



## Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 10:27 PM UTC

PDB ID : 5LMO / pdb\_00005lmo  
EMDB ID : EMD-4074  
Title : Structure of bacterial 30S-IF1-IF3-mRNA translation pre-initiation complex (state-1B)  
Authors : Hussain, T.; Llacer, J.L.; Wimberly, B.T.; Ramakrishnan, V.  
Deposited on : 2016-08-01  
Resolution : 4.30 Å(reported)

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>.

---

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

EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
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

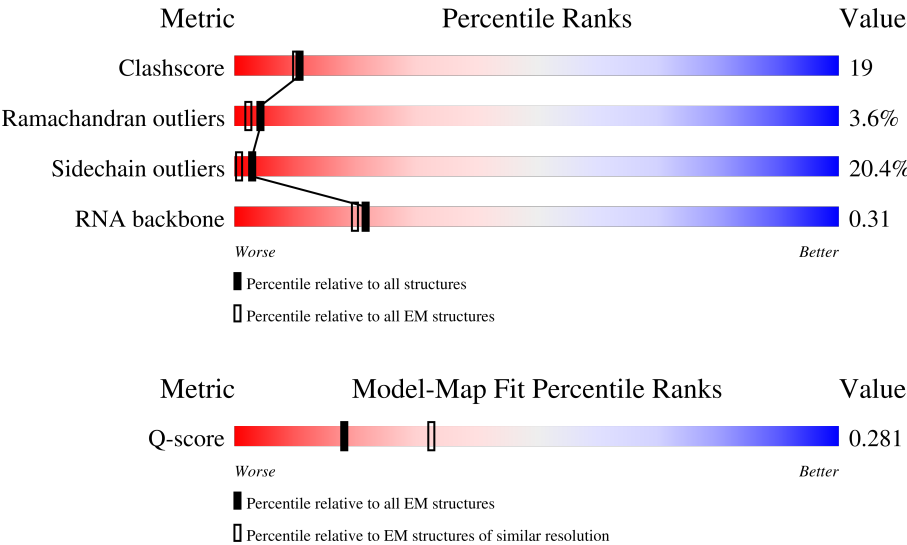
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.30 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                       | 4585 ( 3.80 - 4.80 )                                     |

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   | A     | 1522   | <div> <div>25%</div> <div>54%</div> <div>18%</div> <div>..</div> </div>               |
| 2   | B     | 256    | <div> <div>18%</div> <div>51%</div> <div>33%</div> <div>7%</div> <div>9%</div> </div> |
| 3   | C     | 239    | <div> <div>54%</div> <div>26%</div> <div>5%</div> <div>14%</div> </div>               |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | D     | 209    |                  |
| 5   | E     | 162    |                  |
| 6   | F     | 101    |                  |
| 7   | G     | 156    |                  |
| 8   | H     | 138    |                  |
| 9   | I     | 128    |                  |
| 10  | J     | 105    |                  |
| 11  | K     | 129    |                  |
| 12  | L     | 132    |                  |
| 13  | M     | 126    |                  |
| 14  | N     | 61     |                  |
| 15  | O     | 89     |                  |
| 16  | P     | 88     |                  |
| 17  | Q     | 105    |                  |
| 18  | R     | 88     |                  |
| 19  | S     | 93     |                  |
| 20  | T     | 106    |                  |
| 21  | V     | 27     |                  |
| 22  | W     | 72     |                  |
| 23  | X     | 171    |                  |
| 24  | Y     | 45     |                  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 26  | ZN   | D     | 300 | -         | -        | X       | -                |

## 2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 54110 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 16S rRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 1   | A     | 1514     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 32525 | 14481 | 6019 | 10514 | 1511 |         |       |

- Molecule 2 is a protein called 30S ribosomal protein S2.

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

- Molecule 3 is a protein called 30S ribosomal protein S3.

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

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | M     | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 933   | 577 | 192 | 162 | 2 |         |       |

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|-------|
| 18  | R     | 73       | Total | C   | N   | O  | 0       | 0     |
|     |       |          | 598   | 381 | 118 | 99 |         |       |

- Molecule 19 is a protein called 30S ribosomal protein S19.

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

- Molecule 20 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | T     | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 763   | 470 | 162 | 129 | 2 |         |       |

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

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

- Molecule 22 is a protein called Translation initiation factor IF-1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | W     | 71       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 570   | 362 | 103 | 103 | 2 |         |       |

- Molecule 23 is a protein called Translation initiation factor IF-3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | X     | 168      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1356  | 853 | 249 | 245 | 9 |         |       |

- Molecule 24 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |     |    |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 24  | Y     | 19       | Total | C   | N  | O   | P  | 0       | 0     |
|     |       |          | 417   | 186 | 84 | 128 | 19 |         |       |

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

| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 25  | A     | 107      | Total | Mg  | 0       |
|     |       |          | 107   | 107 |         |
| 25  | W     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |

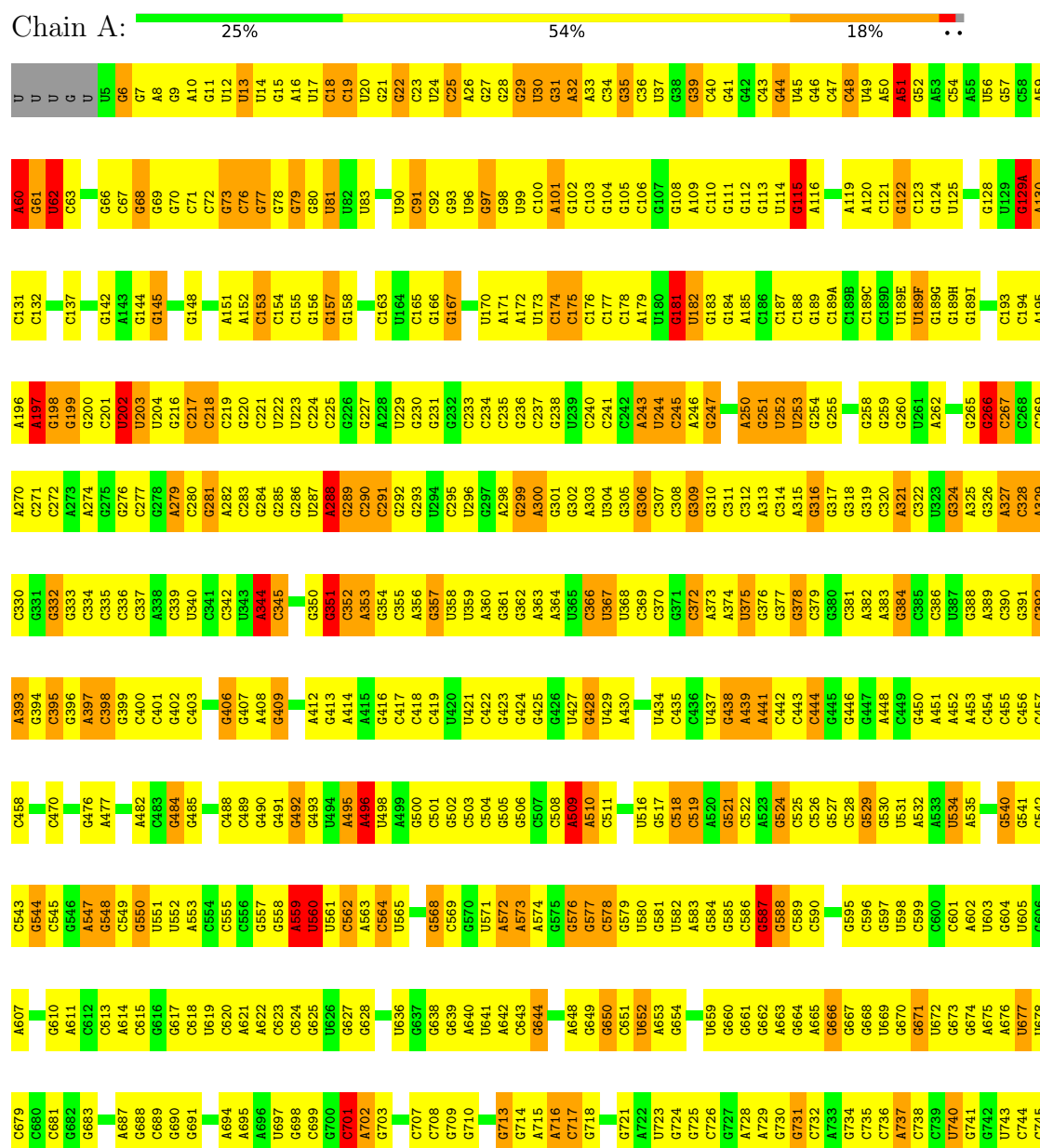
- Molecule 26 is ZINC ION (CCD ID: ZN) (formula: Zn).

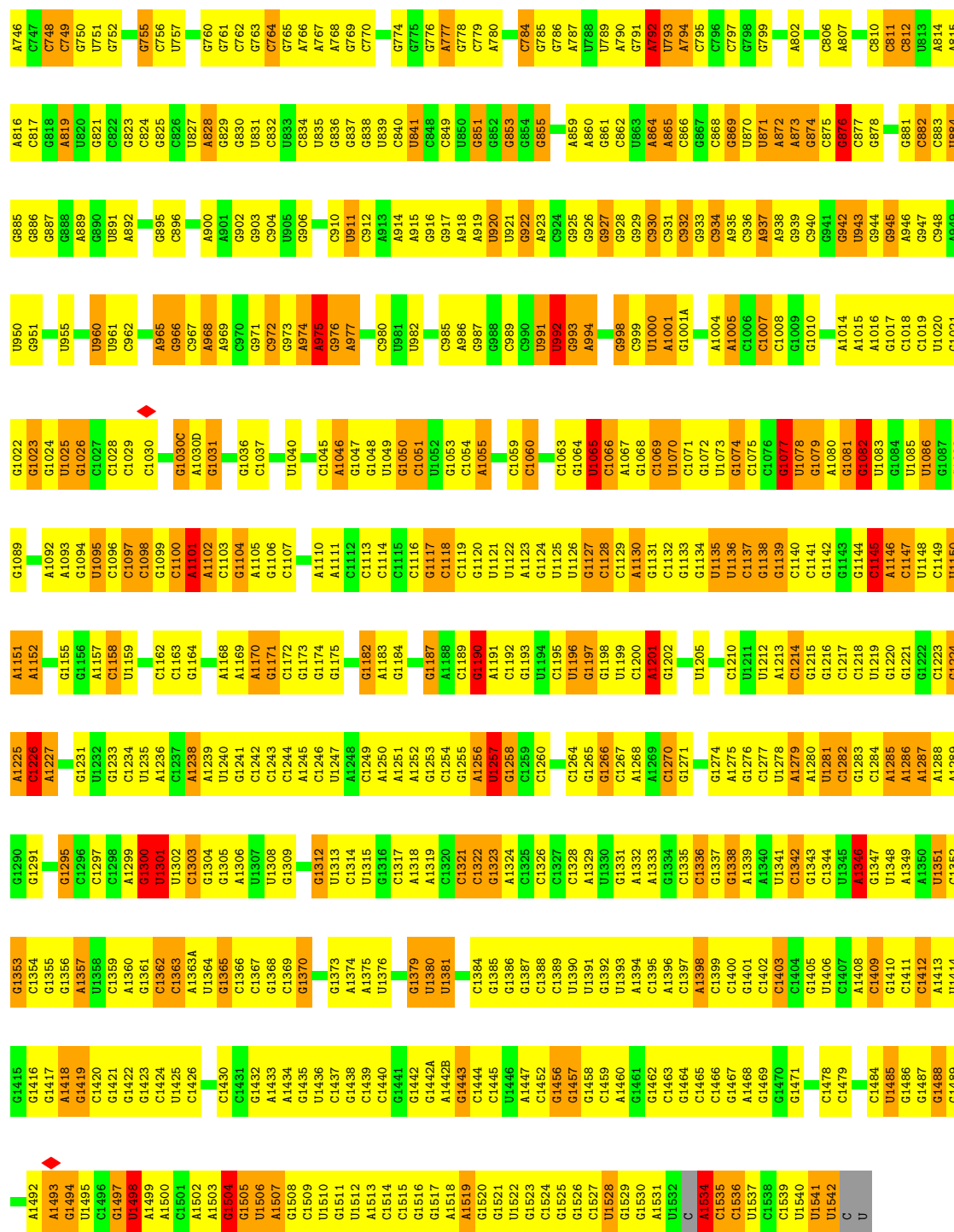
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 26  | D     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 26  | N     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

### 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.

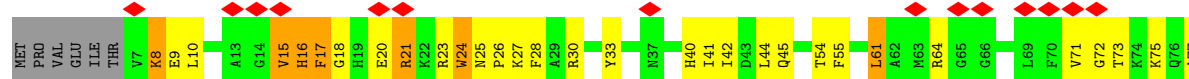
#### • Molecule 1: 16S rRNA

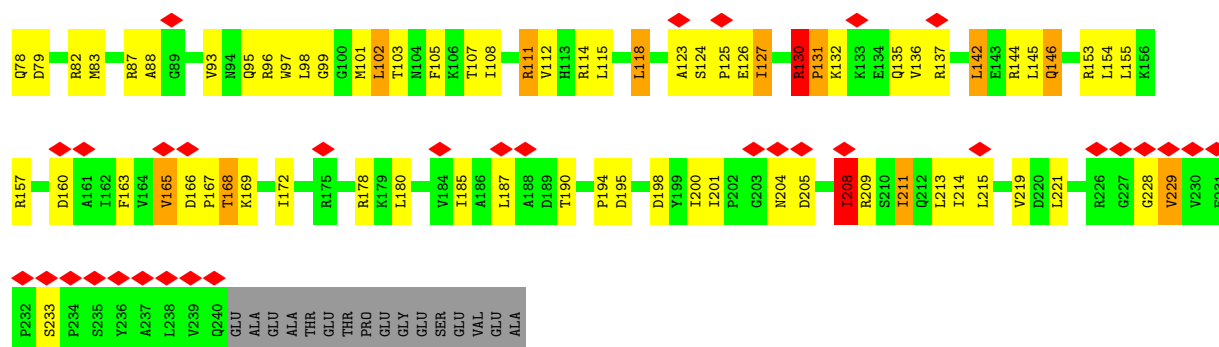




• Molecule 2: 30S ribosomal protein S2

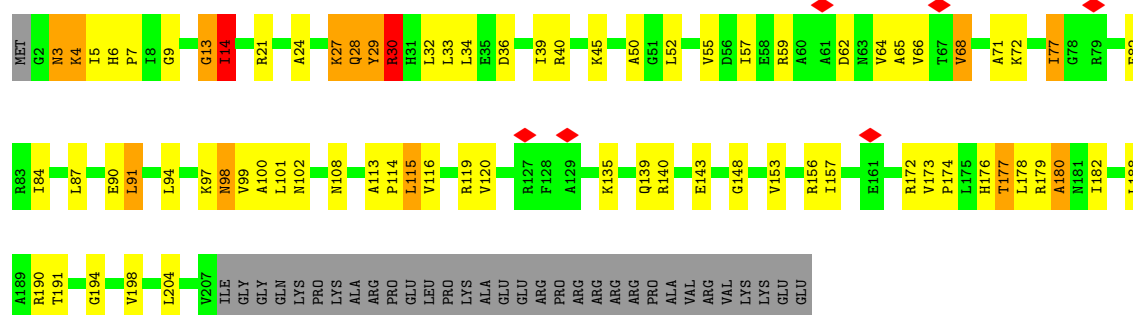
Chain B:





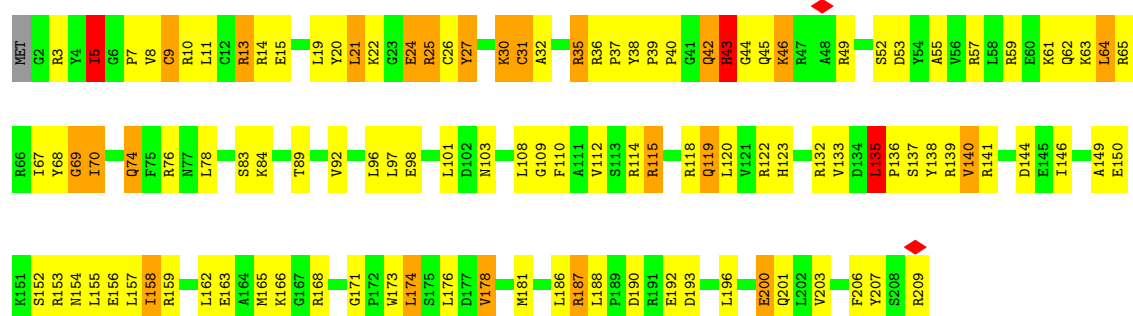
• Molecule 3: 30S ribosomal protein S3

Chain C: 54% 26% 5% 14%



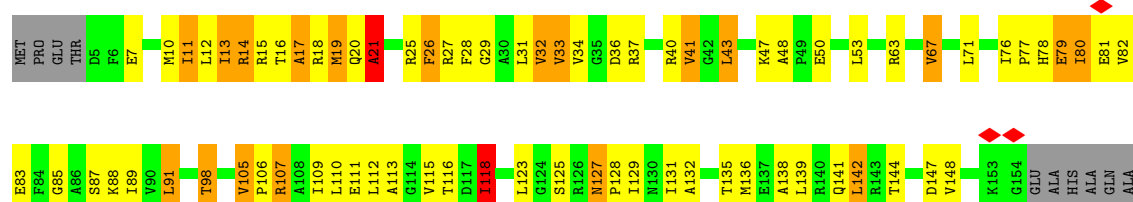
• Molecule 4: 30S ribosomal protein S4

Chain D: 44% 43% 11%



• Molecule 5: 30S ribosomal protein S5

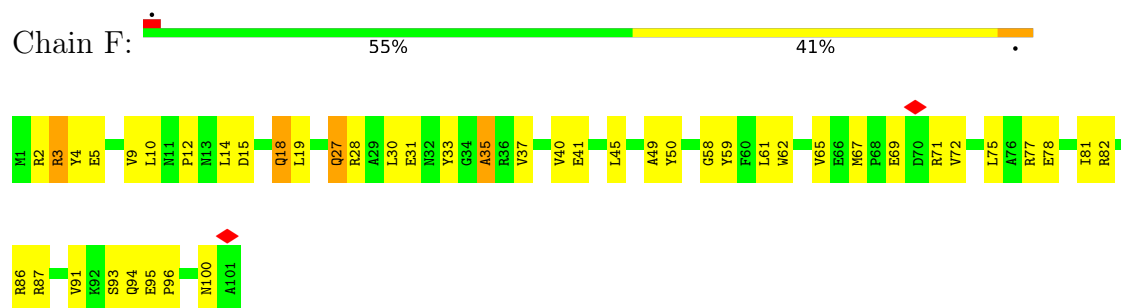
Chain E: 46% 33% 12% 7%



GLN  
GLY

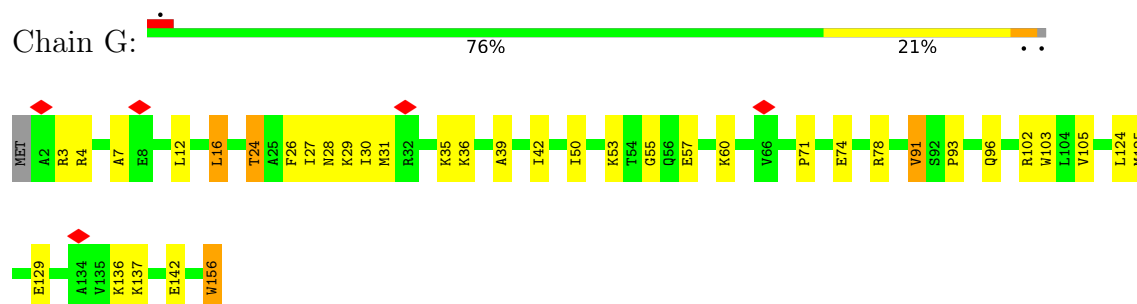
- Molecule 6: 30S ribosomal protein S6

Chain F:



