



## Full wwPDB EM Validation Report ⓘ

Mar 14, 2026 – 02:40 AM UTC

PDB ID : 9H9H / pdb\_00009h9h  
EMDB ID : EMD-51964  
Title : Complex 1 30S-IF1-IF2-IF3-GE81112  
Authors : Schedlbauer, A.; Han, X.; van Bakel, W.; Kaminishi, T.; Ochoa-Lizarralde, B.; Iturrioz, I.; Capuni, R.; Parry, R.; Zegarra, R.; Gil-Carton, D.; Lopez-Alonso, J.P.; Barragan Sanz, K.; Brandi, L.; Gualerzi, C.O.; Fucini, P.; Connell, S.R.  
Deposited on : 2024-10-31  
Resolution : 3.80 Å (reported)  
Based on initial model : 4YBB

This is a Full wwPDB EM 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/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

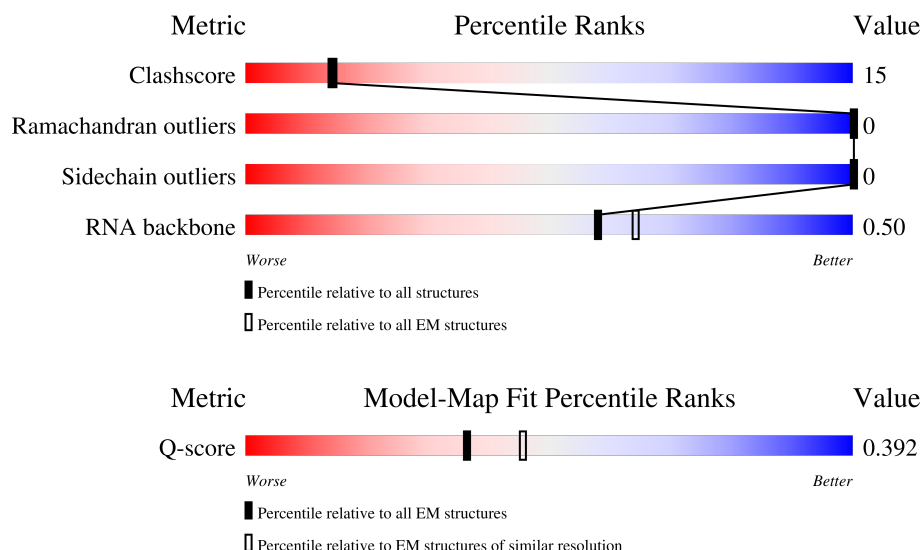
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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.








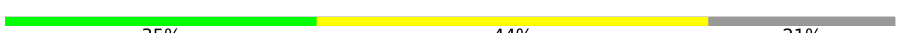




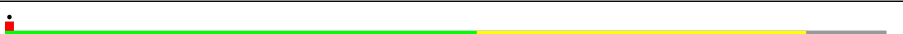



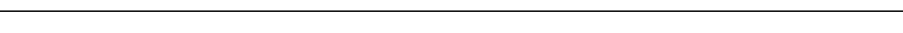
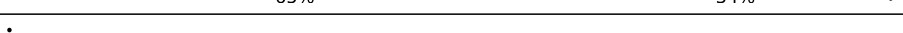








| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|--|
| Clashscore            | 229148                      | 23984                       | -  |
| Ramachandran outliers | 224038                      | 23583                       | -  |
| Sidechain outliers    | 223484                      | 23102                       | -  |
| RNA backbone          | 8273                        | 3508                        | -  |
| Q-score               | -                           | 25397                       | 10198 ( 3.30 - 4.30 )                                    |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 2     | 4      |                  |
| 2   | 3     | 77     |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 3   | A     | 1542   |    |
| 4   | B     | 241    |    |
| 5   | C     | 233    |    |
| 6   | D     | 206    |    |
| 7   | E     | 167    |    |
| 8   | F     | 135    |    |
| 9   | G     | 179    |    |
| 10  | H     | 130    |    |
| 11  | I     | 130    |    |
| 12  | J     | 103    |    |
| 13  | K     | 129    |    |
| 14  | L     | 124    |    |
| 15  | M     | 118    |  |
| 16  | N     | 101    |  |
| 17  | O     | 89     |  |
| 18  | P     | 82     |  |
| 19  | Q     | 84     |  |
| 20  | R     | 75     |  |
| 21  | S     | 92     |  |
| 22  | T     | 87     |  |
| 23  | U     | 71     |  |
| 24  | X     | 72     |  |
| 25  | Y     | 890    |  |
| 26  | Z     | 180    |  |

## 2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 58815 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 mRNA (5'-R(P\*AP\*AP\*UP\*G)-3').

| Mol | Chain | Residues | Atoms |    |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 1   | 2     | 4        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 87    | 39 | 17 | 27 | 4 |         |       |

- Molecule 2 is a RNA chain called t-RNA (77-MER).

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 2   | 3     | 77       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1646  | 732 | 293 | 544 | 77 |         |       |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference     |
|-------|---------|----------|--------|-----------|---------------|
| 3     | 34      | C        | G      | conflict  | GB 2208028712 |
| 3     | 35      | A        | -      | insertion | GB 2208028712 |
| 3     | 37      | A        | C      | conflict  | GB 2208028712 |
| 3     | ?       | -        | G      | deletion  | GB 2208028712 |
| 3     | 69      | U        | C      | conflict  | GB 2208028712 |

- Molecule 3 is a RNA chain called 16S RNA (1534-MER).

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 3   | A     | 1534     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 32930 | 14694 | 6041 | 10661 | 1534 |         |       |

- Molecule 4 is a protein called Small ribosomal subunit protein uS2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4   | B     | 224      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1753  | 1109 | 315 | 321 | 8 |         |       |

- Molecule 5 is a protein called Small ribosomal subunit protein uS3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5   | C     | 211      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1653  | 1046 | 310 | 293 | 4 |         |       |

- Molecule 6 is a protein called Small ribosomal subunit protein uS4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6   | D     | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1643  | 1026 | 315 | 298 | 4 |         |       |

- Molecule 7 is a protein called Small ribosomal subunit protein uS5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | E     | 156      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1152  | 717 | 217 | 212 | 6 |         |       |

- Molecule 8 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | F     | 106      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 862   | 545 | 156 | 154 | 7 |         |       |

- Molecule 9 is a protein called Small ribosomal subunit protein uS7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | G     | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1181  | 735 | 227 | 215 | 4 |         |       |

- Molecule 10 is a protein called Small ribosomal subunit protein uS8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | H     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 979   | 616 | 173 | 184 | 6 |         |       |

- Molecule 11 is a protein called Small ribosomal subunit protein uS9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | I     | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1021  | 634 | 206 | 178 | 3 |         |       |

- Molecule 12 is a protein called Small ribosomal subunit protein uS10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | J     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 803   | 502 | 154 | 146 | 1 |         |       |

- Molecule 13 is a protein called Small ribosomal subunit protein uS11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | K     | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 877   | 540 | 174 | 160 | 3 |         |       |

- Molecule 14 is a protein called Small ribosomal subunit protein uS12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | L     | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 955   | 590 | 196 | 165 | 4 |         |       |

- Molecule 15 is a protein called Small ribosomal subunit protein uS13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | M     | 115      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 891   | 552 | 179 | 157 | 3 |         |       |

- Molecule 16 is a protein called Small ribosomal subunit protein uS14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | N     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 805   | 499 | 164 | 139 | 3 |         |       |

- Molecule 17 is a protein called Small ribosomal subunit protein uS15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | O     | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 714   | 439 | 144 | 130 | 1 |         |       |

- Molecule 18 is a protein called Small ribosomal subunit protein bS16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | P     | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 649   | 406 | 128 | 114 | 1 |         |       |

- Molecule 19 is a protein called Small ribosomal subunit protein uS17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | Q     | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 648   | 411 | 121 | 113 | 3 |         |       |

- Molecule 20 is a protein called Small ribosomal subunit protein bS18.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 20  | R     | 56       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 464   | 293 | 88 | 83 |         |       |

- Molecule 21 is a protein called Small ribosomal subunit protein uS19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | S     | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 663   | 424 | 126 | 111 | 2 |         |       |

- Molecule 22 is a protein called Small ribosomal subunit protein bS20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | T     | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 670   | 414 | 138 | 115 | 3 |         |       |

- Molecule 23 is a protein called Small ribosomal subunit protein bS21.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 23  | U     | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 430   | 269 | 89 | 71 | 1 |         |       |

- Molecule 24 is a protein called Translation initiation factor IF-1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | X     | 70       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 563   | 353 | 102 | 105 | 3 |         |       |

- Molecule 25 is a protein called Translation initiation factor IF-2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 25  | Y     | 488      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3651  | 2278 | 640 | 716 | 17 |         |       |

- Molecule 26 is a protein called Translation initiation factor IF-3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | Z     | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 923   | 586 | 166 | 167 | 4 |         |       |

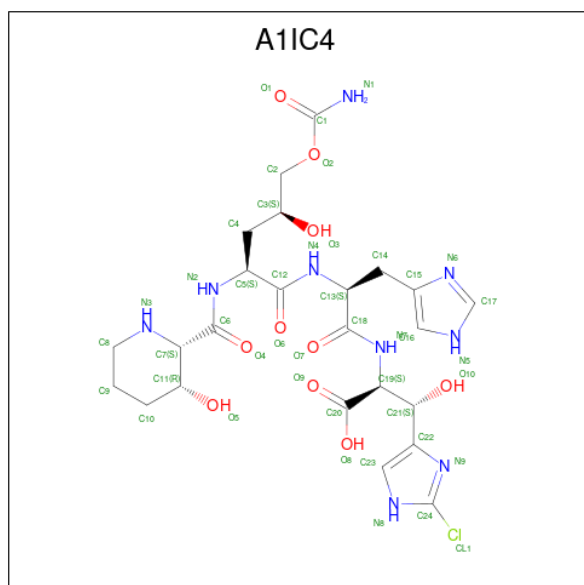
- Molecule 27 is POTASSIUM ION (CCD ID: K) (formula: K).

| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 27  | 2     | 1        | Total | K | 0       |
|     |       |          | 1     | 1 |         |
| 27  | A     | 4        | Total | K | 0       |
|     |       |          | 4     | 4 |         |

- Molecule 28 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 28  | 3     | 3        | Total | Mg  | 0       |
|     |       |          | 3     | 3   |         |
| 28  | A     | 148      | Total | Mg  | 0       |
|     |       |          | 148   | 148 |         |
| 28  | K     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |

- Molecule 29 is (2S,3S)-2-[[[(2S)-2-[[[(2S,4S)-5-aminocarbonyloxy-4-oxidanyl-2-[[[(2S,3R)-3-oxidanylpiperidin-2-yl]carbonylamino]pentanoyl]amino]-3-(1H-imidazol-4-yl)propanoyl]amino]-3-(2-chloranyl-1H-imidazol-4-yl)-3-oxidanyl-propanoic acid (CCD ID: A1IC4) (formula: C<sub>24</sub>H<sub>34</sub>ClN<sub>9</sub>O<sub>10</sub>) (labeled as "Ligand of Interest" by depositor).





| Mol | Chain | Residues | Atoms |    |    |   |    | AltConf |
|-----|-------|----------|-------|----|----|---|----|---------|
| 29  | A     | 1        | Total | C  | Cl | N | O  | 0       |
|     |       |          | 44    | 24 | 1  | 9 | 10 |         |

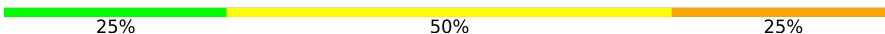
- Molecule 30 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 30  | B     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

### 3 Residue-property plots

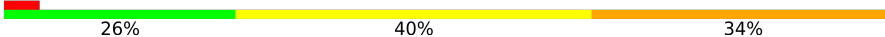
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

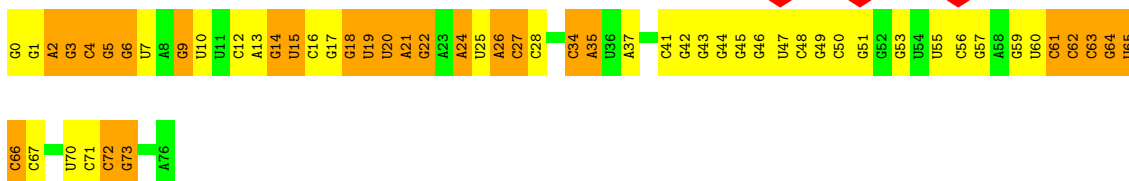
- Molecule 1: mRNA (5'-R(P\*AP\*AP\*UP\*G)-3')

Chain 2: 



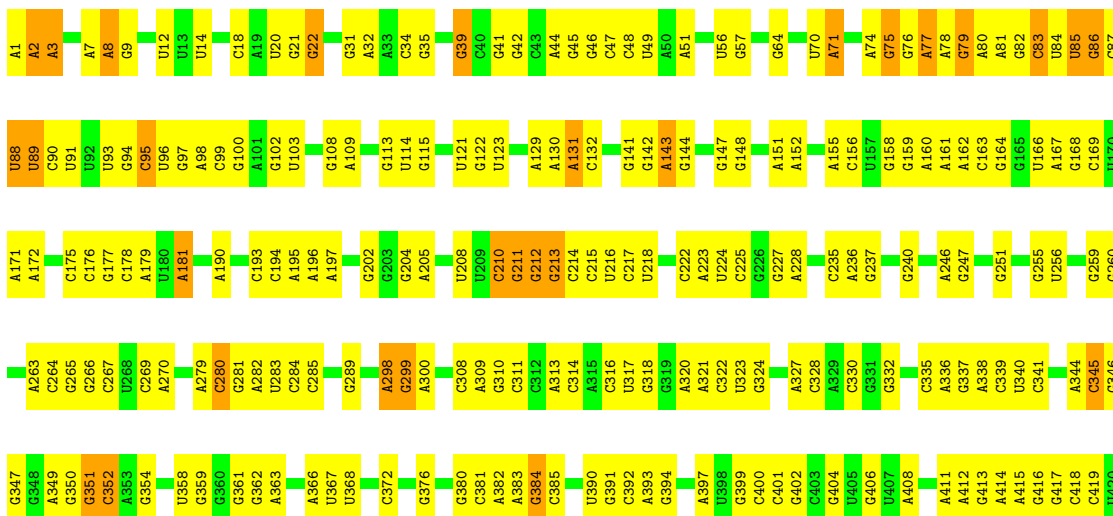
- Molecule 2: t-RNA (77-MER)

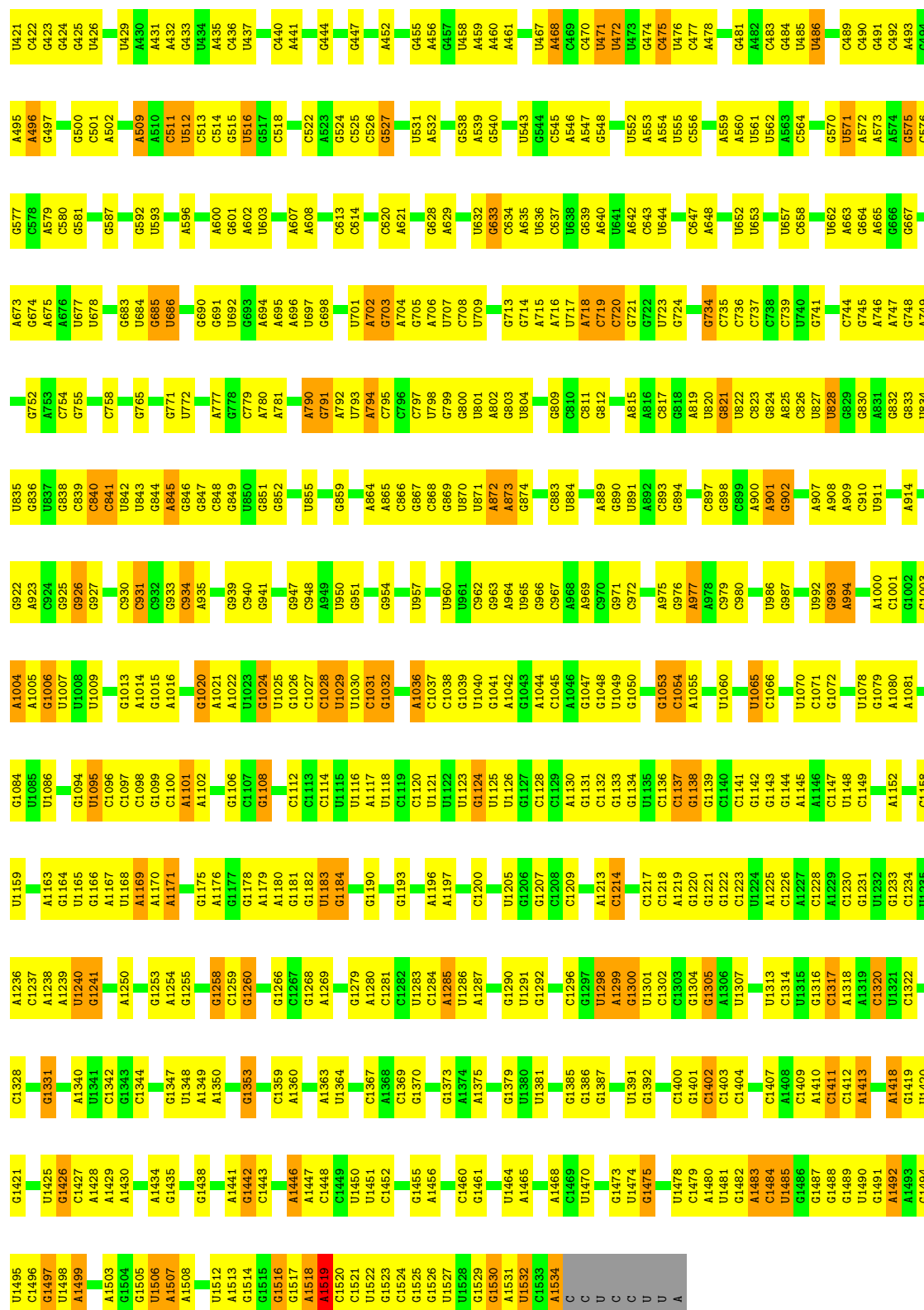
Chain 3: 



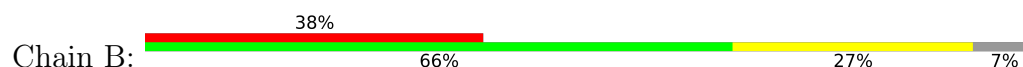
- Molecule 3: 16S RNA (1534-MER)

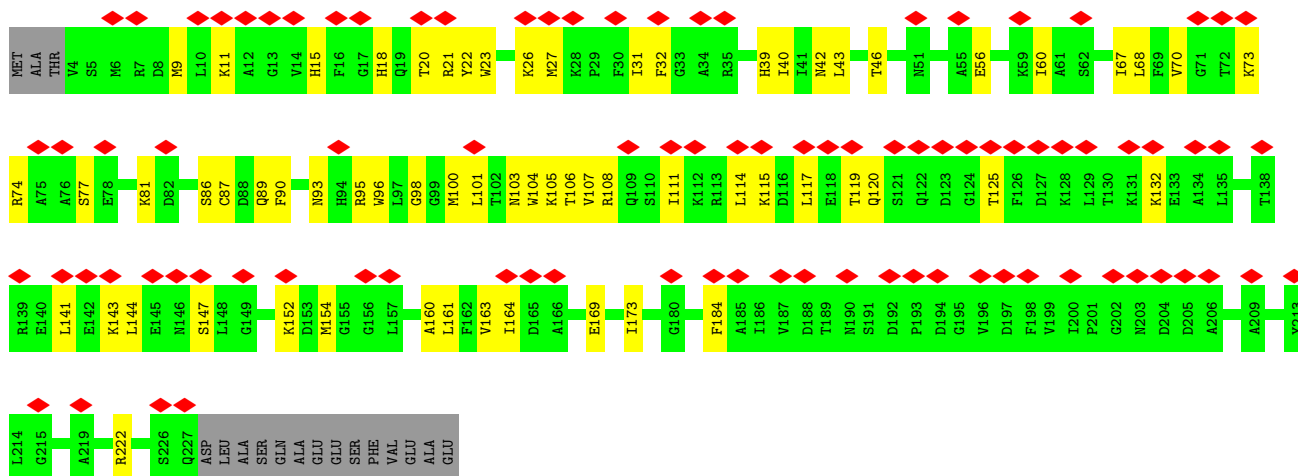
Chain A: 





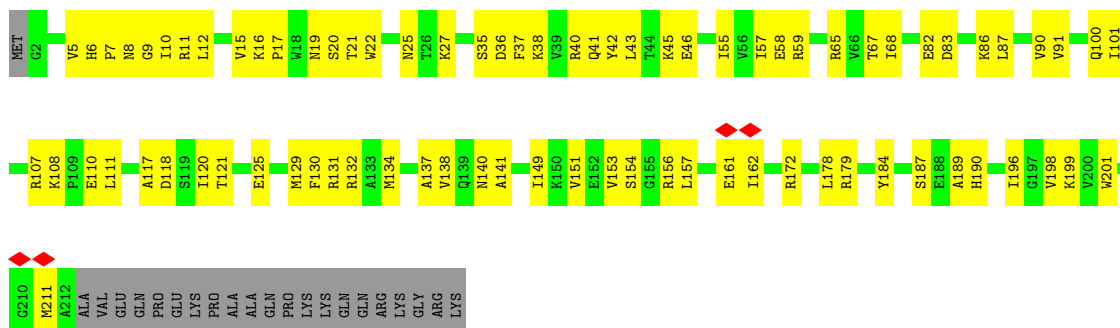
● Molecule 4: Small ribosomal subunit protein uS2





- Molecule 5: Small ribosomal subunit protein uS3

Chain C: 56% 34% 9%



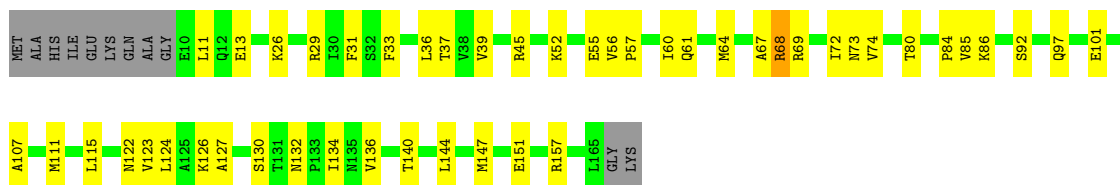
- Molecule 6: Small ribosomal subunit protein uS4

Chain D: 68% 32%

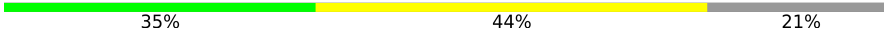


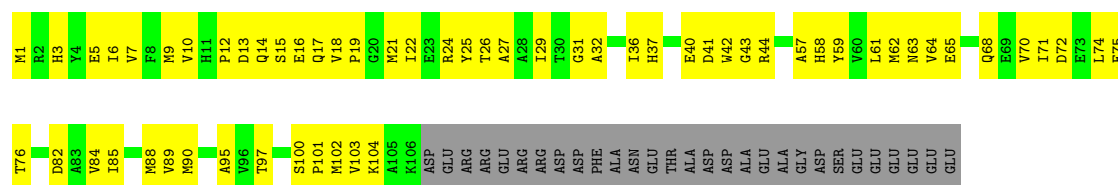
- Molecule 7: Small ribosomal subunit protein uS5

Chain E: 65% 28% 7%



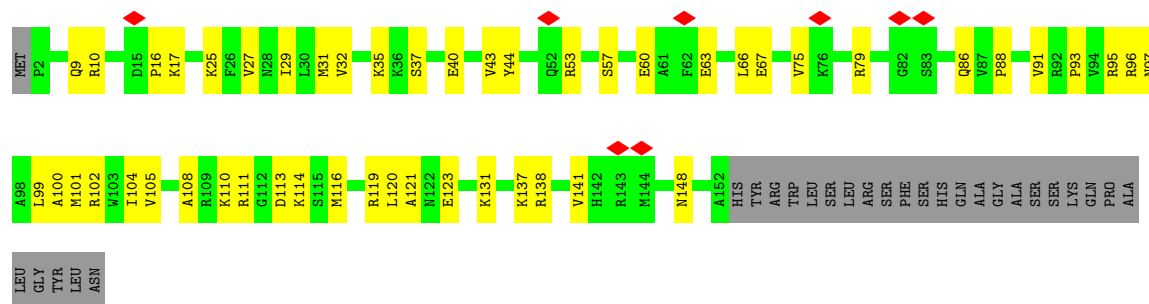
- Molecule 8: Small ribosomal subunit protein bS6, fully modified isoform

Chain F:  35% 44% 21%



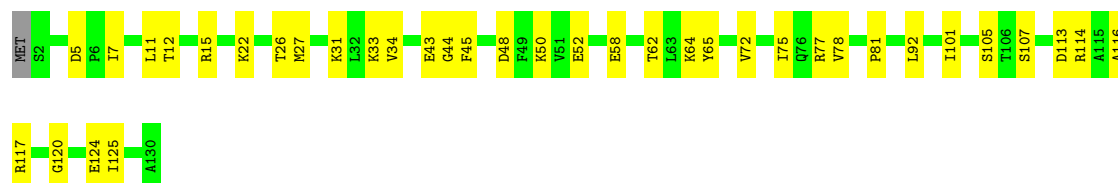
• Molecule 9: Small ribosomal subunit protein uS7

Chain G:  56% 28% 16%



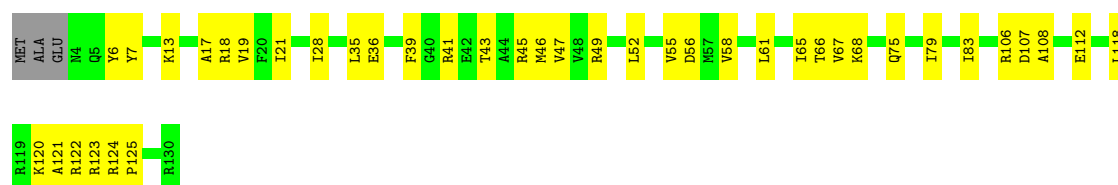
• Molecule 10: Small ribosomal subunit protein uS8

Chain H:  71% 28%



• Molecule 11: Small ribosomal subunit protein uS9

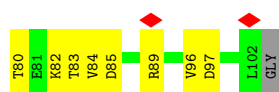
Chain I:  67% 31%



• Molecule 12: Small ribosomal subunit protein uS10

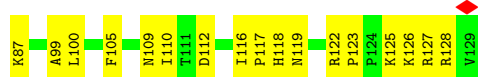
Chain J:  54% 43%





- Molecule 13: Small ribosomal subunit protein uS11

Chain K: 53% 37% 9%



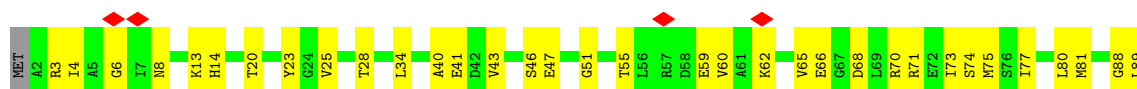
- Molecule 14: Small ribosomal subunit protein uS12

Chain L: 77% 23%



- Molecule 15: Small ribosomal subunit protein uS13

Chain M: 58% 38%



- Molecule 16: Small ribosomal subunit protein uS14

Chain N: 72% 27%



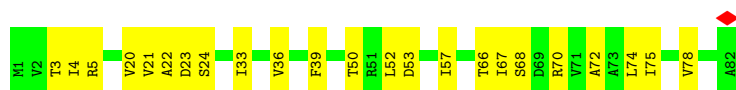
- Molecule 17: Small ribosomal subunit protein uS15

Chain O: 65% 34%



- Molecule 18: Small ribosomal subunit protein bS16

Chain P: 72% 28%



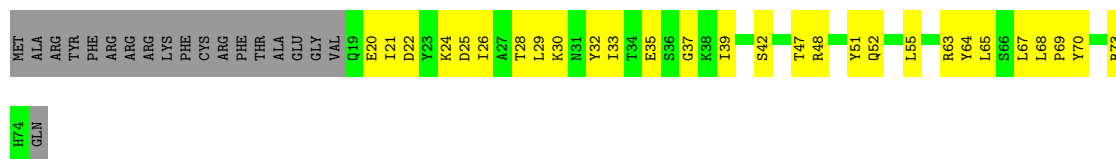
- Molecule 19: Small ribosomal subunit protein uS17

Chain Q: 64% 30% 5%



- Molecule 20: Small ribosomal subunit protein bS18

Chain R: 37% 37% 25%



- Molecule 21: Small ribosomal subunit protein uS19

Chain S: 64% 26% 10%



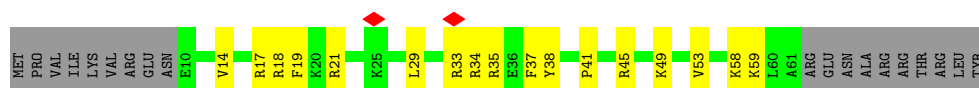
- Molecule 22: Small ribosomal subunit protein bS20

Chain T: 60% 39% 1%



- Molecule 23: Small ribosomal subunit protein bS21

Chain U: 49% 24% 27%



- Molecule 24: Translation initiation factor IF-1

Chain X: 68% 29% 3%



- Molecule 25: Translation initiation factor IF-2







## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 46163                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 51                                      | Depositor |
| Minimum defocus (nm)                 | 400                                     | Depositor |
| Maximum defocus (nm)                 | 3800                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 0.037                                   | Depositor |
| Minimum map value                    | -0.012                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.002                                   | Depositor |
| Recommended contour level            | 0.005                                   | Depositor |
| Map size (Å)                         | 325.8, 325.8, 325.8                     | wwPDB     |
| Map dimensions                       | 300, 300, 300                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.086, 1.086, 1.086                     | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UR3, PSU, 4OC, MA6, K, G7M, 5MC, 2MG, A1IC4, MG, ZN

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   | 2     | 0.40         | 0/97    | 0.45        | 0/149          |
| 2   | 3     | 0.19         | 0/1838  | 0.33        | 0/2863         |
| 3   | A     | 0.25         | 0/36593 | 0.31        | 0/57081        |
| 4   | B     | 0.25         | 0/1784  | 0.47        | 0/2403         |
| 5   | C     | 0.22         | 0/1680  | 0.40        | 0/2263         |
| 6   | D     | 0.31         | 0/1665  | 0.48        | 0/2227         |
| 7   | E     | 0.33         | 0/1165  | 0.53        | 0/1568         |
| 8   | F     | 0.22         | 0/881   | 0.49        | 0/1189         |
| 9   | G     | 0.24         | 0/1195  | 0.46        | 0/1602         |
| 10  | H     | 0.28         | 0/989   | 0.52        | 0/1326         |
| 11  | I     | 0.21         | 0/1033  | 0.49        | 1/1375 (0.1%)  |
| 12  | J     | 0.38         | 0/813   | 0.59        | 0/1100         |
| 13  | K     | 0.48         | 0/893   | 0.63        | 0/1205         |
| 14  | L     | 0.49         | 0/969   | 0.60        | 0/1300         |
| 15  | M     | 0.37         | 0/900   | 0.58        | 0/1204         |
| 16  | N     | 0.15         | 0/817   | 0.42        | 0/1088         |
| 17  | O     | 0.34         | 0/722   | 0.55        | 0/964          |
| 18  | P     | 0.47         | 0/659   | 0.55        | 0/884          |
| 19  | Q     | 0.57         | 0/657   | 0.72        | 0/881          |
| 20  | R     | 0.43         | 0/471   | 0.63        | 0/633          |
| 21  | S     | 0.20         | 0/680   | 0.47        | 0/915          |
| 22  | T     | 0.26         | 0/676   | 0.46        | 0/895          |
| 23  | U     | 0.34         | 0/436   | 0.54        | 0/577          |
| 24  | X     | 0.42         | 0/570   | 0.67        | 0/766          |
| 25  | Y     | 0.43         | 0/3691  | 0.59        | 0/4988         |
| 26  | Z     | 0.28         | 0/934   | 0.58        | 0/1238         |
| All | All   | 0.29         | 0/62808 | 0.41        | 1/92684 (0.0%) |

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

sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 7   | E     | 0                   | 2                   |
| 15  | M     | 0                   | 2                   |
| 19  | Q     | 0                   | 1                   |
| 20  | R     | 0                   | 1                   |
| 25  | Y     | 0                   | 2                   |
| All | All   | 0                   | 8                   |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | I     | 13  | LYS  | CB-CA-C | -5.36 | 110.38      | 116.54   |

There are no chirality outliers.

