the first position of the tRNA anticodon stabilize U-G wobble pairing during decoding  
Authors : Kurata, S.; Weixlbaumer, A.; Ohtsuki, T.; Shimazaki, T.; Wada, T.; Kirino, Y.; Takai, K.; Watanabe, K.; Ramakrishnan, V.; Suzuki, T.  
Deposited on : 2008-03-13  
Resolution : 2.50 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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031633  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031633

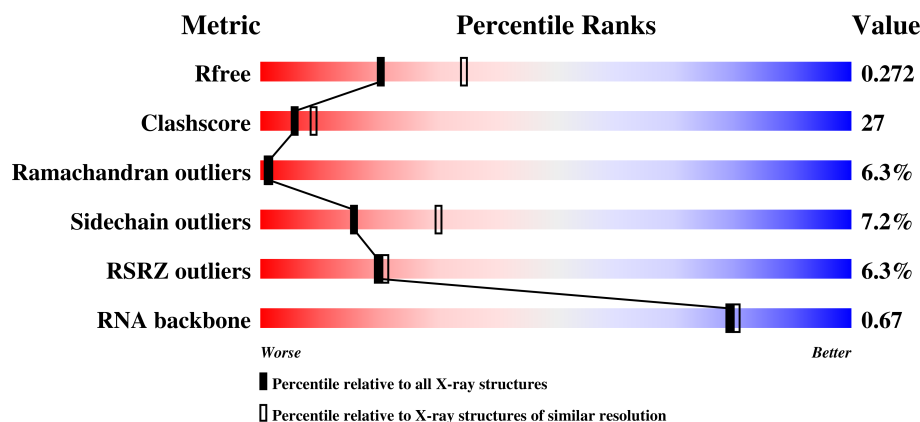
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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






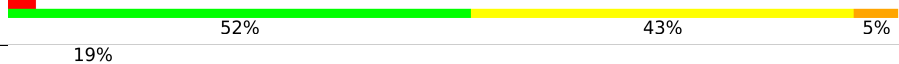
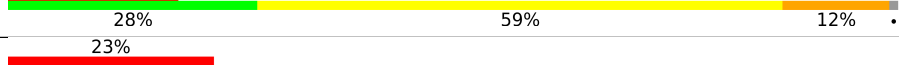
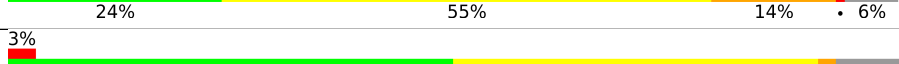
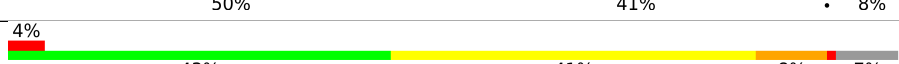
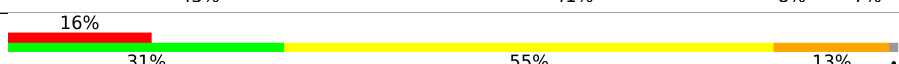
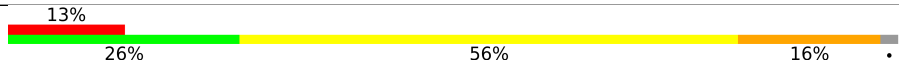
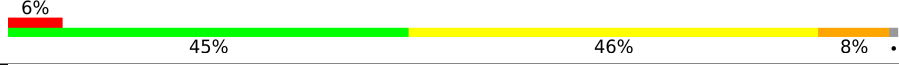
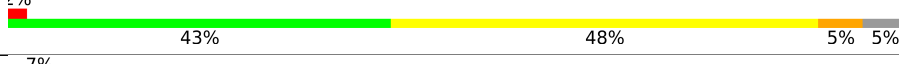
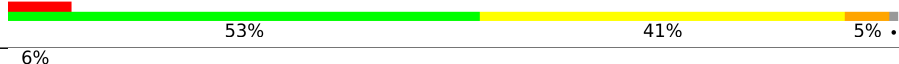
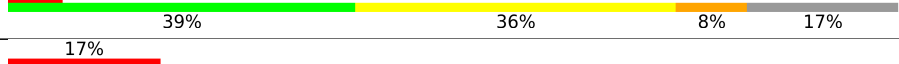

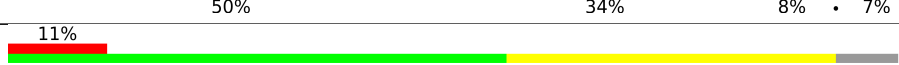
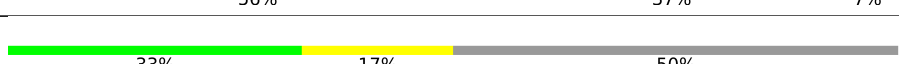
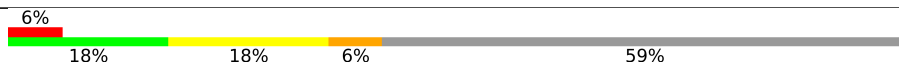

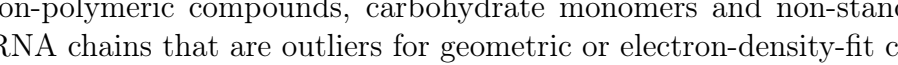
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 111664                      | 4155 (2.50-2.50)                                      |
| Clashscore            | 122126                      | 4827 (2.50-2.50)                                      |
| Ramachandran outliers | 120053                      | 4735 (2.50-2.50)                                      |
| Sidechain outliers    | 120020                      | 4737 (2.50-2.50)                                      |
| RSRZ outliers         | 108989                      | 4058 (2.50-2.50)                                      |
| RNA backbone          | 2636                        | 1092 (2.90-2.10)                                      |

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

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | A     | 1522   | <div> <div>2%</div> <div> <div></div> <div>39%</div> <div>48%</div> <div>10%</div> <div>..</div> </div> </div>  |
| 2   | B     | 256    | <div> <div>9%</div> <div> <div></div> <div>29%</div> <div>50%</div> <div>12%</div> <div>8%</div> </div> </div>  |
| 3   | C     | 239    | <div> <div>9%</div> <div> <div></div> <div>27%</div> <div>46%</div> <div>13%</div> <div>13%</div> </div> </div> |
| 4   | D     | 209    | <div> <div>10%</div> <div> <div></div> <div>53%</div> <div>43%</div> <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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 24  | MG   | A     | 1603 | -         | -        | -       | X                |
| 24  | MG   | A     | 1610 | -         | -        | -       | X                |
| 24  | MG   | A     | 1626 | -         | -        | -       | X                |
| 24  | MG   | A     | 1632 | -         | -        | -       | X                |
| 24  | MG   | A     | 1641 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 24  | MG   | A     | 1643 | -         | -        | -       | X                |
| 24  | MG   | A     | 1658 | -         | -        | -       | X                |
| 24  | MG   | A     | 1665 | -         | -        | -       | X                |
| 24  | MG   | A     | 1678 | -         | -        | -       | X                |
| 24  | MG   | A     | 1709 | -         | -        | -       | X                |
| 24  | MG   | A     | 1710 | -         | -        | -       | X                |
| 24  | MG   | A     | 1715 | -         | -        | -       | X                |
| 24  | MG   | A     | 1731 | -         | -        | -       | X                |
| 24  | MG   | A     | 1758 | -         | -        | -       | X                |
| 24  | MG   | A     | 1773 | -         | -        | -       | X                |
| 25  | K    | A     | 1819 | -         | -        | -       | X                |
| 25  | K    | A     | 1851 | -         | -        | -       | X                |

## 2 Entry composition [i](#)

There are 27 unique types of molecules in this entry. The entry contains 52245 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1   | A     | 1513     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32511 | 14472 | 6016 | 10511 | 1512 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | B     | 236      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1874  | 1195 | 336 | 338 | 5 |         |         |       |

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | J     | 99       | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 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 TYPE Z.

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

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | S     | 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     |
|     |       |          | 762   | 469 | 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(\*UP\*UP\*AP\*AP\*AP\*AP)-3'.

| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---|---------|---------|-------|
| 22  | X     | 3        | Total | C  | N | O  | P | 0       | 0       | 0     |
|     |       |          | 59    | 28 | 9 | 20 | 2 |         |         |       |

- Molecule 23 is a RNA chain called 5'-R(\*GP\*CP\*AP\*UP\*GP\*CP\*UP\*TM2P\*AP\*AP\*AP\*AP\*CP\*AP\*UP\*GP\*CP)-3'.

| Mol | Chain | Residues | Atoms |    |    |    |   |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---|---------|---------|-------|
| 23  | Y     | 7        | Total | C  | N  | O  | P | S | 0       | 0       | 0     |
|     |       |          | 153   | 70 | 28 | 48 | 6 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 24  | Q     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 24  | D     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 24  | E     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 24  | B     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 24  | I     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 24  | A     | 199      | Total | Mg  | 0       | 0       |
|     |       |          | 199   | 199 |         |         |
| 24  | N     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 24  | M     | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |

- Molecule 25 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 25  | P     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 25  | E     | 3        | Total | K | 0       | 0       |
|     |       |          | 3     | 3 |         |         |

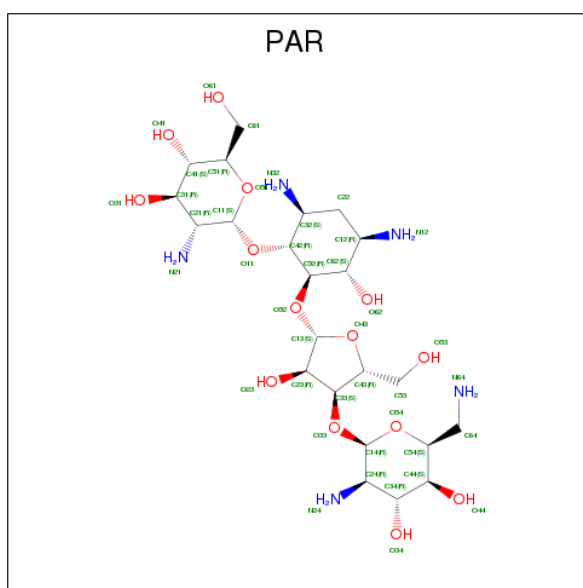
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| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 25  | I     | 1        | Total K<br>1 1   | 0       | 0       |
| 25  | A     | 54       | Total K<br>54 54 | 0       | 0       |
| 25  | T     | 1        | Total K<br>1 1   | 0       | 0       |
| 25  | N     | 1        | Total K<br>1 1   | 0       | 0       |
| 25  | R     | 1        | Total K<br>1 1   | 0       | 0       |

- Molecule 26 is PAROMOMYCIN (three-letter code: PAR) (formula:  $C_{23}H_{45}N_5O_{14}$ ).



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

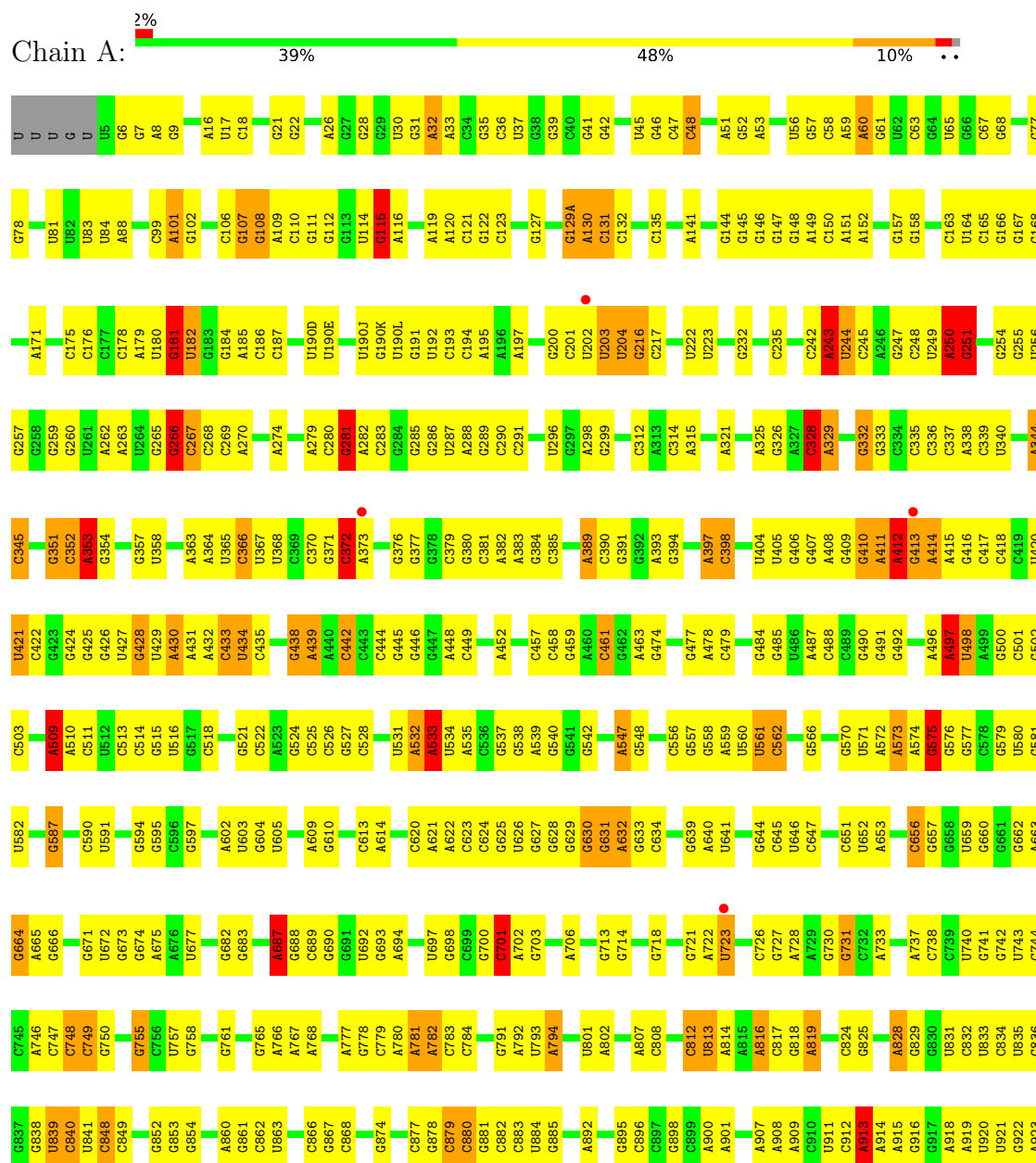
- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

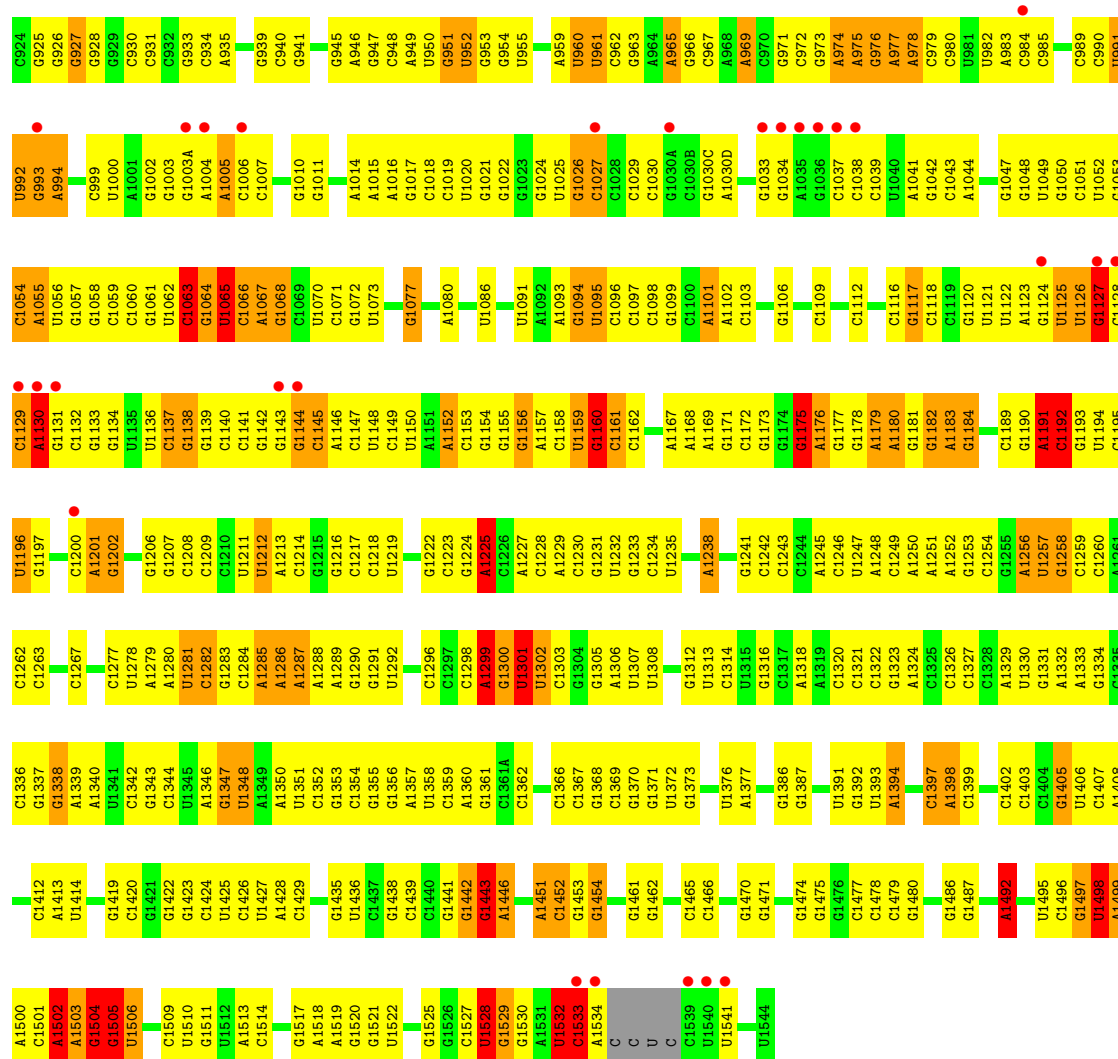
| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 27  | D     | 1        | Total Zn<br>1 1 | 0       | 0       |
| 27  | N     | 1        | Total Zn<br>1 1 | 0       | 0       |

### 3 Residue-property plots

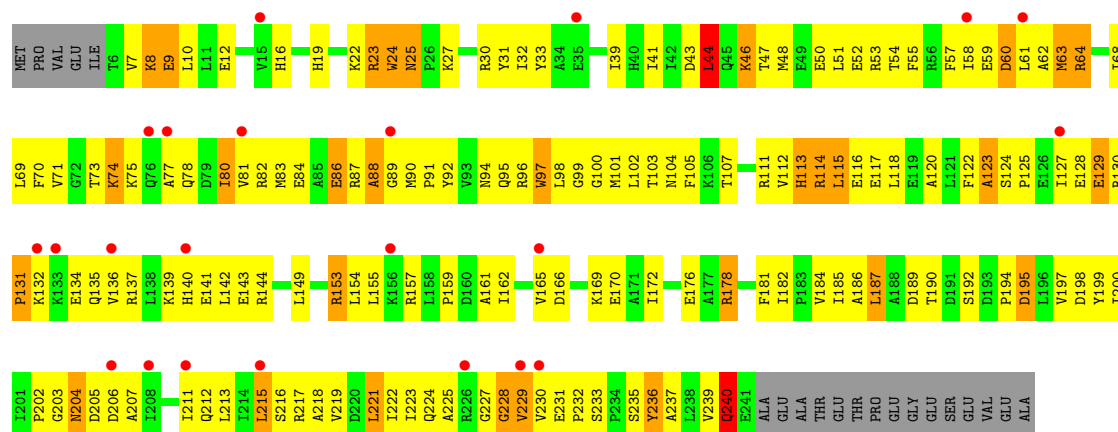
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

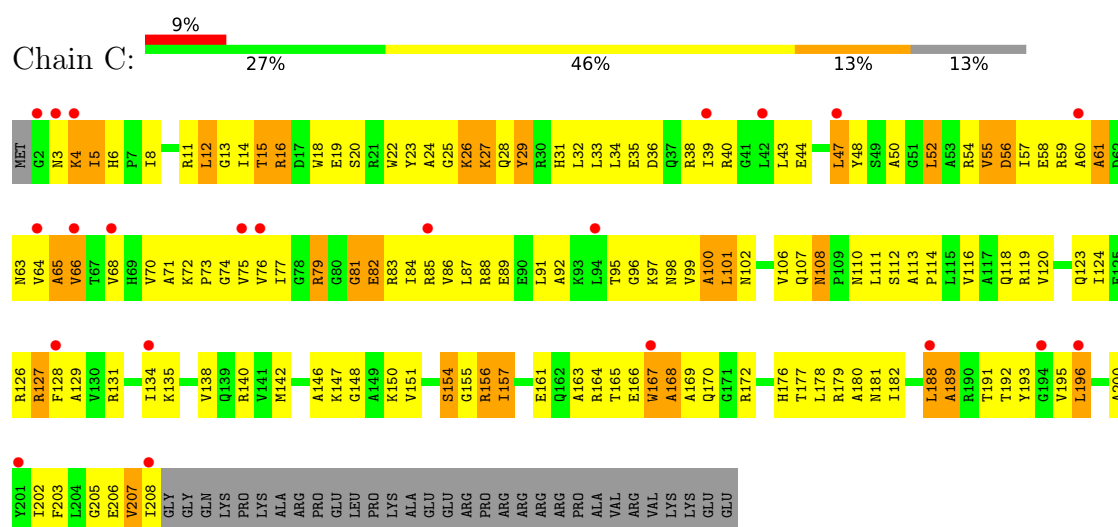
#### • Molecule 1: 16S rRNA



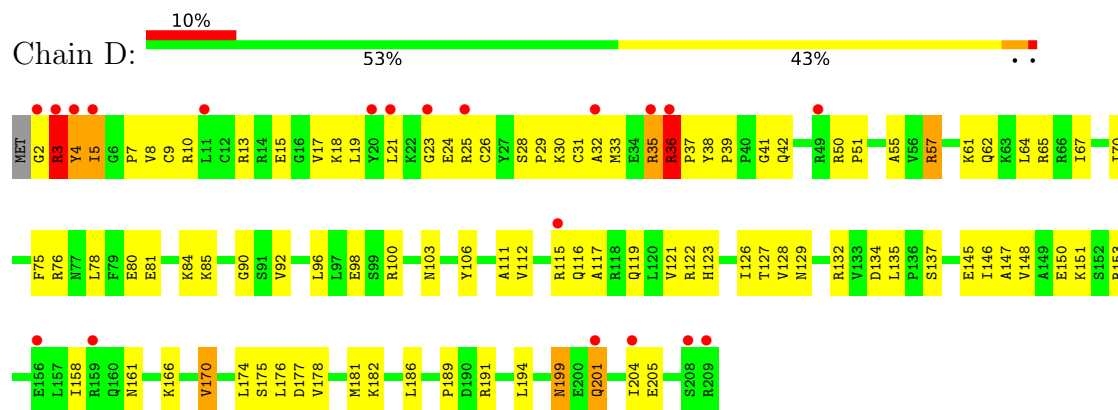


### • Molecule 2: 30S RIBOSOMAL PROTEIN S2

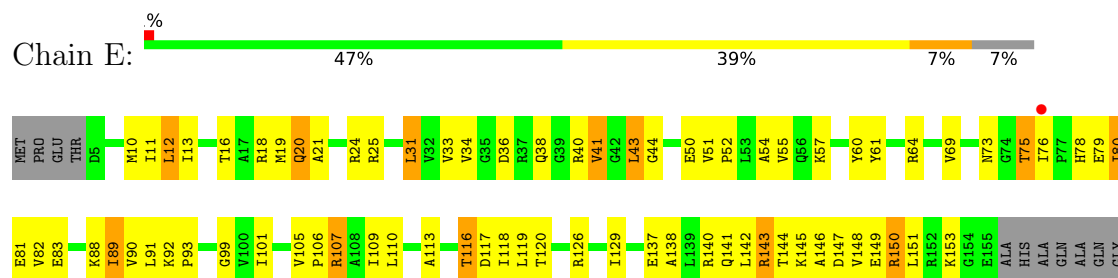


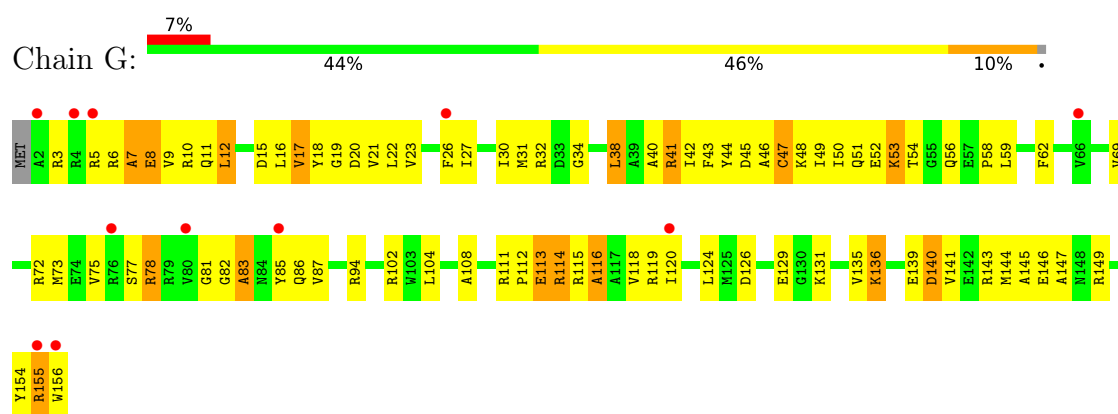


• Molecule 4: 30S RIBOSOMAL PROTEIN S4

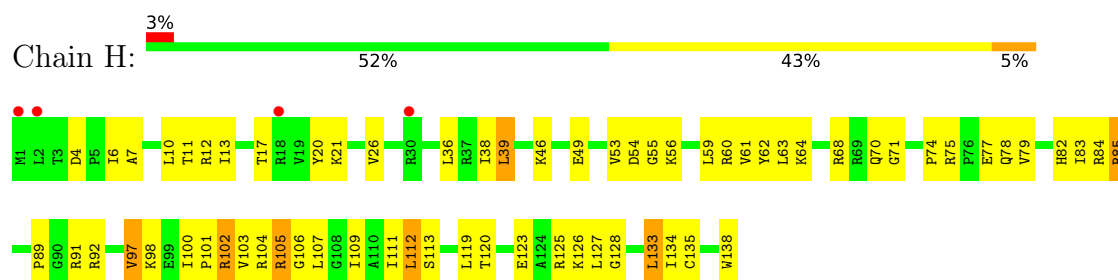


• Molecule 5: 30S RIBOSOMAL PROTEIN S5

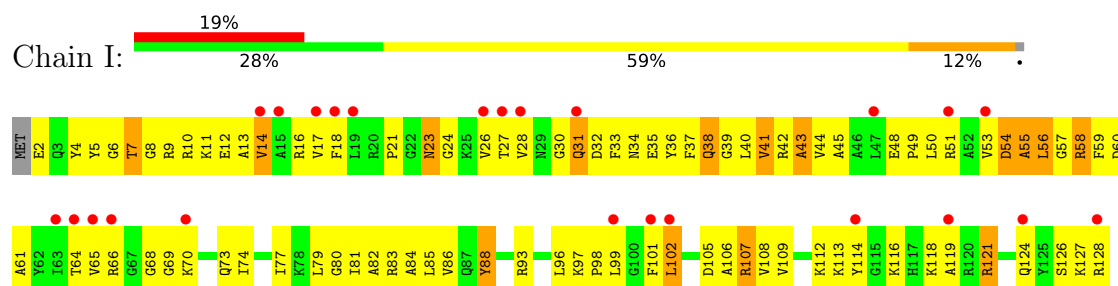




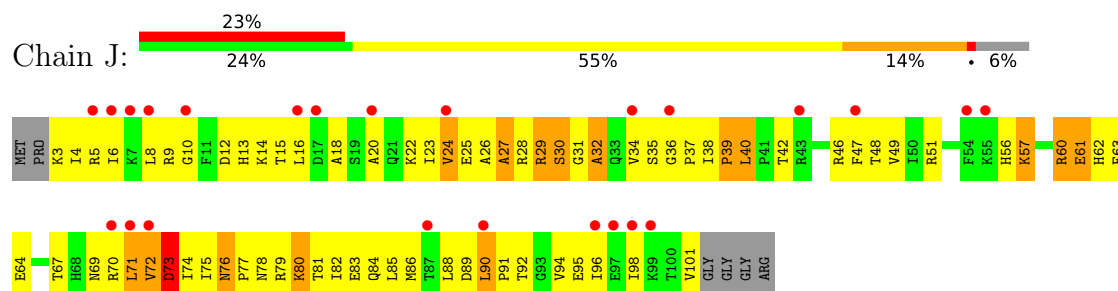
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



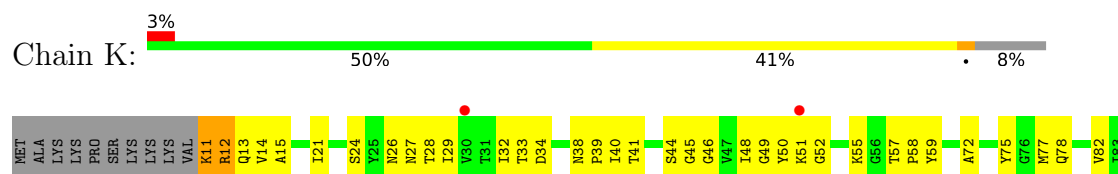
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



• Molecule 10: 30S RIBOSOMAL PROTEIN S10

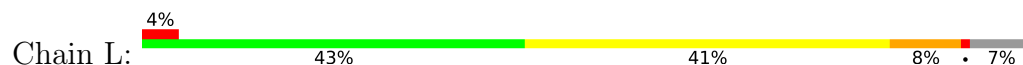


• Molecule 11: 30S RIBOSOMAL PROTEIN S11





• Molecule 12: 30S RIBOSOMAL PROTEIN S12



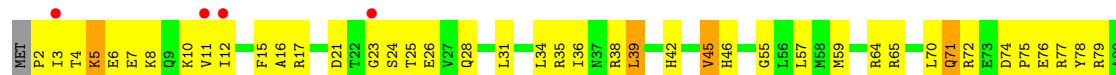
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



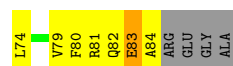
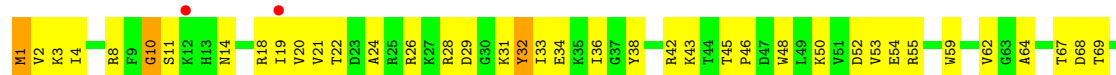
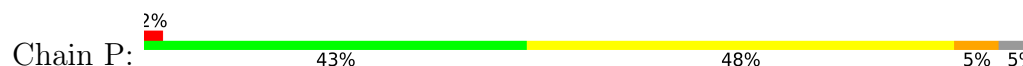
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z



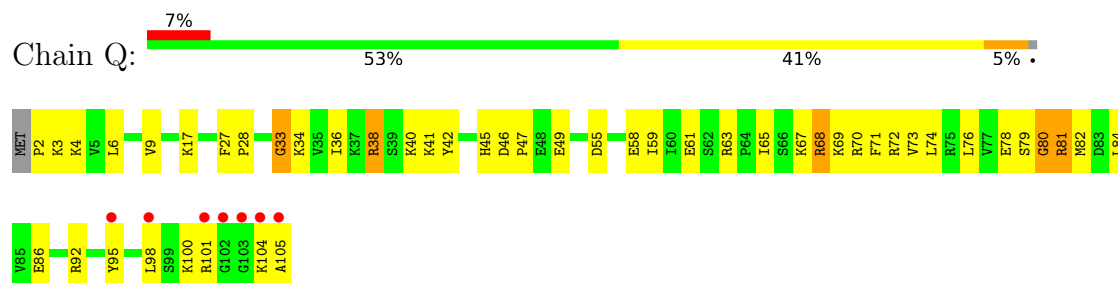
• Molecule 15: 30S RIBOSOMAL PROTEIN S15



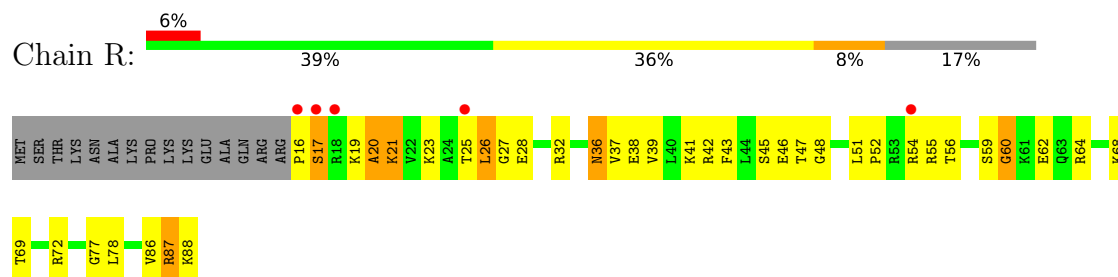
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



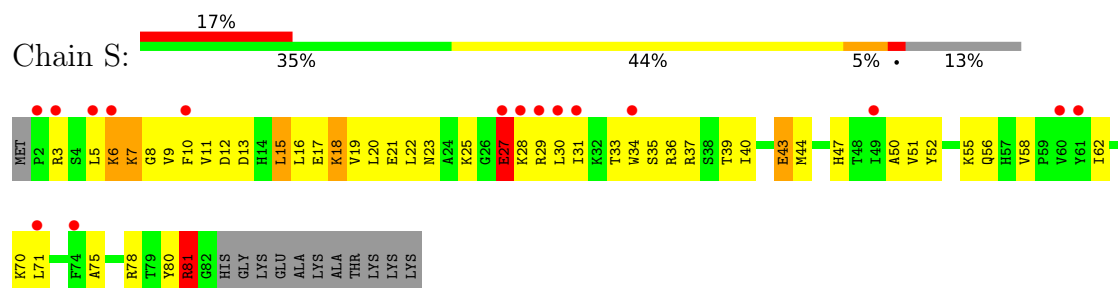
- Molecule 17: 30S RIBOSOMAL PROTEIN S17



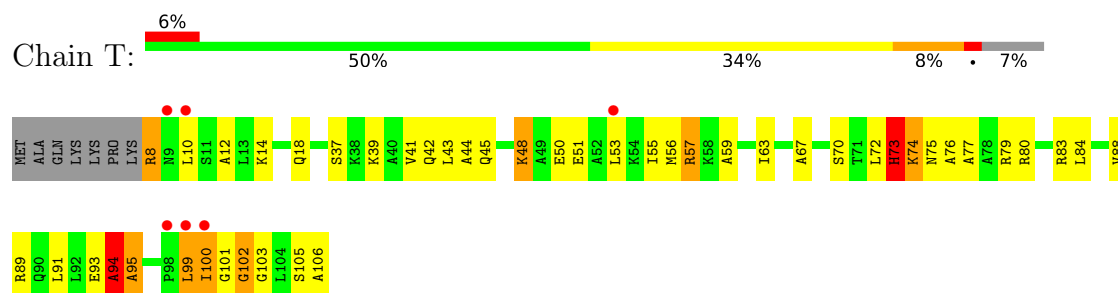
- Molecule 18: 30S RIBOSOMAL PROTEIN S18



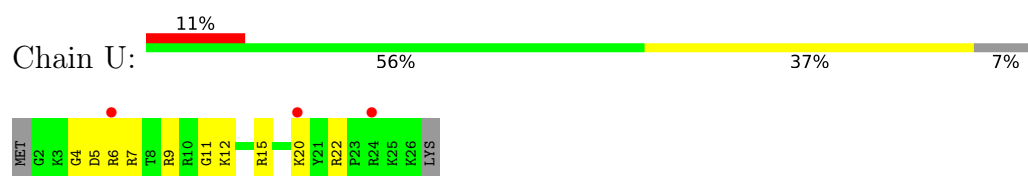
- Molecule 19: 30S RIBOSOMAL PROTEIN S19



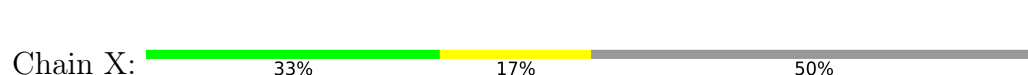
- Molecule 20: 30S RIBOSOMAL PROTEIN S20



- Molecule 21: 30S RIBOSOMAL PROTEIN THX

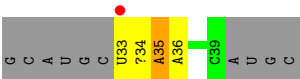
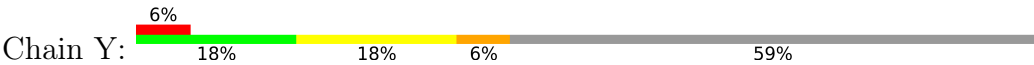


- Molecule 22: 5'-R(\*UP\*UP\*AP\*AP\*AP\*AP)-3'





● Molecule 23: 5'-R(\*GP\*CP\*AP\*UP\*GP\*CP\*UP\*TM2P\*AP\*AP\*AP \*AP\*CP\*AP\*UP\*GP\*CP)-3'





## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 41 21 2   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 402.00Å 402.00Å 175.65Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 49.50 – 2.50<br>284.26 – 2.35                               | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.8 (49.50-2.50)<br>99.0 (284.26-2.35)                     | Depositor<br>EDS |
| $R_{merge}$   | 0.16  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.83 (at 2.34Å)   | Xtriage          |
| Refinement program  | CNS 1.1   | Depositor        |
| R, $R_{free}$   | 0.257 , 0.283<br>0.250 , 0.272                              | Depositor<br>DCC |
| $R_{free}$ test set   | 29655 reflections (5.05%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 36.2  | Xtriage          |
| Anisotropy  | 0.023   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.25 , 50.2   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.91  | EDS              |
| Total number of atoms   | 52245   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 59.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% 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: MG, K, PAR, ZN, TM2

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

| Mol | Chain | Bond lengths |                 | Bond angles |                 |
|-----|-------|--------------|-----------------|-------------|-----------------|
|     |       | RMSZ         | $\# Z  > 5$     | RMSZ        | $\# Z  > 5$     |
| 1   | A     | 1.17         | 15/36390 (0.0%) | 0.88        | 71/56793 (0.1%) |
| 2   | B     | 29.07        | 1/1909 (0.1%)   | 1.16        | 2/2579 (0.1%)   |
| 3   | C     | 0.35         | 0/1637          | 0.59        | 0/2207          |
| 4   | D     | 0.34         | 0/1733          | 0.57        | 0/2318          |
| 5   | E     | 0.45         | 0/1163          | 0.71        | 0/1566          |
| 6   | F     | 0.32         | 0/856           | 0.59        | 0/1154          |
| 7   | G     | 0.33         | 0/1276          | 0.63        | 0/1709          |
| 8   | H     | 0.43         | 0/1136          | 0.75        | 0/1527          |
| 9   | I     | 0.35         | 0/1029          | 0.63        | 0/1378          |
| 10  | J     | 0.37         | 0/806           | 0.63        | 0/1084          |
| 11  | K     | 0.38         | 0/900           | 0.70        | 0/1213          |
| 12  | L     | 0.43         | 0/987           | 0.75        | 0/1322          |
| 13  | M     | 0.33         | 0/1008          | 0.60        | 0/1347          |
| 14  | N     | 0.35         | 0/501           | 0.62        | 0/664           |
| 15  | O     | 0.36         | 0/745           | 0.61        | 1/992 (0.1%)    |
| 16  | P     | 0.45         | 0/717           | 0.70        | 0/965           |
| 17  | Q     | 0.42         | 0/870           | 0.73        | 1/1159 (0.1%)   |
| 18  | R     | 0.37         | 0/603           | 0.61        | 0/799           |
| 19  | S     | 0.33         | 0/662           | 0.61        | 0/892           |
| 20  | T     | 0.37         | 0/764           | 0.72        | 1/1006 (0.1%)   |
| 21  | U     | 0.48         | 0/213           | 0.65        | 0/279           |
| 22  | X     | 0.53         | 0/65            | 0.60        | 0/99            |
| 23  | Y     | 0.43         | 0/140           | 0.65        | 0/216           |
| All | All   | 5.45         | 16/56110 (0.0%) | 0.83        | 76/83268 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 11                  | 31                  |
| 2   | B     | 0                   | 1                   |
| 16  | P     | 0                   | 1                   |
| All | All   | 11                  | 33                  |

All (16) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z       | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|---------|-------------|----------|
| 2   | B     | 240  | GLN  | CD-OE1 | 1270.14 | 29.18       | 1.24     |
| 1   | A     | 1127 | G    | O3'-P  | -95.85  | 0.46        | 1.61     |
| 1   | A     | 1063 | C    | O3'-P  | -75.59  | 0.70        | 1.61     |
| 1   | A     | 1160 | G    | O3'-P  | -73.55  | 0.72        | 1.61     |
| 1   | A     | 1532 | U    | O3'-P  | -64.97  | 0.83        | 1.61     |
| 1   | A     | 1156 | G    | O3'-P  | -59.43  | 0.89        | 1.61     |
| 1   | A     | 1191 | A    | O3'-P  | -52.33  | 0.98        | 1.61     |
| 1   | A     | 1175 | G    | O3'-P  | -51.28  | 0.99        | 1.61     |
| 1   | A     | 1179 | A    | O3'-P  | -44.13  | 1.08        | 1.61     |
| 1   | A     | 1192 | C    | O3'-P  | -42.03  | 1.10        | 1.61     |
| 1   | A     | 1144 | G    | O3'-P  | -30.47  | 1.24        | 1.61     |
| 1   | A     | 1064 | G    | O3'-P  | -25.75  | 1.30        | 1.61     |
| 1   | A     | 1533 | C    | O3'-P  | 9.56    | 1.72        | 1.61     |
| 1   | A     | 1541 | U    | O3'-P  | -5.55   | 1.54        | 1.61     |
| 1   | A     | 1505 | G    | P-O5'  | -5.23   | 1.54        | 1.59     |
| 1   | A     | 813  | U    | P-O5'  | -5.11   | 1.54        | 1.59     |

All (76) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 2   | B     | 240  | GLN  | CG-CD-OE1 | -49.40 | 22.81       | 121.60   |
| 1   | A     | 1160 | G    | P-O3'-C3' | -45.24 | 65.41       | 119.70   |
| 1   | A     | 1064 | G    | OP1-P-O3' | -36.76 | 24.33       | 105.20   |
| 1   | A     | 1192 | C    | OP2-P-O3' | -35.85 | 26.34       | 105.20   |
| 1   | A     | 1144 | G    | P-O3'-C3' | -33.90 | 79.02       | 119.70   |
| 1   | A     | 1160 | G    | O3'-P-O5' | 31.41  | 163.69      | 104.00   |
| 1   | A     | 1179 | A    | OP2-P-O3' | -28.19 | 43.18       | 105.20   |
| 1   | A     | 1144 | G    | OP1-P-O3' | 26.60  | 163.72      | 105.20   |
| 1   | A     | 1179 | A    | P-O3'-C3' | -23.60 | 91.38       | 119.70   |
| 1   | A     | 1179 | A    | O3'-P-O5' | 22.44  | 146.64      | 104.00   |
| 1   | A     | 1533 | C    | P-O3'-C3' | -21.79 | 93.55       | 119.70   |
| 1   | A     | 1160 | G    | OP1-P-O3' | -20.98 | 59.03       | 105.20   |
| 1   | A     | 1127 | G    | P-O3'-C3' | 20.38  | 144.15      | 119.70   |
| 1   | A     | 1144 | G    | O3'-P-O5' | -19.92 | 66.15       | 104.00   |
| 1   | A     | 1191 | A    | P-O3'-C3' | 19.44  | 143.02      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 1   | A     | 1532 | U    | OP2-P-O3'   | -19.31 | 62.72       | 105.20   |
| 1   | A     | 1063 | C    | P-O3'-C3'   | 17.18  | 140.31      | 119.70   |
| 1   | A     | 1532 | U    | O3'-P-O5'   | 15.76  | 133.94      | 104.00   |
| 1   | A     | 1156 | G    | P-O3'-C3'   | 14.91  | 137.59      | 119.70   |
| 1   | A     | 1144 | G    | OP2-P-O3'   | -13.77 | 74.90       | 105.20   |
| 1   | A     | 1064 | G    | OP2-P-O3'   | 13.43  | 134.75      | 105.20   |
| 1   | A     | 1533 | C    | O3'-P-O5'   | 12.94  | 128.58      | 104.00   |
| 1   | A     | 1175 | G    | O3'-P-O5'   | 12.42  | 127.61      | 104.00   |
| 1   | A     | 1498 | U    | C2'-C3'-O3' | 10.61  | 132.84      | 109.50   |
| 1   | A     | 1179 | A    | OP1-P-O3'   | -10.35 | 82.43       | 105.20   |
| 1   | A     | 115  | G    | C2'-C3'-O3' | 9.98   | 131.45      | 109.50   |
| 1   | A     | 1192 | C    | OP1-P-O3'   | 9.79   | 126.75      | 105.20   |
| 1   | A     | 1503 | A    | C2'-C3'-O3' | 9.65   | 130.74      | 109.50   |
| 1   | A     | 1443 | G    | C2'-C3'-O3' | 9.42   | 130.22      | 109.50   |
| 1   | A     | 1192 | C    | O3'-P-O5'   | 9.40   | 121.86      | 104.00   |
| 1   | A     | 243  | A    | C2'-C3'-O3' | 9.32   | 130.01      | 109.50   |
| 1   | A     | 1301 | U    | C2'-C3'-O3' | 9.28   | 129.93      | 109.50   |
| 1   | A     | 1127 | G    | OP1-P-O3'   | 9.17   | 125.38      | 105.20   |
| 1   | A     | 701  | C    | C2'-C3'-O3' | 9.05   | 129.41      | 109.50   |
| 1   | A     | 1528 | U    | C2'-C3'-O3' | 8.97   | 129.23      | 109.50   |
| 1   | A     | 575  | G    | C2'-C3'-O3' | 8.93   | 129.14      | 109.50   |
| 1   | A     | 1175 | G    | OP2-P-O3'   | -8.93  | 85.56       | 105.20   |
| 1   | A     | 281  | G    | C2'-C3'-O3' | 8.74   | 128.74      | 109.50   |
| 1   | A     | 1160 | G    | OP2-P-O3'   | -8.54  | 86.40       | 105.20   |
| 1   | A     | 1532 | U    | P-O3'-C3'   | -8.53  | 109.46      | 119.70   |
| 2   | B     | 240  | GLN  | OE1-CD-NE2  | -8.37  | 102.66      | 121.90   |
| 1   | A     | 812  | C    | C2'-C3'-O3' | 8.21   | 127.55      | 109.50   |
| 1   | A     | 412  | A    | N9-C1'-C2'  | 8.16   | 124.60      | 114.00   |
| 1   | A     | 687  | A    | C2'-C3'-O3' | 7.93   | 126.96      | 109.50   |
| 1   | A     | 60   | A    | C2'-C3'-O3' | 7.64   | 126.31      | 109.50   |
| 1   | A     | 328  | C    | C2'-C3'-O3' | 7.55   | 126.11      | 109.50   |
| 1   | A     | 1191 | A    | O3'-P-O5'   | -7.50  | 89.74       | 104.00   |
| 1   | A     | 410  | G    | C2'-C3'-O3' | 7.46   | 125.91      | 109.50   |
| 1   | A     | 181  | G    | C2'-C3'-O3' | 7.24   | 125.43      | 109.50   |
| 1   | A     | 497  | A    | C2'-C3'-O3' | 7.16   | 125.24      | 109.50   |
| 1   | A     | 266  | G    | C2'-C3'-O3' | 7.13   | 125.19      | 109.50   |
| 1   | A     | 372  | C    | C2'-C3'-O3' | 7.08   | 125.07      | 109.50   |
| 1   | A     | 1505 | G    | C2'-C3'-O3' | 7.06   | 125.03      | 109.50   |
| 1   | A     | 366  | C    | C2'-C3'-O3' | 7.05   | 125.01      | 109.50   |
| 1   | A     | 533  | A    | C2'-C3'-O3' | 6.85   | 124.67      | 113.70   |
| 1   | A     | 1299 | A    | N9-C1'-C2'  | 6.76   | 122.79      | 114.00   |
| 1   | A     | 965  | A    | C2'-C3'-O3' | 6.68   | 124.39      | 113.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 913  | A    | C2'-C3'-O3' | 6.59  | 124.24      | 113.70   |
| 1   | A     | 1502 | A    | N9-C1'-C2'  | 6.35  | 122.25      | 114.00   |
| 1   | A     | 1191 | A    | OP1-P-O3'   | 6.25  | 118.96      | 105.20   |
| 1   | A     | 353  | A    | C5'-C4'-O4' | -6.21 | 101.65      | 109.10   |
| 1   | A     | 1065 | U    | C2'-C3'-O3' | 6.05  | 123.38      | 113.70   |
| 1   | A     | 428  | G    | C2'-C3'-O3' | 5.74  | 122.89      | 113.70   |
| 1   | A     | 509  | A    | C2'-C3'-O3' | 5.71  | 122.84      | 113.70   |
| 1   | A     | 281  | G    | C4'-C3'-O3' | 5.67  | 124.34      | 113.00   |
| 1   | A     | 63   | C    | C5'-C4'-C3' | -5.59 | 107.06      | 116.00   |
| 1   | A     | 328  | C    | O4'-C1'-N1  | -5.47 | 103.83      | 108.20   |
| 17  | Q     | 98   | LEU  | CA-CB-CG    | 5.32  | 127.54      | 115.30   |
| 1   | A     | 748  | C    | C2'-C3'-O3' | 5.26  | 122.12      | 113.70   |
| 1   | A     | 1504 | G    | C2'-C3'-O3' | 5.24  | 122.09      | 113.70   |
| 1   | A     | 1533 | C    | OP1-P-O3'   | -5.22 | 93.72       | 105.20   |
| 1   | A     | 575  | G    | O4'-C1'-N9  | -5.22 | 104.03      | 108.20   |
| 15  | O     | 45   | VAL  | N-CA-C      | -5.09 | 97.25       | 111.00   |
| 1   | A     | 1225 | A    | N9-C1'-C2'  | 5.07  | 120.58      | 114.00   |
| 1   | A     | 389  | A    | C5'-C4'-C3' | 5.06  | 124.09      | 116.00   |
| 20  | T     | 94   | ALA  | N-CA-C      | -5.02 | 97.44       | 111.00   |

All (11) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 1   | A     | 115  | G    | C3'  |
| 1   | A     | 243  | A    | C3'  |
| 1   | A     | 281  | G    | C3'  |
| 1   | A     | 410  | G    | C3'  |
| 1   | A     | 412  | A    | C1'  |
| 1   | A     | 701  | C    | C3'  |
| 1   | A     | 812  | C    | C3'  |
| 1   | A     | 1443 | G    | C3'  |
| 1   | A     | 1498 | U    | C3'  |
| 1   | A     | 1503 | A    | C3'  |
| 1   | A     | 1528 | U    | C3'  |

All (33) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | A     | 107  | G    | Sidechain |
| 1   | A     | 1077 | G    | Sidechain |
| 1   | A     | 108  | G    | Sidechain |
| 1   | A     | 1130 | A    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | A     | 1299 | A    | Sidechain |
| 1   | A     | 1405 | G    | Sidechain |
| 1   | A     | 1414 | U    | Sidechain |
| 1   | A     | 1454 | G    | Sidechain |
| 1   | A     | 1492 | A    | Sidechain |
| 1   | A     | 250  | A    | Sidechain |
| 1   | A     | 251  | G    | Sidechain |
| 1   | A     | 274  | A    | Sidechain |
| 1   | A     | 37   | U    | Sidechain |
| 1   | A     | 380  | G    | Sidechain |
| 1   | A     | 561  | U    | Sidechain |
| 1   | A     | 566  | G    | Sidechain |
| 1   | A     | 575  | G    | Sidechain |
| 1   | A     | 587  | G    | Sidechain |
| 1   | A     | 597  | G    | Sidechain |
| 1   | A     | 656  | C    | Sidechain |
| 1   | A     | 664  | G    | Sidechain |
| 1   | A     | 682  | G    | Sidechain |
| 1   | A     | 727  | G    | Sidechain |
| 1   | A     | 733  | A    | Sidechain |
| 1   | A     | 852  | G    | Sidechain |
| 1   | A     | 879  | C    | Sidechain |
| 1   | A     | 880  | C    | Sidechain |
| 1   | A     | 898  | G    | Sidechain |
| 1   | A     | 951  | G    | Sidechain |
| 1   | A     | 952  | U    | Sidechain |
| 1   | A     | 982  | U    | Sidechain |
| 2   | B     | 240  | GLN  | Sidechain |
| 16  | P     | 32   | TYR  | Sidechain |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 32511 | 0        | 16411    | 950     | 0            |
| 2   | B     | 1874  | 0        | 1887     | 190     | 0            |
| 3   | C     | 1613  | 0        | 1677     | 200     | 0            |
| 4   | D     | 1703  | 0        | 1767     | 93      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5   | E     | 1147  | 0        | 1207     | 85      | 0            |
| 6   | F     | 843   | 0        | 857      | 58      | 0            |
| 7   | G     | 1257  | 0        | 1296     | 102     | 0            |
| 8   | H     | 1116  | 0        | 1177     | 54      | 0            |
| 9   | I     | 1011  | 0        | 1041     | 120     | 0            |
| 10  | J     | 793   | 0        | 835      | 127     | 1            |
| 11  | K     | 885   | 0        | 904      | 51      | 0            |
| 12  | L     | 971   | 0        | 1057     | 79      | 0            |
| 13  | M     | 997   | 0        | 1072     | 122     | 0            |
| 14  | N     | 492   | 0        | 531      | 66      | 0            |
| 15  | O     | 734   | 0        | 771      | 44      | 0            |
| 16  | P     | 701   | 0        | 720      | 45      | 0            |
| 17  | Q     | 857   | 0        | 930      | 56      | 0            |
| 18  | R     | 597   | 0        | 668      | 47      | 0            |
| 19  | S     | 648   | 0        | 673      | 57      | 0            |
| 20  | T     | 762   | 0        | 859      | 61      | 0            |
| 21  | U     | 209   | 0        | 221      | 15      | 0            |
| 22  | X     | 59    | 0        | 33       | 1       | 0            |
| 23  | Y     | 153   | 0        | 83       | 8       | 0            |
| 24  | A     | 199   | 0        | 0        | 0       | 0            |
| 24  | B     | 1     | 0        | 0        | 0       | 0            |
| 24  | D     | 1     | 0        | 0        | 0       | 0            |
| 24  | E     | 1     | 0        | 0        | 0       | 0            |
| 24  | I     | 1     | 0        | 0        | 0       | 0            |
| 24  | M     | 1     | 0        | 0        | 0       | 0            |
| 24  | N     | 1     | 0        | 0        | 0       | 0            |
| 24  | Q     | 1     | 0        | 0        | 0       | 0            |
| 25  | A     | 54    | 0        | 0        | 0       | 0            |
| 25  | E     | 3     | 0        | 0        | 0       | 0            |
| 25  | I     | 1     | 0        | 0        | 0       | 0            |
| 25  | N     | 1     | 0        | 0        | 0       | 0            |
| 25  | P     | 1     | 0        | 0        | 0       | 0            |
| 25  | R     | 1     | 0        | 0        | 0       | 0            |
| 25  | T     | 1     | 0        | 0        | 0       | 0            |
| 26  | A     | 42    | 0        | 45       | 1       | 0            |
| 27  | D     | 1     | 0        | 0        | 0       | 0            |
| 27  | N     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 52245 | 0        | 36722    | 2401    | 1            |

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 27.