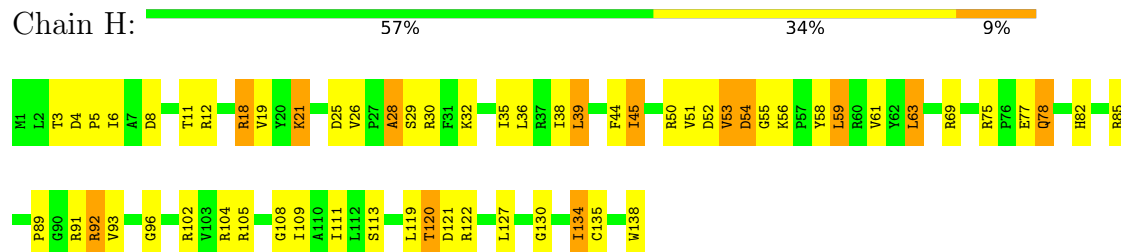
- Molecule 7: 30S ribosomal protein S7

Chain G:



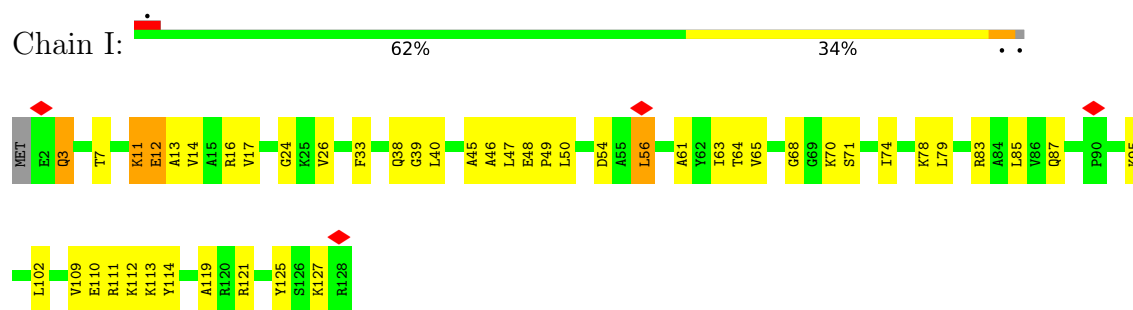
- Molecule 8: 30S ribosomal protein S8

Chain H:



- Molecule 9: 30S ribosomal protein S9

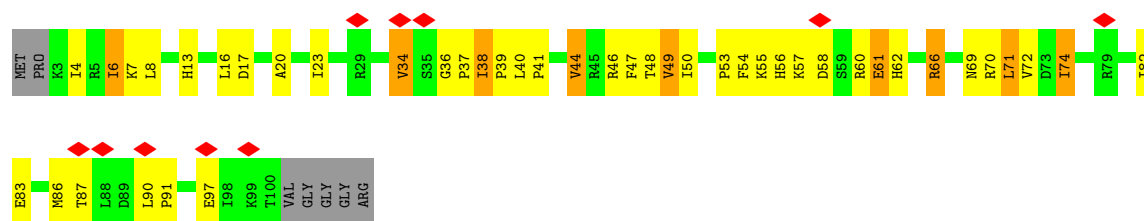
Chain I:



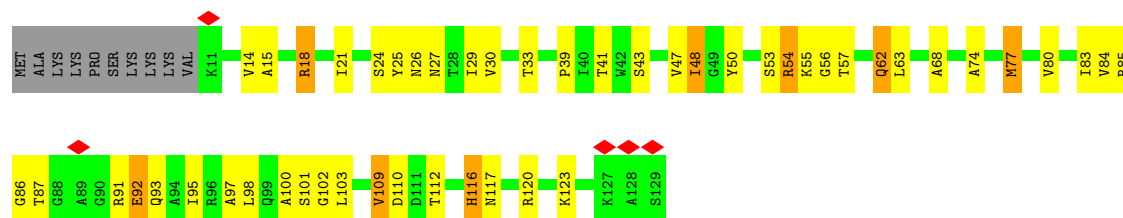
- Molecule 10: 30S ribosomal protein S10

Chain J:

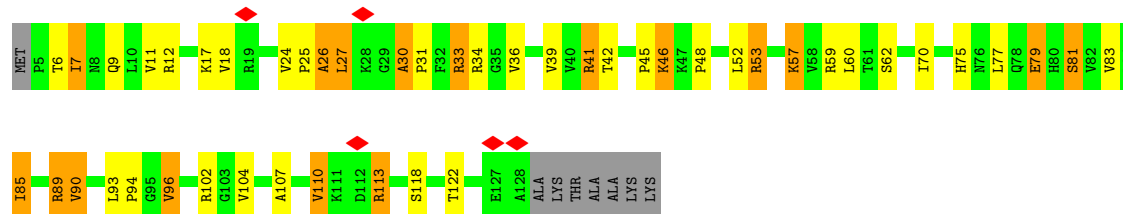




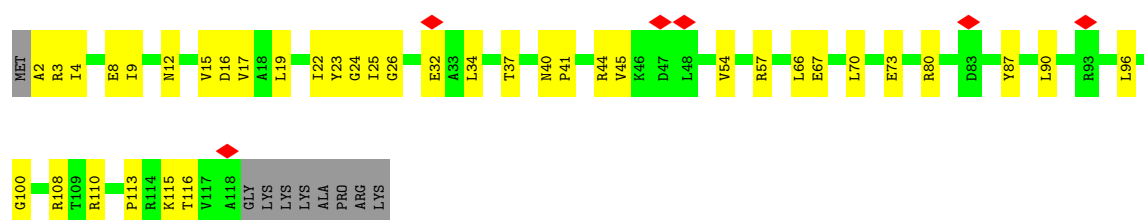
- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12



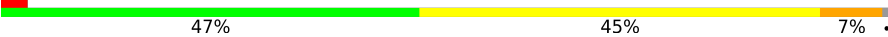
- Molecule 13: 30S ribosomal protein S13

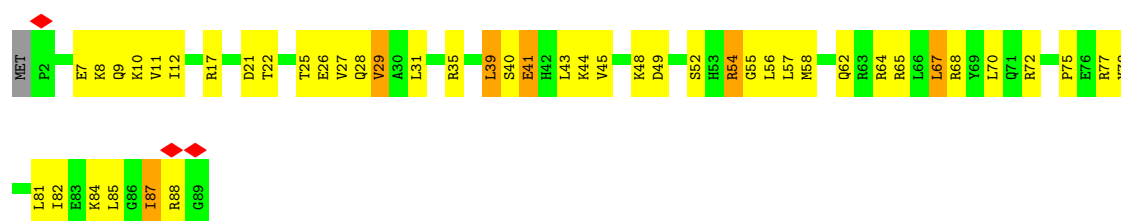


- Molecule 14: 30S ribosomal protein S14 type Z



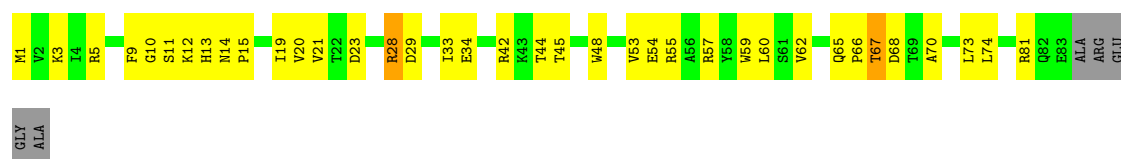
- Molecule 15: 30S ribosomal protein S15

Chain O: 



- Molecule 16: 30S ribosomal protein S16

Chain P: 



- Molecule 17: 30S ribosomal protein S17

Chain Q: 



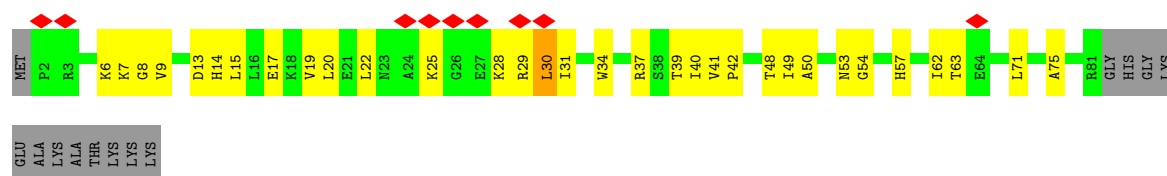
- Molecule 18: 30S ribosomal protein S18

Chain R: 



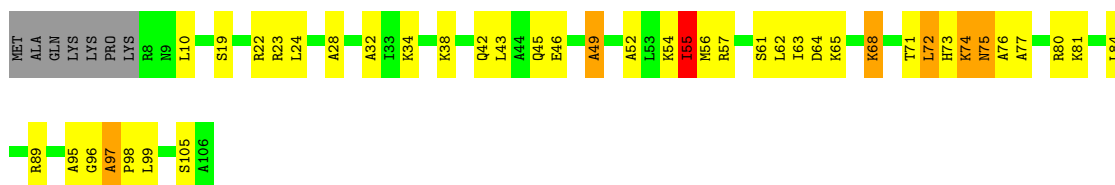
- Molecule 19: 30S ribosomal protein S19

Chain S: 

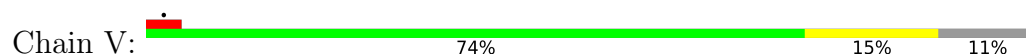


- Molecule 20: 30S ribosomal protein S20

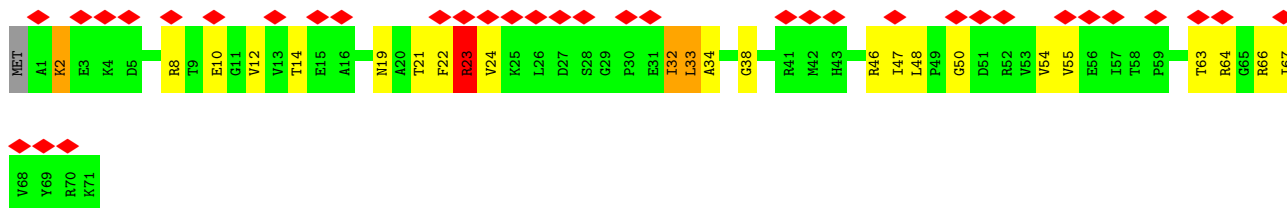
Chain T: 



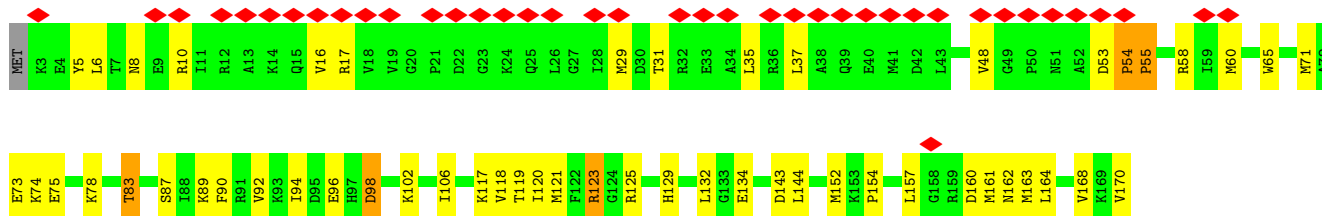
- Molecule 21: 30S ribosomal protein Thx



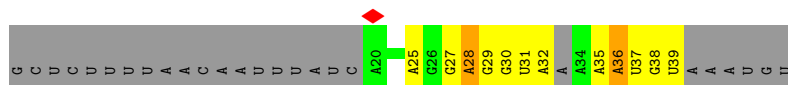
- Molecule 22: Translation initiation factor IF-1



- Molecule 23: Translation initiation factor IF-3



- Molecule 24: mRNA



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 57382                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI POLARA 300                          | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 30                                      | Depositor |
| Minimum defocus (nm)                 | 1500                                    | Depositor |
| Maximum defocus (nm)                 | 3500                                    | Depositor |
| Magnification                        | 104478                                  | Depositor |
| Image detector                       | OTHER                                   | Depositor |
| Maximum map value                    | 0.377                                   | Depositor |
| Minimum map value                    | -0.084                                  | Depositor |
| Average map value                    | -0.000                                  | Depositor |
| Map value standard deviation         | 0.017                                   | Depositor |
| Recommended contour level            | 0.05                                    | Depositor |
| Map size ( $\text{\AA}$ )            | 348.4, 348.4, 348.4                     | wwPDB     |
| Map dimensions                       | 260, 260, 260                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.34, 1.34, 1.34                        | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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   | A     | 0.46         | 0/36397     | 0.86        | 78/56783 (0.1%)  |
| 2   | B     | 0.78         | 0/1935      | 1.21        | 6/2609 (0.2%)    |
| 3   | C     | 0.75         | 0/1636      | 1.26        | 6/2205 (0.3%)    |
| 4   | D     | 0.62         | 0/1733      | 1.20        | 7/2318 (0.3%)    |
| 5   | E     | 0.63         | 0/1162      | 1.21        | 4/1564 (0.3%)    |
| 6   | F     | 0.55         | 0/856       | 1.18        | 3/1154 (0.3%)    |
| 7   | G     | 0.80         | 0/1276      | 1.19        | 1/1709 (0.1%)    |
| 8   | H     | 0.56         | 0/1136      | 1.13        | 3/1527 (0.2%)    |
| 9   | I     | 0.70         | 0/1029      | 1.26        | 4/1379 (0.3%)    |
| 10  | J     | 0.85         | 0/805       | 1.12        | 1/1082 (0.1%)    |
| 11  | K     | 0.74         | 0/900       | 1.15        | 1/1213 (0.1%)    |
| 12  | L     | 0.52         | 0/986       | 1.09        | 3/1320 (0.2%)    |
| 13  | M     | 0.85         | 0/943       | 1.23        | 4/1265 (0.3%)    |
| 14  | N     | 0.66         | 0/501       | 1.06        | 0/664            |
| 15  | O     | 0.65         | 0/745       | 1.29        | 1/992 (0.1%)     |
| 16  | P     | 0.52         | 0/716       | 1.05        | 0/963            |
| 17  | Q     | 0.53         | 0/836       | 1.08        | 0/1117           |
| 18  | R     | 0.69         | 0/604       | 1.21        | 1/801 (0.1%)     |
| 19  | S     | 0.94         | 0/661       | 1.12        | 2/890 (0.2%)     |
| 20  | T     | 0.65         | 0/765       | 1.39        | 6/1007 (0.6%)    |
| 21  | V     | 0.61         | 0/212       | 0.96        | 0/277            |
| 22  | W     | 0.83         | 0/580       | 1.25        | 2/782 (0.3%)     |
| 23  | X     | 0.78         | 0/1373      | 1.18        | 2/1838 (0.1%)    |
| 24  | Y     | 0.61         | 0/468       | 0.84        | 0/727            |
| All | All   | 0.57         | 0/58255     | 0.98        | 135/86186 (0.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 5   | E     | 1                   | 0                   |
| 12  | L     | 0                   | 1                   |
| 16  | P     | 0                   | 1                   |
| 23  | X     | 0                   | 1                   |
| All | All   | 1                   | 3                   |

There are no bond length outliers.