All (8) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 7   | E     | 68  | ARG  | Sidechain |
| 7   | E     | 69  | ARG  | Sidechain |
| 15  | M     | 92  | ARG  | Sidechain |
| 15  | M     | 93  | ARG  | Sidechain |
| 19  | Q     | 65  | ARG  | Sidechain |
| 20  | R     | 73  | ARG  | Sidechain |
| 25  | Y     | 381 | ARG  | Sidechain |
| 25  | Y     | 455 | ARG  | Sidechain |

## 5.2 Too-close contacts [i](#)

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   | 2     | 87    | 0        | 44       | 4       | 0            |
| 2   | 3     | 1646  | 0        | 832      | 41      | 0            |
| 3   | A     | 32930 | 0        | 16588    | 630     | 0            |
| 4   | B     | 1753  | 0        | 1780     | 56      | 0            |
| 5   | C     | 1653  | 0        | 1722     | 61      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6   | D     | 1643  | 0        | 1707     | 60      | 0            |
| 7   | E     | 1152  | 0        | 1192     | 39      | 0            |
| 8   | F     | 862   | 0        | 864      | 51      | 0            |
| 9   | G     | 1181  | 0        | 1238     | 42      | 0            |
| 10  | H     | 979   | 0        | 1031     | 29      | 0            |
| 11  | I     | 1021  | 0        | 1070     | 31      | 0            |
| 12  | J     | 803   | 0        | 842      | 38      | 0            |
| 13  | K     | 877   | 0        | 887      | 50      | 0            |
| 14  | L     | 955   | 0        | 1016     | 28      | 0            |
| 15  | M     | 891   | 0        | 952      | 38      | 0            |
| 16  | N     | 805   | 0        | 844      | 24      | 0            |
| 17  | O     | 714   | 0        | 734      | 24      | 0            |
| 18  | P     | 649   | 0        | 666      | 18      | 0            |
| 19  | Q     | 648   | 0        | 691      | 19      | 0            |
| 20  | R     | 464   | 0        | 486      | 27      | 0            |
| 21  | S     | 663   | 0        | 688      | 21      | 0            |
| 22  | T     | 670   | 0        | 719      | 26      | 0            |
| 23  | U     | 430   | 0        | 458      | 25      | 0            |
| 24  | X     | 563   | 0        | 581      | 15      | 0            |
| 25  | Y     | 3651  | 0        | 3726     | 162     | 0            |
| 26  | Z     | 923   | 0        | 976      | 46      | 0            |
| 27  | 2     | 1     | 0        | 0        | 0       | 0            |
| 27  | A     | 4     | 0        | 0        | 0       | 0            |
| 28  | 3     | 3     | 0        | 0        | 0       | 0            |
| 28  | A     | 148   | 0        | 0        | 0       | 0            |
| 28  | K     | 1     | 0        | 0        | 0       | 0            |
| 29  | A     | 44    | 0        | 0        | 2       | 0            |
| 30  | B     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 58815 | 0        | 42334    | 1472    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (1472) 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) |
|------------------|------------------|--------------------------|-------------------|
| 13:K:35:THR:HG22 | 13:K:41:ALA:HA   | 1.18                     | 1.16              |
| 13:K:21:ALA:HB3  | 13:K:84:VAL:HG22 | 1.39                     | 1.00              |
| 15:M:4:ILE:HD11  | 15:M:60:VAL:HG21 | 1.48                     | 0.94              |
| 18:P:3:THR:HG22  | 18:P:66:THR:OG1  | 1.69                     | 0.93              |
| 6:D:110:THR:HG23 | 6:D:113:GLU:H    | 1.34                     | 0.91              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 26:Z:86:LYS:O    | 26:Z:90:VAL:HG23  | 1.74                     | 0.88              |
| 12:J:59:LYS:HG2  | 12:J:60:ASP:H     | 1.41                     | 0.85              |
| 12:J:14:ASP:OD2  | 12:J:17:LEU:HG    | 1.77                     | 0.85              |
| 2:3:27:C:H2'     | 2:3:28:C:C6       | 2.13                     | 0.84              |
| 10:H:48:ASP:HB3  | 10:H:62:THR:HB    | 1.60                     | 0.83              |
| 2:3:27:C:H6      | 2:3:27:C:H5'      | 1.44                     | 0.83              |
| 21:S:19:VAL:HG21 | 21:S:44:MET:HG2   | 1.59                     | 0.83              |
| 6:D:124:MET:SD   | 6:D:127:GLY:HA2   | 2.20                     | 0.82              |
| 3:A:718:A:O2'    | 23:U:35:ARG:NH2   | 2.12                     | 0.81              |
| 13:K:21:ALA:CB   | 13:K:84:VAL:HG22  | 2.10                     | 0.81              |
| 25:Y:401:ASP:HA  | 25:Y:404:LYS:HD2  | 1.61                     | 0.81              |
| 25:Y:329:GLY:O   | 25:Y:333:ILE:HG13 | 1.82                     | 0.80              |
| 3:A:1438:G:OP1   | 22:T:29:ARG:HD3   | 1.81                     | 0.80              |
| 19:Q:69:LYS:HG2  | 19:Q:70:THR:HG23  | 1.63                     | 0.79              |
| 3:A:685:G:N2     | 3:A:705:G:O6      | 2.16                     | 0.79              |
| 25:Y:779:LYS:HA  | 25:Y:782:MET:HE3  | 1.64                     | 0.79              |
| 3:A:1298:U:H3    | 9:G:114:LYS:HA    | 1.44                     | 0.79              |
| 3:A:908:A:H2'    | 3:A:909:A:H8      | 1.47                     | 0.79              |
| 9:G:37:SER:HB2   | 11:I:41:ARG:HD2   | 1.64                     | 0.78              |
| 5:C:134:MET:HE3  | 5:C:151:VAL:CG1   | 2.12                     | 0.78              |
| 11:I:55:VAL:O    | 11:I:56:ASP:OD1   | 2.01                     | 0.78              |
| 5:C:134:MET:HE3  | 5:C:151:VAL:HG12  | 1.64                     | 0.78              |
| 3:A:368:U:OP1    | 25:Y:605:ARG:NH2  | 2.17                     | 0.78              |
| 3:A:744:C:H2'    | 3:A:745:G:H8      | 1.49                     | 0.77              |
| 25:Y:409:ASP:HB3 | 25:Y:415:LYS:HG3  | 1.65                     | 0.77              |
| 25:Y:665:LYS:HA  | 25:Y:668:ARG:HE   | 1.50                     | 0.77              |
| 26:Z:93:VAL:HG22 | 26:Z:123:LYS:HB2  | 1.65                     | 0.77              |
| 12:J:6:ILE:HG22  | 12:J:76:ILE:HB    | 1.66                     | 0.77              |
| 24:X:46:ARG:O    | 24:X:70:ARG:NH1   | 2.18                     | 0.77              |
| 14:L:21:VAL:HG12 | 14:L:24:LEU:HB2   | 1.65                     | 0.76              |
| 22:T:35:VAL:O    | 22:T:39:ILE:HG12  | 1.85                     | 0.76              |
| 26:Z:143:GLU:OE1 | 26:Z:143:GLU:N    | 2.19                     | 0.76              |
| 7:E:55:GLU:HG3   | 7:E:57:PRO:HD2    | 1.68                     | 0.76              |
| 15:M:90:ARG:HD2  | 15:M:95:LEU:HB2   | 1.68                     | 0.76              |
| 6:D:95:GLU:HA    | 6:D:100:ASN:HD22  | 1.51                     | 0.75              |
| 3:A:390:U:H2'    | 3:A:391:G:H8      | 1.52                     | 0.75              |
| 3:A:1516:2MG:N2  | 3:A:1519:MA6:OP2  | 2.20                     | 0.75              |
| 22:T:80:THR:O    | 22:T:84:ASN:ND2   | 2.20                     | 0.74              |
| 4:B:23:TRP:HB3   | 4:B:39:HIS:NE2    | 2.03                     | 0.74              |
| 6:D:188:ARG:HH22 | 6:D:193:ALA:HA    | 1.52                     | 0.74              |
| 3:A:1474:U:H2'   | 3:A:1475:G:H8     | 1.53                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:F:22:ILE:O      | 8:F:26:THR:OG1    | 2.05                     | 0.73              |
| 11:I:120:LYS:HG2  | 11:I:123:ARG:HB3  | 1.70                     | 0.73              |
| 14:L:21:VAL:HG13  | 14:L:95:TYR:HE1   | 1.54                     | 0.73              |
| 15:M:77:ILE:HB    | 15:M:91:HIS:HE1   | 1.53                     | 0.73              |
| 3:A:950:U:H3      | 3:A:1231:G:H1     | 1.37                     | 0.72              |
| 12:J:59:LYS:HG2   | 12:J:60:ASP:N     | 2.03                     | 0.72              |
| 2:3:27:C:H2'      | 2:3:28:C:H6       | 1.52                     | 0.72              |
| 3:A:1029:U:O2     | 3:A:1032:G:N1     | 2.18                     | 0.72              |
| 7:E:11:LEU:HD12   | 7:E:39:VAL:HG22   | 1.72                     | 0.72              |
| 3:A:1086:U:H3     | 3:A:1099:G:H1     | 1.38                     | 0.71              |
| 25:Y:575:ASP:HB3  | 25:Y:578:ARG:HB2  | 1.72                     | 0.71              |
| 3:A:1302:C:OP1    | 15:M:13:LYS:NZ    | 2.23                     | 0.71              |
| 6:D:156:LYS:HA    | 6:D:159:LEU:HD12  | 1.72                     | 0.71              |
| 3:A:1240:U:H5''   | 3:A:1241:G:C8     | 2.25                     | 0.71              |
| 17:O:89:ARG:OXT   | 17:O:89:ARG:NH1   | 2.23                     | 0.71              |
| 3:A:222:C:H2'     | 3:A:223:A:H8      | 1.54                     | 0.71              |
| 25:Y:309:ASP:HB3  | 25:Y:364:LYS:HD3  | 1.72                     | 0.70              |
| 25:Y:688:GLU:HG3  | 25:Y:717:LYS:HD2  | 1.74                     | 0.70              |
| 7:E:136:VAL:O     | 7:E:140:THR:HG23  | 1.92                     | 0.70              |
| 12:J:26:VAL:HG23  | 12:J:36:VAL:HG11  | 1.74                     | 0.70              |
| 3:A:1255:G:O2'    | 3:A:1258:G:N3     | 2.24                     | 0.70              |
| 9:G:66:LEU:HD21   | 9:G:97:ASN:OD1    | 1.91                     | 0.70              |
| 13:K:18:ASP:OD2   | 13:K:37:ARG:NH1   | 2.24                     | 0.69              |
| 13:K:116:ILE:HG22 | 13:K:118:HIS:CD2  | 2.26                     | 0.69              |
| 15:M:34:LEU:HD21  | 15:M:41:GLU:HA    | 1.73                     | 0.69              |
| 26:Z:177:LYS:NZ   | 26:Z:178:LYS:O    | 2.22                     | 0.69              |
| 3:A:1218:C:H2'    | 3:A:1219:A:H8     | 1.57                     | 0.69              |
| 25:Y:599:CYS:HB3  | 25:Y:641:VAL:HG22 | 1.74                     | 0.69              |
| 26:Z:177:LYS:HG2  | 26:Z:178:LYS:N    | 2.07                     | 0.69              |
| 3:A:1409:C:H2'    | 3:A:1410:A:H8     | 1.57                     | 0.69              |
| 25:Y:394:VAL:HG21 | 25:Y:548:ILE:HD11 | 1.75                     | 0.69              |
| 13:K:117:PRO:HD2  | 23:U:35:ARG:HH11  | 1.58                     | 0.69              |
| 25:Y:436:GLU:O    | 25:Y:437:ASN:ND2  | 2.26                     | 0.69              |
| 9:G:93:PRO:HA     | 9:G:96:ARG:HD3    | 1.75                     | 0.69              |
| 26:Z:89:LYS:HE3   | 26:Z:89:LYS:HA    | 1.75                     | 0.69              |
| 26:Z:141:GLY:O    | 26:Z:144:VAL:HG22 | 1.92                     | 0.69              |
| 3:A:358:U:O2'     | 25:Y:576:LYS:O    | 2.11                     | 0.68              |
| 3:A:1101:A:OP2    | 4:B:95:ARG:NH1    | 2.27                     | 0.68              |
| 3:A:1513:A:H2'    | 3:A:1514:G:H8     | 1.56                     | 0.68              |
| 3:A:178:C:H2'     | 3:A:179:A:H8      | 1.59                     | 0.68              |
| 8:F:13:ASP:OD1    | 8:F:14:GLN:NE2    | 2.27                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:1328:C:H5''   | 15:M:28:THR:HG21  | 1.76                     | 0.68              |
| 25:Y:514:LEU:CD1  | 25:Y:530:PHE:CE1  | 2.76                     | 0.68              |
| 3:A:166:U:H2'     | 3:A:167:A:C8      | 2.29                     | 0.68              |
| 14:L:65:SER:HG    | 14:L:97:THR:HG1   | 1.41                     | 0.68              |
| 3:A:673:A:H2'     | 3:A:674:G:C8      | 2.29                     | 0.68              |
| 3:A:1158:C:H4'    | 4:B:132:LYS:HD3   | 1.76                     | 0.68              |
| 25:Y:388:GLU:HB2  | 25:Y:561:ARG:HG3  | 1.75                     | 0.67              |
| 3:A:1427:C:H2'    | 3:A:1428:A:H8     | 1.59                     | 0.67              |
| 3:A:166:U:H2'     | 3:A:167:A:H8      | 1.58                     | 0.67              |
| 3:A:1522:U:H2'    | 3:A:1523:G:H8     | 1.59                     | 0.67              |
| 6:D:163:GLU:O     | 6:D:167:LYS:NZ    | 2.27                     | 0.67              |
| 8:F:40:GLU:N      | 8:F:40:GLU:OE1    | 2.27                     | 0.67              |
| 25:Y:586:VAL:O    | 25:Y:623:SER:N    | 2.27                     | 0.67              |
| 10:H:26:THR:HB    | 10:H:58:GLU:OE2   | 1.95                     | 0.67              |
| 14:L:42:PRO:HG3   | 14:L:47:SER:HA    | 1.77                     | 0.67              |
| 26:Z:111:LEU:O    | 26:Z:115:ILE:HG12 | 1.94                     | 0.67              |
| 3:A:1534:A:N6     | 23:U:58:LYS:HE2   | 2.09                     | 0.67              |
| 9:G:91:VAL:HG12   | 9:G:96:ARG:HG3    | 1.75                     | 0.67              |
| 2:3:49:G:N2       | 2:3:66:C:O2       | 2.28                     | 0.67              |
| 11:I:52:LEU:HB3   | 11:I:58:VAL:HG22  | 1.77                     | 0.67              |
| 3:A:745:G:H2'     | 3:A:746:A:H8      | 1.60                     | 0.66              |
| 8:F:12:PRO:O      | 8:F:15:SER:OG     | 2.09                     | 0.66              |
| 16:N:12:LYS:O     | 16:N:16:LEU:HD12  | 1.95                     | 0.66              |
| 25:Y:400:VAL:O    | 25:Y:404:LYS:N    | 2.24                     | 0.66              |
| 25:Y:596:ILE:HD11 | 25:Y:647:GLU:HG3  | 1.77                     | 0.66              |
| 8:F:1:MET:HE2     | 8:F:65:GLU:HG2    | 1.77                     | 0.66              |
| 13:K:110:ILE:HG22 | 23:U:19:PHE:CD1   | 2.30                     | 0.66              |
| 20:R:20:GLU:OE1   | 20:R:20:GLU:N     | 2.23                     | 0.66              |
| 3:A:1530:G:H2'    | 3:A:1531:A:H8     | 1.59                     | 0.66              |
| 3:A:910:C:H2'     | 3:A:911:U:C6      | 2.30                     | 0.66              |
| 26:Z:177:LYS:HG2  | 26:Z:178:LYS:H    | 1.60                     | 0.66              |
| 3:A:900:A:H2'     | 3:A:901:A:C8      | 2.31                     | 0.66              |
| 6:D:110:THR:CG2   | 6:D:113:GLU:H     | 2.05                     | 0.66              |
| 3:A:1350:A:OP1    | 11:I:123:ARG:NH1  | 2.28                     | 0.66              |
| 25:Y:587:ARG:HG3  | 25:Y:588:GLU:HG3  | 1.77                     | 0.66              |
| 3:A:1305:G:N2     | 3:A:1331:G:O2'    | 2.25                     | 0.66              |
| 3:A:1411:C:H42    | 3:A:1489:G:H1     | 1.44                     | 0.66              |
| 15:M:65:VAL:HG12  | 15:M:68:ASP:HB2   | 1.76                     | 0.66              |
| 25:Y:583:THR:HG22 | 25:Y:627:GLU:HG3  | 1.76                     | 0.66              |
| 3:A:1385:G:H2'    | 3:A:1386:G:C8     | 2.31                     | 0.66              |
| 17:O:8:THR:O      | 17:O:12:VAL:HG12  | 1.96                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:Q:48:ASP:OD1   | 19:Q:75:LEU:HD13  | 1.96                     | 0.66              |
| 3:A:458:U:H2'     | 3:A:459:A:H8      | 1.60                     | 0.66              |
| 3:A:745:G:H2'     | 3:A:746:A:C8      | 2.31                     | 0.66              |
| 3:A:1128:C:O2'    | 3:A:1147:C:N3     | 2.28                     | 0.66              |
| 25:Y:426:GLN:OE1  | 25:Y:427:HIS:ND1  | 2.26                     | 0.66              |
| 9:G:57:SER:HB2    | 9:G:60:GLU:HB2    | 1.77                     | 0.65              |
| 13:K:35:THR:CG2   | 13:K:41:ALA:HA    | 2.12                     | 0.65              |
| 2:3:49:G:H1       | 2:3:65:U:H3       | 1.44                     | 0.65              |
| 3:A:1413:A:H2     | 3:A:1487:G:H1     | 1.41                     | 0.65              |
| 8:F:41:ASP:OD1    | 8:F:43:GLY:N      | 2.29                     | 0.65              |
| 20:R:28:THR:HG23  | 20:R:29:LEU:HD12  | 1.78                     | 0.65              |
| 25:Y:397:MET:HE1  | 25:Y:479:THR:HG23 | 1.78                     | 0.65              |
| 3:A:939:G:H4'     | 9:G:102:ARG:HH22  | 1.60                     | 0.65              |
| 10:H:113:ASP:OD1  | 10:H:114:ARG:N    | 2.29                     | 0.65              |
| 25:Y:447:GLY:HA2  | 25:Y:455:ARG:HD3  | 1.77                     | 0.65              |
| 4:B:20:THR:HA     | 4:B:39:HIS:CE1    | 2.32                     | 0.65              |
| 3:A:335:C:H2'     | 3:A:336:A:H8      | 1.60                     | 0.65              |
| 3:A:951:G:OP2     | 15:M:101:ARG:NH1  | 2.29                     | 0.65              |
| 4:B:81:LYS:HZ2    | 4:B:93:ASN:HB2    | 1.62                     | 0.65              |
| 23:U:41:PRO:HB2   | 23:U:45:ARG:HH21  | 1.61                     | 0.65              |
| 4:B:154:MET:SD    | 4:B:154:MET:N     | 2.70                     | 0.65              |
| 25:Y:617:VAL:HG12 | 25:Y:619:GLU:H    | 1.63                     | 0.64              |
| 3:A:664:G:H22     | 3:A:741:G:H1      | 1.45                     | 0.64              |
| 6:D:90:LEU:HD12   | 6:D:91:LEU:HD22   | 1.80                     | 0.64              |
| 4:B:70:VAL:HB     | 4:B:163:VAL:HG12  | 1.79                     | 0.64              |
| 5:C:110:GLU:OE2   | 5:C:140:ASN:OD1   | 2.15                     | 0.64              |
| 3:A:1507:A:H2'    | 3:A:1508:A:C8     | 2.32                     | 0.64              |
| 8:F:21:MET:HA     | 8:F:24:ARG:HB3    | 1.80                     | 0.64              |
| 12:J:37:ARG:N     | 12:J:75:ASP:O     | 2.30                     | 0.64              |
| 10:H:45:PHE:CD1   | 10:H:72:VAL:HG22  | 2.32                     | 0.64              |
| 17:O:36:ILE:HD13  | 17:O:60:VAL:HG12  | 1.79                     | 0.64              |
| 20:R:26:ILE:HG22  | 20:R:30:LYS:HD3   | 1.80                     | 0.64              |
| 25:Y:673:LYS:HG2  | 25:Y:677:MET:HE2  | 1.80                     | 0.64              |
| 3:A:1451:U:OP2    | 3:A:1452:C:N4     | 2.31                     | 0.64              |
| 8:F:6:ILE:HB      | 8:F:62:MET:HG3    | 1.79                     | 0.64              |
| 3:A:1492:A:N6     | 14:L:44:LYS:O     | 2.31                     | 0.64              |
| 3:A:492:C:H2'     | 3:A:493:A:C8      | 2.33                     | 0.63              |
| 3:A:1314:C:N4     | 21:S:2:PRO:O      | 2.32                     | 0.63              |
| 8:F:16:GLU:CD     | 8:F:16:GLU:H      | 2.05                     | 0.63              |
| 3:A:1222:G:OP2    | 3:A:1322:C:N4     | 2.22                     | 0.63              |
| 6:D:90:LEU:CD1    | 6:D:91:LEU:HD22   | 2.29                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:198:HIS:O     | 6:D:202:GLU:HG2   | 1.97                     | 0.63              |
| 13:K:126:LYS:HA   | 23:U:37:PHE:CE1   | 2.33                     | 0.63              |
| 3:A:552:U:H2'     | 3:A:553:A:H8      | 1.64                     | 0.63              |
| 18:P:72:ALA:HA    | 18:P:75:ILE:HD12  | 1.81                     | 0.63              |
| 25:Y:343:ALA:HB1  | 25:Y:347:GLN:HG2  | 1.81                     | 0.63              |
| 19:Q:26:GLU:N     | 19:Q:26:GLU:OE1   | 2.32                     | 0.63              |
| 23:U:59:LYS:O     | 23:U:59:LYS:NZ    | 2.25                     | 0.62              |
| 3:A:1137:C:O2     | 3:A:1138:G:N2     | 2.32                     | 0.62              |
| 14:L:73:ASN:HB3   | 25:Y:670:GLN:HG2  | 1.80                     | 0.62              |
| 3:A:433:G:H21     | 25:Y:300:GLN:HE22 | 1.48                     | 0.62              |
| 3:A:908:A:H2'     | 3:A:909:A:C8      | 2.32                     | 0.62              |
| 3:A:1391:U:H2'    | 3:A:1392:G:H8     | 1.64                     | 0.62              |
| 19:Q:38:ILE:HG22  | 19:Q:39:LYS:N     | 2.14                     | 0.62              |
| 24:X:55:VAL:HA    | 24:X:66:ARG:O     | 2.00                     | 0.62              |
| 25:Y:564:MET:HE1  | 25:Y:566:SER:HB2  | 1.80                     | 0.62              |
| 3:A:18:C:OP1      | 7:E:132:ASN:ND2   | 2.29                     | 0.62              |
| 3:A:77:A:H2'      | 3:A:78:A:C8       | 2.35                     | 0.62              |
| 3:A:408:A:OP1     | 6:D:110:THR:HG21  | 1.99                     | 0.62              |
| 7:E:45:ARG:HH21   | 7:E:72:ILE:C      | 2.07                     | 0.62              |
| 9:G:75:VAL:HB     | 9:G:148:ASN:HD22  | 1.64                     | 0.62              |
| 14:L:70:GLU:N     | 14:L:70:GLU:OE1   | 2.33                     | 0.61              |
| 17:O:29:VAL:HG21  | 17:O:67:LEU:HD21  | 1.82                     | 0.61              |
| 22:T:22:ALA:O     | 22:T:26:SER:OG    | 2.18                     | 0.61              |
| 3:A:1015:G:N2     | 3:A:1218:C:O2     | 2.31                     | 0.61              |
| 2:3:53:G:N2       | 2:3:62:C:O4'      | 2.33                     | 0.61              |
| 9:G:108:ALA:HA    | 9:G:123:GLU:HG3   | 1.81                     | 0.61              |
| 18:P:3:THR:CG2    | 18:P:66:THR:OG1   | 2.47                     | 0.61              |
| 25:Y:321:LEU:HD11 | 25:Y:325:MET:HE3  | 1.82                     | 0.61              |
| 3:A:1166:G:O2'    | 3:A:1170:A:N6     | 2.34                     | 0.61              |
| 6:D:170:TRP:CD2   | 6:D:186:PRO:HG3   | 2.35                     | 0.61              |
| 7:E:36:LEU:HD22   | 7:E:134:ILE:HG22  | 1.82                     | 0.61              |
| 3:A:1427:C:H2'    | 3:A:1428:A:C8     | 2.34                     | 0.61              |
| 3:A:1488:G:H2'    | 3:A:1489:G:C8     | 2.36                     | 0.61              |
| 21:S:63:THR:N     | 21:S:66:MET:HE3   | 2.14                     | 0.61              |
| 25:Y:733:ALA:HA   | 25:Y:743:LEU:HD11 | 1.82                     | 0.61              |
| 4:B:20:THR:HA     | 4:B:39:HIS:HE1    | 1.65                     | 0.61              |
| 9:G:97:ASN:O      | 9:G:101:MET:HG3   | 2.00                     | 0.61              |
| 15:M:8:ASN:ND2    | 15:M:66:GLU:OE2   | 2.34                     | 0.61              |
| 3:A:1513:A:H2'    | 3:A:1514:G:C8     | 2.35                     | 0.61              |
| 13:K:29:ASN:OD1   | 13:K:30:THR:N     | 2.34                     | 0.61              |
| 26:Z:159:GLU:OE1  | 26:Z:160:SER:N    | 2.34                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:X:52:LYS:O     | 24:X:71:SER:OG    | 2.19                     | 0.61              |
| 3:A:824:G:H2'     | 3:A:825:A:C8      | 2.36                     | 0.61              |
| 13:K:110:ILE:CG2  | 23:U:19:PHE:CD1   | 2.83                     | 0.61              |
| 3:A:404:G:OP2     | 6:D:115:ARG:NH2   | 2.32                     | 0.60              |
| 5:C:140:ASN:OD1   | 5:C:141:ALA:N     | 2.34                     | 0.60              |
| 3:A:1114:C:O2'    | 16:N:100:SER:O    | 2.18                     | 0.60              |
| 5:C:40:ARG:HH11   | 5:C:57:ILE:HD13   | 1.67                     | 0.60              |
| 10:H:124:GLU:N    | 10:H:124:GLU:OE1  | 2.33                     | 0.60              |
| 13:K:116:ILE:HG22 | 13:K:118:HIS:HD2  | 1.66                     | 0.60              |
| 22:T:24:ARG:HD3   | 22:T:61:GLN:HE22  | 1.66                     | 0.60              |
| 3:A:930:C:H3'     | 3:A:931:C:H5''    | 1.82                     | 0.60              |
| 21:S:63:THR:H     | 21:S:66:MET:HE3   | 1.67                     | 0.60              |
| 3:A:716:A:H1'     | 13:K:119:ASN:O    | 2.02                     | 0.60              |
| 5:C:108:LYS:HB3   | 5:C:111:LEU:HD12  | 1.83                     | 0.60              |
| 7:E:72:ILE:HD12   | 7:E:73:ASN:H      | 1.67                     | 0.60              |
| 11:I:79:ILE:O     | 11:I:83:ILE:HG22  | 2.02                     | 0.60              |
| 25:Y:609:MET:SD   | 25:Y:619:GLU:HA   | 2.42                     | 0.60              |
| 3:A:71:A:H61      | 3:A:99:C:H1'      | 1.65                     | 0.60              |
| 25:Y:506:ASP:HB3  | 25:Y:509:ARG:HB2  | 1.82                     | 0.60              |
| 3:A:1348:U:H4'    | 11:I:122:ARG:HD2  | 1.83                     | 0.60              |
| 13:K:16:VAL:HG22  | 13:K:79:ILE:HD13  | 1.84                     | 0.60              |
| 15:M:40:ALA:HB3   | 15:M:43:VAL:HG13  | 1.83                     | 0.60              |
| 8:F:15:SER:OG     | 8:F:44:ARG:NH2    | 2.34                     | 0.60              |
| 8:F:68:GLN:O      | 8:F:71:ILE:HG12   | 2.02                     | 0.60              |
| 25:Y:479:THR:O    | 25:Y:483:ILE:HG13 | 2.02                     | 0.60              |
| 1:2:16:A:P        | 3:A:926:G:H22     | 2.26                     | 0.59              |
| 3:A:1239:A:H1'    | 3:A:1241:G:C5     | 2.37                     | 0.59              |
| 14:L:21:VAL:HG11  | 14:L:24:LEU:HD22  | 1.84                     | 0.59              |
| 19:Q:50:ASN:HB2   | 19:Q:52:GLU:HG2   | 1.84                     | 0.59              |
| 3:A:1048:G:N2     | 3:A:1209:C:O2     | 2.29                     | 0.59              |
| 3:A:1118:U:OP1    | 11:I:106:ARG:NH1  | 2.35                     | 0.59              |
| 3:A:1183:U:O2'    | 3:A:1184:G:OP1    | 2.19                     | 0.59              |
| 5:C:11:ARG:HB3    | 5:C:15:VAL:HG22   | 1.85                     | 0.59              |
| 6:D:197:GLU:OE1   | 6:D:197:GLU:N     | 2.27                     | 0.59              |
| 8:F:12:PRO:HD3    | 8:F:57:ALA:HA     | 1.84                     | 0.59              |
| 16:N:41:ARG:O     | 16:N:45:VAL:HG23  | 2.02                     | 0.59              |
| 25:Y:687:HIS:ND1  | 25:Y:715:GLU:O    | 2.36                     | 0.59              |
| 3:A:841:C:H2'     | 3:A:842:U:C5      | 2.37                     | 0.59              |
| 24:X:32:VAL:HG13  | 24:X:63:SER:O     | 2.03                     | 0.59              |
| 2:3:4:C:H2'       | 2:3:5:G:H4'       | 1.82                     | 0.59              |
| 3:A:1124:G:N2     | 3:A:1125:U:O4     | 2.24                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:1165:U:H3     | 3:A:1171:A:H61    | 1.50                     | 0.59              |
| 8:F:9:MET:HG3     | 8:F:85:ILE:HB     | 1.83                     | 0.59              |
| 4:B:73:LYS:HE2    | 4:B:164:ILE:HD11  | 1.83                     | 0.59              |
| 10:H:45:PHE:HD1   | 10:H:72:VAL:HG22  | 1.66                     | 0.59              |
| 19:Q:14:SER:HB2   | 19:Q:22:VAL:HB    | 1.83                     | 0.59              |
| 2:3:27:C:O2       | 2:3:44:G:N2       | 2.36                     | 0.59              |
| 3:A:947:G:H5''    | 15:M:107:ARG:HB2  | 1.84                     | 0.59              |
| 7:E:92:SER:OG     | 7:E:130:SER:O     | 2.18                     | 0.59              |
| 16:N:80:SER:HB2   | 16:N:83:LYS:HD3   | 1.85                     | 0.59              |
| 8:F:29:ILE:HD11   | 8:F:74:LEU:HD11   | 1.85                     | 0.59              |
| 9:G:86:GLN:N      | 9:G:86:GLN:OE1    | 2.36                     | 0.59              |
| 17:O:26:GLU:OE1   | 17:O:26:GLU:N     | 2.31                     | 0.59              |
| 26:Z:70:TYR:HB2   | 26:Z:72:LYS:HZ2   | 1.67                     | 0.59              |
| 3:A:235:C:H2'     | 3:A:236:A:C8      | 2.38                     | 0.58              |
| 3:A:1385:G:H2'    | 3:A:1386:G:H8     | 1.68                     | 0.58              |
| 4:B:117:LEU:HB3   | 4:B:141:LEU:HD21  | 1.84                     | 0.58              |
| 7:E:151:GLU:CD    | 7:E:151:GLU:H     | 2.10                     | 0.58              |
| 11:I:112:GLU:N    | 11:I:112:GLU:OE1  | 2.35                     | 0.58              |
| 25:Y:395:THR:HB   | 25:Y:462:THR:HG21 | 1.83                     | 0.58              |
| 3:A:160:A:H2'     | 3:A:161:A:C8      | 2.37                     | 0.58              |
| 3:A:208:U:O2'     | 3:A:211:G:O6      | 2.20                     | 0.58              |
| 3:A:235:C:H2'     | 3:A:236:A:H8      | 1.67                     | 0.58              |
| 3:A:390:U:H2'     | 3:A:391:G:C8      | 2.37                     | 0.58              |
| 3:A:1240:U:H5''   | 3:A:1241:G:H8     | 1.65                     | 0.58              |
| 4:B:77:SER:O      | 4:B:81:LYS:HG3    | 2.02                     | 0.58              |
| 3:A:1446:A:H2'    | 3:A:1447:A:C8     | 2.38                     | 0.58              |
| 14:L:21:VAL:CG1   | 14:L:24:LEU:HB2   | 2.32                     | 0.58              |
| 2:3:34:C:O2'      | 2:3:35:A:OP1      | 2.21                     | 0.58              |
| 5:C:107:ARG:HD3   | 5:C:107:ARG:N     | 2.18                     | 0.58              |
| 7:E:26:LYS:HD2    | 7:E:26:LYS:O      | 2.04                     | 0.58              |
| 7:E:57:PRO:HA     | 7:E:60:ILE:HG12   | 1.86                     | 0.58              |
| 3:A:210:C:H1'     | 3:A:211:G:N1      | 2.17                     | 0.58              |
| 3:A:399:G:H2'     | 3:A:400:C:C6      | 2.38                     | 0.58              |
| 5:C:21:THR:OG1    | 5:C:58:GLU:OE2    | 2.20                     | 0.58              |
| 3:A:382:A:H2'     | 3:A:383:A:C8      | 2.38                     | 0.58              |
| 3:A:1299:A:N3     | 3:A:1299:A:H2'    | 2.19                     | 0.58              |
| 7:E:29:ARG:HH21   | 7:E:31:PHE:HZ     | 1.51                     | 0.58              |
| 8:F:102:MET:HE2   | 20:R:25:ASP:HA    | 1.85                     | 0.58              |
| 12:J:37:ARG:HB2   | 12:J:75:ASP:HB3   | 1.85                     | 0.58              |
| 13:K:21:ALA:HB3   | 13:K:84:VAL:CG2   | 2.24                     | 0.58              |
| 26:Z:114:LEU:HD11 | 26:Z:152:LEU:HD22 | 1.85                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:941:G:N2      | 3:A:1342:C:O2     | 2.33                     | 0.58              |
| 7:E:101:GLU:N     | 7:E:101:GLU:OE1   | 2.36                     | 0.58              |
| 3:A:1494:G:N2     | 26:Z:103:ASP:OD2  | 2.30                     | 0.58              |
| 18:P:36:VAL:HG11  | 18:P:57:ILE:HD11  | 1.85                     | 0.58              |
| 3:A:376:G:H5''    | 18:P:5:ARG:HB2    | 1.85                     | 0.58              |
| 3:A:1317:C:OP1    | 16:N:24:ARG:NH2   | 2.37                     | 0.58              |
| 3:A:1534:A:H62    | 23:U:58:LYS:HE2   | 1.67                     | 0.58              |
| 6:D:50:ASP:O      | 6:D:54:GLN:HG3    | 2.03                     | 0.58              |
| 10:H:7:ILE:H      | 10:H:7:ILE:HD12   | 1.67                     | 0.58              |
| 2:3:12:C:H5'      | 26:Z:87:LYS:HZ1   | 1.68                     | 0.57              |
| 6:D:90:LEU:HD12   | 6:D:91:LEU:N      | 2.19                     | 0.57              |
| 13:K:46:THR:HG23  | 13:K:49:GLY:H     | 1.69                     | 0.57              |
| 7:E:107:ALA:HB1   | 7:E:111:MET:HE3   | 1.86                     | 0.57              |
| 8:F:42:TRP:HB2    | 8:F:59:TYR:HB2    | 1.85                     | 0.57              |
| 6:D:101:VAL:O     | 6:D:105:MET:HG2   | 2.04                     | 0.57              |
| 18:P:4:ILE:HG13   | 18:P:21:VAL:HG22  | 1.86                     | 0.57              |
| 6:D:197:GLU:H     | 6:D:197:GLU:CD    | 2.12                     | 0.57              |
| 13:K:82:LEU:HD22  | 13:K:105:PHE:HB3  | 1.86                     | 0.57              |
| 25:Y:432:HIS:CG   | 25:Y:432:HIS:O    | 2.58                     | 0.57              |
| 3:A:477:C:H2'     | 3:A:478:A:C8      | 2.39                     | 0.57              |
| 5:C:11:ARG:NH1    | 5:C:178:LEU:HA    | 2.19                     | 0.57              |
| 12:J:85:ASP:O     | 12:J:89:ARG:HG2   | 2.05                     | 0.57              |
| 25:Y:377:VAL:HG21 | 25:Y:653:VAL:HG21 | 1.86                     | 0.57              |
| 3:A:167:A:H2'     | 3:A:168:G:H8      | 1.69                     | 0.57              |
| 3:A:1098:C:OP2    | 4:B:143:LYS:NZ    | 2.38                     | 0.57              |
| 3:A:1223:C:OP2    | 21:S:78:ARG:NH2   | 2.32                     | 0.57              |
| 3:A:1375:A:OP1    | 9:G:25:LYS:NZ     | 2.30                     | 0.57              |
| 9:G:113:ASP:H     | 9:G:119:ARG:HG2   | 1.70                     | 0.57              |
| 15:M:46:SER:OG    | 15:M:47:GLU:N     | 2.33                     | 0.57              |
| 15:M:71:ARG:O     | 15:M:74:SER:OG    | 2.19                     | 0.57              |
| 3:A:34:C:H2'      | 3:A:35:G:H8       | 1.69                     | 0.57              |
| 3:A:1005:A:N7     | 3:A:1024:G:O2'    | 2.36                     | 0.57              |
| 3:A:1013:G:N2     | 3:A:1016:A:OP2    | 2.26                     | 0.57              |
| 9:G:137:LYS:O     | 9:G:141:VAL:HG13  | 2.04                     | 0.57              |
| 17:O:29:VAL:HG23  | 17:O:63:ARG:HG2   | 1.87                     | 0.57              |
| 3:A:1007:U:OP1    | 16:N:19:LYS:NZ    | 2.24                     | 0.57              |
| 3:A:1237:C:H3'    | 3:A:1238:A:H5'    | 1.86                     | 0.57              |
| 3:A:1494:G:C8     | 24:X:18:PRO:HB3   | 2.39                     | 0.57              |
| 15:M:93:ARG:HG3   | 15:M:95:LEU:HG    | 1.86                     | 0.57              |
| 3:A:147:G:H2'     | 3:A:148:G:C8      | 2.39                     | 0.57              |
| 3:A:643:C:OP1     | 10:H:31:LYS:NZ    | 2.37                     | 0.57              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:A:1219:A:H5''   | 16:N:53:ARG:HH11 | 1.70                     | 0.57              |
| 20:R:48:ARG:HD2   | 20:R:48:ARG:N    | 2.19                     | 0.57              |
| 25:Y:329:GLY:HA3  | 25:Y:332:VAL:HB  | 1.86                     | 0.57              |
| 3:A:8:A:N7        | 6:D:206:LYS:HA   | 2.19                     | 0.56              |
| 3:A:1316:G:O6     | 21:S:7:LYS:NZ    | 2.38                     | 0.56              |
| 3:A:1367:C:OP1    | 12:J:62:ARG:NH2  | 2.37                     | 0.56              |
| 25:Y:482:ALA:HA   | 25:Y:485:HIS:CE1 | 2.40                     | 0.56              |
| 3:A:471:U:H2'     | 3:A:472:U:H6     | 1.69                     | 0.56              |
| 3:A:790:A:H2'     | 3:A:791:G:C8     | 2.40                     | 0.56              |
| 3:A:1412:C:H2'    | 3:A:1413:A:O4'   | 2.05                     | 0.56              |
| 3:A:337:G:H2'     | 3:A:338:A:C8     | 2.41                     | 0.56              |
| 3:A:500:G:H2'     | 3:A:501:C:C6     | 2.41                     | 0.56              |
| 3:A:993:G:O2'     | 3:A:994:A:N7     | 2.38                     | 0.56              |
| 8:F:100:SER:HB3   | 8:F:103:VAL:HG22 | 1.87                     | 0.56              |
| 19:Q:59:VAL:HG12  | 19:Q:78:VAL:HG13 | 1.87                     | 0.56              |
| 25:Y:314:GLU:HA   | 25:Y:351:GLN:HB2 | 1.87                     | 0.56              |
| 25:Y:514:LEU:HD13 | 25:Y:530:PHE:HE1 | 1.70                     | 0.56              |
| 3:A:811:C:O2'     | 3:A:901:A:N1     | 2.39                     | 0.56              |
| 6:D:118:VAL:HA    | 6:D:123:ILE:HD13 | 1.86                     | 0.56              |
| 23:U:29:LEU:O     | 23:U:33:ARG:HG2  | 2.05                     | 0.56              |
| 2:3:0:G:O2'       | 2:3:1:G:O5'      | 2.23                     | 0.56              |
| 3:A:181:A:O2'     | 3:A:194:C:N4     | 2.39                     | 0.56              |
| 3:A:299:G:H2'     | 3:A:300:A:C8     | 2.40                     | 0.56              |
| 3:A:458:U:H2'     | 3:A:459:A:C8     | 2.40                     | 0.56              |
| 3:A:1041:G:H2'    | 3:A:1042:A:H8    | 1.69                     | 0.56              |
| 3:A:1060:U:H3     | 3:A:1197:A:H61   | 1.53                     | 0.56              |
| 3:A:1147:C:H2'    | 3:A:1148:U:H6    | 1.71                     | 0.56              |
| 11:I:19:VAL:HG22  | 11:I:65:ILE:HG23 | 1.87                     | 0.56              |
| 16:N:66:GLN:CD    | 16:N:66:GLN:H    | 2.14                     | 0.56              |
| 3:A:868:C:H2'     | 3:A:869:G:O4'    | 2.05                     | 0.56              |
| 3:A:1391:U:H2'    | 3:A:1392:G:C8    | 2.41                     | 0.56              |
| 4:B:26:LYS:H      | 4:B:26:LYS:HD2   | 1.69                     | 0.56              |
| 9:G:16:PRO:HG3    | 11:I:43:THR:HG22 | 1.86                     | 0.56              |
| 17:O:55:GLY:O     | 17:O:59:MET:HG3  | 2.05                     | 0.56              |
| 3:A:171:A:H2'     | 3:A:172:A:C8     | 2.40                     | 0.56              |
| 3:A:824:G:H2'     | 3:A:825:A:H8     | 1.69                     | 0.56              |
| 24:X:56:GLU:OE1   | 24:X:56:GLU:N    | 2.37                     | 0.56              |
| 3:A:986:U:H3      | 3:A:1219:A:H61   | 1.54                     | 0.55              |
| 3:A:1259:C:O2'    | 3:A:1283:U:O2    | 2.24                     | 0.55              |
| 5:C:125:GLU:HG3   | 5:C:189:ALA:HB1  | 1.88                     | 0.55              |
| 14:L:65:SER:OG    | 14:L:97:THR:OG1  | 2.14                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:512:U:H2'     | 3:A:513:C:C6      | 2.41                     | 0.55              |
| 3:A:794:A:H2'     | 3:A:795:C:C6      | 2.42                     | 0.55              |
| 7:E:60:ILE:HG13   | 7:E:61:GLN:N      | 2.20                     | 0.55              |
| 20:R:21:ILE:HG21  | 20:R:55:LEU:HD23  | 1.88                     | 0.55              |
| 3:A:1147:C:O2'    | 11:I:7:TYR:OH     | 2.20                     | 0.55              |
| 3:A:56:U:H2'      | 3:A:57:G:H8       | 1.72                     | 0.55              |
| 3:A:1134:G:N1     | 3:A:1141:C:N3     | 2.54                     | 0.55              |
| 10:H:11:LEU:HD22  | 10:H:75:ILE:HG23  | 1.89                     | 0.55              |
| 16:N:98:LYS:NZ    | 16:N:99:ALA:O     | 2.37                     | 0.55              |
| 21:S:50:ALA:HB1   | 21:S:57:HIS:HB3   | 1.88                     | 0.55              |
| 3:A:739:C:O2'     | 17:O:42:HIS:ND1   | 2.39                     | 0.55              |
| 5:C:7:PRO:HG2     | 5:C:201:TRP:HE1   | 1.71                     | 0.55              |
| 7:E:64:MET:O      | 7:E:68:ARG:HG3    | 2.07                     | 0.55              |
| 25:Y:414:THR:HG23 | 25:Y:416:VAL:HG22 | 1.88                     | 0.55              |
| 25:Y:511:LYS:HA   | 25:Y:514:LEU:HG   | 1.88                     | 0.55              |
| 26:Z:127:THR:HB   | 26:Z:169:GLN:HE21 | 1.72                     | 0.55              |
| 1:2:16:A:OP2      | 3:A:926:G:N1      | 2.35                     | 0.55              |
| 25:Y:321:LEU:HD11 | 25:Y:325:MET:CE   | 2.36                     | 0.55              |
| 25:Y:665:LYS:HA   | 25:Y:668:ARG:NE   | 2.18                     | 0.55              |
| 3:A:634:C:H2'     | 3:A:635:A:H8      | 1.71                     | 0.55              |
| 3:A:1178:G:N2     | 3:A:1181:G:OP2    | 2.39                     | 0.55              |
| 11:I:36:GLU:N     | 11:I:36:GLU:OE1   | 2.38                     | 0.55              |
| 20:R:68:LEU:HG    | 20:R:69:PRO:HD2   | 1.88                     | 0.55              |
| 25:Y:371:ASN:O    | 25:Y:374:GLU:HG2  | 2.06                     | 0.55              |
| 3:A:714:G:H2'     | 3:A:715:A:C8      | 2.41                     | 0.55              |
| 3:A:1320:C:N3     | 21:S:36:ARG:NH2   | 2.55                     | 0.55              |
| 17:O:87:LEU:HD23  | 17:O:87:LEU:H     | 1.70                     | 0.55              |
| 25:Y:522:GLU:HA   | 25:Y:526:GLY:H    | 1.70                     | 0.55              |
| 3:A:539:A:H2'     | 3:A:540:G:C8      | 2.42                     | 0.55              |
| 4:B:86:SER:O      | 4:B:222:ARG:NH1   | 2.38                     | 0.55              |
| 12:J:42:LEU:HB2   | 12:J:71:LEU:HB3   | 1.89                     | 0.55              |
| 25:Y:514:LEU:CD1  | 25:Y:530:PHE:HE1  | 2.19                     | 0.55              |
| 2:3:25:U:H2'      | 2:3:26:A:O4'      | 2.06                     | 0.54              |
| 3:A:1480:A:H2'    | 3:A:1481:U:C6     | 2.42                     | 0.54              |
| 3:A:865:A:H2'     | 3:A:866:C:C6      | 2.43                     | 0.54              |
| 3:A:1426:G:C6     | 3:A:1475:G:C5     | 2.95                     | 0.54              |
| 9:G:111:ARG:HD2   | 9:G:123:GLU:HG2   | 1.89                     | 0.54              |
| 25:Y:321:LEU:CD1  | 25:Y:325:MET:HE3  | 2.38                     | 0.54              |
| 25:Y:528:SER:O    | 25:Y:529:GLN:NE2  | 2.40                     | 0.54              |
| 20:R:42:SER:OG    | 20:R:47:THR:O     | 2.26                     | 0.54              |
| 24:X:35:HIS:O     | 24:X:67:ILE:HG12  | 2.07                     | 0.54              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 2:3:50:C:N4         | 2:3:51:G:O6        | 2.41                     | 0.54              |
| 3:A:1359:C:OP1      | 16:N:62:ASN:ND2    | 2.40                     | 0.54              |
| 8:F:9:MET:HE2       | 8:F:59:TYR:CE2     | 2.43                     | 0.54              |
| 14:L:42:PRO:HD3     | 14:L:48:ALA:O      | 2.08                     | 0.54              |
| 2:3:6:G:N2          | 2:3:67:C:O2        | 2.41                     | 0.54              |
| 3:A:781:A:OP2       | 3:A:800:G:N1       | 2.29                     | 0.54              |
| 3:A:1005:A:N6       | 3:A:1024:G:O3'     | 2.41                     | 0.54              |
| 8:F:27:ALA:O        | 8:F:31:GLY:N       | 2.39                     | 0.54              |
| 3:A:555:U:H2'       | 3:A:556:C:C6       | 2.42                     | 0.54              |
| 20:R:65:LEU:HB3     | 20:R:67:LEU:HG     | 1.90                     | 0.54              |
| 13:K:126:LYS:HD3    | 23:U:37:PHE:CD1    | 2.43                     | 0.54              |
| 3:A:1474:U:O2'      | 3:A:1475:G:H5'     | 2.08                     | 0.54              |
| 19:Q:49:GLU:OE1     | 19:Q:49:GLU:N      | 2.36                     | 0.54              |
| 20:R:35:GLU:OE1     | 20:R:35:GLU:N      | 2.35                     | 0.54              |
| 29:A:1601:A1IC4:O10 | 29:A:1601:A1IC4:N3 | 2.41                     | 0.54              |
| 3:A:440:C:C2        | 3:A:441:A:C8       | 2.95                     | 0.53              |
| 12:J:80:THR:HB      | 12:J:83:THR:HG23   | 1.90                     | 0.53              |
| 6:D:57:GLU:HG2      | 6:D:199:LEU:HD12   | 1.90                     | 0.53              |
| 9:G:86:GLN:HB3      | 9:G:148:ASN:HD21   | 1.73                     | 0.53              |
| 20:R:33:ILE:HD11    | 20:R:37:GLY:HA2    | 1.89                     | 0.53              |
| 3:A:167:A:H2'       | 3:A:168:G:C8       | 2.42                     | 0.53              |
| 3:A:948:C:H3'       | 15:M:105:ASN:HD21  | 1.74                     | 0.53              |
| 3:A:1447:A:H5''     | 3:A:1448:C:H5      | 1.73                     | 0.53              |
| 10:H:116:ALA:O      | 10:H:120:GLY:N     | 2.41                     | 0.53              |
| 4:B:105:LYS:HZ1     | 4:B:106:THR:HG22   | 1.73                     | 0.53              |
| 6:D:50:ASP:OD1      | 6:D:51:TYR:N       | 2.39                     | 0.53              |
| 19:Q:38:ILE:CG2     | 19:Q:39:LYS:N      | 2.72                     | 0.53              |
| 3:A:555:U:H2'       | 3:A:556:C:H6       | 1.74                     | 0.53              |
| 3:A:1009:U:H3       | 3:A:1020:G:H1      | 1.55                     | 0.53              |
| 3:A:1279:G:O2'      | 3:A:1281:C:OP2     | 2.23                     | 0.53              |
| 4:B:114:LEU:HD13    | 4:B:144:LEU:HG     | 1.90                     | 0.53              |
| 12:J:63:ASP:OD2     | 16:N:85:ARG:NH1    | 2.41                     | 0.53              |
| 3:A:392:C:O2'       | 3:A:483:C:O2'      | 2.26                     | 0.53              |
| 3:A:647:C:H2'       | 3:A:648:A:H8       | 1.74                     | 0.53              |
| 3:A:1284:C:H3'      | 3:A:1285:A:H2'     | 1.90                     | 0.53              |
| 3:A:1506:U:O2       | 13:K:128:ARG:NH1   | 2.41                     | 0.53              |
| 6:D:61:VAL:O        | 6:D:64:ILE:HG22    | 2.08                     | 0.53              |
| 8:F:72:ASP:HA       | 8:F:75:GLU:HG2     | 1.90                     | 0.53              |
| 10:H:5:ASP:OD2      | 10:H:77:ARG:NH2    | 2.42                     | 0.53              |
| 12:J:32:THR:HG23    | 12:J:83:THR:HG22   | 1.91                     | 0.53              |
| 26:Z:74:LEU:H       | 26:Z:74:LEU:HD12   | 1.74                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:838:G:H2'     | 3:A:839:C:H6      | 1.73                     | 0.53              |
| 7:E:157:ARG:NH2   | 10:H:43:GLU:OE2   | 2.33                     | 0.53              |
| 8:F:32:ALA:HB2    | 8:F:70:VAL:HG21   | 1.91                     | 0.53              |
| 20:R:29:LEU:HD12  | 20:R:29:LEU:H     | 1.73                     | 0.53              |
| 3:A:436:C:H2'     | 3:A:437:U:C6      | 2.44                     | 0.53              |
| 3:A:1530:G:H2'    | 3:A:1531:A:C8     | 2.43                     | 0.53              |
| 8:F:10:VAL:HG22   | 8:F:84:VAL:HG12   | 1.89                     | 0.53              |
| 11:I:75:GLN:O     | 11:I:79:ILE:HG12  | 2.09                     | 0.53              |
| 12:J:80:THR:HG22  | 12:J:82:LYS:HE2   | 1.91                     | 0.53              |
| 13:K:19:GLY:N     | 13:K:79:ILE:HD11  | 2.24                     | 0.53              |