All (2401) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1192:C:O3'   | 1:A:1193:G:P     | 1.10                     | 1.49              |
| 1:A:1175:G:O3'   | 1:A:1176:A:P     | 0.99                     | 1.39              |
| 1:A:1191:A:O3'   | 1:A:1192:C:P     | 0.98                     | 1.37              |
| 1:A:1175:G:C3'   | 1:A:1176:A:P     | 2.14                     | 1.34              |
| 1:A:1156:G:C3'   | 1:A:1157:A:P     | 2.17                     | 1.32              |
| 1:A:1118:C:O2    | 1:A:1179:A:C6    | 1.83                     | 1.32              |
| 1:A:1533:C:O2'   | 1:A:1534:A:H5'   | 1.25                     | 1.31              |
| 1:A:1156:G:O3'   | 1:A:1157:A:P     | 0.89                     | 1.29              |
| 1:A:1532:U:O2    | 1:A:1534:A:OP2   | 1.52                     | 1.27              |
| 1:A:1191:A:HO3'  | 1:A:1192:C:P     | 0.89                     | 1.26              |
| 1:A:1192:C:HO3'  | 1:A:1193:G:P     | 1.10                     | 1.19              |
| 1:A:1191:A:C3'   | 1:A:1192:C:P     | 2.31                     | 1.18              |
| 1:A:1192:C:C4'   | 1:A:1193:G:OP2   | 1.95                     | 1.13              |
| 1:A:1192:C:C3'   | 1:A:1193:G:OP2   | 0.79                     | 1.09              |
| 1:A:243:A:H4'    | 1:A:244:U:H5'    | 1.34                     | 1.08              |
| 19:S:33:THR:HG22 | 19:S:35:SER:H    | 1.21                     | 1.03              |
| 1:A:1533:C:O2'   | 1:A:1534:A:C5'   | 2.07                     | 1.03              |
| 1:A:1192:C:H3'   | 1:A:1193:G:OP2   | 1.22                     | 1.01              |
| 13:M:88:ARG:HD2  | 19:S:3:ARG:HH21  | 1.26                     | 1.00              |
| 1:A:1128:C:H5'   | 9:I:16:ARG:HH12  | 1.23                     | 1.00              |
| 1:A:1356:G:H2'   | 1:A:1357:A:C8    | 1.98                     | 0.99              |
| 14:N:26:ARG:HH21 | 14:N:47:LEU:HG   | 1.26                     | 0.99              |
| 1:A:1175:G:O3'   | 1:A:1176:A:OP2   | 1.72                     | 0.98              |
| 1:A:1192:C:C2'   | 1:A:1193:G:OP2   | 2.11                     | 0.98              |
| 1:A:266:G:H5''   | 1:A:268:C:H41    | 1.28                     | 0.98              |
| 19:S:28:LYS:HG2  | 19:S:29:ARG:H    | 1.26                     | 0.98              |
| 1:A:1118:C:O2    | 1:A:1179:A:C5    | 2.17                     | 0.97              |
| 1:A:1065:U:H5''  | 1:A:1190:G:N2    | 1.78                     | 0.97              |
| 3:C:14:ILE:HG22  | 3:C:15:THR:H     | 1.29                     | 0.97              |
| 14:N:6:LEU:HD12  | 14:N:23:ARG:HH21 | 1.26                     | 0.97              |
| 13:M:49:THR:HG22 | 13:M:51:ALA:H    | 1.28                     | 0.96              |
| 12:L:47:LYS:HB3  | 12:L:48:PRO:HD3  | 1.43                     | 0.96              |
| 1:A:1190:G:H3'   | 3:C:3:ASN:ND2    | 1.80                     | 0.96              |
| 1:A:1152:A:H5''  | 10:J:13:HIS:HD2  | 1.28                     | 0.96              |
| 11:K:14:VAL:HG21 | 11:K:40:ILE:HD11 | 1.47                     | 0.96              |
| 1:A:1156:G:O3'   | 1:A:1157:A:OP2   | 1.83                     | 0.95              |
| 8:H:64:LYS:HG2   | 8:H:79:VAL:HG21  | 1.47                     | 0.95              |
| 1:A:975:A:H5'    | 1:A:975:A:H8     | 1.32                     | 0.94              |
| 2:B:132:LYS:HD2  | 2:B:135:GLN:HB2  | 1.46                     | 0.94              |
| 13:M:10:PRO:HB2  | 13:M:18:ALA:HB1  | 1.49                     | 0.94              |
| 1:A:1086:U:H3    | 1:A:1099:G:H22   | 1.10                     | 0.93              |
| 1:A:1533:C:HO2'  | 1:A:1534:A:H5'   | 1.33                     | 0.92              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:23:GLY:HA3   | 4:D:112:VAL:HG22 | 1.49                     | 0.92              |
| 1:A:1128:C:C5'   | 9:I:16:ARG:HH12  | 1.83                     | 0.92              |
| 19:S:15:LEU:HA   | 19:S:18:LYS:HB3  | 1.52                     | 0.92              |
| 1:A:1026:G:H3'   | 1:A:1027:C:H5''  | 1.52                     | 0.91              |
| 1:A:664:G:H22    | 1:A:741:G:H1     | 1.18                     | 0.91              |
| 13:M:108:ARG:HE  | 13:M:108:ARG:HA  | 1.35                     | 0.91              |
| 3:C:64:VAL:HB    | 3:C:99:VAL:HG21  | 1.50                     | 0.91              |
| 1:A:1175:G:O2'   | 1:A:1176:A:H5'   | 1.72                     | 0.90              |
| 3:C:6:HIS:HD2    | 3:C:8:ILE:H      | 1.18                     | 0.90              |
| 5:E:80:ILE:HD12  | 5:E:91:LEU:HB2   | 1.53                     | 0.90              |
| 1:A:1156:G:HO3'  | 1:A:1157:A:P     | 1.10                     | 0.90              |
| 18:R:17:SER:HB3  | 18:R:54:ARG:HH11 | 1.36                     | 0.89              |
| 1:A:129(A):G:O2' | 1:A:190(E):U:H2' | 1.72                     | 0.89              |
| 5:E:79:GLU:HG3   | 5:E:93:PRO:HD2   | 1.54                     | 0.89              |
| 10:J:4:ILE:HD11  | 10:J:74:ILE:HD12 | 1.54                     | 0.89              |
| 10:J:32:ALA:HB2  | 10:J:76:ASN:HD22 | 1.37                     | 0.89              |
| 1:A:1250:A:H4'   | 9:I:68:GLY:H     | 1.37                     | 0.89              |
| 1:A:1152:A:H5''  | 10:J:13:HIS:CD2  | 2.07                     | 0.89              |
| 1:A:1533:C:H2'   | 1:A:1534:A:O5'   | 1.73                     | 0.89              |
| 1:A:1367:C:H5'   | 10:J:60:ARG:NH1  | 1.88                     | 0.89              |
| 5:E:80:ILE:CD1   | 5:E:91:LEU:HB2   | 2.03                     | 0.88              |
| 20:T:43:LEU:HD13 | 20:T:51:GLU:HG3  | 1.56                     | 0.88              |
| 1:A:328:C:O2     | 1:A:328:C:H2'    | 1.74                     | 0.88              |
| 7:G:54:THR:HG22  | 7:G:56:GLN:H     | 1.37                     | 0.88              |
| 2:B:48:MET:HA    | 2:B:51:LEU:HD12  | 1.55                     | 0.88              |
| 20:T:8:ARG:HH11  | 20:T:8:ARG:HB3   | 1.37                     | 0.88              |
| 5:E:50:GLU:HG3   | 5:E:52:PRO:HD2   | 1.56                     | 0.87              |
| 9:I:53:VAL:HG21  | 9:I:85:LEU:HD21  | 1.57                     | 0.87              |
| 2:B:97:TRP:HZ2   | 2:B:102:LEU:HD13 | 1.40                     | 0.87              |
| 3:C:64:VAL:HG23  | 3:C:99:VAL:HG11  | 1.57                     | 0.87              |
| 3:C:58:GLU:HB3   | 10:J:92:THR:HG21 | 1.56                     | 0.87              |
| 19:S:5:LEU:O     | 19:S:6:LYS:HB2   | 1.75                     | 0.87              |
| 5:E:150:ARG:HH11 | 5:E:150:ARG:HG3  | 1.40                     | 0.86              |
| 1:A:1532:U:O2'   | 1:A:1533:C:O5'   | 1.66                     | 0.86              |
| 12:L:111:LYS:HE3 | 12:L:112:ASP:H   | 1.40                     | 0.86              |
| 2:B:118:LEU:HB2  | 2:B:142:LEU:HD21 | 1.57                     | 0.86              |
| 2:B:83:MET:HA    | 2:B:86:GLU:HB2   | 1.56                     | 0.86              |
| 5:E:51:VAL:HB    | 5:E:52:PRO:HD3   | 1.58                     | 0.85              |
| 2:B:103:THR:HG23 | 2:B:176:GLU:HB2  | 1.56                     | 0.85              |
| 1:A:1137:C:H4'   | 1:A:1138:G:C2    | 2.12                     | 0.85              |
| 1:A:1532:U:H2'   | 1:A:1533:C:C5'   | 2.02                     | 0.85              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:2:ARG:NE     | 6:F:69:GLU:HG2   | 1.90                     | 0.85              |
| 11:K:40:ILE:HG22 | 11:K:41:THR:HG23 | 1.57                     | 0.85              |
| 2:B:44:LEU:H     | 2:B:44:LEU:HD12  | 1.42                     | 0.85              |
| 7:G:136:LYS:HA   | 7:G:136:LYS:HE2  | 1.57                     | 0.85              |
| 13:M:37:THR:HG23 | 13:M:55:ARG:HD2  | 1.59                     | 0.85              |
| 1:A:1250:A:H4'   | 9:I:68:GLY:N     | 1.91                     | 0.84              |
| 17:Q:67:LYS:HA   | 17:Q:70:ARG:HH12 | 1.42                     | 0.84              |
| 12:L:55:VAL:HG12 | 12:L:56:ALA:H    | 1.42                     | 0.84              |
| 10:J:46:ARG:HG2  | 10:J:46:ARG:HH11 | 1.42                     | 0.84              |
| 9:I:93:ARG:HB3   | 9:I:93:ARG:NH1   | 1.92                     | 0.84              |
| 1:A:1116:C:H2'   | 1:A:1117:G:H5''  | 1.60                     | 0.84              |
| 19:S:13:ASP:HA   | 19:S:16:LEU:HB3  | 1.58                     | 0.84              |
| 1:A:1190:G:OP1   | 3:C:4:LYS:HA     | 1.78                     | 0.84              |
| 2:B:211:ILE:O    | 2:B:215:LEU:HB2  | 1.75                     | 0.84              |
| 11:K:57:THR:HG22 | 11:K:59:TYR:H    | 1.43                     | 0.84              |
| 1:A:1369:C:H2'   | 1:A:1370:G:C8    | 2.13                     | 0.83              |
| 2:B:46:LYS:HE3   | 2:B:46:LYS:HA    | 1.59                     | 0.83              |
| 1:A:975:A:H4'    | 1:A:976:G:H5''   | 1.58                     | 0.83              |
| 9:I:97:LYS:HB3   | 9:I:98:PRO:HD3   | 1.60                     | 0.83              |
| 6:F:80:ARG:NH1   | 6:F:88:VAL:HB    | 1.93                     | 0.83              |
| 4:D:7:PRO:HB2    | 4:D:10:ARG:HD2   | 1.58                     | 0.83              |
| 1:A:432:A:H3'    | 1:A:433:C:H5''   | 1.60                     | 0.83              |
| 7:G:155:ARG:HA   | 7:G:155:ARG:HH11 | 1.42                     | 0.83              |
| 19:S:17:GLU:HA   | 19:S:20:LEU:HG   | 1.61                     | 0.82              |
| 1:A:1178:G:N2    | 1:A:1180:A:C8    | 2.47                     | 0.82              |
| 1:A:203:U:H5''   | 1:A:204:U:OP1    | 1.78                     | 0.82              |
| 1:A:1160:G:O2'   | 1:A:1161:C:H5'   | 1.79                     | 0.82              |
| 1:A:250:A:H4'    | 1:A:251:G:O5'    | 1.78                     | 0.82              |
| 2:B:77:ALA:HB2   | 2:B:211:ILE:HD13 | 1.61                     | 0.82              |
| 18:R:32:ARG:HA   | 18:R:69:THR:HG21 | 1.60                     | 0.82              |
| 5:E:144:THR:O    | 5:E:148:VAL:HG23 | 1.79                     | 0.81              |
| 12:L:111:LYS:HA  | 12:L:111:LYS:HE3 | 1.59                     | 0.81              |
| 1:A:946:A:H2'    | 1:A:947:G:C8     | 2.15                     | 0.81              |
| 14:N:26:ARG:HE   | 14:N:47:LEU:HD11 | 1.45                     | 0.81              |
| 20:T:74:LYS:HZ3  | 20:T:74:LYS:HA   | 1.44                     | 0.81              |
| 3:C:14:ILE:HG22  | 3:C:15:THR:N     | 1.96                     | 0.81              |
| 1:A:1128:C:H5'   | 9:I:16:ARG:NH1   | 1.95                     | 0.81              |
| 13:M:4:ILE:HG22  | 13:M:5:ALA:H     | 1.45                     | 0.81              |
| 2:B:114:ARG:HA   | 2:B:117:GLU:HB3  | 1.62                     | 0.81              |
| 12:L:111:LYS:CE  | 12:L:112:ASP:H   | 1.93                     | 0.81              |
| 4:D:24:GLU:HG2   | 4:D:25:ARG:H     | 1.46                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 15:O:16:ALA:HB1  | 15:O:21:ASP:HB3  | 1.62                     | 0.81              |
| 2:B:124:SER:HB2  | 2:B:125:PRO:HD2  | 1.63                     | 0.80              |
| 13:M:11:ARG:HG3  | 13:M:12:ASN:N    | 1.97                     | 0.80              |
| 1:A:1118:C:O2    | 1:A:1179:A:N1    | 2.13                     | 0.80              |
| 1:A:243:A:C4'    | 1:A:244:U:H5'    | 2.09                     | 0.80              |
| 12:L:27:LEU:O    | 12:L:29:GLY:N    | 2.13                     | 0.80              |
| 1:A:1477:C:H2'   | 1:A:1478:C:H6    | 1.46                     | 0.80              |
| 2:B:161:ALA:HB1  | 2:B:185:ILE:HD11 | 1.62                     | 0.80              |
| 13:M:4:ILE:HG22  | 13:M:5:ALA:N     | 1.97                     | 0.80              |
| 1:A:975:A:H5'    | 1:A:975:A:C8     | 2.16                     | 0.80              |
| 1:A:1292:U:P     | 7:G:41:ARG:HH22  | 2.05                     | 0.80              |
| 15:O:8:LYS:O     | 15:O:11:VAL:HG12 | 1.81                     | 0.80              |
| 2:B:231:GLU:HB3  | 2:B:232:PRO:HD2  | 1.62                     | 0.80              |
| 1:A:1175:G:O2'   | 1:A:1176:A:C5'   | 2.31                     | 0.79              |
| 1:A:1192:C:C3'   | 1:A:1193:G:P     | 2.13                     | 0.79              |
| 2:B:25:ASN:HD22  | 2:B:27:LYS:H     | 1.29                     | 0.79              |
| 1:A:1281:U:H5'   | 1:A:1282:C:H5    | 1.46                     | 0.79              |
| 1:A:972:C:H4'    | 10:J:57:LYS:HG2  | 1.65                     | 0.79              |
| 9:I:106:ALA:O    | 9:I:108:VAL:HG23 | 1.81                     | 0.79              |
| 13:M:11:ARG:O    | 13:M:13:LYS:HG2  | 1.81                     | 0.79              |
| 1:A:1435:G:H2'   | 1:A:1436:U:C6    | 2.17                     | 0.79              |
| 1:A:579:G:H5'    | 1:A:728:A:H1'    | 1.64                     | 0.79              |
| 4:D:150:GLU:CD   | 4:D:150:GLU:H    | 1.85                     | 0.79              |
| 3:C:147:LYS:HE2  | 3:C:205:GLY:HA2  | 1.65                     | 0.79              |
| 1:A:1175:G:H2'   | 1:A:1176:A:H8    | 1.48                     | 0.78              |
| 8:H:119:LEU:HB3  | 8:H:123:GLU:HB2  | 1.65                     | 0.78              |
| 9:I:6:GLY:H      | 9:I:84:ALA:HB2   | 1.48                     | 0.78              |
| 1:A:1116:C:C2'   | 1:A:1117:G:H5''  | 2.13                     | 0.78              |
| 1:A:1057:G:H5''  | 3:C:154:SER:HB2  | 1.65                     | 0.78              |
| 1:A:1179:A:N6    | 1:A:1180:A:C2    | 2.52                     | 0.78              |
| 3:C:34:LEU:HD23  | 3:C:34:LEU:O     | 1.83                     | 0.78              |
| 12:L:28:LYS:C    | 12:L:30:ALA:H    | 1.85                     | 0.78              |
| 1:A:1123:A:H4'   | 10:J:37:PRO:HD2  | 1.66                     | 0.78              |
| 9:I:6:GLY:N      | 9:I:84:ALA:HB2   | 1.99                     | 0.78              |
| 6:F:9:VAL:HB     | 6:F:87:ARG:HB2   | 1.65                     | 0.77              |
| 1:A:1175:G:O3'   | 1:A:1176:A:OP1   | 2.01                     | 0.77              |
| 12:L:28:LYS:O    | 12:L:30:ALA:N    | 2.15                     | 0.77              |
| 9:I:48:GLU:HG2   | 9:I:51:ARG:NH2   | 2.00                     | 0.77              |
| 1:A:1175:G:HO3'  | 1:A:1176:A:P     | 1.24                     | 0.77              |
| 5:E:144:THR:HG22 | 5:E:146:ALA:H    | 1.49                     | 0.77              |
| 1:A:1191:A:O3'   | 1:A:1192:C:OP2   | 2.02                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1532:U:C2    | 1:A:1534:A:OP2   | 2.38                     | 0.77              |
| 1:A:35:G:H2'     | 1:A:36:C:C6      | 2.20                     | 0.77              |
| 2:B:103:THR:CG2  | 2:B:176:GLU:HB2  | 2.14                     | 0.77              |
| 2:B:223:ILE:HD12 | 2:B:224:GLN:N    | 1.99                     | 0.77              |
| 6:F:46:ARG:HB3   | 6:F:46:ARG:NH1   | 2.00                     | 0.77              |
| 1:A:1127:G:H21   | 1:A:1146:A:N6    | 1.83                     | 0.76              |
| 1:A:1502:A:H2    | 1:A:1505:G:H1    | 1.32                     | 0.76              |
| 10:J:64:GLU:HG2  | 14:N:59:ALA:HB2  | 1.66                     | 0.76              |
| 2:B:111:ARG:HB3  | 2:B:149:LEU:HD11 | 1.65                     | 0.76              |
| 14:N:6:LEU:HD12  | 14:N:23:ARG:NH2  | 2.00                     | 0.76              |
| 1:A:1160:G:O2'   | 1:A:1161:C:C5'   | 2.28                     | 0.76              |
| 14:N:12:ARG:HD3  | 14:N:12:ARG:H    | 1.51                     | 0.76              |
| 1:A:1175:G:C2'   | 1:A:1176:A:P     | 2.73                     | 0.76              |
| 7:G:75:VAL:HG21  | 7:G:86:GLN:HB3   | 1.67                     | 0.76              |
| 1:A:1080:A:H5''  | 5:E:16:THR:HG21  | 1.68                     | 0.76              |
| 1:A:1352:C:H2'   | 1:A:1353:G:C8    | 2.20                     | 0.76              |
| 1:A:1532:U:HO2'  | 1:A:1533:C:H6    | 1.31                     | 0.75              |
| 1:A:1127:G:N2    | 1:A:1146:A:H62   | 1.85                     | 0.75              |
| 2:B:124:SER:O    | 2:B:127:ILE:HG13 | 1.85                     | 0.75              |
| 1:A:1189:C:P     | 10:J:51:ARG:HH22 | 2.09                     | 0.75              |
| 1:A:1443:G:H4'   | 1:A:1446:A:H5'   | 1.68                     | 0.75              |
| 6:F:22:GLU:OE2   | 6:F:82:ARG:HD3   | 1.86                     | 0.75              |
| 1:A:1127:G:H21   | 1:A:1146:A:H62   | 1.35                     | 0.75              |
| 1:A:1356:G:H2'   | 1:A:1357:A:H8    | 1.46                     | 0.75              |
| 13:M:37:THR:HG22 | 13:M:39:ILE:HG13 | 1.68                     | 0.75              |
| 1:A:1060:C:H2'   | 1:A:1061:G:H8    | 1.52                     | 0.75              |
| 11:K:87:THR:HA   | 11:K:91:ARG:HH21 | 1.52                     | 0.75              |
| 16:P:67:THR:HG22 | 16:P:69:THR:H    | 1.51                     | 0.75              |
| 1:A:371:G:O2'    | 1:A:372:C:H5'    | 1.87                     | 0.75              |
| 5:E:92:LYS:HB3   | 5:E:119:LEU:HB2  | 1.68                     | 0.75              |
| 13:M:11:ARG:HG3  | 13:M:12:ASN:H    | 1.52                     | 0.75              |
| 1:A:438:G:H4'    | 1:A:439:A:OP1    | 1.87                     | 0.74              |
| 7:G:62:PHE:HD1   | 7:G:124:LEU:HD11 | 1.49                     | 0.74              |
| 13:M:14:ARG:HB3  | 13:M:16:ASP:OD1  | 1.86                     | 0.74              |
| 19:S:52:TYR:HA   | 19:S:56:GLN:O    | 1.87                     | 0.74              |
| 1:A:141:A:H1'    | 1:A:182:U:O2     | 1.87                     | 0.74              |
| 1:A:984:C:H2'    | 1:A:985:C:H6     | 1.51                     | 0.74              |
| 13:M:88:ARG:HD2  | 19:S:3:ARG:NH2   | 2.03                     | 0.74              |
| 19:S:7:LYS:HD2   | 19:S:7:LYS:O     | 1.87                     | 0.74              |
| 19:S:33:THR:HG22 | 19:S:35:SER:N    | 2.02                     | 0.74              |
| 16:P:81:ARG:HG2  | 16:P:83:GLU:HG2  | 1.69                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:44:LEU:H     | 2:B:44:LEU:CD1   | 1.99                     | 0.74              |
| 7:G:136:LYS:NZ   | 7:G:143:ARG:HH12 | 1.85                     | 0.74              |
| 1:A:629:G:H2'    | 1:A:630:G:O4'    | 1.88                     | 0.74              |
| 15:O:87:ILE:HG22 | 15:O:88:ARG:N    | 2.03                     | 0.74              |
| 1:A:1190:G:H3'   | 3:C:3:ASN:HD22   | 1.49                     | 0.74              |
| 1:A:351:G:H4'    | 1:A:352:C:OP1    | 1.88                     | 0.74              |
| 12:L:38:THR:O    | 12:L:79:GLU:HG3  | 1.87                     | 0.74              |
| 3:C:91:LEU:HD21  | 3:C:99:VAL:H     | 1.52                     | 0.73              |
| 10:J:46:ARG:NH1  | 10:J:64:GLU:HB3  | 2.03                     | 0.73              |
| 7:G:155:ARG:HA   | 7:G:155:ARG:NH1  | 2.02                     | 0.73              |
| 6:F:46:ARG:HB3   | 6:F:46:ARG:HH11  | 1.52                     | 0.73              |
| 11:K:72:ALA:HB1  | 11:K:77:MET:HE2  | 1.71                     | 0.73              |
| 17:Q:67:LYS:CA   | 17:Q:70:ARG:HH12 | 2.00                     | 0.73              |
| 1:A:390:C:H2'    | 1:A:391:G:H8     | 1.53                     | 0.73              |
| 5:E:107:ARG:HH11 | 5:E:107:ARG:HB2  | 1.54                     | 0.73              |
| 9:I:93:ARG:HB3   | 9:I:93:ARG:HH11  | 1.52                     | 0.73              |
| 1:A:1193:G:O2'   | 1:A:1194:U:H5'   | 1.88                     | 0.73              |
| 1:A:1533:C:C2'   | 1:A:1534:A:O5'   | 2.36                     | 0.73              |
| 6:F:44:GLY:HA2   | 6:F:59:TYR:CE1   | 2.23                     | 0.73              |
| 1:A:1133:G:H2'   | 1:A:1134:G:H8    | 1.52                     | 0.73              |
| 20:T:8:ARG:NH1   | 20:T:8:ARG:HB3   | 2.04                     | 0.73              |
| 1:A:382:A:H2'    | 1:A:383:A:C8     | 2.23                     | 0.73              |
| 23:Y:33:U:H2'    | 23:Y:34:TM2:H3'  | 1.69                     | 0.73              |
| 2:B:88:ALA:CB    | 2:B:90:MET:HG2   | 2.19                     | 0.73              |
| 1:A:390:C:H2'    | 1:A:391:G:C8     | 2.24                     | 0.73              |
| 13:M:34:LEU:HD13 | 13:M:41:PRO:HA   | 1.71                     | 0.73              |
| 14:N:44:LEU:O    | 14:N:44:LEU:HD12 | 1.87                     | 0.73              |
| 14:N:12:ARG:H    | 14:N:12:ARG:CD   | 2.02                     | 0.72              |
| 1:A:1016:A:H2'   | 1:A:1017:G:O4'   | 1.89                     | 0.72              |
| 2:B:218:ALA:O    | 2:B:222:ILE:HG13 | 1.88                     | 0.72              |
| 10:J:38:ILE:HB   | 10:J:71:LEU:HB3  | 1.71                     | 0.72              |
| 3:C:70:VAL:HG12  | 3:C:72:LYS:H     | 1.54                     | 0.72              |
| 5:E:144:THR:HG22 | 5:E:146:ALA:N    | 2.04                     | 0.72              |
| 19:S:50:ALA:HA   | 19:S:58:VAL:O    | 1.89                     | 0.72              |
| 2:B:130:ARG:HB3  | 2:B:131:PRO:HD2  | 1.72                     | 0.72              |
| 10:J:90:LEU:H    | 10:J:91:PRO:CD   | 2.03                     | 0.72              |
| 1:A:1286:A:H2'   | 1:A:1287:A:H4'   | 1.70                     | 0.72              |
| 10:J:49:VAL:HG23 | 14:N:41:ARG:HB2  | 1.70                     | 0.72              |
| 10:J:35:SER:HB2  | 10:J:72:VAL:O    | 1.89                     | 0.72              |
| 15:O:25:THR:HG21 | 15:O:70:LEU:HG   | 1.72                     | 0.72              |
| 2:B:60:ASP:O     | 2:B:64:ARG:HG3   | 1.89                     | 0.72              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:84:GLU:OE1   | 2:B:216:SER:HA    | 1.89                     | 0.72              |
| 3:C:101:LEU:HD23 | 3:C:102:ASN:N     | 2.04                     | 0.72              |
| 1:A:496:A:H4'    | 1:A:497:A:O5'     | 1.89                     | 0.71              |
| 10:J:30:SER:HB3  | 10:J:84:GLN:HE21  | 1.53                     | 0.71              |
| 1:A:1497:G:O2'   | 1:A:1498:U:H5'    | 1.90                     | 0.71              |
| 10:J:5:ARG:HA    | 10:J:73:ASP:OD1   | 1.90                     | 0.71              |
| 1:A:434:U:H2'    | 1:A:435:C:C6      | 2.25                     | 0.71              |
| 2:B:197:VAL:HB   | 2:B:200:ILE:HG12  | 1.72                     | 0.71              |
| 17:Q:59:ILE:HG22 | 17:Q:71:PHE:CD1   | 2.24                     | 0.71              |
| 1:A:1156:G:C3'   | 1:A:1157:A:OP2    | 2.38                     | 0.71              |
| 1:A:1191:A:P     | 3:C:3:ASN:HD21    | 2.12                     | 0.71              |
| 9:I:128:ARG:HG2  | 13:M:126:LYS:HZ3  | 1.55                     | 0.71              |
| 1:A:1054:C:H3'   | 1:A:1054:C:O2     | 1.90                     | 0.71              |
| 1:A:1086:U:H3    | 1:A:1099:G:N2     | 1.87                     | 0.71              |
| 1:A:1504:G:H3'   | 1:A:1504:G:OP2    | 1.90                     | 0.71              |
| 3:C:79:ARG:HG2   | 3:C:82:GLU:HG2    | 1.73                     | 0.71              |
| 10:J:38:ILE:HB   | 10:J:71:LEU:CB    | 2.20                     | 0.71              |
| 1:A:1281:U:H5'   | 1:A:1282:C:C5     | 2.25                     | 0.71              |
| 2:B:166:ASP:OD2  | 2:B:169:LYS:HB2   | 1.91                     | 0.71              |
| 7:G:140:ASP:HA   | 7:G:143:ARG:HH22  | 1.54                     | 0.71              |
| 1:A:1343:G:H1'   | 9:I:121:ARG:HH12  | 1.56                     | 0.71              |
| 9:I:70:LYS:O     | 9:I:74:ILE:HG13   | 1.91                     | 0.71              |
| 11:K:99:GLN:HG2  | 11:K:105:VAL:HG21 | 1.72                     | 0.71              |
| 18:R:88:LYS:HG2  | 18:R:88:LYS:OXT   | 1.90                     | 0.71              |
| 2:B:139:LYS:O    | 2:B:139:LYS:HD3   | 1.90                     | 0.71              |
| 15:O:87:ILE:HG22 | 15:O:88:ARG:H     | 1.56                     | 0.71              |
| 18:R:36:ASN:HD21 | 18:R:38:GLU:HG2   | 1.55                     | 0.70              |
| 1:A:524:G:H2'    | 1:A:525:C:C6      | 2.26                     | 0.70              |
| 13:M:40:ASN:HD22 | 13:M:41:PRO:HD2   | 1.56                     | 0.70              |
| 19:S:22:LEU:HD11 | 19:S:31:ILE:HD11  | 1.72                     | 0.70              |
| 1:A:1095:U:H2'   | 1:A:1096:C:C6     | 2.25                     | 0.70              |
| 2:B:204:ASN:ND2  | 2:B:206:ASP:H     | 1.89                     | 0.70              |
| 2:B:116:GLU:HB3  | 2:B:153:ARG:HH22  | 1.56                     | 0.70              |
| 4:D:35:ARG:O     | 4:D:36:ARG:HB2    | 1.90                     | 0.70              |
| 7:G:85:TYR:HD1   | 7:G:154:TYR:HE1   | 1.39                     | 0.70              |
| 3:C:110:ASN:O    | 3:C:111:LEU:HD23  | 1.90                     | 0.70              |
| 1:A:1178:G:N2    | 1:A:1180:A:H8     | 1.89                     | 0.70              |
| 1:A:1492:A:OP1   | 12:L:47:LYS:N     | 2.19                     | 0.70              |
| 1:A:353:A:H5'    | 1:A:353:A:H8      | 1.57                     | 0.70              |
| 1:A:1366:C:H2'   | 1:A:1367:C:H6     | 1.54                     | 0.70              |
| 4:D:24:GLU:HG2   | 4:D:25:ARG:N      | 2.05                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:G:120:ILE:O    | 7:G:124:LEU:HD23 | 1.91                     | 0.70              |
| 2:B:88:ALA:C     | 2:B:90:MET:H     | 1.95                     | 0.70              |
| 16:P:52:ASP:OD1  | 16:P:54:GLU:HG2  | 1.92                     | 0.70              |
| 10:J:24:VAL:O    | 10:J:28:ARG:HG3  | 1.92                     | 0.70              |
| 1:A:187:C:O2     | 20:T:105:SER:HB3 | 1.91                     | 0.70              |
| 9:I:55:ALA:O     | 9:I:56:LEU:HB2   | 1.92                     | 0.70              |
| 9:I:10:ARG:HD3   | 9:I:105:ASP:HB3  | 1.72                     | 0.69              |
| 10:J:39:PRO:O    | 10:J:40:LEU:HB2  | 1.91                     | 0.69              |
| 10:J:8:LEU:HB2   | 10:J:70:ARG:HB2  | 1.73                     | 0.69              |
| 20:T:53:LEU:O    | 20:T:57:ARG:HD2  | 1.92                     | 0.69              |
| 3:C:14:ILE:CG2   | 3:C:15:THR:H     | 2.04                     | 0.69              |
| 1:A:673:G:H2'    | 1:A:674:G:C8     | 2.26                     | 0.69              |
| 2:B:97:TRP:CZ2   | 2:B:102:LEU:HD13 | 2.25                     | 0.69              |
| 2:B:178:ARG:HB3  | 2:B:178:ARG:HH11 | 1.56                     | 0.69              |
| 2:B:64:ARG:HH11  | 2:B:64:ARG:HB3   | 1.58                     | 0.69              |
| 13:M:40:ASN:HD22 | 13:M:41:PRO:CD   | 2.05                     | 0.69              |
| 12:L:111:LYS:HE3 | 12:L:112:ASP:N   | 2.07                     | 0.69              |
| 13:M:17:VAL:O    | 13:M:20:THR:HB   | 1.92                     | 0.69              |
| 19:S:15:LEU:O    | 19:S:19:VAL:HG12 | 1.93                     | 0.69              |
| 20:T:50:GLU:HB2  | 20:T:99:LEU:HD12 | 1.75                     | 0.69              |
| 1:A:1160:G:O6    | 1:A:1181:G:O6    | 2.10                     | 0.69              |
| 1:A:254:G:OP1    | 17:Q:67:LYS:O    | 2.09                     | 0.69              |
| 1:A:1477:C:H2'   | 1:A:1478:C:C6    | 2.28                     | 0.69              |
| 5:E:10:MET:SD    | 5:E:13:ILE:HD11  | 2.33                     | 0.69              |
| 1:A:1497:G:C2'   | 1:A:1498:U:H5'   | 2.23                     | 0.69              |
| 9:I:27:THR:HG23  | 9:I:30:GLY:O     | 1.93                     | 0.69              |
| 1:A:1529:G:H3'   | 1:A:1529:G:OP2   | 1.93                     | 0.69              |
| 2:B:25:ASN:ND2   | 2:B:27:LYS:H     | 1.91                     | 0.69              |
| 5:E:126:ARG:HG3  | 5:E:126:ARG:HH11 | 1.58                     | 0.69              |
| 7:G:149:ARG:HB3  | 7:G:149:ARG:NH2  | 2.08                     | 0.69              |
| 10:J:6:ILE:HA    | 10:J:98:ILE:HG12 | 1.75                     | 0.68              |
| 7:G:140:ASP:HA   | 7:G:143:ARG:NH2  | 2.09                     | 0.68              |
| 14:N:32:SER:HB3  | 14:N:41:ARG:HB3  | 1.74                     | 0.68              |
| 19:S:28:LYS:HG2  | 19:S:29:ARG:N    | 2.05                     | 0.68              |
| 6:F:26:ILE:O     | 6:F:30:LEU:HG    | 1.94                     | 0.68              |
| 3:C:150:LYS:HG3  | 3:C:169:ALA:HB2  | 1.75                     | 0.68              |
| 10:J:23:ILE:O    | 10:J:23:ILE:HG22 | 1.92                     | 0.68              |
| 15:O:17:ARG:HH11 | 15:O:17:ARG:HG3  | 1.59                     | 0.68              |
| 9:I:102:LEU:HD12 | 9:I:102:LEU:H    | 1.59                     | 0.68              |
| 1:A:433:C:H5''   | 1:A:433:C:H6     | 1.59                     | 0.68              |
| 13:M:15:VAL:HG23 | 13:M:43:THR:O    | 1.93                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1149:C:H2'   | 1:A:1150:U:C6    | 2.29                     | 0.68              |
| 1:A:1366:C:H2'   | 1:A:1367:C:C6    | 2.28                     | 0.68              |
| 2:B:115:LEU:HG   | 2:B:153:ARG:HH21 | 1.56                     | 0.68              |
| 12:L:25:PRO:C    | 12:L:27:LEU:H    | 1.95                     | 0.68              |
| 1:A:1142:G:H2'   | 1:A:1143:G:O4'   | 1.93                     | 0.68              |
| 1:A:1175:G:C3'   | 1:A:1176:A:OP2   | 2.33                     | 0.68              |
| 1:A:731:G:OP1    | 1:A:766:A:H1'    | 1.94                     | 0.68              |
| 2:B:22:LYS:HG3   | 2:B:23:ARG:N     | 2.08                     | 0.68              |
| 11:K:15:ALA:HA   | 11:K:77:MET:HA   | 1.76                     | 0.68              |
| 21:U:6:ARG:HG3   | 21:U:15:ARG:NH1  | 2.09                     | 0.68              |
| 1:A:1026:G:H3'   | 1:A:1027:C:C5'   | 2.22                     | 0.67              |
| 1:A:35:G:H2'     | 1:A:36:C:H6      | 1.59                     | 0.67              |
| 13:M:22:ILE:HB   | 13:M:25:ILE:HB   | 1.75                     | 0.67              |
| 15:O:79:ARG:CZ   | 15:O:83:GLU:HB2  | 2.24                     | 0.67              |
| 6:F:60:PHE:CE2   | 18:R:78:LEU:HD21 | 2.28                     | 0.67              |
| 10:J:57:LYS:O    | 10:J:57:LYS:HD2  | 1.94                     | 0.67              |
| 13:M:11:ARG:CG   | 13:M:12:ASN:H    | 2.07                     | 0.67              |
| 20:T:74:LYS:HB3  | 20:T:74:LYS:HZ2  | 1.59                     | 0.67              |
| 1:A:1062:U:H2'   | 1:A:1063:C:C6    | 2.29                     | 0.67              |
| 1:A:1211:U:H5'   | 1:A:1212:U:OP1   | 1.94                     | 0.67              |
| 1:A:364:A:N6     | 12:L:28:LYS:HE3  | 2.09                     | 0.67              |
| 9:I:118:LYS:O    | 9:I:119:ALA:HB3  | 1.93                     | 0.67              |
| 1:A:1057:G:H5''  | 3:C:154:SER:CB   | 2.24                     | 0.67              |
| 11:K:57:THR:HG22 | 11:K:59:TYR:N    | 2.09                     | 0.67              |
| 17:Q:68:ARG:N    | 17:Q:70:ARG:NH1  | 2.43                     | 0.67              |
| 3:C:155:GLY:O    | 3:C:156:ARG:HB2  | 1.94                     | 0.67              |
| 1:A:1257:U:H4'   | 1:A:1258:G:OP2   | 1.95                     | 0.67              |
| 1:A:1521:G:H2'   | 1:A:1522:U:C6    | 2.30                     | 0.67              |
| 1:A:1502:A:H2    | 1:A:1505:G:N1    | 1.93                     | 0.67              |
| 9:I:21:PRO:HA    | 9:I:58:ARG:O     | 1.94                     | 0.67              |
| 1:A:1080:A:C5'   | 5:E:16:THR:HG21  | 2.25                     | 0.67              |
| 1:A:1117:G:N2    | 1:A:1180:A:H1'   | 2.09                     | 0.67              |
| 1:A:1521:G:H2'   | 1:A:1522:U:H6    | 1.60                     | 0.67              |
| 2:B:98:LEU:O     | 2:B:101:MET:HG3  | 1.95                     | 0.67              |
| 2:B:215:LEU:O    | 2:B:219:VAL:HG23 | 1.94                     | 0.67              |
| 4:D:80:GLU:O     | 4:D:84:LYS:HG3   | 1.95                     | 0.67              |
| 10:J:49:VAL:O    | 10:J:60:ARG:O    | 2.13                     | 0.67              |
| 1:A:235:C:H5'    | 17:Q:70:ARG:HG2  | 1.74                     | 0.67              |
| 2:B:77:ALA:HB2   | 2:B:211:ILE:HG21 | 1.75                     | 0.66              |
| 3:C:119:ARG:HG2  | 3:C:140:ARG:NH2  | 2.11                     | 0.66              |
| 9:I:24:GLY:HA2   | 9:I:59:PHE:O     | 1.95                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1250:A:H4'   | 9:I:68:GLY:CA    | 2.24                     | 0.66              |
| 11:K:33:THR:HG22 | 11:K:39:PRO:HA   | 1.77                     | 0.66              |
| 1:A:1126:U:H2'   | 1:A:1127:G:C8    | 2.30                     | 0.66              |
| 1:A:664:G:OP1    | 18:R:64:ARG:HD2  | 1.94                     | 0.66              |
| 20:T:56:MET:HE3  | 20:T:88:VAL:HG11 | 1.77                     | 0.66              |
| 3:C:195:VAL:C    | 3:C:196:LEU:HD22 | 2.15                     | 0.66              |
| 1:A:853:G:O2'    | 1:A:854:G:H5'    | 1.95                     | 0.66              |
| 1:A:127:G:HO2'   | 17:Q:2:PRO:N     | 1.94                     | 0.66              |
| 1:A:1412:C:H2'   | 1:A:1413:A:C8    | 2.31                     | 0.66              |
| 1:A:1392:G:O2'   | 1:A:1502:A:H5''  | 1.96                     | 0.66              |
| 12:L:55:VAL:HG12 | 12:L:56:ALA:N    | 2.11                     | 0.66              |
| 10:J:10:GLY:N    | 10:J:16:LEU:HD11 | 2.11                     | 0.66              |
| 13:M:37:THR:O    | 13:M:37:THR:HG22 | 1.95                     | 0.66              |
| 2:B:239:VAL:O    | 2:B:240:GLN:HG3  | 1.96                     | 0.66              |
| 3:C:180:ALA:O    | 3:C:181:ASN:HB3  | 1.96                     | 0.66              |
| 1:A:1062:U:H2'   | 1:A:1063:C:C5    | 2.30                     | 0.66              |
| 1:A:1068:G:H8    | 1:A:1068:G:OP2   | 1.80                     | 0.65              |
| 1:A:1527:C:O2'   | 1:A:1528:U:H5'   | 1.96                     | 0.65              |
| 3:C:23:TYR:CD2   | 3:C:24:ALA:N     | 2.63                     | 0.65              |
| 10:J:15:THR:HG22 | 10:J:94:VAL:HG23 | 1.78                     | 0.65              |
| 9:I:128:ARG:HA   | 13:M:126:LYS:NZ  | 2.10                     | 0.65              |
| 18:R:38:GLU:CD   | 18:R:38:GLU:H    | 1.99                     | 0.65              |
| 21:U:5:ASP:O     | 21:U:11:GLY:HA3  | 1.96                     | 0.65              |
| 1:A:575:G:OP1    | 1:A:575:G:H4'    | 1.97                     | 0.65              |
| 13:M:62:ASN:O    | 13:M:63:THR:HB   | 1.97                     | 0.65              |
| 1:A:780:A:O2'    | 1:A:781:A:H5''   | 1.96                     | 0.65              |
| 3:C:3:ASN:O      | 3:C:4:LYS:HB2    | 1.96                     | 0.65              |
| 3:C:84:ILE:HD11  | 3:C:88:ARG:HH21  | 1.61                     | 0.65              |
| 7:G:111:ARG:NH2  | 7:G:126:ASP:OD2  | 2.29                     | 0.65              |
| 1:A:1347:G:N2    | 1:A:1373:G:H2'   | 2.12                     | 0.65              |
| 1:A:1443:G:H4'   | 1:A:1446:A:C5'   | 2.25                     | 0.65              |
| 3:C:110:ASN:ND2  | 3:C:140:ARG:HB3  | 2.12                     | 0.65              |
| 9:I:65:VAL:HG21  | 9:I:77:ILE:HD11  | 1.77                     | 0.65              |
| 10:J:15:THR:HG22 | 10:J:94:VAL:CG2  | 2.27                     | 0.65              |
| 13:M:4:ILE:CG2   | 13:M:5:ALA:H     | 2.10                     | 0.65              |
| 1:A:1048:G:H5''  | 14:N:3:ARG:HG3   | 1.79                     | 0.65              |
| 1:A:1128:C:O2'   | 1:A:1130:A:C8    | 2.50                     | 0.65              |
| 1:A:1256:A:O2'   | 1:A:1257:U:H5'   | 1.97                     | 0.65              |
| 1:A:556:C:O2'    | 1:A:557:G:H5'    | 1.95                     | 0.65              |
| 1:A:163:C:O2'    | 1:A:164:U:H5'    | 1.97                     | 0.65              |
| 1:A:537:G:H2'    | 1:A:538:G:H8     | 1.60                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:G:111:ARG:HB2  | 7:G:119:ARG:HG2  | 1.79                     | 0.65              |
| 9:I:53:VAL:CG1   | 9:I:96:LEU:HD11  | 2.27                     | 0.65              |
| 18:R:36:ASN:ND2  | 18:R:38:GLU:HG2  | 2.11                     | 0.65              |
| 18:R:46:GLU:CD   | 18:R:46:GLU:H    | 2.00                     | 0.65              |
| 2:B:139:LYS:C    | 2:B:139:LYS:HD3  | 2.17                     | 0.65              |
| 5:E:143:ARG:NH1  | 8:H:77:GLU:OE2   | 2.30                     | 0.65              |
| 1:A:1066:C:O2'   | 1:A:1067:A:H5'   | 1.97                     | 0.65              |
| 1:A:683:G:H21    | 11:K:38:ASN:HD22 | 1.43                     | 0.65              |
| 15:O:78:TYR:CZ   | 15:O:82:ILE:HD11 | 2.31                     | 0.65              |
| 21:U:12:LYS:HB3  | 21:U:22:ARG:HD2  | 1.78                     | 0.65              |
| 1:A:1156:G:O3'   | 1:A:1157:A:OP1   | 2.03                     | 0.64              |
| 1:A:1305:G:H5'   | 21:U:4:GLY:HA3   | 1.78                     | 0.64              |
| 5:E:82:VAL:HG21  | 5:E:138:ALA:HA   | 1.78                     | 0.64              |
| 6:F:33:TYR:HA    | 6:F:71:ARG:CZ    | 2.27                     | 0.64              |
| 1:A:1152:A:C5'   | 10:J:13:HIS:HD2  | 2.07                     | 0.64              |
| 1:A:1229:A:OP2   | 13:M:114:ARG:HD3 | 1.97                     | 0.64              |
| 1:A:421:U:H5'    | 1:A:422:C:C5     | 2.32                     | 0.64              |
| 1:A:840:C:H4'    | 1:A:848:C:O2     | 1.97                     | 0.64              |
| 8:H:113:SER:HB2  | 8:H:134:ILE:HD11 | 1.78                     | 0.64              |
| 11:K:110:ASP:HB2 | 18:R:88:LYS:HD2  | 1.79                     | 0.64              |
| 12:L:79:GLU:O    | 12:L:79:GLU:HG2  | 1.97                     | 0.64              |
| 16:P:22:THR:HA   | 16:P:33:ILE:HG13 | 1.79                     | 0.64              |
| 17:Q:27:PHE:CE1  | 17:Q:36:ILE:HD11 | 2.32                     | 0.64              |
| 19:S:28:LYS:CG   | 19:S:29:ARG:H    | 2.06                     | 0.64              |
| 1:A:1300:G:O2'   | 1:A:1301:U:H6    | 1.80                     | 0.64              |
| 1:A:1367:C:H5'   | 10:J:60:ARG:HH12 | 1.61                     | 0.64              |
| 3:C:64:VAL:H     | 3:C:99:VAL:HB    | 1.61                     | 0.64              |
| 1:A:1021:G:O2'   | 1:A:1022:G:H5'   | 1.96                     | 0.64              |
| 2:B:74:LYS:NZ    | 2:B:206:ASP:HA   | 2.12                     | 0.64              |
| 8:H:112:LEU:HD23 | 8:H:112:LEU:N    | 2.13                     | 0.64              |
| 12:L:54:LYS:HD2  | 12:L:54:LYS:N    | 2.12                     | 0.64              |
| 13:M:9:ILE:N     | 13:M:9:ILE:HD12  | 2.13                     | 0.64              |
| 14:N:29:ARG:HH11 | 14:N:29:ARG:HG2  | 1.61                     | 0.64              |
| 1:A:99:C:H2'     | 1:A:101:A:C8     | 2.33                     | 0.64              |
| 1:A:1026:G:C3'   | 1:A:1027:C:H5''  | 2.26                     | 0.64              |
| 1:A:1286:A:C8    | 1:A:1287:A:H4'   | 2.31                     | 0.64              |
| 3:C:127:ARG:HG2  | 3:C:127:ARG:HH11 | 1.62                     | 0.64              |
| 6:F:47:ARG:N     | 6:F:47:ARG:HD3   | 2.13                     | 0.64              |
| 1:A:1392:G:N2    | 1:A:1502:A:H8    | 1.96                     | 0.64              |
| 1:A:397:A:H5'    | 1:A:398:C:OP1    | 1.98                     | 0.64              |
| 1:A:1147:C:H4'   | 9:I:5:TYR:HE2    | 1.63                     | 0.64              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 9:I:7:THR:HG22   | 9:I:8:GLY:N       | 2.12                     | 0.64              |
| 1:A:946:A:H2'    | 1:A:947:G:H8      | 1.63                     | 0.64              |
| 2:B:129:GLU:O    | 2:B:130:ARG:HB2   | 1.97                     | 0.64              |
| 1:A:363:A:H62    | 12:L:28:LYS:HE2   | 1.61                     | 0.64              |
| 19:S:17:GLU:O    | 19:S:21:GLU:HG3   | 1.97                     | 0.64              |
| 1:A:1392:G:H21   | 1:A:1502:A:H8     | 1.46                     | 0.63              |
| 10:J:32:ALA:H    | 10:J:78:ASN:HD21  | 1.44                     | 0.63              |
| 3:C:58:GLU:HB3   | 10:J:92:THR:CG2   | 2.28                     | 0.63              |
| 11:K:29:ILE:HG22 | 11:K:44:SER:HB2   | 1.80                     | 0.63              |
| 19:S:17:GLU:HA   | 19:S:20:LEU:CG    | 2.29                     | 0.63              |
| 19:S:6:LYS:HG2   | 19:S:7:LYS:HG3    | 1.79                     | 0.63              |
| 20:T:10:LEU:HG   | 20:T:12:ALA:HB3   | 1.80                     | 0.63              |
| 1:A:1251:A:H1'   | 1:A:1369:C:HO2'   | 1.62                     | 0.63              |
| 2:B:114:ARG:CA   | 2:B:117:GLU:HB3   | 2.29                     | 0.63              |
| 2:B:185:ILE:H    | 2:B:185:ILE:HD12  | 1.63                     | 0.63              |
| 2:B:88:ALA:HB3   | 2:B:90:MET:HG2    | 1.80                     | 0.63              |
| 3:C:32:LEU:HD22  | 3:C:59:ARG:NH1    | 2.13                     | 0.63              |
| 7:G:38:LEU:HD12  | 7:G:38:LEU:O      | 1.98                     | 0.63              |
| 16:P:67:THR:HG22 | 16:P:68:ASP:N     | 2.13                     | 0.63              |
| 1:A:1305:G:C5'   | 21:U:4:GLY:HA3    | 2.28                     | 0.63              |
| 1:A:948:C:OP1    | 13:M:109:THR:HG22 | 1.98                     | 0.63              |
| 5:E:149:GLU:O    | 5:E:153:LYS:HG2   | 1.99                     | 0.63              |
| 10:J:32:ALA:CB   | 10:J:76:ASN:HD22  | 2.11                     | 0.63              |
| 1:A:109:A:H2'    | 1:A:326:G:N2      | 2.13                     | 0.63              |
| 2:B:77:ALA:CB    | 2:B:211:ILE:HG21  | 2.28                     | 0.63              |
| 1:A:1161:C:H2'   | 1:A:1162:C:C6     | 2.33                     | 0.63              |
| 1:A:1435:G:H2'   | 1:A:1436:U:H6     | 1.64                     | 0.63              |
| 15:O:36:ILE:HG12 | 15:O:59:MET:HE3   | 1.81                     | 0.63              |
| 1:A:1407:C:O2'   | 1:A:1408:A:H5'    | 1.99                     | 0.63              |