All (135) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 9   | I     | 11   | LYS  | CB-CA-C     | 21.29  | 152.79      | 110.42   |
| 22  | W     | 23   | ARG  | N-CA-C      | -19.22 | 79.83       | 110.20   |
| 3   | C     | 14   | ILE  | N-CA-C      | 15.16  | 124.78      | 110.53   |
| 1   | A     | 266  | G    | C2'-C3'-O3' | 14.17  | 130.75      | 109.50   |
| 3   | C     | 28   | GLN  | N-CA-C      | 12.93  | 125.46      | 111.36   |
| 5   | E     | 21   | ALA  | CB-CA-C     | 12.73  | 135.76      | 110.42   |
| 3   | C     | 29   | TYR  | N-CA-C      | 12.29  | 124.67      | 111.28   |
| 1   | A     | 792  | A    | C2'-C3'-O3' | 12.20  | 127.80      | 109.50   |
| 9   | I     | 12   | GLU  | N-CA-C      | -12.13 | 95.46       | 111.71   |
| 1   | A     | 1346 | A    | C2'-C3'-O3' | 10.46  | 125.19      | 109.50   |
| 1   | A     | 1498 | U    | C2'-C3'-O3' | 10.13  | 124.69      | 109.50   |
| 1   | A     | 1301 | U    | C2'-C3'-O3' | 9.95   | 124.43      | 109.50   |
| 12  | L     | 30   | ALA  | CA-C-N      | 9.80   | 129.56      | 119.56   |
| 12  | L     | 30   | ALA  | C-N-CA      | 9.80   | 129.56      | 119.56   |
| 1   | A     | 1145 | C    | C2'-C3'-O3' | 9.67   | 124.01      | 109.50   |
| 1   | A     | 197  | A    | C2'-C3'-O3' | 9.56   | 123.84      | 109.50   |
| 1   | A     | 115  | G    | C4'-C3'-O3' | 9.44   | 123.56      | 109.40   |
| 1   | A     | 181  | G    | C2'-C3'-O3' | 9.36   | 123.54      | 109.50   |
| 1   | A     | 1182 | G    | C2'-C3'-O3' | 9.28   | 123.42      | 109.50   |
| 1   | A     | 51   | A    | C4'-C3'-O3' | 9.04   | 122.96      | 109.40   |
| 9   | I     | 11   | LYS  | N-CA-C      | -8.87  | 91.91       | 110.80   |
| 1   | A     | 328  | C    | C2'-C3'-O3' | 8.87   | 122.80      | 109.50   |
| 6   | F     | 95   | GLU  | CA-C-N      | 8.83   | 130.88      | 119.84   |
| 6   | F     | 95   | GLU  | C-N-CA      | 8.83   | 130.88      | 119.84   |
| 1   | A     | 1534 | A    | C2'-C3'-O3' | 8.60   | 126.60      | 113.70   |
| 1   | A     | 960  | U    | C2'-C3'-O3' | 8.38   | 122.06      | 109.50   |
| 1   | A     | 1190 | G    | C2'-C3'-O3' | 8.35   | 126.22      | 113.70   |
| 1   | A     | 748  | C    | C2'-C3'-O3' | 8.33   | 122.00      | 109.50   |
| 1   | A     | 965  | A    | C2'-C3'-O3' | 8.17   | 121.76      | 109.50   |
| 1   | A     | 1285 | A    | C4'-C3'-O3' | 7.96   | 121.34      | 109.40   |
| 20  | T     | 97   | ALA  | CA-C-N      | 7.88   | 129.69      | 119.84   |
| 20  | T     | 97   | ALA  | C-N-CA      | 7.88   | 129.69      | 119.84   |
| 1   | A     | 1257 | U    | C2'-C3'-O3' | 7.74   | 121.11      | 109.50   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 1   | A     | 181    | G    | C4'-C3'-O3' | 7.70  | 120.95      | 109.40   |
| 1   | A     | 496    | A    | C4'-C3'-O3' | 7.60  | 120.80      | 109.40   |
| 1   | A     | 1380   | U    | C2'-C3'-O3' | 7.52  | 120.78      | 109.50   |
| 1   | A     | 1101   | A    | C4'-C3'-O3' | 7.49  | 120.63      | 109.40   |
| 1   | A     | 281    | G    | C2'-C3'-O3' | 7.44  | 124.86      | 113.70   |
| 1   | A     | 509    | A    | C4'-C3'-O3' | 7.42  | 124.12      | 113.00   |
| 1   | A     | 1201   | A    | C4'-C3'-O3' | 7.33  | 120.39      | 109.40   |
| 20  | T     | 71     | THR  | N-CA-C      | 7.33  | 119.27      | 111.28   |
| 11  | K     | 80     | VAL  | N-CA-C      | 7.25  | 118.25      | 108.11   |
| 1   | A     | 372    | C    | C2'-C3'-O3' | 7.14  | 120.21      | 109.50   |
| 1   | A     | 484    | G    | C2'-C3'-O3' | 7.03  | 120.05      | 109.50   |
| 1   | A     | 428    | G    | C2'-C3'-O3' | 6.96  | 119.94      | 109.50   |
| 1   | A     | 202    | U    | C4'-C3'-O3' | 6.93  | 119.80      | 109.40   |
| 1   | A     | 776    | G    | C4'-C3'-O3' | -6.92 | 102.62      | 113.00   |
| 4   | D     | 135    | LEU  | CA-C-N      | 6.88  | 127.45      | 119.47   |
| 4   | D     | 135    | LEU  | C-N-CA      | 6.88  | 127.45      | 119.47   |
| 2   | B     | 24     | TRP  | N-CA-C      | 6.78  | 125.23      | 110.80   |
| 1   | A     | 1214   | C    | C4'-C3'-O3' | 6.74  | 119.50      | 109.40   |
| 20  | T     | 74     | LYS  | N-CA-C      | 6.71  | 118.25      | 111.07   |
| 3   | C     | 98     | ASN  | N-CA-C      | -6.62 | 99.62       | 109.15   |
| 6   | F     | 50     | TYR  | N-CA-C      | -6.62 | 102.17      | 108.13   |
| 1   | A     | 876    | G    | C4'-C3'-O3' | -6.56 | 103.16      | 113.00   |
| 1   | A     | 115    | G    | C2'-C3'-O3' | 6.53  | 119.30      | 109.50   |
| 1   | A     | 560    | U    | C2'-C3'-O3' | 6.53  | 119.30      | 109.50   |
| 1   | A     | 1300   | G    | C2'-C3'-O3' | 6.45  | 119.18      | 109.50   |
| 1   | A     | 1403   | C    | C4'-C3'-O3' | -6.40 | 103.40      | 113.00   |
| 1   | A     | 587    | G    | C4'-C3'-O3' | -6.35 | 103.47      | 113.00   |
| 1   | A     | 1201   | A    | C2'-C3'-O3' | 6.35  | 119.03      | 109.50   |
| 1   | A     | 243    | A    | C2'-C3'-O3' | 6.32  | 118.98      | 109.50   |
| 1   | A     | 1065   | U    | C2'-C3'-O3' | 6.28  | 118.92      | 109.50   |
| 22  | W     | 24     | VAL  | N-CA-CB     | -6.27 | 104.19      | 112.34   |
| 8   | H     | 54     | ASP  | N-CA-C      | 6.24  | 120.00      | 111.39   |
| 1   | A     | 559    | A    | C2'-C3'-O3' | 6.24  | 123.06      | 113.70   |
| 1   | A     | 218    | C    | C4'-C3'-O3' | -6.22 | 103.67      | 113.00   |
| 1   | A     | 1504   | G    | C2'-C3'-O3' | 6.22  | 118.83      | 109.50   |
| 1   | A     | 60     | A    | C2'-C3'-O3' | 6.21  | 118.82      | 109.50   |
| 1   | A     | 484    | G    | C4'-C3'-O3' | 6.19  | 118.69      | 109.40   |
| 1   | A     | 1147   | C    | C3'-C2'-O2' | 6.18  | 119.96      | 110.70   |
| 1   | A     | 129(A) | G    | C2'-C3'-O3' | 6.17  | 118.75      | 109.50   |
| 1   | A     | 344    | A    | C2'-C3'-O3' | 6.13  | 118.70      | 109.50   |
| 8   | H     | 119    | LEU  | N-CA-C      | 6.13  | 118.10      | 108.96   |
| 1   | A     | 1380   | U    | C4'-C3'-O3' | 6.12  | 118.58      | 109.40   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 1196 | U    | C4'-C3'-O3' | 6.12  | 118.57      | 109.40   |
| 1   | A     | 48   | C    | C4'-C3'-O3' | 6.11  | 118.57      | 109.40   |
| 5   | E     | 118  | ILE  | N-CA-C      | 6.06  | 115.81      | 108.06   |
| 1   | A     | 992  | U    | C2'-C3'-O3' | 6.02  | 118.53      | 109.50   |
| 1   | A     | 1000 | U    | C2'-C3'-O3' | 6.00  | 122.70      | 113.70   |
| 10  | J     | 6    | ILE  | N-CA-C      | 5.97  | 116.21      | 106.72   |
| 1   | A     | 1069 | C    | C2'-C3'-O3' | -5.92 | 104.81      | 113.70   |
| 15  | O     | 85   | LEU  | N-CA-C      | 5.89  | 120.60      | 113.41   |
| 12  | L     | 26   | ALA  | N-CA-C      | -5.89 | 106.44      | 113.21   |
| 1   | A     | 62   | U    | C4'-C3'-O3' | -5.89 | 104.17      | 113.00   |
| 1   | A     | 960  | U    | C4'-C3'-O3' | 5.85  | 118.17      | 109.40   |
| 4   | D     | 171  | GLY  | CA-C-N      | 5.81  | 127.10      | 119.84   |
| 4   | D     | 171  | GLY  | C-N-CA      | 5.81  | 127.10      | 119.84   |
| 13  | M     | 66   | LEU  | N-CA-C      | 5.80  | 118.56      | 108.76   |
| 2   | B     | 208  | ILE  | N-CA-C      | 5.77  | 121.35      | 109.34   |
| 1   | A     | 701  | C    | C2'-C3'-O3' | 5.77  | 118.16      | 109.50   |
| 9   | I     | 70   | LYS  | N-CA-C      | 5.76  | 118.05      | 111.02   |
| 1   | A     | 812  | C    | C4'-C3'-O3' | -5.71 | 104.43      | 113.00   |
| 4   | D     | 188  | LEU  | CA-C-N      | 5.71  | 125.72      | 119.89   |
| 4   | D     | 188  | LEU  | C-N-CA      | 5.71  | 125.72      | 119.89   |
| 1   | A     | 428  | G    | C4'-C3'-O3' | 5.70  | 117.95      | 109.40   |
| 7   | G     | 91   | VAL  | N-CA-C      | 5.70  | 116.09      | 108.11   |
| 1   | A     | 1226 | C    | C4'-C3'-O3' | 5.68  | 117.92      | 109.40   |
| 3   | C     | 180  | ALA  | N-CA-C      | 5.64  | 117.12      | 110.97   |
| 1   | A     | 25   | C    | C4'-C3'-O3' | -5.63 | 104.56      | 113.00   |
| 5   | E     | 142  | LEU  | N-CA-C      | 5.52  | 118.08      | 110.35   |
| 20  | T     | 75   | ASN  | N-CA-C      | 5.49  | 117.07      | 111.14   |
| 1   | A     | 1197 | G    | C4'-C3'-O3' | -5.47 | 104.79      | 113.00   |
| 19  | S     | 54   | GLY  | N-CA-C      | -5.46 | 107.82      | 114.92   |
| 13  | M     | 4    | ILE  | N-CA-C      | 5.44  | 117.85      | 111.05   |
| 1   | A     | 351  | G    | C2'-C3'-O3' | 5.39  | 117.59      | 109.50   |
| 2   | B     | 130  | ARG  | CA-C-N      | 5.38  | 126.57      | 119.84   |
| 2   | B     | 130  | ARG  | C-N-CA      | 5.38  | 126.57      | 119.84   |
| 1   | A     | 448  | A    | C4'-C3'-O3' | -5.35 | 104.98      | 113.00   |
| 2   | B     | 27   | LYS  | N-CA-C      | -5.30 | 106.66      | 113.23   |
| 1   | A     | 1082 | G    | C4'-C3'-O3' | -5.29 | 105.06      | 113.00   |
| 1   | A     | 288  | A    | C2'-C3'-O3' | 5.27  | 121.61      | 113.70   |
| 1   | A     | 991  | U    | C4'-C3'-O3' | -5.27 | 105.10      | 113.00   |
| 4   | D     | 24   | GLU  | N-CA-C      | -5.25 | 103.59      | 110.53   |
| 1   | A     | 975  | A    | C2'-C3'-O3' | 5.24  | 117.35      | 109.50   |
| 1   | A     | 6    | G    | C4'-C3'-O3' | -5.23 | 105.15      | 113.00   |
| 1   | A     | 1196 | U    | C2'-C3'-O3' | 5.23  | 117.34      | 109.50   |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 544  | G    | C2'-C3'-O3' | -5.21 | 105.88      | 113.70   |
| 13  | M     | 40   | ASN  | CA-C-N      | 5.21  | 125.28      | 119.87   |
| 13  | M     | 40   | ASN  | C-N-CA      | 5.21  | 125.28      | 119.87   |
| 8   | H     | 28   | ALA  | N-CA-C      | 5.20  | 116.99      | 108.52   |
| 1   | A     | 811  | C    | C2'-C3'-O3' | -5.19 | 105.92      | 113.70   |
| 23  | X     | 129  | HIS  | O-C-N       | 5.17  | 125.46      | 120.55   |
| 1   | A     | 1077 | G    | C3'-C2'-O2' | 5.17  | 118.45      | 110.70   |
| 5   | E     | 26   | PHE  | N-CA-C      | 5.16  | 117.37      | 110.35   |
| 1   | A     | 60   | A    | C4'-C3'-O3' | 5.15  | 117.12      | 109.40   |
| 1   | A     | 145  | G    | C4'-C3'-O3' | 5.15  | 120.72      | 113.00   |
| 3   | C     | 30   | ARG  | N-CA-C      | 5.15  | 116.89      | 111.28   |
| 1   | A     | 553  | A    | C4'-C3'-O3' | -5.14 | 105.30      | 113.00   |
| 19  | S     | 34   | TRP  | N-CA-C      | -5.13 | 107.40      | 113.97   |
| 23  | X     | 168  | VAL  | N-CA-C      | 5.13  | 115.27      | 110.30   |
| 2   | B     | 118  | LEU  | N-CA-C      | 5.11  | 117.75      | 111.82   |
| 1   | A     | 508  | C    | C2'-C3'-O3' | -5.11 | 101.84      | 109.50   |
| 20  | T     | 55   | ILE  | CB-CA-C     | 5.06  | 118.98      | 112.14   |
| 18  | R     | 17   | SER  | N-CA-C      | 5.00  | 121.45      | 110.80   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 5   | E     | 21  | ALA  | CA   |

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 12  | L     | 89  | ARG  | Peptide |
| 16  | P     | 67  | THR  | Peptide |
| 23  | X     | 53  | ASP  | Peptide |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 32525 | 0        | 16435    | 1141    | 0            |
| 2   | B     | 1900  | 0        | 1951     | 39      | 0            |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | C     | 1612  | 0        | 1677     | 95      | 0            |
| 4   | D     | 1703  | 0        | 1764     | 83      | 0            |
| 5   | E     | 1146  | 0        | 1207     | 63      | 0            |
| 6   | F     | 843   | 0        | 857      | 20      | 0            |
| 7   | G     | 1257  | 0        | 1296     | 24      | 0            |
| 8   | H     | 1116  | 0        | 1177     | 38      | 0            |
| 9   | I     | 1010  | 0        | 1035     | 25      | 0            |
| 10  | J     | 792   | 0        | 832      | 73      | 0            |
| 11  | K     | 885   | 0        | 903      | 40      | 0            |
| 12  | L     | 970   | 0        | 1057     | 24      | 0            |
| 13  | M     | 933   | 0        | 992      | 15      | 0            |
| 14  | N     | 492   | 0        | 533      | 35      | 0            |
| 15  | O     | 734   | 0        | 771      | 15      | 0            |
| 16  | P     | 700   | 0        | 720      | 22      | 0            |
| 17  | Q     | 823   | 0        | 891      | 32      | 0            |
| 18  | R     | 598   | 0        | 670      | 24      | 0            |
| 19  | S     | 647   | 0        | 673      | 12      | 0            |
| 20  | T     | 763   | 0        | 861      | 35      | 0            |
| 21  | V     | 208   | 0        | 221      | 1       | 0            |
| 22  | W     | 570   | 0        | 599      | 33      | 0            |
| 23  | X     | 1356  | 0        | 1399     | 22      | 0            |
| 24  | Y     | 417   | 0        | 208      | 11      | 0            |
| 25  | A     | 107   | 0        | 0        | 1       | 0            |
| 25  | W     | 1     | 0        | 0        | 0       | 0            |
| 26  | D     | 1     | 0        | 0        | 3       | 0            |
| 26  | N     | 1     | 0        | 0        | 1       | 0            |
| All | All   | 54110 | 0        | 38729    | 1712    | 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 19.