| 3:A:962:C:H2'     | 3:A:963:G:H8      | 1.74                     | 0.53              |
| 3:A:1496:C:N4     | 3:A:1497:G:O6     | 2.42                     | 0.53              |
| 4:B:31:ILE:HD12   | 4:B:39:HIS:HB3    | 1.90                     | 0.53              |
| 15:M:59:GLU:HA    | 15:M:62:LYS:HE2   | 1.90                     | 0.53              |
| 21:S:10:PHE:HE1   | 21:S:37:ARG:HG3   | 1.74                     | 0.53              |
| 25:Y:471:ALA:HB1  | 25:Y:506:ASP:H    | 1.74                     | 0.53              |
| 3:A:893:C:H2'     | 3:A:894:G:H8      | 1.74                     | 0.52              |
| 4:B:100:MET:HB3   | 4:B:107:VAL:HG11  | 1.90                     | 0.52              |
| 5:C:137:ALA:HA    | 5:C:140:ASN:HD21  | 1.74                     | 0.52              |
| 13:K:13:ARG:CZ    | 13:K:77:TYR:HA    | 2.40                     | 0.52              |
| 13:K:126:LYS:HA   | 23:U:37:PHE:HE1   | 1.72                     | 0.52              |
| 22:T:80:THR:O     | 22:T:83:ILE:HG22  | 2.09                     | 0.52              |
| 6:D:110:THR:HG23  | 6:D:113:GLU:N     | 2.14                     | 0.52              |
| 12:J:80:THR:CG2   | 12:J:82:LYS:HE2   | 2.39                     | 0.52              |
| 15:M:71:ARG:HH12  | 15:M:75:MET:HE3   | 1.74                     | 0.52              |
| 25:Y:394:VAL:HG22 | 25:Y:464:ILE:HB   | 1.90                     | 0.52              |
| 25:Y:397:MET:HE3  | 25:Y:467:LEU:HB2  | 1.91                     | 0.52              |
| 3:A:1526:G:H2'    | 3:A:1527:U:C6     | 2.43                     | 0.52              |
| 4:B:18:HIS:HB3    | 4:B:22:TYR:HD2    | 1.74                     | 0.52              |
| 12:J:22:THR:O     | 12:J:26:VAL:HG12  | 2.10                     | 0.52              |
| 23:U:17:ARG:O     | 23:U:21:ARG:HG2   | 2.10                     | 0.52              |
| 25:Y:399:HIS:ND1  | 25:Y:447:GLY:HA3  | 2.24                     | 0.52              |
| 25:Y:565:ALA:HA   | 25:Y:589:GLY:HA3  | 1.90                     | 0.52              |
| 25:Y:574:LEU:HD21 | 25:Y:634:VAL:HG22 | 1.91                     | 0.52              |
| 3:A:707:U:H2'     | 3:A:708:C:C6      | 2.45                     | 0.52              |
| 3:A:1413:A:N1     | 3:A:1487:G:O6     | 2.43                     | 0.52              |
| 3:A:1507:A:H2'    | 3:A:1508:A:H8     | 1.74                     | 0.52              |
| 5:C:65:ARG:NH1    | 5:C:67:THR:OG1    | 2.42                     | 0.52              |
| 14:L:25:GLU:O     | 14:L:25:GLU:HG2   | 2.09                     | 0.52              |
| 22:T:58:VAL:HG23  | 22:T:59:ASP:OD1   | 2.09                     | 0.52              |
| 25:Y:696:ASP:OD1  | 25:Y:696:ASP:N    | 2.41                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:Z:156:ALA:C    | 26:Z:177:LYS:HE3  | 2.35                     | 0.52              |
| 3:A:78:A:N6       | 3:A:79:G:H21      | 2.08                     | 0.52              |
| 3:A:780:A:H5''    | 13:K:125:LYS:HE2  | 1.91                     | 0.52              |
| 3:A:1027:C:H2'    | 3:A:1028:C:C6     | 2.45                     | 0.52              |
| 4:B:115:LYS:O     | 4:B:119:THR:HG23  | 2.09                     | 0.52              |
| 6:D:13:ARG:HB3    | 6:D:38:PRO:HD3    | 1.91                     | 0.52              |
| 3:A:399:G:H2'     | 3:A:400:C:H6      | 1.72                     | 0.52              |
| 3:A:511:C:OP1     | 6:D:44:ARG:NH1    | 2.42                     | 0.52              |
| 3:A:744:C:H2'     | 3:A:745:G:C8      | 2.37                     | 0.52              |
| 3:A:979:C:OP1     | 3:A:1223:C:N4     | 2.42                     | 0.52              |
| 9:G:101:MET:O     | 9:G:105:VAL:HG13  | 2.09                     | 0.52              |
| 13:K:112:ASP:OD1  | 13:K:112:ASP:O    | 2.28                     | 0.52              |
| 3:A:380:G:N2      | 3:A:383:A:OP2     | 2.42                     | 0.52              |
| 3:A:779:C:H2'     | 3:A:780:A:C8      | 2.44                     | 0.52              |
| 3:A:972:C:OP2     | 12:J:59:LYS:HE2   | 2.09                     | 0.52              |
| 3:A:1236:A:H2'    | 3:A:1237:C:H6     | 1.75                     | 0.52              |
| 5:C:6:HIS:CE1     | 5:C:8:ASN:HB3     | 2.45                     | 0.52              |
| 8:F:21:MET:HB2    | 8:F:25:TYR:CE1    | 2.45                     | 0.52              |
| 13:K:22:HIS:HB2   | 13:K:33:THR:HG23  | 1.91                     | 0.52              |
| 21:S:24:GLU:OE1   | 21:S:24:GLU:N     | 2.28                     | 0.52              |
| 25:Y:311:VAL:HA   | 25:Y:366:ILE:HB   | 1.90                     | 0.52              |
| 25:Y:480:ILE:HA   | 25:Y:483:ILE:HD12 | 1.92                     | 0.52              |
| 25:Y:609:MET:SD   | 25:Y:619:GLU:CA   | 2.98                     | 0.52              |
| 2:3:7:U:O2'       | 2:3:46:G:N2       | 2.34                     | 0.52              |
| 3:A:501:C:H2'     | 3:A:502:A:H8      | 1.74                     | 0.52              |
| 5:C:55:ILE:HG12   | 5:C:68:ILE:HG23   | 1.90                     | 0.52              |
| 5:C:91:VAL:HG11   | 5:C:101:ILE:HD11  | 1.90                     | 0.52              |
| 10:H:31:LYS:HA    | 10:H:34:VAL:HG22  | 1.92                     | 0.52              |
| 25:Y:606:VAL:HG13 | 25:Y:628:ILE:HB   | 1.91                     | 0.52              |
| 25:Y:749:ARG:HA   | 25:Y:749:ARG:NH1  | 2.25                     | 0.52              |
| 9:G:63:GLU:O      | 9:G:67:GLU:HG3    | 2.10                     | 0.52              |
| 12:J:34:ALA:HB2   | 12:J:83:THR:HG21  | 1.91                     | 0.52              |
| 3:A:202:G:HO2'    | 3:A:468:A:H8      | 1.57                     | 0.51              |
| 3:A:1410:A:H2'    | 3:A:1411:C:C6     | 2.45                     | 0.51              |
| 4:B:103:ASN:ND2   | 4:B:106:THR:HG23  | 2.24                     | 0.51              |
| 15:M:23:TYR:HB3   | 15:M:66:GLU:HB3   | 1.92                     | 0.51              |
| 17:O:3:LEU:HD23   | 17:O:38:HIS:CD2   | 2.45                     | 0.51              |
| 25:Y:316:ILE:HB   | 25:Y:320:GLU:OE2  | 2.10                     | 0.51              |
| 12:J:66:GLU:OE2   | 12:J:68:ARG:NH1   | 2.43                     | 0.51              |
| 3:A:791:G:H22     | 3:A:1497:G:H4'    | 1.75                     | 0.51              |
| 3:A:1419:G:H2'    | 3:A:1420:U:O4'    | 2.11                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 17:O:32:LEU:O    | 17:O:36:ILE:HG13  | 2.09                     | 0.51              |
| 26:Z:139:GLN:H   | 26:Z:139:GLN:CD   | 2.14                     | 0.51              |
| 2:3:5:G:O2'      | 2:3:6:G:H5'       | 2.10                     | 0.51              |
| 3:A:1081:A:OP2   | 7:E:52:LYS:NZ     | 2.42                     | 0.51              |
| 4:B:77:SER:HB2   | 4:B:81:LYS:HZ1    | 1.74                     | 0.51              |
| 19:Q:17:MET:HE3  | 19:Q:20:SER:OG    | 2.10                     | 0.51              |
| 12:J:15:HIS:CE1  | 12:J:16:ARG:HG3   | 2.45                     | 0.51              |
| 2:3:34:C:H2'     | 2:3:35:A:H8       | 1.74                     | 0.51              |
| 3:A:1130:A:H61   | 3:A:1144:G:H1'    | 1.75                     | 0.51              |
| 16:N:85:ARG:O    | 16:N:89:MET:HG2   | 2.11                     | 0.51              |
| 25:Y:594:GLY:HA2 | 25:Y:605:ARG:HH12 | 1.74                     | 0.51              |
| 26:Z:71:GLY:HA2  | 26:Z:74:LEU:HD13  | 1.92                     | 0.51              |
| 2:3:72:C:O2'     | 2:3:73:G:H8       | 1.94                     | 0.51              |
| 3:A:161:A:H2'    | 3:A:162:A:C8      | 2.46                     | 0.51              |
| 3:A:515:G:H2'    | 3:A:516:PSU:H6    | 1.76                     | 0.51              |
| 7:E:126:LYS:HD2  | 7:E:127:ALA:H     | 1.76                     | 0.51              |
| 22:T:9:LYS:O     | 22:T:13:GLN:HG2   | 2.09                     | 0.51              |
| 3:A:471:U:H2'    | 3:A:472:U:C6      | 2.45                     | 0.51              |
| 3:A:1481:U:H2'   | 3:A:1482:G:C8     | 2.46                     | 0.51              |
| 8:F:21:MET:HB2   | 8:F:25:TYR:CZ     | 2.46                     | 0.51              |
| 14:L:54:ARG:NH1  | 14:L:62:GLU:HG3   | 2.24                     | 0.51              |
| 3:A:632:U:H5''   | 3:A:633:G:H8      | 1.75                     | 0.51              |
| 3:A:1080:A:OP1   | 7:E:52:LYS:HD3    | 2.11                     | 0.51              |
| 12:J:12:ALA:HB2  | 12:J:96:VAL:HG23  | 1.93                     | 0.51              |
| 25:Y:401:ASP:OD1 | 25:Y:402:HIS:N    | 2.43                     | 0.51              |
| 25:Y:534:SER:HB3 | 25:Y:538:GLY:H    | 1.75                     | 0.51              |
| 3:A:193:C:H2'    | 3:A:194:C:C6      | 2.46                     | 0.51              |
| 3:A:690:G:H2'    | 3:A:691:G:C8      | 2.46                     | 0.51              |
| 3:A:1065:U:H5''  | 3:A:1190:G:H22    | 1.75                     | 0.51              |
| 9:G:37:SER:O     | 9:G:40:GLU:HG2    | 2.11                     | 0.51              |
| 25:Y:309:ASP:OD1 | 25:Y:309:ASP:N    | 2.41                     | 0.51              |
| 25:Y:715:GLU:OE1 | 25:Y:715:GLU:N    | 2.36                     | 0.51              |
| 3:A:707:U:H2'    | 3:A:708:C:H6      | 1.76                     | 0.50              |
| 3:A:1381:U:H1'   | 9:G:79:ARG:HB2    | 1.92                     | 0.50              |
| 4:B:42:ASN:O     | 4:B:46:THR:OG1    | 2.29                     | 0.50              |
| 6:D:147:GLU:HA   | 6:D:150:LYS:HB2   | 1.94                     | 0.50              |
| 9:G:9:GLN:OE1    | 9:G:10:ARG:N      | 2.44                     | 0.50              |
| 25:Y:549:LEU:O   | 25:Y:553:GLU:HG2  | 2.12                     | 0.50              |
| 3:A:298:A:O2'    | 3:A:299:G:OP1     | 2.24                     | 0.50              |
| 3:A:713:G:H2'    | 3:A:714:G:C8      | 2.46                     | 0.50              |
| 7:E:33:PHE:CD2   | 7:E:56:VAL:HG22   | 2.45                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:E:84:PRO:HB3   | 7:E:97:GLN:HB2    | 1.93                     | 0.50              |
| 7:E:144:LEU:O    | 7:E:147:MET:HG2   | 2.11                     | 0.50              |
| 25:Y:425:THR:HB  | 25:Y:446:PRO:HA   | 1.92                     | 0.50              |
| 3:A:358:U:H2'    | 3:A:359:G:H8      | 1.77                     | 0.50              |
| 11:I:107:ASP:OD1 | 11:I:108:ALA:N    | 2.44                     | 0.50              |
| 13:K:68:GLU:OE2  | 13:K:99:ALA:HB1   | 2.11                     | 0.50              |
| 3:A:950:U:H2'    | 3:A:951:G:C8      | 2.47                     | 0.50              |
| 4:B:152:LYS:HG2  | 4:B:152:LYS:O     | 2.11                     | 0.50              |
| 25:Y:327:VAL:HB  | 25:Y:333:ILE:HG12 | 1.92                     | 0.50              |
| 25:Y:408:LEU:O   | 25:Y:412:ARG:N    | 2.25                     | 0.50              |
| 3:A:404:G:P      | 6:D:115:ARG:HH21  | 2.35                     | 0.50              |
| 3:A:893:C:H2'    | 3:A:894:G:C8      | 2.46                     | 0.50              |
| 3:A:948:C:H3'    | 15:M:105:ASN:ND2  | 2.26                     | 0.50              |
| 9:G:75:VAL:HG12  | 9:G:88:PRO:HB3    | 1.94                     | 0.50              |
| 12:J:27:GLU:OE1  | 12:J:27:GLU:HA    | 2.11                     | 0.50              |
| 19:Q:49:GLU:HG2  | 19:Q:50:ASN:OD1   | 2.11                     | 0.50              |
| 2:3:14:G:O2'     | 2:3:15:U:OP1      | 2.24                     | 0.50              |
| 3:A:344:A:O2'    | 3:A:346:G:N7      | 2.41                     | 0.50              |
| 3:A:940:C:H2'    | 3:A:941:G:C8      | 2.46                     | 0.50              |
| 3:A:1175:G:H2'   | 3:A:1176:A:H8     | 1.77                     | 0.50              |
| 6:D:105:MET:HE3  | 6:D:180:GLY:HA3   | 1.93                     | 0.50              |
| 13:K:79:ILE:HG23 | 13:K:105:PHE:CE1  | 2.46                     | 0.50              |
| 3:A:56:U:H2'     | 3:A:57:G:C8       | 2.47                     | 0.50              |
| 3:A:418:C:H2'    | 3:A:419:C:C6      | 2.46                     | 0.50              |
| 3:A:979:C:O2     | 16:N:59:ARG:NH1   | 2.44                     | 0.50              |
| 6:D:188:ARG:NH2  | 6:D:193:ALA:HA    | 2.22                     | 0.50              |
| 9:G:66:LEU:HD11  | 9:G:100:ALA:CB    | 2.42                     | 0.50              |
| 21:S:80:TYR:CZ   | 21:S:82:GLY:HA2   | 2.47                     | 0.50              |
| 3:A:12:U:H4'     | 3:A:526:C:H4'     | 1.93                     | 0.50              |
| 3:A:384:G:H2'    | 3:A:385:C:H6      | 1.76                     | 0.50              |
| 3:A:736:C:H2'    | 3:A:737:C:H6      | 1.76                     | 0.50              |
| 3:A:963:G:H21    | 12:J:57:VAL:HG11  | 1.77                     | 0.50              |
| 5:C:36:ASP:HB3   | 5:C:40:ARG:HH12   | 1.77                     | 0.50              |
| 6:D:110:THR:HG22 | 6:D:113:GLU:HB2   | 1.94                     | 0.50              |
| 10:H:44:GLY:O    | 10:H:64:LYS:NZ    | 2.23                     | 0.50              |
| 3:A:222:C:H2'    | 3:A:223:A:C8      | 2.42                     | 0.49              |
| 3:A:263:A:H2'    | 3:A:264:C:C5      | 2.47                     | 0.49              |
| 3:A:897:C:N4     | 3:A:898:G:O6      | 2.45                     | 0.49              |
| 3:A:1116:U:H2'   | 3:A:1117:A:C8     | 2.47                     | 0.49              |
| 20:R:48:ARG:HD2  | 20:R:48:ARG:H     | 1.75                     | 0.49              |
| 3:A:79:G:N2      | 3:A:80:A:H62      | 2.10                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:A:269:C:H2'    | 3:A:270:A:C8      | 2.47                     | 0.49              |
| 3:A:1038:C:H2'   | 3:A:1039:G:C8     | 2.47                     | 0.49              |
| 3:A:1166:G:N2    | 3:A:1169:A:OP2    | 2.45                     | 0.49              |
| 4:B:77:SER:HB2   | 4:B:81:LYS:NZ     | 2.27                     | 0.49              |
| 9:G:100:ALA:O    | 9:G:104:ILE:HG12  | 2.12                     | 0.49              |
| 17:O:15:PHE:HE1  | 17:O:84:ARG:HH12  | 1.58                     | 0.49              |
| 19:Q:68:SER:HB3  | 19:Q:71:LYS:HB2   | 1.94                     | 0.49              |
| 3:A:195:A:H2'    | 3:A:196:A:C8      | 2.47                     | 0.49              |
| 3:A:255:G:H2'    | 3:A:256:U:C6      | 2.47                     | 0.49              |
| 3:A:496:A:H5'    | 3:A:497:G:OP2     | 2.12                     | 0.49              |
| 3:A:546:A:H4'    | 3:A:548:G:H4'     | 1.94                     | 0.49              |
| 3:A:840:C:H1'    | 3:A:847:G:N2      | 2.27                     | 0.49              |
| 3:A:842:U:H2'    | 3:A:843:U:C6      | 2.47                     | 0.49              |
| 3:A:1426:G:H2'   | 3:A:1427:C:H6     | 1.77                     | 0.49              |
| 6:D:150:LYS:HD3  | 6:D:178:MET:HE3   | 1.93                     | 0.49              |
| 18:P:39:PHE:HD1  | 18:P:74:LEU:HD11  | 1.77                     | 0.49              |
| 3:A:108:G:O6     | 22:T:10:ARG:HG2   | 2.13                     | 0.49              |
| 3:A:1283:U:H2'   | 3:A:1284:C:C6     | 2.46                     | 0.49              |
| 7:E:101:GLU:O    | 7:E:122:ASN:ND2   | 2.45                     | 0.49              |
| 10:H:27:MET:HE2  | 10:H:33:LYS:HD3   | 1.94                     | 0.49              |
| 13:K:67:ALA:HB1  | 13:K:100:LEU:HD22 | 1.93                     | 0.49              |
| 25:Y:664:VAL:O   | 25:Y:668:ARG:HG3  | 2.13                     | 0.49              |
| 3:A:39:G:C4      | 3:A:404:G:N2      | 2.80                     | 0.49              |
| 3:A:130:A:O2'    | 3:A:131:A:O5'     | 2.27                     | 0.49              |
| 3:A:313:A:H2'    | 3:A:314:C:C6      | 2.48                     | 0.49              |
| 3:A:950:U:H2'    | 3:A:951:G:H8      | 1.78                     | 0.49              |
| 3:A:1044:A:N6    | 3:A:1045:C:O2     | 2.45                     | 0.49              |
| 3:A:1095:U:OP1   | 3:A:1108:G:N2     | 2.32                     | 0.49              |
| 4:B:32:PHE:HB2   | 4:B:42:ASN:HB3    | 1.94                     | 0.49              |
| 5:C:137:ALA:HA   | 5:C:140:ASN:ND2   | 2.28                     | 0.49              |
| 13:K:116:ILE:CG2 | 13:K:118:HIS:CD2  | 2.93                     | 0.49              |
| 3:A:323:U:H2'    | 3:A:324:G:O4'     | 2.12                     | 0.49              |
| 3:A:440:C:H2'    | 3:A:441:A:H8      | 1.76                     | 0.49              |
| 3:A:501:C:H2'    | 3:A:502:A:C8      | 2.47                     | 0.49              |
| 3:A:513:C:H2'    | 3:A:514:C:C6      | 2.47                     | 0.49              |
| 12:J:24:GLU:O    | 12:J:28:THR:HG22  | 2.11                     | 0.49              |
| 15:M:3:ARG:NH2   | 15:M:4:ILE:O      | 2.46                     | 0.49              |
| 18:P:3:THR:HG22  | 18:P:66:THR:HG1   | 1.74                     | 0.49              |
| 3:A:236:A:H2'    | 3:A:237:G:H8      | 1.77                     | 0.49              |
| 3:A:475:C:H2'    | 3:A:476:U:C6      | 2.47                     | 0.49              |
| 3:A:509:A:N3     | 3:A:543:U:O2'     | 2.45                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:E:85:VAL:HG12   | 7:E:86:LYS:N      | 2.28                     | 0.49              |
| 15:M:4:ILE:HD11   | 15:M:60:VAL:CG2   | 2.31                     | 0.49              |
| 3:A:691:G:H2'     | 3:A:692:U:C6      | 2.48                     | 0.49              |
| 3:A:1418:A:H62    | 3:A:1482:G:H1'    | 1.78                     | 0.49              |
| 8:F:15:SER:O      | 8:F:18:VAL:HB     | 2.13                     | 0.49              |
| 8:F:88:MET:SD     | 20:R:64:TYR:HE2   | 2.36                     | 0.49              |
| 9:G:116:MET:O     | 9:G:120:LEU:HG    | 2.13                     | 0.49              |
| 21:S:66:MET:SD    | 21:S:74:PHE:HE2   | 2.36                     | 0.49              |
| 22:T:81:ALA:O     | 22:T:85:LYS:HG2   | 2.13                     | 0.49              |
| 25:Y:457:ARG:CZ   | 25:Y:637:ALA:HB1  | 2.43                     | 0.49              |
| 25:Y:522:GLU:N    | 25:Y:528:SER:OG   | 2.46                     | 0.49              |
| 26:Z:114:LEU:HD11 | 26:Z:152:LEU:CD2  | 2.41                     | 0.49              |
| 3:A:142:G:H2'     | 3:A:143:A:C8      | 2.48                     | 0.49              |
| 3:A:628:G:H2'     | 3:A:629:A:C8      | 2.48                     | 0.49              |
| 3:A:811:C:H4'     | 3:A:901:A:H61     | 1.77                     | 0.49              |
| 3:A:1401:G:H2'    | 3:A:1402:4OC:O4'  | 2.12                     | 0.49              |
| 10:H:5:ASP:HB2    | 10:H:81:PRO:HG2   | 1.95                     | 0.49              |
| 12:J:31:ARG:HA    | 12:J:31:ARG:NE    | 2.27                     | 0.49              |
| 17:O:86:GLY:C     | 17:O:88:ARG:HH12  | 2.20                     | 0.49              |
| 25:Y:594:GLY:HA2  | 25:Y:605:ARG:NH1  | 2.28                     | 0.49              |
| 3:A:129:A:H1'     | 3:A:130:A:C8      | 2.48                     | 0.49              |
| 3:A:1521:C:H2'    | 3:A:1522:U:C6     | 2.48                     | 0.49              |
| 4:B:68:LEU:HB3    | 4:B:161:LEU:HD12  | 1.95                     | 0.49              |
| 5:C:134:MET:SD    | 5:C:153:VAL:HG21  | 2.53                     | 0.49              |
| 8:F:37:HIS:CD2    | 8:F:95:ALA:HB1    | 2.48                     | 0.49              |
| 3:A:500:G:H2'     | 3:A:501:C:H6      | 1.75                     | 0.48              |
| 3:A:652:U:O4      | 3:A:752:G:O2'     | 2.24                     | 0.48              |
| 3:A:1041:G:H2'    | 3:A:1042:A:C8     | 2.47                     | 0.48              |
| 17:O:28:GLN:O     | 17:O:32:LEU:HG    | 2.13                     | 0.48              |
| 3:A:737:C:H5'     | 8:F:89:VAL:HG23   | 1.94                     | 0.48              |
| 10:H:105:SER:OG   | 10:H:124:GLU:HB2  | 2.13                     | 0.48              |
| 15:M:70:ARG:HA    | 15:M:73:ILE:HD12  | 1.93                     | 0.48              |
| 16:N:80:SER:O     | 16:N:84:VAL:HG12  | 2.13                     | 0.48              |
| 3:A:674:G:H2'     | 3:A:675:A:C8      | 2.49                     | 0.48              |
| 4:B:56:GLU:O      | 4:B:60:ILE:HG12   | 2.12                     | 0.48              |
| 7:E:45:ARG:NH2    | 7:E:72:ILE:O      | 2.42                     | 0.48              |
| 9:G:75:VAL:HA     | 9:G:88:PRO:HA     | 1.95                     | 0.48              |
| 25:Y:695:ALA:HB3  | 25:Y:701:VAL:HG22 | 1.94                     | 0.48              |
| 25:Y:756:LYS:HD3  | 25:Y:756:LYS:N    | 2.27                     | 0.48              |
| 3:A:175:C:H2'     | 3:A:176:C:C6      | 2.49                     | 0.48              |
| 3:A:212:G:H2'     | 3:A:213:G:O4'     | 2.12                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:575:G:O2'     | 3:A:821:G:H5'     | 2.13                     | 0.48              |
| 3:A:632:U:H5''    | 3:A:633:G:C8      | 2.48                     | 0.48              |
| 3:A:1328:C:OP1    | 15:M:28:THR:OG1   | 2.26                     | 0.48              |
| 25:Y:320:GLU:OE1  | 25:Y:324:LYS:HE2  | 2.13                     | 0.48              |
| 3:A:1455:G:H2'    | 3:A:1456:A:H8     | 1.78                     | 0.48              |
| 4:B:96:TRP:CZ2    | 4:B:98:GLY:HA2    | 2.49                     | 0.48              |
| 8:F:19:PRO:HA     | 8:F:22:ILE:HG12   | 1.96                     | 0.48              |
| 9:G:40:GLU:HA     | 9:G:43:VAL:HG12   | 1.94                     | 0.48              |
| 12:J:18:ILE:O     | 12:J:22:THR:HG22  | 2.13                     | 0.48              |
| 22:T:29:ARG:HA    | 22:T:32:ILE:CG1   | 2.43                     | 0.48              |
| 25:Y:611:ASN:OD1  | 25:Y:615:GLN:N    | 2.38                     | 0.48              |
| 1:2:18:G:C6       | 3:A:1400:C:O4'    | 2.67                     | 0.48              |
| 3:A:412:A:C6      | 3:A:414:A:H1'     | 2.48                     | 0.48              |
| 3:A:825:A:H2'     | 3:A:826:C:C6      | 2.48                     | 0.48              |
| 3:A:1009:U:O2     | 3:A:1020:G:N2     | 2.28                     | 0.48              |
| 3:A:1260:G:H4'    | 3:A:1283:U:O2'    | 2.14                     | 0.48              |
| 6:D:147:GLU:HA    | 6:D:150:LYS:HE3   | 1.95                     | 0.48              |
| 13:K:116:ILE:CG2  | 13:K:118:HIS:HD2  | 2.26                     | 0.48              |
| 22:T:66:LEU:HD23  | 22:T:67:ILE:HG23  | 1.95                     | 0.48              |
| 3:A:662:U:H2'     | 3:A:663:A:C8      | 2.49                     | 0.48              |
| 3:A:719:C:O2      | 20:R:39:ILE:HG13  | 2.14                     | 0.48              |
| 3:A:1031:C:H4'    | 3:A:1032:G:O5'    | 2.14                     | 0.48              |
| 3:A:1053:G:H4'    | 3:A:1054:C:H3'    | 1.95                     | 0.48              |
| 3:A:1190:G:OP1    | 5:C:5:VAL:N       | 2.39                     | 0.48              |
| 4:B:96:TRP:CH2    | 4:B:100:MET:HG3   | 2.48                     | 0.48              |
| 5:C:117:ALA:HB1   | 5:C:187:SER:HB2   | 1.96                     | 0.48              |
| 5:C:161:GLU:HG3   | 5:C:162:ILE:HG13  | 1.96                     | 0.48              |
| 6:D:4:TYR:CZ      | 6:D:11:LEU:HD21   | 2.49                     | 0.48              |
| 8:F:7:VAL:HG12    | 8:F:88:MET:HB2    | 1.96                     | 0.48              |
| 22:T:32:ILE:HA    | 22:T:35:VAL:HG12  | 1.95                     | 0.48              |
| 26:Z:169:GLN:HE22 | 26:Z:171:ILE:HD13 | 1.79                     | 0.48              |
| 3:A:452:A:H1'     | 18:P:70:ARG:HD3   | 1.95                     | 0.48              |
| 3:A:512:U:H2'     | 3:A:513:C:H6      | 1.79                     | 0.48              |
| 3:A:538:G:H2'     | 3:A:539:A:H8      | 1.79                     | 0.48              |
| 3:A:701:U:H4'     | 3:A:703:G:C8      | 2.48                     | 0.48              |
| 3:A:1220:G:P      | 16:N:53:ARG:HH12  | 2.37                     | 0.48              |
| 8:F:100:SER:HA    | 20:R:24:LYS:HZ1   | 1.78                     | 0.48              |
| 11:I:39:PHE:O     | 11:I:45:ARG:NH2   | 2.42                     | 0.48              |
| 17:O:3:LEU:HG     | 17:O:35:GLN:OE1   | 2.13                     | 0.48              |
| 5:C:83:ASP:HA     | 5:C:86:LYS:HG3    | 1.96                     | 0.48              |
| 7:E:45:ARG:NE     | 7:E:45:ARG:HA     | 2.29                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:O:24:SER:HB2   | 17:O:26:GLU:OE1   | 2.14                     | 0.48              |
| 3:A:855:U:OP2     | 3:A:871:U:N3      | 2.40                     | 0.48              |
| 3:A:1291:U:H5''   | 11:I:41:ARG:HE    | 1.77                     | 0.48              |
| 3:A:1464:U:H2'    | 3:A:1465:A:H8     | 1.79                     | 0.48              |
| 5:C:9:GLY:O       | 5:C:12:LEU:HG     | 2.14                     | 0.48              |
| 5:C:42:TYR:CZ     | 5:C:46:GLU:HG3    | 2.49                     | 0.48              |
| 4:B:20:THR:CA     | 4:B:39:HIS:HE1    | 2.26                     | 0.47              |
| 9:G:27:VAL:HG12   | 9:G:43:VAL:HG11   | 1.96                     | 0.47              |
| 13:K:13:ARG:NH2   | 13:K:15:GLN:HE22  | 2.12                     | 0.47              |
| 24:X:56:GLU:OE2   | 24:X:66:ARG:HB3   | 2.14                     | 0.47              |
| 3:A:1047:G:H5''   | 16:N:4:GLN:HG3    | 1.96                     | 0.47              |
| 3:A:1147:C:H2'    | 3:A:1148:U:C6     | 2.50                     | 0.47              |
| 3:A:1298:U:N3     | 9:G:114:LYS:HA    | 2.19                     | 0.47              |
| 3:A:1426:G:H2'    | 3:A:1427:C:C6     | 2.49                     | 0.47              |
| 3:A:1489:G:H2'    | 3:A:1490:U:C6     | 2.48                     | 0.47              |
| 5:C:129:MET:HE1   | 5:C:132:ARG:HG2   | 1.96                     | 0.47              |
| 8:F:3:HIS:CE1     | 8:F:95:ALA:HB2    | 2.49                     | 0.47              |
| 13:K:61:PHE:O     | 13:K:65:VAL:HG23  | 2.15                     | 0.47              |
| 18:P:50:THR:HG21  | 18:P:74:LEU:HD12  | 1.96                     | 0.47              |
| 3:A:216:U:H2'     | 3:A:217:C:C6      | 2.48                     | 0.47              |
| 3:A:460:A:H2'     | 3:A:461:A:C8      | 2.50                     | 0.47              |
| 3:A:592:G:H2'     | 3:A:593:U:H6      | 1.78                     | 0.47              |
| 3:A:736:C:H2'     | 3:A:737:C:C6      | 2.50                     | 0.47              |
| 3:A:791:G:N2      | 3:A:1497:G:H4'    | 2.29                     | 0.47              |
| 14:L:80:ILE:C     | 14:L:102:LEU:HD12 | 2.39                     | 0.47              |
| 17:O:89:ARG:HH11  | 17:O:89:ARG:C     | 2.22                     | 0.47              |
| 3:A:83:C:O2       | 3:A:85:U:N3       | 2.47                     | 0.47              |
| 3:A:820:U:H4'     | 3:A:821:G:OP2     | 2.13                     | 0.47              |
| 3:A:1434:A:H2'    | 3:A:1435:G:O4'    | 2.14                     | 0.47              |
| 13:K:110:ILE:HG22 | 23:U:19:PHE:CE1   | 2.49                     | 0.47              |
| 24:X:46:ARG:C     | 24:X:47:ILE:HD12  | 2.39                     | 0.47              |
| 25:Y:309:ASP:HA   | 25:Y:364:LYS:HB3  | 1.95                     | 0.47              |
| 2:3:1:G:H1'       | 2:3:2:A:C8        | 2.50                     | 0.47              |
| 3:A:431:A:C4      | 3:A:432:A:C8      | 3.03                     | 0.47              |
| 4:B:104:TRP:HE3   | 4:B:108:ARG:HH21  | 1.63                     | 0.47              |
| 5:C:41:GLN:HG2    | 5:C:45:LYS:NZ     | 2.30                     | 0.47              |
| 15:M:20:THR:HA    | 15:M:25:VAL:HG13  | 1.97                     | 0.47              |
| 3:A:636:U:H2'     | 3:A:637:C:C6      | 2.49                     | 0.47              |
| 3:A:843:U:H2'     | 3:A:844:G:H8      | 1.78                     | 0.47              |
| 3:A:872:A:C5      | 3:A:874:G:C8      | 3.02                     | 0.47              |
| 3:A:910:C:H2'     | 3:A:911:U:H6      | 1.78                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:169:GLU:N     | 4:B:169:GLU:OE1   | 2.48                     | 0.47              |
| 2:3:34:C:HO2'     | 2:3:35:A:P        | 2.35                     | 0.47              |
| 2:3:61:C:O2'      | 2:3:62:C:H5'      | 2.15                     | 0.47              |
| 3:A:790:A:O2'     | 26:Z:95:GLU:O     | 2.32                     | 0.47              |
| 3:A:890:G:H1'     | 3:A:891:U:H5      | 1.80                     | 0.47              |
| 3:A:1123:U:O2'    | 12:J:39:PRO:O     | 2.31                     | 0.47              |
| 3:A:1130:A:H2'    | 3:A:1131:G:C8     | 2.49                     | 0.47              |
| 3:A:1240:U:C4     | 9:G:116:MET:HE2   | 2.50                     | 0.47              |
| 3:A:1360:A:OP2    | 16:N:75:ARG:NH2   | 2.48                     | 0.47              |
| 6:D:128:ARG:HA    | 6:D:128:ARG:NH1   | 2.29                     | 0.47              |
| 7:E:13:GLU:OE1    | 7:E:13:GLU:N      | 2.48                     | 0.47              |
| 8:F:32:ALA:CB     | 8:F:70:VAL:HG21   | 2.43                     | 0.47              |
| 8:F:36:ILE:HG22   | 8:F:64:VAL:HG13   | 1.96                     | 0.47              |
| 15:M:77:ILE:HB    | 15:M:91:HIS:CE1   | 2.40                     | 0.47              |
| 25:Y:435:THR:HB   | 25:Y:545:LEU:HD11 | 1.96                     | 0.47              |
| 26:Z:103:ASP:C    | 26:Z:105:GLY:H    | 2.23                     | 0.47              |
| 3:A:384:G:H2'     | 3:A:385:C:C6      | 2.49                     | 0.47              |
| 3:A:719:C:O2'     | 3:A:720:C:O4'     | 2.33                     | 0.47              |
| 3:A:748:G:H2'     | 3:A:749:A:H8      | 1.79                     | 0.47              |
| 25:Y:533:VAL:HB   | 25:Y:541:ILE:HG12 | 1.96                     | 0.47              |
| 25:Y:689:VAL:HG23 | 25:Y:718:VAL:HA   | 1.97                     | 0.47              |
| 3:A:320:A:H2'     | 3:A:321:A:C8      | 2.50                     | 0.47              |
| 3:A:1072:G:O6     | 3:A:1102:A:N6     | 2.48                     | 0.47              |
| 5:C:87:LEU:HD11   | 5:C:101:ILE:HG21  | 1.97                     | 0.47              |
| 5:C:154:SER:O     | 5:C:196:ILE:HD12  | 2.15                     | 0.47              |
| 6:D:105:MET:SD    | 6:D:171:LEU:HD13  | 2.55                     | 0.47              |
| 13:K:126:LYS:HA   | 23:U:37:PHE:CD1   | 2.50                     | 0.47              |
| 21:S:15:LEU:O     | 21:S:19:VAL:HG12  | 2.15                     | 0.47              |
| 24:X:38:GLY:HA2   | 24:X:41:ARG:HG3   | 1.97                     | 0.47              |
| 25:Y:603:TYR:CD1  | 25:Y:603:TYR:C    | 2.92                     | 0.47              |
| 2:3:12:C:H5'      | 26:Z:87:LYS:NZ    | 2.30                     | 0.47              |
| 2:3:63:C:H2'      | 2:3:64:G:C8       | 2.50                     | 0.47              |
| 3:A:930:C:C3'     | 3:A:931:C:H5''    | 2.45                     | 0.47              |
| 3:A:1152:A:OP1    | 12:J:70:HIS:ND1   | 2.45                     | 0.47              |
| 5:C:137:ALA:O     | 5:C:140:ASN:OD1   | 2.33                     | 0.47              |
| 24:X:5:ASP:OD1    | 24:X:5:ASP:N      | 2.47                     | 0.47              |
| 3:A:246:A:C2      | 3:A:282:A:C5      | 3.03                     | 0.46              |
| 3:A:838:G:H2'     | 3:A:839:C:C6      | 2.50                     | 0.46              |
| 3:A:864:A:H2'     | 3:A:865:A:C8      | 2.49                     | 0.46              |
| 3:A:1446:A:H2'    | 3:A:1447:A:H8     | 1.80                     | 0.46              |
| 3:A:1460:C:C2     | 3:A:1461:G:C8     | 3.03                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:C:41:GLN:HG2    | 5:C:45:LYS:HZ3    | 1.80                     | 0.46              |
| 5:C:65:ARG:HA     | 5:C:100:GLN:HG2   | 1.96                     | 0.46              |
| 13:K:20:VAL:HA    | 13:K:83:GLU:O     | 2.15                     | 0.46              |
| 14:L:108:LYS:HD3  | 14:L:108:LYS:N    | 2.30                     | 0.46              |
| 3:A:309:A:H2'     | 3:A:310:G:H8      | 1.78                     | 0.46              |
| 3:A:513:C:H2'     | 3:A:514:C:H6      | 1.79                     | 0.46              |
| 3:A:664:G:N2      | 3:A:741:G:H1      | 2.12                     | 0.46              |
| 3:A:708:C:H2'     | 3:A:709:U:H6      | 1.80                     | 0.46              |
| 3:A:1163:A:H2'    | 3:A:1164:G:H8     | 1.79                     | 0.46              |
| 3:A:1236:A:H2'    | 3:A:1237:C:C6     | 2.50                     | 0.46              |
| 3:A:1250:A:H2     | 3:A:1353:G:H21    | 1.62                     | 0.46              |
| 6:D:71:GLN:OE1    | 6:D:97:ARG:NH1    | 2.37                     | 0.46              |
| 25:Y:390:ARG:HD3  | 25:Y:559:ALA:HB2  | 1.97                     | 0.46              |
| 3:A:393:A:C2      | 3:A:394:G:C8      | 3.03                     | 0.46              |
| 3:A:925:G:C2      | 3:A:927:G:C8      | 3.03                     | 0.46              |
| 3:A:1495:U:H2'    | 3:A:1496:C:C6     | 2.50                     | 0.46              |
| 5:C:138:VAL:HA    | 5:C:149:ILE:HD13  | 1.96                     | 0.46              |
| 2:3:2:A:O2'       | 2:3:3:G:OP1       | 2.33                     | 0.46              |
| 2:3:18:G:H4'      | 2:3:19:U:OP2      | 2.15                     | 0.46              |
| 3:A:825:A:H2'     | 3:A:826:C:H6      | 1.80                     | 0.46              |
| 3:A:1531:A:H2'    | 3:A:1532:U:C6     | 2.50                     | 0.46              |
| 5:C:25:ASN:HD22   | 5:C:27:LYS:HZ1    | 1.63                     | 0.46              |
| 6:D:95:GLU:HA     | 6:D:100:ASN:ND2   | 2.23                     | 0.46              |
| 18:P:74:LEU:O     | 18:P:78:VAL:HG23  | 2.16                     | 0.46              |
| 3:A:418:C:H2'     | 3:A:419:C:H6      | 1.80                     | 0.46              |
| 3:A:833:G:H2'     | 3:A:834:U:C6      | 2.50                     | 0.46              |
| 3:A:979:C:H2'     | 16:N:59:ARG:HH12  | 1.80                     | 0.46              |
| 3:A:1291:U:H2'    | 3:A:1292:G:H8     | 1.81                     | 0.46              |
| 3:A:1429:A:H2'    | 3:A:1430:A:C8     | 2.51                     | 0.46              |
| 3:A:1446:A:C6     | 3:A:1447:A:C6     | 3.03                     | 0.46              |
| 3:A:1478:U:H2'    | 3:A:1479:C:C6     | 2.50                     | 0.46              |
| 6:D:69:GLU:HA     | 6:D:69:GLU:OE1    | 2.14                     | 0.46              |
| 11:I:17:ALA:HB2   | 11:I:67:VAL:HG23  | 1.96                     | 0.46              |
| 25:Y:721:ILE:HG21 | 25:Y:735:LEU:HD11 | 1.96                     | 0.46              |
| 26:Z:75:TYR:O     | 26:Z:79:LYS:HG2   | 2.15                     | 0.46              |
| 3:A:204:G:C4      | 3:A:205:A:C8      | 3.04                     | 0.46              |
| 3:A:1455:G:H2'    | 3:A:1456:A:C8     | 2.51                     | 0.46              |
| 12:J:67:ILE:HG12  | 16:N:96:LEU:HA    | 1.97                     | 0.46              |
| 25:Y:425:THR:O    | 25:Y:446:PRO:HB3  | 2.16                     | 0.46              |
| 3:A:1479:C:H2'    | 3:A:1480:A:H8     | 1.80                     | 0.46              |
| 8:F:18:VAL:HG11   | 8:F:58:HIS:CE1    | 2.51                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:G:31:MET:SD     | 9:G:32:VAL:N      | 2.89                     | 0.46              |
| 14:L:30:LYS:O     | 14:L:81:LEU:HD12  | 2.16                     | 0.46              |
| 21:S:35:SER:O     | 21:S:38:SER:OG    | 2.23                     | 0.46              |
| 25:Y:694:LYS:HD3  | 25:Y:732:ASP:OD1  | 2.16                     | 0.46              |
| 3:A:470:C:H2'     | 3:A:471:U:H6      | 1.80                     | 0.46              |
| 3:A:803:G:H2'     | 3:A:804:U:C6      | 2.51                     | 0.46              |
| 3:A:830:G:H5''    | 4:B:21:ARG:HB3    | 1.98                     | 0.46              |
| 3:A:1418:A:C4     | 3:A:1483:A:C8     | 3.03                     | 0.46              |
| 3:A:1425:U:H2'    | 3:A:1426:G:C8     | 2.51                     | 0.46              |
| 13:K:127:ARG:HG3  | 23:U:37:PHE:CZ    | 2.51                     | 0.46              |
| 17:O:27:VAL:O     | 17:O:31:LEU:HD23  | 2.15                     | 0.46              |
| 23:U:34:ARG:NH1   | 23:U:35:ARG:HB2   | 2.30                     | 0.46              |
| 23:U:49:LYS:O     | 23:U:53:VAL:HG12  | 2.15                     | 0.46              |
| 25:Y:480:ILE:HG13 | 25:Y:483:ILE:HD12 | 1.98                     | 0.46              |
| 25:Y:693:LEU:O    | 25:Y:694:LYS:HD2  | 2.16                     | 0.46              |
| 3:A:41:G:H2'      | 3:A:42:G:H8       | 1.79                     | 0.46              |
| 3:A:867:G:O2'     | 3:A:873:A:N1      | 2.44                     | 0.46              |
| 3:A:1205:U:H4'    | 5:C:190:HIS:HE1   | 1.81                     | 0.46              |
| 3:A:1450:U:N3     | 3:A:1452:C:O2     | 2.49                     | 0.46              |
| 9:G:53:ARG:HH21   | 9:G:121:ALA:HB1   | 1.81                     | 0.46              |
| 13:K:30:THR:O     | 13:K:31:ILE:HD13  | 2.16                     | 0.46              |
| 14:L:75:GLN:NE2   | 25:Y:670:GLN:HE21 | 2.14                     | 0.46              |
| 18:P:23:ASP:OD1   | 18:P:24:SER:N     | 2.49                     | 0.46              |
| 25:Y:522:GLU:HB2  | 25:Y:528:SER:O    | 2.16                     | 0.46              |
| 25:Y:604:GLY:HA3  | 25:Y:630:GLY:O    | 2.15                     | 0.46              |
| 3:A:447:G:N1      | 3:A:486:U:OP2     | 2.29                     | 0.46              |
| 3:A:600:A:H2'     | 3:A:601:G:H8      | 1.80                     | 0.46              |
| 3:A:780:A:H5''    | 13:K:125:LYS:CE   | 2.46                     | 0.46              |
| 3:A:1133:G:H2'    | 3:A:1134:G:C8     | 2.51                     | 0.46              |
| 3:A:1425:U:H2'    | 3:A:1426:G:H8     | 1.81                     | 0.46              |
| 3:A:1484:C:O2'    | 3:A:1485:U:OP1    | 2.27                     | 0.46              |
| 3:A:1488:G:H2'    | 3:A:1489:G:H8     | 1.78                     | 0.46              |
| 7:E:39:VAL:HG12   | 7:E:67:ALA:HB1    | 1.97                     | 0.46              |
| 25:Y:357:VAL:O    | 25:Y:361:MET:HG2  | 2.15                     | 0.46              |
| 25:Y:569:VAL:HG13 | 25:Y:569:VAL:O    | 2.16                     | 0.46              |
| 25:Y:576:LYS:HA   | 25:Y:576:LYS:HD3  | 1.63                     | 0.46              |
| 3:A:1120:C:H2'    | 3:A:1121:U:C6     | 2.50                     | 0.45              |
| 5:C:25:ASN:HD22   | 5:C:27:LYS:NZ     | 2.13                     | 0.45              |
| 6:D:102:VAL:HG13  | 6:D:114:ALA:HB1   | 1.98                     | 0.45              |
| 9:G:25:LYS:O      | 9:G:29:ILE:HG23   | 2.16                     | 0.45              |
| 23:U:14:VAL:O     | 23:U:18:ARG:HG3   | 2.16                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:A:151:A:C5      | 3:A:152:A:C8     | 3.04                     | 0.45              |
| 3:A:227:G:H2'     | 3:A:228:A:C8     | 2.52                     | 0.45              |
| 3:A:539:A:H2'     | 3:A:540:G:H8     | 1.81                     | 0.45              |
| 6:D:50:ASP:O      | 6:D:53:VAL:HG12  | 2.17                     | 0.45              |
| 6:D:164:GLN:OE1   | 6:D:164:GLN:N    | 2.40                     | 0.45              |
| 25:Y:452:THR:HA   | 25:Y:455:ARG:HE  | 1.81                     | 0.45              |
| 3:A:88:U:O2'      | 3:A:89:U:OP2     | 2.28                     | 0.45              |
| 3:A:177:G:H5'     | 22:T:60:ARG:NH1  | 2.31                     | 0.45              |
| 3:A:1524:C:H2'    | 3:A:1525:G:H8    | 1.81                     | 0.45              |
| 4:B:67:ILE:H      | 4:B:89:GLN:NE2   | 2.15                     | 0.45              |
| 22:T:28:MET:HE3   | 22:T:28:MET:HA   | 1.98                     | 0.45              |
| 3:A:71:A:N1       | 3:A:99:C:O2'     | 2.49                     | 0.45              |
| 3:A:717:U:O2'     | 3:A:734:G:O4'    | 2.25                     | 0.45              |
| 4:B:26:LYS:C      | 4:B:27:MET:HE2   | 2.41                     | 0.45              |
| 5:C:35:SER:HB2    | 5:C:59:ARG:HH22  | 1.81                     | 0.45              |
| 22:T:34:LYS:HE3   | 22:T:34:LYS:HB3  | 1.69                     | 0.45              |
| 25:Y:646:ASP:H    | 25:Y:649:LYS:NZ  | 2.14                     | 0.45              |
| 25:Y:749:ARG:HA   | 25:Y:749:ARG:CZ  | 2.47                     | 0.45              |
| 3:A:554:A:H2'     | 3:A:555:U:C6     | 2.51                     | 0.45              |
| 3:A:1349:A:H61    | 3:A:1373:G:H1'   | 1.82                     | 0.45              |
| 4:B:15:HIS:O      | 4:B:40:ILE:HA    | 2.17                     | 0.45              |
| 8:F:29:ILE:HG21   | 8:F:36:ILE:HG23  | 1.99                     | 0.45              |
| 10:H:50:LYS:HG3   | 10:H:52:GLU:OE1  | 2.15                     | 0.45              |
| 12:J:59:LYS:CG    | 12:J:60:ASP:N    | 2.78                     | 0.45              |
| 20:R:29:LEU:O     | 20:R:33:ILE:HG22 | 2.16                     | 0.45              |
| 21:S:11:ILE:HG13  | 21:S:38:SER:HB2  | 1.97                     | 0.45              |
| 24:X:10:GLN:OE1   | 24:X:54:THR:HG22 | 2.17                     | 0.45              |
| 25:Y:695:ALA:HB3  | 25:Y:701:VAL:CG2 | 2.47                     | 0.45              |
| 25:Y:697:VAL:HG23 | 25:Y:700:SER:H   | 1.81                     | 0.45              |
| 26:Z:139:GLN:OE1  | 26:Z:139:GLN:N   | 2.34                     | 0.45              |
| 3:A:872:A:C4      | 3:A:874:G:N7     | 2.84                     | 0.45              |
| 4:B:9:MET:HB2     | 4:B:43:LEU:HD13  | 1.98                     | 0.45              |
| 11:I:68:LYS:HE3   | 11:I:68:LYS:HB3  | 1.80                     | 0.45              |
| 18:P:53:ASP:O     | 18:P:57:ILE:HG12 | 2.17                     | 0.45              |
| 19:Q:77:ARG:HH12  | 19:Q:79:VAL:HG13 | 1.81                     | 0.45              |
| 20:R:65:LEU:HD23  | 20:R:65:LEU:HA   | 1.73                     | 0.45              |
| 25:Y:356:LEU:O    | 25:Y:360:GLU:HG3 | 2.16                     | 0.45              |
| 25:Y:668:ARG:HB2  | 25:Y:668:ARG:CZ  | 2.46                     | 0.45              |
| 2:3:21:A:H4'      | 2:3:22:G:OP2     | 2.15                     | 0.45              |
| 3:A:49:U:C2       | 3:A:361:G:N2     | 2.85                     | 0.45              |
| 3:A:114:U:H2'     | 3:A:115:G:C8     | 2.52                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:707:U:C2      | 3:A:708:C:C5      | 3.04                     | 0.45              |
| 3:A:821:G:H2'     | 3:A:822:U:H6      | 1.82                     | 0.45              |
| 3:A:836:G:C5      | 3:A:851:G:C6      | 3.05                     | 0.45              |
| 3:A:1147:C:O2     | 11:I:18:ARG:NH1   | 2.50                     | 0.45              |
| 7:E:115:LEU:HD13  | 7:E:123:VAL:HG11  | 1.99                     | 0.45              |
| 11:I:46:MET:O     | 11:I:49:ARG:HG2   | 2.17                     | 0.45              |
| 11:I:121:ALA:O    | 11:I:122:ARG:HG2  | 2.16                     | 0.45              |
| 11:I:124:ARG:HG3  | 11:I:125:PRO:HD2  | 1.99                     | 0.45              |
| 14:L:30:LYS:HD2   | 14:L:30:LYS:HA    | 1.79                     | 0.45              |
| 25:Y:306:VAL:O    | 25:Y:363:HIS:ND1  | 2.48                     | 0.45              |
| 25:Y:591:LEU:HB2  | 25:Y:620:ALA:HB3  | 1.98                     | 0.45              |
| 25:Y:603:TYR:CE2  | 25:Y:651:ARG:HA   | 2.51                     | 0.45              |
| 3:A:155:A:H2'     | 3:A:156:C:O4'     | 2.17                     | 0.45              |
| 3:A:176:C:H2'     | 3:A:177:G:N3      | 2.32                     | 0.45              |
| 3:A:323:U:OP1     | 22:T:21:ASN:ND2   | 2.31                     | 0.45              |
| 3:A:1028:C:HO2'   | 3:A:1029:U:H6     | 1.62                     | 0.45              |
| 3:A:1296:C:H5''   | 15:M:14:HIS:CE1   | 2.51                     | 0.45              |
| 6:D:34:ILE:H      | 6:D:34:ILE:HD12   | 1.81                     | 0.45              |
| 6:D:44:ARG:HD2    | 6:D:46:PRO:HG3    | 1.98                     | 0.45              |
| 22:T:48:GLN:HG3   | 22:T:83:ILE:HD11  | 1.99                     | 0.45              |
| 25:Y:534:SER:O    | 25:Y:541:ILE:HD11 | 2.17                     | 0.45              |