| 3:C:156:ARG:HH21 | 3:C:161:GLU:HA    | 1.63                     | 0.63              |
| 3:C:52:LEU:H     | 3:C:52:LEU:CD2    | 2.11                     | 0.63              |
| 7:G:26:PHE:CE2   | 7:G:30:ILE:HD11   | 2.34                     | 0.63              |
| 7:G:50:ILE:O     | 7:G:54:THR:HB     | 1.99                     | 0.63              |
| 10:J:49:VAL:HG22 | 14:N:41:ARG:HD2   | 1.81                     | 0.63              |
| 15:O:8:LYS:O     | 15:O:12:ILE:HG13  | 1.99                     | 0.63              |
| 1:A:1053:G:C3'   | 1:A:1054:C:H5'    | 2.29                     | 0.63              |
| 5:E:101:ILE:HD12 | 5:E:119:LEU:HD23  | 1.79                     | 0.63              |
| 1:A:1121:U:H2'   | 1:A:1122:U:H6     | 1.64                     | 0.63              |
| 1:A:1125:U:H5'   | 1:A:1126:U:H5     | 1.63                     | 0.63              |
| 1:A:991:U:O4     | 1:A:1212:U:H1'    | 1.98                     | 0.63              |
| 1:A:1250:A:H2'   | 1:A:1251:A:C8     | 2.33                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 10:J:89:ASP:HB2  | 10:J:91:PRO:HD2  | 1.81                     | 0.63              |
| 3:C:15:THR:O     | 3:C:16:ARG:HB2   | 1.97                     | 0.63              |
| 10:J:32:ALA:H    | 10:J:78:ASN:ND2  | 1.97                     | 0.63              |
| 12:L:111:LYS:HE3 | 12:L:111:LYS:CA  | 2.29                     | 0.63              |
| 1:A:1141:C:H2'   | 1:A:1142:G:H8    | 1.64                     | 0.62              |
| 1:A:1533:C:C2'   | 1:A:1534:A:C5'   | 2.76                     | 0.62              |
| 2:B:91:PRO:HG3   | 2:B:154:LEU:HB2  | 1.81                     | 0.62              |
| 1:A:537:G:H2'    | 1:A:538:G:C8     | 2.34                     | 0.62              |
| 3:C:70:VAL:HG12  | 3:C:71:ALA:N     | 2.13                     | 0.62              |
| 5:E:24:ARG:HH11  | 5:E:24:ARG:HG2   | 1.63                     | 0.62              |
| 10:J:30:SER:CB   | 10:J:84:GLN:HE21 | 2.11                     | 0.62              |
| 10:J:90:LEU:H    | 10:J:91:PRO:HD2  | 1.64                     | 0.62              |
| 10:J:47:PHE:CZ   | 14:N:37:PHE:HE1  | 2.17                     | 0.62              |
| 19:S:51:VAL:O    | 19:S:58:VAL:HG22 | 1.98                     | 0.62              |
| 1:A:1305:G:N2    | 1:A:1331:G:O2'   | 2.33                     | 0.62              |
| 4:D:17:VAL:HG12  | 4:D:18:LYS:N     | 2.14                     | 0.62              |
| 7:G:85:TYR:HD1   | 7:G:154:TYR:CE1  | 2.15                     | 0.62              |
| 10:J:94:VAL:HG12 | 10:J:95:GLU:N    | 2.14                     | 0.62              |
| 16:P:20:VAL:HG11 | 16:P:32:TYR:HB3  | 1.82                     | 0.62              |
| 19:S:5:LEU:O     | 19:S:6:LYS:CB    | 2.47                     | 0.62              |
| 1:A:107:G:C2'    | 1:A:108:G:H5'    | 2.29                     | 0.62              |
| 1:A:1132:C:H2'   | 1:A:1133:G:C8    | 2.34                     | 0.62              |
| 1:A:839:U:O2     | 1:A:839:U:H2'    | 1.97                     | 0.62              |
| 1:A:1014:A:C2    | 1:A:1219:U:H1'   | 2.34                     | 0.62              |
| 1:A:1369:C:H2'   | 1:A:1370:G:H8    | 1.61                     | 0.62              |
| 1:A:314:C:O2'    | 1:A:315:A:H5'    | 1.99                     | 0.62              |
| 1:A:287:U:O2'    | 1:A:288:A:H5'    | 2.00                     | 0.62              |
| 1:A:421:U:H5'    | 1:A:422:C:H5     | 1.64                     | 0.62              |
| 1:A:657:G:H4'    | 15:O:28:GLN:HG2  | 1.82                     | 0.62              |
| 3:C:13:GLY:HA3   | 14:N:57:ARG:HH21 | 1.65                     | 0.62              |
| 10:J:49:VAL:CG2  | 14:N:41:ARG:HB2  | 2.28                     | 0.62              |
| 13:M:14:ARG:NH1  | 13:M:16:ASP:OD2  | 2.33                     | 0.62              |
| 13:M:25:ILE:HD11 | 13:M:60:VAL:HG11 | 1.82                     | 0.62              |
| 2:B:54:THR:O     | 2:B:57:PHE:HB3   | 2.00                     | 0.62              |
| 9:I:58:ARG:HD2   | 9:I:59:PHE:CE1   | 2.34                     | 0.62              |
| 16:P:74:LEU:O    | 16:P:79:VAL:HG23 | 1.98                     | 0.62              |
| 3:C:14:ILE:HG22  | 3:C:15:THR:HG23  | 1.81                     | 0.62              |
| 12:L:33:ARG:HG2  | 12:L:62:SER:HB2  | 1.82                     | 0.62              |
| 14:N:9:LYS:HD2   | 14:N:9:LYS:C     | 2.19                     | 0.62              |
| 1:A:192:U:C1'    | 20:T:103:GLY:HA2 | 2.30                     | 0.62              |
| 1:A:1216:G:H5''  | 14:N:5:ALA:HB2   | 1.82                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:19:GLU:HA    | 3:C:54:ARG:HH21  | 1.65                     | 0.62              |
| 3:C:70:VAL:O     | 3:C:106:VAL:HG23 | 1.99                     | 0.62              |
| 4:D:119:GLN:HG2  | 4:D:123:HIS:CD2  | 2.34                     | 0.62              |
| 4:D:176:LEU:HD12 | 4:D:177:ASP:H    | 1.64                     | 0.62              |
| 13:M:31:LYS:O    | 13:M:35:GLU:HB2  | 2.00                     | 0.62              |
| 15:O:6:GLU:CD    | 15:O:6:GLU:H     | 2.04                     | 0.62              |
| 1:A:266:G:C8     | 1:A:266:G:H5'    | 2.35                     | 0.61              |
| 1:A:562:C:H1'    | 12:L:15:ARG:HG3  | 1.81                     | 0.61              |
| 1:A:1128:C:C4'   | 9:I:16:ARG:HH12  | 2.11                     | 0.61              |
| 1:A:1106:G:OP1   | 3:C:172:ARG:HD3  | 2.00                     | 0.61              |
| 1:A:1160:G:C6    | 1:A:1181:G:O6    | 2.53                     | 0.61              |
| 3:C:19:GLU:HB3   | 3:C:40:ARG:HH21  | 1.64                     | 0.61              |
| 9:I:97:LYS:HA    | 9:I:102:LEU:HD11 | 1.82                     | 0.61              |
| 10:J:90:LEU:N    | 10:J:91:PRO:HD2  | 2.15                     | 0.61              |
| 1:A:371:G:C2'    | 1:A:372:C:H5'    | 2.29                     | 0.61              |
| 1:A:828:A:H2'    | 1:A:829:G:O4'    | 2.00                     | 0.61              |
| 7:G:43:PHE:O     | 7:G:47:CYS:HB2   | 2.00                     | 0.61              |
| 12:L:47:LYS:HB3  | 12:L:48:PRO:CD   | 2.25                     | 0.61              |
| 1:A:1251:A:H2'   | 1:A:1252:A:C8    | 2.36                     | 0.61              |
| 1:A:112:G:H4'    | 1:A:389:A:H5''   | 1.82                     | 0.61              |
| 7:G:18:TYR:CE2   | 7:G:59:LEU:HB2   | 2.35                     | 0.61              |
| 7:G:51:GLN:O     | 7:G:52:GLU:HG2   | 2.01                     | 0.61              |
| 13:M:50:GLU:O    | 13:M:54:VAL:HG23 | 1.99                     | 0.61              |
| 1:A:1241:G:H2'   | 1:A:1242:C:C6    | 2.34                     | 0.61              |
| 1:A:631:G:H5'    | 1:A:632:A:OP1    | 2.00                     | 0.61              |
| 1:A:969:A:H61    | 13:M:126:LYS:HB2 | 1.65                     | 0.61              |
| 9:I:108:VAL:HG12 | 9:I:109:VAL:N    | 2.16                     | 0.61              |
| 13:M:22:ILE:HG13 | 13:M:25:ILE:HD12 | 1.83                     | 0.61              |
| 20:T:45:GLN:HB2  | 20:T:91:LEU:HD13 | 1.81                     | 0.61              |
| 1:A:1128:C:O2'   | 1:A:1130:A:H8    | 1.84                     | 0.61              |
| 1:A:1286:A:H8    | 1:A:1287:A:H4'   | 1.65                     | 0.61              |
| 1:A:1300:G:HO2'  | 1:A:1301:U:H6    | 1.46                     | 0.61              |
| 1:A:983:A:H5'    | 1:A:984:C:OP2    | 2.00                     | 0.61              |
| 3:C:50:ALA:HB1   | 3:C:70:VAL:HG11  | 1.81                     | 0.61              |
| 12:L:24:VAL:O    | 12:L:26:ALA:N    | 2.32                     | 0.61              |
| 2:B:195:ASP:O    | 8:H:74:PRO:HG3   | 2.00                     | 0.61              |
| 3:C:107:GLN:O    | 3:C:108:ASN:HB3  | 2.01                     | 0.61              |
| 4:D:146:ILE:HD12 | 4:D:146:ILE:N    | 2.15                     | 0.61              |
| 7:G:75:VAL:CG2   | 7:G:86:GLN:HB3   | 2.29                     | 0.61              |
| 10:J:46:ARG:HG2  | 10:J:46:ARG:NH1  | 2.15                     | 0.61              |
| 10:J:71:LEU:O    | 10:J:72:VAL:HB   | 2.00                     | 0.61              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:701:C:H5''    | 1:A:703:G:O4'    | 2.00                     | 0.61              |
| 13:M:102:ARG:HH11 | 13:M:102:ARG:HB2 | 1.66                     | 0.61              |
| 1:A:243:A:H4'     | 1:A:244:U:C5'    | 2.20                     | 0.61              |
| 1:A:818:G:C3'     | 1:A:819:A:H5''   | 2.30                     | 0.61              |
| 2:B:69:LEU:HD12   | 2:B:155:LEU:HD11 | 1.82                     | 0.61              |
| 12:L:70:ILE:HD13  | 12:L:77:LEU:HD12 | 1.82                     | 0.61              |
| 1:A:376:G:OP2     | 16:P:67:THR:HG21 | 2.01                     | 0.61              |
| 1:A:538:G:OP2     | 12:L:115:LYS:HG3 | 1.99                     | 0.61              |
| 5:E:126:ARG:HG3   | 5:E:126:ARG:NH1  | 2.16                     | 0.61              |
| 6:F:30:LEU:HB3    | 6:F:35:ALA:HB3   | 1.82                     | 0.61              |
| 12:L:24:VAL:HG12  | 12:L:24:VAL:O    | 2.01                     | 0.61              |
| 1:A:1318:A:H1'    | 19:S:37:ARG:HH11 | 1.66                     | 0.61              |
| 7:G:12:LEU:N      | 7:G:12:LEU:HD12  | 2.15                     | 0.60              |
| 9:I:82:ALA:O      | 9:I:86:VAL:HG23  | 2.01                     | 0.60              |
| 10:J:9:ARG:HB3    | 10:J:9:ARG:NH1   | 2.16                     | 0.60              |
| 1:A:1343:G:H2'    | 1:A:1344:C:C6    | 2.35                     | 0.60              |
| 1:A:364:A:H61     | 12:L:28:LYS:HE3  | 1.65                     | 0.60              |
| 12:L:126:LYS:HG3  | 12:L:127:GLU:H   | 1.66                     | 0.60              |
| 1:A:818:G:O2'     | 1:A:819:A:H5''   | 2.01                     | 0.60              |
| 6:F:38:GLU:O      | 6:F:39:LYS:HB3   | 2.00                     | 0.60              |
| 13:M:49:THR:HB    | 13:M:52:GLU:HG3  | 1.83                     | 0.60              |
| 16:P:4:ILE:HG13   | 16:P:64:ALA:HB1  | 1.83                     | 0.60              |
| 1:A:539:A:H2'     | 1:A:540:G:C8     | 2.36                     | 0.60              |
| 10:J:9:ARG:C      | 10:J:16:LEU:HD11 | 2.22                     | 0.60              |
| 20:T:43:LEU:HD11  | 20:T:55:ILE:HD12 | 1.82                     | 0.60              |
| 12:L:40:VAL:HG11  | 12:L:77:LEU:O    | 2.01                     | 0.60              |
| 16:P:20:VAL:HG11  | 16:P:32:TYR:CB   | 2.32                     | 0.60              |
| 17:Q:65:ILE:N     | 17:Q:65:ILE:HD12 | 2.15                     | 0.60              |
| 1:A:1132:C:H2'    | 1:A:1133:G:H8    | 1.66                     | 0.60              |
| 1:A:433:C:C5'     | 1:A:433:C:H6     | 2.14                     | 0.60              |
| 1:A:539:A:H2'     | 1:A:540:G:H8     | 1.66                     | 0.60              |
| 1:A:973:G:H3'     | 1:A:974:A:H5''   | 1.84                     | 0.60              |
| 10:J:49:VAL:O     | 10:J:60:ARG:HA   | 2.01                     | 0.60              |
| 10:J:90:LEU:N     | 10:J:91:PRO:CD   | 2.63                     | 0.60              |
| 3:C:188:LEU:O     | 3:C:189:ALA:HB2  | 2.02                     | 0.60              |
| 1:A:405:U:H3'     | 1:A:406:G:H5'    | 1.84                     | 0.60              |
| 10:J:36:GLY:O     | 10:J:72:VAL:HA   | 2.01                     | 0.60              |
| 1:A:1291:G:H4'    | 9:I:39:GLY:HA3   | 1.84                     | 0.60              |
| 1:A:26:A:N6       | 1:A:558:G:H1'    | 2.17                     | 0.60              |
| 1:A:427:U:OP1     | 4:D:13:ARG:NH2   | 2.35                     | 0.60              |
| 10:J:23:ILE:N     | 10:J:23:ILE:HD12 | 2.17                     | 0.60              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 17:Q:69:LYS:C    | 17:Q:70:ARG:HD2   | 2.22                     | 0.60              |
| 19:S:18:LYS:HD3  | 19:S:18:LYS:O     | 2.02                     | 0.60              |
| 1:A:1305:G:H22   | 1:A:1331:G:C2'    | 2.15                     | 0.60              |
| 1:A:1298:C:H2'   | 7:G:114:ARG:NH1   | 2.17                     | 0.60              |
| 13:M:125:ARG:HD2 | 13:M:125:ARG:C    | 2.22                     | 0.60              |
| 3:C:14:ILE:O     | 3:C:16:ARG:N      | 2.35                     | 0.59              |
| 9:I:93:ARG:CB    | 9:I:93:ARG:HH11   | 2.13                     | 0.59              |
| 1:A:1323:G:H2'   | 1:A:1324:A:C8     | 2.37                     | 0.59              |
| 1:A:353:A:H5'    | 1:A:353:A:C8      | 2.37                     | 0.59              |
| 10:J:6:ILE:HG23  | 10:J:98:ILE:HD11  | 1.84                     | 0.59              |
| 11:K:126:ARG:O   | 11:K:127:LYS:HB2  | 2.03                     | 0.59              |
| 1:A:1156:G:H3'   | 1:A:1157:A:P      | 2.34                     | 0.59              |
| 1:A:639:G:O2'    | 1:A:640:A:H5'     | 2.02                     | 0.59              |
| 1:A:382:A:H2'    | 1:A:383:A:H8      | 1.63                     | 0.59              |
| 1:A:412:A:N6     | 4:D:35:ARG:HB2    | 2.17                     | 0.59              |
| 2:B:88:ALA:HB1   | 2:B:90:MET:HG2    | 1.84                     | 0.59              |
| 11:K:108:ILE:N   | 11:K:108:ILE:HD12 | 2.17                     | 0.59              |
| 2:B:204:ASN:HD22 | 2:B:206:ASP:H     | 1.50                     | 0.59              |
| 3:C:82:GLU:O     | 3:C:85:ARG:HB3    | 2.03                     | 0.59              |
| 1:A:1063:C:H3'   | 1:A:1064:G:H2'    | 1.84                     | 0.59              |
| 1:A:107:G:H2'    | 1:A:108:G:H5'     | 1.84                     | 0.59              |
| 3:C:156:ARG:NH2  | 3:C:161:GLU:HA    | 2.17                     | 0.59              |
| 12:L:124:LYS:HD3 | 12:L:125:PRO:HD2  | 1.85                     | 0.59              |
| 17:Q:27:PHE:HB2  | 17:Q:28:PRO:HD2   | 1.84                     | 0.59              |
| 17:Q:59:ILE:HG22 | 17:Q:71:PHE:HD1   | 1.65                     | 0.59              |
| 12:L:28:LYS:C    | 12:L:30:ALA:N     | 2.53                     | 0.59              |
| 20:T:43:LEU:CD1  | 20:T:55:ILE:HD12  | 2.33                     | 0.59              |
| 1:A:1176:A:H2'   | 1:A:1177:G:C8     | 2.38                     | 0.59              |
| 6:F:45:LEU:HD12  | 6:F:45:LEU:O      | 2.03                     | 0.59              |
| 9:I:126:SER:O    | 9:I:127:LYS:HB3   | 2.02                     | 0.59              |
| 1:A:1148:U:H2'   | 1:A:1149:C:O4'    | 2.03                     | 0.59              |
| 1:A:818:G:C2'    | 1:A:819:A:H5''    | 2.33                     | 0.59              |
| 12:L:43:VAL:HG12 | 12:L:44:THR:N     | 2.18                     | 0.59              |
| 13:M:90:LEU:HA   | 13:M:93:ARG:HB2   | 1.85                     | 0.59              |
| 1:A:1190:G:H3'   | 3:C:3:ASN:HD21    | 1.62                     | 0.59              |
| 1:A:860:A:H2'    | 1:A:861:G:O4'     | 2.03                     | 0.59              |
| 2:B:129:GLU:N    | 2:B:129:GLU:OE2   | 2.36                     | 0.59              |
| 9:I:53:VAL:CG2   | 9:I:85:LEU:HD21   | 2.30                     | 0.59              |
| 1:A:1153:C:P     | 10:J:13:HIS:HE2   | 2.26                     | 0.59              |
| 10:J:5:ARG:O     | 10:J:98:ILE:HG23  | 2.03                     | 0.59              |
| 10:J:76:ASN:O    | 10:J:78:ASN:N     | 2.33                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1347:G:O2'   | 1:A:1348:U:P     | 2.60                     | 0.58              |
| 1:A:1479:C:H2'   | 1:A:1480:G:H8    | 1.66                     | 0.58              |
| 1:A:984:C:H2'    | 1:A:985:C:C6     | 2.37                     | 0.58              |
| 2:B:53:ARG:HH12  | 2:B:199:TYR:HA   | 1.67                     | 0.58              |
| 2:B:88:ALA:O     | 2:B:90:MET:N     | 2.36                     | 0.58              |
| 4:D:126:ILE:HG22 | 4:D:127:THR:N    | 2.18                     | 0.58              |
| 5:E:150:ARG:NH1  | 5:E:150:ARG:HG3  | 2.09                     | 0.58              |
| 1:A:1168:A:H2'   | 1:A:1169:A:C8    | 2.37                     | 0.58              |
| 1:A:908:A:H2'    | 1:A:909:A:C8     | 2.39                     | 0.58              |
| 2:B:204:ASN:HD22 | 2:B:204:ASN:C    | 2.04                     | 0.58              |
| 2:B:74:LYS:HZ2   | 2:B:206:ASP:HA   | 1.68                     | 0.58              |
| 3:C:123:GLN:O    | 3:C:126:ARG:HG2  | 2.02                     | 0.58              |
| 1:A:1128:C:C5'   | 9:I:16:ARG:NH1   | 2.59                     | 0.58              |
| 6:F:100:ASN:HB3  | 18:R:27:GLY:O    | 2.03                     | 0.58              |
| 1:A:961:U:C2'    | 1:A:962:C:H5'    | 2.34                     | 0.58              |
| 8:H:120:THR:OG1  | 8:H:123:GLU:HG3  | 2.03                     | 0.58              |
| 9:I:48:GLU:HA    | 9:I:51:ARG:HE    | 1.68                     | 0.58              |
| 1:A:1038:C:H2'   | 1:A:1039:C:C6    | 2.39                     | 0.58              |
| 1:A:1125:U:H3    | 10:J:5:ARG:HH21  | 1.50                     | 0.58              |
| 1:A:1247:U:O2'   | 1:A:1248:A:H5'   | 2.03                     | 0.58              |
| 1:A:1330:U:OP1   | 13:M:23:TYR:O    | 2.21                     | 0.58              |
| 1:A:269:C:H2'    | 1:A:270:A:C8     | 2.39                     | 0.58              |
| 4:D:189:PRO:HB2  | 4:D:194:LEU:HD21 | 1.84                     | 0.58              |
| 5:E:36:ASP:OD2   | 5:E:40:ARG:HB2   | 2.03                     | 0.58              |
| 7:G:136:LYS:NZ   | 7:G:143:ARG:NH1  | 2.51                     | 0.58              |
| 8:H:83:ILE:O     | 8:H:83:ILE:HG23  | 2.03                     | 0.58              |
| 14:N:9:LYS:O     | 14:N:11:LYS:N    | 2.36                     | 0.58              |
| 19:S:33:THR:HG22 | 19:S:34:TRP:N    | 2.19                     | 0.58              |
| 1:A:1029:C:H2'   | 1:A:1030:C:C6    | 2.39                     | 0.58              |
| 1:A:1277:C:HO2'  | 1:A:1279:A:H8    | 1.51                     | 0.58              |
| 1:A:1368:G:OP2   | 9:I:112:LYS:HD2  | 2.04                     | 0.58              |
| 4:D:10:ARG:HG3   | 4:D:10:ARG:HH11  | 1.69                     | 0.58              |
| 9:I:48:GLU:N     | 9:I:49:PRO:CD    | 2.67                     | 0.58              |
| 13:M:40:ASN:ND2  | 13:M:42:ALA:H    | 2.01                     | 0.58              |
| 1:A:1003(A):G:C2 | 1:A:1004:A:H1'   | 2.38                     | 0.58              |
| 1:A:1042:G:O2'   | 1:A:1043:C:H5'   | 2.03                     | 0.58              |
| 1:A:1316:G:N2    | 1:A:1318:A:H3'   | 2.18                     | 0.58              |
| 1:A:1391:U:H2'   | 1:A:1392:G:C8    | 2.39                     | 0.58              |
| 2:B:114:ARG:HA   | 2:B:117:GLU:CB   | 2.33                     | 0.58              |
| 2:B:223:ILE:HD12 | 2:B:224:GLN:H    | 1.68                     | 0.58              |
| 1:A:1250:A:C4'   | 9:I:68:GLY:H     | 2.12                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 16:P:38:TYR:HE2  | 16:P:50:LYS:HE2  | 1.68                     | 0.58              |
| 1:A:1118:C:H1'   | 1:A:1179:A:C4    | 2.39                     | 0.58              |
| 1:A:192:U:H1'    | 20:T:103:GLY:HA2 | 1.85                     | 0.58              |
| 1:A:1190:G:C3'   | 3:C:3:ASN:ND2    | 2.64                     | 0.58              |
| 3:C:64:VAL:CG2   | 3:C:99:VAL:HG11  | 2.31                     | 0.58              |
| 4:D:199:ASN:HD21 | 4:D:201:GLN:HB2  | 1.68                     | 0.58              |
| 14:N:3:ARG:HB2   | 14:N:3:ARG:HH11  | 1.68                     | 0.58              |
| 1:A:1175:G:H3'   | 1:A:1176:A:OP2   | 2.03                     | 0.58              |
| 1:A:1232:U:P     | 9:I:124:GLN:HE21 | 2.27                     | 0.58              |
| 3:C:27:LYS:HD3   | 3:C:27:LYS:N     | 2.19                     | 0.58              |
| 6:F:46:ARG:HH11  | 6:F:46:ARG:CB    | 2.16                     | 0.58              |
| 23:Y:34:TM2:H2'  | 23:Y:35:A:C8     | 2.39                     | 0.58              |
| 1:A:939:G:H2'    | 1:A:940:C:C6     | 2.39                     | 0.58              |
| 3:C:32:LEU:HD22  | 3:C:59:ARG:HH11  | 1.69                     | 0.58              |
| 1:A:407:G:O2'    | 4:D:116:GLN:HG3  | 2.03                     | 0.58              |
| 5:E:76:ILE:HG13  | 5:E:142:LEU:CD1  | 2.34                     | 0.58              |
| 5:E:81:GLU:CD    | 5:E:88:LYS:HE2   | 2.25                     | 0.58              |
| 6:F:3:ARG:HG2    | 6:F:93:SER:OG    | 2.04                     | 0.58              |
| 8:H:4:ASP:OD2    | 8:H:85:ARG:NH1   | 2.35                     | 0.58              |
| 1:A:1251:A:H4'   | 9:I:12:GLU:OE2   | 2.03                     | 0.58              |
| 10:J:27:ALA:HA   | 10:J:81:THR:HG23 | 1.86                     | 0.58              |
| 14:N:26:ARG:HH21 | 14:N:47:LEU:CG   | 2.11                     | 0.58              |
| 3:C:29:TYR:OH    | 14:N:54:PRO:HG2  | 2.03                     | 0.58              |
| 17:Q:45:HIS:HB3  | 17:Q:72:ARG:HG2  | 1.86                     | 0.58              |
| 18:R:42:ARG:NH1  | 18:R:42:ARG:HB3  | 2.18                     | 0.58              |
| 1:A:1137:C:H4'   | 1:A:1138:G:N1    | 2.19                     | 0.57              |
| 2:B:141:GLU:O    | 2:B:144:ARG:HG3  | 2.04                     | 0.57              |
| 3:C:34:LEU:HD21  | 3:C:38:ARG:NE    | 2.19                     | 0.57              |
| 7:G:31:MET:HG2   | 7:G:32:ARG:H     | 1.68                     | 0.57              |
| 7:G:5:ARG:NE     | 7:G:7:ALA:HA     | 2.19                     | 0.57              |
| 1:A:1251:A:H1'   | 1:A:1369:C:O2'   | 2.02                     | 0.57              |
| 1:A:1397:C:H4'   | 1:A:1398:A:OP2   | 2.04                     | 0.57              |
| 3:C:64:VAL:HG12  | 3:C:66:VAL:HG23  | 1.86                     | 0.57              |
| 3:C:91:LEU:HD23  | 3:C:92:ALA:N     | 2.17                     | 0.57              |
| 1:A:972:C:P      | 10:J:57:LYS:HE2  | 2.44                     | 0.57              |
| 12:L:57:LYS:HD3  | 12:L:67:THR:HG23 | 1.86                     | 0.57              |
| 15:O:87:ILE:CG2  | 15:O:88:ARG:H    | 2.17                     | 0.57              |
| 19:S:80:TYR:CZ   | 19:S:81:ARG:HD3  | 2.39                     | 0.57              |
| 1:A:1160:G:HO2'  | 1:A:1161:C:H5'   | 1.70                     | 0.57              |
| 3:C:79:ARG:HG2   | 3:C:82:GLU:CG    | 2.34                     | 0.57              |
| 1:A:620:C:N1     | 4:D:135:LEU:HD13 | 2.19                     | 0.57              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:D:31:CYS:O     | 4:D:31:CYS:SG     | 2.62                     | 0.57              |
| 1:A:666:G:H5'    | 1:A:726:C:H1'     | 1.86                     | 0.57              |
| 9:I:4:TYR:CE1    | 9:I:88:TYR:HA     | 2.39                     | 0.57              |
| 12:L:34:ARG:O    | 12:L:61:THR:HG23  | 2.05                     | 0.57              |
| 13:M:8:GLU:OE1   | 13:M:22:ILE:HG23  | 2.04                     | 0.57              |
| 1:A:1320:C:O2'   | 1:A:1321:C:H5'    | 2.05                     | 0.57              |
| 9:I:107:ARG:HH11 | 9:I:107:ARG:HB3   | 1.68                     | 0.57              |
| 17:Q:40:LYS:HD2  | 17:Q:42:TYR:CZ    | 2.39                     | 0.57              |
| 1:A:1157:A:C5    | 1:A:1180:A:N6     | 2.73                     | 0.57              |
| 1:A:457:C:H2'    | 1:A:458:C:H6      | 1.69                     | 0.57              |
| 5:E:110:LEU:HD13 | 5:E:118:ILE:HG21  | 1.85                     | 0.57              |
| 12:L:113:ARG:NH1 | 12:L:116:SER:H    | 2.02                     | 0.57              |
| 12:L:58:VAL:O    | 12:L:65:GLU:HA    | 2.04                     | 0.57              |
| 6:F:100:ASN:ND2  | 18:R:23:LYS:HG2   | 2.20                     | 0.57              |
| 3:C:6:HIS:CD2    | 3:C:8:ILE:H       | 2.09                     | 0.57              |
| 3:C:23:TYR:OH    | 10:J:9:ARG:HD3    | 2.03                     | 0.57              |
| 12:L:89:ARG:HA   | 12:L:97:ARG:HA    | 1.86                     | 0.57              |
| 13:M:3:ARG:HB2   | 13:M:9:ILE:HG13   | 1.86                     | 0.57              |
| 1:A:337:C:H2'    | 1:A:338:A:H8      | 1.69                     | 0.57              |
| 1:A:832:C:O2'    | 1:A:833:U:H5'     | 2.04                     | 0.57              |
| 2:B:114:ARG:NH1  | 2:B:118:LEU:HD21  | 2.20                     | 0.57              |
| 3:C:6:HIS:CD2    | 3:C:8:ILE:HB      | 2.40                     | 0.57              |
| 7:G:69:VAL:HG21  | 7:G:104:LEU:HD21  | 1.87                     | 0.57              |
| 9:I:45:ALA:O     | 9:I:48:GLU:HB2    | 2.04                     | 0.57              |
| 12:L:27:LEU:HG   | 12:L:28:LYS:H     | 1.70                     | 0.57              |
| 1:A:1024:G:C3'   | 1:A:1025:U:H5''   | 2.34                     | 0.57              |
| 1:A:746:A:O2'    | 1:A:747:C:H5'     | 2.05                     | 0.57              |
| 3:C:154:SER:OG   | 3:C:155:GLY:N     | 2.37                     | 0.57              |
| 10:J:84:GLN:O    | 10:J:88:LEU:HD12  | 2.05                     | 0.57              |
| 12:L:83:VAL:HG13 | 12:L:100:ILE:HG23 | 1.86                     | 0.57              |
| 1:A:1175:G:C2'   | 1:A:1176:A:O5'    | 2.53                     | 0.57              |
| 1:A:646:U:H2'    | 1:A:647:C:C6      | 2.39                     | 0.57              |
| 1:A:918:A:H2'    | 1:A:919:A:C8      | 2.40                     | 0.57              |
| 3:C:126:ARG:NH2  | 3:C:128:PHE:CD1   | 2.73                     | 0.57              |
| 5:E:146:ALA:O    | 5:E:150:ARG:HB2   | 2.05                     | 0.57              |
| 16:P:38:TYR:CE2  | 16:P:50:LYS:HE2   | 2.39                     | 0.57              |
| 19:S:5:LEU:HD11  | 19:S:70:LYS:NZ    | 2.20                     | 0.57              |
| 1:A:1112:C:C4    | 3:C:178:LEU:HD23  | 2.40                     | 0.56              |
| 1:A:1121:U:H2'   | 1:A:1122:U:C6     | 2.39                     | 0.56              |
| 1:A:895:G:H2'    | 1:A:896:C:H6      | 1.70                     | 0.56              |
| 4:D:17:VAL:CG1   | 4:D:18:LYS:N      | 2.69                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:H:103:VAL:HG21 | 8:H:109:ILE:O    | 2.05                     | 0.56              |
| 19:S:40:ILE:CG2  | 19:S:62:ILE:HD11 | 2.35                     | 0.56              |
| 1:A:834:C:H2'    | 1:A:835:U:H6     | 1.70                     | 0.56              |
| 4:D:170:VAL:HG13 | 4:D:174:LEU:HB2  | 1.86                     | 0.56              |
| 17:Q:59:ILE:HD13 | 17:Q:73:VAL:HA   | 1.87                     | 0.56              |
| 1:A:1424:C:O2'   | 1:A:1425:U:H5'   | 2.05                     | 0.56              |
| 1:A:344:A:H4'    | 1:A:345:C:OP2    | 2.06                     | 0.56              |
| 2:B:87:ARG:O     | 2:B:88:ALA:CB    | 2.52                     | 0.56              |
| 10:J:47:PHE:CE2  | 14:N:37:PHE:HE1  | 2.22                     | 0.56              |
| 13:M:79:LYS:HE2  | 13:M:83:ASP:OD2  | 2.06                     | 0.56              |
| 17:Q:40:LYS:HG2  | 17:Q:41:LYS:N    | 2.20                     | 0.56              |
| 20:T:74:LYS:CB   | 20:T:74:LYS:NZ   | 2.68                     | 0.56              |
| 23:Y:34:TM2:H2'  | 23:Y:35:A:H8     | 1.70                     | 0.56              |
| 7:G:31:MET:HG2   | 7:G:32:ARG:N     | 2.20                     | 0.56              |
| 1:A:1101:A:H8    | 2:B:172:ILE:HD13 | 1.71                     | 0.56              |
| 5:E:60:TYR:CE1   | 5:E:64:ARG:NH2   | 2.73                     | 0.56              |
| 11:K:57:THR:HG23 | 11:K:58:PRO:HD2  | 1.87                     | 0.56              |
| 16:P:10:GLY:HA3  | 16:P:14:ASN:O    | 2.05                     | 0.56              |
| 19:S:47:HIS:O    | 19:S:62:ILE:HG22 | 2.06                     | 0.56              |
| 1:A:1065:U:H5''  | 1:A:1190:G:H21   | 1.64                     | 0.56              |
| 1:A:1347:G:H2'   | 1:A:1373:G:H1    | 1.70                     | 0.56              |
| 4:D:62:GLN:HE22  | 4:D:65:ARG:NH1   | 2.03                     | 0.56              |
| 17:Q:4:LYS:HD2   | 17:Q:6:LEU:HD21  | 1.87                     | 0.56              |
| 1:A:1161:C:H2'   | 1:A:1162:C:C5    | 2.40                     | 0.56              |
| 1:A:409:G:H1     | 1:A:433:C:H42    | 1.54                     | 0.56              |
| 13:M:65:LYS:O    | 13:M:66:LEU:HD23 | 2.05                     | 0.56              |
| 20:T:50:GLU:HG3  | 20:T:100:ILE:HB  | 1.87                     | 0.56              |
| 1:A:1496:C:H2'   | 1:A:1497:G:C8    | 2.41                     | 0.56              |
| 2:B:130:ARG:CB   | 2:B:131:PRO:HD2  | 2.36                     | 0.56              |
| 2:B:207:ALA:O    | 2:B:211:ILE:HG13 | 2.05                     | 0.56              |
| 3:C:11:ARG:O     | 3:C:14:ILE:O     | 2.23                     | 0.56              |
| 3:C:131:ARG:O    | 3:C:135:LYS:HB2  | 2.06                     | 0.56              |
| 13:M:90:LEU:O    | 13:M:94:ARG:HD2  | 2.05                     | 0.56              |
| 17:Q:67:LYS:HA   | 17:Q:70:ARG:NH1  | 2.15                     | 0.56              |
| 19:S:13:ASP:HA   | 19:S:16:LEU:CB   | 2.32                     | 0.56              |
| 20:T:74:LYS:HB3  | 20:T:74:LYS:NZ   | 2.20                     | 0.56              |
| 1:A:1118:C:C2    | 1:A:1179:A:N1    | 2.74                     | 0.56              |
| 1:A:1427:U:H2'   | 1:A:1428:A:C8    | 2.41                     | 0.56              |
| 1:A:17:U:H2'     | 1:A:18:C:C6      | 2.40                     | 0.56              |
| 1:A:895:G:H2'    | 1:A:896:C:C6     | 2.40                     | 0.56              |
| 18:R:17:SER:HB3  | 18:R:54:ARG:NH1  | 2.16                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:915:A:H2'    | 1:A:916:G:H5'    | 1.88                     | 0.56              |
| 2:B:204:ASN:HD21 | 2:B:206:ASP:HB3  | 1.68                     | 0.56              |
| 3:C:73:PRO:O     | 3:C:76:VAL:HG22  | 2.06                     | 0.56              |
| 6:F:25:ILE:HD12  | 6:F:82:ARG:HD2   | 1.88                     | 0.56              |
| 11:K:33:THR:HG22 | 11:K:39:PRO:CA   | 2.36                     | 0.56              |
| 13:M:66:LEU:O    | 13:M:69:GLU:HB2  | 2.05                     | 0.56              |
| 20:T:67:ALA:HA   | 20:T:73:HIS:H    | 1.71                     | 0.56              |
| 1:A:1015:A:H2'   | 1:A:1016:A:C8    | 2.41                     | 0.55              |
| 1:A:1041:A:H2'   | 1:A:1042:G:C8    | 2.41                     | 0.55              |
| 1:A:1126:U:H2'   | 1:A:1127:G:H8    | 1.67                     | 0.55              |
| 5:E:33:VAL:HG11  | 5:E:109:ILE:HA   | 1.88                     | 0.55              |
| 5:E:75:THR:HG23  | 5:E:76:ILE:N     | 2.21                     | 0.55              |
| 7:G:135:VAL:O    | 7:G:139:GLU:HG3  | 2.06                     | 0.55              |
| 10:J:4:ILE:HG12  | 10:J:74:ILE:HB   | 1.87                     | 0.55              |
| 1:A:1159:U:C4    | 1:A:1182:G:C6    | 2.94                     | 0.55              |
| 1:A:807:A:H2'    | 1:A:808:C:C6     | 2.41                     | 0.55              |
| 14:N:24:CYS:SG   | 14:N:40:CYS:N    | 2.79                     | 0.55              |
| 14:N:6:LEU:C     | 14:N:8:GLU:H     | 2.07                     | 0.55              |
| 18:R:47:THR:HG22 | 18:R:48:GLY:H    | 1.70                     | 0.55              |
| 1:A:1072:G:H2'   | 1:A:1073:U:C6    | 2.42                     | 0.55              |
| 1:A:1370:G:O2'   | 1:A:1371:G:H5'   | 2.07                     | 0.55              |
| 13:M:59:TYR:O    | 13:M:63:THR:HG22 | 2.06                     | 0.55              |
| 15:O:87:ILE:CG2  | 15:O:88:ARG:N    | 2.69                     | 0.55              |
| 18:R:47:THR:HG22 | 18:R:48:GLY:N    | 2.20                     | 0.55              |
| 1:A:1038:C:H2'   | 1:A:1039:C:H6    | 1.70                     | 0.55              |
| 2:B:70:PHE:HB3   | 2:B:81:VAL:HG13  | 1.87                     | 0.55              |
| 9:I:126:SER:HB2  | 9:I:128:ARG:O    | 2.07                     | 0.55              |
| 1:A:269:C:H2'    | 1:A:270:A:H8     | 1.72                     | 0.55              |
| 1:A:357:G:O2'    | 1:A:358:U:H5'    | 2.06                     | 0.55              |
| 1:A:478:A:O2'    | 1:A:479:C:H5'    | 2.07                     | 0.55              |
| 1:A:834:C:H2'    | 1:A:835:U:C6     | 2.41                     | 0.55              |
| 1:A:1206:G:H1'   | 3:C:193:TYR:O    | 2.06                     | 0.55              |
| 3:C:56:ASP:O     | 3:C:57:ILE:HG13  | 2.06                     | 0.55              |
| 7:G:120:ILE:H    | 7:G:120:ILE:HD12 | 1.71                     | 0.55              |
| 1:A:953:G:H1'    | 13:M:125:ARG:CB  | 2.36                     | 0.55              |
| 13:M:40:ASN:HD22 | 13:M:41:PRO:N    | 2.05                     | 0.55              |
| 19:S:19:VAL:HG13 | 19:S:20:LEU:N    | 2.21                     | 0.55              |
| 1:A:1160:G:N2    | 1:A:1161:C:C1'   | 2.66                     | 0.55              |
| 1:A:1216:G:H5''  | 14:N:5:ALA:CB    | 2.37                     | 0.55              |
| 1:A:1258:G:O2'   | 1:A:1259:C:H5'   | 2.07                     | 0.55              |
| 1:A:1438:G:H2'   | 1:A:1439:C:C6    | 2.42                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:21:G:H2'     | 1:A:22:G:C8       | 2.42                     | 0.55              |
| 1:A:268:C:H2'    | 1:A:269:C:H6      | 1.72                     | 0.55              |
| 1:A:337:C:H2'    | 1:A:338:A:C8      | 2.42                     | 0.55              |
| 1:A:862:C:O2'    | 1:A:863:U:H5'     | 2.06                     | 0.55              |
| 1:A:1103:C:OP1   | 2:B:96:ARG:NH1    | 2.40                     | 0.55              |
| 3:C:60:ALA:O     | 3:C:61:ALA:HB2    | 2.06                     | 0.55              |
| 9:I:128:ARG:HA   | 13:M:126:LYS:HZ3  | 1.71                     | 0.55              |
| 12:L:126:LYS:C   | 12:L:127:GLU:HG3  | 2.27                     | 0.55              |
| 13:M:25:ILE:HD11 | 13:M:60:VAL:CG1   | 2.37                     | 0.55              |
| 15:O:4:THR:OG1   | 15:O:7:GLU:HG3    | 2.06                     | 0.55              |
| 1:A:1175:G:H2'   | 1:A:1176:A:C8     | 2.36                     | 0.55              |
| 1:A:328:C:O2     | 1:A:328:C:C2'     | 2.47                     | 0.55              |
| 3:C:79:ARG:HG3   | 3:C:79:ARG:O      | 2.07                     | 0.55              |
| 18:R:19:LYS:O    | 18:R:20:ALA:HB2   | 2.07                     | 0.55              |
| 3:C:107:GLN:H    | 3:C:107:GLN:CD    | 2.10                     | 0.55              |
| 13:M:34:LEU:CD1  | 13:M:41:PRO:HA    | 2.37                     | 0.55              |
| 1:A:411:A:O2'    | 1:A:412:A:H5'     | 2.06                     | 0.55              |
| 20:T:57:ARG:HE   | 20:T:102:GLY:HA3  | 1.71                     | 0.55              |
| 1:A:1091:U:O2    | 1:A:1093:A:C8     | 2.60                     | 0.55              |
| 1:A:268:C:O2'    | 1:A:269:C:H5'     | 2.07                     | 0.55              |
| 1:A:991:U:C4     | 1:A:1212:U:H1'    | 2.42                     | 0.55              |
| 3:C:110:ASN:HD21 | 3:C:140:ARG:HB3   | 1.71                     | 0.55              |
| 18:R:87:ARG:O    | 18:R:88:LYS:HB3   | 2.06                     | 0.55              |
| 2:B:97:TRP:CZ2   | 2:B:101:MET:HB2   | 2.42                     | 0.54              |
| 12:L:68:ALA:HB3  | 12:L:100:ILE:HD11 | 1.89                     | 0.54              |
| 20:T:100:ILE:O   | 20:T:101:GLY:C    | 2.45                     | 0.54              |
| 1:A:1123:A:H2    | 10:J:39:PRO:HG2   | 1.71                     | 0.54              |
| 1:A:1152:A:H5'   | 10:J:70:ARG:NH2   | 2.23                     | 0.54              |
| 2:B:113:HIS:O    | 2:B:117:GLU:HB2   | 2.07                     | 0.54              |
| 1:A:921:U:O2     | 5:E:19:MET:HB2    | 2.07                     | 0.54              |
| 20:T:76:ALA:O    | 20:T:80:ARG:HG3   | 2.07                     | 0.54              |
| 22:X:3:A:N1      | 23:Y:34:TM2:O4    | 2.39                     | 0.54              |
| 1:A:1024:G:H3'   | 1:A:1025:U:H5''   | 1.90                     | 0.54              |
| 1:A:1159:U:C5    | 1:A:1182:G:C5     | 2.96                     | 0.54              |
| 1:A:1218:C:H2'   | 1:A:1219:U:C6     | 2.42                     | 0.54              |
| 1:A:431:A:O2'    | 1:A:432:A:H5'     | 2.07                     | 0.54              |
| 1:A:594:G:C2'    | 1:A:595:G:H5'     | 2.37                     | 0.54              |
| 1:A:755:G:OP2    | 15:O:65:ARG:HD2   | 2.08                     | 0.54              |
| 1:A:818:G:H3'    | 1:A:819:A:C5'     | 2.37                     | 0.54              |
| 3:C:134:ILE:HG22 | 3:C:168:ALA:HB3   | 1.88                     | 0.54              |
| 4:D:64:LEU:HD12  | 4:D:75:PHE:CZ     | 2.41                     | 0.54              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 7:G:18:TYR:CD2    | 7:G:59:LEU:HB2   | 2.42                     | 0.54              |
| 9:I:26:VAL:HG13   | 9:I:61:ALA:HB3   | 1.89                     | 0.54              |
| 11:K:21:ILE:HD12  | 11:K:95:ILE:HD13 | 1.90                     | 0.54              |
| 1:A:1030(C):G:H2' | 1:A:1030(D):A:C8 | 2.42                     | 0.54              |
| 1:A:1106:G:H5''   | 3:C:172:ARG:HG2  | 1.88                     | 0.54              |
| 1:A:1192:C:C2'    | 1:A:1193:G:P     | 2.89                     | 0.54              |
| 1:A:1228:C:H4'    | 13:M:116:THR:HA  | 1.90                     | 0.54              |
| 1:A:1283:G:O2'    | 1:A:1284:C:H5'   | 2.07                     | 0.54              |
| 1:A:1498:U:H4'    | 1:A:1519:A:C2    | 2.42                     | 0.54              |
| 2:B:83:MET:SD     | 2:B:235:SER:HB3  | 2.47                     | 0.54              |
| 9:I:17:VAL:CG2    | 9:I:80:GLY:HA3   | 2.37                     | 0.54              |
| 10:J:38:ILE:HB    | 10:J:71:LEU:HB2  | 1.90                     | 0.54              |
| 14:N:37:PHE:CE2   | 14:N:53:LEU:HD13 | 2.42                     | 0.54              |
| 1:A:1060:C:H2'    | 1:A:1061:G:C8    | 2.40                     | 0.54              |
| 1:A:1054:C:H5     | 1:A:1196:U:C5    | 2.26                     | 0.54              |
| 1:A:1479:C:H2'    | 1:A:1480:G:C8    | 2.41                     | 0.54              |
| 1:A:954:G:H2'     | 1:A:955:U:C6     | 2.42                     | 0.54              |
| 3:C:147:LYS:HE2   | 3:C:205:GLY:CA   | 2.37                     | 0.54              |
| 10:J:4:ILE:CG1    | 10:J:74:ILE:HB   | 2.37                     | 0.54              |
| 10:J:63:PHE:HE1   | 14:N:45:ARG:HG3  | 1.71                     | 0.54              |
| 1:A:1118:C:C2     | 1:A:1179:A:C2    | 2.96                     | 0.54              |
| 1:A:1201:A:H4'    | 1:A:1202:G:O5'   | 2.07                     | 0.54              |
| 1:A:424:G:O2'     | 1:A:425:G:H5'    | 2.06                     | 0.54              |
| 1:A:838:G:H2'     | 1:A:839:U:H5''   | 1.89                     | 0.54              |
| 1:A:912:C:O2'     | 1:A:913:A:H5'    | 2.07                     | 0.54              |
| 2:B:224:GLN:O     | 2:B:224:GLN:HG2  | 2.08                     | 0.54              |
| 4:D:201:GLN:HA    | 4:D:201:GLN:HE21 | 1.73                     | 0.54              |
| 1:A:1059:C:O2'    | 1:A:1060:C:H5'   | 2.07                     | 0.54              |
| 1:A:1253:G:H2'    | 1:A:1254:C:C6    | 2.42                     | 0.54              |
| 1:A:1392:G:N2     | 1:A:1502:A:C8    | 2.75                     | 0.54              |
| 2:B:187:LEU:HD21  | 2:B:203:GLY:HA3  | 1.90                     | 0.54              |
| 2:B:22:LYS:C      | 2:B:24:TRP:H     | 2.09                     | 0.54              |
| 3:C:91:LEU:HD11   | 3:C:99:VAL:HG23  | 1.88                     | 0.54              |
| 4:D:127:THR:CG2   | 4:D:147:ALA:HB3  | 2.38                     | 0.54              |
| 1:A:430:A:OP1     | 4:D:9:CYS:HB2    | 2.08                     | 0.54              |
| 6:F:22:GLU:HA     | 6:F:22:GLU:OE2   | 2.08                     | 0.54              |
| 6:F:67:MET:HB2    | 6:F:68:PRO:HD2   | 1.87                     | 0.54              |
| 1:A:106:C:O2      | 1:A:379:C:H4'    | 2.08                     | 0.54              |
| 1:A:1147:C:H4'    | 9:I:5:TYR:CE2    | 2.42                     | 0.54              |
| 1:A:1154:G:H2'    | 1:A:1155:G:H8    | 1.73                     | 0.54              |
| 1:A:547:A:H4'     | 1:A:548:G:O5'    | 2.07                     | 0.54              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:167:TRP:O    | 3:C:168:ALA:HB3   | 2.07                     | 0.54              |
| 10:J:18:ALA:C    | 10:J:20:ALA:H     | 2.11                     | 0.54              |
| 16:P:74:LEU:HB3  | 16:P:79:VAL:HG21  | 1.89                     | 0.54              |
| 1:A:45:U:H2'     | 1:A:46:G:C8       | 2.43                     | 0.54              |
| 1:A:740:U:O2'    | 1:A:741:G:H5'     | 2.08                     | 0.54              |
| 2:B:88:ALA:C     | 2:B:90:MET:N      | 2.60                     | 0.54              |
| 5:E:116:THR:HG22 | 5:E:117:ASP:OD2   | 2.08                     | 0.54              |
| 9:I:107:ARG:HH11 | 9:I:107:ARG:CB    | 2.21                     | 0.54              |
| 13:M:108:ARG:NE  | 13:M:108:ARG:HA   | 2.16                     | 0.54              |
| 14:N:18:VAL:HG23 | 14:N:19:ARG:H     | 1.73                     | 0.54              |
| 5:E:137:GLU:O    | 5:E:141:GLN:HG3   | 2.07                     | 0.54              |
| 12:L:83:VAL:HG11 | 12:L:100:ILE:HG13 | 1.88                     | 0.54              |
| 17:Q:67:LYS:CA   | 17:Q:70:ARG:NH1   | 2.71                     | 0.54              |
| 1:A:1306:A:N6    | 1:A:1331:G:H1'    | 2.24                     | 0.53              |
| 1:A:1425:U:H2'   | 1:A:1426:C:C6     | 2.44                     | 0.53              |