All (1712) 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) |
|------------------|-----------------|--------------------------|-------------------|
| 20:T:72:LEU:CD2  | 20:T:77:ALA:HB2 | 1.20                     | 1.68              |
| 1:A:1080:A:C5'   | 5:E:16:THR:HG21 | 1.11                     | 1.57              |
| 20:T:72:LEU:HD21 | 20:T:77:ALA:CA  | 1.35                     | 1.54              |
| 20:T:72:LEU:HD21 | 20:T:77:ALA:CB  | 1.33                     | 1.53              |
| 1:A:1080:A:C5'   | 5:E:16:THR:CG2  | 1.84                     | 1.53              |
| 1:A:1080:A:H5''  | 5:E:16:THR:CG2  | 1.45                     | 1.44              |
| 20:T:72:LEU:CD2  | 20:T:77:ALA:CB  | 1.91                     | 1.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 10:J:38:ILE:CG2  | 10:J:71:LEU:O    | 1.71                     | 1.38              |
| 1:A:279:A:C4     | 17:Q:98:LEU:HD23 | 1.59                     | 1.35              |
| 1:A:279:A:C4     | 17:Q:98:LEU:CD2  | 2.12                     | 1.30              |
| 3:C:59:ARG:CG    | 3:C:64:VAL:CG2   | 2.11                     | 1.29              |
| 3:C:57:ILE:CG1   | 3:C:66:VAL:HG22  | 1.60                     | 1.28              |
| 1:A:247:G:OP2    | 17:Q:100:LYS:CE  | 1.85                     | 1.23              |
| 10:J:17:ASP:OD1  | 10:J:70:ARG:NH2  | 1.68                     | 1.23              |
| 3:C:57:ILE:HG12  | 3:C:66:VAL:CG2   | 1.69                     | 1.22              |
| 1:A:1113:C:H4'   | 3:C:14:ILE:CD1   | 1.67                     | 1.22              |
| 4:D:36:ARG:HD2   | 4:D:38:TYR:CZ    | 1.73                     | 1.21              |
| 10:J:38:ILE:HG23 | 10:J:71:LEU:O    | 1.05                     | 1.20              |
| 1:A:262:A:C5'    | 20:T:73:HIS:HE1  | 1.54                     | 1.20              |
| 3:C:59:ARG:HG3   | 3:C:64:VAL:CG2   | 1.68                     | 1.18              |
| 1:A:1080:A:H5'   | 5:E:16:THR:CG2   | 1.58                     | 1.18              |
| 1:A:262:A:C5'    | 20:T:73:HIS:CE1  | 2.27                     | 1.17              |
| 1:A:1398:A:N6    | 5:E:21:ALA:O     | 1.75                     | 1.17              |
| 3:C:59:ARG:CG    | 3:C:64:VAL:HG23  | 1.72                     | 1.15              |
| 22:W:21:THR:HG21 | 22:W:33:LEU:CD1  | 1.76                     | 1.14              |
| 1:A:827:U:N3     | 1:A:872:A:N6     | 1.96                     | 1.13              |
| 1:A:1081:G:H2'   | 1:A:1082:G:H8    | 1.08                     | 1.12              |
| 14:N:24:CYS:SG   | 26:N:101:ZN:ZN   | 1.40                     | 1.10              |
| 3:C:59:ARG:HG3   | 3:C:64:VAL:HG22  | 1.32                     | 1.10              |
| 10:J:20:ALA:HB2  | 10:J:70:ARG:CD   | 1.81                     | 1.10              |
| 1:A:1079:G:H5'   | 5:E:14:ARG:HH22  | 0.97                     | 1.09              |
| 1:A:1113:C:C4'   | 3:C:14:ILE:HD12  | 1.82                     | 1.09              |
| 4:D:36:ARG:CD    | 4:D:38:TYR:CZ    | 2.36                     | 1.09              |
| 1:A:262:A:H5'    | 20:T:73:HIS:CE1  | 1.84                     | 1.08              |
| 1:A:1113:C:H4'   | 3:C:14:ILE:HD12  | 1.09                     | 1.08              |
| 3:C:59:ARG:NE    | 3:C:64:VAL:CG2   | 2.15                     | 1.08              |
| 3:C:59:ARG:CG    | 3:C:64:VAL:HG22  | 1.79                     | 1.08              |
| 1:A:1081:G:H2'   | 1:A:1082:G:C8    | 1.89                     | 1.08              |
| 3:C:59:ARG:HG2   | 3:C:64:VAL:HG23  | 1.36                     | 1.08              |
| 20:T:72:LEU:HD21 | 20:T:77:ALA:HA   | 1.35                     | 1.07              |
| 8:H:54:ASP:O     | 8:H:56:LYS:HE3   | 1.51                     | 1.07              |
| 3:C:59:ARG:CZ    | 3:C:64:VAL:HG21  | 1.84                     | 1.07              |
| 10:J:20:ALA:CB   | 10:J:70:ARG:CD   | 2.32                     | 1.07              |
| 10:J:20:ALA:HB2  | 10:J:70:ARG:HD2  | 1.31                     | 1.07              |
| 1:A:1077:G:N2    | 1:A:1079:G:H3'   | 1.69                     | 1.06              |
| 1:A:1079:G:C5'   | 5:E:14:ARG:HH22  | 1.68                     | 1.06              |
| 1:A:279:A:C5     | 17:Q:98:LEU:HD23 | 1.90                     | 1.05              |
| 1:A:864:A:H2'    | 1:A:865:A:C8     | 1.92                     | 1.05              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 22:W:21:THR:HG21 | 22:W:33:LEU:HD11 | 1.38                     | 1.03              |
| 10:J:50:ILE:HG12 | 10:J:60:ARG:HH21 | 1.24                     | 1.03              |
| 1:A:1219:U:H2'   | 1:A:1220:G:H8    | 1.24                     | 1.02              |
| 1:A:827:U:H3     | 1:A:872:A:N6     | 1.52                     | 1.02              |
| 3:C:24:ALA:HB1   | 3:C:28:GLN:HG2   | 1.38                     | 1.02              |
| 1:A:664:G:H22    | 1:A:741:G:H1     | 1.05                     | 1.01              |
| 10:J:48:THR:HG22 | 10:J:60:ARG:HG2  | 1.42                     | 1.01              |
| 1:A:920:U:H2'    | 1:A:921:U:C6     | 1.95                     | 1.01              |
| 20:T:72:LEU:CD2  | 20:T:77:ALA:CA   | 2.31                     | 1.01              |
| 1:A:279:A:N3     | 17:Q:98:LEU:CD2  | 2.24                     | 1.01              |
| 3:C:59:ARG:CD    | 3:C:64:VAL:HG22  | 1.91                     | 1.00              |
| 10:J:50:ILE:HG13 | 10:J:60:ARG:NE   | 1.77                     | 1.00              |
| 10:J:37:PRO:HA   | 10:J:72:VAL:HG22 | 1.42                     | 1.00              |
| 1:A:920:U:H2'    | 1:A:921:U:H6     | 1.21                     | 1.00              |
| 1:A:247:G:OP2    | 17:Q:100:LYS:HE3 | 1.58                     | 0.99              |
| 1:A:80:G:H3'     | 1:A:81:U:H5''    | 1.44                     | 0.99              |
| 1:A:1080:A:C5'   | 5:E:16:THR:HG23  | 1.91                     | 0.98              |
| 1:A:17:U:H2'     | 1:A:18:C:C6      | 1.98                     | 0.98              |
| 3:C:59:ARG:NE    | 3:C:64:VAL:HG22  | 1.78                     | 0.98              |
| 10:J:50:ILE:HG13 | 10:J:60:ARG:HE   | 1.26                     | 0.98              |
| 1:A:1256:A:H3'   | 3:C:27:LYS:NZ    | 1.79                     | 0.97              |
| 1:A:279:A:N3     | 17:Q:98:LEU:HD23 | 1.79                     | 0.97              |
| 1:A:1070:U:H2'   | 1:A:1071:C:C6    | 1.98                     | 0.97              |
| 1:A:1103:C:H2'   | 1:A:1104:G:O4'   | 1.64                     | 0.97              |
| 1:A:1113:C:C4'   | 3:C:14:ILE:CD1   | 2.41                     | 0.97              |
| 4:D:9:CYS:SG     | 26:D:300:ZN:ZN   | 1.53                     | 0.97              |
| 1:A:1322:C:H5''  | 13:M:100:GLY:HA2 | 1.45                     | 0.96              |
| 1:A:45:U:H2'     | 1:A:46:G:C8      | 1.99                     | 0.96              |
| 1:A:45:U:H2'     | 1:A:46:G:H8      | 1.29                     | 0.96              |
| 1:A:745:C:H2'    | 1:A:746:A:C8     | 2.01                     | 0.96              |
| 5:E:107:ARG:HH11 | 5:E:107:ARG:HB2  | 1.28                     | 0.96              |
| 16:P:59:TRP:O    | 16:P:62:VAL:HG22 | 1.65                     | 0.95              |
| 1:A:1219:U:H2'   | 1:A:1220:G:C8    | 2.01                     | 0.95              |
| 3:C:59:ARG:NE    | 3:C:64:VAL:HG21  | 1.81                     | 0.94              |
| 1:A:266:G:H3'    | 17:Q:67:LYS:HB2  | 1.48                     | 0.94              |
| 3:C:64:VAL:O     | 3:C:99:VAL:HG23  | 1.67                     | 0.94              |
| 1:A:1077:G:H22   | 1:A:1079:G:H3'   | 1.26                     | 0.94              |
| 1:A:279:A:C2     | 17:Q:98:LEU:HD23 | 2.02                     | 0.94              |
| 1:A:1080:A:H5'   | 5:E:16:THR:HG21  | 1.13                     | 0.93              |
| 10:J:20:ALA:CB   | 10:J:70:ARG:HD3  | 1.95                     | 0.93              |
| 20:T:72:LEU:HD23 | 20:T:77:ALA:HB2  | 0.94                     | 0.93              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1079:G:H5'   | 5:E:14:ARG:NH2   | 1.82                     | 0.93              |
| 3:C:28:GLN:HE21  | 3:C:32:LEU:HD11  | 1.29                     | 0.93              |
| 1:A:247:G:OP2    | 17:Q:100:LYS:CD  | 2.16                     | 0.93              |
| 1:A:262:A:H5''   | 20:T:73:HIS:HE1  | 1.35                     | 0.92              |
| 11:K:91:ARG:NH2  | 11:K:110:ASP:OD2 | 2.03                     | 0.92              |
| 1:A:1158:C:H4'   | 2:B:132:LYS:HB2  | 1.54                     | 0.90              |
| 1:A:1356:G:H2'   | 1:A:1357:A:C8    | 2.07                     | 0.90              |
| 1:A:827:U:O4     | 1:A:872:A:N1     | 2.05                     | 0.90              |
| 1:A:1101:A:H5''  | 2:B:99:GLY:HA3   | 1.54                     | 0.89              |
| 10:J:50:ILE:CG1  | 10:J:60:ARG:HH21 | 1.85                     | 0.89              |
| 10:J:36:GLY:O    | 10:J:72:VAL:HG13 | 1.73                     | 0.89              |
| 1:A:729:A:H2'    | 1:A:730:G:H8     | 1.37                     | 0.89              |
| 1:A:1070:U:H2'   | 1:A:1071:C:H6    | 1.35                     | 0.88              |
| 11:K:91:ARG:HH21 | 18:R:88:LYS:HZ2  | 1.16                     | 0.88              |
| 1:A:1022:G:H2'   | 1:A:1023:G:H8    | 1.38                     | 0.88              |
| 22:W:33:LEU:HD21 | 22:W:64:ARG:NH1  | 1.89                     | 0.88              |
| 1:A:662:G:H2'    | 1:A:663:A:C8     | 2.09                     | 0.88              |
| 1:A:917:G:H2'    | 1:A:918:A:C8     | 2.09                     | 0.87              |
| 4:D:35:ARG:HB3   | 4:D:35:ARG:HH21  | 1.37                     | 0.87              |
| 3:C:30:ARG:NH1   | 3:C:30:ARG:HB2   | 1.89                     | 0.87              |
| 10:J:50:ILE:CG1  | 10:J:60:ARG:HE   | 1.87                     | 0.87              |
| 14:N:24:CYS:HB3  | 14:N:29:ARG:H    | 1.40                     | 0.86              |
| 3:C:30:ARG:HG2   | 14:N:37:PHE:C    | 2.00                     | 0.86              |
| 10:J:38:ILE:HG22 | 10:J:71:LEU:O    | 1.76                     | 0.86              |
| 1:A:247:G:OP2    | 17:Q:100:LYS:NZ  | 2.08                     | 0.86              |
| 1:A:868:C:H2'    | 1:A:869:G:O4'    | 1.75                     | 0.86              |
| 1:A:1106:G:H5''  | 3:C:172:ARG:HG3  | 1.58                     | 0.86              |
| 8:H:45:ILE:HG22  | 8:H:63:LEU:HA    | 1.57                     | 0.86              |
| 4:D:26:CYS:SG    | 26:D:300:ZN:ZN   | 1.64                     | 0.85              |
| 22:W:21:THR:CG2  | 22:W:33:LEU:CD1  | 2.54                     | 0.85              |
| 1:A:247:G:OP2    | 17:Q:100:LYS:HD2 | 1.74                     | 0.85              |
| 3:C:59:ARG:CD    | 3:C:64:VAL:CG2   | 2.53                     | 0.85              |
| 1:A:1190:G:H5'   | 3:C:176:HIS:HE1  | 1.41                     | 0.85              |
| 1:A:17:U:O2'     | 1:A:1079:G:H1'   | 1.77                     | 0.85              |
| 10:J:20:ALA:HB1  | 10:J:70:ARG:HD3  | 1.55                     | 0.85              |
| 1:A:15:G:H2'     | 1:A:16:A:H8      | 1.41                     | 0.84              |
| 1:A:745:C:H2'    | 1:A:746:A:H8     | 1.40                     | 0.84              |
| 1:A:662:G:H2'    | 1:A:663:A:H8     | 1.42                     | 0.83              |
| 11:K:91:ARG:HH21 | 18:R:88:LYS:NZ   | 1.76                     | 0.83              |
| 1:A:1099:G:C6    | 1:A:1100:C:N3    | 2.47                     | 0.83              |
| 22:W:32:ILE:O    | 22:W:32:ILE:HD13 | 1.78                     | 0.82              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:30:ARG:CD    | 14:N:35:ARG:O    | 2.28                     | 0.82              |
| 1:A:170:U:H2'    | 1:A:171:A:H8     | 1.44                     | 0.82              |
| 10:J:38:ILE:HG23 | 10:J:71:LEU:C    | 2.05                     | 0.82              |
| 1:A:1022:G:H2'   | 1:A:1023:G:C8    | 2.14                     | 0.82              |
| 4:D:36:ARG:CD    | 4:D:38:TYR:OH    | 2.27                     | 0.82              |
| 1:A:262:A:C4'    | 20:T:73:HIS:CE1  | 2.62                     | 0.82              |
| 1:A:269:C:H2'    | 1:A:270:A:C8     | 2.14                     | 0.82              |
| 1:A:279:A:N3     | 17:Q:98:LEU:HD21 | 1.93                     | 0.82              |
| 1:A:1101:A:H4'   | 1:A:1102:A:O5'   | 1.79                     | 0.81              |
| 1:A:777:A:H2'    | 1:A:778:G:C8     | 2.14                     | 0.81              |
| 1:A:398:C:H2'    | 1:A:399:G:H8     | 1.44                     | 0.81              |
| 1:A:1256:A:H3'   | 3:C:27:LYS:CE    | 2.10                     | 0.81              |
| 9:I:13:ALA:HB2   | 9:I:68:GLY:HA3   | 1.62                     | 0.81              |
| 22:W:33:LEU:CD2  | 22:W:64:ARG:NH1  | 2.43                     | 0.81              |
| 1:A:124:G:H2'    | 1:A:125:U:O4'    | 1.79                     | 0.81              |
| 6:F:49:ALA:HB1   | 18:R:80:PRO:HA   | 1.62                     | 0.81              |
| 1:A:870:U:H4'    | 1:A:871:U:H5''   | 1.62                     | 0.81              |
| 1:A:16:A:N3      | 1:A:1080:A:H1'   | 1.96                     | 0.80              |
| 1:A:101:A:H2'    | 1:A:102:G:H8     | 1.45                     | 0.80              |
| 4:D:26:CYS:HA    | 4:D:31:CYS:HB2   | 1.63                     | 0.80              |
| 1:A:1096:C:H2'   | 1:A:1097:C:C6    | 2.17                     | 0.80              |
| 1:A:16:A:C2      | 1:A:1080:A:H1'   | 2.18                     | 0.80              |
| 1:A:303:A:H2'    | 1:A:304:U:H6     | 1.44                     | 0.80              |
| 1:A:1073:U:H3    | 1:A:1102:A:H61   | 1.30                     | 0.79              |
| 1:A:729:A:H2'    | 1:A:730:G:C8     | 2.16                     | 0.79              |
| 1:A:925:G:H1     | 1:A:1391:U:H3    | 1.28                     | 0.79              |
| 4:D:36:ARG:HG3   | 4:D:38:TYR:CE2   | 2.17                     | 0.79              |
| 11:K:87:THR:HG23 | 11:K:91:ARG:HD3  | 1.65                     | 0.78              |
| 1:A:309:G:H2'    | 1:A:310:G:H8     | 1.48                     | 0.78              |
| 1:A:299:G:H2'    | 1:A:300:A:C8     | 2.18                     | 0.78              |
| 1:A:1190:G:H5'   | 3:C:176:HIS:CE1  | 2.17                     | 0.78              |
| 1:A:1390:U:H2'   | 1:A:1391:U:C6    | 2.18                     | 0.78              |
| 6:F:49:ALA:CB    | 18:R:80:PRO:HA   | 2.13                     | 0.78              |
| 1:A:1096:C:H2'   | 1:A:1097:C:H6    | 1.49                     | 0.78              |
| 1:A:1128:C:H2'   | 1:A:1139:G:N7    | 1.99                     | 0.78              |
| 11:K:87:THR:HA   | 11:K:91:ARG:HD2  | 1.65                     | 0.78              |
| 1:A:21:G:H2'     | 1:A:22:G:C8      | 2.18                     | 0.78              |
| 1:A:1127:G:H21   | 1:A:1147:C:H41   | 1.29                     | 0.78              |
| 20:T:72:LEU:HD21 | 20:T:77:ALA:N    | 1.97                     | 0.77              |
| 1:A:1435:G:H2'   | 1:A:1436:U:C6    | 2.19                     | 0.77              |
| 1:A:728:A:H2'    | 1:A:729:A:C8     | 2.19                     | 0.77              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:59:ARG:HG3   | 3:C:64:VAL:HG23  | 1.46                     | 0.77              |
| 5:E:43:LEU:HD11  | 5:E:132:ALA:HB1  | 1.67                     | 0.77              |
| 1:A:1507:A:H2'   | 1:A:1508:G:C8    | 2.19                     | 0.77              |
| 16:P:59:TRP:O    | 16:P:62:VAL:CG2  | 2.31                     | 0.77              |
| 4:D:26:CYS:SG    | 4:D:31:CYS:SG    | 2.81                     | 0.77              |
| 4:D:35:ARG:HH21  | 4:D:35:ARG:CB    | 1.98                     | 0.77              |
| 1:A:302:G:H2'    | 1:A:303:A:C8     | 2.19                     | 0.77              |
| 1:A:914:A:H2'    | 1:A:915:A:H8     | 1.48                     | 0.76              |
| 8:H:91:ARG:HD3   | 12:L:7:ILE:HG21  | 1.67                     | 0.76              |
| 1:A:1367:C:H4'   | 10:J:48:THR:HG21 | 1.66                     | 0.76              |
| 1:A:24:U:H2'     | 1:A:25:C:C6      | 2.20                     | 0.76              |
| 1:A:279:A:C4     | 17:Q:98:LEU:HD21 | 2.18                     | 0.76              |
| 1:A:303:A:H2'    | 1:A:304:U:C6     | 2.21                     | 0.76              |
| 10:J:37:PRO:O    | 10:J:70:ARG:CG   | 2.34                     | 0.76              |
| 4:D:36:ARG:HD3   | 4:D:38:TYR:OH    | 1.85                     | 0.76              |
| 5:E:107:ARG:HB2  | 5:E:107:ARG:NH1  | 2.01                     | 0.76              |
| 1:A:728:A:H2'    | 1:A:729:A:H8     | 1.48                     | 0.75              |
| 10:J:60:ARG:HB2  | 10:J:60:ARG:CZ   | 2.14                     | 0.75              |
| 1:A:262:A:H4'    | 20:T:73:HIS:CE1  | 2.20                     | 0.75              |
| 1:A:1080:A:H5'   | 5:E:16:THR:CB    | 2.15                     | 0.75              |
| 1:A:1080:A:H5''  | 5:E:16:THR:HG21  | 0.77                     | 0.75              |
| 1:A:1256:A:H3'   | 3:C:27:LYS:HZ2   | 1.49                     | 0.75              |
| 1:A:1102:A:H2'   | 1:A:1103:C:C6    | 2.21                     | 0.75              |
| 1:A:56:U:H2'     | 1:A:57:G:C8      | 2.21                     | 0.74              |
| 1:A:919:A:C2     | 1:A:1080:A:H2    | 2.05                     | 0.74              |
| 1:A:701:C:H4'    | 1:A:702:A:O5'    | 1.87                     | 0.74              |
| 10:J:17:ASP:OD1  | 10:J:70:ARG:CZ   | 2.35                     | 0.74              |