| 3:A:316:C:OP2     | 3:A:351:G:O2'     | 2.32                     | 0.45              |
| 3:A:476:U:H2'     | 3:A:477:C:C6      | 2.52                     | 0.45              |
| 3:A:1124:G:O2'    | 3:A:1145:A:N6     | 2.49                     | 0.45              |
| 3:A:1496:C:OP1    | 26:Z:99:ARG:HG3   | 2.17                     | 0.45              |
| 4:B:11:LYS:HA     | 4:B:11:LYS:HD2    | 1.77                     | 0.45              |
| 4:B:169:GLU:O     | 4:B:173:ILE:HG13  | 2.17                     | 0.45              |
| 6:D:128:ARG:HA    | 6:D:128:ARG:CZ    | 2.46                     | 0.45              |
| 25:Y:380:ASP:O    | 25:Y:645:ARG:NH2  | 2.49                     | 0.45              |
| 25:Y:617:VAL:HG12 | 25:Y:618:LEU:N    | 2.32                     | 0.45              |
| 25:Y:668:ARG:HB2  | 25:Y:668:ARG:NH1  | 2.32                     | 0.45              |
| 3:A:97:G:H2'      | 3:A:98:A:O4'      | 2.16                     | 0.45              |
| 3:A:412:A:N1      | 3:A:414:A:H1'     | 2.32                     | 0.45              |
| 3:A:634:C:H2'     | 3:A:635:A:C8      | 2.51                     | 0.45              |
| 3:A:643:C:C2      | 3:A:644:U:C5      | 3.05                     | 0.45              |
| 3:A:987:G:H1      | 3:A:1218:C:H42    | 1.64                     | 0.45              |
| 3:A:1181:G:O2'    | 3:A:1182:G:N7     | 2.44                     | 0.45              |
| 8:F:61:LEU:HD12   | 8:F:62:MET:N      | 2.32                     | 0.45              |
| 3:A:339:C:H2'     | 3:A:340:U:C6      | 2.53                     | 0.44              |
| 3:A:432:A:C4      | 3:A:433:G:C8      | 3.05                     | 0.44              |
| 3:A:559:A:H4'     | 3:A:560:A:H3'     | 2.00                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:A:1369:C:H2'     | 3:A:1370:G:C8      | 2.52                     | 0.44              |
| 6:D:99:ASP:OD1     | 6:D:99:ASP:N       | 2.50                     | 0.44              |
| 9:G:138:ARG:O      | 9:G:141:VAL:HG22   | 2.17                     | 0.44              |
| 19:Q:9:GLN:HE21    | 19:Q:58:VAL:HG12   | 1.82                     | 0.44              |
| 25:Y:396:ILE:HA    | 25:Y:466:VAL:O     | 2.17                     | 0.44              |
| 26:Z:157:VAL:N     | 26:Z:177:LYS:HE3   | 2.32                     | 0.44              |
| 3:A:223:A:H2'      | 3:A:224:U:C6       | 2.52                     | 0.44              |
| 3:A:587:G:N2       | 3:A:754:C:OP2      | 2.38                     | 0.44              |
| 3:A:827:U:H2'      | 3:A:870:U:O4       | 2.18                     | 0.44              |
| 3:A:1014:A:C2      | 3:A:1219:A:H1'     | 2.52                     | 0.44              |
| 3:A:1100:C:OP2     | 4:B:95:ARG:NE      | 2.50                     | 0.44              |
| 29:A:1601:A1IC4:O4 | 29:A:1601:A1IC4:O5 | 2.32                     | 0.44              |
| 10:H:113:ASP:HB2   | 10:H:117:ARG:HH12  | 1.82                     | 0.44              |
| 11:I:19:VAL:HG22   | 11:I:65:ILE:HD12   | 1.99                     | 0.44              |
| 12:J:7:ARG:HG2     | 12:J:73:LEU:HD11   | 1.99                     | 0.44              |
| 17:O:26:GLU:H      | 17:O:26:GLU:CD     | 2.14                     | 0.44              |
| 3:A:212:G:C4       | 3:A:213:G:C8       | 3.06                     | 0.44              |
| 3:A:308:C:C2       | 3:A:309:A:C8       | 3.06                     | 0.44              |
| 3:A:977:A:O3'      | 3:A:980:C:N4       | 2.51                     | 0.44              |
| 3:A:1521:C:H2'     | 3:A:1522:U:H6      | 1.82                     | 0.44              |
| 4:B:68:LEU:HD13    | 4:B:90:PHE:HB2     | 1.99                     | 0.44              |
| 8:F:9:MET:O        | 8:F:85:ILE:N       | 2.44                     | 0.44              |
| 12:J:27:GLU:O      | 12:J:31:ARG:HG2    | 2.17                     | 0.44              |
| 13:K:109:ASN:O     | 13:K:110:ILE:HD13  | 2.17                     | 0.44              |
| 25:Y:346:ASN:C     | 25:Y:346:ASN:OD1   | 2.59                     | 0.44              |
| 25:Y:559:ALA:HB1   | 25:Y:588:GLU:HG2   | 1.98                     | 0.44              |
| 26:Z:77:LYS:HD3    | 26:Z:77:LYS:HA     | 1.82                     | 0.44              |
| 26:Z:91:ILE:O      | 26:Z:93:VAL:HG23   | 2.18                     | 0.44              |
| 2:3:27:C:O2        | 2:3:44:G:C2        | 2.71                     | 0.44              |
| 3:A:210:C:H1'      | 3:A:211:G:H1       | 1.82                     | 0.44              |
| 3:A:215:C:H2'      | 3:A:216:U:C6       | 2.53                     | 0.44              |
| 3:A:1347:G:O2'     | 3:A:1373:G:O6      | 2.26                     | 0.44              |
| 10:H:43:GLU:HG2    | 10:H:101:ILE:HD13  | 1.98                     | 0.44              |
| 25:Y:454:MET:HA    | 25:Y:457:ARG:HD3   | 1.99                     | 0.44              |
| 25:Y:531:VAL:HG21  | 25:Y:544:LEU:HD13  | 1.98                     | 0.44              |
| 3:A:318:G:C6       | 3:A:336:A:C6       | 3.05                     | 0.44              |
| 3:A:677:U:H2'      | 3:A:678:U:H6       | 1.82                     | 0.44              |
| 3:A:898:G:N1       | 3:A:902:G:C6       | 2.86                     | 0.44              |
| 3:A:1230:C:H2'     | 3:A:1231:G:C8      | 2.53                     | 0.44              |
| 3:A:1239:A:H1'     | 3:A:1241:G:N7      | 2.33                     | 0.44              |
| 6:D:90:LEU:HD12    | 6:D:90:LEU:C       | 2.43                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:E:36:LEU:HD12   | 7:E:37:THR:N      | 2.32                     | 0.44              |
| 12:J:51:VAL:HB    | 16:N:81:ARG:HB2   | 2.00                     | 0.44              |
| 24:X:13:VAL:HG13  | 24:X:50:GLY:H     | 1.83                     | 0.44              |
| 25:Y:514:LEU:HD12 | 25:Y:530:PHE:CE1  | 2.51                     | 0.44              |
| 2:3:20:U:O2'      | 2:3:22:G:OP2      | 2.28                     | 0.44              |
| 3:A:349:A:H2'     | 3:A:350:G:H8      | 1.82                     | 0.44              |
| 3:A:490:C:H2'     | 3:A:491:G:H8      | 1.82                     | 0.44              |
| 3:A:511:C:H4'     | 6:D:44:ARG:HH12   | 1.83                     | 0.44              |
| 3:A:684:U:C4      | 3:A:685:G:C6      | 3.06                     | 0.44              |
| 3:A:1266:G:N2     | 3:A:1269:A:OP2    | 2.26                     | 0.44              |
| 8:F:104:LYS:HD2   | 8:F:104:LYS:O     | 2.17                     | 0.44              |
| 9:G:17:LYS:HB2    | 9:G:44:TYR:CZ     | 2.53                     | 0.44              |
| 3:A:113:G:H2'     | 3:A:114:U:C6      | 2.52                     | 0.44              |
| 3:A:175:C:H2'     | 3:A:176:C:H6      | 1.83                     | 0.44              |
| 4:B:87:CYS:SG     | 4:B:89:GLN:HB2    | 2.57                     | 0.44              |
| 25:Y:335:ALA:O    | 25:Y:339:LEU:HG   | 2.18                     | 0.44              |
| 25:Y:687:HIS:HD1  | 25:Y:716:VAL:HG22 | 1.83                     | 0.44              |
| 26:Z:108:GLN:O    | 26:Z:112:ARG:HG3  | 2.18                     | 0.44              |
| 2:3:42:G:H2'      | 2:3:43:G:C8       | 2.52                     | 0.44              |
| 3:A:337:G:H2'     | 3:A:338:A:H8      | 1.81                     | 0.44              |
| 3:A:401:C:P       | 6:D:70:ARG:HH21   | 2.41                     | 0.44              |
| 3:A:720:C:O2'     | 20:R:52:GLN:NE2   | 2.51                     | 0.44              |
| 3:A:840:C:H2'     | 3:A:840:C:O2      | 2.18                     | 0.44              |
| 13:K:19:GLY:H     | 13:K:79:ILE:HD11  | 1.82                     | 0.44              |
| 25:Y:578:ARG:CZ   | 25:Y:629:LEU:HD11 | 2.47                     | 0.44              |
| 26:Z:166:GLU:OE2  | 26:Z:171:ILE:HG22 | 2.17                     | 0.44              |
| 3:A:21:G:H2'      | 3:A:22:G:C8       | 2.53                     | 0.44              |
| 3:A:560:A:H4'     | 3:A:561:U:H5''    | 1.99                     | 0.44              |
| 3:A:847:G:H2'     | 3:A:848:C:O4'     | 2.18                     | 0.44              |
| 3:A:1096:C:H2'    | 3:A:1097:C:C6     | 2.53                     | 0.44              |
| 3:A:1474:U:H2'    | 3:A:1475:G:C8     | 2.43                     | 0.44              |
| 4:B:27:MET:O      | 4:B:31:ILE:HG12   | 2.17                     | 0.44              |
| 4:B:101:LEU:H     | 4:B:101:LEU:HD23  | 1.83                     | 0.44              |
| 20:R:22:ASP:OD2   | 20:R:24:LYS:HB2   | 2.17                     | 0.44              |
| 21:S:52:HIS:HB2   | 21:S:57:HIS:NE2   | 2.32                     | 0.44              |
| 22:T:28:MET:SD    | 22:T:57:ILE:HG22  | 2.57                     | 0.44              |
| 2:3:34:C:H2'      | 2:3:35:A:C8       | 2.52                     | 0.43              |
| 3:A:20:U:H2'      | 3:A:21:G:O4'      | 2.18                     | 0.43              |
| 3:A:217:C:H2'     | 3:A:218:U:C6      | 2.53                     | 0.43              |
| 3:A:363:A:OP2     | 14:L:31:ARG:NH1   | 2.50                     | 0.43              |
| 3:A:381:C:H2'     | 3:A:382:A:O4'     | 2.18                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:A:417:G:H2'     | 3:A:418:C:C6     | 2.53                     | 0.43              |
| 3:A:613:C:H2'     | 3:A:614:C:C6     | 2.52                     | 0.43              |
| 7:E:11:LEU:HD12   | 7:E:39:VAL:CG2   | 2.46                     | 0.43              |
| 8:F:5:GLU:OE1     | 8:F:63:ASN:ND2   | 2.28                     | 0.43              |
| 10:H:11:LEU:HD22  | 10:H:75:ILE:CG2  | 2.47                     | 0.43              |
| 13:K:13:ARG:NH2   | 13:K:77:TYR:HA   | 2.33                     | 0.43              |
| 13:K:110:ILE:HG21 | 23:U:19:PHE:CD1  | 2.52                     | 0.43              |
| 15:M:113:ARG:C    | 15:M:114:LYS:HD2 | 2.43                     | 0.43              |
| 16:N:83:LYS:HD2   | 16:N:83:LYS:N    | 2.33                     | 0.43              |
| 21:S:41:PHE:H     | 21:S:44:MET:CE   | 2.31                     | 0.43              |
| 22:T:49:LYS:O     | 22:T:53:GLU:HG2  | 2.16                     | 0.43              |
| 25:Y:312:ILE:HG21 | 25:Y:354:ALA:HB1 | 1.99                     | 0.43              |
| 25:Y:562:LYS:HD2  | 25:Y:563:GLY:N   | 2.33                     | 0.43              |
| 25:Y:756:LYS:HA   | 25:Y:759:GLU:OE1 | 2.17                     | 0.43              |
| 2:3:27:C:C2       | 2:3:28:C:C5      | 3.06                     | 0.43              |
| 2:3:63:C:H2'      | 2:3:64:G:H8      | 1.81                     | 0.43              |
| 3:A:702:A:H5''    | 3:A:703:G:N7     | 2.33                     | 0.43              |
| 5:C:10:ILE:CD1    | 5:C:178:LEU:HD21 | 2.48                     | 0.43              |
| 8:F:37:HIS:HB3    | 8:F:97:THR:HG22  | 1.99                     | 0.43              |
| 11:I:18:ARG:HB2   | 11:I:66:THR:HG22 | 2.00                     | 0.43              |
| 11:I:118:LEU:HD22 | 11:I:124:ARG:HA  | 1.99                     | 0.43              |
| 12:J:9:ARG:HG2    | 12:J:73:LEU:HD13 | 1.99                     | 0.43              |
| 13:K:79:ILE:HD12  | 13:K:80:LYS:H    | 1.84                     | 0.43              |
| 13:K:123:PRO:HD2  | 23:U:38:TYR:HD2  | 1.82                     | 0.43              |
| 14:L:73:ASN:CB    | 25:Y:670:GLN:HG2 | 2.47                     | 0.43              |
| 3:A:190:A:O5'     | 3:A:190:A:H8     | 2.01                     | 0.43              |
| 3:A:491:G:OP1     | 6:D:148:LYS:NZ   | 2.31                     | 0.43              |
| 3:A:570:G:H2'     | 3:A:571:U:C6     | 2.53                     | 0.43              |
| 3:A:592:G:H2'     | 3:A:593:U:C6     | 2.53                     | 0.43              |
| 3:A:657:U:H2'     | 3:A:658:C:H6     | 1.83                     | 0.43              |
| 3:A:683:G:C6      | 3:A:684:U:C4     | 3.07                     | 0.43              |
| 3:A:1112:C:H1'    | 5:C:179:ARG:NH1  | 2.32                     | 0.43              |
| 3:A:1305:G:H22    | 3:A:1331:G:HO2'  | 1.57                     | 0.43              |
| 4:B:20:THR:C      | 4:B:39:HIS:HE1   | 2.26                     | 0.43              |
| 5:C:108:LYS:HD2   | 5:C:111:LEU:HD12 | 1.99                     | 0.43              |
| 18:P:22:ALA:HA    | 18:P:33:ILE:HD12 | 1.99                     | 0.43              |
| 25:Y:312:ILE:HA   | 25:Y:324:LYS:NZ  | 2.33                     | 0.43              |
| 25:Y:514:LEU:HD13 | 25:Y:530:PHE:CE1 | 2.49                     | 0.43              |
| 3:A:212:G:C5      | 3:A:213:G:C8     | 3.06                     | 0.43              |
| 3:A:361:G:H2'     | 3:A:362:G:O4'    | 2.18                     | 0.43              |
| 3:A:455:G:H2'     | 3:A:456:A:H8     | 1.83                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:A:601:G:H2'    | 3:A:602:A:H8      | 1.84                     | 0.43              |
| 3:A:1230:C:H2'   | 3:A:1231:G:H8     | 1.82                     | 0.43              |
| 3:A:1253:G:H2'   | 3:A:1254:A:C8     | 2.54                     | 0.43              |
| 3:A:1512:U:H2'   | 3:A:1513:A:C8     | 2.53                     | 0.43              |
| 13:K:64:GLN:O    | 13:K:68:GLU:HG2   | 2.19                     | 0.43              |
| 21:S:40:ILE:HG21 | 21:S:66:MET:HG3   | 2.00                     | 0.43              |
| 3:A:75:G:C2      | 3:A:96:U:C2       | 3.07                     | 0.43              |
| 3:A:102:G:H2'    | 3:A:103:U:H6      | 1.84                     | 0.43              |
| 3:A:401:C:H2'    | 3:A:402:G:C8      | 2.54                     | 0.43              |
| 3:A:415:A:C6     | 3:A:416:G:C5      | 3.06                     | 0.43              |
| 3:A:843:U:H2'    | 3:A:844:G:C8      | 2.53                     | 0.43              |
| 3:A:1209:C:O2'   | 3:A:1214:C:N4     | 2.51                     | 0.43              |
| 3:A:298:A:HO2'   | 3:A:299:G:P       | 2.42                     | 0.43              |
| 3:A:1182:G:H4'   | 3:A:1183:U:H5''   | 1.98                     | 0.43              |
| 3:A:1237:C:O2'   | 3:A:1300:G:N1     | 2.41                     | 0.43              |
| 3:A:1307:U:H5'   | 15:M:108:THR:HG21 | 2.00                     | 0.43              |
| 7:E:157:ARG:HD2  | 10:H:45:PHE:CZ    | 2.53                     | 0.43              |
| 13:K:127:ARG:HG3 | 23:U:37:PHE:HZ    | 1.84                     | 0.43              |
| 26:Z:148:VAL:O   | 26:Z:152:LEU:HG   | 2.18                     | 0.43              |
| 3:A:236:A:H2'    | 3:A:237:G:C8      | 2.54                     | 0.43              |
| 3:A:321:A:H2'    | 3:A:322:C:H6      | 1.84                     | 0.43              |
| 3:A:1386:G:O2'   | 3:A:1387:G:H5'    | 2.18                     | 0.43              |
| 3:A:1418:A:N6    | 3:A:1482:G:H1'    | 2.33                     | 0.43              |
| 3:A:1518:MA6:O2' | 3:A:1519:MA6:O4'  | 2.31                     | 0.43              |
| 6:D:165:ARG:O    | 6:D:167:LYS:NZ    | 2.40                     | 0.43              |
| 6:D:168:PRO:HB3  | 6:D:170:TRP:CZ3   | 2.53                     | 0.43              |
| 8:F:6:ILE:HD12   | 8:F:89:VAL:HG12   | 2.01                     | 0.43              |
| 25:Y:476:MET:HB2 | 25:Y:479:THR:OG1  | 2.19                     | 0.43              |
| 25:Y:519:ILE:HB  | 25:Y:527:GLU:OE1  | 2.19                     | 0.43              |
| 26:Z:81:SER:HA   | 26:Z:84:GLN:HB2   | 2.00                     | 0.43              |
| 26:Z:107:TYR:HD2 | 26:Z:108:GLN:NE2  | 2.17                     | 0.43              |
| 3:A:284:C:C2     | 3:A:285:C:C5      | 3.07                     | 0.43              |
| 3:A:489:C:H2'    | 3:A:490:C:H6      | 1.84                     | 0.43              |
| 3:A:704:A:C4     | 3:A:705:G:C8      | 3.06                     | 0.43              |
| 3:A:771:G:H2'    | 3:A:772:U:C6      | 2.54                     | 0.43              |
| 3:A:1049:U:H4'   | 3:A:1050:G:H5''   | 2.01                     | 0.43              |
| 14:L:99:ARG:HD3  | 14:L:104:CYS:SG   | 2.58                     | 0.43              |
| 18:P:4:ILE:HA    | 18:P:20:VAL:O     | 2.18                     | 0.43              |
| 3:A:259:G:C4     | 3:A:260:G:C8      | 3.06                     | 0.43              |
| 3:A:269:C:H2'    | 3:A:270:A:H8      | 1.83                     | 0.43              |
| 3:A:1004:A:H1'   | 3:A:1036:A:H2     | 1.84                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:1316:G:N2     | 3:A:1318:A:H3'    | 2.34                     | 0.43              |
| 3:A:1426:G:C6     | 3:A:1475:G:C6     | 3.07                     | 0.43              |
| 4:B:32:PHE:HB3    | 4:B:40:ILE:HG22   | 2.00                     | 0.43              |
| 5:C:130:PHE:CZ    | 5:C:131:ARG:HG2   | 2.54                     | 0.43              |
| 7:E:97:GLN:OE1    | 7:E:124:LEU:HB2   | 2.19                     | 0.43              |
| 8:F:17:GLN:C      | 8:F:21:MET:HE3    | 2.43                     | 0.43              |
| 8:F:102:MET:CE    | 20:R:25:ASP:HA    | 2.48                     | 0.43              |
| 23:U:49:LYS:HE3   | 23:U:49:LYS:HB2   | 1.64                     | 0.43              |
| 3:A:216:U:H2'     | 3:A:217:C:H6      | 1.83                     | 0.43              |
| 3:A:1163:A:H2'    | 3:A:1164:G:C8     | 2.54                     | 0.43              |
| 3:A:1381:U:O2'    | 9:G:79:ARG:NH2    | 2.50                     | 0.43              |
| 3:A:1520:C:H2'    | 3:A:1521:C:C6     | 2.54                     | 0.43              |
| 5:C:19:ASN:OD1    | 5:C:19:ASN:C      | 2.62                     | 0.43              |
| 5:C:25:ASN:HB3    | 5:C:27:LYS:HZ3    | 1.84                     | 0.43              |
| 8:F:72:ASP:O      | 8:F:76:THR:HG22   | 2.18                     | 0.43              |
| 9:G:95:ARG:O      | 9:G:99:LEU:HG     | 2.19                     | 0.43              |
| 11:I:21:ILE:HG21  | 11:I:61:LEU:HD13  | 2.01                     | 0.43              |
| 19:Q:79:VAL:HB    | 19:Q:80:GLU:OE1   | 2.19                     | 0.43              |
| 25:Y:404:LYS:NZ   | 25:Y:424:ILE:HA   | 2.34                     | 0.43              |
| 25:Y:743:LEU:HD23 | 25:Y:743:LEU:HA   | 1.86                     | 0.43              |
| 3:A:335:C:H2'     | 3:A:336:A:C8      | 2.49                     | 0.42              |
| 3:A:339:C:H2'     | 3:A:340:U:H6      | 1.83                     | 0.42              |
| 3:A:401:C:H2'     | 3:A:402:G:H8      | 1.84                     | 0.42              |
| 3:A:705:G:C4      | 3:A:706:A:C8      | 3.07                     | 0.42              |
| 3:A:843:U:H5      | 3:A:845:A:H62     | 1.66                     | 0.42              |
| 3:A:963:G:H2'     | 3:A:964:A:H8      | 1.84                     | 0.42              |
| 5:C:120:ILE:HG21  | 5:C:198:VAL:HG11  | 2.01                     | 0.42              |
| 6:D:177:LYS:HB2   | 6:D:179:GLU:OE1   | 2.18                     | 0.42              |
| 7:E:80:THR:OG1    | 7:E:122:ASN:O     | 2.29                     | 0.42              |
| 8:F:90:MET:HE3    | 8:F:90:MET:HA     | 2.00                     | 0.42              |
| 15:M:23:TYR:CE1   | 15:M:70:ARG:HG3   | 2.55                     | 0.42              |
| 3:A:214:C:C2      | 3:A:215:C:C5      | 3.07                     | 0.42              |
| 3:A:321:A:H2'     | 3:A:322:C:C6      | 2.54                     | 0.42              |
| 3:A:718:A:C4      | 3:A:719:C:C5      | 3.07                     | 0.42              |
| 3:A:1517:G:C6     | 3:A:1518:MA6:H103 | 2.55                     | 0.42              |
| 4:B:105:LYS:HE3   | 4:B:105:LYS:HB3   | 1.93                     | 0.42              |
| 7:E:55:GLU:HG3    | 7:E:56:VAL:N      | 2.34                     | 0.42              |
| 9:G:131:LYS:HA    | 9:G:131:LYS:HD3   | 1.61                     | 0.42              |
| 11:I:35:LEU:HD11  | 11:I:45:ARG:HG2   | 2.01                     | 0.42              |
| 14:L:21:VAL:HG12  | 14:L:21:VAL:O     | 2.18                     | 0.42              |
| 25:Y:511:LYS:HA   | 25:Y:514:LEU:CD1  | 2.49                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:3:0:G:H2'      | 2:3:1:G:C8       | 2.54                     | 0.42              |
| 3:A:95:C:H2'     | 3:A:96:U:H6      | 1.84                     | 0.42              |
| 3:A:647:C:H2'    | 3:A:648:A:C8     | 2.51                     | 0.42              |
| 3:A:718:A:HO2'   | 23:U:35:ARG:NH2  | 2.17                     | 0.42              |
| 3:A:1269:A:C4    | 3:A:1313:U:H1'   | 2.53                     | 0.42              |
| 12:J:11:LYS:HZ3  | 12:J:97:ASP:HB3  | 1.84                     | 0.42              |
| 16:N:27:LEU:O    | 16:N:30:ILE:HG22 | 2.18                     | 0.42              |
| 26:Z:179:LYS:HE2 | 26:Z:179:LYS:HB3 | 1.85                     | 0.42              |
| 3:A:368:U:OP2    | 25:Y:607:ARG:NH1 | 2.47                     | 0.42              |
| 3:A:522:C:H41    | 14:L:50:ARG:NH2  | 2.16                     | 0.42              |
| 3:A:1038:C:N4    | 3:A:1039:G:O6    | 2.53                     | 0.42              |
| 3:A:1404:C:C2    | 3:A:1499:A:C6    | 3.07                     | 0.42              |
| 3:A:1520:C:H2'   | 3:A:1521:C:H6    | 1.85                     | 0.42              |
| 5:C:11:ARG:HH12  | 5:C:178:LEU:HA   | 1.85                     | 0.42              |
| 8:F:82:ASP:OD1   | 8:F:82:ASP:C     | 2.62                     | 0.42              |
| 15:M:107:ARG:NH2 | 15:M:111:GLY:O   | 2.53                     | 0.42              |
| 3:A:524:G:H2'    | 3:A:525:C:C6     | 2.55                     | 0.42              |
| 3:A:545:C:P      | 6:D:62:ARG:HH12  | 2.43                     | 0.42              |
| 3:A:696:A:H2'    | 3:A:697:U:H6     | 1.85                     | 0.42              |
| 3:A:716:A:C6     | 3:A:717:U:C4     | 3.08                     | 0.42              |
| 3:A:734:G:H2'    | 3:A:735:C:H6     | 1.83                     | 0.42              |
| 3:A:1118:U:H1'   | 3:A:1179:A:C4    | 2.55                     | 0.42              |
| 3:A:1298:U:H5''  | 3:A:1299:A:O4'   | 2.19                     | 0.42              |
| 3:A:1483:A:H2'   | 3:A:1484:C:O4'   | 2.19                     | 0.42              |
| 4:B:111:ILE:HD13 | 4:B:111:ILE:HA   | 1.83                     | 0.42              |
| 10:H:92:LEU:HD23 | 10:H:92:LEU:HA   | 1.75                     | 0.42              |
| 20:R:63:ARG:HD2  | 20:R:70:TYR:HA   | 2.01                     | 0.42              |
| 25:Y:357:VAL:HA  | 25:Y:360:GLU:CD  | 2.45                     | 0.42              |
| 25:Y:661:PHE:O   | 25:Y:665:LYS:HG2 | 2.18                     | 0.42              |
| 3:A:828:U:C4     | 3:A:859:G:C4     | 3.08                     | 0.42              |
| 3:A:1013:G:N2    | 3:A:1015:G:H3'   | 2.34                     | 0.42              |
| 3:A:1071:C:H2'   | 3:A:1072:G:C8    | 2.54                     | 0.42              |
| 6:D:58:LYS:HZ3   | 6:D:62:ARG:HD3   | 1.84                     | 0.42              |
| 17:O:28:GLN:H    | 17:O:28:GLN:HG2  | 1.60                     | 0.42              |
| 3:A:34:C:H2'     | 3:A:35:G:C8      | 2.52                     | 0.42              |
| 3:A:338:A:H2'    | 3:A:339:C:C6     | 2.55                     | 0.42              |
| 3:A:639:G:C2     | 3:A:640:A:C5     | 3.07                     | 0.42              |
| 3:A:642:A:C8     | 10:H:107:SER:HA  | 2.55                     | 0.42              |
| 5:C:157:LEU:HD23 | 5:C:157:LEU:HA   | 1.74                     | 0.42              |
| 19:Q:58:VAL:HB   | 19:Q:80:GLU:OE1  | 2.20                     | 0.42              |
| 22:T:56:PRO:O    | 22:T:60:ARG:HG3  | 2.20                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:X:19:ASN:N     | 24:X:19:ASN:HD22  | 2.18                     | 0.42              |
| 25:Y:694:LYS:HG3  | 25:Y:728:ILE:HG12 | 2.01                     | 0.42              |
| 25:Y:757:VAL:O    | 25:Y:761:GLU:HB3  | 2.20                     | 0.42              |
| 3:A:113:G:H2'     | 3:A:114:U:H6      | 1.84                     | 0.42              |
| 3:A:602:A:H2'     | 3:A:603:U:C6      | 2.55                     | 0.42              |
| 3:A:801:U:H2'     | 3:A:802:A:H8      | 1.84                     | 0.42              |
| 3:A:1078:U:H2'    | 3:A:1079:G:C8     | 2.55                     | 0.42              |
| 3:A:1428:A:C6     | 3:A:1473:G:N1     | 2.88                     | 0.42              |
| 4:B:103:ASN:HD21  | 4:B:105:LYS:HE3   | 1.84                     | 0.42              |
| 9:G:110:LYS:HA    | 9:G:110:LYS:HD3   | 1.80                     | 0.42              |
| 10:H:27:MET:O     | 10:H:58:GLU:HG2   | 2.19                     | 0.42              |
| 18:P:39:PHE:CD1   | 18:P:74:LEU:HD11  | 2.53                     | 0.42              |
| 22:T:37:ALA:O     | 22:T:40:GLU:HG3   | 2.18                     | 0.42              |
| 25:Y:486:ALA:HA   | 25:Y:489:ALA:HB3  | 2.01                     | 0.42              |
| 26:Z:112:ARG:O    | 26:Z:115:ILE:HG13 | 2.19                     | 0.42              |
| 2:3:25:U:C2       | 2:3:26:A:C8       | 3.08                     | 0.42              |
| 3:A:123:U:H5''    | 3:A:311:C:O2'     | 2.19                     | 0.42              |
| 3:A:279:A:H5''    | 3:A:280:C:H3'     | 2.01                     | 0.42              |
| 3:A:607:A:H2'     | 3:A:608:A:H8      | 1.85                     | 0.42              |
| 4:B:144:LEU:O     | 4:B:147:SER:OG    | 2.32                     | 0.42              |
| 7:E:85:VAL:CG1    | 7:E:86:LYS:N      | 2.83                     | 0.42              |
| 14:L:21:VAL:CG1   | 14:L:24:LEU:HD22  | 2.50                     | 0.42              |
| 15:M:51:GLY:O     | 15:M:55:THR:HG22  | 2.19                     | 0.42              |
| 25:Y:317:THR:HB   | 25:Y:348:VAL:HG12 | 2.02                     | 0.42              |
| 25:Y:499:LYS:HA   | 25:Y:499:LYS:HD2  | 1.83                     | 0.42              |
| 2:3:24:A:C6       | 2:3:25:U:C2       | 3.07                     | 0.42              |
| 2:3:27:C:H5'      | 2:3:27:C:C6       | 2.36                     | 0.42              |
| 3:A:71:A:C6       | 3:A:100:G:C8      | 3.08                     | 0.42              |
| 3:A:264:C:H2'     | 3:A:265:G:C8      | 2.55                     | 0.42              |
| 3:A:324:G:N1      | 3:A:327:A:OP2     | 2.52                     | 0.42              |
| 3:A:344:A:OP2     | 3:A:345:C:N4      | 2.53                     | 0.42              |
| 3:A:380:G:N2      | 3:A:384:G:C5      | 2.88                     | 0.42              |
| 3:A:747:A:H2'     | 3:A:748:G:C8      | 2.55                     | 0.42              |
| 3:A:1411:C:N4     | 3:A:1489:G:H1     | 2.14                     | 0.42              |
| 5:C:16:LYS:HD3    | 5:C:17:PRO:HD2    | 2.02                     | 0.42              |
| 5:C:156:ARG:NH2   | 5:C:161:GLU:HA    | 2.35                     | 0.42              |
| 15:M:89:LEU:O     | 15:M:92:ARG:HG2   | 2.20                     | 0.42              |
| 16:N:4:GLN:HA     | 16:N:7:LYS:HE2    | 2.01                     | 0.42              |
| 18:P:52:LEU:HD13  | 18:P:78:VAL:HG21  | 2.02                     | 0.42              |
| 25:Y:399:HIS:CE1  | 25:Y:447:GLY:HA3  | 2.55                     | 0.42              |
| 25:Y:709:LEU:HD23 | 25:Y:709:LEU:HA   | 1.65                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:3:62:C:H2'      | 2:3:63:C:C4'     | 2.50                     | 0.41              |
| 3:A:41:G:N1       | 3:A:402:G:C6     | 2.88                     | 0.41              |
| 3:A:158:G:C6      | 3:A:164:G:C5     | 3.08                     | 0.41              |
| 3:A:580:C:H2'     | 3:A:581:G:O4'    | 2.20                     | 0.41              |
| 3:A:792:A:C4      | 3:A:794:A:C6     | 3.07                     | 0.41              |
| 3:A:1226:C:C5     | 15:M:103:LYS:HA  | 2.55                     | 0.41              |
| 3:A:1233:G:C2     | 3:A:1234:C:C2    | 3.09                     | 0.41              |
| 4:B:120:GLN:HG3   | 4:B:125:THR:OG1  | 2.19                     | 0.41              |
| 4:B:160:ALA:HB1   | 4:B:184:PHE:HE1  | 1.85                     | 0.41              |
| 7:E:74:VAL:HG21   | 7:E:144:LEU:HB3  | 2.02                     | 0.41              |
| 9:G:66:LEU:HD11   | 9:G:100:ALA:HB1  | 2.02                     | 0.41              |
| 10:H:22:LYS:N     | 10:H:65:TYR:OH   | 2.53                     | 0.41              |
| 17:O:86:GLY:O     | 17:O:88:ARG:NH2  | 2.36                     | 0.41              |
| 19:Q:9:GLN:HE22   | 19:Q:79:VAL:HG11 | 1.85                     | 0.41              |
| 19:Q:47:HIS:HB2   | 19:Q:67:LEU:HD11 | 2.02                     | 0.41              |
| 2:3:9:G:N2        | 2:3:26:A:H1'     | 2.34                     | 0.41              |
| 3:A:352:C:O2'     | 3:A:354:G:OP1    | 2.32                     | 0.41              |
| 3:A:600:A:H2'     | 3:A:601:G:C8     | 2.55                     | 0.41              |
| 3:A:823:C:H2'     | 3:A:824:G:H8     | 1.85                     | 0.41              |
| 3:A:927:G:OP1     | 3:A:1505:G:N2    | 2.49                     | 0.41              |
| 3:A:1491:G:H5'    | 3:A:1492:A:OP1   | 2.19                     | 0.41              |
| 4:B:115:LYS:HB2   | 4:B:115:LYS:HE2  | 1.68                     | 0.41              |
| 5:C:82:GLU:N      | 5:C:82:GLU:OE1   | 2.53                     | 0.41              |
| 14:L:34:CYS:HB2   | 14:L:78:SER:H    | 1.85                     | 0.41              |
| 15:M:81:MET:O     | 15:M:92:ARG:NH2  | 2.53                     | 0.41              |
| 16:N:86:GLU:OE1   | 16:N:87:ALA:N    | 2.53                     | 0.41              |
| 25:Y:460:GLN:HG2  | 25:Y:489:ALA:HB2 | 2.02                     | 0.41              |
| 25:Y:514:LEU:HA   | 25:Y:517:TYR:CD1 | 2.55                     | 0.41              |
| 25:Y:522:GLU:HA   | 25:Y:526:GLY:N   | 2.33                     | 0.41              |
| 25:Y:713:THR:HG22 | 25:Y:714:ASP:H   | 1.84                     | 0.41              |
| 26:Z:89:LYS:O     | 26:Z:92:GLN:HB3  | 2.19                     | 0.41              |
| 26:Z:103:ASP:O    | 26:Z:104:GLU:HB2 | 2.19                     | 0.41              |
| 3:A:425:G:H2'     | 3:A:426:U:C6     | 2.55                     | 0.41              |
| 3:A:620:C:H2'     | 3:A:621:A:O4'    | 2.21                     | 0.41              |
| 3:A:931:C:H42     | 3:A:1386:G:H1    | 1.68                     | 0.41              |
| 3:A:1039:G:H2'    | 3:A:1040:U:C6    | 2.55                     | 0.41              |
| 3:A:1479:C:H2'    | 3:A:1480:A:C8    | 2.55                     | 0.41              |
| 4:B:105:LYS:NZ    | 4:B:106:THR:HG22 | 2.35                     | 0.41              |
| 5:C:153:VAL:HG12  | 5:C:196:ILE:HD11 | 2.01                     | 0.41              |
| 6:D:13:ARG:NH2    | 6:D:38:PRO:HA    | 2.35                     | 0.41              |
| 6:D:90:LEU:HD11   | 6:D:91:LEU:HD22  | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:K:24:HIS:NE2   | 13:K:87:LYS:HE2   | 2.35                     | 0.41              |
| 15:M:3:ARG:HB2    | 15:M:6:GLY:O      | 2.20                     | 0.41              |
| 22:T:8:LYS:O      | 22:T:12:ILE:HG12  | 2.20                     | 0.41              |
| 23:U:41:PRO:HB2   | 23:U:45:ARG:NH2   | 2.31                     | 0.41              |
| 25:Y:397:MET:HE2  | 25:Y:467:LEU:HD22 | 2.02                     | 0.41              |
| 26:Z:144:VAL:HG23 | 26:Z:145:LEU:N    | 2.35                     | 0.41              |
| 3:A:259:G:OP2     | 22:T:78:ASN:ND2   | 2.53                     | 0.41              |
| 3:A:471:U:HO2'    | 3:A:472:U:P       | 2.42                     | 0.41              |
| 3:A:954:G:N2      | 3:A:1228:C:N3     | 2.68                     | 0.41              |
| 5:C:37:PHE:CE1    | 5:C:38:LYS:HD3    | 2.55                     | 0.41              |
| 5:C:118:ASP:HA    | 5:C:121:THR:OG1   | 2.20                     | 0.41              |
| 6:D:45:LYS:O      | 6:D:45:LYS:HD3    | 2.20                     | 0.41              |
| 8:F:16:GLU:O      | 8:F:19:PRO:HD2    | 2.20                     | 0.41              |
| 8:F:40:GLU:OE2    | 8:F:61:LEU:HG     | 2.20                     | 0.41              |
| 25:Y:665:LYS:HB2  | 25:Y:668:ARG:HH21 | 1.85                     | 0.41              |
| 3:A:45:G:H2'      | 3:A:46:G:H8       | 1.86                     | 0.41              |
| 3:A:340:U:H2'     | 3:A:341:C:H6      | 1.86                     | 0.41              |
| 3:A:717:U:C2      | 3:A:734:G:C8      | 3.09                     | 0.41              |
| 3:A:771:G:C6      | 3:A:809:G:C6      | 3.09                     | 0.41              |
| 3:A:833:G:H2'     | 3:A:834:U:H6      | 1.85                     | 0.41              |
| 3:A:841:C:C4      | 3:A:846:G:C4      | 3.09                     | 0.41              |
| 5:C:20:SER:OG     | 5:C:22:TRP:NE1    | 2.53                     | 0.41              |
| 5:C:184:TYR:HE1   | 5:C:199:LYS:HB3   | 1.86                     | 0.41              |
| 14:L:34:CYS:SG    | 14:L:78:SER:HB2   | 2.61                     | 0.41              |
| 25:Y:513:GLU:O    | 25:Y:516:GLN:N    | 2.54                     | 0.41              |
| 3:A:131:A:H2'     | 3:A:132:C:C6      | 2.56                     | 0.41              |
| 3:A:283:U:C2      | 3:A:284:C:C6      | 3.09                     | 0.41              |
| 3:A:745:G:C2      | 3:A:746:A:C5      | 3.09                     | 0.41              |
| 3:A:748:G:H2'     | 3:A:749:A:C8      | 2.56                     | 0.41              |
| 3:A:851:G:C2      | 3:A:852:G:C8      | 3.09                     | 0.41              |
| 3:A:962:C:H2'     | 3:A:963:G:C8      | 2.55                     | 0.41              |
| 3:A:1148:U:H2'    | 3:A:1149:C:O4'    | 2.20                     | 0.41              |
| 14:L:71:GLY:O     | 14:L:99:ARG:NH2   | 2.46                     | 0.41              |
| 20:R:21:ILE:HD13  | 20:R:55:LEU:HD23  | 2.01                     | 0.41              |
| 20:R:21:ILE:HD11  | 20:R:51:TYR:HD1   | 1.86                     | 0.41              |
| 22:T:59:ASP:OD1   | 22:T:59:ASP:N     | 2.53                     | 0.41              |
| 25:Y:347:GLN:OE1  | 25:Y:349:ILE:HG23 | 2.21                     | 0.41              |
| 25:Y:564:MET:HG2  | 25:Y:643:VAL:HB   | 2.02                     | 0.41              |
| 3:A:224:U:H2'     | 3:A:225:C:C6      | 2.56                     | 0.41              |
| 3:A:345:C:H1'     | 3:A:346:G:C2      | 2.56                     | 0.41              |
| 3:A:652:U:C2      | 3:A:752:G:N2      | 2.89                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:705:G:C5      | 3:A:706:A:C8      | 3.09                     | 0.41              |
| 5:C:43:LEU:HD23   | 5:C:43:LEU:HA     | 1.86                     | 0.41              |
| 5:C:121:THR:HB    | 5:C:189:ALA:HB2   | 2.02                     | 0.41              |
| 8:F:42:TRP:CZ2    | 20:R:24:LYS:HE3   | 2.55                     | 0.41              |
| 12:J:36:VAL:HA    | 12:J:76:ILE:HA    | 2.03                     | 0.41              |
| 13:K:22:HIS:HB2   | 13:K:33:THR:CG2   | 2.50                     | 0.41              |
| 13:K:122:ARG:HA   | 13:K:123:PRO:HD3  | 1.97                     | 0.41              |
| 17:O:48:LYS:HE3   | 17:O:50:HIS:CE1   | 2.56                     | 0.41              |
| 25:Y:766:ARG:HH21 | 25:Y:777:GLU:HG3  | 1.85                     | 0.41              |
| 25:Y:771:ILE:HG12 | 25:Y:775:ILE:HD11 | 2.02                     | 0.41              |
| 3:A:338:A:H2'     | 3:A:339:C:H6      | 1.86                     | 0.41              |
| 3:A:1290:G:H5'    | 9:G:35:LYS:NZ     | 2.36                     | 0.41              |
| 8:F:101:PRO:HD2   | 20:R:24:LYS:HE2   | 2.02                     | 0.41              |
| 26:Z:114:LEU:HD12 | 26:Z:114:LEU:C    | 2.46                     | 0.41              |
| 1:2:15:A:N1       | 2:3:37:A:H2       | 2.19                     | 0.41              |
| 3:A:86:G:H1'      | 3:A:87:C:H5       | 1.86                     | 0.41              |
| 3:A:279:A:H5'     | 3:A:281:G:O4'     | 2.21                     | 0.41              |
| 3:A:415:A:C4      | 3:A:416:G:C8      | 3.09                     | 0.41              |
| 3:A:907:A:H2'     | 3:A:908:A:H8      | 1.86                     | 0.41              |
| 3:A:922:G:H2'     | 3:A:923:A:C8      | 2.56                     | 0.41              |
| 3:A:1005:A:C6     | 3:A:1006:G:H1'    | 2.56                     | 0.41              |
| 3:A:1132:C:H2'    | 3:A:1133:G:H8     | 1.86                     | 0.41              |
| 3:A:1217:C:H2'    | 3:A:1218:C:C6     | 2.55                     | 0.41              |
| 3:A:1442:G:H2'    | 3:A:1443:C:C6     | 2.56                     | 0.41              |
| 3:A:1484:C:C4     | 3:A:1485:U:C4     | 3.09                     | 0.41              |
| 3:A:1518:MA6:C5   | 3:A:1519:MA6:H103 | 2.51                     | 0.41              |
| 5:C:86:LYS:O      | 5:C:90:VAL:HG23   | 2.20                     | 0.41              |
| 5:C:117:ALA:O     | 5:C:120:ILE:HG22  | 2.21                     | 0.41              |
| 7:E:126:LYS:HD2   | 7:E:127:ALA:N     | 2.35                     | 0.41              |
| 11:I:43:THR:O     | 11:I:47:VAL:HG12  | 2.21                     | 0.41              |
| 14:L:44:LYS:HG3   | 14:L:89:ASP:HA    | 2.02                     | 0.41              |
| 15:M:3:ARG:O      | 15:M:3:ARG:HG3    | 2.20                     | 0.41              |
| 25:Y:729:THR:C    | 25:Y:754:ALA:HB2  | 2.46                     | 0.41              |
| 3:A:159:G:N2      | 3:A:162:A:OP2     | 2.54                     | 0.41              |
| 3:A:667:G:H4'     | 17:O:51:HIS:CE1   | 2.56                     | 0.41              |
| 3:A:992:U:H4'     | 3:A:993:G:O4'     | 2.21                     | 0.41              |
| 4:B:74:ARG:O      | 4:B:77:SER:OG     | 2.38                     | 0.41              |
| 10:H:78:VAL:HB    | 10:H:125:ILE:HG22 | 2.03                     | 0.41              |
| 15:M:23:TYR:HB3   | 15:M:66:GLU:HG2   | 2.03                     | 0.41              |
| 25:Y:455:ARG:O    | 25:Y:459:ALA:N    | 2.54                     | 0.41              |
| 3:A:1:A:H2'       | 3:A:2:A:O4'       | 2.21                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:122:G:H2'     | 3:A:123:U:O4'     | 2.21                     | 0.40              |
| 3:A:204:G:H2'     | 3:A:205:A:H8      | 1.85                     | 0.40              |
| 3:A:613:C:H2'     | 3:A:614:C:H6      | 1.86                     | 0.40              |
| 3:A:697:U:C4      | 3:A:698:G:C8      | 3.10                     | 0.40              |
| 3:A:714:G:H2'     | 3:A:715:A:H8      | 1.85                     | 0.40              |
| 3:A:1178:G:N2     | 3:A:1180:A:H3'    | 2.36                     | 0.40              |
| 10:H:7:ILE:HB     | 10:H:77:ARG:HH21  | 1.85                     | 0.40              |
| 11:I:28:ILE:HD11  | 11:I:35:LEU:HD22  | 2.03                     | 0.40              |
| 13:K:38:GLN:OE1   | 13:K:40:ASN:N     | 2.53                     | 0.40              |
| 17:O:70:LEU:HD22  | 17:O:78:TYR:HB2   | 2.03                     | 0.40              |
| 18:P:67:ILE:HG22  | 18:P:68:SER:O     | 2.21                     | 0.40              |
| 25:Y:472:ASP:OD1  | 25:Y:473:ASP:N    | 2.54                     | 0.40              |
| 25:Y:523:GLU:HG2  | 25:Y:530:PHE:HE2  | 1.84                     | 0.40              |
| 25:Y:740:ASN:OD1  | 25:Y:740:ASN:N    | 2.54                     | 0.40              |
| 26:Z:154:GLU:H    | 26:Z:154:GLU:HG2  | 1.67                     | 0.40              |
| 3:A:284:C:H2'     | 3:A:285:C:H6      | 1.86                     | 0.40              |
| 3:A:538:G:H2'     | 3:A:539:A:C8      | 2.56                     | 0.40              |
| 3:A:635:A:H2'     | 3:A:636:U:C6      | 2.56                     | 0.40              |
| 3:A:652:U:C4      | 3:A:752:G:N3      | 2.90                     | 0.40              |
| 3:A:677:U:H2'     | 3:A:678:U:C6      | 2.56                     | 0.40              |
| 3:A:797:C:H2'     | 3:A:798:U:H6      | 1.86                     | 0.40              |
| 3:A:834:U:H2'     | 3:A:835:U:C6      | 2.56                     | 0.40              |
| 3:A:907:A:H2'     | 3:A:908:A:C8      | 2.57                     | 0.40              |
| 3:A:1106:G:P      | 5:C:172:ARG:HH21  | 2.44                     | 0.40              |
| 3:A:1221:G:H4'    | 21:S:77:THR:HG21  | 2.02                     | 0.40              |
| 3:A:1266:G:N2     | 3:A:1268:G:H3'    | 2.36                     | 0.40              |
| 3:A:1420:U:H2'    | 3:A:1421:G:C8     | 2.57                     | 0.40              |
| 6:D:59:GLN:OE1    | 6:D:63:ARG:NH2    | 2.53                     | 0.40              |
| 6:D:185:LYS:HA    | 6:D:186:PRO:HD3   | 1.96                     | 0.40              |
| 10:H:12:THR:HA    | 10:H:15:ARG:NH1   | 2.36                     | 0.40              |
| 12:J:11:LYS:HG2   | 12:J:71:LEU:CD1   | 2.51                     | 0.40              |
| 20:R:29:LEU:HA    | 20:R:32:TYR:HD1   | 1.86                     | 0.40              |
| 26:Z:92:GLN:HG2   | 26:Z:122:ASP:OD2  | 2.20                     | 0.40              |
| 26:Z:113:SER:HA   | 26:Z:116:ARG:NH2  | 2.36                     | 0.40              |
| 26:Z:128:LEU:HD23 | 26:Z:145:LEU:HD21 | 2.03                     | 0.40              |
| 3:A:264:C:O2'     | 19:Q:65:ARG:NH1   | 2.54                     | 0.40              |
| 3:A:317:U:N3      | 3:A:318:G:N7      | 2.70                     | 0.40              |
| 3:A:601:G:H2'     | 3:A:602:A:C8      | 2.56                     | 0.40              |
| 3:A:800:G:H2'     | 3:A:801:U:C5      | 2.56                     | 0.40              |
| 3:A:883:C:H2'     | 3:A:884:U:C6      | 2.56                     | 0.40              |
| 3:A:1226:C:H4'    | 21:S:80:TYR:CZ    | 2.57                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:1322:C:OP1    | 21:S:78:ARG:NH2   | 2.47                     | 0.40              |
| 3:A:1413:A:N1     | 3:A:1487:G:C6     | 2.90                     | 0.40              |
| 15:M:80:LEU:O     | 15:M:88:GLY:HA3   | 2.21                     | 0.40              |
| 22:T:28:MET:O     | 22:T:32:ILE:HG12  | 2.21                     | 0.40              |
| 24:X:56:GLU:CD    | 24:X:66:ARG:HB3   | 2.46                     | 0.40              |
| 25:Y:404:LYS:HZ3  | 25:Y:424:ILE:HA   | 1.86                     | 0.40              |
| 26:Z:121:GLY:HA2  | 26:Z:176:PRO:HG3  | 2.03                     | 0.40              |
| 3:A:2:A:H4'       | 3:A:3:A:OP1       | 2.21                     | 0.40              |
| 3:A:210:C:O2'     | 3:A:211:G:N2      | 2.54                     | 0.40              |
| 3:A:571:U:H5'     | 3:A:819:A:N7      | 2.36                     | 0.40              |
| 3:A:685:G:C2      | 3:A:686:U:C4      | 3.09                     | 0.40              |
| 3:A:765:G:N1      | 3:A:812:G:O2'     | 2.50                     | 0.40              |
| 3:A:799:G:H2'     | 3:A:800:G:O4'     | 2.21                     | 0.40              |
| 3:A:934:C:H5      | 3:A:1344:C:H2'    | 1.87                     | 0.40              |
| 3:A:1000:A:H2'    | 3:A:1001:C:C6     | 2.57                     | 0.40              |
| 3:A:1070:U:H2'    | 3:A:1071:C:C6     | 2.56                     | 0.40              |
| 3:A:1298:U:H4'    | 3:A:1299:A:C4     | 2.56                     | 0.40              |
| 5:C:211:MET:H     | 5:C:211:MET:HG2   | 1.76                     | 0.40              |
| 25:Y:397:MET:CE   | 25:Y:479:THR:HG23 | 2.49                     | 0.40              |
| 25:Y:693:LEU:HB3  | 25:Y:723:SER:HB3  | 2.03                     | 0.40              |
| 25:Y:770:VAL:HG12 | 25:Y:772:TYR:H    | 1.87                     | 0.40              |
| 2:3:27:C:H1'      | 2:3:44:G:H22      | 1.87                     | 0.40              |
| 3:A:71:A:N6       | 3:A:99:C:HO2'     | 2.19                     | 0.40              |
| 3:A:168:G:C6      | 3:A:169:C:C2      | 3.09                     | 0.40              |
| 3:A:408:A:C6      | 3:A:435:A:C6      | 3.10                     | 0.40              |
| 3:A:459:A:C6      | 3:A:474:G:C6      | 3.10                     | 0.40              |
| 3:A:840:C:H2'     | 3:A:841:C:H5''    | 2.03                     | 0.40              |
| 3:A:1233:G:H2'    | 3:A:1234:C:C6     | 2.57                     | 0.40              |
| 3:A:1284:C:OP2    | 3:A:1285:A:O2'    | 2.29                     | 0.40              |
| 3:A:1518:MA6:C6   | 3:A:1519:MA6:H103 | 2.51                     | 0.40              |
| 11:I:6:TYR:HB2    | 11:I:21:ILE:HB    | 2.04                     | 0.40              |
| 12:J:80:THR:O     | 12:J:84:VAL:HG23  | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