| 1:A:167:G:O2'    | 1:A:168:G:H5'     | 2.08                     | 0.53              |
| 1:A:77:G:O2'     | 1:A:78:G:H5'      | 2.08                     | 0.53              |
| 1:A:791:G:C6     | 1:A:792:A:N7      | 2.76                     | 0.53              |
| 3:C:95:THR:C     | 3:C:97:LYS:H      | 2.11                     | 0.53              |
| 4:D:70:ILE:HD11  | 4:D:100:ARG:NE    | 2.23                     | 0.53              |
| 12:L:75:HIS:HD2  | 12:L:77:LEU:H     | 1.55                     | 0.53              |
| 14:N:12:ARG:N    | 14:N:12:ARG:CD    | 2.71                     | 0.53              |
| 17:Q:81:ARG:O    | 17:Q:81:ARG:HG3   | 2.07                     | 0.53              |
| 1:A:1053:G:H3'   | 1:A:1054:C:H5'    | 1.90                     | 0.53              |
| 1:A:1167:A:H2'   | 1:A:1168:A:C8     | 2.44                     | 0.53              |
| 1:A:1230:C:H1'   | 13:M:126:LYS:HA   | 1.90                     | 0.53              |
| 1:A:1347:G:C2'   | 1:A:1348:U:OP2    | 2.55                     | 0.53              |
| 1:A:1419:G:O2'   | 1:A:1420:C:H5'    | 2.08                     | 0.53              |
| 1:A:975:A:H4'    | 1:A:976:G:C5'     | 2.33                     | 0.53              |
| 2:B:162:ILE:HD11 | 2:B:184:VAL:HG22  | 1.91                     | 0.53              |
| 3:C:142:MET:HG3  | 3:C:170:GLN:HB2   | 1.90                     | 0.53              |
| 1:A:542:G:OP1    | 4:D:10:ARG:NH2    | 2.41                     | 0.53              |
| 5:E:76:ILE:CG2   | 5:E:78:HIS:O      | 2.57                     | 0.53              |
| 1:A:1054:C:C3'   | 1:A:1054:C:O2     | 2.57                     | 0.53              |
| 5:E:36:ASP:OD1   | 5:E:38:GLN:N      | 2.36                     | 0.53              |
| 8:H:54:ASP:CG    | 8:H:55:GLY:N      | 2.62                     | 0.53              |
| 6:F:100:ASN:HD22 | 18:R:23:LYS:HG2   | 1.72                     | 0.53              |
| 2:B:230:VAL:HG12 | 2:B:231:GLU:N     | 2.23                     | 0.53              |
| 4:D:4:TYR:O      | 4:D:5:ILE:HB      | 2.07                     | 0.53              |
| 6:F:19:LEU:HD23  | 6:F:19:LEU:C      | 2.29                     | 0.53              |
| 8:H:10:LEU:HD22  | 8:H:83:ILE:HD11   | 1.89                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:I:36:TYR:HD2   | 9:I:37:PHE:CE2   | 2.27                     | 0.53              |
| 9:I:99:LEU:HB3   | 9:I:101:PHE:CD1  | 2.44                     | 0.53              |
| 18:R:43:PHE:HD2  | 18:R:56:THR:HG22 | 1.74                     | 0.53              |
| 1:A:1532:U:O2'   | 1:A:1533:C:H6    | 1.91                     | 0.53              |
| 2:B:27:LYS:HD3   | 2:B:195:ASP:OD2  | 2.08                     | 0.53              |
| 3:C:77:ILE:C     | 3:C:83:ARG:HB3   | 2.29                     | 0.53              |
| 7:G:15:ASP:O     | 7:G:19:GLY:HA2   | 2.08                     | 0.53              |
| 9:I:48:GLU:HG2   | 9:I:51:ARG:HH21  | 1.71                     | 0.53              |
| 12:L:47:LYS:CB   | 12:L:48:PRO:HD3  | 2.28                     | 0.53              |
| 9:I:128:ARG:CG   | 13:M:126:LYS:HZ3 | 2.21                     | 0.53              |
| 1:A:1004:A:N7    | 1:A:1037:C:N3    | 2.56                     | 0.53              |
| 13:M:49:THR:HG22 | 13:M:51:ALA:N    | 2.10                     | 0.53              |
| 14:N:46:GLU:O    | 14:N:49:HIS:HB2  | 2.08                     | 0.53              |
| 20:T:72:LEU:O    | 20:T:73:HIS:O    | 2.26                     | 0.53              |
| 1:A:1101:A:H4'   | 1:A:1102:A:O5'   | 2.09                     | 0.53              |
| 1:A:831:U:OP1    | 2:B:22:LYS:HE3   | 2.08                     | 0.53              |
| 3:C:134:ILE:HG21 | 3:C:167:TRP:O    | 2.09                     | 0.53              |
| 3:C:54:ARG:CG    | 3:C:55:VAL:H     | 2.22                     | 0.53              |
| 5:E:82:VAL:HG21  | 5:E:138:ALA:CA   | 2.39                     | 0.53              |
| 15:O:45:VAL:HG12 | 15:O:46:HIS:N    | 2.24                     | 0.53              |
| 17:Q:68:ARG:HH11 | 17:Q:68:ARG:HG2  | 1.73                     | 0.53              |
| 1:A:32:A:H2'     | 1:A:33:A:C8      | 2.44                     | 0.53              |
| 3:C:52:LEU:H     | 3:C:52:LEU:HD23  | 1.73                     | 0.53              |
| 7:G:5:ARG:HG3    | 7:G:7:ALA:H      | 1.74                     | 0.53              |
| 1:A:1326:C:C5    | 21:U:6:ARG:NH2   | 2.77                     | 0.53              |
| 1:A:1260:C:O5'   | 1:A:1284:C:H4'   | 2.08                     | 0.53              |
| 1:A:1238:A:OP1   | 1:A:1336:C:H5    | 1.92                     | 0.53              |
| 2:B:132:LYS:HG3  | 2:B:136:VAL:HG23 | 1.89                     | 0.53              |
| 7:G:16:LEU:N     | 7:G:16:LEU:HD22  | 2.24                     | 0.53              |
| 19:S:17:GLU:CA   | 19:S:20:LEU:HG   | 2.37                     | 0.53              |
| 1:A:1181:G:O2'   | 1:A:1184:G:H5'   | 2.09                     | 0.53              |
| 1:A:1525:G:OP1   | 11:K:120:ARG:NH2 | 2.41                     | 0.53              |
| 1:A:501:C:H2'    | 1:A:502:G:C8     | 2.44                     | 0.53              |
| 1:A:570:G:H2'    | 1:A:571:U:C6     | 2.44                     | 0.53              |
| 1:A:625:G:H2'    | 1:A:626:U:C6     | 2.44                     | 0.53              |
| 1:A:833:U:H2'    | 1:A:834:C:C6     | 2.44                     | 0.53              |
| 3:C:126:ARG:C    | 3:C:127:ARG:HD2  | 2.28                     | 0.53              |
| 7:G:44:TYR:HE1   | 9:I:41:VAL:HG11  | 1.73                     | 0.53              |
| 1:A:1249:C:O2'   | 9:I:73:GLN:NE2   | 2.42                     | 0.53              |
| 12:L:54:LYS:CD   | 12:L:54:LYS:N    | 2.72                     | 0.53              |
| 19:S:22:LEU:CD1  | 19:S:31:ILE:HD11 | 2.38                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:28:G:O2'     | 1:A:296:U:OP1    | 2.25                     | 0.52              |
| 1:A:961:U:H2'    | 1:A:962:C:H5'    | 1.91                     | 0.52              |
| 3:C:207:VAL:HG12 | 3:C:207:VAL:O    | 2.08                     | 0.52              |
| 12:L:42:THR:HG21 | 12:L:52:LEU:HB3  | 1.90                     | 0.52              |
| 1:A:1486:G:H2'   | 1:A:1487:G:O4'   | 2.09                     | 0.52              |
| 2:B:115:LEU:HG   | 2:B:153:ARG:NH2  | 2.22                     | 0.52              |
| 4:D:28:SER:C     | 4:D:30:LYS:H     | 2.12                     | 0.52              |
| 4:D:36:ARG:HG3   | 4:D:38:TYR:CZ    | 2.44                     | 0.52              |
| 8:H:111:ILE:O    | 8:H:134:ILE:HB   | 2.08                     | 0.52              |
| 20:T:39:LYS:HD3  | 20:T:55:ILE:HD13 | 1.92                     | 0.52              |
| 1:A:1342:C:O2'   | 1:A:1343:G:H5'   | 2.09                     | 0.52              |
| 1:A:1372:U:H2'   | 1:A:1373:G:O4'   | 2.10                     | 0.52              |
| 2:B:44:LEU:HD12  | 2:B:44:LEU:N     | 2.18                     | 0.52              |
| 7:G:18:TYR:HD2   | 7:G:59:LEU:HD22  | 1.74                     | 0.52              |
| 10:J:6:ILE:HB    | 10:J:72:VAL:HB   | 1.90                     | 0.52              |
| 1:A:1116:C:H2'   | 1:A:1117:G:C5'   | 2.36                     | 0.52              |
| 2:B:185:ILE:HD12 | 2:B:185:ILE:N    | 2.24                     | 0.52              |
| 3:C:44:GLU:HG2   | 3:C:52:LEU:HD11  | 1.91                     | 0.52              |
| 3:C:54:ARG:CG    | 3:C:55:VAL:N     | 2.72                     | 0.52              |
| 11:K:78:GLN:O    | 11:K:103:LEU:HA  | 2.08                     | 0.52              |
| 12:L:56:ALA:HB2  | 12:L:70:ILE:HD11 | 1.90                     | 0.52              |
| 1:A:1005:A:H2'   | 1:A:1006:C:H5'   | 1.92                     | 0.52              |
| 1:A:1393:U:O4'   | 1:A:1502:A:H5'   | 2.08                     | 0.52              |
| 1:A:178:C:O2'    | 1:A:179:A:H5'    | 2.08                     | 0.52              |
| 2:B:64:ARG:NH1   | 2:B:64:ARG:HB3   | 2.23                     | 0.52              |
| 4:D:170:VAL:CG1  | 4:D:174:LEU:HB2  | 2.40                     | 0.52              |
| 8:H:36:LEU:CD1   | 8:H:59:LEU:HD13  | 2.40                     | 0.52              |
| 17:Q:63:ARG:O    | 17:Q:65:ILE:HD12 | 2.10                     | 0.52              |
| 18:R:54:ARG:HH21 | 18:R:54:ARG:HG2  | 1.75                     | 0.52              |
| 18:R:86:VAL:O    | 18:R:87:ARG:HB2  | 2.09                     | 0.52              |
| 1:A:1405:G:O2'   | 1:A:1406:U:H5'   | 2.09                     | 0.52              |
| 3:C:72:LYS:O     | 3:C:75:VAL:HG23  | 2.09                     | 0.52              |
| 2:B:181:PHE:CD2  | 8:H:70:GLN:HB3   | 2.44                     | 0.52              |
| 1:A:1123:A:C2    | 10:J:39:PRO:HG2  | 2.44                     | 0.52              |
| 15:O:79:ARG:O    | 15:O:79:ARG:HD2  | 2.10                     | 0.52              |
| 1:A:187:C:C2     | 20:T:105:SER:HB3 | 2.44                     | 0.52              |
| 1:A:1156:G:O3'   | 1:A:1157:A:O5'   | 2.06                     | 0.52              |
| 1:A:1329:A:O2'   | 1:A:1330:U:H5'   | 2.09                     | 0.52              |
| 14:N:14:PRO:O    | 14:N:15:LYS:CB   | 2.58                     | 0.52              |
| 14:N:47:LEU:HD23 | 14:N:50:LYS:HD3  | 1.91                     | 0.52              |
| 16:P:19:ILE:HG22 | 16:P:36:ILE:HG13 | 1.92                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 16:P:4:ILE:HG23  | 16:P:36:ILE:HD11  | 1.92                     | 0.52              |
| 20:T:67:ALA:O    | 20:T:73:HIS:ND1   | 2.43                     | 0.52              |
| 1:A:1161:C:N4    | 1:A:1182:G:H22    | 2.08                     | 0.52              |
| 1:A:824:C:H2'    | 1:A:825:G:H8      | 1.75                     | 0.52              |
| 8:H:101:PRO:HA   | 8:H:102:ARG:HE    | 1.74                     | 0.52              |
| 13:M:98:VAL:O    | 13:M:98:VAL:HG12  | 2.09                     | 0.52              |
| 1:A:1190:G:C3'   | 3:C:3:ASN:HD21    | 2.22                     | 0.52              |
| 1:A:67:C:O2'     | 1:A:171:A:H1'     | 2.10                     | 0.52              |
| 1:A:640:A:O2'    | 1:A:641:U:H5'     | 2.09                     | 0.52              |
| 3:C:54:ARG:HG2   | 3:C:55:VAL:N      | 2.25                     | 0.52              |
| 7:G:136:LYS:HD3  | 7:G:140:ASP:OD1   | 2.09                     | 0.52              |
| 9:I:10:ARG:HD2   | 9:I:11:LYS:N      | 2.25                     | 0.52              |
| 10:J:49:VAL:HG21 | 14:N:41:ARG:O     | 2.10                     | 0.52              |
| 18:R:55:ARG:HB3  | 18:R:55:ARG:CZ    | 2.40                     | 0.52              |
| 18:R:87:ARG:O    | 18:R:88:LYS:CB    | 2.58                     | 0.52              |
| 1:A:1497:G:H2'   | 1:A:1498:U:H5'    | 1.92                     | 0.52              |
| 1:A:627:G:H2'    | 1:A:628:G:H8      | 1.74                     | 0.52              |
| 1:A:977:A:H2'    | 1:A:978:A:H5'     | 1.92                     | 0.52              |
| 2:B:122:PHE:HE2  | 2:B:139:LYS:HG2   | 1.75                     | 0.52              |
| 10:J:60:ARG:O    | 10:J:61:GLU:HB3   | 2.10                     | 0.52              |
| 1:A:761:G:O2'    | 17:Q:105:ALA:HB2  | 2.10                     | 0.52              |
| 17:Q:4:LYS:HD2   | 17:Q:6:LEU:CD2    | 2.40                     | 0.52              |
| 18:R:59:SER:H    | 18:R:62:GLU:HB2   | 1.75                     | 0.52              |
| 1:A:1003(A):G:N3 | 1:A:1004:A:H1'    | 2.25                     | 0.51              |
| 1:A:1305:G:H5''  | 21:U:4:GLY:C      | 2.30                     | 0.51              |
| 1:A:131:C:H2'    | 1:A:132:C:C6      | 2.44                     | 0.51              |
| 1:A:332:G:O2'    | 1:A:333:G:H5'     | 2.10                     | 0.51              |
| 2:B:91:PRO:HG2   | 2:B:155:LEU:HG    | 1.91                     | 0.51              |
| 11:K:107:SER:C   | 11:K:108:ILE:HD12 | 2.31                     | 0.51              |
| 12:L:125:PRO:O   | 12:L:126:LYS:O    | 2.27                     | 0.51              |
| 1:A:1292:U:P     | 7:G:41:ARG:NH2    | 2.80                     | 0.51              |
| 4:D:36:ARG:H     | 4:D:37:PRO:CD     | 2.23                     | 0.51              |
| 5:E:57:LYS:HG2   | 5:E:61:TYR:CE2    | 2.46                     | 0.51              |
| 7:G:45:ASP:O     | 7:G:48:LYS:HG2    | 2.10                     | 0.51              |
| 19:S:20:LEU:HA   | 19:S:23:ASN:HD22  | 1.75                     | 0.51              |
| 7:G:113:GLU:CG   | 7:G:119:ARG:HG3   | 2.39                     | 0.51              |
| 7:G:23:VAL:O     | 7:G:27:ILE:HG12   | 2.10                     | 0.51              |
| 8:H:7:ALA:HB2    | 8:H:85:ARG:HD2    | 1.92                     | 0.51              |
| 12:L:126:LYS:O   | 12:L:127:GLU:OE1  | 2.28                     | 0.51              |
| 17:Q:55:ASP:HB3  | 17:Q:76:LEU:CD1   | 2.40                     | 0.51              |
| 20:T:94:ALA:O    | 20:T:95:ALA:HB2   | 2.10                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1118:C:O2    | 1:A:1179:A:C2     | 2.63                     | 0.51              |
| 1:A:1510:U:H2'   | 1:A:1511:G:C8     | 2.46                     | 0.51              |
| 1:A:526:C:OP2    | 12:L:91:LYS:HE3   | 2.10                     | 0.51              |
| 1:A:814:A:H2'    | 1:A:816:A:H5''    | 1.92                     | 0.51              |
| 1:A:1101:A:C8    | 2:B:172:ILE:HD13  | 2.44                     | 0.51              |
| 2:B:78:GLN:O     | 2:B:94:ASN:OD1    | 2.28                     | 0.51              |
| 3:C:48:TYR:HE1   | 3:C:118:GLN:HE21  | 1.58                     | 0.51              |
| 14:N:29:ARG:NH1  | 14:N:29:ARG:HG2   | 2.24                     | 0.51              |
| 15:O:17:ARG:HG3  | 15:O:17:ARG:NH1   | 2.25                     | 0.51              |
| 16:P:20:VAL:CG1  | 16:P:32:TYR:HB2   | 2.41                     | 0.51              |
| 1:A:961:U:O2'    | 1:A:962:C:H5'     | 2.10                     | 0.51              |
| 1:A:992:U:H4'    | 1:A:993:G:O5'     | 2.10                     | 0.51              |
| 9:I:69:GLY:O     | 9:I:73:GLN:HG3    | 2.10                     | 0.51              |
| 11:K:99:GLN:CG   | 11:K:105:VAL:HG21 | 2.39                     | 0.51              |
| 11:K:34:ASP:OD2  | 11:K:38:ASN:HB2   | 2.10                     | 0.51              |
| 12:L:113:ARG:NH1 | 12:L:115:LYS:HB2  | 2.25                     | 0.51              |
| 13:M:4:ILE:O     | 13:M:5:ALA:C      | 2.48                     | 0.51              |
| 4:D:70:ILE:HD11  | 4:D:100:ARG:CZ    | 2.40                     | 0.51              |
| 9:I:6:GLY:HA3    | 9:I:83:ARG:HB2    | 1.93                     | 0.51              |
| 10:J:48:THR:OG1  | 10:J:62:HIS:CD2   | 2.64                     | 0.51              |
| 11:K:110:ASP:OD1 | 18:R:88:LYS:NZ    | 2.41                     | 0.51              |
| 10:J:64:GLU:CG   | 14:N:59:ALA:HB2   | 2.36                     | 0.51              |
| 20:T:70:SER:HA   | 20:T:73:HIS:CD2   | 2.46                     | 0.51              |
| 1:A:1179:A:O2'   | 1:A:1180:A:H5'    | 2.10                     | 0.51              |
| 1:A:908:A:H2'    | 1:A:909:A:H8      | 1.74                     | 0.51              |
| 2:B:213:LEU:C    | 2:B:213:LEU:HD23  | 2.30                     | 0.51              |
| 4:D:24:GLU:O     | 4:D:25:ARG:HB3    | 2.11                     | 0.51              |
| 5:E:12:LEU:HD13  | 5:E:31:LEU:HB2    | 1.92                     | 0.51              |
| 12:L:29:GLY:O    | 12:L:30:ALA:O     | 2.29                     | 0.51              |
| 10:J:61:GLU:OE1  | 14:N:45:ARG:HD2   | 2.10                     | 0.51              |
| 1:A:1208:C:H2'   | 1:A:1209:C:C6     | 2.46                     | 0.51              |
| 1:A:1208:C:H2'   | 1:A:1209:C:H6     | 1.76                     | 0.51              |
| 1:A:959:A:C2     | 1:A:1222:G:O4'    | 2.64                     | 0.51              |
| 1:A:1238:A:N7    | 1:A:1303:C:H1'    | 2.25                     | 0.51              |
| 1:A:976:G:C8     | 1:A:1358:U:O2     | 2.64                     | 0.51              |
| 1:A:532:A:O2'    | 1:A:533:A:P       | 2.69                     | 0.51              |
| 3:C:73:PRO:C     | 3:C:75:VAL:H      | 2.14                     | 0.51              |
| 5:E:51:VAL:HB    | 5:E:52:PRO:CD     | 2.38                     | 0.51              |
| 7:G:113:GLU:HG2  | 7:G:119:ARG:HG3   | 1.92                     | 0.51              |
| 1:A:1307:U:H5'   | 13:M:109:THR:HG21 | 1.93                     | 0.51              |
| 14:N:44:LEU:C    | 14:N:44:LEU:HD12  | 2.30                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:120:VAL:O    | 3:C:124:ILE:HG13 | 2.11                     | 0.51              |
| 4:D:191:ARG:O    | 4:D:191:ARG:HD2  | 2.11                     | 0.51              |
| 7:G:5:ARG:CZ     | 7:G:7:ALA:HA     | 2.40                     | 0.51              |
| 1:A:689:C:P      | 11:K:46:GLY:HA3  | 2.51                     | 0.51              |
| 12:L:92:ASP:O    | 12:L:94:PRO:HD3  | 2.11                     | 0.51              |
| 16:P:8:ARG:HH11  | 16:P:8:ARG:HG2   | 1.76                     | 0.51              |
| 2:B:48:MET:O     | 2:B:51:LEU:HB2   | 2.10                     | 0.50              |
| 7:G:6:ARG:O      | 7:G:6:ARG:HG2    | 2.10                     | 0.50              |
| 13:M:13:LYS:HA   | 13:M:44:ARG:NE   | 2.26                     | 0.50              |
| 20:T:74:LYS:HZ3  | 20:T:74:LYS:CA   | 2.18                     | 0.50              |
| 1:A:112:G:H5'    | 1:A:389:A:H4'    | 1.93                     | 0.50              |
| 1:A:255:G:O6     | 1:A:266:G:O6     | 2.30                     | 0.50              |
| 1:A:383:A:H2'    | 1:A:384:G:H5'    | 1.94                     | 0.50              |
| 2:B:114:ARG:C    | 2:B:117:GLU:HB3  | 2.32                     | 0.50              |
| 11:K:15:ALA:CA   | 11:K:77:MET:HA   | 2.41                     | 0.50              |
| 17:Q:104:LYS:HD3 | 17:Q:105:ALA:N   | 2.26                     | 0.50              |
| 1:A:1223:C:P     | 19:S:78:ARG:NH1  | 2.85                     | 0.50              |
| 3:C:154:SER:O    | 3:C:165:THR:HA   | 2.10                     | 0.50              |
| 4:D:70:ILE:HG22  | 4:D:75:PHE:HB2   | 1.93                     | 0.50              |
| 5:E:81:GLU:CG    | 5:E:88:LYS:HE2   | 2.42                     | 0.50              |
| 7:G:15:ASP:HB3   | 7:G:20:ASP:H     | 1.77                     | 0.50              |
| 10:J:42:THR:HG23 | 10:J:67:THR:O    | 2.10                     | 0.50              |
| 1:A:521:G:OP1    | 12:L:73:GLU:O    | 2.29                     | 0.50              |
| 18:R:59:SER:O    | 18:R:60:GLY:C    | 2.49                     | 0.50              |
| 1:A:1133:G:H2'   | 1:A:1134:G:C8    | 2.41                     | 0.50              |
| 1:A:1143:G:H2'   | 1:A:1144:G:C8    | 2.46                     | 0.50              |
| 1:A:1262:C:O2'   | 1:A:1263:C:H5'   | 2.11                     | 0.50              |
| 1:A:26:A:H61     | 1:A:558:G:H1'    | 1.76                     | 0.50              |
| 1:A:370:C:O2'    | 1:A:371:G:H5'    | 2.11                     | 0.50              |
| 1:A:501:C:H2'    | 1:A:502:G:H8     | 1.75                     | 0.50              |
| 1:A:538:G:H2'    | 1:A:539:A:C8     | 2.47                     | 0.50              |
| 1:A:594:G:H2'    | 1:A:595:G:H5'    | 1.92                     | 0.50              |
| 6:F:83:ASP:C     | 6:F:85:VAL:H     | 2.13                     | 0.50              |
| 7:G:143:ARG:O    | 7:G:147:ALA:HB2  | 2.12                     | 0.50              |
| 16:P:67:THR:CG2  | 16:P:68:ASP:N    | 2.74                     | 0.50              |
| 17:Q:68:ARG:N    | 17:Q:70:ARG:HH12 | 2.08                     | 0.50              |
| 1:A:1327:C:OP1   | 21:U:20:LYS:HB3  | 2.12                     | 0.50              |
| 1:A:1168:A:C6    | 1:A:1169:A:C6    | 3.00                     | 0.50              |
| 2:B:46:LYS:CA    | 2:B:46:LYS:HE3   | 2.37                     | 0.50              |
| 5:E:11:ILE:CG2   | 5:E:105:VAL:HG22 | 2.41                     | 0.50              |
| 6:F:33:TYR:HA    | 6:F:71:ARG:NH2   | 2.27                     | 0.50              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 7:G:15:ASP:OD2    | 7:G:44:TYR:OH    | 2.29                     | 0.50              |
| 17:Q:59:ILE:CG2   | 17:Q:71:PHE:HB3  | 2.42                     | 0.50              |
| 1:A:384:G:H2'     | 1:A:385:C:C6     | 2.47                     | 0.50              |
| 1:A:644:G:O2'     | 1:A:645:C:H5'    | 2.11                     | 0.50              |
| 1:A:1346:A:C4     | 7:G:10:ARG:NH2   | 2.79                     | 0.50              |
| 7:G:52:GLU:O      | 7:G:53:LYS:HG2   | 2.12                     | 0.50              |
| 8:H:36:LEU:HD12   | 8:H:59:LEU:HD13  | 1.92                     | 0.50              |
| 10:J:39:PRO:HA    | 10:J:70:ARG:HH11 | 1.77                     | 0.50              |
| 10:J:46:ARG:HH11  | 10:J:64:GLU:HB3  | 1.74                     | 0.50              |
| 10:J:71:LEU:O     | 10:J:72:VAL:CB   | 2.59                     | 0.50              |
| 19:S:55:LYS:HG2   | 19:S:56:GLN:HG3  | 1.92                     | 0.50              |
| 1:A:1149:C:H2'    | 1:A:1150:U:H6    | 1.75                     | 0.50              |
| 1:A:1288:A:H1'    | 1:A:1352:C:O2'   | 2.11                     | 0.50              |
| 1:A:1532:U:H2'    | 1:A:1533:C:H5''  | 1.87                     | 0.50              |
| 1:A:192:U:O4'     | 20:T:103:GLY:HA2 | 2.12                     | 0.50              |
| 4:D:8:VAL:HB      | 4:D:21:LEU:CD1   | 2.41                     | 0.50              |
| 4:D:78:LEU:HD22   | 4:D:96:LEU:HB3   | 1.93                     | 0.50              |
| 12:L:113:ARG:HH12 | 12:L:116:SER:H   | 1.58                     | 0.50              |
| 13:M:19:LEU:HD11  | 13:M:34:LEU:HD21 | 1.94                     | 0.50              |
| 13:M:73:GLU:O     | 13:M:76:ALA:HB3  | 2.12                     | 0.50              |
| 1:A:656:C:O2'     | 15:O:28:GLN:OE1  | 2.29                     | 0.50              |
| 16:P:42:ARG:O     | 16:P:43:LYS:C    | 2.50                     | 0.50              |
| 17:Q:17:LYS:HA    | 17:Q:46:ASP:O    | 2.12                     | 0.50              |
| 1:A:1182:G:O2'    | 1:A:1183:A:P     | 2.70                     | 0.50              |
| 1:A:397:A:N3      | 1:A:397:A:H3'    | 2.26                     | 0.50              |
| 1:A:818:G:C3'     | 1:A:819:A:C5'    | 2.90                     | 0.50              |
| 6:F:40:VAL:HG22   | 6:F:41:GLU:N     | 2.27                     | 0.50              |
| 8:H:60:ARG:HG3    | 8:H:60:ARG:HH11  | 1.77                     | 0.50              |
| 20:T:14:LYS:O     | 20:T:18:GLN:HG3  | 2.11                     | 0.50              |
| 5:E:76:ILE:HG13   | 5:E:142:LEU:HD11 | 1.92                     | 0.50              |
| 1:A:1060:C:H5''   | 10:J:51:ARG:HB3  | 1.94                     | 0.49              |
| 1:A:900:A:H2'     | 1:A:901:A:C8     | 2.47                     | 0.49              |
| 2:B:87:ARG:NH1    | 2:B:233:SER:HA   | 2.26                     | 0.49              |
| 6:F:15:ASP:OD1    | 6:F:17:SER:HB2   | 2.12                     | 0.49              |
| 1:A:939:G:H5''    | 7:G:102:ARG:NH2  | 2.26                     | 0.49              |
| 9:I:83:ARG:O      | 9:I:86:VAL:HB    | 2.11                     | 0.49              |
| 13:M:37:THR:CG2   | 13:M:55:ARG:HD2  | 2.38                     | 0.49              |
| 10:J:63:PHE:CE1   | 14:N:45:ARG:HG3  | 2.46                     | 0.49              |
| 17:Q:3:LYS:HD3    | 17:Q:61:GLU:O    | 2.12                     | 0.49              |
| 18:R:86:VAL:O     | 18:R:87:ARG:CB   | 2.60                     | 0.49              |
| 1:A:580:U:H2'     | 1:A:581:G:O4'    | 2.12                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:659:U:O2'    | 1:A:660:G:H5'     | 2.12                     | 0.49              |
| 1:A:911:U:H2'    | 1:A:912:C:C6      | 2.47                     | 0.49              |
| 2:B:83:MET:O     | 2:B:86:GLU:N      | 2.45                     | 0.49              |
| 3:C:63:ASN:HA    | 3:C:99:VAL:HG12   | 1.94                     | 0.49              |
| 19:S:40:ILE:HG21 | 19:S:62:ILE:HD11  | 1.94                     | 0.49              |
| 20:T:8:ARG:N     | 20:T:8:ARG:HD2    | 2.26                     | 0.49              |
| 1:A:1006:C:H2'   | 1:A:1007:C:C6     | 2.48                     | 0.49              |
| 1:A:1230:C:O2'   | 1:A:1231:G:H5'    | 2.13                     | 0.49              |
| 1:A:1509:C:H2'   | 1:A:1510:U:O4'    | 2.12                     | 0.49              |
| 1:A:1525:G:P     | 11:K:120:ARG:HH22 | 2.35                     | 0.49              |
| 1:A:945:G:C2     | 1:A:946:A:C8      | 3.00                     | 0.49              |
| 4:D:61:LYS:NZ    | 4:D:62:GLN:NE2    | 2.60                     | 0.49              |
| 6:F:19:LEU:O     | 6:F:23:LYS:HG3    | 2.11                     | 0.49              |
| 8:H:112:LEU:CD2  | 8:H:112:LEU:N     | 2.75                     | 0.49              |
| 10:J:6:ILE:HG23  | 10:J:98:ILE:CD1   | 2.42                     | 0.49              |
| 13:M:23:TYR:HB2  | 13:M:67:GLU:OE2   | 2.11                     | 0.49              |
| 1:A:1359:C:OP2   | 14:N:35:ARG:HD2   | 2.13                     | 0.49              |
| 14:N:53:LEU:HB3  | 14:N:56:VAL:HG21  | 1.93                     | 0.49              |
| 19:S:43:GLU:CD   | 19:S:43:GLU:H     | 2.15                     | 0.49              |
| 1:A:1004:A:P     | 1:A:1025:U:H3     | 2.35                     | 0.49              |
| 1:A:1179:A:C6    | 1:A:1180:A:C2     | 3.00                     | 0.49              |
| 1:A:1296:C:H4'   | 1:A:1302:U:C5     | 2.46                     | 0.49              |
| 1:A:390:C:O3'    | 16:P:28:ARG:NH2   | 2.45                     | 0.49              |
| 1:A:426:G:O2'    | 1:A:427:U:H5'     | 2.13                     | 0.49              |
| 2:B:162:ILE:HG13 | 2:B:162:ILE:O     | 2.12                     | 0.49              |
| 4:D:148:VAL:HG11 | 4:D:158:ILE:HD13  | 1.94                     | 0.49              |
| 4:D:189:PRO:HB2  | 4:D:194:LEU:CD2   | 2.43                     | 0.49              |
| 5:E:20:GLN:NE2   | 5:E:21:ALA:O      | 2.45                     | 0.49              |
| 7:G:12:LEU:H     | 7:G:12:LEU:HD12   | 1.78                     | 0.49              |
| 13:M:37:THR:O    | 13:M:39:ILE:HG13  | 2.12                     | 0.49              |
| 13:M:40:ASN:HD22 | 13:M:40:ASN:C     | 2.15                     | 0.49              |
| 15:O:87:ILE:O    | 15:O:88:ARG:HB2   | 2.12                     | 0.49              |
| 16:P:21:VAL:HG21 | 16:P:59:TRP:CD1   | 2.46                     | 0.49              |
| 1:A:1189:C:OP1   | 10:J:51:ARG:NH2   | 2.44                     | 0.49              |
| 1:A:528:C:H5'    | 1:A:535:A:C6      | 2.48                     | 0.49              |
| 1:A:882:C:O2'    | 1:A:883:C:H5'     | 2.11                     | 0.49              |
| 2:B:55:PHE:HD2   | 2:B:221:LEU:HG    | 1.77                     | 0.49              |
| 2:B:25:ASN:C     | 2:B:25:ASN:HD22   | 2.15                     | 0.49              |
| 3:C:206:GLU:O    | 3:C:208:ILE:N     | 2.44                     | 0.49              |
| 6:F:100:ASN:HD22 | 18:R:23:LYS:CG    | 2.24                     | 0.49              |
| 6:F:19:LEU:O     | 6:F:19:LEU:HD23   | 2.13                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 10:J:39:PRO:O    | 10:J:40:LEU:CB   | 2.60                     | 0.49              |
| 10:J:94:VAL:CG1  | 10:J:95:GLU:N    | 2.75                     | 0.49              |
| 12:L:40:VAL:O    | 12:L:40:VAL:HG12 | 2.12                     | 0.49              |
| 13:M:4:ILE:O     | 13:M:5:ALA:O     | 2.29                     | 0.49              |
| 20:T:99:LEU:C    | 20:T:101:GLY:H   | 2.16                     | 0.49              |
| 1:A:48:C:H5''    | 1:A:365:U:O4     | 2.13                     | 0.49              |
| 3:C:34:LEU:HD23  | 3:C:34:LEU:C     | 2.32                     | 0.49              |
| 7:G:120:ILE:N    | 7:G:120:ILE:HD12 | 2.28                     | 0.49              |
| 1:A:1006:C:H2'   | 1:A:1007:C:H6    | 1.77                     | 0.49              |
| 2:B:111:ARG:CB   | 2:B:149:LEU:HD11 | 2.38                     | 0.49              |
| 4:D:150:GLU:N    | 4:D:150:GLU:CD   | 2.61                     | 0.49              |
| 14:N:4:LYS:C     | 14:N:6:LEU:H     | 2.15                     | 0.49              |
| 16:P:20:VAL:CG1  | 16:P:32:TYR:CB   | 2.90                     | 0.49              |
| 1:A:1192:C:O3'   | 1:A:1193:G:OP2   | 0.71                     | 0.49              |
| 1:A:1499:A:H1'   | 1:A:1520:G:H5'   | 1.95                     | 0.49              |
| 3:C:11:ARG:NH1   | 3:C:177:THR:O    | 2.46                     | 0.49              |
| 4:D:19:LEU:HD22  | 4:D:67:ILE:CG1   | 2.43                     | 0.49              |
| 8:H:54:ASP:CG    | 8:H:55:GLY:H     | 2.16                     | 0.49              |
| 16:P:11:SER:OG   | 16:P:14:ASN:HB3  | 2.13                     | 0.49              |
| 1:A:1127:G:N2    | 1:A:1146:A:N6    | 2.51                     | 0.49              |
| 1:A:1314:C:OP2   | 19:S:6:LYS:HG3   | 2.12                     | 0.49              |
| 1:A:1443:G:H5''  | 1:A:1443:G:N3    | 2.28                     | 0.49              |
| 1:A:513:C:H2'    | 1:A:514:C:C6     | 2.48                     | 0.49              |
| 2:B:194:PRO:O    | 2:B:197:VAL:N    | 2.35                     | 0.49              |
| 2:B:96:ARG:O     | 2:B:98:LEU:HD23  | 2.13                     | 0.49              |
| 3:C:134:ILE:CG2  | 3:C:168:ALA:HB3  | 2.43                     | 0.49              |
| 5:E:75:THR:HG23  | 5:E:76:ILE:O     | 2.12                     | 0.49              |
| 8:H:104:ARG:O    | 8:H:105:ARG:C    | 2.52                     | 0.49              |
| 13:M:81:LEU:HD13 | 13:M:88:ARG:HD3  | 1.93                     | 0.49              |
| 15:O:39:LEU:O    | 15:O:39:LEU:HD23 | 2.13                     | 0.49              |
| 1:A:1052:U:H2'   | 1:A:1055:A:OP1   | 2.13                     | 0.49              |
| 1:A:1350:A:C6    | 1:A:1351:U:N3    | 2.81                     | 0.49              |
| 1:A:1474:G:O2'   | 1:A:1475:G:H5'   | 2.13                     | 0.49              |
| 5:E:144:THR:CG2  | 5:E:145:LYS:N    | 2.75                     | 0.49              |
| 7:G:16:LEU:H     | 7:G:16:LEU:HD22  | 1.78                     | 0.49              |
| 14:N:25:VAL:HG12 | 14:N:38:GLY:O    | 2.13                     | 0.49              |
| 17:Q:67:LYS:C    | 17:Q:70:ARG:NH1  | 2.66                     | 0.49              |
| 1:A:157:G:O2'    | 1:A:158:G:H5'    | 2.13                     | 0.48              |
| 1:A:432:A:H2'    | 1:A:433:C:O4'    | 2.13                     | 0.48              |
| 1:A:438:G:C4'    | 1:A:439:A:OP1    | 2.59                     | 0.48              |
| 1:A:706:A:C4'    | 11:K:29:ILE:HD11 | 2.43                     | 0.48              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:132:LYS:HD2   | 2:B:135:GLN:CB   | 2.32                     | 0.48              |
| 2:B:9:GLU:HA      | 2:B:48:MET:SD    | 2.52                     | 0.48              |
| 3:C:128:PHE:CD2   | 3:C:129:ALA:N    | 2.79                     | 0.48              |
| 3:C:155:GLY:O     | 3:C:196:LEU:HD13 | 2.13                     | 0.48              |
| 4:D:24:GLU:C      | 4:D:26:CYS:H     | 2.16                     | 0.48              |
| 4:D:65:ARG:HG3    | 4:D:75:PHE:CG    | 2.48                     | 0.48              |
| 8:H:56:LYS:N      | 8:H:56:LYS:HD2   | 2.28                     | 0.48              |
| 9:I:99:LEU:HB3    | 9:I:101:PHE:CE1  | 2.48                     | 0.48              |
| 11:K:117:ASN:HD22 | 11:K:117:ASN:N   | 2.11                     | 0.48              |
| 1:A:1347:G:O2'    | 1:A:1348:U:C6    | 2.66                     | 0.48              |
| 1:A:457:C:H2'     | 1:A:458:C:C6     | 2.47                     | 0.48              |
| 1:A:56:U:H2'      | 1:A:57:G:C8      | 2.48                     | 0.48              |
| 1:A:792:A:C4      | 1:A:794:A:C6     | 3.01                     | 0.48              |
| 3:C:14:ILE:O      | 3:C:15:THR:C     | 2.50                     | 0.48              |
| 4:D:145:GLU:OE2   | 4:D:182:LYS:HD2  | 2.13                     | 0.48              |
| 4:D:50:ARG:HD2    | 4:D:51:PRO:O     | 2.13                     | 0.48              |
| 8:H:103:VAL:HG21  | 8:H:109:ILE:C    | 2.33                     | 0.48              |
| 8:H:59:LEU:O      | 8:H:61:VAL:HG23  | 2.13                     | 0.48              |
| 10:J:30:SER:HB3   | 10:J:84:GLN:NE2  | 2.26                     | 0.48              |
| 20:T:99:LEU:O     | 20:T:101:GLY:N   | 2.47                     | 0.48              |
| 1:A:474:G:H5''    | 16:P:81:ARG:NH1  | 2.28                     | 0.48              |
| 3:C:155:GLY:CA    | 3:C:164:ARG:H    | 2.26                     | 0.48              |
| 4:D:28:SER:O      | 4:D:30:LYS:N     | 2.46                     | 0.48              |
| 6:F:23:LYS:O      | 6:F:27:GLN:HG2   | 2.12                     | 0.48              |
| 6:F:45:LEU:HA     | 6:F:59:TYR:HA    | 1.95                     | 0.48              |
| 7:G:112:PRO:O     | 7:G:113:GLU:C    | 2.50                     | 0.48              |
| 1:A:1343:G:H1'    | 9:I:121:ARG:NH1  | 2.25                     | 0.48              |
| 9:I:37:PHE:O      | 9:I:38:GLN:O     | 2.32                     | 0.48              |
| 1:A:706:A:O4'     | 11:K:29:ILE:HD11 | 2.13                     | 0.48              |
| 16:P:45:THR:HB    | 16:P:46:PRO:HD2  | 1.94                     | 0.48              |
| 18:R:25:THR:O     | 18:R:26:LEU:HB2  | 2.14                     | 0.48              |
| 1:A:1425:U:H3     | 1:A:1475:G:H1    | 1.60                     | 0.48              |
| 2:B:170:GLU:OE2   | 2:B:170:GLU:HA   | 2.13                     | 0.48              |
| 2:B:74:LYS:HD3    | 2:B:205:ASP:O    | 2.12                     | 0.48              |
| 3:C:3:ASN:O       | 3:C:4:LYS:CB     | 2.61                     | 0.48              |
| 4:D:57:ARG:NH2    | 5:E:107:ARG:HE   | 2.11                     | 0.48              |
| 6:F:27:GLN:C      | 6:F:29:ALA:H     | 2.16                     | 0.48              |
| 1:A:1249:C:H4'    | 9:I:36:TYR:OH    | 2.13                     | 0.48              |
| 11:K:124:LYS:HZ2  | 11:K:125:PHE:HZ  | 1.58                     | 0.48              |
| 19:S:15:LEU:HD12  | 19:S:16:LEU:N    | 2.28                     | 0.48              |
| 19:S:20:LEU:HD12  | 19:S:21:GLU:N    | 2.28                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 20:T:37:SER:O    | 20:T:41:VAL:HG23 | 2.13                     | 0.48              |
| 1:A:1125:U:H5'   | 1:A:1126:U:C5    | 2.47                     | 0.48              |
| 1:A:1284:C:H3'   | 1:A:1285:A:H8    | 1.77                     | 0.48              |
| 1:A:135:C:O2     | 16:P:1:MET:N     | 2.42                     | 0.48              |
| 1:A:814:A:H2'    | 1:A:816:A:C5'    | 2.43                     | 0.48              |
| 2:B:60:ASP:OD2   | 2:B:64:ARG:HD2   | 2.13                     | 0.48              |
| 3:C:11:ARG:O     | 3:C:14:ILE:N     | 2.47                     | 0.48              |
| 3:C:148:GLY:HA3  | 3:C:172:ARG:O    | 2.13                     | 0.48              |
| 7:G:141:VAL:O    | 7:G:144:MET:HB2  | 2.13                     | 0.48              |
| 9:I:114:TYR:C    | 9:I:116:LYS:H    | 2.17                     | 0.48              |
| 1:A:1232:U:OP1   | 9:I:124:GLN:NE2  | 2.46                     | 0.48              |
| 10:J:29:ARG:NH1  | 10:J:84:GLN:OE1  | 2.46                     | 0.48              |
| 12:L:111:LYS:HA  | 12:L:111:LYS:CE  | 2.37                     | 0.48              |
| 15:O:15:PHE:CE2  | 15:O:84:LYS:HD2  | 2.48                     | 0.48              |
| 17:Q:67:LYS:HG2  | 17:Q:68:ARG:N    | 2.28                     | 0.48              |
| 1:A:1124:G:H2'   | 1:A:1145:C:H5    | 1.79                     | 0.48              |
| 1:A:1194:U:O2'   | 1:A:1195:C:H5'   | 2.13                     | 0.48              |
| 1:A:1277:C:H2'   | 1:A:1278:U:H5'   | 1.94                     | 0.48              |
| 1:A:477:G:O2'    | 1:A:478:A:H5'    | 2.13                     | 0.48              |
| 2:B:122:PHE:O    | 2:B:123:ALA:HB2  | 2.13                     | 0.48              |
| 2:B:159:PRO:HB2  | 2:B:161:ALA:O    | 2.13                     | 0.48              |
| 1:A:1109:C:OP2   | 3:C:176:HIS:CD2  | 2.66                     | 0.48              |
| 3:C:47:LEU:N     | 3:C:47:LEU:HD12  | 2.29                     | 0.48              |
| 6:F:8:ILE:HG22   | 6:F:10:LEU:CD1   | 2.44                     | 0.48              |
| 10:J:16:LEU:HD21 | 10:J:94:VAL:HG13 | 1.96                     | 0.48              |
| 12:L:18:VAL:O    | 12:L:18:VAL:HG23 | 2.13                     | 0.48              |
| 13:M:94:ARG:HD2  | 13:M:94:ARG:N    | 2.29                     | 0.48              |
| 19:S:15:LEU:HD12 | 19:S:16:LEU:H    | 1.78                     | 0.48              |
| 1:A:1156:G:H21   | 1:A:1179:A:H61   | 1.61                     | 0.48              |
| 1:A:1347:G:N7    | 9:I:107:ARG:NH1  | 2.60                     | 0.48              |
| 2:B:33:TYR:HB2   | 2:B:43:ASP:HA    | 1.95                     | 0.48              |
| 2:B:84:GLU:HB3   | 2:B:219:VAL:HG21 | 1.95                     | 0.48              |
| 11:K:48:ILE:HG22 | 11:K:49:GLY:H    | 1.79                     | 0.48              |
| 1:A:1300:G:O2'   | 1:A:1301:U:P     | 2.71                     | 0.48              |
| 1:A:1505:G:H3'   | 1:A:1505:G:C8    | 2.49                     | 0.48              |
| 3:C:70:VAL:C     | 3:C:106:VAL:HG23 | 2.34                     | 0.48              |
| 5:E:144:THR:H    | 5:E:147:ASP:HB2  | 1.79                     | 0.48              |
| 9:I:55:ALA:O     | 9:I:56:LEU:CB    | 2.61                     | 0.48              |
| 12:L:27:LEU:C    | 12:L:29:GLY:N    | 2.66                     | 0.48              |
| 13:M:96:LEU:O    | 13:M:97:PRO:C    | 2.52                     | 0.48              |
| 18:R:42:ARG:HH11 | 18:R:42:ARG:HB3  | 1.78                     | 0.48              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 19:S:27:GLU:CD    | 19:S:27:GLU:N    | 2.67                     | 0.48              |
| 1:A:1278:U:H5''   | 1:A:1279:A:O4'   | 2.14                     | 0.48              |
| 1:A:627:G:H2'     | 1:A:628:G:C8     | 2.49                     | 0.48              |
| 1:A:838:G:N2      | 1:A:849:C:C2     | 2.81                     | 0.48              |
| 1:A:839:U:C2'     | 1:A:839:U:O2     | 2.62                     | 0.48              |
| 1:A:945:G:H2'     | 1:A:945:G:N3     | 2.29                     | 0.48              |
| 5:E:81:GLU:HG2    | 5:E:88:LYS:HE2   | 1.96                     | 0.48              |
| 7:G:136:LYS:HE2   | 7:G:136:LYS:CA   | 2.38                     | 0.48              |
| 10:J:3:LYS:O      | 10:J:101:VAL:N   | 2.47                     | 0.48              |
| 1:A:1241:G:H2'    | 1:A:1242:C:H6    | 1.77                     | 0.48              |
| 1:A:1370:G:C2     | 1:A:1371:G:C8    | 3.02                     | 0.48              |
| 1:A:1465:C:H2'    | 1:A:1466:C:O4'   | 2.14                     | 0.48              |
| 1:A:930:C:C2'     | 1:A:931:C:H5'    | 2.44                     | 0.48              |
| 11:K:101:SER:O    | 11:K:103:LEU:N   | 2.40                     | 0.48              |
| 11:K:14:VAL:O     | 11:K:15:ALA:HB3  | 2.14                     | 0.48              |
| 12:L:77:LEU:HD21  | 12:L:107:ALA:HB2 | 1.95                     | 0.48              |
| 13:M:102:ARG:NH1  | 13:M:102:ARG:HB2 | 2.29                     | 0.48              |
| 13:M:14:ARG:N     | 13:M:44:ARG:HD2  | 2.28                     | 0.48              |
| 1:A:1003(A):G:H2' | 1:A:1004:A:C4'   | 2.44                     | 0.47              |
| 1:A:1054:C:O2'    | 1:A:1055:A:H5''  | 2.13                     | 0.47              |
| 1:A:1178:G:N2     | 1:A:1180:A:H3'   | 2.29                     | 0.47              |
| 1:A:411:A:O2'     | 1:A:413:G:H5'    | 2.14                     | 0.47              |
| 4:D:92:VAL:O      | 4:D:96:LEU:HD13  | 2.14                     | 0.47              |
| 5:E:79:GLU:HG3    | 5:E:93:PRO:CD    | 2.37                     | 0.47              |
| 9:I:51:ARG:HG2    | 9:I:56:LEU:HD11  | 1.97                     | 0.47              |
| 14:N:4:LYS:C      | 14:N:6:LEU:N     | 2.67                     | 0.47              |
| 17:Q:9:VAL:HG21   | 17:Q:84:LEU:HD13 | 1.95                     | 0.47              |
| 1:A:1156:G:H3'    | 1:A:1157:A:OP2   | 2.12                     | 0.47              |
| 1:A:1191:A:HO3'   | 1:A:1192:C:C5'   | 2.15                     | 0.47              |
| 1:A:1402:C:H2'    | 1:A:1403:C:O4'   | 2.14                     | 0.47              |
| 1:A:404:U:H2'     | 1:A:405:U:C6     | 2.49                     | 0.47              |
| 1:A:457:C:O2'     | 1:A:458:C:H5'    | 2.14                     | 0.47              |
| 6:F:4:TYR:CZ      | 6:F:72:VAL:HG21  | 2.49                     | 0.47              |
| 7:G:18:TYR:OH     | 7:G:58:PRO:HG2   | 2.14                     | 0.47              |
| 14:N:8:GLU:O      | 14:N:9:LYS:C     | 2.52                     | 0.47              |
| 1:A:101:A:O2'     | 1:A:102:G:H5'    | 2.14                     | 0.47              |
| 1:A:200:G:H2'     | 1:A:201:C:O4'    | 2.15                     | 0.47              |
| 1:A:640:A:C2'     | 1:A:641:U:H5'    | 2.44                     | 0.47              |
| 1:A:861:G:O2'     | 1:A:862:C:H5'    | 2.14                     | 0.47              |
| 2:B:186:ALA:HB3   | 2:B:197:VAL:HG11 | 1.96                     | 0.47              |
| 6:F:10:LEU:HD12   | 6:F:10:LEU:N     | 2.29                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:67:MET:CE    | 6:F:75:LEU:HD12  | 2.43                     | 0.47              |
| 6:F:86:ARG:O     | 6:F:87:ARG:HG2   | 2.13                     | 0.47              |