| 1:A:90:U:H2'     | 1:A:91:C:C6      | 2.22                     | 0.74              |
| 1:A:224:C:H2'    | 1:A:225:C:C6     | 2.21                     | 0.74              |
| 1:A:398:C:H2'    | 1:A:399:G:C8     | 2.23                     | 0.74              |
| 1:A:1080:A:C4'   | 5:E:16:THR:HG23  | 2.17                     | 0.74              |
| 3:C:30:ARG:HD2   | 14:N:35:ARG:O    | 1.87                     | 0.74              |
| 10:J:50:ILE:CD1  | 10:J:60:ARG:HE   | 2.00                     | 0.74              |
| 1:A:313:A:H2'    | 1:A:314:C:C6     | 2.22                     | 0.74              |
| 8:H:54:ASP:O     | 8:H:56:LYS:CE    | 2.35                     | 0.74              |
| 4:D:36:ARG:HD2   | 4:D:38:TYR:CE1   | 2.23                     | 0.73              |
| 1:A:1077:G:H2'   | 1:A:1078:U:H2'   | 1.71                     | 0.73              |
| 1:A:269:C:H2'    | 1:A:270:A:H8     | 1.52                     | 0.73              |
| 1:A:1113:C:H4'   | 3:C:14:ILE:HD13  | 1.69                     | 0.73              |
| 1:A:1521:G:H2'   | 1:A:1522:U:C6    | 2.22                     | 0.73              |
| 10:J:50:ILE:HG13 | 10:J:60:ARG:CZ   | 2.18                     | 0.73              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 22:W:23:ARG:HH21 | 22:W:33:LEU:HB2  | 1.53                     | 0.73              |
| 1:A:439:A:OP2    | 1:A:493:G:N1     | 2.19                     | 0.73              |
| 1:A:1348:U:H2'   | 1:A:1349:A:H8    | 1.52                     | 0.73              |
| 1:A:1390:U:H2'   | 1:A:1391:U:H6    | 1.54                     | 0.73              |
| 3:C:30:ARG:HD3   | 14:N:35:ARG:O    | 1.88                     | 0.72              |
| 1:A:279:A:C6     | 17:Q:98:LEU:HD23 | 2.25                     | 0.72              |
| 4:D:36:ARG:CD    | 4:D:38:TYR:CE2   | 2.72                     | 0.72              |
| 1:A:262:A:C4'    | 20:T:73:HIS:HE1  | 1.98                     | 0.72              |
| 2:B:15:VAL:HG11  | 2:B:209:ARG:HB3  | 1.70                     | 0.72              |
| 1:A:1287:A:H2'   | 1:A:1288:A:C8    | 2.24                     | 0.72              |
| 11:K:54:ARG:H    | 11:K:54:ARG:HD2  | 1.55                     | 0.72              |
| 1:A:973:G:H3'    | 1:A:974:A:H5''   | 1.72                     | 0.72              |
| 3:C:30:ARG:HG3   | 14:N:36:PHE:O    | 1.90                     | 0.72              |
| 1:A:1256:A:C3'   | 3:C:27:LYS:NZ    | 2.51                     | 0.72              |
| 1:A:1386:G:H2'   | 1:A:1387:G:H8    | 1.54                     | 0.72              |
| 10:J:50:ILE:CG1  | 10:J:60:ARG:NH2  | 2.53                     | 0.72              |
| 10:J:53:PRO:HA   | 14:N:41:ARG:HH21 | 1.54                     | 0.71              |
| 1:A:13:U:N3      | 1:A:915:A:N6     | 2.38                     | 0.71              |
| 1:A:113:G:H2'    | 1:A:114:U:C6     | 2.25                     | 0.71              |
| 4:D:9:CYS:HG     | 26:D:300:ZN:ZN   | 1.02                     | 0.71              |
| 10:J:38:ILE:O    | 10:J:71:LEU:N    | 2.23                     | 0.71              |
| 10:J:40:LEU:HB2  | 10:J:69:ASN:HB3  | 1.73                     | 0.71              |
| 1:A:562:C:H41    | 1:A:884:U:H2'    | 1.55                     | 0.71              |
| 10:J:48:THR:HG22 | 10:J:60:ARG:CG   | 2.18                     | 0.71              |
| 20:T:72:LEU:CD2  | 20:T:77:ALA:HA   | 2.11                     | 0.71              |
| 22:W:21:THR:CG2  | 22:W:33:LEU:HG   | 2.20                     | 0.71              |
| 1:A:1080:A:H4'   | 5:E:16:THR:HG23  | 1.70                     | 0.71              |
| 1:A:1256:A:C3'   | 3:C:27:LYS:HZ2   | 2.03                     | 0.71              |
| 1:A:524:G:C6     | 1:A:525:C:N4     | 2.58                     | 0.71              |
| 1:A:1443:G:C6    | 1:A:1444:C:N4    | 2.58                     | 0.71              |
| 1:A:403:C:H5''   | 4:D:136:PRO:HD2  | 1.71                     | 0.71              |
| 1:A:664:G:N2     | 1:A:741:G:H1     | 1.87                     | 0.71              |
| 1:A:769:G:N2     | 1:A:770:C:C2     | 2.59                     | 0.71              |
| 1:A:1500:A:H5''  | 1:A:1508:G:H5''  | 1.73                     | 0.71              |
| 1:A:302:G:H2'    | 1:A:303:A:H8     | 1.53                     | 0.70              |
| 1:A:316:G:H1     | 1:A:337:C:H42    | 1.38                     | 0.70              |
| 1:A:1081:G:OP2   | 5:E:16:THR:HG22  | 1.91                     | 0.70              |
| 1:A:69:G:H1      | 1:A:100:C:N4     | 1.89                     | 0.70              |
| 10:J:37:PRO:HA   | 10:J:72:VAL:CG2  | 2.18                     | 0.70              |
| 1:A:69:G:H1      | 1:A:100:C:H42    | 1.36                     | 0.70              |
| 1:A:18:C:H2'     | 1:A:19:C:C6      | 2.27                     | 0.70              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 10:J:17:ASP:CG   | 10:J:70:ARG:NH2  | 2.49                     | 0.69              |
| 1:A:406:G:H4'    | 4:D:5:ILE:HD11   | 1.73                     | 0.69              |
| 1:A:24:U:H2'     | 1:A:25:C:H6      | 1.56                     | 0.69              |
| 1:A:424:G:H2'    | 1:A:425:G:C8     | 2.27                     | 0.69              |
| 5:E:14:ARG:O     | 5:E:14:ARG:HG2   | 1.92                     | 0.69              |
| 1:A:10:A:H2'     | 1:A:11:G:C8      | 2.27                     | 0.69              |
| 1:A:10:A:H2'     | 1:A:11:G:H8      | 1.56                     | 0.69              |
| 1:A:584:G:H2'    | 1:A:585:G:H8     | 1.58                     | 0.69              |
| 5:E:105:VAL:HB   | 5:E:106:PRO:HD3  | 1.74                     | 0.69              |
| 22:W:21:THR:HG21 | 22:W:33:LEU:HD12 | 1.71                     | 0.69              |
| 22:W:33:LEU:HD23 | 22:W:64:ARG:HG2  | 1.72                     | 0.69              |
| 1:A:312:C:H2'    | 1:A:313:A:C8     | 2.28                     | 0.69              |
| 1:A:1095:U:H2'   | 1:A:1096:C:C6    | 2.27                     | 0.69              |
| 1:A:1445:C:C2    | 1:A:1458:G:C2    | 2.81                     | 0.69              |
| 1:A:584:G:H2'    | 1:A:585:G:C8     | 2.27                     | 0.69              |
| 1:A:56:U:H2'     | 1:A:57:G:H8      | 1.58                     | 0.68              |
| 14:N:41:ARG:HE   | 14:N:42:ILE:HG13 | 1.58                     | 0.68              |
| 24:Y:28:A:H3'    | 24:Y:29:G:C8     | 2.27                     | 0.68              |
| 1:A:13:U:H3      | 1:A:915:A:N6     | 1.91                     | 0.68              |
| 1:A:67:C:H2'     | 1:A:68:G:H8      | 1.57                     | 0.68              |
| 1:A:543:C:H2'    | 1:A:544:G:C8     | 2.28                     | 0.68              |
| 1:A:1079:G:H2'   | 1:A:1080:A:C8    | 2.28                     | 0.68              |
| 10:J:40:LEU:HG   | 10:J:71:LEU:HB2  | 1.76                     | 0.68              |
| 23:X:48:VAL:HG21 | 23:X:58:ARG:HE   | 1.58                     | 0.68              |
| 1:A:16:A:C2      | 1:A:17:U:C6      | 2.82                     | 0.68              |
| 1:A:1536:C:H42   | 24:Y:29:G:H1     | 1.41                     | 0.68              |
| 1:A:67:C:H2'     | 1:A:68:G:C8      | 2.28                     | 0.68              |
| 1:A:524:G:C2     | 1:A:525:C:N3     | 2.61                     | 0.68              |
| 1:A:576:G:H3'    | 1:A:577:G:H5''   | 1.75                     | 0.68              |
| 1:A:1256:A:H3'   | 3:C:27:LYS:HE3   | 1.74                     | 0.68              |
| 10:J:37:PRO:CA   | 10:J:72:VAL:HG22 | 2.21                     | 0.68              |
| 1:A:1410:G:H2'   | 1:A:1411:C:C6    | 2.29                     | 0.68              |
| 3:C:71:ALA:HB2   | 3:C:115:LEU:HD11 | 1.75                     | 0.68              |
| 1:A:860:A:H3'    | 1:A:861:G:H8     | 1.59                     | 0.68              |
| 1:A:1264:C:H2'   | 1:A:1265:G:H8    | 1.58                     | 0.68              |
| 1:A:279:A:C2     | 17:Q:98:LEU:CD2  | 2.74                     | 0.67              |
| 1:A:521:G:N2     | 1:A:522:C:C2     | 2.62                     | 0.67              |
| 1:A:1016:A:H2'   | 1:A:1017:G:O4'   | 1.95                     | 0.67              |
| 11:K:33:THR:HA   | 11:K:39:PRO:HA   | 1.76                     | 0.67              |
| 1:A:564:C:O2     | 1:A:564:C:H2'    | 1.94                     | 0.67              |
| 1:A:588:G:N2     | 1:A:589:C:C2     | 2.63                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:234:C:H2'    | 1:A:235:C:C6     | 2.29                     | 0.67              |
| 1:A:690:G:OP2    | 11:K:27:ASN:HB3  | 1.94                     | 0.67              |
| 23:X:5:TYR:HE2   | 23:X:65:TRP:CH2  | 2.12                     | 0.67              |
| 22:W:33:LEU:HD21 | 22:W:64:ARG:HH11 | 1.59                     | 0.67              |
| 1:A:1132:C:H2'   | 1:A:1133:G:C8    | 2.30                     | 0.66              |
| 8:H:29:SER:HB3   | 8:H:32:LYS:HG3   | 1.78                     | 0.66              |
| 15:O:31:LEU:O    | 15:O:35:ARG:HG3  | 1.96                     | 0.66              |
| 1:A:610:G:H2'    | 1:A:611:A:H8     | 1.59                     | 0.66              |
| 3:C:57:ILE:CD1   | 3:C:66:VAL:HG22  | 2.25                     | 0.66              |
| 16:P:67:THR:HG22 | 16:P:68:ASP:H    | 1.59                     | 0.66              |
| 1:A:16:A:H1'     | 1:A:1080:A:H4'   | 1.77                     | 0.66              |
| 1:A:568:G:N2     | 1:A:883:C:C2     | 2.63                     | 0.66              |
| 20:T:72:LEU:HD23 | 20:T:77:ALA:CB   | 1.90                     | 0.66              |
| 3:C:24:ALA:CB    | 3:C:28:GLN:HG2   | 2.22                     | 0.66              |
| 1:A:543:C:H2'    | 1:A:544:G:H8     | 1.60                     | 0.66              |
| 5:E:139:LEU:HA   | 5:E:142:LEU:HD12 | 1.77                     | 0.66              |
| 4:D:36:ARG:HD3   | 4:D:38:TYR:CZ    | 2.26                     | 0.66              |
| 1:A:522:C:H41    | 12:L:53:ARG:HH21 | 1.44                     | 0.66              |
| 1:A:1079:G:C5'   | 5:E:14:ARG:NH2   | 2.51                     | 0.66              |
| 3:C:66:VAL:HG12  | 3:C:68:VAL:HG22  | 1.77                     | 0.65              |
| 1:A:955:U:H1'    | 1:A:1227:A:H61   | 1.61                     | 0.65              |
| 1:A:1244:C:H2'   | 1:A:1245:A:H8    | 1.60                     | 0.65              |
| 8:H:121:ASP:CG   | 8:H:122:ARG:H    | 2.04                     | 0.65              |
| 1:A:19:C:H2'     | 1:A:20:U:C6      | 2.32                     | 0.65              |
| 4:D:63:LYS:O     | 4:D:67:ILE:HG13  | 1.97                     | 0.65              |
| 1:A:1328:C:H2'   | 1:A:1329:A:O4'   | 1.97                     | 0.65              |
| 9:I:46:ALA:HB2   | 9:I:74:ILE:HG23  | 1.78                     | 0.65              |
| 1:A:253:U:H2'    | 1:A:254:G:H8     | 1.62                     | 0.65              |
| 1:A:1163:C:H2'   | 1:A:1164:G:H8    | 1.60                     | 0.65              |
| 3:C:39:ILE:HG21  | 3:C:66:VAL:HG21  | 1.77                     | 0.65              |
| 9:I:114:TYR:HD2  | 10:J:58:ASP:O    | 1.80                     | 0.65              |
| 10:J:37:PRO:O    | 10:J:70:ARG:HG3  | 1.97                     | 0.64              |
| 4:D:7:PRO:HB2    | 4:D:10:ARG:HD2   | 1.78                     | 0.64              |
| 1:A:1020:U:H2'   | 1:A:1021:G:H8    | 1.63                     | 0.64              |
| 6:F:9:VAL:HB     | 6:F:87:ARG:HB2   | 1.79                     | 0.64              |
| 1:A:777:A:H2'    | 1:A:778:G:H8     | 1.59                     | 0.64              |
| 1:A:1504:G:H5''  | 1:A:1505:G:O4'   | 1.98                     | 0.64              |
| 24:Y:28:A:H3'    | 24:Y:29:G:H8     | 1.62                     | 0.64              |
| 1:A:930:C:H2'    | 1:A:931:C:O4'    | 1.97                     | 0.64              |
| 1:A:172:A:H2'    | 1:A:174:C:H5     | 1.62                     | 0.64              |
| 1:A:587:G:O2'    | 1:A:588:G:H5'    | 1.97                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1073:U:H3    | 1:A:1102:A:N6    | 1.94                     | 0.64              |
| 1:A:1264:C:H2'   | 1:A:1265:G:C8    | 2.33                     | 0.64              |
| 16:P:65:GLN:HE21 | 16:P:66:PRO:HD2  | 1.62                     | 0.64              |
| 4:D:30:LYS:C     | 4:D:32:ALA:H     | 2.03                     | 0.64              |
| 1:A:312:C:H2'    | 1:A:313:A:H8     | 1.62                     | 0.63              |
| 1:A:1255:G:H2'   | 1:A:1279:A:N6    | 2.13                     | 0.63              |
| 3:C:30:ARG:HB2   | 3:C:30:ARG:HH11  | 1.63                     | 0.63              |
| 1:A:335:C:H2'    | 1:A:336:C:C6     | 2.33                     | 0.63              |
| 1:A:424:G:H2'    | 1:A:425:G:H8     | 1.60                     | 0.63              |
| 19:S:22:LEU:HD13 | 19:S:28:LYS:HB3  | 1.78                     | 0.63              |
| 1:A:864:A:O2'    | 1:A:1078:U:C4    | 2.52                     | 0.63              |
| 1:A:1402:C:H2'   | 1:A:1403:C:H6    | 1.62                     | 0.63              |
| 12:L:46:LYS:HB3  | 12:L:48:PRO:HD2  | 1.80                     | 0.63              |
| 1:A:878:G:H5'    | 8:H:89:PRO:HG2   | 1.79                     | 0.63              |
| 1:A:1071:C:H2'   | 1:A:1072:G:H8    | 1.64                     | 0.63              |
| 1:A:1536:C:N4    | 24:Y:29:G:H1     | 1.96                     | 0.63              |
| 1:A:370:C:C2     | 1:A:392:G:N2     | 2.66                     | 0.63              |
| 1:A:1443:G:C2    | 1:A:1444:C:N3    | 2.67                     | 0.63              |
| 1:A:914:A:H2'    | 1:A:915:A:C8     | 2.32                     | 0.62              |
| 3:C:29:TYR:OH    | 14:N:37:PHE:CE1  | 2.51                     | 0.62              |
| 20:T:34:LYS:HG3  | 20:T:80:ARG:HH12 | 1.64                     | 0.62              |
| 1:A:1241:G:N2    | 1:A:1242:C:C2    | 2.67                     | 0.62              |
| 1:A:1515:C:H2'   | 1:A:1516:G:C8    | 2.34                     | 0.62              |
| 5:E:87:SER:HA    | 5:E:125:SER:HB3  | 1.80                     | 0.62              |
| 1:A:678:U:H2'    | 1:A:679:C:C6     | 2.34                     | 0.62              |
| 10:J:37:PRO:O    | 10:J:70:ARG:HG2  | 1.98                     | 0.62              |
| 15:O:8:LYS:HG2   | 15:O:31:LEU:HD11 | 1.80                     | 0.62              |
| 1:A:919:A:C2     | 1:A:1079:G:N2    | 2.68                     | 0.62              |
| 10:J:50:ILE:HG12 | 10:J:60:ARG:NH2  | 2.06                     | 0.62              |
| 23:X:89:LYS:HD2  | 24:Y:36:A:H61    | 1.64                     | 0.62              |
| 1:A:946:A:H2'    | 1:A:947:G:C8     | 2.35                     | 0.62              |
| 1:A:1152:A:H5'   | 10:J:13:HIS:HB2  | 1.81                     | 0.62              |
| 1:A:110:C:H2'    | 1:A:111:G:O4'    | 1.98                     | 0.62              |
| 16:P:13:HIS:O    | 16:P:15:PRO:HD3  | 1.99                     | 0.62              |
| 22:W:21:THR:CG2  | 22:W:33:LEU:HD12 | 2.27                     | 0.62              |
| 1:A:1342:C:H2'   | 1:A:1343:G:C8    | 2.35                     | 0.62              |
| 1:A:1387:G:O3'   | 1:A:1388:C:H5'   | 1.99                     | 0.62              |
| 1:A:1505:G:H4'   | 1:A:1506:U:H5''  | 1.81                     | 0.62              |
| 1:A:610:G:H2'    | 1:A:611:A:C8     | 2.35                     | 0.61              |
| 1:A:1313:U:H2'   | 1:A:1314:C:C6    | 2.35                     | 0.61              |
| 4:D:36:ARG:CG    | 4:D:38:TYR:CE2   | 2.83                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 12:L:102:ARG:HG2 | 12:L:107:ALA:HB1 | 1.82                     | 0.61              |
| 23:X:5:TYR:HE2   | 23:X:65:TRP:HH2  | 1.48                     | 0.61              |
| 1:A:671:G:N2     | 1:A:736:C:C2     | 2.68                     | 0.61              |
| 1:A:911:U:H2'    | 1:A:912:C:C6     | 2.35                     | 0.61              |
| 1:A:112:G:H21    | 1:A:354:G:H5'    | 1.64                     | 0.61              |
| 1:A:259:G:H2'    | 1:A:260:G:C8     | 2.35                     | 0.61              |
| 1:A:442:C:H2'    | 1:A:443:C:C6     | 2.35                     | 0.61              |
| 1:A:725:G:N2     | 1:A:726:C:C2     | 2.69                     | 0.61              |
| 4:D:36:ARG:HD2   | 4:D:38:TYR:OH    | 1.90                     | 0.61              |
| 1:A:123:C:H2'    | 1:A:124:G:H8     | 1.64                     | 0.61              |
| 1:A:974:A:H4'    | 1:A:975:A:H3'    | 1.83                     | 0.61              |
| 1:A:1098:C:H1'   | 1:A:1168:A:H2    | 1.66                     | 0.61              |
| 10:J:49:VAL:O    | 10:J:60:ARG:HG3  | 2.00                     | 0.61              |
| 3:C:57:ILE:HG12  | 3:C:66:VAL:HG22  | 0.72                     | 0.61              |
| 22:W:32:ILE:HB   | 22:W:63:THR:O    | 2.01                     | 0.61              |
| 1:A:1080:A:H5'   | 5:E:16:THR:OG1   | 2.01                     | 0.61              |
| 1:A:1353:G:N2    | 1:A:1354:C:C2    | 2.68                     | 0.61              |
| 2:B:111:ARG:HD3  | 2:B:145:LEU:HD21 | 1.82                     | 0.61              |
| 1:A:27:G:H2'     | 1:A:28:G:C8      | 2.36                     | 0.61              |
| 1:A:827:U:C2     | 1:A:872:A:N6     | 2.69                     | 0.61              |
| 1:A:1355:G:H2'   | 1:A:1356:G:H8    | 1.65                     | 0.61              |
| 2:B:71:VAL:HA    | 2:B:93:VAL:HG12  | 1.82                     | 0.61              |