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 |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 4   | B     | 222/241 (92%)   | 215 (97%)  | 7 (3%)  | 0        | 100         | 100 |
| 5   | C     | 209/233 (90%)   | 206 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 6   | D     | 203/206 (98%)   | 199 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 7   | E     | 154/167 (92%)   | 151 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 8   | F     | 104/135 (77%)   | 103 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 9   | G     | 149/179 (83%)   | 146 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 10  | H     | 127/130 (98%)   | 124 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 11  | I     | 125/130 (96%)   | 120 (96%)  | 5 (4%)  | 0        | 100         | 100 |
| 12  | J     | 98/103 (95%)    | 96 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 13  | K     | 115/129 (89%)   | 112 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 14  | L     | 121/124 (98%)   | 117 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 15  | M     | 113/118 (96%)   | 108 (96%)  | 5 (4%)  | 0        | 100         | 100 |
| 16  | N     | 98/101 (97%)    | 96 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 17  | O     | 86/89 (97%)     | 86 (100%)  | 0       | 0        | 100         | 100 |
| 18  | P     | 80/82 (98%)     | 80 (100%)  | 0       | 0        | 100         | 100 |
| 19  | Q     | 78/84 (93%)     | 73 (94%)   | 5 (6%)  | 0        | 100         | 100 |
| 20  | R     | 54/75 (72%)     | 53 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 21  | S     | 81/92 (88%)     | 78 (96%)   | 3 (4%)  | 0        | 100         | 100 |
| 22  | T     | 84/87 (97%)     | 84 (100%)  | 0       | 0        | 100         | 100 |
| 23  | U     | 50/71 (70%)     | 50 (100%)  | 0       | 0        | 100         | 100 |
| 24  | X     | 68/72 (94%)     | 67 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 25  | Y     | 486/890 (55%)   | 466 (96%)  | 20 (4%) | 0        | 100         | 100 |
| 26  | Z     | 110/180 (61%)   | 105 (96%)  | 5 (4%)  | 0        | 100         | 100 |
| All | All   | 3015/3718 (81%) | 2935 (97%) | 80 (3%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 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 PDB entries followed by that with respect to all EM