| 1:A:1091:U:O2    | 1:A:1093:A:H8    | 1.98                     | 0.47              |
| 1:A:1128:C:H4'   | 9:I:16:ARG:NH1   | 2.29                     | 0.47              |
| 1:A:1161:C:H2'   | 1:A:1162:C:H6    | 1.79                     | 0.47              |
| 1:A:129(A):G:O2' | 1:A:130:A:OP2    | 2.33                     | 0.47              |
| 1:A:179:A:O2'    | 1:A:180:U:H5'    | 2.15                     | 0.47              |
| 2:B:118:LEU:HB2  | 2:B:142:LEU:CD2  | 2.37                     | 0.47              |
| 2:B:96:ARG:HG3   | 2:B:96:ARG:O     | 2.13                     | 0.47              |
| 3:C:25:GLY:O     | 3:C:27:LYS:N     | 2.47                     | 0.47              |
| 4:D:166:LYS:HG3  | 4:D:178:VAL:HG11 | 1.96                     | 0.47              |
| 5:E:90:VAL:O     | 5:E:120:THR:HA   | 2.13                     | 0.47              |
| 10:J:12:ASP:HB3  | 10:J:15:THR:HB   | 1.96                     | 0.47              |
| 11:K:27:ASN:OD1  | 11:K:28:THR:N    | 2.47                     | 0.47              |
| 1:A:1066:C:C2'   | 1:A:1067:A:H5'   | 2.45                     | 0.47              |
| 1:A:1128:C:H4'   | 9:I:16:ARG:HH12  | 1.78                     | 0.47              |
| 1:A:713:G:H2'    | 1:A:714:G:C8     | 2.50                     | 0.47              |
| 1:A:757:U:H2'    | 1:A:758:G:O4'    | 2.14                     | 0.47              |
| 2:B:73:THR:HG23  | 2:B:95:GLN:O     | 2.15                     | 0.47              |
| 3:C:155:GLY:O    | 3:C:156:ARG:CB   | 2.61                     | 0.47              |
| 1:A:1112:C:O2    | 3:C:179:ARG:HG2  | 2.14                     | 0.47              |
| 4:D:31:CYS:C     | 4:D:33:MET:H     | 2.18                     | 0.47              |
| 9:I:4:TYR:CZ     | 9:I:88:TYR:HD1   | 2.32                     | 0.47              |
| 11:K:110:ASP:HB2 | 18:R:88:LYS:CD   | 2.43                     | 0.47              |
| 1:A:953:G:H1'    | 13:M:125:ARG:HA  | 1.96                     | 0.47              |
| 15:O:5:LYS:HD2   | 15:O:5:LYS:H     | 1.80                     | 0.47              |
| 18:R:37:VAL:O    | 18:R:41:LYS:HB2  | 2.14                     | 0.47              |
| 1:A:1112:C:N3    | 3:C:178:LEU:HD23 | 2.29                     | 0.47              |
| 1:A:1339:A:H2'   | 1:A:1340:A:O4'   | 2.13                     | 0.47              |
| 1:A:175:C:H2'    | 1:A:176:C:H6     | 1.80                     | 0.47              |
| 1:A:487:A:H2'    | 1:A:488:C:O4'    | 2.14                     | 0.47              |
| 1:A:490:G:H2'    | 1:A:491:G:H8     | 1.80                     | 0.47              |
| 1:A:522:C:OP2    | 12:L:69:TYR:OH   | 2.24                     | 0.47              |
| 1:A:730:G:N2     | 1:A:765:G:H5''   | 2.29                     | 0.47              |
| 3:C:127:ARG:HG2  | 3:C:127:ARG:NH1  | 2.29                     | 0.47              |
| 4:D:19:LEU:HD22  | 4:D:67:ILE:HG12  | 1.96                     | 0.47              |
| 5:E:12:LEU:C     | 5:E:12:LEU:HD22  | 2.35                     | 0.47              |
| 6:F:2:ARG:CD     | 6:F:69:GLU:HG2   | 2.45                     | 0.47              |
| 7:G:51:GLN:O     | 7:G:52:GLU:C     | 2.53                     | 0.47              |
| 8:H:53:VAL:O     | 8:H:54:ASP:HB3   | 2.15                     | 0.47              |
| 12:L:57:LYS:HD3  | 12:L:67:THR:CG2  | 2.45                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 13:M:91:ARG:CB   | 13:M:98:VAL:HG22 | 2.44                     | 0.47              |
| 1:A:1470:G:O2'   | 1:A:1471:G:H5'   | 2.14                     | 0.47              |
| 1:A:1474:G:H2'   | 1:A:1475:G:H8    | 1.80                     | 0.47              |
| 1:A:459:G:C6     | 1:A:461:C:H5''   | 2.49                     | 0.47              |
| 3:C:27:LYS:H     | 3:C:27:LYS:HD3   | 1.80                     | 0.47              |
| 3:C:87:LEU:C     | 3:C:89:GLU:H     | 2.18                     | 0.47              |
| 7:G:75:VAL:HG11  | 7:G:144:MET:CE   | 2.44                     | 0.47              |
| 9:I:126:SER:O    | 9:I:127:LYS:CB   | 2.62                     | 0.47              |
| 10:J:6:ILE:HD12  | 10:J:72:VAL:CG1  | 2.44                     | 0.47              |
| 13:M:65:LYS:CG   | 13:M:69:GLU:HB3  | 2.45                     | 0.47              |
| 13:M:8:GLU:C     | 13:M:9:ILE:HD12  | 2.35                     | 0.47              |
| 14:N:24:CYS:HB2  | 14:N:40:CYS:HB3  | 1.95                     | 0.47              |
| 19:S:80:TYR:OH   | 19:S:81:ARG:HD3  | 2.14                     | 0.47              |
| 1:A:1201:A:O2'   | 1:A:1202:G:OP2   | 2.29                     | 0.47              |
| 1:A:1234:C:O2'   | 1:A:1235:U:H5'   | 2.15                     | 0.47              |
| 1:A:1305:G:H22   | 1:A:1331:G:H2'   | 1.77                     | 0.47              |
| 1:A:783:C:O2'    | 1:A:784:C:H5'    | 2.14                     | 0.47              |
| 1:A:989:C:O2'    | 1:A:990:C:H5'    | 2.14                     | 0.47              |
| 3:C:123:GLN:O    | 3:C:128:PHE:HB2  | 2.15                     | 0.47              |
| 3:C:23:TYR:CD1   | 10:J:10:GLY:HA2  | 2.49                     | 0.47              |
| 3:C:70:VAL:HG12  | 3:C:71:ALA:H     | 1.76                     | 0.47              |
| 4:D:153:ARG:HG2  | 4:D:181:MET:SD   | 2.55                     | 0.47              |
| 13:M:4:ILE:CG2   | 13:M:5:ALA:N     | 2.65                     | 0.47              |
| 17:Q:68:ARG:HH11 | 17:Q:68:ARG:CG   | 2.27                     | 0.47              |
| 1:A:325:A:OP2    | 20:T:70:SER:HB3  | 2.15                     | 0.47              |
| 1:A:1002:G:H2'   | 1:A:1003:G:C8    | 2.50                     | 0.47              |
| 1:A:1065:U:H1'   | 1:A:1066:C:OP2   | 2.15                     | 0.47              |
| 1:A:1175:G:O2'   | 1:A:1176:A:O5'   | 2.32                     | 0.47              |
| 1:A:1422:G:O2'   | 1:A:1423:G:H5'   | 2.14                     | 0.47              |
| 1:A:1451:A:O2'   | 1:A:1452:C:OP1   | 2.31                     | 0.47              |
| 1:A:147:G:O2'    | 1:A:148:G:H5'    | 2.15                     | 0.47              |
| 1:A:409:G:H1     | 1:A:433:C:N4     | 2.11                     | 0.47              |
| 1:A:620:C:C2     | 4:D:135:LEU:HD13 | 2.50                     | 0.47              |
| 3:C:23:TYR:C     | 3:C:23:TYR:CD2   | 2.88                     | 0.47              |
| 11:K:11:LYS:HD2  | 11:K:11:LYS:O    | 2.14                     | 0.47              |
| 17:Q:78:GLU:HG3  | 17:Q:78:GLU:O    | 2.14                     | 0.47              |
| 20:T:10:LEU:HG   | 20:T:12:ALA:CB   | 2.44                     | 0.47              |
| 20:T:74:LYS:NZ   | 20:T:74:LYS:HA   | 2.24                     | 0.47              |
| 1:A:1399:C:C2    | 1:A:1502:A:N6    | 2.82                     | 0.47              |
| 1:A:417:C:H2'    | 1:A:418:C:H6     | 1.79                     | 0.47              |
| 1:A:421:U:O2     | 1:A:421:U:O4'    | 2.33                     | 0.47              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:41:G:H2'      | 1:A:42:G:C8      | 2.50                     | 0.47              |
| 1:A:620:C:H2'     | 1:A:621:A:O4'    | 2.15                     | 0.47              |
| 1:A:818:G:H3'     | 1:A:819:A:H5''   | 1.97                     | 0.47              |
| 3:C:195:VAL:O     | 3:C:196:LEU:HD22 | 2.15                     | 0.47              |
| 5:E:20:GLN:O      | 5:E:21:ALA:C     | 2.53                     | 0.47              |
| 8:H:102:ARG:NE    | 8:H:102:ARG:H    | 2.13                     | 0.47              |
| 10:J:8:LEU:CD2    | 10:J:96:ILE:HG12 | 2.45                     | 0.47              |
| 12:L:55:VAL:CG1   | 12:L:56:ALA:H    | 2.22                     | 0.47              |
| 3:C:29:TYR:CZ     | 14:N:54:PRO:HG2  | 2.50                     | 0.47              |
| 14:N:9:LYS:HD2    | 14:N:9:LYS:O     | 2.15                     | 0.47              |
| 16:P:28:ARG:HG3   | 16:P:29:ASP:OD2  | 2.14                     | 0.47              |
| 16:P:20:VAL:HG13  | 16:P:32:TYR:HB2  | 1.97                     | 0.47              |
| 16:P:34:GLU:OE2   | 16:P:55:ARG:HD3  | 2.15                     | 0.47              |
| 17:Q:6:LEU:O      | 17:Q:59:ILE:N    | 2.48                     | 0.47              |
| 1:A:1003(A):G:H2' | 1:A:1004:A:O4'   | 2.14                     | 0.47              |
| 2:B:115:LEU:HD21  | 2:B:153:ARG:HE   | 1.79                     | 0.47              |
| 2:B:62:ALA:C      | 2:B:64:ARG:H     | 2.18                     | 0.47              |
| 2:B:75:LYS:HA     | 2:B:78:GLN:HB2   | 1.96                     | 0.47              |
| 4:D:31:CYS:O      | 4:D:33:MET:N     | 2.43                     | 0.47              |
| 7:G:49:ILE:HG22   | 7:G:49:ILE:O     | 2.15                     | 0.47              |
| 8:H:46:LYS:HG3    | 8:H:64:LYS:HB2   | 1.96                     | 0.47              |
| 12:L:26:ALA:O     | 12:L:27:LEU:O    | 2.33                     | 0.47              |
| 13:M:108:ARG:HH21 | 13:M:111:LYS:HB2 | 1.80                     | 0.47              |
| 15:O:36:ILE:CG1   | 15:O:59:MET:HE3  | 2.43                     | 0.47              |
| 1:A:1117:G:H5'    | 1:A:1117:G:H8    | 1.80                     | 0.46              |
| 1:A:1157:A:H4'    | 1:A:1158:C:O5'   | 2.15                     | 0.46              |
| 1:A:1256:A:H5'    | 1:A:1258:G:C1'   | 2.44                     | 0.46              |
| 1:A:1355:G:O2'    | 1:A:1356:G:H5'   | 2.14                     | 0.46              |
| 1:A:1394:A:C5     | 1:A:1501:C:H4'   | 2.50                     | 0.46              |
| 1:A:414:A:H2'     | 1:A:415:A:H8     | 1.80                     | 0.46              |
| 1:A:915:A:C2'     | 1:A:916:G:H5'    | 2.45                     | 0.46              |
| 2:B:102:LEU:HD12  | 2:B:102:LEU:N    | 2.30                     | 0.46              |
| 9:I:32:ASP:O      | 9:I:35:GLU:HB3   | 2.15                     | 0.46              |
| 13:M:21:TYR:N     | 13:M:21:TYR:CD1  | 2.82                     | 0.46              |
| 1:A:442:C:H42     | 1:A:492:G:H1     | 1.62                     | 0.46              |
| 1:A:960:U:O2      | 1:A:960:U:H2'    | 2.14                     | 0.46              |
| 2:B:69:LEU:CD1    | 2:B:155:LEU:HD11 | 2.45                     | 0.46              |
| 2:B:69:LEU:HD23   | 2:B:70:PHE:N     | 2.31                     | 0.46              |
| 3:C:36:ASP:O      | 3:C:39:ILE:HB    | 2.15                     | 0.46              |
| 3:C:6:HIS:HD2     | 3:C:8:ILE:N      | 2.00                     | 0.46              |
| 3:C:84:ILE:HD11   | 3:C:88:ARG:NH2   | 2.29                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:101:ALA:HB2  | 18:R:28:GLU:OE1  | 2.15                     | 0.46              |
| 10:J:96:ILE:HG22 | 10:J:98:ILE:HG13 | 1.97                     | 0.46              |
| 11:K:124:LYS:HD2 | 11:K:125:PHE:CZ  | 2.50                     | 0.46              |
| 1:A:950:U:H5     | 13:M:102:ARG:HE  | 1.62                     | 0.46              |
| 14:N:18:VAL:HG23 | 14:N:19:ARG:N    | 2.30                     | 0.46              |
| 1:A:1129:C:O2'   | 1:A:1130:A:P     | 2.74                     | 0.46              |
| 1:A:1461:G:O2'   | 1:A:1462:G:H5'   | 2.15                     | 0.46              |
| 1:A:411:A:C2'    | 1:A:412:A:H5'    | 2.45                     | 0.46              |
| 1:A:824:C:H2'    | 1:A:825:G:C8     | 2.50                     | 0.46              |
| 5:E:89:ILE:HD13  | 5:E:90:VAL:H     | 1.80                     | 0.46              |
| 7:G:85:TYR:O     | 7:G:87:VAL:HG23  | 2.14                     | 0.46              |
| 7:G:8:GLU:OE1    | 7:G:8:GLU:O      | 2.33                     | 0.46              |
| 10:J:80:LYS:HZ3  | 10:J:80:LYS:HB2  | 1.79                     | 0.46              |
| 13:M:106:ASN:O   | 13:M:107:ALA:HB3 | 2.16                     | 0.46              |
| 16:P:3:LYS:O     | 16:P:21:VAL:HA   | 2.16                     | 0.46              |
| 1:A:1160:G:N2    | 1:A:1161:C:H1'   | 2.31                     | 0.46              |
| 1:A:1305:G:OP2   | 1:A:1305:G:C8    | 2.69                     | 0.46              |
| 1:A:1238:A:H5'   | 1:A:1336:C:H41   | 1.80                     | 0.46              |
| 1:A:1406:U:O2'   | 1:A:1407:C:H5'   | 2.16                     | 0.46              |
| 1:A:513:C:O2'    | 1:A:514:C:H5'    | 2.15                     | 0.46              |
| 1:A:778:G:O2'    | 1:A:779:C:H5'    | 2.15                     | 0.46              |
| 2:B:100:GLY:O    | 2:B:104:ASN:N    | 2.43                     | 0.46              |
| 2:B:61:LEU:HD12  | 2:B:68:ILE:HD11  | 1.96                     | 0.46              |
| 4:D:148:VAL:CG1  | 4:D:158:ILE:HD13 | 2.45                     | 0.46              |
| 5:E:107:ARG:HH11 | 5:E:107:ARG:CB   | 2.26                     | 0.46              |
| 16:P:18:ARG:NH1  | 16:P:32:TYR:OH   | 2.48                     | 0.46              |
| 1:A:448:A:H2'    | 1:A:449:C:C6     | 2.51                     | 0.46              |
| 1:A:604:G:O2'    | 1:A:605:U:H5'    | 2.16                     | 0.46              |
| 2:B:102:LEU:CD1  | 2:B:102:LEU:N    | 2.79                     | 0.46              |
| 2:B:137:ARG:HB3  | 2:B:137:ARG:HH11 | 1.80                     | 0.46              |
| 2:B:50:GLU:HB3   | 2:B:200:ILE:O    | 2.15                     | 0.46              |
| 6:F:25:ILE:CD1   | 6:F:82:ARG:HD2   | 2.46                     | 0.46              |
| 8:H:68:ARG:HH11  | 8:H:68:ARG:HG2   | 1.81                     | 0.46              |
| 13:M:37:THR:CG2  | 13:M:37:THR:O    | 2.62                     | 0.46              |
| 1:A:1019:C:O2'   | 1:A:1020:U:H5'   | 2.16                     | 0.46              |
| 1:A:1095:U:H2'   | 1:A:1096:C:H6    | 1.72                     | 0.46              |
| 1:A:1343:G:H2'   | 1:A:1344:C:H6    | 1.81                     | 0.46              |
| 1:A:556:C:C2'    | 1:A:557:G:H5'    | 2.45                     | 0.46              |
| 1:A:689:C:H2'    | 1:A:690:G:O4'    | 2.14                     | 0.46              |
| 1:A:947:G:H2'    | 1:A:948:C:O4'    | 2.16                     | 0.46              |
| 2:B:128:GLU:O    | 2:B:129:GLU:O    | 2.34                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:108:ASN:ND2  | 3:C:111:LEU:HG   | 2.31                     | 0.46              |
| 4:D:57:ARG:NE    | 4:D:205:GLU:OE2  | 2.48                     | 0.46              |
| 5:E:147:ASP:O    | 5:E:151:LEU:HG   | 2.16                     | 0.46              |
| 8:H:101:PRO:HG2  | 8:H:133:LEU:HD11 | 1.97                     | 0.46              |
| 13:M:13:LYS:O    | 13:M:14:ARG:C    | 2.53                     | 0.46              |
| 17:Q:45:HIS:CD2  | 17:Q:47:PRO:HD3  | 2.51                     | 0.46              |
| 1:A:1157:A:C6    | 1:A:1180:A:N6    | 2.84                     | 0.46              |
| 1:A:1229:A:H2'   | 1:A:1230:C:H6    | 1.81                     | 0.46              |
| 1:A:1326:C:OP1   | 21:U:12:LYS:NZ   | 2.48                     | 0.46              |
| 1:A:408:A:H4'    | 4:D:112:VAL:HG11 | 1.97                     | 0.46              |
| 1:A:954:G:H2'    | 1:A:955:U:H6     | 1.81                     | 0.46              |
| 2:B:59:GLU:O     | 2:B:63:MET:HG2   | 2.16                     | 0.46              |
| 3:C:113:ALA:N    | 3:C:114:PRO:CD   | 2.78                     | 0.46              |
| 3:C:95:THR:O     | 3:C:95:THR:OG1   | 2.33                     | 0.46              |
| 4:D:90:GLY:N     | 4:D:204:ILE:HD11 | 2.31                     | 0.46              |
| 5:E:143:ARG:HA   | 5:E:143:ARG:HD3  | 1.55                     | 0.46              |
| 7:G:111:ARG:HB3  | 7:G:113:GLU:HG2  | 1.97                     | 0.46              |
| 12:L:50:SER:O    | 12:L:51:ALA:HB2  | 2.15                     | 0.46              |
| 18:R:20:ALA:O    | 18:R:21:LYS:C    | 2.53                     | 0.46              |
| 20:T:53:LEU:HD13 | 20:T:102:GLY:H   | 1.81                     | 0.46              |
| 1:A:1124:G:H2'   | 1:A:1145:C:C5    | 2.51                     | 0.46              |
| 1:A:1154:G:O2'   | 1:A:1155:G:H5'   | 2.16                     | 0.46              |
| 1:A:1256:A:H5'   | 1:A:1258:G:H1'   | 1.98                     | 0.46              |
| 1:A:1299:A:C5    | 1:A:1301:U:O2    | 2.69                     | 0.46              |
| 1:A:1354:C:H2'   | 1:A:1355:G:H8    | 1.79                     | 0.46              |
| 1:A:180:U:H2'    | 1:A:181:G:H5'    | 1.96                     | 0.46              |
| 1:A:509:A:H5''   | 4:D:55:ALA:HB2   | 1.98                     | 0.46              |
| 5:E:18:ARG:NH1   | 5:E:25:ARG:HB2   | 2.31                     | 0.46              |
| 8:H:6:ILE:O      | 8:H:10:LEU:HG    | 2.14                     | 0.46              |
| 12:L:86:ARG:HG3  | 12:L:86:ARG:HH11 | 1.80                     | 0.46              |
| 20:T:39:LYS:CD   | 20:T:55:ILE:HD13 | 2.46                     | 0.46              |
| 1:A:1024:G:H2'   | 1:A:1025:U:H5''  | 1.97                     | 0.46              |
| 1:A:1130:A:OP2   | 1:A:1130:A:H3'   | 2.16                     | 0.46              |
| 1:A:1169:A:H2'   | 1:A:1171:G:O4'   | 2.16                     | 0.46              |
| 1:A:1428:A:H2'   | 1:A:1429:C:C6    | 2.50                     | 0.46              |
| 1:A:497:A:H1'    | 1:A:498:U:OP1    | 2.16                     | 0.46              |
| 3:C:11:ARG:O     | 3:C:12:LEU:C     | 2.54                     | 0.46              |
| 7:G:46:ALA:O     | 7:G:50:ILE:HG12  | 2.16                     | 0.46              |
| 10:J:25:GLU:C    | 10:J:27:ALA:H    | 2.19                     | 0.46              |
| 13:M:60:VAL:CG1  | 13:M:66:LEU:HD11 | 2.46                     | 0.46              |
| 16:P:20:VAL:CG1  | 16:P:21:VAL:N    | 2.79                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1250:A:H5'   | 9:I:68:GLY:O     | 2.16                     | 0.46              |
| 1:A:979:C:H2'    | 1:A:980:C:H5'    | 1.97                     | 0.46              |
| 3:C:58:GLU:HB2   | 3:C:65:ALA:HB2   | 1.98                     | 0.46              |
| 5:E:91:LEU:HD23  | 5:E:120:THR:HG22 | 1.98                     | 0.46              |
| 7:G:18:TYR:OH    | 7:G:58:PRO:CG    | 2.64                     | 0.46              |
| 9:I:108:VAL:CG1  | 9:I:109:VAL:N    | 2.78                     | 0.46              |
| 9:I:118:LYS:O    | 9:I:119:ALA:CB   | 2.58                     | 0.46              |
| 13:M:13:LYS:HD3  | 13:M:17:VAL:CG1  | 2.45                     | 0.46              |
| 19:S:36:ARG:NH2  | 19:S:75:ALA:HB3  | 2.31                     | 0.46              |
| 1:A:114:U:O2'    | 1:A:115:G:H5'    | 2.16                     | 0.45              |
| 1:A:1289:A:H2'   | 1:A:1290:G:H5'   | 1.98                     | 0.45              |
| 1:A:131:C:H2'    | 1:A:132:C:H6     | 1.81                     | 0.45              |
| 1:A:285:G:O2'    | 1:A:286:G:H5'    | 2.15                     | 0.45              |
| 2:B:97:TRP:HZ3   | 2:B:100:GLY:H    | 1.64                     | 0.45              |
| 3:C:11:ARG:O     | 3:C:13:GLY:N     | 2.49                     | 0.45              |
| 1:A:1279:A:H61   | 3:C:26:LYS:NZ    | 2.14                     | 0.45              |
| 3:C:34:LEU:HG    | 14:N:25:VAL:HG21 | 1.98                     | 0.45              |
| 3:C:95:THR:O     | 3:C:97:LYS:N     | 2.49                     | 0.45              |
| 4:D:64:LEU:HD12  | 4:D:75:PHE:HZ    | 1.81                     | 0.45              |
| 7:G:77:SER:O     | 7:G:78:ARG:HB2   | 2.16                     | 0.45              |
| 12:L:113:ARG:NH1 | 12:L:116:SER:N   | 2.63                     | 0.45              |
| 21:U:6:ARG:HD2   | 21:U:15:ARG:HH12 | 1.81                     | 0.45              |
| 1:A:1054:C:H42   | 23:Y:34:TM2:C1'  | 2.28                     | 0.45              |
| 1:A:1152:A:H2'   | 1:A:1153:C:C6    | 2.50                     | 0.45              |
| 1:A:1191:A:H3'   | 1:A:1192:C:P     | 2.45                     | 0.45              |
| 1:A:149:A:H2'    | 1:A:150:C:C6     | 2.51                     | 0.45              |
| 1:A:1533:C:H2'   | 1:A:1534:A:C5'   | 2.42                     | 0.45              |
| 1:A:393:A:O2'    | 1:A:394:G:H5'    | 2.16                     | 0.45              |
| 1:A:721:G:H4'    | 1:A:722:A:O4'    | 2.17                     | 0.45              |
| 3:C:107:GLN:O    | 3:C:108:ASN:CB   | 2.64                     | 0.45              |
| 7:G:51:GLN:HB2   | 7:G:52:GLU:OE1   | 2.16                     | 0.45              |
| 13:M:44:ARG:O    | 13:M:45:VAL:C    | 2.53                     | 0.45              |
| 18:R:16:PRO:O    | 18:R:54:ARG:NH1  | 2.49                     | 0.45              |
| 1:A:110:C:H2'    | 1:A:111:G:O4'    | 2.16                     | 0.45              |
| 1:A:928:G:O2'    | 1:A:1533:C:OP1   | 2.34                     | 0.45              |
| 1:A:633:G:H2'    | 1:A:634:C:C6     | 2.52                     | 0.45              |
| 2:B:80:ILE:O     | 2:B:84:GLU:HB2   | 2.16                     | 0.45              |
| 5:E:11:ILE:HD11  | 5:E:33:VAL:CG2   | 2.46                     | 0.45              |
| 11:K:13:GLN:HA   | 11:K:75:TYR:O    | 2.16                     | 0.45              |
| 13:M:65:LYS:HG3  | 13:M:69:GLU:HB3  | 1.98                     | 0.45              |
| 13:M:60:VAL:HG12 | 13:M:66:LEU:HD11 | 1.99                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 15:O:3:ILE:HG12  | 15:O:38:ARG:NH1   | 2.31                     | 0.45              |
| 1:A:377:G:OP1    | 16:P:3:LYS:HD3    | 2.17                     | 0.45              |
| 19:S:12:ASP:O    | 19:S:15:LEU:HD12  | 2.16                     | 0.45              |
| 1:A:1141:C:O2'   | 1:A:1142:G:H5'    | 2.16                     | 0.45              |
| 1:A:1347:G:C8    | 9:I:107:ARG:NH1   | 2.84                     | 0.45              |
| 1:A:1347:G:O2'   | 1:A:1348:U:H6     | 1.99                     | 0.45              |
| 1:A:151:A:H2'    | 1:A:152:A:O4'     | 2.16                     | 0.45              |
| 1:A:184:G:H2'    | 1:A:185:A:H8      | 1.80                     | 0.45              |
| 1:A:280:C:O2     | 17:Q:38:ARG:HG3   | 2.17                     | 0.45              |
| 1:A:781:A:C5     | 1:A:802:A:C2      | 3.05                     | 0.45              |
| 2:B:10:LEU:C     | 2:B:12:GLU:H      | 2.19                     | 0.45              |
| 3:C:44:GLU:HA    | 3:C:52:LEU:HD11   | 1.97                     | 0.45              |
| 3:C:73:PRO:O     | 3:C:75:VAL:N      | 2.49                     | 0.45              |
| 7:G:62:PHE:HA    | 7:G:124:LEU:HD12  | 1.98                     | 0.45              |
| 9:I:4:TYR:CE2    | 9:I:88:TYR:HD1    | 2.34                     | 0.45              |
| 9:I:53:VAL:HG13  | 9:I:96:LEU:HD11   | 1.99                     | 0.45              |
| 1:A:1207:G:H2'   | 1:A:1208:C:H6     | 1.82                     | 0.45              |
| 1:A:742:G:P      | 15:O:35:ARG:HH22  | 2.39                     | 0.45              |
| 2:B:118:LEU:C    | 2:B:120:ALA:N     | 2.69                     | 0.45              |
| 4:D:98:GLU:HG2   | 4:D:189:PRO:HG3   | 1.98                     | 0.45              |
| 1:A:1080:A:H4'   | 5:E:16:THR:HG21   | 1.99                     | 0.45              |
| 7:G:82:GLY:O     | 7:G:83:ALA:HB2    | 2.16                     | 0.45              |
| 9:I:12:GLU:O     | 9:I:12:GLU:HG2    | 2.16                     | 0.45              |
| 13:M:11:ARG:CD   | 13:M:12:ASN:H     | 2.28                     | 0.45              |
| 1:A:163:C:H2'    | 1:A:164:U:H6      | 1.80                     | 0.45              |
| 1:A:245:C:O2     | 1:A:283:C:N3      | 2.49                     | 0.45              |
| 1:A:961:U:H2'    | 1:A:962:C:C5'     | 2.47                     | 0.45              |
| 4:D:128:VAL:O    | 4:D:129:ASN:HB2   | 2.17                     | 0.45              |
| 1:A:922:G:H4'    | 5:E:20:GLN:HA     | 1.98                     | 0.45              |
| 9:I:102:LEU:HD12 | 9:I:102:LEU:N     | 2.30                     | 0.45              |
| 9:I:43:ALA:HA    | 9:I:74:ILE:HD13   | 1.98                     | 0.45              |
| 10:J:46:ARG:HH12 | 10:J:64:GLU:HB3   | 1.81                     | 0.45              |
| 11:K:78:GLN:O    | 11:K:103:LEU:HD23 | 2.16                     | 0.45              |
| 1:A:1229:A:H2'   | 1:A:1230:C:C6     | 2.52                     | 0.45              |
| 3:C:20:SER:HB3   | 3:C:22:TRP:HE1    | 1.82                     | 0.45              |
| 4:D:81:GLU:O     | 4:D:85:LYS:HG3    | 2.16                     | 0.45              |
| 5:E:137:GLU:OE2  | 5:E:140:ARG:HD2   | 2.16                     | 0.45              |
| 6:F:10:LEU:HA    | 6:F:84:ASN:O      | 2.17                     | 0.45              |
| 7:G:72:ARG:O     | 7:G:73:MET:HG2    | 2.17                     | 0.45              |
| 8:H:82:HIS:HB3   | 8:H:138:TRP:CD2   | 2.52                     | 0.45              |
| 2:B:178:ARG:NH1  | 8:H:71:GLY:O      | 2.50                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 13:M:33:ALA:HA    | 13:M:59:TYR:CE2  | 2.51                     | 0.45              |
| 1:A:1127:G:N2     | 1:A:1147:C:N4    | 2.64                     | 0.45              |
| 1:A:978:A:O2'     | 1:A:1322:C:N3    | 2.47                     | 0.45              |
| 1:A:1386:G:O2'    | 1:A:1387:G:H5'   | 2.17                     | 0.45              |
| 1:A:222:U:H2'     | 1:A:223:U:C6     | 2.51                     | 0.45              |
| 1:A:262:A:H5'     | 20:T:74:LYS:HG3  | 1.99                     | 0.45              |
| 2:B:101:MET:O     | 2:B:105:PHE:HA   | 2.16                     | 0.45              |
| 2:B:204:ASN:C     | 2:B:204:ASN:ND2  | 2.70                     | 0.45              |
| 2:B:51:LEU:O      | 2:B:55:PHE:HD1   | 2.00                     | 0.45              |
| 3:C:108:ASN:C     | 3:C:110:ASN:H    | 2.19                     | 0.45              |
| 3:C:40:ARG:HG2    | 3:C:55:VAL:HG11  | 1.98                     | 0.45              |
| 12:L:6:THR:OG1    | 12:L:9:GLN:HG3   | 2.16                     | 0.45              |
| 1:A:190(D):U:O2'  | 1:A:190(E):U:H5' | 2.16                     | 0.45              |
| 1:A:433:C:C5'     | 1:A:433:C:C6     | 2.98                     | 0.45              |
| 1:A:538:G:OP2     | 12:L:115:LYS:CG  | 2.65                     | 0.45              |
| 2:B:184:VAL:HG12  | 2:B:197:VAL:HG13 | 1.99                     | 0.45              |
| 2:B:97:TRP:CH2    | 2:B:101:MET:HB2  | 2.52                     | 0.45              |
| 3:C:112:SER:C     | 3:C:114:PRO:HD2  | 2.37                     | 0.45              |
| 6:F:8:ILE:HG22    | 6:F:10:LEU:HD12  | 1.99                     | 0.45              |
| 8:H:84:ARG:O      | 8:H:135:CYS:HB2  | 2.17                     | 0.45              |
| 9:I:37:PHE:HD1    | 9:I:43:ALA:HB1   | 1.82                     | 0.45              |
| 15:O:2:PRO:HB2    | 15:O:3:ILE:H     | 1.63                     | 0.45              |
| 18:R:88:LYS:CG    | 18:R:88:LYS:OXT  | 2.64                     | 0.45              |
| 20:T:105:SER:O    | 20:T:106:ALA:C   | 2.55                     | 0.45              |
| 1:A:662:G:H2'     | 1:A:663:A:C8     | 2.52                     | 0.45              |
| 1:A:81:U:H2'      | 1:A:83:U:OP2     | 2.17                     | 0.45              |
| 3:C:172:ARG:HB3   | 3:C:172:ARG:HH11 | 1.82                     | 0.45              |
| 3:C:5:ILE:N       | 3:C:5:ILE:HD12   | 2.32                     | 0.45              |
| 4:D:117:ALA:O     | 4:D:121:VAL:HG23 | 2.16                     | 0.45              |
| 7:G:15:ASP:OD2    | 7:G:16:LEU:N     | 2.50                     | 0.45              |
| 13:M:108:ARG:HH21 | 13:M:111:LYS:CB  | 2.29                     | 0.45              |
| 13:M:14:ARG:H     | 13:M:44:ARG:HE   | 1.64                     | 0.45              |
| 1:A:974:A:OP2     | 14:N:41:ARG:NH1  | 2.50                     | 0.45              |
| 15:O:74:ASP:CG    | 15:O:77:ARG:HG3  | 2.38                     | 0.45              |
| 17:Q:101:ARG:NE   | 17:Q:101:ARG:HA  | 2.31                     | 0.45              |
| 18:R:45:SER:O     | 18:R:47:THR:O    | 2.34                     | 0.45              |
| 1:A:165:C:O2'     | 1:A:166:G:H5'    | 2.16                     | 0.44              |
| 1:A:290:C:O2'     | 1:A:291:C:H5'    | 2.17                     | 0.44              |
| 1:A:513:C:H2'     | 1:A:514:C:H6     | 1.81                     | 0.44              |
| 1:A:67:C:H2'      | 1:A:68:G:C8      | 2.52                     | 0.44              |
| 2:B:189:ASP:HB2   | 2:B:205:ASP:OD2  | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:G:48:LYS:CG    | 7:G:49:ILE:N     | 2.79                     | 0.44              |
| 10:J:31:GLY:HA3  | 10:J:78:ASN:ND2  | 2.32                     | 0.44              |
| 10:J:60:ARG:HD3  | 10:J:60:ARG:HA   | 1.90                     | 0.44              |
| 10:J:39:PRO:O    | 10:J:69:ASN:O    | 2.35                     | 0.44              |
| 15:O:26:GLU:HG3  | 15:O:81:LEU:HG   | 1.98                     | 0.44              |
| 1:A:1054:C:H2'   | 1:A:1055:A:H5''  | 2.00                     | 0.44              |
| 1:A:1057:G:O2'   | 1:A:1058:G:H5'   | 2.17                     | 0.44              |
| 1:A:1129:C:O2'   | 1:A:1130:A:OP2   | 2.34                     | 0.44              |
| 1:A:1257:U:H5''  | 1:A:1258:G:O5'   | 2.17                     | 0.44              |
| 1:A:1312:G:O2'   | 1:A:1313:U:H5'   | 2.17                     | 0.44              |
| 1:A:500:G:H2'    | 1:A:501:C:C6     | 2.52                     | 0.44              |
| 1:A:674:G:O2'    | 1:A:675:A:H5'    | 2.17                     | 0.44              |
| 1:A:723:U:O2     | 1:A:723:U:H2'    | 2.16                     | 0.44              |
| 1:A:940:C:H2'    | 1:A:941:G:H8     | 1.82                     | 0.44              |
| 1:A:977:A:C2'    | 1:A:978:A:H5'    | 2.47                     | 0.44              |
| 2:B:153:ARG:HG3  | 2:B:153:ARG:HH11 | 1.82                     | 0.44              |
| 2:B:73:THR:O     | 2:B:75:LYS:N     | 2.50                     | 0.44              |
| 6:F:67:MET:HE1   | 6:F:75:LEU:HD12  | 2.00                     | 0.44              |
| 12:L:75:HIS:CD2  | 12:L:77:LEU:H    | 2.34                     | 0.44              |
| 13:M:37:THR:HG23 | 13:M:55:ARG:CD   | 2.38                     | 0.44              |
| 13:M:40:ASN:ND2  | 13:M:40:ASN:C    | 2.71                     | 0.44              |
| 14:N:11:LYS:C    | 14:N:13:THR:N    | 2.70                     | 0.44              |
| 15:O:21:ASP:OD2  | 15:O:24:SER:HB3  | 2.16                     | 0.44              |
| 18:R:87:ARG:HH21 | 18:R:87:ARG:HG3  | 1.82                     | 0.44              |
| 19:S:39:THR:HG22 | 19:S:40:ILE:N    | 2.32                     | 0.44              |
| 1:A:1242:C:O2'   | 1:A:1243:C:H5'   | 2.17                     | 0.44              |
| 1:A:1238:A:C8    | 1:A:1303:C:H1'   | 2.52                     | 0.44              |
| 1:A:831:U:O2'    | 1:A:832:C:H5'    | 2.17                     | 0.44              |
| 2:B:64:ARG:HH11  | 2:B:64:ARG:CB    | 2.28                     | 0.44              |
| 3:C:19:GLU:HG2   | 3:C:54:ARG:HE    | 1.82                     | 0.44              |
| 3:C:70:VAL:CG1   | 3:C:71:ALA:N     | 2.79                     | 0.44              |
| 4:D:103:ASN:O    | 4:D:106:TYR:HB3  | 2.17                     | 0.44              |
| 4:D:126:ILE:CG2  | 4:D:127:THR:N    | 2.80                     | 0.44              |
| 4:D:31:CYS:O     | 4:D:32:ALA:HB3   | 2.16                     | 0.44              |
| 11:K:32:ILE:HG21 | 11:K:77:MET:CE   | 2.47                     | 0.44              |
| 18:R:43:PHE:C    | 18:R:51:LEU:HD12 | 2.37                     | 0.44              |
| 23:Y:34:TM2:O3S  | 23:Y:36:A:N6     | 2.50                     | 0.44              |
| 1:A:1229:A:C2    | 1:A:1230:C:C4    | 3.05                     | 0.44              |
| 1:A:1307:U:H2'   | 1:A:1308:U:C6    | 2.53                     | 0.44              |
| 1:A:1318:A:O2'   | 19:S:37:ARG:HD2  | 2.17                     | 0.44              |
| 1:A:1329:A:OP1   | 13:M:26:GLY:HA3  | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:145:G:O2'    | 1:A:146:G:H5'    | 2.17                     | 0.44              |
| 2:B:30:ARG:C     | 2:B:32:ILE:H     | 2.20                     | 0.44              |
| 2:B:95:GLN:OE1   | 2:B:95:GLN:HA    | 2.16                     | 0.44              |
| 3:C:126:ARG:O    | 3:C:127:ARG:HB2  | 2.18                     | 0.44              |
| 3:C:167:TRP:O    | 3:C:168:ALA:CB   | 2.66                     | 0.44              |
| 6:F:33:TYR:C     | 6:F:71:ARG:NH2   | 2.71                     | 0.44              |
| 7:G:149:ARG:CZ   | 7:G:149:ARG:HB3  | 2.46                     | 0.44              |
| 17:Q:67:LYS:C    | 17:Q:70:ARG:HH12 | 2.19                     | 0.44              |
| 20:T:12:ALA:C    | 20:T:14:LYS:N    | 2.70                     | 0.44              |
| 1:A:1329:A:N7    | 21:U:7:ARG:NH2   | 2.65                     | 0.44              |
| 1:A:697:U:H2'    | 1:A:698:G:H5'    | 1.98                     | 0.44              |
| 1:A:892:A:C2     | 1:A:907:A:C4     | 3.06                     | 0.44              |
| 1:A:994:A:H2'    | 1:A:994:A:N3     | 2.32                     | 0.44              |
| 2:B:124:SER:CB   | 2:B:125:PRO:HD2  | 2.43                     | 0.44              |
| 2:B:213:LEU:O    | 2:B:217:ARG:HG2  | 2.17                     | 0.44              |
| 2:B:223:ILE:C    | 2:B:225:ALA:H    | 2.20                     | 0.44              |
| 2:B:130:ARG:NH2  | 3:C:207:VAL:HG11 | 2.33                     | 0.44              |
| 1:A:542:G:H5'    | 4:D:41:GLY:HA3   | 1.99                     | 0.44              |
| 6:F:36:ARG:NH1   | 6:F:38:GLU:HG2   | 2.32                     | 0.44              |
| 7:G:145:ALA:C    | 7:G:147:ALA:H    | 2.21                     | 0.44              |
| 8:H:55:GLY:C     | 8:H:56:LYS:HD2   | 2.37                     | 0.44              |
| 2:B:178:ARG:O    | 8:H:71:GLY:HA2   | 2.17                     | 0.44              |
| 13:M:108:ARG:CA  | 13:M:108:ARG:HE  | 2.14                     | 0.44              |
| 13:M:40:ASN:HB3  | 13:M:43:THR:HG23 | 1.99                     | 0.44              |
| 13:M:61:GLU:C    | 13:M:62:ASN:HD22 | 2.20                     | 0.44              |
| 20:T:74:LYS:NZ   | 20:T:74:LYS:CA   | 2.81                     | 0.44              |
| 1:A:1353:G:H2'   | 1:A:1354:C:C6    | 2.52                     | 0.44              |
| 1:A:1495:U:H2'   | 1:A:1496:C:C6    | 2.52                     | 0.44              |
| 1:A:123:C:OP1    | 1:A:312:C:H5'    | 2.17                     | 0.44              |
| 1:A:339:C:H2'    | 1:A:340:U:C6     | 2.53                     | 0.44              |
| 1:A:975:A:C5'    | 1:A:975:A:C8     | 2.95                     | 0.44              |
| 3:C:134:ILE:HG23 | 3:C:151:VAL:HB   | 2.00                     | 0.44              |
| 4:D:61:LYS:NZ    | 4:D:62:GLN:HE21  | 2.15                     | 0.44              |
| 5:E:150:ARG:CG   | 5:E:150:ARG:NH1  | 2.77                     | 0.44              |
| 5:E:83:GLU:HG3   | 5:E:88:LYS:HG3   | 1.99                     | 0.44              |
| 9:I:113:LYS:H    | 9:I:119:ALA:HA   | 1.81                     | 0.44              |
| 10:J:15:THR:O    | 10:J:15:THR:HG22 | 2.18                     | 0.44              |
| 12:L:77:LEU:HD21 | 12:L:107:ALA:CB  | 2.48                     | 0.44              |
| 1:A:1423:G:O2'   | 1:A:1424:C:H5'   | 2.17                     | 0.44              |
| 1:A:1505:G:H4'   | 1:A:1506:U:O5'   | 2.17                     | 0.44              |
| 1:A:338:A:H2     | 1:A:351:G:H22    | 1.66                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:737:A:H2'    | 1:A:738:C:C6     | 2.52                     | 0.44              |
| 2:B:30:ARG:HG3   | 2:B:31:TYR:CD2   | 2.53                     | 0.44              |
| 5:E:129:ILE:H    | 5:E:129:ILE:HD12 | 1.82                     | 0.44              |
| 5:E:76:ILE:HG13  | 5:E:142:LEU:HD13 | 1.99                     | 0.44              |
| 7:G:129:GLU:OE1  | 7:G:131:LYS:HE2  | 2.18                     | 0.44              |
| 8:H:104:ARG:O    | 8:H:106:GLY:N    | 2.51                     | 0.44              |
| 9:I:31:GLN:HB3   | 9:I:35:GLU:CG    | 2.47                     | 0.44              |
| 10:J:80:LYS:NZ   | 10:J:80:LYS:HB2  | 2.33                     | 0.44              |
| 1:A:1228:C:OP1   | 13:M:115:LYS:HE3 | 2.18                     | 0.44              |
| 13:M:36:LYS:HD2  | 13:M:59:TYR:OH   | 2.18                     | 0.44              |
| 1:A:1320:C:O2    | 19:S:36:ARG:NH1  | 2.50                     | 0.44              |
| 1:A:1441:G:H4'   | 1:A:1442:G:C5    | 2.52                     | 0.44              |
| 1:A:625:G:H2'    | 1:A:626:U:H6     | 1.83                     | 0.44              |
| 2:B:92:TYR:C     | 2:B:92:TYR:CD1   | 2.90                     | 0.44              |
| 3:C:113:ALA:HB1  | 3:C:200:ALA:HB3  | 2.00                     | 0.44              |
| 3:C:18:TRP:HE3   | 3:C:18:TRP:H     | 1.65                     | 0.44              |
| 5:E:69:VAL:HG21  | 5:E:113:ALA:HB1  | 1.98                     | 0.44              |
| 7:G:136:LYS:HZ2  | 7:G:143:ARG:HH12 | 1.64                     | 0.44              |
| 10:J:22:LYS:HB2  | 10:J:22:LYS:NZ   | 2.33                     | 0.44              |
| 13:M:62:ASN:O    | 13:M:63:THR:CB   | 2.66                     | 0.44              |
| 15:O:5:LYS:N     | 15:O:5:LYS:HD2   | 2.32                     | 0.44              |
| 15:O:74:ASP:O    | 15:O:76:GLU:N    | 2.51                     | 0.44              |
| 19:S:18:LYS:HD3  | 19:S:18:LYS:C    | 2.39                     | 0.44              |
| 1:A:1267:C:O2    | 21:U:20:LYS:HD2  | 2.18                     | 0.44              |
| 1:A:1305:G:N2    | 1:A:1331:G:C2'   | 2.81                     | 0.44              |
| 1:A:1360:A:O2'   | 1:A:1361:G:H5'   | 2.18                     | 0.44              |
| 1:A:782:A:H2'    | 1:A:783:C:O4'    | 2.18                     | 0.44              |
| 2:B:22:LYS:O     | 2:B:24:TRP:N     | 2.50                     | 0.44              |
| 3:C:79:ARG:CG    | 3:C:82:GLU:HG2   | 2.45                     | 0.44              |
| 6:F:15:ASP:O     | 6:F:17:SER:N     | 2.51                     | 0.44              |
| 7:G:108:ALA:O    | 7:G:119:ARG:HG2  | 2.18                     | 0.44              |
| 10:J:14:LYS:O    | 10:J:18:ALA:HB3  | 2.18                     | 0.44              |
| 12:L:117:ARG:NH2 | 12:L:124:LYS:HA  | 2.33                     | 0.44              |
| 14:N:22:THR:HG23 | 14:N:33:VAL:HG21 | 2.00                     | 0.44              |
| 18:R:37:VAL:HG22 | 18:R:78:LEU:HB3  | 2.00                     | 0.44              |
| 1:A:999:C:H2'    | 1:A:1000:U:C6    | 2.53                     | 0.43              |
| 1:A:405:U:O4     | 4:D:2:GLY:HA2    | 2.18                     | 0.43              |
| 1:A:630:G:H5'    | 1:A:631:G:OP2    | 2.17                     | 0.43              |
| 2:B:192:SER:O    | 2:B:194:PRO:HD3  | 2.18                     | 0.43              |
| 8:H:38:ILE:N     | 8:H:38:ILE:HD12  | 2.33                     | 0.43              |
| 1:A:1343:G:C1'   | 9:I:121:ARG:HH12 | 2.28                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 10:J:75:ILE:O     | 10:J:76:ASN:HB2    | 2.18                     | 0.43              |
| 12:L:82:VAL:HG23  | 12:L:106:ASP:OD1   | 2.18                     | 0.43              |
| 13:M:44:ARG:O     | 13:M:46:LYS:N      | 2.51                     | 0.43              |
| 15:O:87:ILE:O     | 15:O:88:ARG:CB     | 2.66                     | 0.43              |
| 17:Q:92:ARG:O     | 17:Q:95:TYR:HB2    | 2.18                     | 0.43              |
| 1:A:1157:A:C6     | 1:A:1180:A:C5      | 3.06                     | 0.43              |
| 1:A:1178:G:C2     | 1:A:1180:A:C8      | 3.06                     | 0.43              |
| 1:A:1192:C:H2'    | 1:A:1193:G:O5'     | 2.19                     | 0.43              |
| 26:A:1854:PAR:H43 | 26:A:1854:PAR:H642 | 2.00                     | 0.43              |
| 1:A:967:C:OP1     | 1:A:969:A:H5'      | 2.19                     | 0.43              |
| 3:C:127:ARG:HD2   | 3:C:127:ARG:N      | 2.33                     | 0.43              |
| 3:C:155:GLY:HA3   | 3:C:164:ARG:H      | 1.83                     | 0.43              |
| 3:C:47:LEU:CD2    | 3:C:68:VAL:HG11    | 2.49                     | 0.43              |
| 3:C:52:LEU:N      | 3:C:52:LEU:CD2     | 2.81                     | 0.43              |
| 8:H:13:ILE:O      | 8:H:17:THR:HG23    | 2.19                     | 0.43              |
| 8:H:63:LEU:HD22   | 8:H:63:LEU:H       | 1.82                     | 0.43              |
| 8:H:20:TYR:CE2    | 8:H:75:ARG:HD2     | 2.53                     | 0.43              |
| 9:I:53:VAL:O      | 9:I:54:ASP:CB      | 2.66                     | 0.43              |
| 1:A:1152:A:OP1    | 10:J:13:HIS:HB2    | 2.18                     | 0.43              |
| 16:P:1:MET:O      | 16:P:24:ALA:HB2    | 2.17                     | 0.43              |
| 1:A:1010:G:O2'    | 1:A:1011:G:H5'     | 2.18                     | 0.43              |
| 1:A:1054:C:C2'    | 1:A:1055:A:H5''    | 2.48                     | 0.43              |
| 1:A:344:A:O2'     | 1:A:345:C:OP1      | 2.32                     | 0.43              |
| 1:A:677:U:H3      | 1:A:713:G:H22      | 1.66                     | 0.43              |
| 1:A:920:U:H2'     | 1:A:921:U:C6       | 2.53                     | 0.43              |
| 1:A:1206:G:H4'    | 3:C:192:THR:O      | 2.19                     | 0.43              |
| 4:D:36:ARG:H      | 4:D:37:PRO:HD3     | 1.82                     | 0.43              |
| 4:D:36:ARG:N      | 4:D:37:PRO:CD      | 2.81                     | 0.43              |
| 7:G:145:ALA:O     | 7:G:146:GLU:CB     | 2.63                     | 0.43              |
| 7:G:145:ALA:O     | 7:G:146:GLU:HB3    | 2.18                     | 0.43              |
| 10:J:16:LEU:CD2   | 10:J:94:VAL:HG13   | 2.48                     | 0.43              |
| 1:A:761:G:H1'     | 17:Q:105:ALA:CB    | 2.47                     | 0.43              |