| 11:K:87:THR:HA   | 11:K:91:ARG:CD   | 2.30                     | 0.61              |
| 22:W:32:ILE:HD13 | 22:W:32:ILE:C    | 2.23                     | 0.61              |
| 1:A:1111:A:N1    | 3:C:177:THR:HB   | 2.16                     | 0.60              |
| 1:A:309:G:H2'    | 1:A:310:G:C8     | 2.34                     | 0.60              |
| 1:A:1065:U:H4'   | 1:A:1066:C:O5'   | 2.01                     | 0.60              |
| 1:A:376:G:H2'    | 1:A:377:G:H8     | 1.67                     | 0.60              |
| 1:A:548:G:H2'    | 1:A:549:C:C6     | 2.37                     | 0.60              |
| 1:A:683:G:N2     | 1:A:708:C:C2     | 2.70                     | 0.60              |
| 4:D:20:TYR:HA    | 4:D:26:CYS:HB3   | 1.83                     | 0.60              |
| 8:H:121:ASP:CG   | 8:H:122:ARG:N    | 2.60                     | 0.60              |
| 1:A:181:G:H4'    | 1:A:182:U:H5'    | 1.82                     | 0.60              |
| 1:A:407:G:H1'    | 4:D:119:GLN:HE22 | 1.67                     | 0.60              |
| 1:A:1255:G:H2'   | 1:A:1279:A:H62   | 1.67                     | 0.60              |
| 6:F:94:GLN:HB3   | 18:R:32:ARG:HD3  | 1.82                     | 0.60              |
| 1:A:568:G:C2     | 1:A:883:C:N3     | 2.70                     | 0.60              |
| 1:A:174:C:H2'    | 1:A:175:C:C6     | 2.36                     | 0.60              |
| 1:A:895:G:H1     | 1:A:904:C:H42    | 1.50                     | 0.60              |
| 1:A:1355:G:H1    | 1:A:1367:C:H42   | 1.50                     | 0.60              |
| 1:A:15:G:C5      | 1:A:16:A:N7      | 2.69                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1235:U:H2'   | 1:A:1236:A:O4'   | 2.02                     | 0.60              |
| 1:A:123:C:H2'    | 1:A:124:G:C8     | 2.37                     | 0.60              |
| 1:A:255:G:C2     | 1:A:272:C:C2     | 2.90                     | 0.60              |
| 1:A:279:A:C5     | 17:Q:98:LEU:CD2  | 2.67                     | 0.60              |
| 1:A:453:A:H2'    | 1:A:454:C:C6     | 2.37                     | 0.60              |
| 22:W:33:LEU:HD23 | 22:W:33:LEU:O    | 2.02                     | 0.60              |
| 1:A:266:G:C8     | 1:A:266:G:H5''   | 2.37                     | 0.59              |
| 22:W:21:THR:CG2  | 22:W:33:LEU:CG   | 2.80                     | 0.59              |
| 1:A:46:G:H2'     | 1:A:366:C:C5     | 2.37                     | 0.59              |
| 1:A:1001:A:H2'   | 1:A:1001(A):G:C8 | 2.36                     | 0.59              |
| 3:C:59:ARG:HG2   | 3:C:64:VAL:CG2   | 2.03                     | 0.59              |
| 4:D:109:GLY:HA3  | 4:D:165:MET:HG3  | 1.84                     | 0.59              |
| 1:A:1080:A:C4'   | 5:E:16:THR:CG2   | 2.70                     | 0.59              |
| 1:A:1507:A:H2'   | 1:A:1508:G:H8    | 1.67                     | 0.59              |
| 5:E:18:ARG:HB3   | 5:E:25:ARG:O     | 2.02                     | 0.59              |
| 11:K:62:GLN:HG2  | 11:K:97:ALA:HB2  | 1.83                     | 0.59              |
| 16:P:48:TRP:CD1  | 16:P:48:TRP:H    | 2.21                     | 0.59              |
| 23:X:90:PHE:HD1  | 23:X:94:ILE:HD13 | 1.67                     | 0.59              |
| 1:A:32:A:H2'     | 1:A:33:A:C8      | 2.38                     | 0.59              |
| 1:A:313:A:H2'    | 1:A:314:C:H6     | 1.67                     | 0.59              |
| 1:A:521:G:N1     | 1:A:522:C:C4     | 2.70                     | 0.59              |
| 1:A:1512:U:H2'   | 1:A:1513:A:C8    | 2.37                     | 0.59              |
| 12:L:24:VAL:HG12 | 12:L:26:ALA:H    | 1.67                     | 0.59              |
| 1:A:769:G:N1     | 1:A:770:C:C4     | 2.71                     | 0.59              |
| 1:A:1105:A:H2'   | 1:A:1106:G:H8    | 1.68                     | 0.59              |
| 10:J:50:ILE:HG13 | 10:J:60:ARG:NH2  | 2.18                     | 0.59              |
| 1:A:20:U:H2'     | 1:A:21:G:O4'     | 2.03                     | 0.59              |
| 1:A:183:G:H2'    | 1:A:184:G:O4'    | 2.03                     | 0.59              |
| 1:A:861:G:O6     | 1:A:869:G:N2     | 2.35                     | 0.59              |
| 1:A:1416:G:H2'   | 1:A:1417:G:O4'   | 2.02                     | 0.59              |
| 10:J:50:ILE:CG1  | 10:J:60:ARG:NE   | 2.56                     | 0.59              |
| 1:A:77:G:H3'     | 1:A:77:G:C8      | 2.37                     | 0.59              |
| 1:A:170:U:H2'    | 1:A:171:A:C8     | 2.33                     | 0.59              |
| 1:A:320:C:H2'    | 1:A:321:A:C8     | 2.38                     | 0.59              |
| 1:A:743:U:H2'    | 1:A:744:C:C6     | 2.38                     | 0.59              |
| 1:A:1069:C:H42   | 1:A:1106:G:H1    | 1.51                     | 0.59              |
| 1:A:1162:C:C2    | 1:A:1175:G:N2    | 2.70                     | 0.59              |
| 1:A:13:U:OP1     | 25:A:1606:MG:MG  | 1.45                     | 0.59              |
| 1:A:128:G:N2     | 1:A:234:C:C2     | 2.71                     | 0.59              |
| 4:D:166:LYS:HG3  | 4:D:178:VAL:HG21 | 1.85                     | 0.59              |
| 7:G:93:PRO:O     | 7:G:96:GLN:HG2   | 2.03                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:741:G:H5'    | 15:O:39:LEU:HD21 | 1.84                     | 0.59              |
| 1:A:920:U:O2'    | 1:A:1081:G:O2'   | 2.20                     | 0.59              |
| 1:A:1238:A:H5'   | 1:A:1336:C:H41   | 1.68                     | 0.59              |
| 3:C:66:VAL:CG1   | 3:C:68:VAL:HG22  | 2.32                     | 0.59              |
| 1:A:926:G:H3'    | 1:A:1505:G:N2    | 2.18                     | 0.58              |
| 10:J:34:VAL:HG22 | 10:J:74:ILE:HG23 | 1.85                     | 0.58              |
| 12:L:25:PRO:C    | 12:L:27:LEU:H    | 2.11                     | 0.58              |
| 1:A:222:U:H2'    | 1:A:223:U:C6     | 2.38                     | 0.58              |
| 1:A:363:A:C6     | 12:L:31:PRO:HD2  | 2.38                     | 0.58              |
| 1:A:1074:G:N1    | 1:A:1075:C:C2    | 2.72                     | 0.58              |
| 1:A:1515:C:H2'   | 1:A:1516:G:H8    | 1.68                     | 0.58              |
| 1:A:928:G:H2'    | 1:A:929:G:C8     | 2.38                     | 0.58              |
| 1:A:1099:G:C2    | 1:A:1100:C:O2    | 2.56                     | 0.58              |
| 1:A:34:C:H2'     | 1:A:35:G:C8      | 2.39                     | 0.58              |
| 1:A:1128:C:H1'   | 1:A:1146:A:H61   | 1.67                     | 0.58              |
| 10:J:7:LYS:HB2   | 10:J:97:GLU:HB2  | 1.84                     | 0.58              |
| 23:X:29:MET:HE2  | 23:X:37:LEU:HD11 | 1.86                     | 0.58              |
| 1:A:1456:G:N2    | 1:A:1457:G:C8    | 2.72                     | 0.58              |
| 22:W:23:ARG:NH2  | 22:W:33:LEU:HB2  | 2.19                     | 0.58              |
| 1:A:392:G:H2'    | 1:A:393:A:H8     | 1.67                     | 0.58              |
| 6:F:35:ALA:HA    | 6:F:67:MET:HB3   | 1.84                     | 0.58              |
| 10:J:60:ARG:HB2  | 10:J:60:ARG:NH1  | 2.19                     | 0.58              |
| 1:A:1464:G:N2    | 1:A:1465:C:C2    | 2.72                     | 0.58              |
| 1:A:936:C:H2'    | 1:A:937:A:H8     | 1.69                     | 0.58              |
| 1:A:1118:C:H2'   | 1:A:1119:C:C6    | 2.39                     | 0.58              |
| 1:A:1172:C:H2'   | 1:A:1173:G:H8    | 1.68                     | 0.58              |
| 5:E:81:GLU:HA    | 5:E:89:ILE:O     | 2.04                     | 0.58              |
| 1:A:1369:C:H2'   | 1:A:1370:G:C8    | 2.40                     | 0.57              |
| 1:A:397:A:H3'    | 1:A:397:A:N3     | 2.18                     | 0.57              |
| 1:A:648:A:H2'    | 1:A:649:G:C8     | 2.39                     | 0.57              |
| 1:A:860:A:H3'    | 1:A:861:G:C8     | 2.39                     | 0.57              |
| 1:A:1059:C:H2'   | 1:A:1060:C:C6    | 2.39                     | 0.57              |
| 1:A:128:G:C2     | 1:A:234:C:C2     | 2.93                     | 0.57              |
| 1:A:1097:C:H2'   | 1:A:1098:C:C6    | 2.38                     | 0.57              |
| 11:K:15:ALA:HA   | 11:K:77:MET:HA   | 1.85                     | 0.57              |
| 1:A:689:C:H5''   | 11:K:27:ASN:ND2  | 2.20                     | 0.57              |
| 1:A:1118:C:H4'   | 9:I:83:ARG:HH22  | 1.69                     | 0.57              |
| 1:A:883:C:H2'    | 1:A:884:U:C6     | 2.38                     | 0.57              |
| 10:J:37:PRO:HB2  | 10:J:70:ARG:HH11 | 1.68                     | 0.57              |
| 22:W:21:THR:HG22 | 22:W:33:LEU:HG   | 1.86                     | 0.57              |
| 1:A:401:C:H2'    | 1:A:402:G:H8     | 1.68                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:540:G:H2'    | 1:A:541:G:C8     | 2.39                     | 0.57              |
| 1:A:1379:G:HO2'  | 7:G:156:TRP:CD1  | 2.23                     | 0.57              |
| 1:A:837:G:H8     | 1:A:837:G:O5'    | 1.88                     | 0.57              |
| 4:D:115:ARG:HB3  | 4:D:115:ARG:HH11 | 1.69                     | 0.57              |
| 1:A:549:C:H2'    | 1:A:550:G:H8     | 1.70                     | 0.57              |
| 1:A:681:C:C2     | 1:A:710:G:N2     | 2.72                     | 0.57              |
| 1:A:392:G:H2'    | 1:A:393:A:C8     | 2.40                     | 0.57              |
| 1:A:590:C:H42    | 1:A:649:G:H1     | 1.53                     | 0.57              |
| 1:A:864:A:C2     | 1:A:865:A:C2     | 2.92                     | 0.57              |
| 1:A:877:C:H2'    | 1:A:878:G:C8     | 2.40                     | 0.57              |
| 1:A:1081:G:H5'   | 5:E:18:ARG:HD3   | 1.85                     | 0.57              |
| 2:B:97:TRP:HZ2   | 2:B:102:LEU:HD13 | 1.70                     | 0.57              |
| 8:H:108:GLY:HA3  | 8:H:138:TRP:HB3  | 1.87                     | 0.57              |
| 14:N:41:ARG:NE   | 14:N:42:ILE:HG13 | 2.20                     | 0.57              |
| 1:A:78:G:H2'     | 1:A:79:G:O4'     | 2.05                     | 0.57              |
| 1:A:1132:C:H2'   | 1:A:1133:G:H8    | 1.69                     | 0.57              |
| 1:A:1225:A:H2'   | 1:A:1225:A:N3    | 2.20                     | 0.57              |
| 9:I:26:VAL:HG21  | 9:I:47:LEU:HD21  | 1.88                     | 0.56              |
| 1:A:585:G:H2'    | 1:A:586:C:O4'    | 2.04                     | 0.56              |
| 1:A:1409:C:H2'   | 1:A:1410:G:H8    | 1.70                     | 0.56              |
| 1:A:1409:C:H2'   | 1:A:1410:G:C8    | 2.40                     | 0.56              |
| 1:A:19:C:H2'     | 1:A:20:U:H6      | 1.69                     | 0.56              |
| 1:A:437:U:H3'    | 1:A:438:G:C8     | 2.40                     | 0.56              |
| 1:A:1114:C:C2    | 1:A:1187:G:C2    | 2.93                     | 0.56              |
| 1:A:1300:G:O2'   | 1:A:1303:C:N4    | 2.37                     | 0.56              |
| 5:E:83:GLU:HA    | 5:E:87:SER:O     | 2.04                     | 0.56              |
| 19:S:50:ALA:HB1  | 19:S:57:HIS:HB3  | 1.87                     | 0.56              |
| 22:W:22:PHE:HB2  | 22:W:67:ILE:HD11 | 1.87                     | 0.56              |
| 1:A:579:G:H2'    | 1:A:580:U:C6     | 2.41                     | 0.56              |
| 1:A:582:U:H2'    | 1:A:583:A:C8     | 2.39                     | 0.56              |
| 1:A:1104:G:H5''  | 1:A:1104:G:H8    | 1.70                     | 0.56              |
| 8:H:113:SER:HB2  | 8:H:134:ILE:HD11 | 1.86                     | 0.56              |
| 12:L:75:HIS:HD2  | 12:L:77:LEU:H    | 1.52                     | 0.56              |
| 1:A:184:G:H2'    | 1:A:185:A:H8     | 1.70                     | 0.56              |
| 1:A:1488:G:H2'   | 1:A:1489:G:H8    | 1.70                     | 0.56              |
| 22:W:32:ILE:H    | 22:W:32:ILE:CD1  | 2.18                     | 0.56              |
| 1:A:109:A:H2'    | 1:A:326:G:N2     | 2.21                     | 0.56              |
| 3:C:28:GLN:NE2   | 3:C:32:LEU:HD11  | 2.12                     | 0.56              |
| 3:C:66:VAL:HG12  | 3:C:68:VAL:CG2   | 2.35                     | 0.56              |
| 11:K:91:ARG:NH2  | 18:R:88:LYS:HZ2  | 1.95                     | 0.56              |
| 23:X:157:LEU:HB2 | 23:X:160:ASP:HB2 | 1.87                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:919:A:N3     | 1:A:1080:A:H2    | 2.03                     | 0.56              |
| 1:A:434:U:H2'    | 1:A:435:C:C6     | 2.41                     | 0.56              |
| 1:A:918:A:C2     | 1:A:1079:G:N2    | 2.74                     | 0.56              |
| 1:A:1121:U:H2'   | 1:A:1122:U:C6    | 2.41                     | 0.56              |
| 1:A:153:C:N4     | 1:A:154:C:N4     | 2.54                     | 0.56              |
| 1:A:967:C:H2'    | 1:A:968:A:C8     | 2.40                     | 0.56              |
| 1:A:1355:G:H2'   | 1:A:1356:G:C8    | 2.40                     | 0.56              |
| 2:B:88:ALA:HB2   | 2:B:219:VAL:HG13 | 1.86                     | 0.56              |
| 1:A:165:C:H2'    | 1:A:166:G:H8     | 1.70                     | 0.55              |
| 1:A:409:G:OP1    | 4:D:24:GLU:HB3   | 2.06                     | 0.55              |
| 1:A:671:G:C2     | 1:A:736:C:N3     | 2.74                     | 0.55              |
| 1:A:834:C:C2     | 1:A:853:G:C2     | 2.94                     | 0.55              |
| 1:A:1368:G:N2    | 1:A:1369:C:C2    | 2.74                     | 0.55              |
| 4:D:101:LEU:HB2  | 4:D:138:TYR:HB3  | 1.88                     | 0.55              |
| 5:E:106:PRO:HA   | 5:E:109:ILE:HD12 | 1.87                     | 0.55              |
| 10:J:20:ALA:CB   | 10:J:70:ARG:NE   | 2.69                     | 0.55              |
| 17:Q:56:VAL:HG13 | 17:Q:77:VAL:HB   | 1.87                     | 0.55              |
| 1:A:1121:U:H2'   | 1:A:1122:U:H6    | 1.71                     | 0.55              |
| 1:A:1244:C:H2'   | 1:A:1245:A:C8    | 2.40                     | 0.55              |
| 3:C:178:LEU:C    | 3:C:180:ALA:H    | 2.14                     | 0.55              |
| 1:A:877:C:H2'    | 1:A:878:G:H8     | 1.71                     | 0.55              |
| 1:A:1163:C:C2    | 1:A:1174:G:N2    | 2.75                     | 0.55              |
| 10:J:48:THR:O    | 10:J:60:ARG:HD3  | 2.05                     | 0.55              |
| 1:A:253:U:H2'    | 1:A:254:G:C8     | 2.41                     | 0.55              |
| 1:A:1071:C:H2'   | 1:A:1072:G:C8    | 2.40                     | 0.55              |
| 1:A:1106:G:N2    | 1:A:1107:C:C2    | 2.74                     | 0.55              |
| 1:A:1323:G:H2'   | 1:A:1324:A:C8    | 2.41                     | 0.55              |
| 3:C:57:ILE:CG1   | 3:C:66:VAL:CG2   | 2.54                     | 0.55              |
| 5:E:17:ALA:HA    | 5:E:26:PHE:HA    | 1.88                     | 0.55              |
| 5:E:20:GLN:O     | 5:E:21:ALA:C     | 2.49                     | 0.55              |
| 22:W:23:ARG:HH21 | 22:W:33:LEU:CB   | 2.18                     | 0.55              |
| 1:A:1346:A:C8    | 1:A:1348:U:C2    | 2.94                     | 0.55              |
| 3:C:30:ARG:HG2   | 14:N:37:PHE:CA   | 2.37                     | 0.55              |
| 1:A:80:G:H3'     | 1:A:81:U:C5'     | 2.26                     | 0.55              |
| 1:A:636:U:H5'    | 17:Q:2:PRO:HG3   | 1.88                     | 0.55              |
| 4:D:32:ALA:O     | 4:D:36:ARG:N     | 2.39                     | 0.55              |
| 8:H:120:THR:HG22 | 8:H:121:ASP:H    | 1.70                     | 0.55              |
| 14:N:24:CYS:CB   | 14:N:29:ARG:H    | 2.17                     | 0.55              |
| 22:W:14:THR:HB   | 22:W:23:ARG:HB3  | 1.89                     | 0.55              |
| 1:A:558:G:H3'    | 1:A:559:A:H5''   | 1.88                     | 0.55              |
| 3:C:29:TYR:OH    | 14:N:37:PHE:HE1  | 1.89                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:59:ARG:CZ    | 3:C:64:VAL:CG2   | 2.64                     | 0.55              |
| 1:A:318:G:N2     | 1:A:336:C:C2     | 2.75                     | 0.55              |
| 1:A:671:G:C2     | 1:A:736:C:C2     | 2.95                     | 0.55              |
| 1:A:939:G:C6     | 1:A:940:C:N4     | 2.75                     | 0.55              |
| 1:A:1511:G:H2'   | 1:A:1512:U:O4'   | 2.07                     | 0.55              |
| 1:A:920:U:C2     | 1:A:1080:A:C2    | 2.94                     | 0.55              |
| 1:A:927:G:O3'    | 1:A:928:G:P      | 2.65                     | 0.55              |
| 1:A:1025:U:H2'   | 1:A:1026:G:C8    | 2.42                     | 0.55              |
| 1:A:383:A:C5     | 1:A:384:G:H1'    | 2.42                     | 0.55              |
| 1:A:652:U:O4     | 1:A:752:G:O2'    | 2.25                     | 0.55              |
| 1:A:1233:G:C6    | 1:A:1234:C:N4    | 2.75                     | 0.55              |
| 9:I:40:LEU:CD2   | 9:I:74:ILE:HD11  | 2.37                     | 0.55              |
| 1:A:266:G:H5''   | 1:A:266:G:H8     | 1.70                     | 0.54              |
| 1:A:455:C:H2'    | 1:A:456:C:C6     | 2.42                     | 0.54              |
| 1:A:28:G:H2'     | 1:A:29:G:O4'     | 2.06                     | 0.54              |
| 1:A:229:U:H2'    | 1:A:230:G:H8     | 1.72                     | 0.54              |
| 1:A:279:A:N9     | 17:Q:98:LEU:CD2  | 2.67                     | 0.54              |