entries.

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 |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 4   | B     | 186/199 (94%)   | 186 (100%)  | 0        | 100         | 100 |
| 5   | C     | 172/190 (90%)   | 172 (100%)  | 0        | 100         | 100 |
| 6   | D     | 172/173 (99%)   | 172 (100%)  | 0        | 100         | 100 |
| 7   | E     | 119/126 (94%)   | 119 (100%)  | 0        | 100         | 100 |
| 8   | F     | 92/116 (79%)    | 92 (100%)   | 0        | 100         | 100 |
| 9   | G     | 124/147 (84%)   | 124 (100%)  | 0        | 100         | 100 |
| 10  | H     | 104/105 (99%)   | 104 (100%)  | 0        | 100         | 100 |
| 11  | I     | 105/107 (98%)   | 105 (100%)  | 0        | 100         | 100 |
| 12  | J     | 88/90 (98%)     | 88 (100%)   | 0        | 100         | 100 |
| 13  | K     | 90/99 (91%)     | 90 (100%)   | 0        | 100         | 100 |
| 14  | L     | 103/104 (99%)   | 103 (100%)  | 0        | 100         | 100 |
| 15  | M     | 93/96 (97%)     | 93 (100%)   | 0        | 100         | 100 |
| 16  | N     | 83/84 (99%)     | 83 (100%)   | 0        | 100         | 100 |
| 17  | O     | 76/77 (99%)     | 76 (100%)   | 0        | 100         | 100 |
| 18  | P     | 65/65 (100%)    | 65 (100%)   | 0        | 100         | 100 |
| 19  | Q     | 74/78 (95%)     | 74 (100%)   | 0        | 100         | 100 |
| 20  | R     | 49/65 (75%)     | 49 (100%)   | 0        | 100         | 100 |
| 21  | S     | 72/79 (91%)     | 72 (100%)   | 0        | 100         | 100 |
| 22  | T     | 65/66 (98%)     | 65 (100%)   | 0        | 100         | 100 |
| 23  | U     | 43/61 (70%)     | 43 (100%)   | 0        | 100         | 100 |
| 24  | X     | 64/65 (98%)     | 64 (100%)   | 0        | 100         | 100 |
| 25  | Y     | 386/713 (54%)   | 386 (100%)  | 0        | 100         | 100 |
| 26  | Z     | 101/156 (65%)   | 101 (100%)  | 0        | 100         | 100 |
| All | All   | 2526/3061 (82%) | 2526 (100%) | 0        | 100         | 100 |

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | B     | 39  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | B     | 51  | ASN  |
| 5   | C     | 3   | GLN  |
| 5   | C     | 25  | ASN  |
| 6   | D     | 54  | GLN  |
| 7   | E     | 78  | ASN  |
| 7   | E     | 121 | HIS  |
| 7   | E     | 135 | ASN  |
| 8   | F     | 37  | HIS  |
| 8   | F     | 68  | GLN  |
| 9   | G     | 68  | ASN  |
| 9   | G     | 122 | ASN  |
| 9   | G     | 148 | ASN  |
| 10  | H     | 16  | ASN  |
| 11  | I     | 5   | GLN  |
| 11  | I     | 32  | GLN  |
| 11  | I     | 50  | GLN  |
| 12  | J     | 58  | ASN  |
| 13  | K     | 15  | GLN  |
| 13  | K     | 64  | GLN  |
| 13  | K     | 118 | HIS  |
| 13  | K     | 119 | ASN  |
| 14  | L     | 96  | HIS  |
| 15  | M     | 14  | HIS  |
| 15  | M     | 91  | HIS  |
| 15  | M     | 105 | ASN  |
| 16  | N     | 4   | GLN  |
| 16  | N     | 35  | ASN  |
| 17  | O     | 20  | ASN  |
| 17  | O     | 38  | HIS  |
| 19  | Q     | 9   | GLN  |
| 20  | R     | 52  | GLN  |
| 20  | R     | 54  | GLN  |
| 22  | T     | 61  | GLN  |
| 22  | T     | 70  | ASN  |
| 22  | T     | 75  | HIS  |
| 22  | T     | 78  | ASN  |
| 22  | T     | 82  | GLN  |
| 24  | X     | 28  | ASN  |
| 25  | Y     | 300 | GLN  |
| 25  | Y     | 331 | GLN  |
| 25  | Y     | 351 | GLN  |
| 25  | Y     | 402 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | Y     | 448 | HIS  |
| 25  | Y     | 485 | HIS  |
| 25  | Y     | 516 | GLN  |
| 25  | Y     | 529 | GLN  |
| 25  | Y     | 669 | GLN  |
| 25  | Y     | 670 | GLN  |
| 25  | Y     | 773 | ASN  |
| 26  | Z     | 92  | GLN  |
| 26  | Z     | 108 | GLN  |
| 26  | Z     | 137 | HIS  |
| 26  | Z     | 169 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | 2     | 3/4 (75%)       | 1 (33%)           | 0               |
| 2   | 3     | 76/77 (98%)     | 38 (50%)          | 6 (7%)          |
| 3   | A     | 1533/1542 (99%) | 249 (16%)         | 13 (0%)         |
| All | All   | 1612/1623 (99%) | 288 (17%)         | 19 (1%)         |

All (288) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 18  | G    |
| 2   | 3     | 2   | A    |
| 2   | 3     | 3   | G    |
| 2   | 3     | 4   | C    |
| 2   | 3     | 5   | G    |
| 2   | 3     | 6   | G    |
| 2   | 3     | 9   | G    |
| 2   | 3     | 10  | U    |
| 2   | 3     | 13  | A    |
| 2   | 3     | 15  | U    |
| 2   | 3     | 16  | C    |
| 2   | 3     | 17  | G    |
| 2   | 3     | 19  | U    |
| 2   | 3     | 20  | U    |
| 2   | 3     | 21  | A    |
| 2   | 3     | 22  | G    |
| 2   | 3     | 24  | A    |
| 2   | 3     | 26  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 3     | 27  | C    |
| 2   | 3     | 35  | A    |
| 2   | 3     | 41  | C    |
| 2   | 3     | 45  | G    |
| 2   | 3     | 47  | U    |
| 2   | 3     | 48  | C    |
| 2   | 3     | 55  | U    |
| 2   | 3     | 56  | C    |
| 2   | 3     | 57  | G    |
| 2   | 3     | 59  | G    |
| 2   | 3     | 60  | U    |
| 2   | 3     | 61  | C    |
| 2   | 3     | 62  | C    |
| 2   | 3     | 63  | C    |
| 2   | 3     | 64  | G    |
| 2   | 3     | 65  | U    |
| 2   | 3     | 66  | C    |
| 2   | 3     | 70  | U    |
| 2   | 3     | 71  | C    |
| 2   | 3     | 72  | C    |
| 2   | 3     | 73  | G    |
| 3   | A     | 3   | A    |
| 3   | A     | 7   | A    |
| 3   | A     | 8   | A    |
| 3   | A     | 9   | G    |
| 3   | A     | 14  | U    |
| 3   | A     | 22  | G    |
| 3   | A     | 31  | G    |
| 3   | A     | 32  | A    |
| 3   | A     | 39  | G    |
| 3   | A     | 44  | A    |
| 3   | A     | 47  | C    |
| 3   | A     | 48  | C    |
| 3   | A     | 51  | A    |
| 3   | A     | 64  | G    |
| 3   | A     | 70  | U    |
| 3   | A     | 71  | A    |
| 3   | A     | 74  | A    |
| 3   | A     | 75  | G    |
| 3   | A     | 76  | G    |
| 3   | A     | 77  | A    |
| 3   | A     | 79  | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | A     | 81  | A    |
| 3   | A     | 82  | G    |
| 3   | A     | 83  | C    |
| 3   | A     | 84  | U    |
| 3   | A     | 85  | U    |
| 3   | A     | 86  | G    |
| 3   | A     | 88  | U    |
| 3   | A     | 89  | U    |
| 3   | A     | 90  | C    |
| 3   | A     | 91  | U    |
| 3   | A     | 93  | U    |
| 3   | A     | 94  | G    |
| 3   | A     | 95  | C    |
| 3   | A     | 109 | A    |
| 3   | A     | 121 | U    |
| 3   | A     | 131 | A    |
| 3   | A     | 141 | G    |
| 3   | A     | 143 | A    |
| 3   | A     | 144 | G    |
| 3   | A     | 163 | C    |
| 3   | A     | 181 | A    |
| 3   | A     | 197 | A    |
| 3   | A     | 210 | C    |
| 3   | A     | 211 | G    |
| 3   | A     | 212 | G    |
| 3   | A     | 213 | G    |
| 3   | A     | 240 | G    |
| 3   | A     | 247 | G    |
| 3   | A     | 251 | G    |
| 3   | A     | 266 | G    |
| 3   | A     | 267 | C    |
| 3   | A     | 280 | C    |
| 3   | A     | 289 | G    |
| 3   | A     | 299 | G    |
| 3   | A     | 328 | C    |
| 3   | A     | 330 | C    |
| 3   | A     | 332 | G    |
| 3   | A     | 345 | C    |
| 3   | A     | 347 | G    |
| 3   | A     | 351 | G    |
| 3   | A     | 352 | C    |
| 3   | A     | 366 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | A     | 367 | U    |
| 3   | A     | 372 | C    |
| 3   | A     | 384 | G    |
| 3   | A     | 397 | A    |
| 3   | A     | 406 | G    |
| 3   | A     | 411 | A    |
| 3   | A     | 413 | G    |
| 3   | A     | 421 | U    |
| 3   | A     | 422 | C    |
| 3   | A     | 423 | G    |
| 3   | A     | 424 | G    |
| 3   | A     | 429 | U    |
| 3   | A     | 444 | G    |
| 3   | A     | 467 | U    |
| 3   | A     | 468 | A    |
| 3   | A     | 472 | U    |
| 3   | A     | 475 | C    |
| 3   | A     | 481 | G    |
| 3   | A     | 484 | G    |
| 3   | A     | 485 | U    |
| 3   | A     | 486 | U    |
| 3   | A     | 495 | A    |
| 3   | A     | 496 | A    |
| 3   | A     | 509 | A    |
| 3   | A     | 511 | C    |
| 3   | A     | 512 | U    |
| 3   | A     | 518 | C    |
| 3   | A     | 527 | G7M  |
| 3   | A     | 531 | U    |
| 3   | A     | 532 | A    |
| 3   | A     | 547 | A    |
| 3   | A     | 562 | U    |
| 3   | A     | 564 | C    |
| 3   | A     | 571 | U    |
| 3   | A     | 572 | A    |
| 3   | A     | 573 | A    |
| 3   | A     | 575 | G    |
| 3   | A     | 576 | C    |
| 3   | A     | 577 | G    |
| 3   | A     | 579 | A    |
| 3   | A     | 596 | A    |
| 3   | A     | 633 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | A     | 653 | U    |
| 3   | A     | 665 | A    |
| 3   | A     | 685 | G    |
| 3   | A     | 686 | U    |
| 3   | A     | 694 | A    |
| 3   | A     | 695 | A    |
| 3   | A     | 702 | A    |
| 3   | A     | 703 | G    |
| 3   | A     | 718 | A    |
| 3   | A     | 719 | C    |
| 3   | A     | 720 | C    |
| 3   | A     | 721 | G    |
| 3   | A     | 723 | U    |
| 3   | A     | 724 | G    |
| 3   | A     | 734 | G    |
| 3   | A     | 755 | G    |
| 3   | A     | 758 | C    |
| 3   | A     | 777 | A    |
| 3   | A     | 790 | A    |
| 3   | A     | 791 | G    |
| 3   | A     | 793 | U    |
| 3   | A     | 794 | A    |
| 3   | A     | 815 | A    |
| 3   | A     | 817 | C    |
| 3   | A     | 821 | G    |
| 3   | A     | 828 | U    |
| 3   | A     | 832 | G    |
| 3   | A     | 840 | C    |
| 3   | A     | 841 | C    |
| 3   | A     | 845 | A    |
| 3   | A     | 849 | G    |
| 3   | A     | 872 | A    |
| 3   | A     | 873 | A    |
| 3   | A     | 889 | A    |
| 3   | A     | 901 | A    |
| 3   | A     | 902 | G    |
| 3   | A     | 914 | A    |
| 3   | A     | 926 | G    |
| 3   | A     | 931 | C    |
| 3   | A     | 933 | G    |
| 3   | A     | 934 | C    |
| 3   | A     | 935 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | A     | 957  | U    |
| 3   | A     | 960  | U    |
| 3   | A     | 965  | U    |
| 3   | A     | 969  | A    |
| 3   | A     | 971  | G    |
| 3   | A     | 975  | A    |
| 3   | A     | 976  | G    |
| 3   | A     | 977  | A    |
| 3   | A     | 993  | G    |
| 3   | A     | 994  | A    |
| 3   | A     | 1003 | G    |
| 3   | A     | 1004 | A    |
| 3   | A     | 1006 | G    |
| 3   | A     | 1020 | G    |
| 3   | A     | 1021 | A    |
| 3   | A     | 1022 | A    |
| 3   | A     | 1024 | G    |
| 3   | A     | 1025 | U    |
| 3   | A     | 1026 | G    |
| 3   | A     | 1028 | C    |
| 3   | A     | 1029 | U    |
| 3   | A     | 1030 | U    |
| 3   | A     | 1031 | C    |
| 3   | A     | 1032 | G    |
| 3   | A     | 1036 | A    |
| 3   | A     | 1037 | C    |
| 3   | A     | 1053 | G    |
| 3   | A     | 1054 | C    |
| 3   | A     | 1055 | A    |
| 3   | A     | 1065 | U    |
| 3   | A     | 1066 | C    |
| 3   | A     | 1084 | G    |
| 3   | A     | 1094 | G    |
| 3   | A     | 1095 | U    |
| 3   | A     | 1101 | A    |
| 3   | A     | 1108 | G    |
| 3   | A     | 1124 | G    |
| 3   | A     | 1126 | U    |
| 3   | A     | 1136 | C    |
| 3   | A     | 1137 | C    |
| 3   | A     | 1138 | G    |
| 3   | A     | 1139 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | A     | 1142 | G    |
| 3   | A     | 1143 | G    |
| 3   | A     | 1159 | U    |
| 3   | A     | 1167 | A    |
| 3   | A     | 1168 | U    |
| 3   | A     | 1169 | A    |
| 3   | A     | 1171 | A    |
| 3   | A     | 1184 | G    |
| 3   | A     | 1193 | G    |
| 3   | A     | 1196 | A    |
| 3   | A     | 1200 | C    |
| 3   | A     | 1213 | A    |
| 3   | A     | 1214 | C    |
| 3   | A     | 1225 | A    |
| 3   | A     | 1240 | U    |
| 3   | A     | 1241 | G    |
| 3   | A     | 1258 | G    |
| 3   | A     | 1260 | G    |
| 3   | A     | 1280 | A    |
| 3   | A     | 1285 | A    |
| 3   | A     | 1286 | U    |
| 3   | A     | 1287 | A    |
| 3   | A     | 1298 | U    |
| 3   | A     | 1299 | A    |
| 3   | A     | 1300 | G    |
| 3   | A     | 1301 | U    |
| 3   | A     | 1304 | G    |
| 3   | A     | 1305 | G    |
| 3   | A     | 1317 | C    |
| 3   | A     | 1320 | C    |
| 3   | A     | 1331 | G    |
| 3   | A     | 1340 | A    |
| 3   | A     | 1353 | G    |
| 3   | A     | 1363 | A    |
| 3   | A     | 1364 | U    |
| 3   | A     | 1379 | G    |
| 3   | A     | 1403 | C    |
| 3   | A     | 1411 | C    |
| 3   | A     | 1413 | A    |
| 3   | A     | 1418 | A    |
| 3   | A     | 1426 | G    |
| 3   | A     | 1441 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | A     | 1442 | G    |
| 3   | A     | 1446 | A    |
| 3   | A     | 1468 | A    |
| 3   | A     | 1470 | U    |
| 3   | A     | 1475 | G    |
| 3   | A     | 1483 | A    |
| 3   | A     | 1485 | U    |
| 3   | A     | 1492 | A    |
| 3   | A     | 1497 | G    |
| 3   | A     | 1499 | A    |
| 3   | A     | 1503 | A    |
| 3   | A     | 1506 | U    |
| 3   | A     | 1507 | A    |
| 3   | A     | 1519 | MA6  |
| 3   | A     | 1529 | G    |
| 3   | A     | 1530 | G    |
| 3   | A     | 1532 | U    |
| 3   | A     | 1534 | A    |