| 17:Q:68:ARG:CG    | 17:Q:68:ARG:NH1    | 2.81                     | 0.43              |
| 20:T:59:ALA:O     | 20:T:63:ILE:HG13   | 2.18                     | 0.43              |
| 20:T:8:ARG:HH11   | 20:T:8:ARG:CB      | 2.21                     | 0.43              |
| 1:A:1097:C:H2'    | 1:A:1098:C:C6      | 2.53                     | 0.43              |
| 1:A:6:G:H4'       | 1:A:298:A:H4'      | 2.00                     | 0.43              |
| 1:A:397:A:H5'     | 1:A:398:C:P        | 2.59                     | 0.43              |
| 1:A:407:G:H2'     | 1:A:408:A:C8       | 2.52                     | 0.43              |
| 1:A:415:A:H2'     | 1:A:416:G:C8       | 2.53                     | 0.43              |
| 1:A:951:G:O2'     | 1:A:952:U:H5'      | 2.19                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:204:ASN:HD21 | 2:B:206:ASP:CB   | 2.30                     | 0.43              |
| 7:G:75:VAL:HG11  | 7:G:144:MET:HE3  | 1.99                     | 0.43              |
| 8:H:77:GLU:CG    | 8:H:78:GLN:N     | 2.81                     | 0.43              |
| 11:K:84:VAL:CG2  | 11:K:95:ILE:HD11 | 2.49                     | 0.43              |
| 9:I:128:ARG:HA   | 13:M:126:LYS:HD2 | 2.00                     | 0.43              |
| 15:O:45:VAL:HG12 | 15:O:46:HIS:H    | 1.83                     | 0.43              |
| 15:O:55:GLY:O    | 15:O:59:MET:HG3  | 2.18                     | 0.43              |
| 20:T:93:GLU:O    | 20:T:94:ALA:HB2  | 2.18                     | 0.43              |
| 1:A:994:A:N7     | 1:A:1216:G:H4'   | 2.34                     | 0.43              |
| 1:A:1402:C:O2    | 1:A:1500:A:N1    | 2.51                     | 0.43              |
| 1:A:1532:U:O2    | 1:A:1534:A:P     | 2.70                     | 0.43              |
| 1:A:186:C:H2'    | 1:A:187:C:C6     | 2.53                     | 0.43              |
| 1:A:644:G:C5     | 1:A:645:C:C5     | 3.06                     | 0.43              |
| 1:A:687:A:H2     | 1:A:700:G:N3     | 2.16                     | 0.43              |
| 2:B:27:LYS:O     | 2:B:194:PRO:HG2  | 2.19                     | 0.43              |
| 3:C:20:SER:HB3   | 3:C:22:TRP:NE1   | 2.33                     | 0.43              |
| 3:C:64:VAL:HB    | 3:C:99:VAL:CG2   | 2.35                     | 0.43              |
| 3:C:35:GLU:HG3   | 3:C:95:THR:HG22  | 2.00                     | 0.43              |
| 12:L:10:LEU:HD22 | 12:L:15:ARG:HD3  | 2.00                     | 0.43              |
| 13:M:40:ASN:ND2  | 13:M:41:PRO:HD2  | 2.31                     | 0.43              |
| 21:U:6:ARG:CG    | 21:U:15:ARG:NH1  | 2.80                     | 0.43              |
| 1:A:1288:A:N1    | 1:A:1371:G:H1'   | 2.33                     | 0.43              |
| 1:A:1346:A:C5    | 7:G:10:ARG:NH2   | 2.86                     | 0.43              |
| 1:A:279:A:H5''   | 1:A:281:G:O4'    | 2.18                     | 0.43              |
| 1:A:590:C:O2'    | 1:A:591:U:H5'    | 2.18                     | 0.43              |
| 5:E:106:PRO:O    | 5:E:110:LEU:HG   | 2.19                     | 0.43              |
| 9:I:23:ASN:HD22  | 9:I:23:ASN:C     | 2.21                     | 0.43              |
| 9:I:32:ASP:OD1   | 9:I:33:PHE:N     | 2.52                     | 0.43              |
| 1:A:1193:G:HO2'  | 1:A:1194:U:H5'   | 1.80                     | 0.43              |
| 1:A:1371:G:O3'   | 9:I:69:GLY:HA3   | 2.18                     | 0.43              |
| 1:A:265:G:H2'    | 1:A:267:C:H5     | 1.82                     | 0.43              |
| 1:A:627:G:O2'    | 1:A:628:G:H5'    | 2.18                     | 0.43              |
| 1:A:757:U:O2'    | 1:A:879:C:H1'    | 2.19                     | 0.43              |
| 2:B:97:TRP:HZ3   | 2:B:100:GLY:N    | 2.17                     | 0.43              |
| 6:F:40:VAL:HG22  | 6:F:41:GLU:H     | 1.83                     | 0.43              |
| 8:H:61:VAL:O     | 8:H:63:LEU:HD22  | 2.17                     | 0.43              |
| 11:K:24:SER:C    | 11:K:26:ASN:H    | 2.20                     | 0.43              |
| 12:L:111:LYS:HE2 | 12:L:112:ASP:H   | 1.75                     | 0.43              |
| 16:P:38:TYR:HE2  | 16:P:50:LYS:CE   | 2.31                     | 0.43              |
| 16:P:43:LYS:HA   | 16:P:48:TRP:HB3  | 2.01                     | 0.43              |
| 19:S:13:ASP:N    | 19:S:13:ASP:OD2  | 2.48                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1018:C:H6    | 1:A:1018:C:O5'   | 2.02                     | 0.43              |
| 1:A:122:G:OP1    | 1:A:122:G:H8     | 2.02                     | 0.43              |
| 1:A:1347:G:H2'   | 1:A:1348:U:OP2   | 2.18                     | 0.43              |
| 1:A:1427:U:H2'   | 1:A:1428:A:H8    | 1.82                     | 0.43              |
| 1:A:254:G:O2'    | 1:A:255:G:H5'    | 2.18                     | 0.43              |
| 1:A:959:A:H3'    | 1:A:960:U:H5''   | 2.00                     | 0.43              |
| 3:C:180:ALA:HB1  | 3:C:182:ILE:HG13 | 2.00                     | 0.43              |
| 7:G:21:VAL:HG23  | 7:G:22:LEU:N     | 2.33                     | 0.43              |
| 10:J:23:ILE:CD1  | 10:J:23:ILE:N    | 2.81                     | 0.43              |
| 14:N:11:LYS:C    | 14:N:13:THR:H    | 2.22                     | 0.43              |
| 15:O:42:HIS:O    | 15:O:45:VAL:O    | 2.37                     | 0.43              |
| 15:O:25:THR:CG2  | 15:O:70:LEU:HG   | 2.46                     | 0.43              |
| 17:Q:101:ARG:HE  | 17:Q:101:ARG:HA  | 1.84                     | 0.43              |
| 20:T:44:ALA:HB2  | 20:T:88:VAL:HG13 | 2.01                     | 0.43              |
| 1:A:1190:G:P     | 3:C:5:ILE:HG13   | 2.58                     | 0.43              |
| 1:A:58:C:O2'     | 1:A:59:A:H5'     | 2.19                     | 0.43              |
| 2:B:140:HIS:O    | 2:B:143:GLU:HB3  | 2.19                     | 0.43              |
| 3:C:47:LEU:HG    | 3:C:76:VAL:HG12  | 2.01                     | 0.43              |
| 3:C:65:ALA:O     | 3:C:66:VAL:HB    | 2.17                     | 0.43              |
| 3:C:68:VAL:HG12  | 3:C:70:VAL:HG23  | 2.01                     | 0.43              |
| 4:D:76:ARG:O     | 4:D:80:GLU:HG2   | 2.18                     | 0.43              |
| 7:G:15:ASP:C     | 7:G:17:VAL:H     | 2.22                     | 0.43              |
| 9:I:17:VAL:HG21  | 9:I:80:GLY:HA3   | 2.01                     | 0.43              |
| 11:K:45:GLY:O    | 11:K:50:TYR:HB2  | 2.18                     | 0.43              |
| 15:O:5:LYS:CD    | 15:O:5:LYS:H     | 2.32                     | 0.43              |
| 18:R:51:LEU:HA   | 18:R:52:PRO:HD3  | 1.87                     | 0.43              |
| 1:A:1058:G:C6    | 1:A:1059:C:N3    | 2.87                     | 0.43              |
| 1:A:1138:G:N1    | 1:A:1140:C:C2    | 2.87                     | 0.43              |
| 1:A:692:U:H2'    | 1:A:694:A:OP2    | 2.19                     | 0.43              |
| 2:B:128:GLU:O    | 2:B:129:GLU:C    | 2.57                     | 0.43              |
| 2:B:97:TRP:CH2   | 2:B:176:GLU:OE2  | 2.72                     | 0.43              |
| 3:C:180:ALA:O    | 3:C:181:ASN:CB   | 2.65                     | 0.43              |
| 5:E:142:LEU:O    | 5:E:143:ARG:NE   | 2.50                     | 0.43              |
| 10:J:22:LYS:HD3  | 10:J:88:LEU:O    | 2.18                     | 0.43              |
| 11:K:48:ILE:HG22 | 11:K:49:GLY:N    | 2.34                     | 0.43              |
| 21:U:6:ARG:HG3   | 21:U:15:ARG:HH11 | 1.81                     | 0.43              |
| 1:A:1223:C:OP2   | 1:A:1224:G:H2'   | 2.19                     | 0.42              |
| 1:A:1305:G:N2    | 1:A:1331:G:HO2'  | 2.15                     | 0.42              |
| 1:A:186:C:H2'    | 1:A:187:C:H6     | 1.84                     | 0.42              |
| 1:A:628:G:O2'    | 1:A:629:G:H5'    | 2.19                     | 0.42              |
| 2:B:22:LYS:C     | 2:B:24:TRP:N     | 2.72                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:74:LYS:O     | 2:B:75:LYS:HB2   | 2.18                     | 0.42              |
| 5:E:51:VAL:O     | 5:E:55:VAL:HG23  | 2.19                     | 0.42              |
| 10:J:6:ILE:HB    | 10:J:71:LEU:O    | 2.19                     | 0.42              |
| 13:M:67:GLU:O    | 13:M:68:GLY:C    | 2.58                     | 0.42              |
| 19:S:51:VAL:HG21 | 19:S:71:LEU:HB3  | 2.00                     | 0.42              |
| 1:A:1225:A:N3    | 1:A:1225:A:H2'   | 2.33                     | 0.42              |
| 1:A:1279:A:O2'   | 1:A:1282:C:N4    | 2.52                     | 0.42              |
| 1:A:1312:G:N7    | 19:S:3:ARG:O     | 2.52                     | 0.42              |
| 1:A:1453:G:H2'   | 1:A:1454:G:O4'   | 2.19                     | 0.42              |
| 1:A:1505:G:H8    | 1:A:1505:G:H3'   | 1.84                     | 0.42              |
| 1:A:490:G:O2'    | 1:A:491:G:H5'    | 2.18                     | 0.42              |
| 2:B:114:ARG:O    | 2:B:117:GLU:HB3  | 2.18                     | 0.42              |
| 3:C:178:LEU:C    | 3:C:180:ALA:H    | 2.21                     | 0.42              |
| 4:D:3:ARG:CZ     | 4:D:5:ILE:HD11   | 2.48                     | 0.42              |
| 5:E:51:VAL:O     | 5:E:54:ALA:HB3   | 2.19                     | 0.42              |
| 7:G:62:PHE:HA    | 7:G:124:LEU:CD1  | 2.49                     | 0.42              |
| 7:G:51:GLN:C     | 7:G:53:LYS:N     | 2.70                     | 0.42              |
| 7:G:9:VAL:HG11   | 7:G:94:ARG:NH1   | 2.34                     | 0.42              |
| 9:I:11:LYS:O     | 9:I:11:LYS:HG2   | 2.19                     | 0.42              |
| 9:I:34:ASN:O     | 9:I:38:GLN:HB2   | 2.19                     | 0.42              |
| 9:I:57:GLY:O     | 9:I:58:ARG:HB2   | 2.20                     | 0.42              |
| 10:J:22:LYS:CD   | 10:J:89:ASP:HA   | 2.50                     | 0.42              |
| 13:M:13:LYS:HD3  | 13:M:17:VAL:HG11 | 2.00                     | 0.42              |
| 1:A:1161:C:O2    | 1:A:1162:C:C5    | 2.72                     | 0.42              |
| 1:A:1495:U:H2'   | 1:A:1496:C:H6    | 1.83                     | 0.42              |
| 1:A:190(J):U:H2' | 1:A:190(K):G:C8  | 2.54                     | 0.42              |
| 1:A:268:C:H2'    | 1:A:269:C:C6     | 2.51                     | 0.42              |
| 1:A:434:U:H2'    | 1:A:435:C:H6     | 1.81                     | 0.42              |
| 1:A:651:C:O2'    | 1:A:652:U:H5'    | 2.19                     | 0.42              |
| 1:A:880:C:O2'    | 1:A:881:G:H5'    | 2.19                     | 0.42              |
| 10:J:29:ARG:O    | 10:J:30:SER:HB3  | 2.19                     | 0.42              |
| 14:N:33:VAL:HA   | 14:N:40:CYS:HA   | 2.01                     | 0.42              |
| 16:P:26:ARG:HD2  | 16:P:31:LYS:O    | 2.19                     | 0.42              |
| 1:A:1251:A:H5'   | 9:I:12:GLU:OE1   | 2.20                     | 0.42              |
| 1:A:1284:C:H3'   | 1:A:1285:A:C8    | 2.53                     | 0.42              |
| 1:A:1376:U:H2'   | 1:A:1377:A:C8    | 2.54                     | 0.42              |
| 1:A:216:G:O2'    | 1:A:217:C:O5'    | 2.38                     | 0.42              |
| 1:A:414:A:H2'    | 1:A:415:A:C8     | 2.54                     | 0.42              |
| 1:A:445:G:O2'    | 1:A:446:G:H5'    | 2.19                     | 0.42              |
| 1:A:624:C:H2'    | 1:A:625:G:H8     | 1.83                     | 0.42              |
| 1:A:663:A:O2'    | 1:A:664:G:H5'    | 2.20                     | 0.42              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:B:47:THR:HA   | 2:B:202:PRO:HG2  | 2.01                     | 0.42              |
| 3:C:14:ILE:CG2  | 3:C:15:THR:N     | 2.66                     | 0.42              |
| 3:C:193:TYR:HE1 | 3:C:196:LEU:HD21 | 1.83                     | 0.42              |
| 6:F:2:ARG:CZ    | 6:F:69:GLU:HG2   | 2.48                     | 0.42              |
| 8:H:49:GLU:HG2  | 8:H:62:TYR:HE2   | 1.84                     | 0.42              |
| 13:M:91:ARG:HB2 | 13:M:98:VAL:HG22 | 2.01                     | 0.42              |
| 16:P:59:TRP:HA  | 16:P:62:VAL:HG22 | 2.02                     | 0.42              |
| 1:A:1047:G:O2'  | 1:A:1048:G:H5'   | 2.19                     | 0.42              |
| 1:A:1442:G:O2'  | 1:A:1443:G:H5'   | 2.20                     | 0.42              |
| 1:A:807:A:H2'   | 1:A:808:C:H6     | 1.85                     | 0.42              |
| 1:A:962:C:H2'   | 1:A:963:G:O4'    | 2.19                     | 0.42              |
| 4:D:17:VAL:CG1  | 4:D:18:LYS:H     | 2.32                     | 0.42              |
| 7:G:31:MET:SD   | 7:G:34:GLY:HA2   | 2.59                     | 0.42              |
| 7:G:38:LEU:HD12 | 7:G:38:LEU:C     | 2.38                     | 0.42              |
| 9:I:17:VAL:HG11 | 9:I:81:ILE:N     | 2.34                     | 0.42              |
| 13:M:23:TYR:HE2 | 13:M:70:LEU:HB3  | 1.84                     | 0.42              |
| 20:T:50:GLU:HB2 | 20:T:99:LEU:CD1  | 2.47                     | 0.42              |
| 1:A:1159:U:C4   | 1:A:1182:G:C5    | 3.08                     | 0.42              |
| 1:A:1300:G:O2'  | 1:A:1301:U:C6    | 2.60                     | 0.42              |
| 1:A:1519:A:C3'  | 1:A:1520:G:H5'   | 2.49                     | 0.42              |
| 1:A:1532:U:H2'  | 1:A:1533:C:H3'   | 2.01                     | 0.42              |
| 1:A:16:A:O2'    | 1:A:17:U:H5'     | 2.19                     | 0.42              |
| 1:A:502:G:H2'   | 1:A:503:C:O4'    | 2.19                     | 0.42              |
| 1:A:622:A:C8    | 1:A:623:C:C6     | 3.08                     | 0.42              |
| 1:A:867:G:C2    | 1:A:868:C:C6     | 3.07                     | 0.42              |
| 2:B:61:LEU:HD13 | 2:B:61:LEU:C     | 2.40                     | 0.42              |
| 7:G:149:ARG:CB  | 7:G:149:ARG:HH21 | 2.32                     | 0.42              |
| 8:H:97:VAL:CG1  | 8:H:98:LYS:N     | 2.81                     | 0.42              |
| 9:I:40:LEU:O    | 9:I:42:ARG:N     | 2.52                     | 0.42              |
| 1:A:1157:A:C8   | 1:A:1181:G:N1    | 2.65                     | 0.42              |
| 1:A:1256:A:C2'  | 1:A:1257:U:OP2   | 2.67                     | 0.42              |
| 1:A:1337:G:H5'' | 1:A:1338:G:OP1   | 2.19                     | 0.42              |
| 1:A:866:C:H2'   | 1:A:867:G:O4'    | 2.19                     | 0.42              |
| 4:D:2:GLY:O     | 4:D:4:TYR:N      | 2.53                     | 0.42              |
| 5:E:91:LEU:CD2  | 5:E:120:THR:HG22 | 2.49                     | 0.42              |
| 5:E:18:ARG:HH12 | 5:E:25:ARG:HD2   | 1.85                     | 0.42              |
| 6:F:83:ASP:C    | 6:F:85:VAL:N     | 2.73                     | 0.42              |
| 1:A:1298:C:N4   | 7:G:114:ARG:HG2  | 2.35                     | 0.42              |
| 8:H:102:ARG:N   | 8:H:102:ARG:NE   | 2.67                     | 0.42              |
| 10:J:9:ARG:HH11 | 10:J:9:ARG:CB    | 2.33                     | 0.42              |
| 14:N:41:ARG:HG3 | 14:N:42:ILE:N    | 2.33                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 14:N:4:LYS:HD3   | 14:N:4:LYS:HA    | 1.82                     | 0.42              |
| 20:T:48:LYS:HB3  | 20:T:51:GLU:HB3  | 2.01                     | 0.42              |
| 20:T:72:LEU:O    | 20:T:73:HIS:C    | 2.58                     | 0.42              |
| 1:A:1120:G:O2'   | 1:A:1121:U:H5'   | 2.19                     | 0.42              |
| 1:A:1260:C:H4'   | 1:A:1283:G:O2'   | 2.19                     | 0.42              |
| 1:A:609:A:C2'    | 1:A:610:G:H5'    | 2.50                     | 0.42              |
| 1:A:767:A:H2'    | 1:A:768:A:C8     | 2.54                     | 0.42              |
| 1:A:925:G:C2     | 1:A:927:G:C8     | 3.08                     | 0.42              |
| 1:A:939:G:H5''   | 7:G:102:ARG:CZ   | 2.50                     | 0.42              |
| 2:B:212:GLN:NE2  | 2:B:216:SER:HB3  | 2.35                     | 0.42              |
| 3:C:54:ARG:HG2   | 3:C:55:VAL:H     | 1.84                     | 0.42              |
| 6:F:33:TYR:HA    | 6:F:71:ARG:NH1   | 2.34                     | 0.42              |
| 7:G:40:ALA:O     | 7:G:41:ARG:C     | 2.58                     | 0.42              |
| 5:E:78:HIS:CD2   | 8:H:107:LEU:HD12 | 2.55                     | 0.42              |
| 9:I:53:VAL:HG12  | 9:I:96:LEU:HD11  | 2.01                     | 0.42              |
| 12:L:27:LEU:C    | 12:L:29:GLY:H    | 2.22                     | 0.42              |
| 17:Q:79:SER:O    | 17:Q:80:GLY:O    | 2.37                     | 0.42              |
| 1:A:1020:U:H2'   | 1:A:1021:G:C8    | 2.55                     | 0.42              |
| 1:A:1077:G:N2    | 1:A:1080:A:OP2   | 2.50                     | 0.42              |
| 1:A:1178:G:C2    | 1:A:1180:A:H8    | 2.38                     | 0.42              |
| 1:A:1286:A:H2'   | 1:A:1287:A:C4'   | 2.45                     | 0.42              |
| 1:A:1333:A:H2'   | 1:A:1334:G:O4'   | 2.20                     | 0.42              |
| 1:A:1355:G:H2'   | 1:A:1356:G:C8    | 2.55                     | 0.42              |
| 1:A:190(E):U:O2' | 17:Q:63:ARG:NH2  | 2.53                     | 0.42              |
| 1:A:960:U:O2     | 1:A:960:U:H5'    | 2.19                     | 0.42              |
| 2:B:16:HIS:O     | 2:B:41:ILE:HG23  | 2.20                     | 0.42              |
| 2:B:50:GLU:O     | 2:B:51:LEU:C     | 2.58                     | 0.42              |
| 3:C:31:HIS:C     | 3:C:33:LEU:H     | 2.23                     | 0.42              |
| 3:C:79:ARG:C     | 3:C:81:GLY:H     | 2.23                     | 0.42              |
| 3:C:79:ARG:NE    | 3:C:82:GLU:HG2   | 2.35                     | 0.42              |
| 4:D:8:VAL:HB     | 4:D:21:LEU:HD12  | 2.00                     | 0.42              |
| 6:F:22:GLU:O     | 6:F:26:ILE:HG13  | 2.19                     | 0.42              |
| 13:M:3:ARG:NH1   | 13:M:7:VAL:HG12  | 2.35                     | 0.42              |
| 13:M:93:ARG:HB3  | 13:M:94:ARG:HD2  | 2.01                     | 0.42              |
| 20:T:56:MET:CE   | 20:T:88:VAL:HG11 | 2.48                     | 0.42              |
| 1:A:1054:C:H42   | 23:Y:34:TM2:C6   | 2.32                     | 0.42              |
| 23:Y:34:TM2:H4'  | 23:Y:35:A:OP1    | 2.20                     | 0.42              |
| 1:A:1518:A:H2'   | 1:A:1519:A:C8    | 2.54                     | 0.42              |
| 1:A:242:C:H2'    | 1:A:243:A:H5'    | 2.02                     | 0.42              |
| 1:A:613:C:O2'    | 1:A:614:A:H5'    | 2.20                     | 0.42              |
| 1:A:749:C:H2'    | 1:A:750:G:H8     | 1.84                     | 0.42              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:930:C:H2'   | 1:A:931:C:H5'    | 2.02                     | 0.42              |
| 2:B:71:VAL:O    | 2:B:165:VAL:HG23 | 2.19                     | 0.42              |
| 3:C:167:TRP:HB3 | 3:C:168:ALA:H    | 1.44                     | 0.42              |
| 3:C:189:ALA:O   | 3:C:191:THR:HG23 | 2.20                     | 0.42              |
| 3:C:39:ILE:O    | 3:C:43:LEU:HB2   | 2.20                     | 0.42              |
| 3:C:86:VAL:O    | 3:C:89:GLU:HB3   | 2.20                     | 0.42              |
| 4:D:121:VAL:O   | 4:D:134:ASP:HA   | 2.20                     | 0.42              |
| 9:I:27:THR:HG22 | 9:I:28:VAL:N     | 2.34                     | 0.42              |
| 14:N:36:PHE:O   | 14:N:36:PHE:CD1  | 2.72                     | 0.42              |
| 16:P:82:GLN:O   | 16:P:84:ALA:N    | 2.53                     | 0.42              |
| 16:P:82:GLN:O   | 16:P:83:GLU:C    | 2.59                     | 0.42              |
| 17:Q:82:MET:O   | 17:Q:86:GLU:HG2  | 2.20                     | 0.42              |
| 20:T:89:ARG:O   | 20:T:93:GLU:HG3  | 2.20                     | 0.42              |
| 1:A:1094:G:O5'  | 1:A:1095:U:H5    | 2.02                     | 0.41              |
| 1:A:1253:G:H2'  | 1:A:1254:C:H6    | 1.85                     | 0.41              |
| 1:A:432:A:C3'   | 1:A:433:C:H5''   | 2.39                     | 0.41              |
| 1:A:444:C:H2'   | 1:A:444:C:O2     | 2.19                     | 0.41              |
| 1:A:573:A:C2    | 1:A:574:A:C2     | 3.08                     | 0.41              |
| 1:A:930:C:O2'   | 1:A:931:C:H5'    | 2.19                     | 0.41              |
| 2:B:19:HIS:O    | 2:B:39:ILE:HG23  | 2.19                     | 0.41              |
| 6:F:34:GLY:N    | 6:F:71:ARG:NH2   | 2.68                     | 0.41              |
| 7:G:149:ARG:CB  | 7:G:149:ARG:NH2  | 2.80                     | 0.41              |
| 9:I:14:VAL:HG23 | 9:I:66:ARG:O     | 2.20                     | 0.41              |
| 10:J:89:ASP:CB  | 10:J:91:PRO:HD2  | 2.49                     | 0.41              |
| 11:K:115:PRO:C  | 11:K:117:ASN:H   | 2.23                     | 0.41              |
| 11:K:51:LYS:O   | 11:K:55:LYS:HE2  | 2.19                     | 0.41              |
| 13:M:62:ASN:N   | 13:M:62:ASN:HD22 | 2.17                     | 0.41              |
| 16:P:59:TRP:HA  | 16:P:62:VAL:CG2  | 2.50                     | 0.41              |
| 17:Q:17:LYS:N   | 17:Q:49:GLU:OE2  | 2.33                     | 0.41              |
| 6:F:50:TYR:CE1  | 18:R:77:GLY:HA2  | 2.54                     | 0.41              |
| 19:S:35:SER:C   | 19:S:37:ARG:H    | 2.23                     | 0.41              |
| 1:A:1041:A:H2'  | 1:A:1042:G:H8    | 1.85                     | 0.41              |
| 1:A:1053:G:C3'  | 1:A:1054:C:C5'   | 2.96                     | 0.41              |
| 1:A:16:A:C2'    | 1:A:17:U:H5'     | 2.49                     | 0.41              |
| 1:A:41:G:H2'    | 1:A:42:G:H8      | 1.85                     | 0.41              |
| 1:A:448:A:C4    | 1:A:487:A:C2     | 3.08                     | 0.41              |
| 1:A:463:A:H4'   | 16:P:80:PHE:O    | 2.20                     | 0.41              |
| 1:A:538:G:H2'   | 1:A:539:A:H8     | 1.84                     | 0.41              |
| 1:A:582:U:OP1   | 15:O:64:ARG:NH2  | 2.45                     | 0.41              |
| 1:A:959:A:H2'   | 1:A:960:U:O4'    | 2.20                     | 0.41              |
| 2:B:122:PHE:CE2 | 2:B:139:LYS:HG2  | 2.55                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:D:151:LYS:H    | 4:D:151:LYS:HD2   | 1.85                     | 0.41              |
| 5:E:31:LEU:HD23  | 5:E:31:LEU:HA     | 1.88                     | 0.41              |
| 5:E:40:ARG:HH11  | 5:E:40:ARG:HG2    | 1.85                     | 0.41              |
| 6:F:69:GLU:C     | 6:F:71:ARG:H      | 2.23                     | 0.41              |
| 1:A:933:G:OP2    | 7:G:3:ARG:HB3     | 2.19                     | 0.41              |
| 10:J:9:ARG:NH1   | 10:J:9:ARG:CB     | 2.82                     | 0.41              |
| 12:L:34:ARG:HG3  | 12:L:105:TYR:CE1  | 2.55                     | 0.41              |
| 17:Q:58:GLU:O    | 17:Q:59:ILE:HD13  | 2.20                     | 0.41              |
| 18:R:36:ASN:O    | 18:R:39:VAL:HG12  | 2.21                     | 0.41              |
| 1:A:1051:C:O2'   | 1:A:1052:U:H5'    | 2.19                     | 0.41              |
| 1:A:256:U:O2'    | 1:A:257:G:H5'     | 2.20                     | 0.41              |
| 1:A:948:C:O2'    | 1:A:949:A:H5'     | 2.20                     | 0.41              |
| 3:C:134:ILE:O    | 3:C:138:VAL:HG23  | 2.20                     | 0.41              |
| 9:I:97:LYS:HB3   | 9:I:98:PRO:CD     | 2.41                     | 0.41              |
| 10:J:39:PRO:HA   | 10:J:70:ARG:NH1   | 2.35                     | 0.41              |
| 10:J:89:ASP:OD2  | 10:J:91:PRO:HD2   | 2.20                     | 0.41              |
| 1:A:881:G:P      | 12:L:12:ARG:HH22  | 2.43                     | 0.41              |
| 14:N:41:ARG:HH11 | 14:N:41:ARG:HG2   | 1.85                     | 0.41              |
| 15:O:36:ILE:HA   | 15:O:59:MET:CE    | 2.51                     | 0.41              |
| 17:Q:59:ILE:HG23 | 17:Q:71:PHE:HB3   | 2.02                     | 0.41              |
| 1:A:191:G:N2     | 20:T:103:GLY:O    | 2.44                     | 0.41              |
| 1:A:1157:A:C5    | 1:A:1180:A:C6     | 3.09                     | 0.41              |
| 1:A:1157:A:H2    | 1:A:1181:G:C1'    | 2.33                     | 0.41              |
| 1:A:1193:G:C2'   | 1:A:1194:U:H5'    | 2.50                     | 0.41              |
| 1:A:730:G:H21    | 1:A:765:G:H5''    | 1.86                     | 0.41              |
| 1:A:780:A:C2     | 1:A:801:U:C5      | 3.09                     | 0.41              |
| 3:C:28:GLN:O     | 3:C:31:HIS:HB2    | 2.21                     | 0.41              |
| 5:E:99:GLY:O     | 5:E:117:ASP:HA    | 2.20                     | 0.41              |
| 7:G:23:VAL:HG13  | 7:G:43:PHE:CE2    | 2.55                     | 0.41              |
| 7:G:51:GLN:HA    | 7:G:54:THR:O      | 2.21                     | 0.41              |
| 11:K:82:VAL:HG23 | 11:K:105:VAL:HG13 | 2.02                     | 0.41              |
| 12:L:27:LEU:O    | 12:L:28:LYS:C     | 2.59                     | 0.41              |
| 17:Q:33:GLY:O    | 17:Q:34:LYS:C     | 2.59                     | 0.41              |
| 1:A:960:U:H1'    | 1:A:1223:C:H5'    | 2.03                     | 0.41              |
| 1:A:1499:A:H1'   | 1:A:1520:G:C5'    | 2.51                     | 0.41              |
| 1:A:602:A:O2'    | 1:A:603:U:H5'     | 2.20                     | 0.41              |
| 2:B:159:PRO:HG2  | 2:B:182:ILE:HD13  | 2.02                     | 0.41              |
| 2:B:90:MET:HE3   | 2:B:222:ILE:HD13  | 2.02                     | 0.41              |
| 2:B:97:TRP:CZ3   | 2:B:176:GLU:OE2   | 2.73                     | 0.41              |
| 2:B:97:TRP:HZ3   | 2:B:99:GLY:HA2    | 1.86                     | 0.41              |
| 7:G:116:ALA:O    | 7:G:120:ILE:HD12  | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:H:126:LYS:C    | 8:H:128:GLY:H    | 2.24                     | 0.41              |
| 9:I:17:VAL:HG11  | 9:I:81:ILE:HG12  | 2.02                     | 0.41              |
| 10:J:23:ILE:O    | 10:J:23:ILE:CG2  | 2.64                     | 0.41              |
| 13:M:44:ARG:HH11 | 13:M:44:ARG:HG2  | 1.86                     | 0.41              |
| 18:R:55:ARG:HB3  | 18:R:55:ARG:NH1  | 2.35                     | 0.41              |
| 1:A:1353:G:H2'   | 1:A:1354:C:H6    | 1.85                     | 0.41              |
| 1:A:415:A:H2'    | 1:A:416:G:H8     | 1.86                     | 0.41              |
| 1:A:52:G:O2'     | 1:A:53:A:H5'     | 2.20                     | 0.41              |
| 4:D:199:ASN:C    | 4:D:199:ASN:HD22 | 2.23                     | 0.41              |
| 8:H:100:ILE:HB   | 8:H:125:ARG:HH12 | 1.86                     | 0.41              |
| 9:I:9:ARG:HD3    | 9:I:14:VAL:CG1   | 2.51                     | 0.41              |
| 10:J:82:ILE:O    | 10:J:82:ILE:HG22 | 2.20                     | 0.41              |
| 11:K:12:ARG:O    | 11:K:13:GLN:HB2  | 2.20                     | 0.41              |
| 13:M:102:ARG:HG3 | 13:M:102:ARG:O   | 2.19                     | 0.41              |
| 13:M:108:ARG:O   | 13:M:112:GLY:N   | 2.48                     | 0.41              |
| 13:M:22:ILE:HG21 | 13:M:25:ILE:HD12 | 2.03                     | 0.41              |
| 15:O:3:ILE:HG13  | 15:O:38:ARG:HD2  | 2.02                     | 0.41              |
| 19:S:20:LEU:HA   | 19:S:23:ASN:ND2  | 2.34                     | 0.41              |
| 19:S:44:MET:O    | 19:S:47:HIS:HB2  | 2.21                     | 0.41              |
| 1:A:109:A:C6     | 1:A:326:G:C6     | 3.09                     | 0.41              |
| 1:A:1172:C:O2'   | 1:A:1173:G:H5'   | 2.20                     | 0.41              |
| 1:A:1157:A:C6    | 1:A:1180:A:N7    | 2.89                     | 0.41              |
| 1:A:1305:G:O2'   | 1:A:1331:G:N2    | 2.54                     | 0.41              |
| 1:A:46:G:O2'     | 1:A:365:U:H1'    | 2.20                     | 0.41              |
| 1:A:743:U:H2'    | 1:A:744:C:C6     | 2.56                     | 0.41              |
| 1:A:993:G:O2'    | 1:A:994:A:P      | 2.78                     | 0.41              |
| 2:B:235:SER:C    | 2:B:237:ALA:N    | 2.73                     | 0.41              |
| 2:B:8:LYS:O      | 2:B:9:GLU:CB     | 2.67                     | 0.41              |
| 3:C:188:LEU:O    | 3:C:189:ALA:CB   | 2.67                     | 0.41              |
| 9:I:16:ARG:HD2   | 9:I:64:THR:CB    | 2.51                     | 0.41              |
| 1:A:718:G:H5'    | 11:K:117:ASN:ND2 | 2.35                     | 0.41              |
| 13:M:8:GLU:OE1   | 13:M:22:ILE:HA   | 2.21                     | 0.41              |
| 13:M:80:ARG:HB3  | 13:M:80:ARG:NH1  | 2.36                     | 0.41              |
| 14:N:30:ALA:O    | 14:N:33:VAL:HG22 | 2.21                     | 0.41              |
| 14:N:4:LYS:HA    | 14:N:7:ILE:HG12  | 2.02                     | 0.41              |
| 1:A:248:C:O2'    | 1:A:249:U:H5'    | 2.21                     | 0.41              |
| 1:A:877:C:O2'    | 1:A:878:G:H5'    | 2.20                     | 0.41              |
| 1:A:940:C:H2'    | 1:A:941:G:C8     | 2.56                     | 0.41              |
| 2:B:104:ASN:OD1  | 2:B:107:THR:HB   | 2.21                     | 0.41              |
| 3:C:108:ASN:HD22 | 3:C:111:LEU:HG   | 1.86                     | 0.41              |
| 3:C:52:LEU:N     | 3:C:52:LEU:HD23  | 2.34                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:91:LEU:C     | 3:C:91:LEU:HD23  | 2.40                     | 0.41              |
| 6:F:23:LYS:NZ    | 6:F:42:GLU:OE2   | 2.53                     | 0.41              |
| 7:G:149:ARG:CA   | 7:G:149:ARG:HH21 | 2.33                     | 0.41              |
| 9:I:9:ARG:HA     | 9:I:13:ALA:O     | 2.20                     | 0.41              |
| 1:A:1147:C:O2    | 9:I:16:ARG:NH2   | 2.54                     | 0.41              |
| 17:Q:68:ARG:O    | 17:Q:68:ARG:HG3  | 2.21                     | 0.41              |
| 2:B:111:ARG:HB3  | 2:B:149:LEU:CD1  | 2.44                     | 0.41              |
| 2:B:112:VAL:C    | 2:B:114:ARG:N    | 2.74                     | 0.41              |
| 2:B:228:GLY:O    | 2:B:229:VAL:C    | 2.58                     | 0.41              |
| 3:C:116:VAL:HG21 | 3:C:202:ILE:HD11 | 2.03                     | 0.41              |
| 3:C:34:LEU:HD21  | 3:C:38:ARG:CZ    | 2.51                     | 0.41              |
| 4:D:112:VAL:HG12 | 4:D:116:GLN:NE2  | 2.36                     | 0.41              |
| 1:A:620:C:C1'    | 4:D:135:LEU:HD13 | 2.51                     | 0.41              |
| 5:E:24:ARG:HG2   | 5:E:24:ARG:NH1   | 2.34                     | 0.41              |
| 6:F:4:TYR:CE1    | 6:F:92:LYS:HG2   | 2.56                     | 0.41              |
| 9:I:42:ARG:O     | 9:I:44:VAL:N     | 2.53                     | 0.41              |
| 9:I:50:LEU:O     | 9:I:53:VAL:HG22  | 2.21                     | 0.41              |
| 10:J:22:LYS:O    | 10:J:26:ALA:HB3  | 2.21                     | 0.41              |
| 10:J:72:VAL:HG12 | 10:J:73:ASP:N    | 2.35                     | 0.41              |
| 17:Q:69:LYS:H    | 17:Q:70:ARG:HH11 | 1.69                     | 0.41              |
| 18:R:37:VAL:CG2  | 18:R:78:LEU:HB3  | 2.51                     | 0.41              |
| 21:U:6:ARG:CD    | 21:U:15:ARG:HH12 | 2.33                     | 0.41              |
| 1:A:1332:A:C2    | 1:A:1333:A:C4    | 3.08                     | 0.41              |
| 1:A:298:A:H2'    | 1:A:299:G:O4'    | 2.21                     | 0.41              |
| 1:A:328:C:H1'    | 1:A:329:A:OP2    | 2.21                     | 0.41              |
| 2:B:134:GLU:HG2  | 2:B:137:ARG:HH21 | 1.85                     | 0.41              |
| 2:B:236:TYR:O    | 2:B:236:TYR:CD2  | 2.74                     | 0.41              |
| 2:B:69:LEU:HD22  | 2:B:71:VAL:CG2   | 2.51                     | 0.41              |
| 4:D:36:ARG:HG3   | 4:D:38:TYR:CE2   | 2.56                     | 0.41              |
| 4:D:42:GLN:O     | 4:D:42:GLN:CG    | 2.69                     | 0.41              |
| 5:E:43:LEU:HD22  | 5:E:44:GLY:N     | 2.36                     | 0.41              |
| 5:E:57:LYS:HG2   | 5:E:61:TYR:HE2   | 1.83                     | 0.41              |
| 6:F:69:GLU:OE1   | 6:F:69:GLU:N     | 2.54                     | 0.41              |
| 8:H:39:LEU:HD12  | 8:H:39:LEU:HA    | 1.80                     | 0.41              |
| 9:I:4:TYR:O      | 9:I:18:PHE:HA    | 2.20                     | 0.41              |
| 10:J:6:ILE:O     | 10:J:71:LEU:O    | 2.39                     | 0.41              |
| 12:L:69:TYR:HB2  | 12:L:90:VAL:HG21 | 2.03                     | 0.41              |
| 14:N:25:VAL:HG13 | 14:N:39:LEU:HD23 | 2.02                     | 0.41              |
| 18:R:68:LYS:O    | 18:R:72:ARG:HG3  | 2.20                     | 0.41              |
| 20:T:45:GLN:NE2  | 20:T:45:GLN:O    | 2.54                     | 0.41              |
| 1:A:1043:C:O2'   | 1:A:1044:A:H5'   | 2.22                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1152:A:H2'   | 1:A:1153:C:H6     | 1.86                     | 0.41              |
| 1:A:1192:C:C2'   | 1:A:1193:G:O5'    | 2.69                     | 0.41              |
| 1:A:335:C:H2'    | 1:A:336:C:C6      | 2.56                     | 0.41              |
| 1:A:408:A:O2'    | 1:A:409:G:H5'     | 2.20                     | 0.41              |
| 2:B:118:LEU:HD11 | 2:B:141:GLU:OE2   | 2.21                     | 0.41              |
| 3:C:100:ALA:O    | 3:C:101:LEU:HB2   | 2.21                     | 0.41              |
| 5:E:78:HIS:HD2   | 8:H:107:LEU:HD12  | 1.86                     | 0.41              |
| 9:I:37:PHE:CD1   | 9:I:43:ALA:HB1    | 2.56                     | 0.41              |
| 9:I:81:ILE:HG22  | 9:I:81:ILE:O      | 2.21                     | 0.41              |
| 1:A:1061:G:H1'   | 10:J:56:HIS:CE1   | 2.56                     | 0.41              |
| 13:M:45:VAL:HA   | 13:M:48:LEU:HG    | 2.02                     | 0.41              |
| 13:M:91:ARG:HB3  | 13:M:98:VAL:HG22  | 2.03                     | 0.41              |
| 16:P:43:LYS:HG3  | 16:P:48:TRP:CD2   | 2.57                     | 0.41              |
| 19:S:10:PHE:O    | 19:S:11:VAL:HG23  | 2.21                     | 0.41              |
| 20:T:53:LEU:HB2  | 20:T:100:ILE:HG22 | 2.02                     | 0.41              |
| 1:A:1377:A:C6    | 7:G:5:ARG:NH2     | 2.89                     | 0.40              |
| 1:A:1498:U:H4'   | 1:A:1519:A:H2     | 1.82                     | 0.40              |
| 1:A:1513:A:H2'   | 1:A:1514:C:C6     | 2.56                     | 0.40              |
| 1:A:693:G:O2'    | 1:A:694:A:H5'     | 2.21                     | 0.40              |
| 1:A:84:U:H2'     | 1:A:88:A:O4'      | 2.21                     | 0.40              |
| 1:A:884:U:H4'    | 1:A:885:G:H5''    | 2.03                     | 0.40              |
| 3:C:36:ASP:OD2   | 3:C:36:ASP:N      | 2.54                     | 0.40              |
| 5:E:80:ILE:HD13  | 5:E:91:LEU:HD12   | 2.02                     | 0.40              |
| 8:H:123:GLU:O    | 8:H:127:LEU:HG    | 2.21                     | 0.40              |
| 9:I:128:ARG:HA   | 13:M:126:LYS:CD   | 2.51                     | 0.40              |
| 14:N:24:CYS:SG   | 14:N:43:CYS:SG    | 3.17                     | 0.40              |
| 1:A:761:G:H1'    | 17:Q:105:ALA:HB2  | 2.03                     | 0.40              |
| 1:A:1033:G:O2'   | 1:A:1034:G:H5'    | 2.21                     | 0.40              |
| 1:A:1047:G:C2'   | 1:A:1048:G:H5'    | 2.50                     | 0.40              |
| 1:A:1056:U:O2    | 1:A:1056:U:H2'    | 2.20                     | 0.40              |
| 1:A:1065:U:H5''  | 1:A:1190:G:H22    | 1.77                     | 0.40              |
| 1:A:1192:C:H3'   | 1:A:1193:G:P      | 2.23                     | 0.40              |
| 1:A:1206:G:C6    | 1:A:1207:G:C5     | 3.09                     | 0.40              |
| 1:A:1217:C:H2'   | 1:A:1218:C:O4'    | 2.21                     | 0.40              |
| 1:A:1367:C:N3    | 1:A:1368:G:C8     | 2.89                     | 0.40              |
| 1:A:344:A:H5''   | 1:A:345:C:H5      | 1.87                     | 0.40              |
| 1:A:420:U:H2'    | 1:A:422:C:C5      | 2.56                     | 0.40              |
| 1:A:502:G:C2     | 1:A:503:C:C2      | 3.09                     | 0.40              |
| 1:A:515:G:C5     | 1:A:516:U:C5      | 3.09                     | 0.40              |
| 1:A:645:C:H2'    | 1:A:646:U:C6      | 2.56                     | 0.40              |
| 1:A:671:G:H2'    | 1:A:672:U:O4'     | 2.21                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:58:GLU:O     | 3:C:64:VAL:HA    | 2.21                     | 0.40              |
| 4:D:100:ARG:HH12 | 4:D:137:SER:HB3  | 1.86                     | 0.40              |
| 4:D:111:ALA:HA   | 4:D:161:ASN:ND2  | 2.36                     | 0.40              |
| 8:H:11:THR:O     | 8:H:12:ARG:C     | 2.59                     | 0.40              |
| 9:I:79:LEU:O     | 9:I:83:ARG:N     | 2.48                     | 0.40              |
| 11:K:101:SER:C   | 11:K:103:LEU:H   | 2.23                     | 0.40              |
| 14:N:6:LEU:C     | 14:N:8:GLU:N     | 2.73                     | 0.40              |
| 1:A:1024:G:C2'   | 1:A:1025:U:H5''  | 2.51                     | 0.40              |
| 1:A:1070:U:O2'   | 1:A:1071:C:H5'   | 2.21                     | 0.40              |
| 1:A:193:C:H2'    | 1:A:194:C:H6     | 1.86                     | 0.40              |
| 1:A:232:G:H1'    | 1:A:262:A:N1     | 2.37                     | 0.40              |
| 1:A:259:G:O2'    | 1:A:260:G:H5'    | 2.21                     | 0.40              |
| 1:A:357:G:H1'    | 1:A:368:U:O2     | 2.22                     | 0.40              |
| 2:B:25:ASN:HD22  | 2:B:27:LYS:N     | 2.08                     | 0.40              |
| 2:B:58:ILE:HG23  | 2:B:68:ILE:CD1   | 2.51                     | 0.40              |
| 2:B:73:THR:O     | 2:B:73:THR:HG22  | 2.21                     | 0.40              |
| 1:A:1056:U:H5'   | 3:C:163:ALA:CB   | 2.51                     | 0.40              |
| 1:A:1279:A:H61   | 3:C:26:LYS:HZ3   | 1.70                     | 0.40              |
| 3:C:36:ASP:OD2   | 3:C:59:ARG:NH2   | 2.55                     | 0.40              |
| 3:C:95:THR:C     | 3:C:97:LYS:N     | 2.74                     | 0.40              |
| 5:E:41:VAL:HG21  | 5:E:113:ALA:HB2  | 2.03                     | 0.40              |
| 1:A:1124:G:O5'   | 10:J:35:SER:O    | 2.39                     | 0.40              |
| 10:J:9:ARG:HB3   | 10:J:9:ARG:CZ    | 2.51                     | 0.40              |
| 13:M:94:ARG:O    | 13:M:95:GLY:C    | 2.60                     | 0.40              |
| 14:N:10:ALA:O    | 14:N:11:LYS:HE3  | 2.20                     | 0.40              |
| 14:N:25:VAL:HG12 | 14:N:38:GLY:C    | 2.41                     | 0.40              |
| 15:O:70:LEU:O    | 15:O:72:ARG:N    | 2.54                     | 0.40              |
| 16:P:43:LYS:HD2  | 16:P:43:LYS:N    | 2.36                     | 0.40              |
| 19:S:19:VAL:CG1  | 19:S:20:LEU:N    | 2.84                     | 0.40              |
| 20:T:57:ARG:HE   | 20:T:102:GLY:CA  | 2.34                     | 0.40              |
| 20:T:79:ARG:O    | 20:T:83:ARG:HG3  | 2.22                     | 0.40              |
| 1:A:190(L):U:H3  | 20:T:105:SER:HG  | 1.70                     | 0.40              |
| 1:A:579:G:H5'    | 1:A:728:A:C1'    | 2.43                     | 0.40              |
| 1:A:750:G:N3     | 15:O:23:GLY:HA3  | 2.37                     | 0.40              |
| 3:C:64:VAL:HG12  | 3:C:66:VAL:CG2   | 2.50                     | 0.40              |
| 4:D:8:VAL:HG11   | 4:D:115:ARG:CZ   | 2.51                     | 0.40              |
| 4:D:146:ILE:N    | 4:D:146:ILE:CD1  | 2.82                     | 0.40              |
| 1:A:587:G:OP1    | 8:H:89:PRO:HB3   | 2.21                     | 0.40              |
| 17:Q:70:ARG:N    | 17:Q:70:ARG:HD2  | 2.37                     | 0.40              |
| 20:T:57:ARG:NE   | 20:T:102:GLY:HA3 | 2.37                     | 0.40              |
| 1:A:949:A:C2     | 1:A:1233:G:N3    | 2.90                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1245:A:H2'   | 1:A:1246:C:C6    | 2.57                     | 0.40              |
| 1:A:262:A:C6     | 1:A:263:A:C6     | 3.09                     | 0.40              |
| 1:A:65:U:C5      | 1:A:381:C:C4     | 3.10                     | 0.40              |
| 1:A:792:A:H1'    | 1:A:794:A:N7     | 2.37                     | 0.40              |
| 1:A:662:G:O2'    | 1:A:836:G:H5'    | 2.21                     | 0.40              |
| 1:A:922:G:C6     | 1:A:923:A:C6     | 3.10                     | 0.40              |
| 2:B:112:VAL:C    | 2:B:114:ARG:H    | 2.23                     | 0.40              |
| 2:B:83:MET:C     | 2:B:86:GLU:H     | 2.23                     | 0.40              |
| 3:C:157:ILE:CD1  | 3:C:166:GLU:HB2  | 2.51                     | 0.40              |
| 3:C:147:LYS:HE3  | 3:C:203:PHE:CE2  | 2.57                     | 0.40              |
| 3:C:39:ILE:HG22  | 3:C:40:ARG:N     | 2.36                     | 0.40              |
| 3:C:47:LEU:HD23  | 3:C:68:VAL:HG11  | 2.03                     | 0.40              |
| 4:D:174:LEU:O    | 4:D:186:LEU:HD11 | 2.22                     | 0.40              |
| 5:E:43:LEU:HD23  | 5:E:43:LEU:HA    | 1.84                     | 0.40              |
| 5:E:76:ILE:CG2   | 5:E:78:HIS:H     | 2.35                     | 0.40              |
| 7:G:115:ARG:HG3  | 7:G:118:VAL:HG23 | 2.02                     | 0.40              |
| 9:I:107:ARG:CB   | 9:I:107:ARG:NH1  | 2.84                     | 0.40              |
| 10:J:14:LYS:HB3  | 10:J:14:LYS:HE2  | 1.91                     | 0.40              |
| 10:J:46:ARG:CG   | 10:J:46:ARG:NH1  | 2.78                     | 0.40              |
| 11:K:84:VAL:HG21 | 11:K:95:ILE:HD11 | 2.04                     | 0.40              |
| 1:A:254:G:OP1    | 17:Q:68:ARG:HB3  | 2.21                     | 0.40              |
| 20:T:63:ILE:HG22 | 20:T:77:ALA:HB1  | 2.03                     | 0.40              |