| 1:A:659:U:H2'    | 1:A:660:G:C8     | 2.42                     | 0.54              |
| 1:A:928:G:H2'    | 1:A:929:G:H8     | 1.72                     | 0.54              |
| 1:A:1512:U:H2'   | 1:A:1513:A:H8    | 1.71                     | 0.54              |
| 1:A:577:G:N2     | 1:A:578:C:C2     | 2.76                     | 0.54              |
| 1:A:1020:U:H2'   | 1:A:1021:G:C8    | 2.43                     | 0.54              |
| 1:A:1162:C:C2    | 1:A:1175:G:C2    | 2.96                     | 0.54              |
| 1:A:1256:A:H2'   | 3:C:27:LYS:HZ1   | 1.72                     | 0.54              |
| 6:F:27:GLN:HA    | 6:F:30:LEU:HD12  | 1.88                     | 0.54              |
| 1:A:761:G:C2     | 1:A:762:C:C2     | 2.95                     | 0.54              |
| 1:A:1135:U:H4'   | 1:A:1136:U:H5    | 1.71                     | 0.54              |
| 1:A:1342:C:H2'   | 1:A:1343:G:H8    | 1.71                     | 0.54              |
| 2:B:61:LEU:HD21  | 2:B:160:ASP:HB3  | 1.88                     | 0.54              |
| 13:M:34:LEU:HD13 | 13:M:41:PRO:HG3  | 1.90                     | 0.54              |
| 23:X:6:LEU:HB3   | 23:X:10:ARG:HB3  | 1.88                     | 0.54              |
| 1:A:333:G:N2     | 1:A:334:C:C2     | 2.75                     | 0.54              |
| 2:B:61:LEU:HD11  | 2:B:160:ASP:HB2  | 1.89                     | 0.54              |
| 4:D:24:GLU:HA    | 4:D:27:TYR:HB2   | 1.88                     | 0.54              |
| 4:D:156:GLU:HA   | 4:D:159:ARG:HD2  | 1.90                     | 0.54              |
| 11:K:87:THR:HG21 | 24:Y:29:G:H4'    | 1.89                     | 0.54              |
| 15:O:26:GLU:O    | 15:O:29:VAL:HG12 | 2.08                     | 0.54              |
| 1:A:101:A:H2'    | 1:A:102:G:C8     | 2.34                     | 0.54              |
| 1:A:223:U:H5'    | 20:T:68:LYS:NZ   | 2.23                     | 0.54              |
| 1:A:500:G:C6     | 1:A:501:C:N4     | 2.76                     | 0.54              |
| 1:A:836:G:H2'    | 1:A:837:G:C8     | 2.43                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 15:O:82:ILE:HA   | 15:O:87:ILE:HD12 | 1.90                     | 0.54              |
| 1:A:197:A:C6     | 1:A:221:C:H4'    | 2.43                     | 0.54              |
| 1:A:262:A:H5''   | 20:T:73:HIS:CE1  | 2.21                     | 0.54              |
| 1:A:568:G:C2     | 1:A:883:C:C2     | 2.95                     | 0.54              |
| 1:A:588:G:N1     | 1:A:589:C:C4     | 2.75                     | 0.54              |
| 1:A:756:C:H2'    | 1:A:757:U:O4'    | 2.07                     | 0.54              |
| 1:A:927:G:OP2    | 1:A:927:G:H4'    | 2.08                     | 0.54              |
| 2:B:17:PHE:HB2   | 2:B:41:ILE:HG12  | 1.89                     | 0.54              |
| 1:A:661:G:C2     | 1:A:745:C:N3     | 2.76                     | 0.54              |
| 1:A:669:U:H2'    | 1:A:670:G:C8     | 2.43                     | 0.54              |
| 1:A:936:C:H2'    | 1:A:937:A:C8     | 2.42                     | 0.54              |
| 1:A:1008:C:C2    | 1:A:1022:G:N2    | 2.76                     | 0.54              |
| 10:J:49:VAL:HG11 | 14:N:44:LEU:HD12 | 1.90                     | 0.54              |
| 20:T:49:ALA:HB3  | 20:T:99:LEU:HD12 | 1.89                     | 0.54              |
| 1:A:934:C:C5     | 1:A:1344:C:H2'   | 2.43                     | 0.54              |
| 1:A:972:C:O3'    | 10:J:57:LYS:HG3  | 2.07                     | 0.54              |
| 1:A:1077:G:N3    | 1:A:1079:G:C8    | 2.75                     | 0.54              |
| 23:X:58:ARG:HD2  | 23:X:60:MET:HE2  | 1.89                     | 0.54              |
| 1:A:166:G:H2'    | 1:A:167:G:C8     | 2.43                     | 0.54              |
| 1:A:730:G:N2     | 1:A:765:G:H5''   | 2.23                     | 0.54              |
| 1:A:1098:C:H1'   | 1:A:1168:A:C2    | 2.43                     | 0.54              |
| 3:C:57:ILE:CD1   | 3:C:66:VAL:CG2   | 2.85                     | 0.54              |
| 10:J:6:ILE:HG13  | 10:J:72:VAL:O    | 2.08                     | 0.54              |
| 12:L:33:ARG:HD3  | 12:L:62:SER:HB3  | 1.89                     | 0.54              |
| 1:A:184:G:H2'    | 1:A:185:A:C8     | 2.42                     | 0.53              |
| 1:A:279:A:C4     | 17:Q:98:LEU:HD22 | 2.31                     | 0.53              |
| 1:A:919:A:N3     | 1:A:1080:A:C2    | 2.76                     | 0.53              |
| 3:C:30:ARG:CB    | 3:C:30:ARG:CZ    | 2.86                     | 0.53              |
| 5:E:127:ASN:ND2  | 5:E:129:ILE:H    | 2.06                     | 0.53              |
| 1:A:790:A:O2'    | 23:X:87:SER:O    | 2.25                     | 0.53              |
| 1:A:994:A:N7     | 1:A:1216:G:H4'   | 2.24                     | 0.53              |
| 1:A:1513:A:H2'   | 1:A:1514:C:C6    | 2.43                     | 0.53              |
| 8:H:12:ARG:NH1   | 8:H:25:ASP:O     | 2.41                     | 0.53              |
| 11:K:84:VAL:CG2  | 11:K:91:ARG:NH2  | 2.71                     | 0.53              |
| 1:A:504:C:C2     | 1:A:542:G:N2     | 2.76                     | 0.53              |
| 1:A:589:C:O2     | 1:A:651:C:O2     | 2.26                     | 0.53              |
| 1:A:872:A:C8     | 1:A:874:G:C8     | 2.96                     | 0.53              |
| 4:D:43:HIS:HB3   | 4:D:46:LYS:HD2   | 1.90                     | 0.53              |
| 17:Q:93:GLN:C    | 17:Q:93:GLN:HE21 | 2.15                     | 0.53              |
| 1:A:114:U:H2'    | 1:A:115:G:C8     | 2.43                     | 0.53              |
| 1:A:229:U:H2'    | 1:A:230:G:C8     | 2.44                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:289:G:N2     | 1:A:290:C:C2     | 2.76                     | 0.53              |
| 1:A:1118:C:H2'   | 1:A:1119:C:H6    | 1.73                     | 0.53              |
| 1:A:1526:G:H2'   | 1:A:1527:C:C6    | 2.43                     | 0.53              |
| 19:S:30:LEU:HD23 | 19:S:50:ALA:HB2  | 1.89                     | 0.53              |
| 1:A:152:A:OP2    | 1:A:153:C:N4     | 2.42                     | 0.53              |
| 1:A:939:G:H2'    | 1:A:940:C:C6     | 2.44                     | 0.53              |
| 1:A:1048:G:H2'   | 1:A:1050:G:H8    | 1.73                     | 0.53              |
| 1:A:35:G:H2'     | 1:A:36:C:C6      | 2.43                     | 0.53              |
| 1:A:44:G:H3'     | 1:A:45:U:C6      | 2.44                     | 0.53              |
| 1:A:509:A:H5'    | 4:D:55:ALA:HB2   | 1.89                     | 0.53              |
| 1:A:576:G:H3'    | 1:A:577:G:C5'    | 2.38                     | 0.53              |
| 3:C:77:ILE:HA    | 3:C:84:ILE:HB    | 1.91                     | 0.53              |
| 1:A:980:C:H1'    | 14:N:19:ARG:HG2  | 1.90                     | 0.53              |
| 1:A:61:G:H2'     | 1:A:62:U:O4'     | 2.08                     | 0.53              |
| 1:A:351:G:H4'    | 1:A:352:C:OP1    | 2.08                     | 0.53              |
| 1:A:669:U:H2'    | 1:A:670:G:H8     | 1.74                     | 0.53              |
| 1:A:1338:G:H2'   | 1:A:1339:A:C8    | 2.44                     | 0.53              |
| 1:A:1348:U:H2'   | 1:A:1349:A:C8    | 2.41                     | 0.53              |
| 1:A:1464:G:N1    | 1:A:1465:C:C4    | 2.77                     | 0.53              |
| 22:W:21:THR:HG21 | 22:W:33:LEU:CG   | 2.37                     | 0.53              |
| 1:A:735:C:H5'    | 18:R:71:LYS:HD3  | 1.91                     | 0.53              |
| 1:A:1088:G:H2'   | 1:A:1089:G:O4'   | 2.09                     | 0.53              |
| 10:J:48:THR:CG2  | 10:J:60:ARG:HG2  | 2.27                     | 0.53              |
| 1:A:316:G:H1     | 1:A:337:C:N4     | 2.05                     | 0.52              |
| 1:A:439:A:C4     | 1:A:496:A:C2     | 2.96                     | 0.52              |
| 1:A:621:A:H2'    | 1:A:622:A:C8     | 2.44                     | 0.52              |
| 1:A:1078:U:O2'   | 1:A:1079:G:O4'   | 2.27                     | 0.52              |
| 1:A:22:G:C6      | 1:A:23:C:C4      | 2.96                     | 0.52              |
| 1:A:598:U:H2'    | 1:A:599:C:C6     | 2.44                     | 0.52              |
| 1:A:1321:C:H5'   | 13:M:87:TYR:CE1  | 2.45                     | 0.52              |
| 4:D:62:GLN:OE1   | 4:D:62:GLN:HA    | 2.09                     | 0.52              |
| 5:E:110:LEU:HD13 | 5:E:118:ILE:HG13 | 1.89                     | 0.52              |
| 10:J:17:ASP:HA   | 10:J:70:ARG:NH2  | 2.24                     | 0.52              |
| 1:A:399:G:C6     | 1:A:400:C:N4     | 2.77                     | 0.52              |
| 1:A:505:G:H2'    | 1:A:506:G:H8     | 1.73                     | 0.52              |
| 1:A:643:C:H2'    | 1:A:644:G:C8     | 2.43                     | 0.52              |
| 1:A:1502:A:H2'   | 1:A:1504:G:C8    | 2.44                     | 0.52              |
| 2:B:142:LEU:HD23 | 2:B:146:GLN:HE22 | 1.74                     | 0.52              |
| 3:C:30:ARG:HB2   | 3:C:30:ARG:CZ    | 2.37                     | 0.52              |
| 1:A:71:C:H2'     | 1:A:72:C:O4'     | 2.10                     | 0.52              |
| 1:A:122:G:N1     | 1:A:123:C:C2     | 2.77                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:598:U:H2'    | 1:A:599:C:H6     | 1.74                     | 0.52              |
| 1:A:1151:A:O2'   | 1:A:1152:A:H8    | 1.92                     | 0.52              |
| 1:A:1291:G:O3'   | 9:I:39:GLY:HA3   | 2.09                     | 0.52              |
| 1:A:1400:C:N3    | 24:Y:38:G:O6     | 2.41                     | 0.52              |
| 1:A:189:G:C2     | 1:A:189(A):C:C2  | 2.98                     | 0.52              |
| 1:A:332:G:C2     | 1:A:333:G:C8     | 2.98                     | 0.52              |
| 1:A:761:G:C6     | 1:A:762:C:C4     | 2.98                     | 0.52              |
| 1:A:779:C:H2'    | 1:A:780:A:O4'    | 2.09                     | 0.52              |
| 1:A:832:C:C2     | 1:A:855:G:C2     | 2.97                     | 0.52              |
| 1:A:872:A:C4     | 1:A:874:G:N7     | 2.77                     | 0.52              |
| 8:H:91:ARG:O     | 8:H:91:ARG:HG3   | 2.08                     | 0.52              |
| 8:H:111:ILE:HG22 | 8:H:134:ILE:HD12 | 1.91                     | 0.52              |
| 1:A:109:A:H5'    | 1:A:110:C:C5     | 2.44                     | 0.52              |
| 1:A:1163:C:N3    | 1:A:1174:G:C2    | 2.78                     | 0.52              |
| 3:C:174:PRO:HB2  | 3:C:177:THR:HG23 | 1.91                     | 0.52              |
| 10:J:17:ASP:CB   | 10:J:70:ARG:NH2  | 2.73                     | 0.52              |
| 1:A:60:A:H4'     | 1:A:61:G:O5'     | 2.10                     | 0.52              |
| 1:A:122:G:C2     | 1:A:123:C:C2     | 2.97                     | 0.52              |
| 1:A:1077:G:N2    | 1:A:1079:G:C3'   | 2.59                     | 0.52              |
| 1:A:1106:G:C6    | 1:A:1107:C:N4    | 2.78                     | 0.52              |
| 1:A:1127:G:H21   | 1:A:1147:C:N4    | 2.02                     | 0.52              |
| 1:A:1217:C:N4    | 1:A:1218:C:N4    | 2.57                     | 0.52              |
| 4:D:200:GLU:OE1  | 4:D:201:GLN:HG3  | 2.09                     | 0.52              |
| 1:A:504:C:N3     | 1:A:542:G:C2     | 2.78                     | 0.52              |
| 1:A:643:C:H2'    | 1:A:644:G:H8     | 1.75                     | 0.52              |
| 1:A:926:G:H3'    | 1:A:1505:G:H21   | 1.74                     | 0.52              |
| 1:A:1030:C:H42   | 1:A:1031:G:H1    | 1.55                     | 0.52              |
| 1:A:1518:A:H2'   | 1:A:1519:A:C8    | 2.44                     | 0.52              |
| 4:D:98:GLU:HA    | 4:D:103:ASN:ND2  | 2.25                     | 0.52              |
| 1:A:99:U:H2'     | 1:A:100:C:C6     | 2.44                     | 0.52              |
| 1:A:360:A:H2'    | 1:A:361:G:O4'    | 2.09                     | 0.52              |
| 1:A:667:G:H2'    | 1:A:668:G:H8     | 1.74                     | 0.52              |
| 1:A:834:C:O2     | 1:A:853:G:C2     | 2.63                     | 0.52              |
| 1:A:1488:G:H2'   | 1:A:1489:G:C8    | 2.44                     | 0.52              |
| 1:A:505:G:H5'    | 1:A:534:U:H2'    | 1.92                     | 0.52              |
| 1:A:955:U:H1'    | 1:A:1227:A:N6    | 2.24                     | 0.52              |
| 1:A:1010:G:H1    | 1:A:1019:C:H42   | 1.57                     | 0.52              |
| 1:A:1068:G:N2    | 1:A:1069:C:C2    | 2.78                     | 0.52              |
| 4:D:36:ARG:HG3   | 4:D:38:TYR:CD2   | 2.44                     | 0.52              |
| 15:O:62:GLN:HA   | 15:O:65:ARG:HH11 | 1.75                     | 0.52              |
| 16:P:1:MET:HE2   | 16:P:3:LYS:HE2   | 1.92                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:558:G:H3'    | 1:A:559:A:C5'    | 2.40                     | 0.51              |
| 1:A:1048:G:H2'   | 1:A:1050:G:C8    | 2.45                     | 0.51              |
| 1:A:1223:C:H5''  | 1:A:1224:G:H5''  | 1.92                     | 0.51              |
| 4:D:42:GLN:C     | 4:D:44:GLY:H     | 2.18                     | 0.51              |
| 1:A:1007:C:H42   | 1:A:1022:G:H1    | 1.57                     | 0.51              |
| 24:Y:27:G:H2'    | 24:Y:28:A:O4'    | 2.10                     | 0.51              |
| 1:A:44:G:H3'     | 1:A:45:U:H6      | 1.75                     | 0.51              |
| 1:A:230:G:H2'    | 1:A:231:G:O4'    | 2.10                     | 0.51              |
| 1:A:766:A:H2'    | 1:A:767:A:O4'    | 2.11                     | 0.51              |
| 1:A:1014:A:H5''  | 19:S:14:HIS:HB3  | 1.92                     | 0.51              |
| 1:A:1379:G:HO2'  | 7:G:156:TRP:HD1  | 1.57                     | 0.51              |
| 15:O:54:ARG:HH21 | 15:O:58:MET:HG3  | 1.74                     | 0.51              |
| 1:A:755:G:N2     | 1:A:756:C:C2     | 2.79                     | 0.51              |
| 11:K:21:ILE:HB   | 11:K:84:VAL:HG12 | 1.91                     | 0.51              |
| 22:W:10:GLU:HG2  | 22:W:54:VAL:HG22 | 1.92                     | 0.51              |
| 1:A:258:G:N2     | 1:A:269:C:C2     | 2.78                     | 0.51              |
| 1:A:1148:U:H5''  | 9:I:7:THR:HG21   | 1.91                     | 0.51              |
| 1:A:1376:U:H5'   | 7:G:102:ARG:HH22 | 1.76                     | 0.51              |
| 1:A:1434:A:H3'   | 1:A:1435:G:C8    | 2.46                     | 0.51              |
| 8:H:18:ARG:HH12  | 8:H:78:GLN:HG3   | 1.76                     | 0.51              |
| 1:A:92:C:H2'     | 1:A:93:G:H8      | 1.76                     | 0.51              |
| 1:A:262:A:H4'    | 20:T:73:HIS:HE1  | 1.66                     | 0.51              |
| 1:A:737:A:H2'    | 1:A:738:C:C6     | 2.45                     | 0.51              |
| 1:A:881:G:OP2    | 12:L:12:ARG:NH2  | 2.41                     | 0.51              |
| 1:A:1081:G:OP2   | 5:E:16:THR:CG2   | 2.58                     | 0.51              |
| 3:C:120:VAL:HB   | 3:C:198:VAL:HG11 | 1.92                     | 0.51              |
| 12:L:41:ARG:HH12 | 12:L:57:LYS:HG3  | 1.74                     | 0.51              |
| 16:P:33:ILE:HG22 | 16:P:34:GLU:HB2  | 1.92                     | 0.51              |
| 1:A:827:U:O2'    | 8:H:19:VAL:HG11  | 2.11                     | 0.51              |
| 1:A:1359:C:H3'   | 14:N:35:ARG:HH21 | 1.76                     | 0.51              |
| 13:M:2:ALA:O     | 13:M:9:ILE:HA    | 2.10                     | 0.51              |
| 1:A:437:U:H3'    | 1:A:438:G:H8     | 1.76                     | 0.51              |
| 1:A:824:C:H2'    | 1:A:825:G:H8     | 1.76                     | 0.51              |
| 1:A:1226:C:H3'   | 13:M:96:LEU:HD21 | 1.92                     | 0.51              |
| 1:A:1312:G:C2    | 1:A:1326:C:C2    | 2.98                     | 0.51              |
| 1:A:1379:G:O2'   | 7:G:156:TRP:HD1  | 1.94                     | 0.51              |
| 4:D:35:ARG:CB    | 4:D:35:ARG:NH2   | 2.73                     | 0.51              |
| 6:F:45:LEU:HG    | 6:F:59:TYR:HD2   | 1.75                     | 0.51              |
| 10:J:44:VAL:HG13 | 10:J:66:ARG:HB3  | 1.93                     | 0.51              |
| 16:P:5:ARG:HH21  | 16:P:28:ARG:HA   | 1.75                     | 0.51              |
| 16:P:48:TRP:H    | 16:P:48:TRP:HD1  | 1.57                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 17:Q:19:VAL:HG23 | 17:Q:44:ALA:HB3  | 1.91                     | 0.51              |
| 1:A:98:G:H2'     | 1:A:99:U:C6      | 2.46                     | 0.51              |
| 1:A:694:A:H5'    | 11:K:53:SER:HB2  | 1.93                     | 0.51              |
| 1:A:914:A:C4     | 1:A:915:A:N7     | 2.78                     | 0.51              |
| 1:A:919:A:C2     | 1:A:1080:A:C2    | 2.92                     | 0.51              |
| 1:A:1086:U:O5'   | 1:A:1086:U:H6    | 1.93                     | 0.51              |
| 1:A:1466:C:H2'   | 1:A:1467:G:O4'   | 2.10                     | 0.51              |
| 5:E:50:GLU:HB2   | 5:E:53:LEU:HB3   | 1.92                     | 0.51              |
| 8:H:28:ALA:HA    | 8:H:59:LEU:HD12  | 1.93                     | 0.51              |
| 1:A:35:G:C6      | 1:A:36:C:N4      | 2.79                     | 0.51              |
| 1:A:77:G:C8      | 1:A:77:G:C3'     | 2.93                     | 0.51              |
| 1:A:122:G:C6     | 1:A:123:C:C4     | 2.99                     | 0.51              |
| 1:A:663:A:H2'    | 1:A:664:G:O4'    | 2.11                     | 0.51              |