All (19) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | 3     | 14   | G    |
| 2   | 3     | 18   | G    |
| 2   | 3     | 21   | A    |
| 2   | 3     | 34   | C    |
| 2   | 3     | 63   | C    |
| 2   | 3     | 70   | U    |
| 3   | A     | 2    | A    |
| 3   | A     | 212  | G    |
| 3   | A     | 298  | A    |
| 3   | A     | 471  | U    |
| 3   | A     | 531  | U    |
| 3   | A     | 685  | G    |
| 3   | A     | 719  | C    |
| 3   | A     | 723  | U    |
| 3   | A     | 790  | A    |
| 3   | A     | 1031 | C    |
| 3   | A     | 1183 | U    |
| 3   | A     | 1240 | U    |
| 3   | A     | 1484 | C    |

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

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

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | 2MG  | A     | 1516 | 3    | 23,26,27     | 1.27 | 4 (17%)  | 33,38,41    | 2.17 | 10 (30%) |
| 3   | 5MC  | A     | 967  | 3    | 19,22,23     | 1.63 | 3 (15%)  | 26,32,35    | 1.14 | 3 (11%)  |
| 3   | 2MG  | A     | 966  | 3    | 23,26,27     | 1.24 | 4 (17%)  | 33,38,41    | 2.19 | 7 (21%)  |
| 3   | MA6  | A     | 1519 | 3    | 23,26,27     | 1.45 | 4 (17%)  | 33,38,41    | 2.41 | 13 (39%) |
| 3   | 4OC  | A     | 1402 | 3    | 20,23,24     | 0.76 | 0        | 25,32,35    | 0.92 | 1 (4%)   |
| 3   | 2MG  | A     | 1207 | 3    | 23,26,27     | 1.26 | 4 (17%)  | 33,38,41    | 2.19 | 5 (15%)  |
| 3   | G7M  | A     | 527  | 3    | 23,26,27     | 0.54 | 0        | 34,39,42    | 0.93 | 1 (2%)   |
| 3   | PSU  | A     | 516  | 3    | 18,21,22     | 1.41 | 4 (22%)  | 21,30,33    | 2.05 | 4 (19%)  |
| 3   | 5MC  | A     | 1407 | 3    | 19,22,23     | 1.48 | 3 (15%)  | 26,32,35    | 1.17 | 3 (11%)  |
| 3   | UR3  | A     | 1498 | 3    | 19,22,23     | 0.92 | 0        | 26,32,35    | 1.71 | 2 (7%)   |
| 3   | MA6  | A     | 1518 | 3    | 23,26,27     | 1.49 | 5 (21%)  | 33,38,41    | 2.34 | 11 (33%) |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 3   | 2MG  | A     | 1516 | 3    | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | 5MC  | A     | 967  | 3    | -       | 1/7/25/26  | 0/2/2/2 |
| 3   | 2MG  | A     | 966  | 3    | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | MA6  | A     | 1519 | 3    | -       | 3/11/29/30 | 0/3/3/3 |
| 3   | 4OC  | A     | 1402 | 3    | -       | 0/9/29/30  | 0/2/2/2 |
| 3   | 2MG  | A     | 1207 | 3    | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | G7M  | A     | 527  | 3    | -       | 2/7/25/26  | 0/3/3/3 |
| 3   | PSU  | A     | 516  | 3    | -       | 4/7/25/26  | 0/2/2/2 |
| 3   | 5MC  | A     | 1407 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | UR3  | A     | 1498 | 3    | -       | 1/7/25/26  | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 3   | MA6  | A     | 1518 | 3    | -       | 1/11/29/30 | 0/3/3/3 |

All (31) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3   | A     | 967  | 5MC  | C5-C4 | 5.87  | 1.48        | 1.44     |
| 3   | A     | 1407 | 5MC  | C5-C4 | 5.07  | 1.48        | 1.44     |
| 3   | A     | 1518 | MA6  | C5-C4 | 4.44  | 1.47        | 1.39     |
| 3   | A     | 1519 | MA6  | C5-C4 | 4.36  | 1.46        | 1.39     |
| 3   | A     | 1207 | 2MG  | C5-C4 | 3.13  | 1.47        | 1.38     |
| 3   | A     | 966  | 2MG  | C5-C4 | 3.02  | 1.47        | 1.38     |
| 3   | A     | 516  | PSU  | C6-C5 | 2.93  | 1.38        | 1.35     |
| 3   | A     | 1516 | 2MG  | C5-C4 | 2.89  | 1.46        | 1.38     |
| 3   | A     | 516  | PSU  | C4-N3 | -2.77 | 1.33        | 1.38     |
| 3   | A     | 967  | 5MC  | C6-C5 | 2.74  | 1.39        | 1.34     |
| 3   | A     | 1407 | 5MC  | C6-N1 | -2.72 | 1.33        | 1.38     |
| 3   | A     | 1518 | MA6  | C5-C6 | 2.66  | 1.48        | 1.41     |
| 3   | A     | 1516 | 2MG  | C6-N1 | -2.64 | 1.33        | 1.38     |
| 3   | A     | 1519 | MA6  | C5-N7 | -2.55 | 1.34        | 1.39     |
| 3   | A     | 1207 | 2MG  | C6-N1 | -2.51 | 1.34        | 1.38     |
| 3   | A     | 1518 | MA6  | C5-N7 | -2.48 | 1.34        | 1.39     |
| 3   | A     | 1519 | MA6  | C5-C6 | 2.48  | 1.47        | 1.41     |
| 3   | A     | 966  | 2MG  | C6-N1 | -2.42 | 1.34        | 1.38     |
| 3   | A     | 1407 | 5MC  | C6-C5 | 2.37  | 1.38        | 1.34     |
| 3   | A     | 967  | 5MC  | C6-N1 | -2.33 | 1.34        | 1.38     |
| 3   | A     | 1516 | 2MG  | C5-N7 | -2.25 | 1.34        | 1.39     |
| 3   | A     | 516  | PSU  | C2-N3 | -2.24 | 1.33        | 1.37     |
| 3   | A     | 1207 | 2MG  | C2-N3 | 2.23  | 1.36        | 1.32     |
| 3   | A     | 1518 | MA6  | C4-N9 | -2.16 | 1.33        | 1.37     |
| 3   | A     | 1519 | MA6  | C4-N9 | -2.15 | 1.33        | 1.37     |
| 3   | A     | 1516 | 2MG  | C4-N9 | -2.15 | 1.32        | 1.38     |
| 3   | A     | 516  | PSU  | C2-N1 | -2.10 | 1.33        | 1.36     |
| 3   | A     | 966  | 2MG  | C2-N3 | 2.09  | 1.35        | 1.32     |
| 3   | A     | 1518 | MA6  | C8-N9 | -2.07 | 1.34        | 1.37     |
| 3   | A     | 1207 | 2MG  | C5-N7 | -2.05 | 1.35        | 1.39     |
| 3   | A     | 966  | 2MG  | C5-N7 | -2.02 | 1.35        | 1.39     |

All (60) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 3   | A     | 1207 | 2MG  | C2-N3-C4 | 7.15 | 120.94      | 112.00   |
| 3   | A     | 966  | 2MG  | C2-N3-C4 | 7.15 | 120.94      | 112.00   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 3   | A     | 1498 | UR3  | C4-N3-C2  | -6.98 | 118.96      | 124.58   |
| 3   | A     | 1516 | 2MG  | C2-N3-C4  | 6.74  | 120.43      | 112.00   |
| 3   | A     | 516  | PSU  | N1-C2-N3  | 6.37  | 121.89      | 115.17   |
| 3   | A     | 1207 | 2MG  | C5-C4-N3  | -6.27 | 118.41      | 128.39   |
| 3   | A     | 966  | 2MG  | C5-C4-N3  | -5.87 | 119.05      | 128.39   |
| 3   | A     | 1516 | 2MG  | C5-C4-N3  | -5.83 | 119.11      | 128.39   |
| 3   | A     | 1519 | MA6  | C5-C4-N3  | -5.75 | 118.80      | 126.72   |
| 3   | A     | 1518 | MA6  | C5-C4-N3  | -5.70 | 118.87      | 126.72   |
| 3   | A     | 1519 | MA6  | C9-N6-C6  | -4.85 | 108.17      | 120.52   |
| 3   | A     | 1207 | 2MG  | N9-C4-N3  | 4.65  | 135.26      | 125.95   |
| 3   | A     | 1519 | MA6  | N3-C4-N9  | 4.63  | 135.05      | 127.17   |
| 3   | A     | 1518 | MA6  | N3-C4-N9  | 4.50  | 134.81      | 127.17   |
| 3   | A     | 1518 | MA6  | C9-N6-C6  | -4.43 | 109.25      | 120.52   |
| 3   | A     | 966  | 2MG  | N9-C4-N3  | 4.37  | 134.70      | 125.95   |
| 3   | A     | 1518 | MA6  | C2-N1-C6  | 4.16  | 121.99      | 111.83   |
| 3   | A     | 1516 | 2MG  | N9-C4-N3  | 4.09  | 134.13      | 125.95   |
| 3   | A     | 1519 | MA6  | C2-N1-C6  | 4.06  | 121.74      | 111.83   |
| 3   | A     | 516  | PSU  | C4-N3-C2  | -3.93 | 120.95      | 126.37   |
| 3   | A     | 516  | PSU  | O2-C2-N1  | -3.83 | 118.84      | 122.79   |
| 3   | A     | 1518 | MA6  | C4-C5-N7  | -3.71 | 106.34      | 110.58   |
| 3   | A     | 1519 | MA6  | C10-N6-C6 | -3.70 | 111.11      | 120.52   |
| 3   | A     | 1519 | MA6  | C2-N3-C4  | 3.62  | 120.67      | 111.83   |
| 3   | A     | 1518 | MA6  | C2-N3-C4  | 3.62  | 120.67      | 111.83   |
| 3   | A     | 1407 | 5MC  | C5-C6-N1  | -3.50 | 119.51      | 123.31   |
| 3   | A     | 1519 | MA6  | C4-C5-N7  | -3.49 | 106.59      | 110.58   |
| 3   | A     | 966  | 2MG  | C6-C5-N7  | 3.41  | 136.49      | 130.29   |
| 3   | A     | 1516 | 2MG  | C6-C5-N7  | 3.34  | 136.38      | 130.29   |
| 3   | A     | 1518 | MA6  | C10-N6-C6 | -3.34 | 112.03      | 120.52   |
| 3   | A     | 1498 | UR3  | C5-C4-N3  | 3.26  | 119.34      | 115.04   |
| 3   | A     | 527  | G7M  | C8-N7-C5  | -3.22 | 103.75      | 107.78   |
| 3   | A     | 1518 | MA6  | N1-C2-N3  | -3.20 | 123.74      | 128.58   |
| 3   | A     | 1519 | MA6  | N1-C2-N3  | -3.19 | 123.75      | 128.58   |
| 3   | A     | 1207 | 2MG  | C6-C5-N7  | 3.18  | 136.07      | 130.29   |
| 3   | A     | 967  | 5MC  | C5-C6-N1  | -3.16 | 119.88      | 123.31   |
| 3   | A     | 1519 | MA6  | N1-C6-N6  | 3.15  | 120.69      | 116.86   |
| 3   | A     | 1519 | MA6  | C4-N9-C8  | 2.81  | 108.69      | 105.74   |
| 3   | A     | 1518 | MA6  | C4-N9-C8  | 2.78  | 108.66      | 105.74   |
| 3   | A     | 967  | 5MC  | C5-C4-N3  | -2.74 | 118.94      | 121.75   |
| 3   | A     | 1518 | MA6  | N1-C6-N6  | 2.72  | 120.17      | 116.86   |
| 3   | A     | 1516 | 2MG  | C4-C5-N7  | -2.65 | 106.47      | 110.67   |
| 3   | A     | 1207 | 2MG  | C4-C5-N7  | -2.60 | 106.54      | 110.67   |
| 3   | A     | 1518 | MA6  | C5-N7-C8  | 2.60  | 107.53      | 103.45   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | A     | 1519 | MA6  | C5-N7-C8    | 2.55  | 107.46      | 103.45   |
| 3   | A     | 966  | 2MG  | C4-C5-N7    | -2.51 | 106.70      | 110.67   |
| 3   | A     | 1407 | 5MC  | C5-C4-N3    | -2.37 | 119.32      | 121.75   |
| 3   | A     | 1516 | 2MG  | N2-C2-N3    | -2.33 | 117.55      | 120.51   |
| 3   | A     | 1519 | MA6  | C5-C6-N6    | -2.32 | 121.67      | 125.33   |
| 3   | A     | 1516 | 2MG  | N1-C2-N2    | 2.32  | 118.92      | 116.56   |
| 3   | A     | 1407 | 5MC  | O2-C2-N3    | -2.27 | 118.75      | 122.33   |
| 3   | A     | 966  | 2MG  | N1-C2-N2    | 2.23  | 118.84      | 116.56   |
| 3   | A     | 966  | 2MG  | O6-C6-C5    | -2.20 | 120.73      | 126.53   |
| 3   | A     | 967  | 5MC  | O2-C2-N3    | -2.19 | 118.88      | 122.33   |
| 3   | A     | 1516 | 2MG  | C2-N1-C6    | -2.17 | 121.93      | 124.55   |
| 3   | A     | 1519 | MA6  | C10-N6-C9   | -2.16 | 109.23      | 116.18   |
| 3   | A     | 1516 | 2MG  | CM2-N2-C2   | -2.12 | 119.09      | 123.65   |
| 3   | A     | 1402 | 4OC  | CM4-N4-C4   | -2.12 | 118.32      | 122.45   |
| 3   | A     | 516  | PSU  | O4'-C1'-C2' | 2.09  | 108.04      | 105.15   |
| 3   | A     | 1516 | 2MG  | O6-C6-C5    | -2.08 | 121.05      | 126.53   |

There are no chirality outliers.

All (12) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | A     | 516  | PSU  | C2'-C1'-C5-C4   |
| 3   | A     | 516  | PSU  | C2'-C1'-C5-C6   |
| 3   | A     | 527  | G7M  | O4'-C4'-C5'-O5' |
| 3   | A     | 1519 | MA6  | O4'-C4'-C5'-O5' |
| 3   | A     | 527  | G7M  | C3'-C4'-C5'-O5' |
| 3   | A     | 1519 | MA6  | C3'-C4'-C5'-O5' |
| 3   | A     | 516  | PSU  | C3'-C4'-C5'-O5' |
| 3   | A     | 516  | PSU  | O4'-C4'-C5'-O5' |
| 3   | A     | 1518 | MA6  | C5-C6-N6-C10    |
| 3   | A     | 1519 | MA6  | C5-C6-N6-C10    |
| 3   | A     | 967  | 5MC  | O4'-C4'-C5'-O5' |
| 3   | A     | 1498 | UR3  | O4'-C4'-C5'-O5' |

There are no ring outliers.

5 monomers are involved in 7 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | A     | 1516 | 2MG  | 1       | 0            |
| 3   | A     | 1519 | MA6  | 4       | 0            |
| 3   | A     | 1402 | 4OC  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | A     | 516  | PSU  | 1       | 0            |
| 3   | A     | 1518 | MA6  | 4       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 159 ligands modelled in this entry, 158 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 |
| 29  | A1IC4 | A     | 1601 | -    | 42,46,46     | 2.29 | 12 (28%) | 47,63,63    | 1.70 | 7 (14%)  |

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   |
|-----|-------|-------|------|------|---------|-------------|---------|
| 29  | A1IC4 | A     | 1601 | -    | -       | 19/49/60/60 | 0/3/3/3 |

All (12) bond length outliers are listed below:

| Mol | Chain | Res  | Type  | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|-------|---------|-------|-------------|----------|
| 29  | A     | 1601 | A1IC4 | C1-N1   | 6.63  | 1.45        | 1.33     |
| 29  | A     | 1601 | A1IC4 | C12-N4  | 5.45  | 1.45        | 1.34     |
| 29  | A     | 1601 | A1IC4 | C6-N2   | 5.24  | 1.45        | 1.34     |
| 29  | A     | 1601 | A1IC4 | C18-N7  | 5.15  | 1.45        | 1.34     |
| 29  | A     | 1601 | A1IC4 | C22-N9  | -3.53 | 1.32        | 1.38     |
| 29  | A     | 1601 | A1IC4 | O2-C1   | 3.22  | 1.40        | 1.35     |
| 29  | A     | 1601 | A1IC4 | C24-CL1 | 2.89  | 1.78        | 1.71     |

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| Mol | Chain | Res  | Type  | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|-------|--------|-------|-------------|----------|
| 29  | A     | 1601 | A1IC4 | O7-C18 | -2.47 | 1.18        | 1.23     |
| 29  | A     | 1601 | A1IC4 | C15-N6 | -2.45 | 1.32        | 1.38     |
| 29  | A     | 1601 | A1IC4 | O6-C12 | -2.40 | 1.18        | 1.23     |
| 29  | A     | 1601 | A1IC4 | O4-C6  | -2.37 | 1.18        | 1.23     |
| 29  | A     | 1601 | A1IC4 | O2-C2  | -2.30 | 1.40        | 1.45     |

All (7) bond angle outliers are listed below:

| Mol | Chain | Res  | Type  | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|-------|-------------|-------|-------------|----------|
| 29  | A     | 1601 | A1IC4 | O2-C1-N1    | 7.26  | 120.14      | 111.11   |
| 29  | A     | 1601 | A1IC4 | O1-C1-N1    | -3.73 | 119.69      | 125.58   |
| 29  | A     | 1601 | A1IC4 | C23-C22-N9  | -3.17 | 106.65      | 110.75   |
| 29  | A     | 1601 | A1IC4 | O2-C1-O1    | -3.16 | 120.16      | 123.08   |
| 29  | A     | 1601 | A1IC4 | C13-C14-C15 | -2.41 | 108.09      | 113.75   |
| 29  | A     | 1601 | A1IC4 | C13-C18-N7  | 2.38  | 121.70      | 116.63   |
| 29  | A     | 1601 | A1IC4 | C19-N7-C18  | -2.05 | 116.83      | 121.90   |

There are no chirality outliers.

All (19) torsion outliers are listed below:

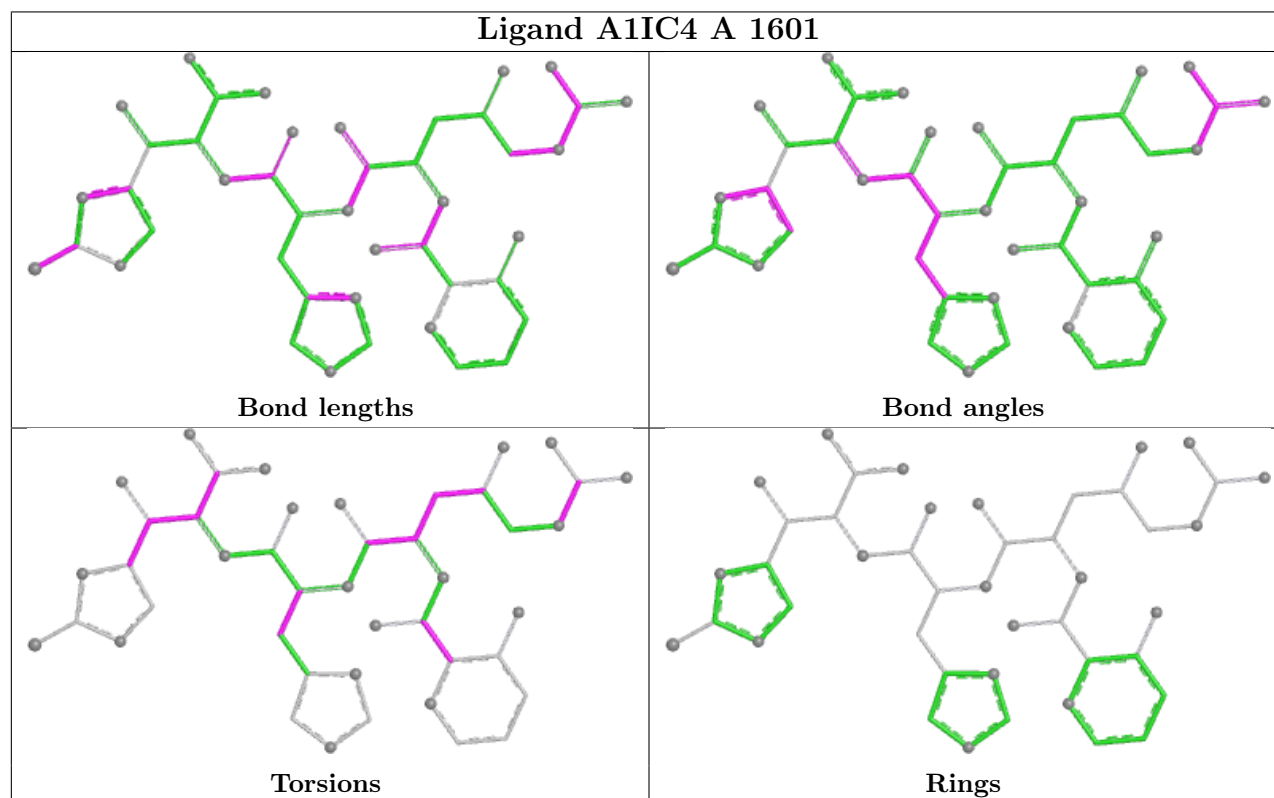
| Mol | Chain | Res  | Type  | Atoms           |
|-----|-------|------|-------|-----------------|
| 29  | A     | 1601 | A1IC4 | N1-C1-O2-C2     |
| 29  | A     | 1601 | A1IC4 | O1-C1-O2-C2     |
| 29  | A     | 1601 | A1IC4 | C2-C3-C4-C5     |
| 29  | A     | 1601 | A1IC4 | O3-C3-C4-C5     |
| 29  | A     | 1601 | A1IC4 | C18-C13-C14-C15 |
| 29  | A     | 1601 | A1IC4 | N7-C19-C21-O10  |
| 29  | A     | 1601 | A1IC4 | N7-C19-C21-C22  |
| 29  | A     | 1601 | A1IC4 | C20-C19-C21-O10 |
| 29  | A     | 1601 | A1IC4 | C20-C19-C21-C22 |
| 29  | A     | 1601 | A1IC4 | O10-C21-C22-N9  |
| 29  | A     | 1601 | A1IC4 | N4-C12-C5-C4    |
| 29  | A     | 1601 | A1IC4 | O6-C12-C5-C4    |
| 29  | A     | 1601 | A1IC4 | N7-C19-C20-O8   |
| 29  | A     | 1601 | A1IC4 | O6-C12-C5-N2    |
| 29  | A     | 1601 | A1IC4 | N4-C12-C5-N2    |
| 29  | A     | 1601 | A1IC4 | N7-C19-C20-O9   |
| 29  | A     | 1601 | A1IC4 | N4-C13-C14-C15  |
| 29  | A     | 1601 | A1IC4 | O4-C6-C7-N3     |
| 29  | A     | 1601 | A1IC4 | C3-C4-C5-N2     |

There are no ring outliers.

1 monomer is involved in 2 short contacts:

| Mol | Chain | Res  | Type  | Clashes | Symm-Clashes |
|-----|-------|------|-------|---------|--------------|
| 29  | A     | 1601 | A1IC4 | 2       | 0            |

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



## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

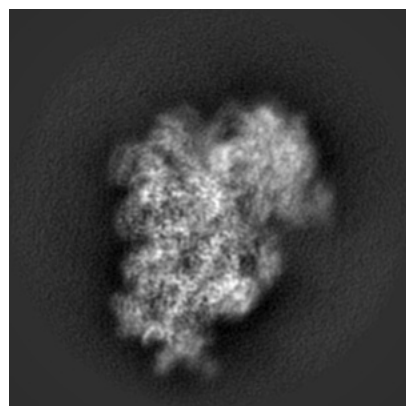
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51964. These allow visual inspection of the internal detail of the map and identification of artifacts.

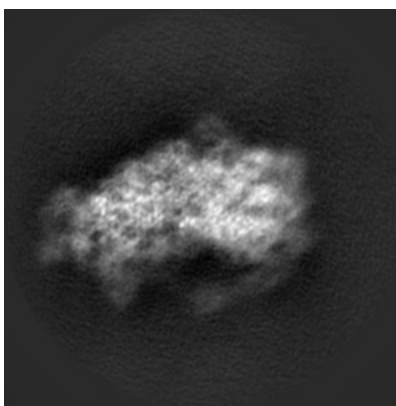
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

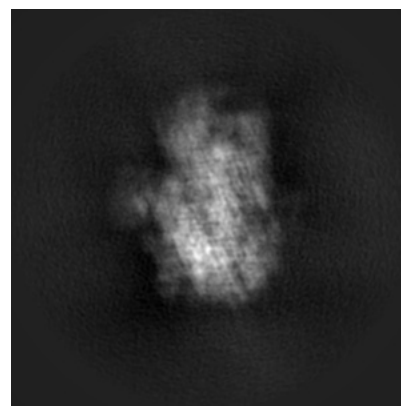
#### 6.1.1 Primary map



X

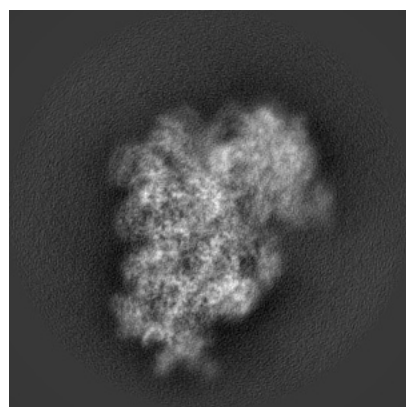


Y

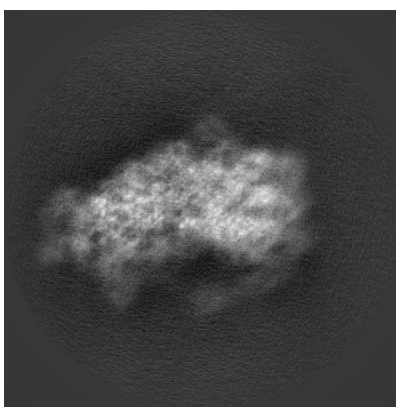


Z

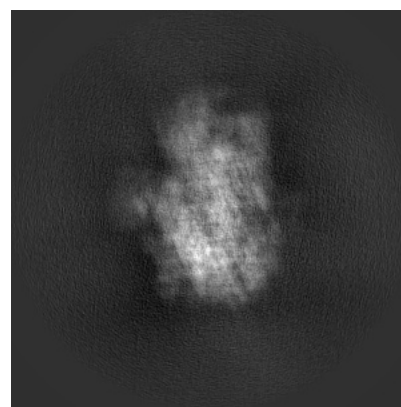
#### 6.1.2 Raw map



X



Y

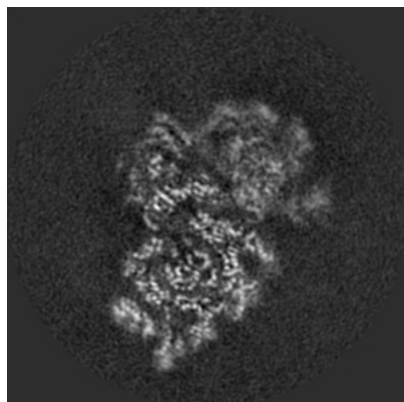


Z

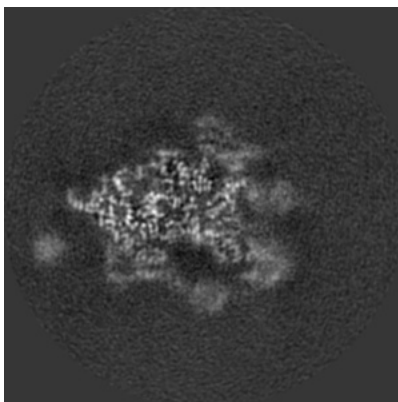
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

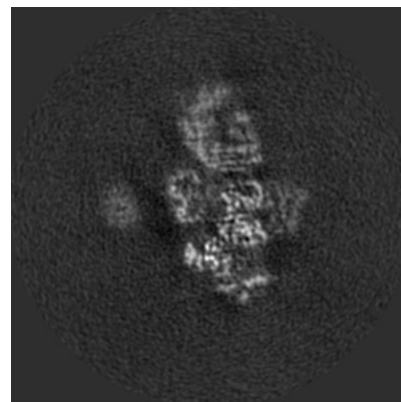
### 6.2.1 Primary map



X Index: 150

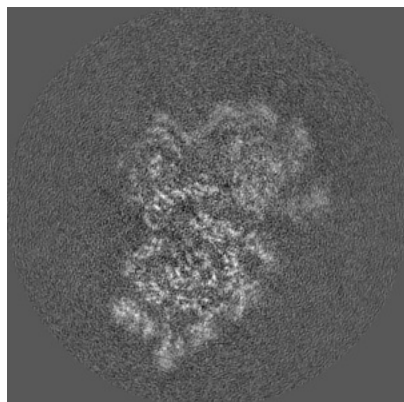


Y Index: 150

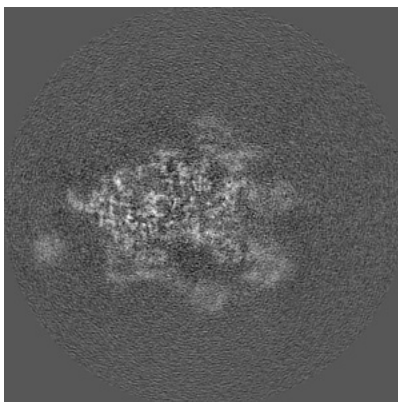


Z Index: 150

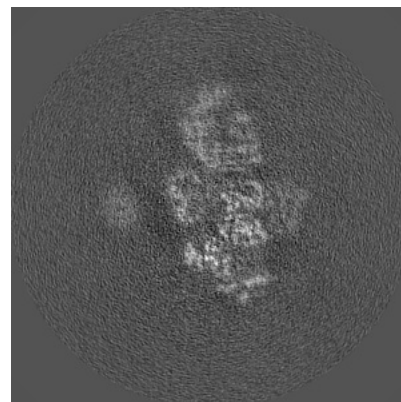
### 6.2.2 Raw map



X Index: 150



Y Index: 150



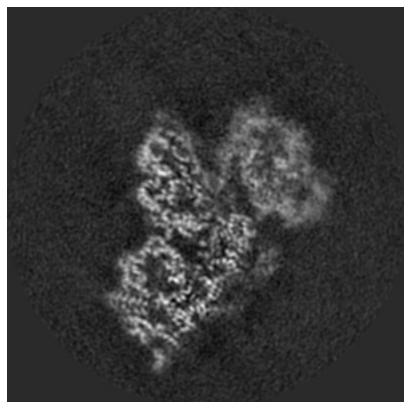
Z Index: 150

The images above show central slices of the map in three orthogonal directions.