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

| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 10:J:79:ARG:NH1 | 10:J:79:ARG:NH1[8_665] | 2.06                     | 0.14              |

## 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     | 234/256 (91%)   | 162 (69%)  | 49 (21%)  | 23 (10%) | 1           | 0   |
| 3   | C     | 205/239 (86%)   | 139 (68%)  | 39 (19%)  | 27 (13%) | 0           | 0   |
| 4   | D     | 206/209 (99%)   | 169 (82%)  | 29 (14%)  | 8 (4%)   | 3           | 4   |
| 5   | E     | 149/162 (92%)   | 135 (91%)  | 14 (9%)   | 0        | 100         | 100 |
| 6   | F     | 99/101 (98%)    | 84 (85%)   | 12 (12%)  | 3 (3%)   | 5           | 7   |
| 7   | G     | 153/156 (98%)   | 129 (84%)  | 14 (9%)   | 10 (6%)  | 1           | 1   |
| 8   | H     | 136/138 (99%)   | 121 (89%)  | 14 (10%)  | 1 (1%)   | 24          | 42  |
| 9   | I     | 125/128 (98%)   | 92 (74%)   | 23 (18%)  | 10 (8%)  | 1           | 1   |
| 10  | J     | 97/105 (92%)    | 60 (62%)   | 21 (22%)  | 16 (16%) | 0           | 0   |
| 11  | K     | 117/129 (91%)   | 100 (86%)  | 15 (13%)  | 2 (2%)   | 10          | 17  |
| 12  | L     | 123/135 (91%)   | 89 (72%)   | 26 (21%)  | 8 (6%)   | 1           | 1   |
| 13  | M     | 123/126 (98%)   | 94 (76%)   | 18 (15%)  | 11 (9%)  | 1           | 1   |
| 14  | N     | 58/61 (95%)     | 49 (84%)   | 7 (12%)   | 2 (3%)   | 4           | 5   |
| 15  | O     | 86/89 (97%)     | 71 (83%)   | 11 (13%)  | 4 (5%)   | 2           | 3   |
| 16  | P     | 82/88 (93%)     | 74 (90%)   | 6 (7%)    | 2 (2%)   | 6           | 10  |
| 17  | Q     | 102/105 (97%)   | 88 (86%)   | 10 (10%)  | 4 (4%)   | 3           | 4   |
| 18  | R     | 71/88 (81%)     | 55 (78%)   | 10 (14%)  | 6 (8%)   | 1           | 1   |
| 19  | S     | 79/93 (85%)     | 58 (73%)   | 14 (18%)  | 7 (9%)   | 1           | 1   |
| 20  | T     | 97/106 (92%)    | 81 (84%)   | 10 (10%)  | 6 (6%)   | 1           | 1   |
| 21  | U     | 23/27 (85%)     | 17 (74%)   | 6 (26%)   | 0        | 100         | 100 |
| All | All   | 2365/2541 (93%) | 1867 (79%) | 348 (15%) | 150 (6%) | 1           | 1   |

All (150) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 88  | ALA  |
| 2   | B     | 123 | ALA  |
| 2   | B     | 129 | GLU  |
| 2   | B     | 229 | VAL  |
| 3   | C     | 15  | THR  |
| 3   | C     | 26  | LYS  |
| 3   | C     | 61  | ALA  |
| 3   | C     | 65  | ALA  |
| 3   | C     | 154 | SER  |
| 3   | C     | 189 | ALA  |
| 3   | C     | 207 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 3   | ARG  |
| 4   | D     | 36  | ARG  |
| 7   | G     | 155 | ARG  |
| 8   | H     | 105 | ARG  |
| 9   | I     | 7   | THR  |
| 9   | I     | 38  | GLN  |
| 9   | I     | 43  | ALA  |
| 9   | I     | 55  | ALA  |
| 9   | I     | 58  | ARG  |
| 9   | I     | 88  | TYR  |
| 10  | J     | 30  | SER  |
| 10  | J     | 39  | PRO  |
| 10  | J     | 72  | VAL  |
| 10  | J     | 85  | LEU  |
| 12  | L     | 27  | LEU  |
| 12  | L     | 28  | LYS  |
| 12  | L     | 30  | ALA  |
| 12  | L     | 47  | LYS  |
| 12  | L     | 126 | LYS  |
| 12  | L     | 127 | GLU  |
| 13  | M     | 5   | ALA  |
| 13  | M     | 12  | ASN  |
| 13  | M     | 45  | VAL  |
| 13  | M     | 63  | THR  |
| 13  | M     | 67  | GLU  |
| 14  | N     | 10  | ALA  |
| 16  | P     | 83  | GLU  |
| 17  | Q     | 80  | GLY  |
| 17  | Q     | 81  | ARG  |
| 18  | R     | 20  | ALA  |
| 19  | S     | 6   | LYS  |
| 19  | S     | 81  | ARG  |
| 20  | T     | 73  | HIS  |
| 20  | T     | 94  | ALA  |
| 20  | T     | 99  | LEU  |
| 2   | B     | 7   | VAL  |
| 2   | B     | 8   | LYS  |
| 2   | B     | 9   | GLU  |
| 2   | B     | 74  | LYS  |
| 2   | B     | 80  | ILE  |
| 2   | B     | 89  | GLY  |
| 2   | B     | 240 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 16  | ARG  |
| 3   | C     | 96  | GLY  |
| 3   | C     | 100 | ALA  |
| 3   | C     | 156 | ARG  |
| 6   | F     | 16  | GLN  |
| 7   | G     | 78  | ARG  |
| 7   | G     | 81  | GLY  |
| 9   | I     | 31  | GLN  |
| 10  | J     | 32  | ALA  |
| 10  | J     | 34  | VAL  |
| 11  | K     | 12  | ARG  |
| 13  | M     | 7   | VAL  |
| 13  | M     | 14  | ARG  |
| 13  | M     | 23  | TYR  |
| 13  | M     | 95  | GLY  |
| 15  | O     | 88  | ARG  |
| 16  | P     | 10  | GLY  |
| 17  | Q     | 100 | LYS  |
| 18  | R     | 87  | ARG  |
| 19  | S     | 9   | VAL  |
| 20  | T     | 95  | ALA  |
| 20  | T     | 100 | ILE  |
| 20  | T     | 102 | GLY  |
| 2   | B     | 44  | LEU  |
| 2   | B     | 131 | PRO  |
| 3   | C     | 12  | LEU  |
| 3   | C     | 29  | TYR  |
| 3   | C     | 81  | GLY  |
| 3   | C     | 98  | ASN  |
| 3   | C     | 146 | ALA  |
| 3   | C     | 168 | ALA  |
| 4   | D     | 29  | PRO  |
| 4   | D     | 35  | ARG  |
| 4   | D     | 39  | PRO  |
| 7   | G     | 7   | ALA  |
| 7   | G     | 53  | LYS  |
| 7   | G     | 83  | ALA  |
| 9   | I     | 56  | LEU  |
| 10  | J     | 40  | LEU  |
| 10  | J     | 60  | ARG  |
| 14  | N     | 15  | LYS  |
| 15  | O     | 71  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19  | S     | 8   | GLY  |
| 19  | S     | 30  | LEU  |
| 19  | S     | 43  | GLU  |
| 2   | B     | 23  | ARG  |
| 2   | B     | 60  | ASP  |
| 2   | B     | 63  | MET  |
| 2   | B     | 190 | THR  |
| 3   | C     | 4   | LYS  |
| 3   | C     | 47  | LEU  |
| 3   | C     | 66  | VAL  |
| 3   | C     | 79  | ARG  |
| 3   | C     | 108 | ASN  |
| 9   | I     | 54  | ASP  |
| 10  | J     | 27  | ALA  |
| 10  | J     | 90  | LEU  |
| 12  | L     | 29  | GLY  |
| 13  | M     | 38  | GLY  |
| 13  | M     | 124 | PRO  |
| 18  | R     | 17  | SER  |
| 18  | R     | 26  | LEU  |
| 19  | S     | 27  | GLU  |
| 2   | B     | 115 | LEU  |
| 2   | B     | 195 | ASP  |
| 3   | C     | 74  | GLY  |
| 3   | C     | 101 | LEU  |
| 3   | C     | 157 | ILE  |
| 3   | C     | 188 | LEU  |
| 4   | D     | 4   | TYR  |
| 4   | D     | 5   | ILE  |
| 4   | D     | 175 | SER  |
| 6   | F     | 39  | LYS  |
| 6   | F     | 70  | ASP  |
| 7   | G     | 17  | VAL  |
| 7   | G     | 42  | ILE  |
| 7   | G     | 116 | ALA  |
| 9   | I     | 41  | VAL  |
| 10  | J     | 61  | GLU  |
| 10  | J     | 73  | ASP  |
| 10  | J     | 86  | MET  |
| 12  | L     | 41  | ARG  |
| 18  | R     | 21  | LYS  |
| 2   | B     | 52  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 198 | ASP  |
| 7   | G     | 41  | ARG  |
| 10  | J     | 76  | ASN  |
| 11  | K     | 52  | GLY  |
| 17  | Q     | 33  | GLY  |
| 10  | J     | 24  | VAL  |
| 3   | C     | 55  | VAL  |
| 15  | O     | 82  | ILE  |
| 2   | B     | 227 | GLY  |
| 2   | B     | 228 | GLY  |
| 18  | R     | 60  | GLY  |
| 10  | J     | 77  | PRO  |
| 15  | O     | 75  | 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     | 194/220 (88%)  | 176 (91%) | 18 (9%)  | 10          | 19 |
| 3   | C     | 160/188 (85%)  | 152 (95%) | 8 (5%)   | 27          | 49 |
| 4   | D     | 180/181 (99%)  | 171 (95%) | 9 (5%)   | 27          | 49 |
| 5   | E     | 115/123 (94%)  | 101 (88%) | 14 (12%) | 5           | 10 |
| 6   | F     | 90/90 (100%)   | 88 (98%)  | 2 (2%)   | 55          | 80 |
| 7   | G     | 126/127 (99%)  | 116 (92%) | 10 (8%)  | 13          | 26 |
| 8   | H     | 119/119 (100%) | 109 (92%) | 10 (8%)  | 12          | 23 |
| 9   | I     | 98/99 (99%)    | 91 (93%)  | 7 (7%)   | 16          | 31 |
| 10  | J     | 87/92 (95%)    | 81 (93%)  | 6 (7%)   | 17          | 32 |
| 11  | K     | 90/99 (91%)    | 87 (97%)  | 3 (3%)   | 41          | 68 |
| 12  | L     | 104/111 (94%)  | 96 (92%)  | 8 (8%)   | 14          | 27 |
| 13  | M     | 100/101 (99%)  | 89 (89%)  | 11 (11%) | 7           | 13 |
| 14  | N     | 49/50 (98%)    | 41 (84%)  | 8 (16%)  | 2           | 4  |
| 15  | O     | 79/80 (99%)    | 71 (90%)  | 8 (10%)  | 8           | 16 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 16  | P     | 72/74 (97%)     | 69 (96%)   | 3 (4%)   | 32          | 57 |
| 17  | Q     | 96/97 (99%)     | 93 (97%)   | 3 (3%)   | 43          | 70 |
| 18  | R     | 64/77 (83%)     | 63 (98%)   | 1 (2%)   | 65          | 86 |
| 19  | S     | 71/80 (89%)     | 65 (92%)   | 6 (8%)   | 12          | 22 |
| 20  | T     | 76/82 (93%)     | 68 (90%)   | 8 (10%)  | 7           | 14 |
| 21  | U     | 19/22 (86%)     | 18 (95%)   | 1 (5%)   | 25          | 46 |
| All | All   | 1989/2112 (94%) | 1845 (93%) | 144 (7%) | 16          | 30 |

All (144) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 24  | TRP  |
| 2   | B     | 25  | ASN  |
| 2   | B     | 44  | LEU  |
| 2   | B     | 46  | LYS  |
| 2   | B     | 64  | ARG  |
| 2   | B     | 82  | ARG  |
| 2   | B     | 86  | GLU  |
| 2   | B     | 97  | TRP  |
| 2   | B     | 113 | HIS  |
| 2   | B     | 114 | ARG  |
| 2   | B     | 153 | ARG  |
| 2   | B     | 157 | ARG  |
| 2   | B     | 178 | ARG  |
| 2   | B     | 187 | LEU  |
| 2   | B     | 204 | ASN  |
| 2   | B     | 215 | LEU  |
| 2   | B     | 221 | LEU  |
| 2   | B     | 236 | TYR  |
| 3   | C     | 5   | ILE  |
| 3   | C     | 27  | LYS  |
| 3   | C     | 52  | LEU  |
| 3   | C     | 56  | ASP  |
| 3   | C     | 82  | GLU  |
| 3   | C     | 127 | ARG  |
| 3   | C     | 167 | TRP  |
| 3   | C     | 196 | LEU  |
| 4   | D     | 3   | ARG  |
| 4   | D     | 15  | GLU  |
| 4   | D     | 36  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 57  | ARG  |
| 4   | D     | 122 | ARG  |
| 4   | D     | 132 | ARG  |
| 4   | D     | 170 | VAL  |
| 4   | D     | 199 | ASN  |
| 4   | D     | 201 | GLN  |
| 5   | E     | 12  | LEU  |
| 5   | E     | 20  | GLN  |
| 5   | E     | 31  | LEU  |
| 5   | E     | 34  | VAL  |
| 5   | E     | 41  | VAL  |
| 5   | E     | 43  | LEU  |
| 5   | E     | 73  | ASN  |
| 5   | E     | 75  | THR  |
| 5   | E     | 80  | ILE  |
| 5   | E     | 89  | ILE  |
| 5   | E     | 107 | ARG  |
| 5   | E     | 116 | THR  |
| 5   | E     | 143 | ARG  |
| 5   | E     | 150 | ARG  |
| 6   | F     | 43  | LEU  |
| 6   | F     | 47  | ARG  |
| 7   | G     | 8   | GLU  |
| 7   | G     | 11  | GLN  |
| 7   | G     | 12  | LEU  |
| 7   | G     | 38  | LEU  |
| 7   | G     | 47  | CYS  |
| 7   | G     | 113 | GLU  |
| 7   | G     | 114 | ARG  |
| 7   | G     | 136 | LYS  |
| 7   | G     | 140 | ASP  |
| 7   | G     | 156 | TRP  |
| 8   | H     | 21  | LYS  |
| 8   | H     | 26  | VAL  |
| 8   | H     | 39  | LEU  |
| 8   | H     | 85  | ARG  |
| 8   | H     | 91  | ARG  |
| 8   | H     | 92  | ARG  |
| 8   | H     | 97  | VAL  |
| 8   | H     | 102 | ARG  |
| 8   | H     | 112 | LEU  |
| 8   | H     | 133 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | I     | 2   | GLU  |
| 9   | I     | 14  | VAL  |
| 9   | I     | 23  | ASN  |
| 9   | I     | 60  | ASP  |
| 9   | I     | 102 | LEU  |
| 9   | I     | 107 | ARG  |
| 9   | I     | 121 | ARG  |
| 10  | J     | 29  | ARG  |
| 10  | J     | 57  | LYS  |
| 10  | J     | 71  | LEU  |
| 10  | J     | 73  | ASP  |
| 10  | J     | 80  | LYS  |
| 10  | J     | 83  | GLU  |
| 11  | K     | 11  | LYS  |
| 11  | K     | 92  | GLU  |
| 11  | K     | 123 | LYS  |
| 12  | L     | 15  | ARG  |
| 12  | L     | 19  | ARG  |
| 12  | L     | 20  | LYS  |
| 12  | L     | 33  | ARG  |
| 12  | L     | 111 | LYS  |
| 12  | L     | 112 | ASP  |
| 12  | L     | 113 | ARG  |
| 12  | L     | 127 | GLU  |
| 13  | M     | 13  | LYS  |
| 13  | M     | 40  | ASN  |
| 13  | M     | 44  | ARG  |
| 13  | M     | 56  | LEU  |
| 13  | M     | 58  | GLU  |
| 13  | M     | 94  | ARG  |
| 13  | M     | 102 | ARG  |
| 13  | M     | 108 | ARG  |
| 13  | M     | 110 | ARG  |
| 13  | M     | 115 | LYS  |
| 13  | M     | 125 | ARG  |
| 14  | N     | 6   | LEU  |
| 14  | N     | 9   | LYS  |
| 14  | N     | 11  | LYS  |
| 14  | N     | 12  | ARG  |
| 14  | N     | 22  | THR  |
| 14  | N     | 26  | ARG  |
| 14  | N     | 41  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | N     | 44  | LEU  |
| 15  | O     | 5   | LYS  |
| 15  | O     | 10  | LYS  |
| 15  | O     | 31  | LEU  |
| 15  | O     | 34  | LEU  |
| 15  | O     | 39  | LEU  |
| 15  | O     | 57  | LEU  |
| 15  | O     | 71  | GLN  |
| 15  | O     | 81  | LEU  |
| 16  | P     | 1   | MET  |
| 16  | P     | 2   | VAL  |
| 16  | P     | 53  | VAL  |
| 17  | Q     | 38  | ARG  |
| 17  | Q     | 68  | ARG  |
| 17  | Q     | 74  | LEU  |
| 18  | R     | 36  | ASN  |
| 19  | S     | 7   | LYS  |
| 19  | S     | 15  | LEU  |
| 19  | S     | 18  | LYS  |
| 19  | S     | 25  | LYS  |
| 19  | S     | 27  | GLU  |
| 19  | S     | 81  | ARG  |
| 20  | T     | 8   | ARG  |
| 20  | T     | 42  | GLN  |
| 20  | T     | 48  | LYS  |
| 20  | T     | 57  | ARG  |
| 20  | T     | 73  | HIS  |
| 20  | T     | 74  | LYS  |
| 20  | T     | 75  | ASN  |
| 20  | T     | 84  | LEU  |
| 21  | U     | 9   | ARG  |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 25  | ASN  |
| 2   | B     | 95  | GLN  |
| 2   | B     | 146 | GLN  |
| 2   | B     | 204 | ASN  |
| 2   | B     | 212 | GLN  |
| 2   | B     | 240 | GLN  |
| 3   | C     | 3   | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 6   | HIS  |
| 3   | C     | 107 | GLN  |
| 3   | C     | 110 | ASN  |
| 3   | C     | 123 | GLN  |
| 4   | D     | 42  | GLN  |
| 4   | D     | 62  | GLN  |
| 4   | D     | 123 | HIS  |
| 4   | D     | 199 | ASN  |
| 4   | D     | 201 | GLN  |
| 5   | E     | 20  | GLN  |
| 5   | E     | 73  | ASN  |
| 6   | F     | 18  | GLN  |
| 6   | F     | 27  | GLN  |
| 6   | F     | 32  | ASN  |
| 6   | F     | 57  | GLN  |
| 6   | F     | 73  | ASN  |
| 6   | F     | 100 | ASN  |
| 7   | G     | 37  | ASN  |
| 7   | G     | 96  | GLN  |
| 7   | G     | 106 | GLN  |
| 7   | G     | 122 | HIS  |
| 9   | I     | 23  | ASN  |
| 9   | I     | 73  | GLN  |
| 9   | I     | 124 | GLN  |
| 10  | J     | 33  | GLN  |
| 10  | J     | 56  | HIS  |
| 10  | J     | 62  | HIS  |
| 10  | J     | 76  | ASN  |
| 10  | J     | 78  | ASN  |
| 11  | K     | 38  | ASN  |
| 11  | K     | 93  | GLN  |
| 11  | K     | 117 | ASN  |
| 12  | L     | 49  | ASN  |
| 12  | L     | 75  | HIS  |
| 13  | M     | 12  | ASN  |
| 13  | M     | 40  | ASN  |
| 13  | M     | 62  | ASN  |
| 15  | O     | 13  | GLN  |
| 15  | O     | 37  | ASN  |
| 16  | P     | 65  | GLN  |
| 16  | P     | 76  | GLN  |
| 17  | Q     | 96  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | R     | 36  | ASN  |
| 19  | S     | 23  | ASN  |
| 19  | S     | 56  | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | A     | 1511/1522 (99%) | 196 (12%)         | 72 (4%)         |
| 22  | X     | 2/6 (33%)       | 0                 | 0               |
| 23  | Y     | 6/17 (35%)      | 1 (16%)           | 0               |
| All | All   | 1519/1545 (98%) | 197 (12%)         | 72 (4%)         |

All (197) 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     | 61  | G    |
| 1   | A     | 101 | A    |
| 1   | A     | 116 | A    |
| 1   | A     | 120 | A    |
| 1   | A     | 121 | C    |
| 1   | A     | 130 | A    |
| 1   | A     | 131 | C    |
| 1   | A     | 144 | G    |
| 1   | A     | 181 | G    |
| 1   | A     | 182 | U    |
| 1   | A     | 195 | A    |
| 1   | A     | 197 | A    |
| 1   | A     | 202 | U    |
| 1   | A     | 204 | U    |
| 1   | A     | 216 | G    |
| 1   | A     | 244 | U    |
| 1   | A     | 247 | G    |
| 1   | A     | 251 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 266 | G    |
| 1   | A     | 267 | C    |
| 1   | A     | 282 | A    |
| 1   | A     | 289 | G    |
| 1   | A     | 321 | A    |
| 1   | A     | 328 | C    |
| 1   | A     | 329 | A    |
| 1   | A     | 332 | G    |
| 1   | A     | 344 | A    |
| 1   | A     | 345 | C    |
| 1   | A     | 352 | C    |
| 1   | A     | 353 | A    |
| 1   | A     | 354 | G    |
| 1   | A     | 367 | U    |
| 1   | A     | 373 | A    |
| 1   | A     | 397 | A    |
| 1   | A     | 398 | C    |
| 1   | A     | 410 | G    |
| 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     | 433 | C    |
| 1   | A     | 434 | U    |
| 1   | A     | 439 | A    |
| 1   | A     | 442 | C    |
| 1   | A     | 452 | A    |
| 1   | A     | 461 | C    |
| 1   | A     | 485 | G    |
| 1   | A     | 497 | A    |
| 1   | A     | 498 | U    |
| 1   | A     | 509 | A    |
| 1   | A     | 510 | A    |
| 1   | A     | 511 | C    |
| 1   | A     | 518 | C    |
| 1   | A     | 527 | G    |
| 1   | A     | 531 | U    |
| 1   | A     | 532 | A    |
| 1   | A     | 533 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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    |
| 1   | A     | 575 | G    |
| 1   | A     | 576 | G    |
| 1   | A     | 577 | G    |
| 1   | A     | 630 | G    |
| 1   | A     | 631 | G    |
| 1   | A     | 632 | A    |
| 1   | A     | 653 | A    |
| 1   | A     | 665 | A    |
| 1   | A     | 688 | G    |
| 1   | A     | 701 | C    |
| 1   | A     | 702 | A    |
| 1   | A     | 723 | U    |
| 1   | A     | 731 | G    |
| 1   | A     | 749 | C    |
| 1   | A     | 755 | G    |
| 1   | A     | 777 | A    |
| 1   | A     | 781 | A    |
| 1   | A     | 782 | A    |
| 1   | A     | 794 | A    |
| 1   | A     | 813 | U    |
| 1   | A     | 816 | A    |
| 1   | A     | 817 | C    |
| 1   | A     | 819 | A    |
| 1   | A     | 828 | A    |
| 1   | A     | 839 | U    |
| 1   | A     | 840 | C    |
| 1   | A     | 841 | U    |
| 1   | A     | 848 | C    |
| 1   | A     | 874 | G    |
| 1   | A     | 914 | A    |
| 1   | A     | 926 | G    |
| 1   | A     | 927 | G    |
| 1   | A     | 934 | C    |
| 1   | A     | 935 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 960  | U    |
| 1   | A     | 961  | U    |
| 1   | A     | 965  | A    |
| 1   | A     | 966  | G    |
| 1   | A     | 969  | A    |
| 1   | A     | 971  | G    |
| 1   | A     | 974  | A    |
| 1   | A     | 975  | A    |
| 1   | A     | 976  | G    |
| 1   | A     | 977  | A    |
| 1   | A     | 978  | A    |
| 1   | A     | 991  | U    |
| 1   | A     | 992  | U    |
| 1   | A     | 993  | G    |
| 1   | A     | 994  | A    |
| 1   | A     | 1005 | A    |
| 1   | A     | 1026 | G    |
| 1   | A     | 1027 | C    |
| 1   | A     | 1050 | G    |
| 1   | A     | 1054 | C    |
| 1   | A     | 1055 | A    |
| 1   | A     | 1065 | U    |
| 1   | A     | 1066 | C    |
| 1   | A     | 1068 | G    |
| 1   | A     | 1094 | G    |
| 1   | A     | 1095 | U    |
| 1   | A     | 1101 | A    |
| 1   | A     | 1117 | G    |
| 1   | A     | 1125 | U    |
| 1   | A     | 1126 | U    |
| 1   | A     | 1127 | G    |
| 1   | A     | 1129 | C    |
| 1   | A     | 1130 | A    |
| 1   | A     | 1131 | G    |
| 1   | A     | 1136 | U    |
| 1   | A     | 1137 | C    |
| 1   | A     | 1138 | G    |
| 1   | A     | 1139 | G    |
| 1   | A     | 1145 | C    |
| 1   | A     | 1152 | A    |
| 1   | A     | 1159 | U    |
| 1   | A     | 1161 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1176 | A    |
| 1   | A     | 1180 | A    |
| 1   | A     | 1183 | A    |
| 1   | A     | 1184 | G    |
| 1   | A     | 1196 | U    |
| 1   | A     | 1197 | G    |
| 1   | A     | 1200 | C    |
| 1   | A     | 1201 | A    |
| 1   | A     | 1202 | G    |
| 1   | A     | 1212 | U    |
| 1   | A     | 1213 | A    |
| 1   | A     | 1214 | C    |
| 1   | A     | 1227 | A    |
| 1   | A     | 1238 | A    |
| 1   | A     | 1257 | U    |
| 1   | A     | 1258 | G    |
| 1   | A     | 1280 | A    |
| 1   | A     | 1281 | U    |
| 1   | A     | 1282 | C    |
| 1   | A     | 1286 | A    |
| 1   | A     | 1287 | A    |
| 1   | A     | 1300 | G    |
| 1   | A     | 1301 | U    |
| 1   | A     | 1302 | U    |
| 1   | A     | 1338 | G    |
| 1   | A     | 1348 | U    |
| 1   | A     | 1362 | C    |
| 1   | A     | 1394 | A    |
| 1   | A     | 1398 | A    |
| 1   | A     | 1442 | G    |
| 1   | A     | 1443 | G    |
| 1   | A     | 1446 | A    |
| 1   | A     | 1452 | C    |
| 1   | A     | 1492 | A    |
| 1   | A     | 1497 | G    |
| 1   | A     | 1499 | A    |
| 1   | A     | 1502 | A    |
| 1   | A     | 1504 | G    |
| 1   | A     | 1505 | G    |
| 1   | A     | 1506 | U    |
| 1   | A     | 1517 | G    |
| 1   | A     | 1529 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1530 | G    |
| 1   | A     | 1533 | C    |
| 23  | Y     | 35   | A    |

All (72) 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     | 203    | U    |
| 1   | A     | 243    | A    |
| 1   | A     | 250    | A    |
| 1   | A     | 266    | G    |
| 1   | A     | 281    | G    |
| 1   | A     | 328    | C    |
| 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     | 433    | C    |
| 1   | A     | 438    | G    |
| 1   | A     | 484    | G    |
| 1   | A     | 497    | 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    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 812  | C    |
| 1   | A     | 819  | A    |
| 1   | A     | 913  | A    |
| 1   | A     | 960  | U    |
| 1   | A     | 965  | A    |
| 1   | A     | 992  | U    |
| 1   | A     | 993  | G    |
| 1   | A     | 1049 | U    |
| 1   | A     | 1063 | C    |
| 1   | A     | 1065 | U    |
| 1   | A     | 1067 | A    |
| 1   | A     | 1127 | G    |
| 1   | A     | 1129 | C    |
| 1   | A     | 1160 | G    |
| 1   | A     | 1175 | G    |
| 1   | A     | 1182 | G    |
| 1   | A     | 1191 | A    |
| 1   | A     | 1192 | C    |
| 1   | A     | 1201 | A    |
| 1   | A     | 1212 | U    |
| 1   | A     | 1225 | A    |
| 1   | A     | 1256 | A    |
| 1   | A     | 1257 | U    |
| 1   | A     | 1281 | U    |
| 1   | A     | 1285 | A    |
| 1   | A     | 1300 | G    |
| 1   | A     | 1301 | U    |
| 1   | A     | 1347 | G    |
| 1   | A     | 1397 | C    |
| 1   | A     | 1443 | G    |
| 1   | A     | 1451 | A    |
| 1   | A     | 1498 | U    |
| 1   | A     | 1503 | A    |
| 1   | A     | 1504 | G    |
| 1   | A     | 1505 | G    |
| 1   | A     | 1528 | U    |
| 1   | A     | 1532 | U    |

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 271 ligands modelled in this entry, 270 are monoatomic - leaving 1 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 26  | PAR  | A     | 1854 | -    | 44,45,45     | 1.30 | 7 (15%)     | 62,67,67    | 1.27 | 5 (8%)      |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 26  | PAR  | A     | 1854 | -    | -       | 0/18/94/94 | 0/4/4/4 |

All (7) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 26  | A     | 1854 | PAR  | O54-C54 | 2.01 | 1.49        | 1.44     |
| 26  | A     | 1854 | PAR  | O51-C51 | 2.08 | 1.49        | 1.44     |
| 26  | A     | 1854 | PAR  | C52-C42 | 2.17 | 1.56        | 1.52     |
| 26  | A     | 1854 | PAR  | O51-C11 | 2.43 | 1.48        | 1.41     |
| 26  | A     | 1854 | PAR  | C11-C21 | 2.50 | 1.57        | 1.52     |
| 26  | A     | 1854 | PAR  | C31-C21 | 2.67 | 1.56        | 1.53     |
| 26  | A     | 1854 | PAR  | O54-C14 | 3.05 | 1.49        | 1.41     |

All (5) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 26  | A     | 1854 | PAR  | O52-C13-O43 | -2.02 | 109.24      | 111.43   |
| 26  | A     | 1854 | PAR  | O52-C13-C23 | 2.83  | 113.82      | 107.96   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 26  | A     | 1854 | PAR  | C14-O54-C54 | 3.77 | 121.15      | 113.71   |
| 26  | A     | 1854 | PAR  | O54-C54-C64 | 3.85 | 113.30      | 106.01   |
| 26  | A     | 1854 | PAR  | O33-C14-C24 | 4.67 | 116.56      | 108.24   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 26  | A     | 1854 | PAR  | 1       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1   | A     | 11               |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | A     | 1064:G    | O3'    | 1065:U    | P      | 1.30         |
| 1     | A     | 1144:G    | O3'    | 1145:C    | P      | 1.24         |
| 1     | A     | 1192:C    | O3'    | 1193:G    | P      | 1.10         |
| 1     | A     | 1179:A    | O3'    | 1180:A    | P      | 1.08         |
| 1     | A     | 1175:G    | O3'    | 1176:A    | P      | 0.99         |
| 1     | A     | 1191:A    | O3'    | 1192:C    | P      | 0.98         |
| 1     | A     | 1156:G    | O3'    | 1157:A    | P      | 0.89         |
| 1     | A     | 1532:U    | O3'    | 1533:C    | P      | 0.83         |
| 1     | A     | 1160:G    | O3'    | 1161:C    | P      | 0.72         |
| 1     | A     | 1063:C    | O3'    | 1064:G    | P      | 0.70         |
| 1     | A     | 1127:G    | O3'    | 1128:C    | P      | 0.46         |