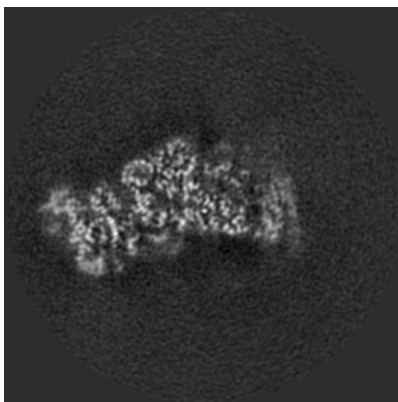


## 6.3 Largest variance slices [i](#)

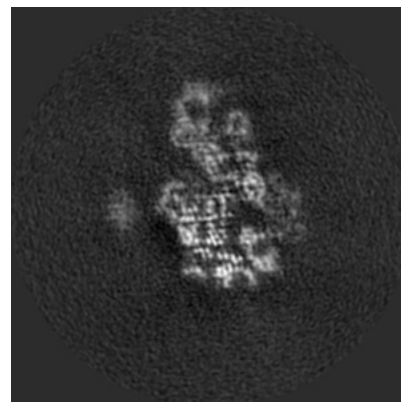
### 6.3.1 Primary map



X Index: 141

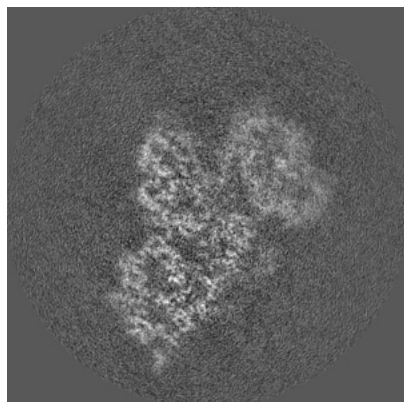


Y Index: 120

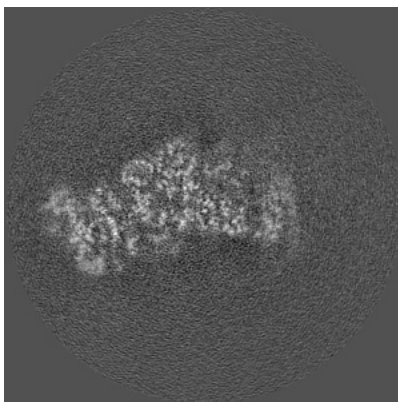


Z Index: 161

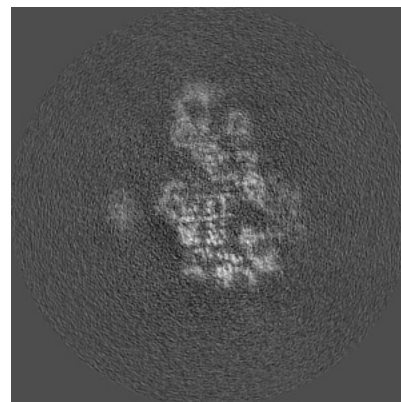
### 6.3.2 Raw map



X Index: 141



Y Index: 120

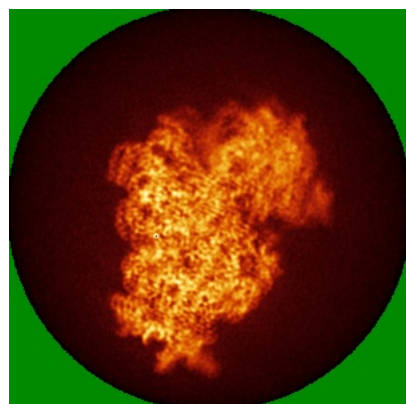


Z Index: 161

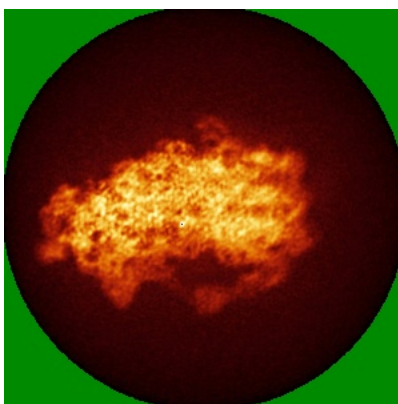
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

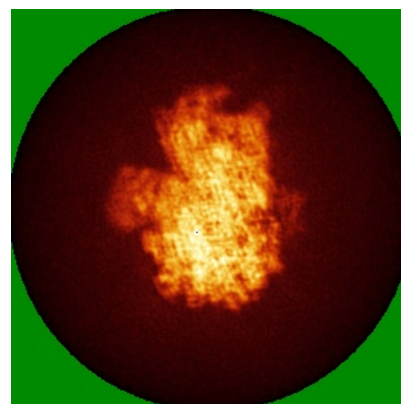
### 6.4.1 Primary map



X

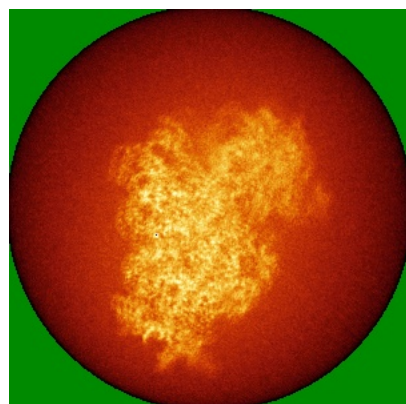


Y

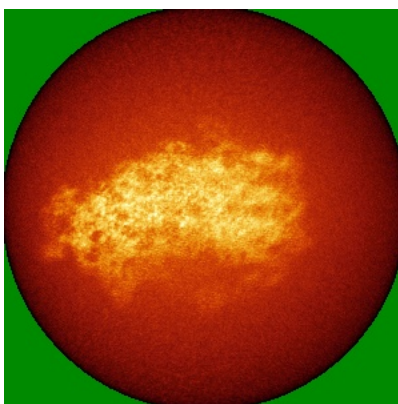


Z

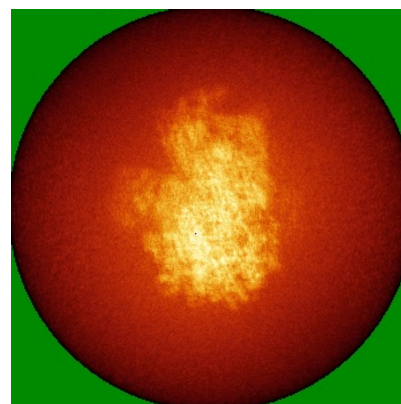
### 6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



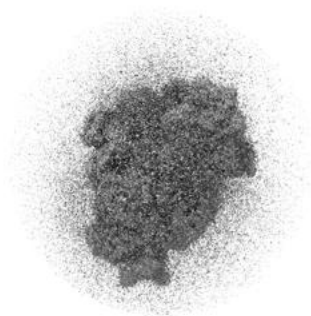
Y



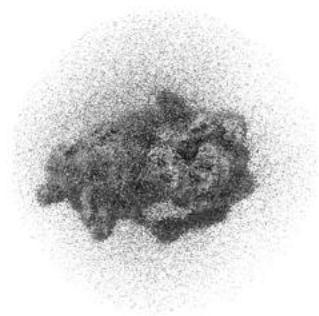
Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

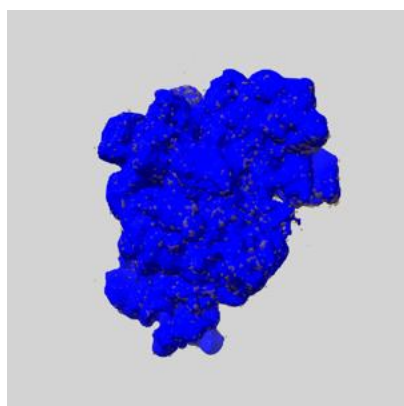
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

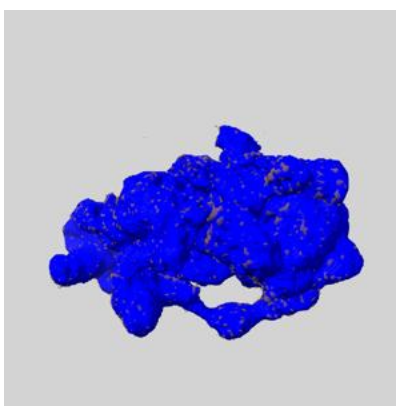
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

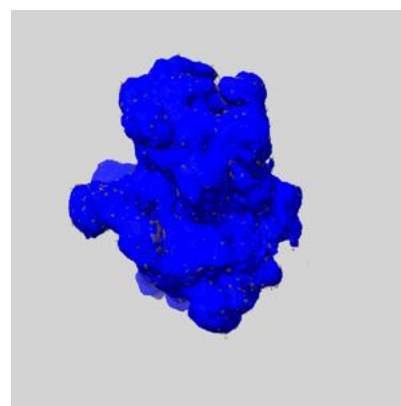
### 6.6.1 emd\_51964\_msk\_1.map [i](#)



X



Y

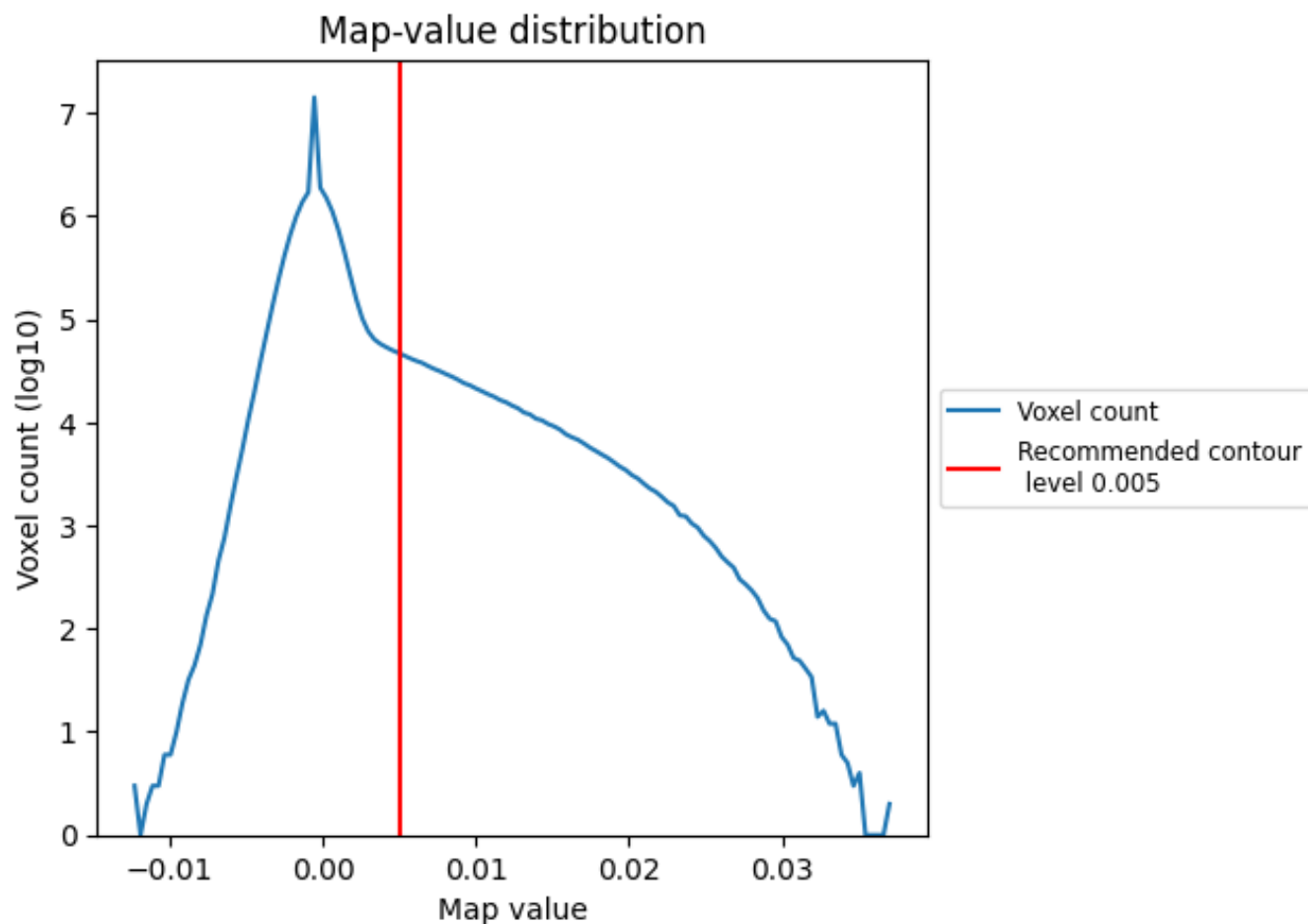


Z

## 7 Map analysis [i](#)

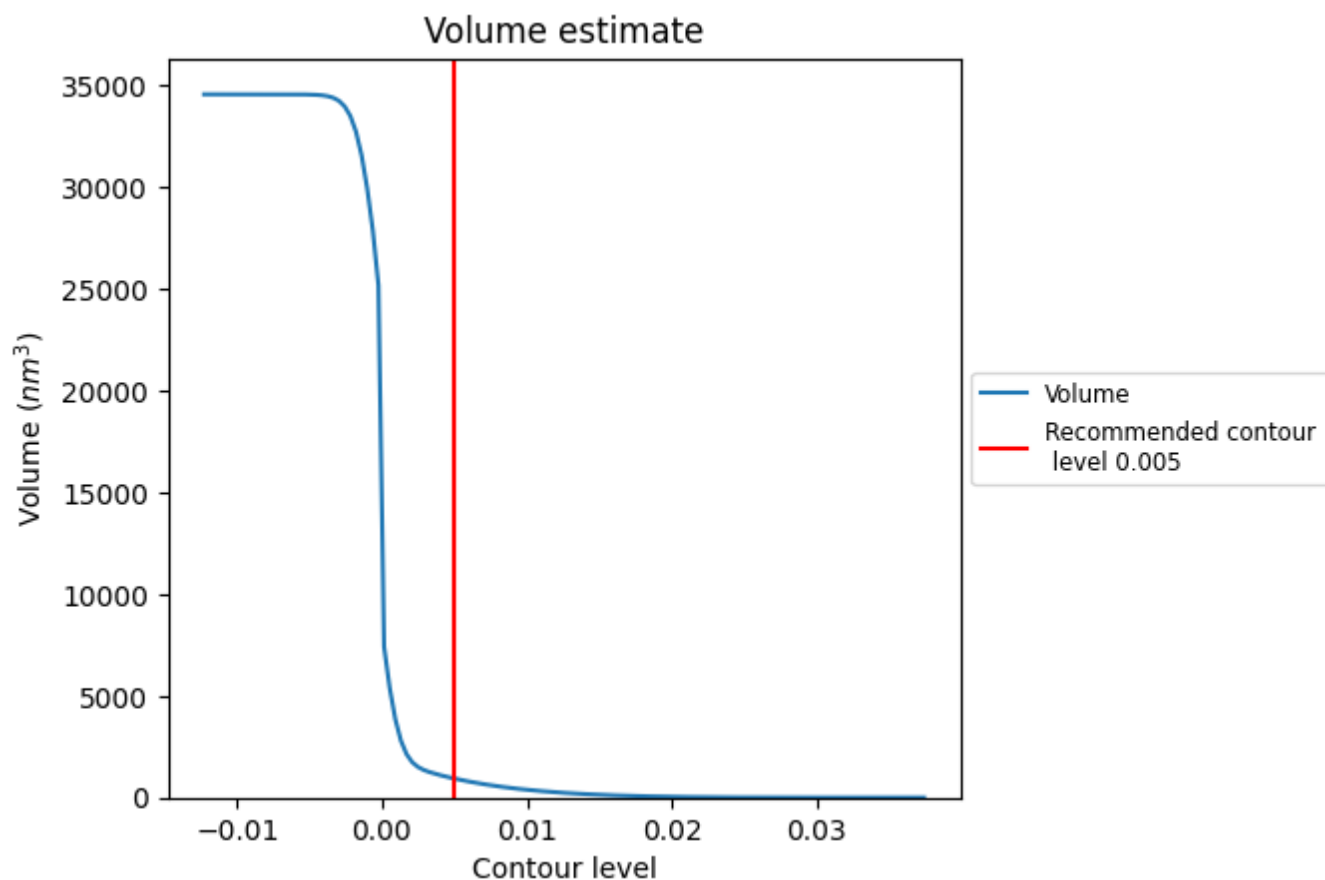
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

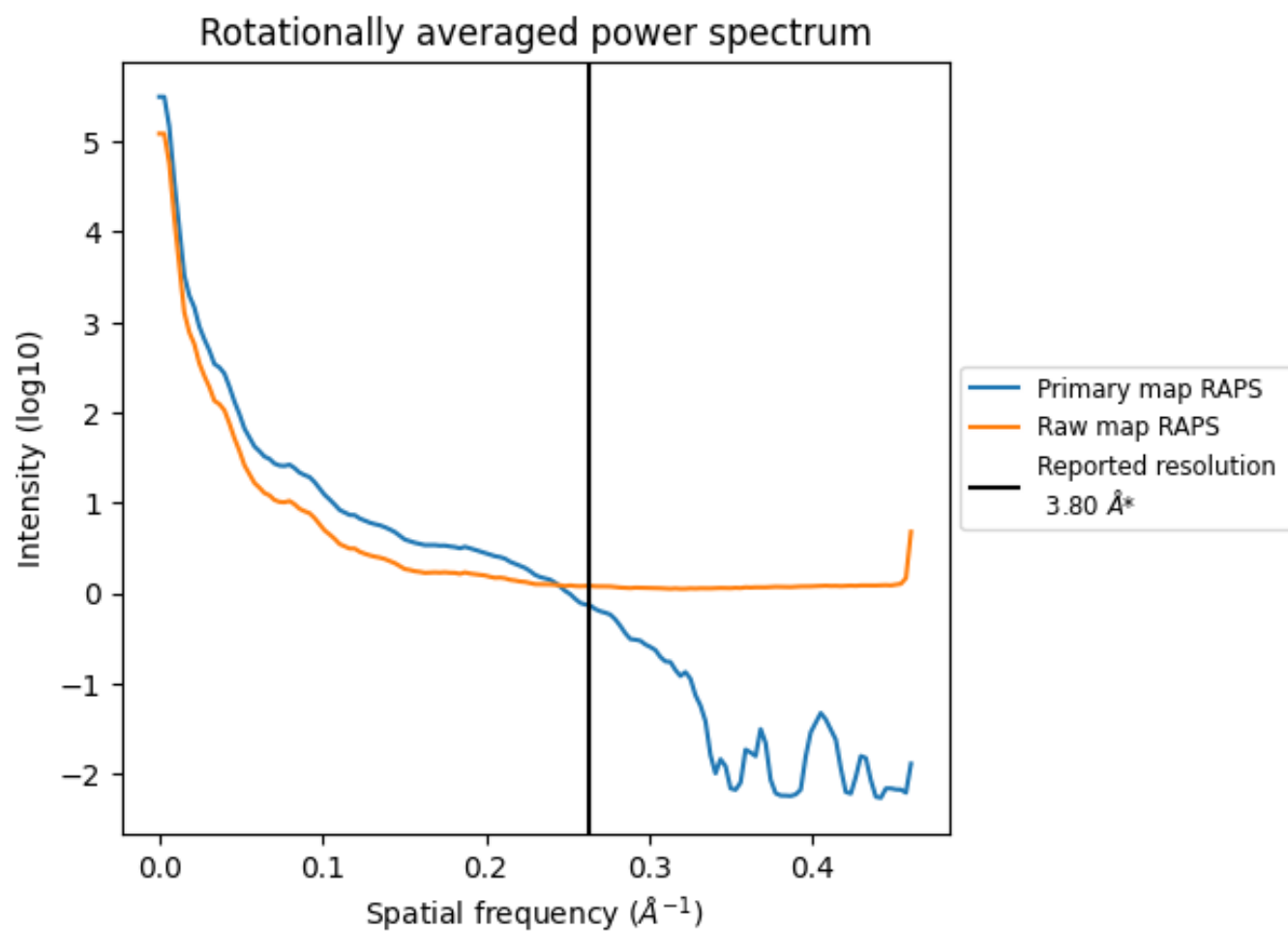
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 934  $\text{nm}^3$ ; this corresponds to an approximate mass of 844 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)

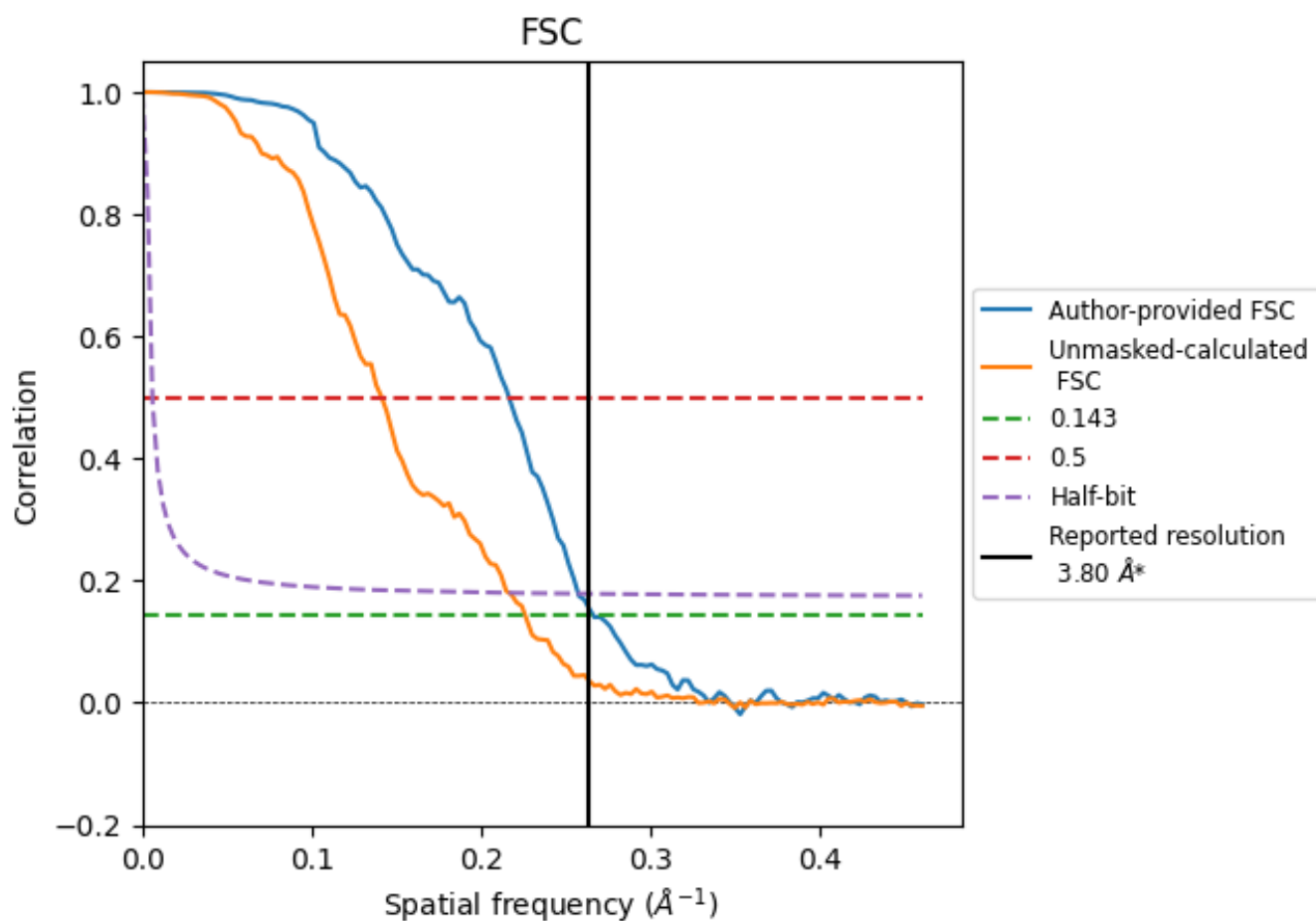


\*Reported resolution corresponds to spatial frequency of 0.263 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.263  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

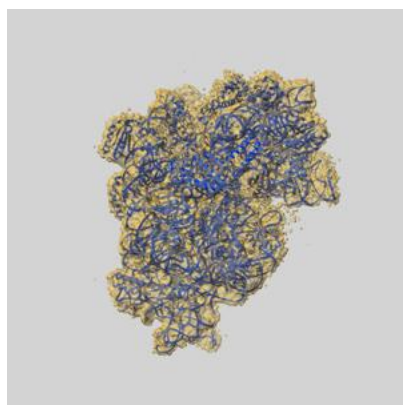
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.80                               | -    | -        |
| Author-provided FSC curve | 3.75                               | 4.62 | 3.89     |
| Unmasked-calculated*      | 4.42                               | 7.07 | 4.62     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.42 differs from the reported value 3.8 by more than 10 %

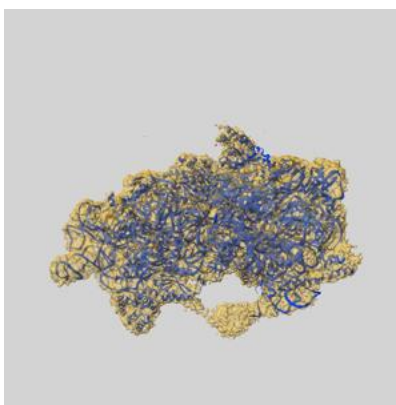
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51964 and PDB model 9H9H. Per-residue inclusion information can be found in section [3](#) on page [10](#).

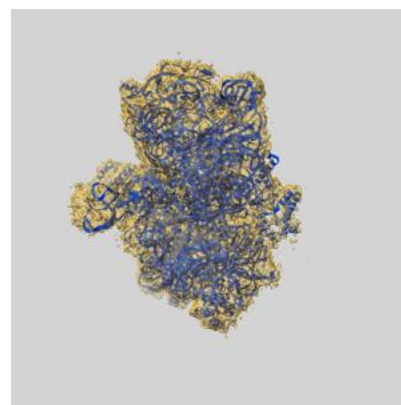
### 9.1 Map-model overlay [i](#)



X



Y

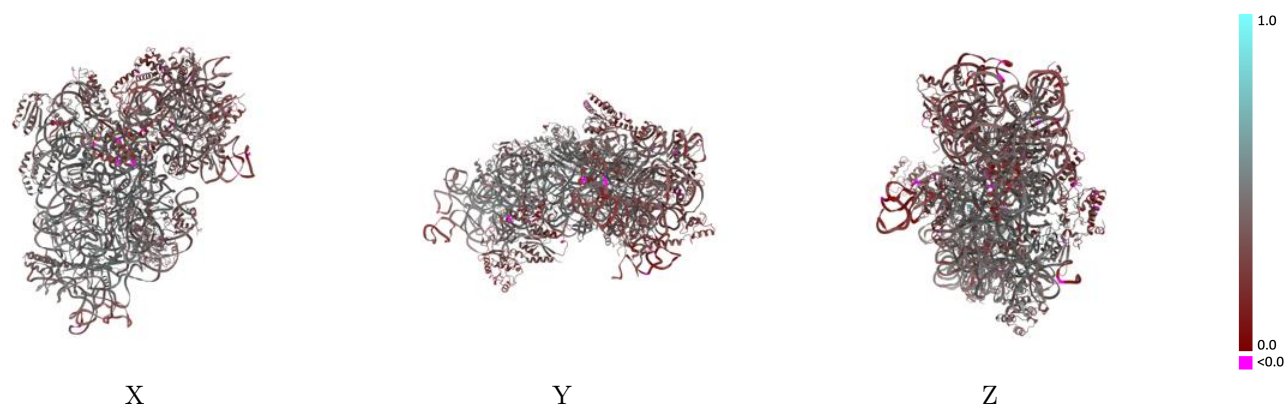


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The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

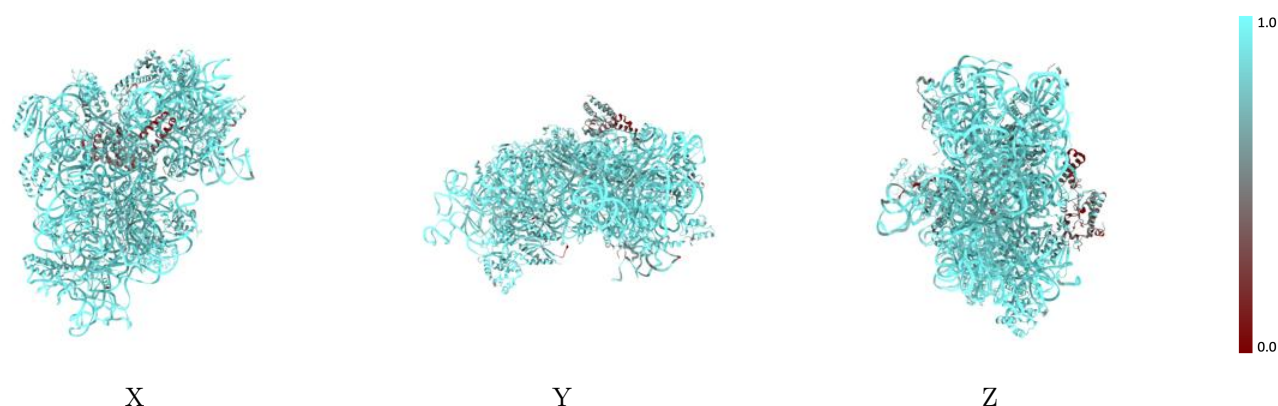


## 9.2 Q-score mapped to coordinate model [i](#)



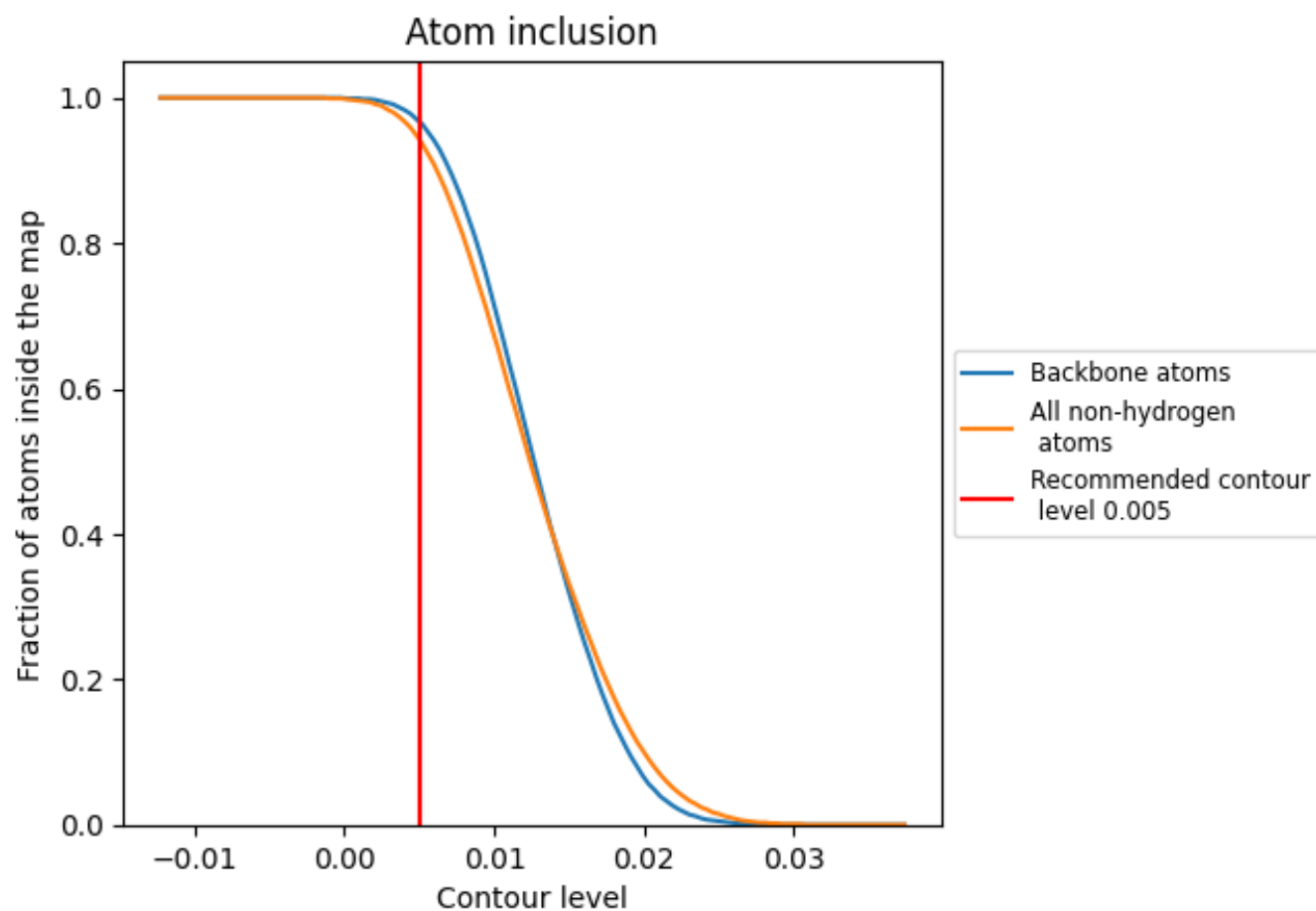
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).























































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 97% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.005) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.9430   |  0.3920   |
| 2     |  0.8980   |  0.3100   |
| 3     |  0.8670   |  0.2470   |
| A     |  0.9910   |  0.4200   |
| B     |  0.4820   |  0.2690   |
| C     |  0.8870   |  0.3820   |
| D     |  0.9480   |  0.4200   |
| E     |  0.9440   |  0.4470   |
| F     |  0.9510   |  0.3890   |
| G     |  0.8140   |  0.2440   |
| H     |  0.9530   |  0.4520   |
| I     |  0.9530   |  0.3450   |
| J     |  0.8520   |  0.3360   |
| K     |  0.9460   |  0.3840   |
| L     |  0.9360  |  0.4690  |
| M     |  0.8870 |  0.2790 |
| N     |  0.9520 |  0.3660 |
| O     |  0.9590 |  0.4220 |
| P     |  0.9550 |  0.4650 |
| Q     |  0.9780 |  0.4510 |
| R     |  0.9460 |  0.4080 |
| S     |  0.8620 |  0.3240 |
| T     |  0.9590 |  0.4130 |
| U     |  0.8420 |  0.3650 |
| X     |  0.9580 |  0.4350 |
| Y     |  0.8720 |  0.3030 |
| Z     |  0.8520 |  0.3490 |