## 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     | 1513/1522 (99%) | -0.08  | 31 (2%) 65 67  | 18, 47, 115, 201      | 0     |
| 2   | B     | 236/256 (92%)   | 0.73   | 22 (9%) 8 8    | 41, 79, 129, 136      | 0     |
| 3   | C     | 207/239 (86%)   | 0.73   | 22 (10%) 6 5   | 48, 74, 118, 125      | 0     |
| 4   | D     | 208/209 (99%)   | 0.65   | 20 (9%) 8 7    | 39, 59, 84, 92        | 0     |
| 5   | E     | 151/162 (93%)   | 0.28   | 1 (0%) 87 88   | 25, 41, 69, 84        | 0     |
| 6   | F     | 101/101 (100%)  | 0.52   | 7 (6%) 17 17   | 49, 77, 92, 96        | 0     |
| 7   | G     | 155/156 (99%)   | 0.54   | 11 (7%) 16 16  | 40, 68, 102, 114      | 0     |
| 8   | H     | 138/138 (100%)  | 0.23   | 4 (2%) 51 55   | 21, 38, 55, 65        | 0     |
| 9   | I     | 127/128 (99%)   | 1.03   | 24 (18%) 1 1   | 39, 82, 103, 112      | 0     |
| 10  | J     | 99/105 (94%)    | 1.27   | 24 (24%) 0 0   | 42, 112, 146, 150     | 0     |
| 11  | K     | 119/129 (92%)   | 0.55   | 4 (3%) 45 48   | 23, 50, 79, 96        | 0     |
| 12  | L     | 125/135 (92%)   | 0.56   | 6 (4%) 30 32   | 17, 52, 74, 109       | 0     |
| 13  | M     | 125/126 (99%)   | 1.87   | 20 (16%) 1 1   | 50, 67, 122, 152      | 0     |
| 14  | N     | 60/61 (98%)     | 1.06   | 8 (13%) 3 2    | 47, 66, 101, 107      | 0     |
| 15  | O     | 88/89 (98%)     | 0.55   | 5 (5%) 24 25   | 36, 54, 82, 109       | 0     |
| 16  | P     | 84/88 (95%)     | 0.27   | 2 (2%) 59 62   | 28, 40, 57, 80        | 0     |
| 17  | Q     | 104/105 (99%)   | 0.72   | 7 (6%) 18 18   | 23, 42, 93, 146       | 0     |
| 18  | R     | 73/88 (82%)     | 0.55   | 5 (6%) 17 18   | 43, 60, 107, 139      | 0     |
| 19  | S     | 81/93 (87%)     | 1.26   | 16 (19%) 1 1   | 56, 90, 123, 134      | 0     |
| 20  | T     | 99/106 (93%)    | 0.44   | 6 (6%) 21 22   | 25, 46, 81, 86        | 0     |
| 21  | U     | 25/27 (92%)     | 1.15   | 3 (12%) 4 4    | 44, 53, 88, 94        | 0     |
| 22  | X     | 3/6 (50%)       | 0.30   | 0 100 100      | 83, 83, 83, 88        | 0     |
| 23  | Y     | 6/17 (35%)      | 0.84   | 1 (16%) 1 1    | 97, 105, 124, 134     | 0     |
| All | All   | 3927/4086 (96%) | 0.41   | 249 (6%) 20 21 | 17, 56, 115, 201      | 0     |

All (249) RSRZ outliers are listed below:

| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 13  | M     | 121     | LYS  | 30.5 |
| 13  | M     | 124     | PRO  | 27.1 |
| 13  | M     | 123     | ALA  | 26.7 |
| 17  | Q     | 105     | ALA  | 25.4 |
| 19  | S     | 3       | ARG  | 24.6 |
| 1   | A     | 1129    | C    | 20.6 |
| 13  | M     | 120     | LYS  | 18.4 |
| 1   | A     | 1534    | A    | 16.3 |
| 13  | M     | 125     | ARG  | 15.8 |
| 13  | M     | 126     | LYS  | 12.6 |
| 13  | M     | 7       | VAL  | 12.3 |
| 17  | Q     | 104     | LYS  | 10.8 |
| 1   | A     | 1540    | U    | 10.7 |
| 14  | N     | 6       | LEU  | 10.3 |
| 11  | K     | 129     | SER  | 9.4  |
| 11  | K     | 128     | ALA  | 7.9  |
| 14  | N     | 3       | ARG  | 7.9  |
| 13  | M     | 122     | LYS  | 7.9  |
| 21  | U     | 6       | ARG  | 6.7  |
| 17  | Q     | 103     | GLY  | 6.6  |
| 1   | A     | 1539    | C    | 6.4  |
| 10  | J     | 24      | VAL  | 6.4  |
| 21  | U     | 24      | ARG  | 6.4  |
| 4   | D     | 23      | GLY  | 6.4  |
| 1   | A     | 1541    | U    | 6.0  |
| 1   | A     | 1004    | A    | 6.0  |
| 12  | L     | 47      | LYS  | 6.0  |
| 14  | N     | 2       | ALA  | 6.0  |
| 2   | B     | 133     | LYS  | 5.9  |
| 10  | J     | 36      | GLY  | 5.9  |
| 1   | A     | 1144    | G    | 5.8  |
| 1   | A     | 1003(A) | G    | 5.7  |
| 3   | C     | 76      | VAL  | 5.7  |
| 13  | M     | 8       | GLU  | 5.6  |
| 2   | B     | 136     | VAL  | 5.6  |
| 23  | Y     | 33      | U    | 5.6  |
| 7   | G     | 5       | ARG  | 5.5  |
| 9   | I     | 66      | ARG  | 5.4  |
| 10  | J     | 10      | GLY  | 5.3  |
| 18  | R     | 16      | PRO  | 5.3  |
| 8   | H     | 1       | MET  | 5.3  |
| 7   | G     | 156     | TRP  | 5.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 10  | J     | 6    | ILE  | 5.0  |
| 4   | D     | 4    | TYR  | 4.9  |
| 9   | I     | 19   | LEU  | 4.9  |
| 1   | A     | 1533 | C    | 4.9  |
| 1   | A     | 1038 | C    | 4.9  |
| 13  | M     | 5    | ALA  | 4.8  |
| 13  | M     | 102  | ARG  | 4.8  |
| 3   | C     | 196  | LEU  | 4.7  |
| 2   | B     | 226  | ARG  | 4.6  |
| 2   | B     | 211  | ILE  | 4.6  |
| 3   | C     | 60   | ALA  | 4.6  |
| 10  | J     | 72   | VAL  | 4.5  |
| 7   | G     | 80   | VAL  | 4.5  |
| 17  | Q     | 102  | GLY  | 4.4  |
| 10  | J     | 34   | VAL  | 4.4  |
| 10  | J     | 90   | LEU  | 4.3  |
| 4   | D     | 5    | ILE  | 4.3  |
| 19  | S     | 49   | ILE  | 4.2  |
| 18  | R     | 17   | SER  | 4.2  |
| 4   | D     | 21   | LEU  | 4.2  |
| 1   | A     | 1034 | G    | 4.1  |
| 4   | D     | 209  | ARG  | 4.1  |
| 10  | J     | 70   | ARG  | 4.1  |
| 19  | S     | 2    | PRO  | 4.0  |
| 10  | J     | 71   | LEU  | 4.0  |
| 19  | S     | 34   | TRP  | 3.9  |
| 2   | B     | 165  | VAL  | 3.9  |
| 1   | A     | 723  | U    | 3.9  |
| 4   | D     | 3    | ARG  | 3.9  |
| 10  | J     | 98   | ILE  | 3.8  |
| 10  | J     | 99   | LYS  | 3.8  |
| 2   | B     | 229  | VAL  | 3.6  |
| 12  | L     | 28   | LYS  | 3.6  |
| 19  | S     | 28   | LYS  | 3.6  |
| 4   | D     | 20   | TYR  | 3.6  |
| 9   | I     | 65   | VAL  | 3.6  |
| 10  | J     | 87   | THR  | 3.6  |
| 1   | A     | 1006 | C    | 3.6  |
| 1   | A     | 1131 | G    | 3.6  |
| 20  | T     | 100  | ILE  | 3.5  |
| 3   | C     | 167  | TRP  | 3.5  |
| 10  | J     | 54   | PHE  | 3.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 1130 | A    | 3.4  |
| 3   | C     | 94   | LEU  | 3.4  |
| 9   | I     | 14   | VAL  | 3.4  |
| 13  | M     | 88   | ARG  | 3.4  |
| 12  | L     | 18   | VAL  | 3.3  |
| 1   | A     | 1033 | G    | 3.3  |
| 15  | O     | 89   | GLY  | 3.3  |
| 6   | F     | 36   | ARG  | 3.3  |
| 9   | I     | 101  | PHE  | 3.2  |
| 19  | S     | 5    | LEU  | 3.2  |
| 13  | M     | 9    | ILE  | 3.2  |
| 7   | G     | 2    | ALA  | 3.2  |
| 10  | J     | 5    | ARG  | 3.2  |
| 9   | I     | 18   | PHE  | 3.2  |
| 1   | A     | 1037 | C    | 3.2  |
| 10  | J     | 96   | ILE  | 3.2  |
| 2   | B     | 35   | GLU  | 3.1  |
| 19  | S     | 31   | ILE  | 3.1  |
| 13  | M     | 25   | ILE  | 3.1  |
| 9   | I     | 70   | LYS  | 3.1  |
| 13  | M     | 56   | LEU  | 3.1  |
| 10  | J     | 43   | ARG  | 3.1  |
| 3   | C     | 2    | GLY  | 3.1  |
| 1   | A     | 1143 | G    | 3.0  |
| 4   | D     | 49   | ARG  | 3.0  |
| 20  | T     | 99   | LEU  | 3.0  |
| 19  | S     | 10   | PHE  | 3.0  |
| 9   | I     | 119  | ALA  | 3.0  |
| 2   | B     | 81   | VAL  | 2.9  |
| 8   | H     | 2    | LEU  | 2.9  |
| 2   | B     | 58   | ILE  | 2.9  |
| 19  | S     | 74   | PHE  | 2.9  |
| 4   | D     | 159  | ARG  | 2.9  |
| 1   | A     | 1127 | G    | 2.9  |
| 4   | D     | 2    | GLY  | 2.9  |
| 3   | C     | 188  | LEU  | 2.9  |
| 17  | Q     | 95   | TYR  | 2.9  |
| 1   | A     | 202  | U    | 2.9  |
| 10  | J     | 97   | GLU  | 2.8  |
| 15  | O     | 3    | ILE  | 2.8  |
| 3   | C     | 201  | TYR  | 2.8  |
| 7   | G     | 4    | ARG  | 2.8  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 7   | G     | 85      | TYR  | 2.8  |
| 1   | A     | 413     | G    | 2.8  |
| 20  | T     | 53      | LEU  | 2.8  |
| 2   | B     | 132     | LYS  | 2.8  |
| 9   | I     | 28      | VAL  | 2.8  |
| 6   | F     | 98      | LEU  | 2.8  |
| 3   | C     | 42      | LEU  | 2.7  |
| 19  | S     | 6       | LYS  | 2.7  |
| 14  | N     | 21      | TYR  | 2.7  |
| 9   | I     | 99      | LEU  | 2.7  |
| 12  | L     | 115     | LYS  | 2.7  |
| 13  | M     | 104     | ARG  | 2.7  |
| 8   | H     | 18      | ARG  | 2.7  |
| 18  | R     | 54      | ARG  | 2.7  |
| 1   | A     | 993     | G    | 2.7  |
| 3   | C     | 66      | VAL  | 2.6  |
| 3   | C     | 75      | VAL  | 2.6  |
| 9   | I     | 26      | VAL  | 2.6  |
| 3   | C     | 208     | ILE  | 2.6  |
| 1   | A     | 1027    | C    | 2.6  |
| 4   | D     | 25      | ARG  | 2.6  |
| 6   | F     | 72      | VAL  | 2.6  |
| 9   | I     | 64      | THR  | 2.6  |
| 14  | N     | 30      | ALA  | 2.6  |
| 13  | M     | 96      | LEU  | 2.6  |
| 12  | L     | 46      | LYS  | 2.6  |
| 19  | S     | 30      | LEU  | 2.6  |
| 20  | T     | 10      | LEU  | 2.6  |
| 2   | B     | 76      | GLN  | 2.5  |
| 10  | J     | 47      | PHE  | 2.5  |
| 7   | G     | 76      | ARG  | 2.5  |
| 4   | D     | 208     | SER  | 2.5  |
| 1   | A     | 1030(A) | G    | 2.5  |
| 2   | B     | 230     | VAL  | 2.5  |
| 3   | C     | 4       | LYS  | 2.5  |
| 2   | B     | 140     | HIS  | 2.5  |
| 12  | L     | 113     | ARG  | 2.5  |
| 4   | D     | 156     | GLU  | 2.5  |
| 4   | D     | 36      | ARG  | 2.4  |
| 9   | I     | 114     | TYR  | 2.4  |
| 6   | F     | 89      | MET  | 2.4  |
| 1   | A     | 1035    | A    | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 10  | J     | 17   | ASP  | 2.4  |
| 19  | S     | 29   | ARG  | 2.4  |
| 7   | G     | 120  | ILE  | 2.4  |
| 4   | D     | 115  | ARG  | 2.4  |
| 3   | C     | 47   | LEU  | 2.4  |
| 10  | J     | 8    | LEU  | 2.4  |
| 21  | U     | 20   | LYS  | 2.4  |
| 4   | D     | 32   | ALA  | 2.4  |
| 1   | A     | 1036 | G    | 2.4  |
| 9   | I     | 128  | ARG  | 2.4  |
| 3   | C     | 39   | ILE  | 2.4  |
| 9   | I     | 15   | ALA  | 2.4  |
| 6   | F     | 14   | LEU  | 2.4  |
| 4   | D     | 201  | GLN  | 2.3  |
| 6   | F     | 101  | ALA  | 2.3  |
| 9   | I     | 47   | LEU  | 2.3  |
| 10  | J     | 16   | LEU  | 2.3  |
| 3   | C     | 85   | ARG  | 2.3  |
| 14  | N     | 35   | ARG  | 2.3  |
| 1   | A     | 984  | C    | 2.3  |
| 3   | C     | 194  | GLY  | 2.3  |
| 2   | B     | 206  | ASP  | 2.3  |
| 17  | Q     | 98   | LEU  | 2.3  |
| 9   | I     | 17   | VAL  | 2.3  |
| 2   | B     | 89   | GLY  | 2.3  |
| 14  | N     | 28   | GLY  | 2.3  |
| 19  | S     | 61   | TYR  | 2.3  |
| 3   | C     | 134  | ILE  | 2.3  |
| 2   | B     | 77   | ALA  | 2.3  |
| 2   | B     | 61   | LEU  | 2.3  |
| 19  | S     | 71   | LEU  | 2.3  |
| 20  | T     | 9    | ASN  | 2.2  |
| 16  | P     | 19   | ILE  | 2.2  |
| 3   | C     | 128  | PHE  | 2.2  |
| 1   | A     | 1128 | C    | 2.2  |
| 15  | O     | 23   | GLY  | 2.2  |
| 7   | G     | 66   | VAL  | 2.2  |
| 19  | S     | 27   | GLU  | 2.2  |
| 3   | C     | 68   | VAL  | 2.2  |
| 6   | F     | 65   | VAL  | 2.2  |
| 2   | B     | 208  | ILE  | 2.2  |
| 15  | O     | 12   | ILE  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 18  | R     | 18   | ARG  | 2.2  |
| 9   | I     | 31   | GLN  | 2.2  |
| 3   | C     | 3    | ASN  | 2.2  |
| 4   | D     | 11   | LEU  | 2.2  |
| 11  | K     | 51   | LYS  | 2.2  |
| 16  | P     | 12   | LYS  | 2.2  |
| 20  | T     | 98   | PRO  | 2.2  |
| 1   | A     | 1124 | G    | 2.2  |
| 9   | I     | 53   | VAL  | 2.2  |
| 11  | K     | 30   | VAL  | 2.1  |
| 13  | M     | 30   | ALA  | 2.1  |
| 7   | G     | 155  | ARG  | 2.1  |
| 4   | D     | 204  | ILE  | 2.1  |
| 9   | I     | 27   | THR  | 2.1  |
| 13  | M     | 11   | ARG  | 2.1  |
| 5   | E     | 76   | ILE  | 2.1  |
| 10  | J     | 55   | LYS  | 2.1  |
| 4   | D     | 35   | ARG  | 2.1  |
| 17  | Q     | 101  | ARG  | 2.1  |
| 2   | B     | 15   | VAL  | 2.1  |
| 14  | N     | 16   | PHE  | 2.1  |
| 10  | J     | 20   | ALA  | 2.1  |
| 15  | O     | 11   | VAL  | 2.1  |
| 9   | I     | 51   | ARG  | 2.1  |
| 2   | B     | 215  | LEU  | 2.1  |
| 9   | I     | 102  | LEU  | 2.1  |
| 3   | C     | 64   | VAL  | 2.1  |
| 10  | J     | 7    | LYS  | 2.1  |
| 13  | M     | 117  | VAL  | 2.0  |
| 2   | B     | 127  | ILE  | 2.0  |
| 8   | H     | 30   | ARG  | 2.0  |
| 18  | R     | 25   | THR  | 2.0  |
| 19  | S     | 60   | VAL  | 2.0  |
| 9   | I     | 124  | GLN  | 2.0  |
| 9   | I     | 63   | ILE  | 2.0  |
| 2   | B     | 156  | LYS  | 2.0  |
| 1   | A     | 1200 | C    | 2.0  |
| 7   | G     | 26   | PHE  | 2.0  |
| 1   | A     | 373  | A    | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 24  | MG   | A     | 1632 | 1/1   | 0.03 | 0.59 | 160,160,160,160             | 0     |
| 25  | K    | R     | 101  | 1/1   | 0.06 | 0.20 | 144,144,144,144             | 0     |
| 24  | MG   | A     | 1676 | 1/1   | 0.32 | 0.21 | 103,103,103,103             | 0     |
| 25  | K    | A     | 1812 | 1/1   | 0.36 | 0.19 | 120,120,120,120             | 0     |
| 24  | MG   | A     | 1627 | 1/1   | 0.39 | 0.35 | 108,108,108,108             | 0     |
| 24  | MG   | A     | 1690 | 1/1   | 0.39 | 0.30 | 91,91,91,91                 | 0     |
| 24  | MG   | A     | 1782 | 1/1   | 0.40 | 0.18 | 132,132,132,132             | 0     |
| 25  | K    | A     | 1836 | 1/1   | 0.46 | 0.27 | 132,132,132,132             | 0     |
| 24  | MG   | A     | 1680 | 1/1   | 0.49 | 0.26 | 85,85,85,85                 | 0     |
| 25  | K    | A     | 1815 | 1/1   | 0.57 | 0.34 | 139,139,139,139             | 0     |
| 24  | MG   | A     | 1797 | 1/1   | 0.58 | 0.18 | 101,101,101,101             | 0     |
| 24  | MG   | A     | 1631 | 1/1   | 0.59 | 0.28 | 100,100,100,100             | 0     |
| 24  | MG   | A     | 1697 | 1/1   | 0.59 | 0.28 | 101,101,101,101             | 0     |
| 25  | K    | A     | 1827 | 1/1   | 0.59 | 0.20 | 122,122,122,122             | 0     |
| 25  | K    | A     | 1825 | 1/1   | 0.59 | 0.27 | 132,132,132,132             | 0     |
| 25  | K    | A     | 1820 | 1/1   | 0.59 | 0.20 | 102,102,102,102             | 0     |
| 25  | K    | A     | 1832 | 1/1   | 0.60 | 0.13 | 101,101,101,101             | 0     |
| 25  | K    | A     | 1821 | 1/1   | 0.60 | 0.19 | 99,99,99,99                 | 0     |
| 25  | K    | A     | 1846 | 1/1   | 0.61 | 0.16 | 118,118,118,118             | 0     |
| 24  | MG   | A     | 1656 | 1/1   | 0.61 | 0.17 | 89,89,89,89                 | 0     |
| 24  | MG   | A     | 1738 | 1/1   | 0.61 | 0.14 | 81,81,81,81                 | 0     |
| 25  | K    | A     | 1806 | 1/1   | 0.63 | 0.11 | 101,101,101,101             | 0     |
| 25  | K    | A     | 1822 | 1/1   | 0.64 | 0.13 | 101,101,101,101             | 0     |
| 24  | MG   | A     | 1726 | 1/1   | 0.65 | 0.28 | 102,102,102,102             | 0     |
| 25  | K    | A     | 1845 | 1/1   | 0.65 | 0.20 | 111,111,111,111             | 0     |
| 25  | K    | A     | 1852 | 1/1   | 0.66 | 0.28 | 120,120,120,120             | 0     |
| 24  | MG   | A     | 1772 | 1/1   | 0.67 | 0.17 | 89,89,89,89                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 24  | MG   | A     | 1784 | 1/1   | 0.68 | 0.19 | 93,93,93,93                 | 0     |
| 24  | MG   | A     | 1610 | 1/1   | 0.68 | 0.45 | 110,110,110,110             | 0     |
| 25  | K    | A     | 1817 | 1/1   | 0.69 | 0.13 | 133,133,133,133             | 0     |
| 24  | MG   | A     | 1652 | 1/1   | 0.71 | 0.17 | 56,56,56,56                 | 0     |
| 24  | MG   | A     | 1673 | 1/1   | 0.72 | 0.15 | 83,83,83,83                 | 0     |
| 24  | MG   | A     | 1714 | 1/1   | 0.72 | 0.32 | 88,88,88,88                 | 0     |
| 24  | MG   | A     | 1779 | 1/1   | 0.72 | 0.19 | 78,78,78,78                 | 0     |
| 24  | MG   | A     | 1716 | 1/1   | 0.73 | 0.36 | 78,78,78,78                 | 0     |
| 24  | MG   | A     | 1641 | 1/1   | 0.73 | 0.49 | 77,77,77,77                 | 0     |
| 24  | MG   | A     | 1678 | 1/1   | 0.73 | 0.49 | 97,97,97,97                 | 0     |
| 24  | MG   | A     | 1611 | 1/1   | 0.73 | 0.22 | 83,83,83,83                 | 0     |
| 24  | MG   | A     | 1710 | 1/1   | 0.73 | 0.48 | 93,93,93,93                 | 0     |
| 24  | MG   | A     | 1773 | 1/1   | 0.74 | 0.43 | 96,96,96,96                 | 0     |
| 24  | MG   | A     | 1692 | 1/1   | 0.74 | 0.16 | 109,109,109,109             | 0     |
| 24  | MG   | A     | 1643 | 1/1   | 0.74 | 0.51 | 88,88,88,88                 | 0     |
| 24  | MG   | A     | 1783 | 1/1   | 0.75 | 0.16 | 91,91,91,91                 | 0     |
| 24  | MG   | A     | 1619 | 1/1   | 0.75 | 0.09 | 72,72,72,72                 | 0     |
| 24  | MG   | A     | 1698 | 1/1   | 0.76 | 0.11 | 69,69,69,69                 | 0     |
| 24  | MG   | A     | 1677 | 1/1   | 0.76 | 0.18 | 95,95,95,95                 | 0     |
| 24  | MG   | A     | 1603 | 1/1   | 0.76 | 0.44 | 104,104,104,104             | 0     |
| 24  | MG   | A     | 1653 | 1/1   | 0.76 | 0.34 | 69,69,69,69                 | 0     |
| 24  | MG   | A     | 1758 | 1/1   | 0.77 | 0.55 | 103,103,103,103             | 0     |
| 25  | K    | A     | 1804 | 1/1   | 0.77 | 0.16 | 107,107,107,107             | 0     |
| 25  | K    | A     | 1829 | 1/1   | 0.77 | 0.09 | 103,103,103,103             | 0     |
| 25  | K    | A     | 1851 | 1/1   | 0.77 | 0.59 | 117,117,117,117             | 0     |
| 24  | MG   | A     | 1614 | 1/1   | 0.77 | 0.36 | 54,54,54,54                 | 0     |
| 25  | K    | A     | 1838 | 1/1   | 0.77 | 0.19 | 94,94,94,94                 | 0     |
| 25  | K    | A     | 1819 | 1/1   | 0.77 | 0.80 | 116,116,116,116             | 0     |
| 24  | MG   | A     | 1709 | 1/1   | 0.78 | 0.49 | 114,114,114,114             | 0     |
| 25  | K    | A     | 1839 | 1/1   | 0.78 | 0.24 | 131,131,131,131             | 0     |
| 24  | MG   | A     | 1766 | 1/1   | 0.78 | 0.32 | 77,77,77,77                 | 0     |
| 24  | MG   | A     | 1715 | 1/1   | 0.78 | 0.44 | 97,97,97,97                 | 0     |
| 25  | K    | A     | 1853 | 1/1   | 0.78 | 0.19 | 119,119,119,119             | 0     |
| 25  | K    | A     | 1813 | 1/1   | 0.79 | 0.25 | 126,126,126,126             | 0     |
| 24  | MG   | A     | 1713 | 1/1   | 0.79 | 0.26 | 86,86,86,86                 | 0     |
| 24  | MG   | A     | 1626 | 1/1   | 0.79 | 0.44 | 79,79,79,79                 | 0     |
| 25  | K    | A     | 1841 | 1/1   | 0.79 | 0.18 | 144,144,144,144             | 0     |
| 24  | MG   | A     | 1687 | 1/1   | 0.79 | 0.12 | 56,56,56,56                 | 0     |
| 25  | K    | A     | 1823 | 1/1   | 0.79 | 0.10 | 118,118,118,118             | 0     |
| 25  | K    | A     | 1844 | 1/1   | 0.79 | 0.28 | 107,107,107,107             | 0     |
| 24  | MG   | A     | 1731 | 1/1   | 0.79 | 0.43 | 73,73,73,73                 | 0     |
| 24  | MG   | A     | 1675 | 1/1   | 0.79 | 0.15 | 69,69,69,69                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 24  | MG   | A     | 1658 | 1/1   | 0.79 | 0.47 | 85,85,85,85                 | 0     |
| 24  | MG   | A     | 1665 | 1/1   | 0.79 | 0.50 | 90,90,90,90                 | 0     |
| 25  | K    | A     | 1816 | 1/1   | 0.80 | 0.16 | 116,116,116,116             | 0     |
| 24  | MG   | A     | 1695 | 1/1   | 0.80 | 0.31 | 90,90,90,90                 | 0     |
| 25  | K    | T     | 201  | 1/1   | 0.80 | 0.19 | 92,92,92,92                 | 0     |
| 24  | MG   | A     | 1660 | 1/1   | 0.80 | 0.46 | 83,83,83,83                 | 0     |
| 24  | MG   | A     | 1629 | 1/1   | 0.81 | 0.15 | 68,68,68,68                 | 0     |
| 25  | K    | A     | 1834 | 1/1   | 0.81 | 0.28 | 115,115,115,115             | 0     |
| 24  | MG   | A     | 1662 | 1/1   | 0.81 | 0.20 | 91,91,91,91                 | 0     |
| 24  | MG   | A     | 1622 | 1/1   | 0.81 | 0.27 | 66,66,66,66                 | 0     |
| 25  | K    | A     | 1805 | 1/1   | 0.81 | 0.14 | 113,113,113,113             | 0     |
| 25  | K    | A     | 1847 | 1/1   | 0.81 | 0.08 | 119,119,119,119             | 0     |
| 24  | MG   | A     | 1620 | 1/1   | 0.81 | 0.20 | 73,73,73,73                 | 0     |
| 24  | MG   | A     | 1759 | 1/1   | 0.82 | 0.47 | 128,128,128,128             | 0     |
| 25  | K    | A     | 1814 | 1/1   | 0.82 | 0.08 | 114,114,114,114             | 0     |
| 25  | K    | A     | 1810 | 1/1   | 0.82 | 0.12 | 113,113,113,113             | 0     |
| 24  | MG   | A     | 1651 | 1/1   | 0.82 | 0.16 | 72,72,72,72                 | 0     |
| 24  | MG   | A     | 1636 | 1/1   | 0.82 | 0.50 | 70,70,70,70                 | 0     |
| 24  | MG   | D     | 302  | 1/1   | 0.82 | 0.34 | 80,80,80,80                 | 0     |
| 24  | MG   | A     | 1767 | 1/1   | 0.82 | 0.19 | 69,69,69,69                 | 0     |
| 25  | K    | E     | 204  | 1/1   | 0.83 | 0.15 | 129,129,129,129             | 0     |
| 24  | MG   | A     | 1706 | 1/1   | 0.83 | 0.25 | 63,63,63,63                 | 0     |
| 24  | MG   | A     | 1683 | 1/1   | 0.83 | 0.45 | 79,79,79,79                 | 0     |
| 25  | K    | A     | 1843 | 1/1   | 0.83 | 0.73 | 80,80,80,80                 | 0     |
| 25  | K    | A     | 1835 | 1/1   | 0.83 | 0.07 | 99,99,99,99                 | 0     |
| 25  | K    | A     | 1831 | 1/1   | 0.83 | 0.15 | 127,127,127,127             | 0     |
| 24  | MG   | A     | 1711 | 1/1   | 0.83 | 0.56 | 104,104,104,104             | 0     |
| 24  | MG   | A     | 1732 | 1/1   | 0.83 | 0.23 | 80,80,80,80                 | 0     |
| 24  | MG   | A     | 1771 | 1/1   | 0.83 | 0.18 | 77,77,77,77                 | 0     |
| 25  | K    | A     | 1808 | 1/1   | 0.84 | 0.18 | 90,90,90,90                 | 0     |
| 24  | MG   | A     | 1637 | 1/1   | 0.84 | 0.43 | 71,71,71,71                 | 0     |
| 24  | MG   | A     | 1780 | 1/1   | 0.84 | 0.15 | 71,71,71,71                 | 0     |
| 24  | MG   | E     | 201  | 1/1   | 0.84 | 0.53 | 78,78,78,78                 | 0     |
| 25  | K    | A     | 1848 | 1/1   | 0.84 | 0.20 | 136,136,136,136             | 0     |
| 24  | MG   | A     | 1718 | 1/1   | 0.85 | 0.33 | 64,64,64,64                 | 0     |
| 24  | MG   | A     | 1735 | 1/1   | 0.85 | 0.21 | 78,78,78,78                 | 0     |
| 24  | MG   | A     | 1763 | 1/1   | 0.85 | 0.35 | 93,93,93,93                 | 0     |
| 24  | MG   | A     | 1722 | 1/1   | 0.85 | 0.55 | 83,83,83,83                 | 0     |
| 24  | MG   | A     | 1756 | 1/1   | 0.85 | 0.29 | 87,87,87,87                 | 0     |
| 24  | MG   | A     | 1707 | 1/1   | 0.85 | 0.21 | 62,62,62,62                 | 0     |
| 24  | MG   | A     | 1625 | 1/1   | 0.85 | 0.19 | 93,93,93,93                 | 0     |
| 24  | MG   | A     | 1757 | 1/1   | 0.85 | 0.47 | 72,72,72,72                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 24  | MG   | A     | 1754 | 1/1   | 0.85 | 0.14 | 80,80,80,80                 | 0     |
| 24  | MG   | A     | 1668 | 1/1   | 0.85 | 0.31 | 85,85,85,85                 | 0     |
| 24  | MG   | A     | 1659 | 1/1   | 0.85 | 0.52 | 84,84,84,84                 | 0     |
| 24  | MG   | A     | 1664 | 1/1   | 0.85 | 0.36 | 107,107,107,107             | 0     |
| 24  | MG   | A     | 1734 | 1/1   | 0.86 | 0.15 | 59,59,59,59                 | 0     |
| 24  | MG   | A     | 1696 | 1/1   | 0.86 | 0.31 | 70,70,70,70                 | 0     |
| 25  | K    | P     | 101  | 1/1   | 0.86 | 0.34 | 94,94,94,94                 | 0     |
| 24  | MG   | A     | 1694 | 1/1   | 0.86 | 0.31 | 71,71,71,71                 | 0     |
| 24  | MG   | A     | 1777 | 1/1   | 0.86 | 0.20 | 75,75,75,75                 | 0     |
| 24  | MG   | A     | 1623 | 1/1   | 0.86 | 0.37 | 92,92,92,92                 | 0     |
| 24  | MG   | A     | 1796 | 1/1   | 0.86 | 0.27 | 68,68,68,68                 | 0     |
| 24  | MG   | A     | 1615 | 1/1   | 0.86 | 0.44 | 107,107,107,107             | 0     |
| 25  | K    | N     | 103  | 1/1   | 0.86 | 0.73 | 111,111,111,111             | 0     |
| 24  | MG   | A     | 1657 | 1/1   | 0.86 | 0.23 | 56,56,56,56                 | 0     |
| 24  | MG   | A     | 1602 | 1/1   | 0.86 | 0.12 | 106,106,106,106             | 0     |
| 25  | K    | A     | 1840 | 1/1   | 0.87 | 0.24 | 96,96,96,96                 | 0     |
| 24  | MG   | A     | 1770 | 1/1   | 0.87 | 0.04 | 105,105,105,105             | 0     |
| 24  | MG   | A     | 1720 | 1/1   | 0.87 | 0.08 | 52,52,52,52                 | 0     |
| 24  | MG   | A     | 1725 | 1/1   | 0.87 | 0.15 | 83,83,83,83                 | 0     |
| 24  | MG   | A     | 1704 | 1/1   | 0.87 | 0.17 | 57,57,57,57                 | 0     |
| 24  | MG   | A     | 1682 | 1/1   | 0.87 | 0.22 | 74,74,74,74                 | 0     |
| 24  | MG   | A     | 1702 | 1/1   | 0.87 | 0.15 | 83,83,83,83                 | 0     |
| 24  | MG   | A     | 1663 | 1/1   | 0.88 | 0.46 | 73,73,73,73                 | 0     |
| 24  | MG   | Q     | 201  | 1/1   | 0.88 | 0.16 | 73,73,73,73                 | 0     |
| 27  | ZN   | D     | 301  | 1/1   | 0.88 | 0.68 | 126,126,126,126             | 0     |
| 24  | MG   | A     | 1736 | 1/1   | 0.88 | 0.48 | 35,35,35,35                 | 0     |
| 24  | MG   | A     | 1728 | 1/1   | 0.88 | 0.17 | 81,81,81,81                 | 0     |
| 24  | MG   | A     | 1749 | 1/1   | 0.88 | 0.28 | 60,60,60,60                 | 0     |
| 24  | MG   | A     | 1761 | 1/1   | 0.88 | 0.23 | 81,81,81,81                 | 0     |
| 24  | MG   | A     | 1671 | 1/1   | 0.88 | 0.54 | 88,88,88,88                 | 0     |
| 25  | K    | A     | 1849 | 1/1   | 0.88 | 0.26 | 117,117,117,117             | 0     |
| 24  | MG   | A     | 1788 | 1/1   | 0.88 | 0.30 | 69,69,69,69                 | 0     |
| 25  | K    | A     | 1850 | 1/1   | 0.88 | 0.46 | 93,93,93,93                 | 0     |
| 24  | MG   | A     | 1778 | 1/1   | 0.88 | 0.20 | 64,64,64,64                 | 0     |
| 24  | MG   | A     | 1789 | 1/1   | 0.88 | 0.19 | 121,121,121,121             | 0     |
| 25  | K    | E     | 203  | 1/1   | 0.88 | 0.36 | 93,93,93,93                 | 0     |
| 25  | K    | A     | 1837 | 1/1   | 0.88 | 0.16 | 122,122,122,122             | 0     |
| 24  | MG   | A     | 1655 | 1/1   | 0.88 | 0.43 | 89,89,89,89                 | 0     |
| 24  | MG   | A     | 1685 | 1/1   | 0.88 | 0.32 | 98,98,98,98                 | 0     |
| 24  | MG   | A     | 1752 | 1/1   | 0.88 | 0.46 | 91,91,91,91                 | 0     |
| 24  | MG   | A     | 1648 | 1/1   | 0.88 | 0.51 | 81,81,81,81                 | 0     |
| 24  | MG   | A     | 1724 | 1/1   | 0.89 | 0.42 | 78,78,78,78                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 24  | MG   | I     | 201  | 1/1   | 0.89 | 0.87 | 62,62,62,62                 | 0     |
| 25  | K    | I     | 202  | 1/1   | 0.89 | 0.52 | 59,59,59,59                 | 0     |
| 24  | MG   | A     | 1634 | 1/1   | 0.89 | 0.24 | 68,68,68,68                 | 0     |
| 24  | MG   | A     | 1755 | 1/1   | 0.89 | 0.12 | 52,52,52,52                 | 0     |
| 24  | MG   | A     | 1638 | 1/1   | 0.89 | 0.22 | 90,90,90,90                 | 0     |
| 24  | MG   | A     | 1606 | 1/1   | 0.90 | 0.16 | 70,70,70,70                 | 0     |
| 25  | K    | A     | 1830 | 1/1   | 0.90 | 0.50 | 93,93,93,93                 | 0     |
| 24  | MG   | A     | 1733 | 1/1   | 0.90 | 0.40 | 56,56,56,56                 | 0     |
| 24  | MG   | A     | 1705 | 1/1   | 0.90 | 0.35 | 74,74,74,74                 | 0     |
| 24  | MG   | A     | 1691 | 1/1   | 0.90 | 0.30 | 68,68,68,68                 | 0     |
| 26  | PAR  | A     | 1854 | 42/42 | 0.91 | 0.23 | 34,38,57,61                 | 0     |
| 25  | K    | A     | 1818 | 1/1   | 0.91 | 0.20 | 107,107,107,107             | 0     |
| 24  | MG   | A     | 1612 | 1/1   | 0.91 | 0.10 | 47,47,47,47                 | 0     |
| 24  | MG   | A     | 1650 | 1/1   | 0.91 | 0.26 | 66,66,66,66                 | 0     |
| 24  | MG   | A     | 1744 | 1/1   | 0.91 | 0.35 | 45,45,45,45                 | 0     |
| 24  | MG   | A     | 1764 | 1/1   | 0.91 | 0.21 | 50,50,50,50                 | 0     |
| 24  | MG   | A     | 1762 | 1/1   | 0.91 | 0.20 | 81,81,81,81                 | 0     |
| 24  | MG   | A     | 1670 | 1/1   | 0.91 | 0.06 | 66,66,66,66                 | 0     |
| 25  | K    | A     | 1833 | 1/1   | 0.91 | 0.38 | 66,66,66,66                 | 0     |
| 24  | MG   | A     | 1689 | 1/1   | 0.91 | 0.53 | 93,93,93,93                 | 0     |
| 24  | MG   | A     | 1719 | 1/1   | 0.91 | 0.17 | 50,50,50,50                 | 0     |
| 24  | MG   | A     | 1721 | 1/1   | 0.91 | 0.39 | 89,89,89,89                 | 0     |
| 24  | MG   | A     | 1669 | 1/1   | 0.91 | 0.36 | 74,74,74,74                 | 0     |
| 24  | MG   | A     | 1717 | 1/1   | 0.92 | 0.07 | 78,78,78,78                 | 0     |
| 24  | MG   | A     | 1775 | 1/1   | 0.92 | 0.20 | 85,85,85,85                 | 0     |
| 24  | MG   | N     | 102  | 1/1   | 0.92 | 0.08 | 66,66,66,66                 | 0     |
| 24  | MG   | A     | 1727 | 1/1   | 0.92 | 0.12 | 63,63,63,63                 | 0     |
| 25  | K    | A     | 1807 | 1/1   | 0.92 | 0.10 | 93,93,93,93                 | 0     |
| 24  | MG   | A     | 1739 | 1/1   | 0.92 | 0.45 | 69,69,69,69                 | 0     |
| 24  | MG   | A     | 1621 | 1/1   | 0.92 | 0.14 | 33,33,33,33                 | 0     |
| 24  | MG   | A     | 1794 | 1/1   | 0.92 | 0.12 | 46,46,46,46                 | 0     |
| 24  | MG   | A     | 1712 | 1/1   | 0.92 | 0.07 | 54,54,54,54                 | 0     |
| 24  | MG   | A     | 1795 | 1/1   | 0.93 | 0.48 | 91,91,91,91                 | 0     |
| 24  | MG   | A     | 1785 | 1/1   | 0.93 | 0.06 | 93,93,93,93                 | 0     |
| 24  | MG   | A     | 1647 | 1/1   | 0.93 | 0.42 | 72,72,72,72                 | 0     |
| 25  | K    | A     | 1824 | 1/1   | 0.93 | 0.05 | 95,95,95,95                 | 0     |
| 24  | MG   | A     | 1740 | 1/1   | 0.93 | 0.42 | 49,49,49,49                 | 0     |
| 24  | MG   | A     | 1640 | 1/1   | 0.93 | 0.33 | 83,83,83,83                 | 0     |
| 25  | K    | A     | 1811 | 1/1   | 0.93 | 0.11 | 123,123,123,123             | 0     |
| 24  | MG   | A     | 1674 | 1/1   | 0.93 | 0.26 | 85,85,85,85                 | 0     |
| 24  | MG   | A     | 1703 | 1/1   | 0.93 | 0.26 | 44,44,44,44                 | 0     |
| 24  | MG   | A     | 1737 | 1/1   | 0.93 | 0.09 | 43,43,43,43                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 24  | MG   | A     | 1630 | 1/1   | 0.93 | 0.45 | 82,82,82,82                 | 0     |
| 24  | MG   | A     | 1624 | 1/1   | 0.93 | 0.31 | 61,61,61,61                 | 0     |
| 24  | MG   | A     | 1688 | 1/1   | 0.93 | 0.39 | 76,76,76,76                 | 0     |
| 24  | MG   | A     | 1786 | 1/1   | 0.93 | 0.39 | 59,59,59,59                 | 0     |
| 24  | MG   | A     | 1708 | 1/1   | 0.93 | 0.35 | 54,54,54,54                 | 0     |
| 24  | MG   | A     | 1700 | 1/1   | 0.94 | 0.29 | 56,56,56,56                 | 0     |
| 24  | MG   | A     | 1790 | 1/1   | 0.94 | 0.47 | 55,55,55,55                 | 0     |
| 24  | MG   | A     | 1799 | 1/1   | 0.94 | 0.23 | 86,86,86,86                 | 0     |
| 24  | MG   | A     | 1635 | 1/1   | 0.94 | 0.45 | 79,79,79,79                 | 0     |
| 24  | MG   | B     | 301  | 1/1   | 0.94 | 0.08 | 38,38,38,38                 | 0     |
| 24  | MG   | A     | 1751 | 1/1   | 0.94 | 0.13 | 70,70,70,70                 | 0     |
| 25  | K    | A     | 1828 | 1/1   | 0.94 | 0.40 | 82,82,82,82                 | 0     |
| 24  | MG   | A     | 1769 | 1/1   | 0.94 | 0.18 | 60,60,60,60                 | 0     |
| 24  | MG   | A     | 1760 | 1/1   | 0.94 | 0.16 | 57,57,57,57                 | 0     |
| 24  | MG   | A     | 1787 | 1/1   | 0.94 | 0.38 | 65,65,65,65                 | 0     |
| 24  | MG   | A     | 1644 | 1/1   | 0.94 | 0.29 | 69,69,69,69                 | 0     |
| 25  | K    | E     | 202  | 1/1   | 0.94 | 0.27 | 69,69,69,69                 | 0     |
| 24  | MG   | A     | 1792 | 1/1   | 0.94 | 0.29 | 57,57,57,57                 | 0     |
| 24  | MG   | A     | 1666 | 1/1   | 0.94 | 0.51 | 87,87,87,87                 | 0     |
| 24  | MG   | A     | 1667 | 1/1   | 0.94 | 0.32 | 40,40,40,40                 | 0     |
| 24  | MG   | A     | 1617 | 1/1   | 0.94 | 0.06 | 55,55,55,55                 | 0     |
| 24  | MG   | A     | 1699 | 1/1   | 0.95 | 0.37 | 31,31,31,31                 | 0     |
| 24  | MG   | A     | 1729 | 1/1   | 0.95 | 0.19 | 53,53,53,53                 | 0     |
| 24  | MG   | A     | 1628 | 1/1   | 0.95 | 0.12 | 59,59,59,59                 | 0     |
| 24  | MG   | A     | 1613 | 1/1   | 0.95 | 0.05 | 35,35,35,35                 | 0     |
| 24  | MG   | A     | 1684 | 1/1   | 0.95 | 0.11 | 55,55,55,55                 | 0     |
| 24  | MG   | A     | 1748 | 1/1   | 0.95 | 0.45 | 79,79,79,79                 | 0     |
| 25  | K    | A     | 1809 | 1/1   | 0.95 | 0.10 | 118,118,118,118             | 0     |
| 24  | MG   | A     | 1781 | 1/1   | 0.95 | 0.32 | 61,61,61,61                 | 0     |
| 24  | MG   | A     | 1798 | 1/1   | 0.95 | 0.04 | 70,70,70,70                 | 0     |
| 24  | MG   | A     | 1616 | 1/1   | 0.95 | 0.11 | 53,53,53,53                 | 0     |
| 24  | MG   | A     | 1723 | 1/1   | 0.95 | 0.09 | 46,46,46,46                 | 0     |
| 24  | MG   | A     | 1730 | 1/1   | 0.95 | 0.24 | 84,84,84,84                 | 0     |
| 24  | MG   | A     | 1681 | 1/1   | 0.95 | 0.26 | 39,39,39,39                 | 0     |
| 25  | K    | A     | 1803 | 1/1   | 0.95 | 0.07 | 97,97,97,97                 | 0     |
| 24  | MG   | A     | 1793 | 1/1   | 0.96 | 0.08 | 36,36,36,36                 | 0     |
| 24  | MG   | A     | 1618 | 1/1   | 0.96 | 0.15 | 40,40,40,40                 | 0     |
| 24  | MG   | A     | 1633 | 1/1   | 0.96 | 0.43 | 86,86,86,86                 | 0     |
| 24  | MG   | A     | 1768 | 1/1   | 0.96 | 0.23 | 66,66,66,66                 | 0     |
| 25  | K    | A     | 1826 | 1/1   | 0.96 | 0.12 | 83,83,83,83                 | 0     |
| 24  | MG   | A     | 1776 | 1/1   | 0.96 | 0.42 | 47,47,47,47                 | 0     |
| 24  | MG   | A     | 1646 | 1/1   | 0.96 | 0.47 | 75,75,75,75                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 24  | MG   | A     | 1753 | 1/1   | 0.96 | 0.14 | 45,45,45,45                 | 0     |
| 24  | MG   | A     | 1701 | 1/1   | 0.96 | 0.07 | 44,44,44,44                 | 0     |
| 24  | MG   | A     | 1741 | 1/1   | 0.96 | 0.28 | 38,38,38,38                 | 0     |
| 25  | K    | A     | 1801 | 1/1   | 0.96 | 0.17 | 76,76,76,76                 | 0     |
| 24  | MG   | A     | 1601 | 1/1   | 0.96 | 0.12 | 56,56,56,56                 | 0     |
| 25  | K    | A     | 1800 | 1/1   | 0.96 | 0.05 | 64,64,64,64                 | 0     |
| 24  | MG   | A     | 1645 | 1/1   | 0.96 | 0.35 | 103,103,103,103             | 0     |
| 24  | MG   | A     | 1607 | 1/1   | 0.97 | 0.46 | 70,70,70,70                 | 0     |
| 24  | MG   | A     | 1654 | 1/1   | 0.97 | 0.50 | 85,85,85,85                 | 0     |
| 24  | MG   | A     | 1747 | 1/1   | 0.97 | 0.30 | 51,51,51,51                 | 0     |
| 24  | MG   | A     | 1605 | 1/1   | 0.97 | 0.36 | 65,65,65,65                 | 0     |
| 24  | MG   | A     | 1661 | 1/1   | 0.97 | 0.26 | 57,57,57,57                 | 0     |
| 24  | MG   | A     | 1639 | 1/1   | 0.97 | 0.17 | 65,65,65,65                 | 0     |
| 24  | MG   | A     | 1686 | 1/1   | 0.97 | 0.34 | 82,82,82,82                 | 0     |
| 24  | MG   | A     | 1608 | 1/1   | 0.97 | 0.28 | 61,61,61,61                 | 0     |
| 24  | MG   | A     | 1693 | 1/1   | 0.97 | 0.28 | 40,40,40,40                 | 0     |
| 24  | MG   | A     | 1746 | 1/1   | 0.97 | 0.30 | 66,66,66,66                 | 0     |
| 24  | MG   | A     | 1609 | 1/1   | 0.97 | 0.26 | 33,33,33,33                 | 0     |
| 24  | MG   | A     | 1672 | 1/1   | 0.97 | 0.15 | 55,55,55,55                 | 0     |
| 24  | MG   | M     | 201  | 1/1   | 0.97 | 0.16 | 49,49,49,49                 | 0     |
| 24  | MG   | A     | 1642 | 1/1   | 0.98 | 0.42 | 67,67,67,67                 | 0     |
| 27  | ZN   | N     | 101  | 1/1   | 0.98 | 0.24 | 73,73,73,73                 | 0     |
| 24  | MG   | A     | 1765 | 1/1   | 0.98 | 0.24 | 59,59,59,59                 | 0     |
| 24  | MG   | A     | 1750 | 1/1   | 0.98 | 0.18 | 52,52,52,52                 | 0     |
| 25  | K    | A     | 1802 | 1/1   | 0.98 | 0.06 | 73,73,73,73                 | 0     |
| 25  | K    | A     | 1842 | 1/1   | 0.98 | 0.42 | 43,43,43,43                 | 0     |
| 24  | MG   | A     | 1743 | 1/1   | 0.98 | 0.26 | 57,57,57,57                 | 0     |
| 24  | MG   | A     | 1774 | 1/1   | 0.98 | 0.14 | 40,40,40,40                 | 0     |
| 24  | MG   | A     | 1679 | 1/1   | 0.98 | 0.22 | 19,19,19,19                 | 0     |
| 24  | MG   | A     | 1649 | 1/1   | 0.98 | 0.16 | 63,63,63,63                 | 0     |
| 24  | MG   | A     | 1745 | 1/1   | 0.98 | 0.27 | 54,54,54,54                 | 0     |
| 24  | MG   | A     | 1742 | 1/1   | 0.99 | 0.11 | 34,34,34,34                 | 0     |
| 24  | MG   | A     | 1791 | 1/1   | 0.99 | 0.08 | 24,24,24,24                 | 0     |
| 24  | MG   | A     | 1604 | 1/1   | 0.99 | 0.10 | 57,57,57,57                 | 0     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.