| 1:A:1281:U:H4'   | 1:A:1282:C:OP2   | 2.10                     | 0.51              |
| 2:B:124:SER:O    | 2:B:127:ILE:HG13 | 2.11                     | 0.51              |
| 2:B:163:PHE:HA   | 2:B:185:ILE:HB   | 1.93                     | 0.51              |
| 7:G:27:ILE:HA    | 7:G:30:ILE:HD12  | 1.93                     | 0.51              |
| 1:A:251:G:C2     | 1:A:266:G:C6     | 3.00                     | 0.50              |
| 1:A:270:A:H2'    | 1:A:271:C:C6     | 2.46                     | 0.50              |
| 1:A:827:U:N3     | 1:A:872:A:C6     | 2.67                     | 0.50              |
| 1:A:1055:A:H2    | 3:C:194:GLY:CA   | 2.24                     | 0.50              |
| 1:A:1348:U:OP1   | 9:I:110:GLU:N    | 2.31                     | 0.50              |
| 6:F:78:GLU:HA    | 6:F:81:ILE:HD12  | 1.92                     | 0.50              |
| 7:G:16:LEU:HD22  | 9:I:45:ALA:HB2   | 1.92                     | 0.50              |
| 1:A:198:G:H2'    | 1:A:199:G:C8     | 2.46                     | 0.50              |
| 1:A:769:G:H4'    | 1:A:1513:A:H4'   | 1.93                     | 0.50              |
| 1:A:1048:G:N2    | 1:A:1210:C:C2    | 2.79                     | 0.50              |
| 1:A:79:G:H2'     | 1:A:80:G:H8      | 1.75                     | 0.50              |
| 1:A:661:G:N2     | 1:A:745:C:C2     | 2.79                     | 0.50              |
| 1:A:1070:U:H2'   | 1:A:1071:C:C5    | 2.43                     | 0.50              |
| 1:A:1103:C:OP1   | 2:B:98:LEU:HD22  | 2.12                     | 0.50              |
| 1:A:1323:G:H2'   | 1:A:1324:A:O4'   | 2.11                     | 0.50              |
| 1:A:1366:C:H2'   | 1:A:1367:C:C6    | 2.46                     | 0.50              |
| 1:A:1399:C:C2    | 1:A:1502:A:N6    | 2.79                     | 0.50              |
| 6:F:45:LEU:HG    | 6:F:59:TYR:CD2   | 2.46                     | 0.50              |
| 6:F:100:ASN:HA   | 18:R:23:LYS:HE2  | 1.93                     | 0.50              |
| 14:N:24:CYS:HB3  | 14:N:29:ARG:N    | 2.19                     | 0.50              |
| 1:A:557:G:C6     | 1:A:558:G:C2     | 2.99                     | 0.50              |
| 1:A:731:G:N2     | 1:A:732:C:C2     | 2.79                     | 0.50              |
| 1:A:1243:C:C2    | 1:A:1295:G:N2    | 2.80                     | 0.50              |
| 4:D:24:GLU:O     | 4:D:25:ARG:HB3   | 2.12                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 9:I:26:VAL:HG22   | 9:I:61:ALA:HB3   | 1.92                     | 0.50              |
| 15:O:41:GLU:O     | 15:O:44:LYS:HB2  | 2.11                     | 0.50              |
| 22:W:33:LEU:HD22  | 22:W:64:ARG:NH1  | 2.24                     | 0.50              |
| 1:A:714:G:H2'     | 1:A:715:A:C8     | 2.47                     | 0.50              |
| 1:A:774:G:N2      | 1:A:806:C:C2     | 2.80                     | 0.50              |
| 1:A:824:C:H2'     | 1:A:825:G:C8     | 2.47                     | 0.50              |
| 1:A:932:C:H5'     | 7:G:3:ARG:CB     | 2.42                     | 0.50              |
| 1:A:13:U:C4       | 1:A:915:A:N6     | 2.79                     | 0.50              |
| 1:A:90:U:H2'      | 1:A:91:C:H6      | 1.71                     | 0.50              |
| 1:A:572:A:N1      | 1:A:864:A:C5     | 2.80                     | 0.50              |
| 1:A:613:C:H2'     | 1:A:614:A:H8     | 1.77                     | 0.50              |
| 1:A:916:G:C2      | 1:A:917:G:C5     | 2.99                     | 0.50              |
| 1:A:946:A:H2'     | 1:A:947:G:H8     | 1.75                     | 0.50              |
| 1:A:1525:G:H2'    | 1:A:1526:G:H8    | 1.76                     | 0.50              |
| 1:A:30:U:H3'      | 1:A:31:G:H5''    | 1.93                     | 0.50              |
| 1:A:354:G:N2      | 1:A:355:C:C2     | 2.79                     | 0.50              |
| 1:A:525:C:H2'     | 1:A:526:C:C6     | 2.46                     | 0.50              |
| 1:A:864:A:C2'     | 1:A:865:A:C8     | 2.83                     | 0.50              |
| 12:L:113:ARG:HH11 | 12:L:113:ARG:HB3 | 1.75                     | 0.50              |
| 1:A:590:C:N4      | 1:A:649:G:H1     | 2.10                     | 0.50              |
| 1:A:987:G:O5'     | 1:A:987:G:H8     | 1.95                     | 0.50              |
| 1:A:1018:C:H2'    | 1:A:1019:C:C6    | 2.47                     | 0.50              |
| 1:A:1059:C:H2'    | 1:A:1060:C:H6    | 1.76                     | 0.50              |
| 1:A:1356:G:C2     | 1:A:1367:C:C2    | 3.00                     | 0.50              |
| 20:T:54:LYS:HA    | 20:T:57:ARG:HH11 | 1.77                     | 0.50              |
| 23:X:5:TYR:CE2    | 23:X:65:TRP:CH2  | 2.96                     | 0.50              |
| 1:A:22:G:C2       | 1:A:23:C:C2      | 3.00                     | 0.50              |
| 1:A:681:C:N3      | 1:A:710:G:C2     | 2.79                     | 0.50              |
| 1:A:827:U:C4      | 1:A:872:A:N1     | 2.79                     | 0.49              |
| 1:A:920:U:C2'     | 1:A:921:U:C6     | 2.83                     | 0.49              |
| 4:D:57:ARG:NE     | 5:E:107:ARG:HE   | 2.10                     | 0.49              |
| 4:D:133:VAL:HG11  | 4:D:138:TYR:HD2  | 1.77                     | 0.49              |
| 22:W:32:ILE:CD1   | 22:W:32:ILE:N    | 2.73                     | 0.49              |
| 1:A:500:G:H2'     | 1:A:501:C:C6     | 2.47                     | 0.49              |
| 1:A:501:C:H2'     | 1:A:502:G:H8     | 1.77                     | 0.49              |
| 1:A:518:C:O2'     | 1:A:519:C:OP2    | 2.28                     | 0.49              |
| 1:A:717:C:H2'     | 1:A:734:G:H5'    | 1.93                     | 0.49              |
| 1:A:876:G:C6      | 1:A:877:C:N4     | 2.79                     | 0.49              |
| 1:A:1365:G:C2     | 1:A:1366:C:C2    | 3.00                     | 0.49              |
| 1:A:1459:C:H2'    | 1:A:1460:A:O4'   | 2.12                     | 0.49              |
| 17:Q:18:THR:HG23  | 17:Q:69:LYS:HE3  | 1.93                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 19:S:22:LEU:CD1  | 19:S:31:ILE:HD11 | 2.43                     | 0.49              |
| 23:X:71:MET:O    | 23:X:75:GLU:HG2  | 2.11                     | 0.49              |
| 1:A:130:A:H8     | 1:A:130:A:OP1    | 1.94                     | 0.49              |
| 1:A:500:G:C2     | 1:A:501:C:N3     | 2.80                     | 0.49              |
| 1:A:562:C:H2'    | 1:A:562:C:OP2    | 2.12                     | 0.49              |
| 1:A:648:A:H2'    | 1:A:649:G:H8     | 1.76                     | 0.49              |
| 1:A:1007:C:O2    | 1:A:1023:G:C2    | 2.65                     | 0.49              |
| 1:A:1393:U:H2'   | 1:A:1395:C:C5    | 2.46                     | 0.49              |
| 2:B:61:LEU:HD11  | 2:B:160:ASP:CB   | 2.42                     | 0.49              |
| 1:A:861:G:N2     | 1:A:862:C:C2     | 2.81                     | 0.49              |
| 1:A:1135:U:H4'   | 1:A:1136:U:C5    | 2.47                     | 0.49              |
| 1:A:366:C:H1'    | 1:A:394:G:H22    | 1.78                     | 0.49              |
| 1:A:725:G:N1     | 1:A:726:C:C4     | 2.81                     | 0.49              |
| 1:A:1023:G:H2'   | 1:A:1023:G:N3    | 2.28                     | 0.49              |
| 4:D:133:VAL:HG11 | 4:D:138:TYR:CD2  | 2.46                     | 0.49              |
| 1:A:92:C:H2'     | 1:A:93:G:C8      | 2.47                     | 0.49              |
| 1:A:1014:A:C5'   | 19:S:14:HIS:HB3  | 2.42                     | 0.49              |
| 1:A:1148:U:O3'   | 9:I:14:VAL:HG11  | 2.13                     | 0.49              |
| 1:A:1354:C:H42   | 1:A:1368:G:H1    | 1.60                     | 0.49              |
| 4:D:19:LEU:HB3   | 4:D:21:LEU:HB2   | 1.93                     | 0.49              |
| 4:D:149:ALA:HB3  | 4:D:152:SER:HB2  | 1.95                     | 0.49              |
| 5:E:82:VAL:O     | 5:E:89:ILE:HG22  | 2.12                     | 0.49              |
| 1:A:548:G:C6     | 1:A:549:C:N4     | 2.80                     | 0.49              |
| 1:A:585:G:C2     | 1:A:586:C:C2     | 3.00                     | 0.49              |
| 1:A:590:C:OP1    | 8:H:30:ARG:N     | 2.45                     | 0.49              |
| 1:A:623:C:H2'    | 1:A:624:C:O4'    | 2.13                     | 0.49              |
| 1:A:1127:G:N2    | 1:A:1145:C:C2    | 2.81                     | 0.49              |
| 1:A:1436:U:H2'   | 1:A:1437:C:O4'   | 2.12                     | 0.49              |
| 11:K:24:SER:C    | 11:K:26:ASN:H    | 2.20                     | 0.49              |
| 11:K:91:ARG:NH2  | 18:R:88:LYS:NZ   | 2.55                     | 0.49              |
| 1:A:358:U:H2'    | 1:A:359:U:O4'    | 2.12                     | 0.49              |
| 1:A:1082:G:H2'   | 1:A:1083:U:O4'   | 2.13                     | 0.49              |
| 9:I:40:LEU:HD21  | 9:I:74:ILE:HD11  | 1.95                     | 0.49              |
| 1:A:233:C:H2'    | 1:A:234:C:H6     | 1.76                     | 0.49              |
| 1:A:505:G:H2'    | 1:A:506:G:C8     | 2.47                     | 0.49              |
| 1:A:549:C:H2'    | 1:A:550:G:C8     | 2.48                     | 0.49              |
| 4:D:3:ARG:HA     | 4:D:3:ARG:CZ     | 2.43                     | 0.49              |
| 18:R:26:LEU:HD21 | 18:R:39:VAL:HG22 | 1.95                     | 0.49              |
| 1:A:582:U:H2'    | 1:A:583:A:H8     | 1.78                     | 0.49              |
| 1:A:1106:G:C2    | 1:A:1107:C:C4    | 3.01                     | 0.49              |
| 1:A:17:U:O2      | 1:A:1079:G:N3    | 2.46                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:21:G:C2      | 1:A:22:G:C5      | 3.01                     | 0.48              |
| 1:A:236:G:C2     | 1:A:237:C:C2     | 3.01                     | 0.48              |
| 18:R:53:ARG:HE   | 18:R:60:ALA:HA   | 1.78                     | 0.48              |
| 1:A:46:G:H2'     | 1:A:366:C:H5     | 1.76                     | 0.48              |
| 1:A:148:G:C2     | 1:A:175:C:C2     | 3.02                     | 0.48              |
| 1:A:590:C:OP1    | 8:H:30:ARG:HG2   | 2.12                     | 0.48              |
| 3:C:174:PRO:HD2  | 3:C:182:ILE:HD11 | 1.95                     | 0.48              |
| 11:K:84:VAL:HG23 | 11:K:91:ARG:HH22 | 1.78                     | 0.48              |
| 18:R:31:LEU:O    | 18:R:69:THR:HG21 | 2.11                     | 0.48              |
| 1:A:216:G:C6     | 1:A:217:C:N4     | 2.81                     | 0.48              |
| 1:A:259:G:H2'    | 1:A:260:G:H8     | 1.74                     | 0.48              |
| 1:A:370:C:N3     | 1:A:392:G:C2     | 2.81                     | 0.48              |
| 1:A:557:G:N1     | 1:A:558:G:C2     | 2.81                     | 0.48              |
| 1:A:707:C:H2'    | 1:A:708:C:C6     | 2.48                     | 0.48              |
| 1:A:1074:G:H4'   | 2:B:103:THR:O    | 2.12                     | 0.48              |
| 1:A:1365:G:C6    | 1:A:1366:C:C4    | 3.01                     | 0.48              |
| 4:D:61:LYS:HD3   | 4:D:206:PHE:CE2  | 2.48                     | 0.48              |
| 5:E:41:VAL:HG13  | 5:E:113:ALA:HA   | 1.95                     | 0.48              |
| 1:A:29:G:H5''    | 1:A:30:U:OP2     | 2.13                     | 0.48              |
| 1:A:189:G:C6     | 1:A:189(A):C:C4  | 3.01                     | 0.48              |
| 1:A:407:G:H2'    | 1:A:408:A:H8     | 1.78                     | 0.48              |
| 1:A:823:G:H2'    | 1:A:824:C:C6     | 2.47                     | 0.48              |
| 1:A:972:C:O2     | 1:A:972:C:H2'    | 2.12                     | 0.48              |
| 1:A:998:G:N2     | 1:A:999:C:C2     | 2.80                     | 0.48              |
| 1:A:295:C:H2'    | 1:A:296:U:O4'    | 2.13                     | 0.48              |
| 1:A:1308:U:H2'   | 1:A:1309:G:C8    | 2.49                     | 0.48              |
| 5:E:80:ILE:HD13  | 5:E:138:ALA:HB1  | 1.95                     | 0.48              |
| 9:I:17:VAL:HG22  | 9:I:63:ILE:HG12  | 1.96                     | 0.48              |
| 10:J:37:PRO:C    | 10:J:72:VAL:HG22 | 2.38                     | 0.48              |
| 1:A:876:G:H2'    | 1:A:877:C:C6     | 2.49                     | 0.48              |
| 1:A:1148:U:C5'   | 9:I:7:THR:HG21   | 2.43                     | 0.48              |
| 2:B:118:LEU:HB3  | 2:B:142:LEU:HD11 | 1.95                     | 0.48              |
| 2:B:166:ASP:C    | 2:B:168:THR:H    | 2.21                     | 0.48              |
| 9:I:47:LEU:HD22  | 9:I:50:LEU:HD12  | 1.96                     | 0.48              |
| 1:A:37:U:O2'     | 1:A:500:G:H4'    | 2.12                     | 0.48              |
| 1:A:165:C:H2'    | 1:A:166:G:C8     | 2.48                     | 0.48              |
| 1:A:734:G:C2     | 1:A:735:C:C2     | 3.01                     | 0.48              |
| 1:A:881:G:C2     | 1:A:882:C:C2     | 3.02                     | 0.48              |
| 1:A:1130:A:H4'   | 9:I:3:GLN:OE1    | 2.13                     | 0.48              |
| 1:A:1218:C:H2'   | 1:A:1219:U:C6    | 2.48                     | 0.48              |
| 17:Q:64:PRO:HB3  | 17:Q:70:ARG:HG3  | 1.96                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:176:C:H2'    | 1:A:177:C:C6     | 2.48                     | 0.48              |
| 1:A:675:A:N3     | 11:K:116:HIS:HB2 | 2.29                     | 0.48              |
| 1:A:1149:C:H2'   | 1:A:1150:U:C6    | 2.49                     | 0.48              |
| 1:A:1256:A:C2'   | 3:C:27:LYS:NZ    | 2.77                     | 0.48              |
| 1:A:1267:C:H2'   | 1:A:1268:A:O4'   | 2.14                     | 0.48              |
| 1:A:1353:G:N1    | 1:A:1354:C:C4    | 2.81                     | 0.48              |
| 8:H:39:LEU:HG    | 8:H:44:PHE:HB2   | 1.95                     | 0.48              |
| 14:N:7:ILE:O     | 14:N:7:ILE:HG22  | 2.14                     | 0.48              |
| 20:T:63:ILE:HG21 | 20:T:81:LYS:HG3  | 1.96                     | 0.48              |
| 23:X:123:ARG:HB2 | 24:Y:38:G:H4'    | 1.94                     | 0.48              |
| 1:A:15:G:C4      | 1:A:16:A:N7      | 2.82                     | 0.48              |
| 1:A:153:C:N4     | 1:A:154:C:H41    | 2.12                     | 0.48              |
| 1:A:362:G:N2     | 1:A:364:A:H3'    | 2.28                     | 0.48              |
| 1:A:945:G:H2'    | 1:A:945:G:N3     | 2.29                     | 0.48              |
| 1:A:1312:G:N2    | 1:A:1326:C:C2    | 2.82                     | 0.48              |
| 4:D:39:PRO:HB2   | 4:D:44:GLY:HA2   | 1.95                     | 0.48              |
| 1:A:39:G:N7      | 1:A:547:A:H2'    | 2.29                     | 0.48              |
| 1:A:218:C:H2'    | 1:A:219:C:C6     | 2.49                     | 0.48              |
| 1:A:962:C:H1'    | 1:A:1201:A:N6    | 2.28                     | 0.48              |
| 1:A:974:A:H8     | 1:A:974:A:OP1    | 1.97                     | 0.48              |
| 1:A:985:C:C2     | 1:A:1221:G:N2    | 2.82                     | 0.48              |
| 2:B:72:GLY:HA2   | 2:B:165:VAL:HB   | 1.96                     | 0.48              |
| 4:D:68:TYR:HB2   | 4:D:70:ILE:HD11  | 1.96                     | 0.48              |
| 8:H:55:GLY:O     | 8:H:56:LYS:HG3   | 2.14                     | 0.48              |
| 14:N:12:ARG:O    | 14:N:14:PRO:HD3  | 2.14                     | 0.48              |
| 15:O:26:GLU:HB3  | 15:O:81:LEU:HD21 | 1.95                     | 0.48              |
| 1:A:718:G:H5'    | 11:K:117:ASN:HB2 | 1.96                     | 0.47              |
| 1:A:992:U:H4'    | 1:A:993:G:O5'    | 2.13                     | 0.47              |
| 1:A:1257:U:H4'   | 1:A:1258:G:O5'   | 2.14                     | 0.47              |
| 1:A:1270:C:H2'   | 1:A:1271:G:H8    | 1.78                     | 0.47              |
| 1:A:18:C:C4      | 1:A:19:C:N4      | 2.82                     | 0.47              |
| 1:A:96:U:H2'     | 1:A:97:G:H8      | 1.77                     | 0.47              |
| 1:A:223:U:H5'    | 20:T:68:LYS:HZ2  | 1.78                     | 0.47              |
| 1:A:504:C:H42    | 1:A:541:G:H1     | 1.62                     | 0.47              |
| 1:A:585:G:C6     | 1:A:586:C:C4     | 3.02                     | 0.47              |
| 1:A:1266:G:N2    | 1:A:1270:C:C2    | 2.82                     | 0.47              |
| 1:A:1504:G:H4'   | 1:A:1505:G:O5'   | 2.14                     | 0.47              |
| 18:R:43:PHE:HD2  | 18:R:56:THR:HG22 | 1.79                     | 0.47              |
| 1:A:70:G:C2      | 1:A:100:C:C2     | 3.03                     | 0.47              |
| 1:A:193:C:H2'    | 1:A:194:C:C6     | 2.49                     | 0.47              |
| 1:A:262:A:H5''   | 20:T:76:ALA:HB2  | 1.95                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:530:G:H8     | 22:W:38:GLY:HA3  | 1.79                     | 0.47              |
| 1:A:874:G:C2     | 1:A:875:C:C2     | 3.03                     | 0.47              |
| 1:A:1017:G:C2    | 1:A:1018:C:C2    | 3.02                     | 0.47              |
| 1:A:1396:A:H4'   | 1:A:1397:C:H5''  | 1.96                     | 0.47              |
| 1:A:1435:G:H2'   | 1:A:1436:U:H6    | 1.71                     | 0.47              |
| 1:A:1444:C:H2'   | 1:A:1445:C:C6    | 2.50                     | 0.47              |
| 4:D:30:LYS:C     | 4:D:32:ALA:N     | 2.72                     | 0.47              |
| 6:F:49:ALA:HB2   | 18:R:80:PRO:HA   | 1.91                     | 0.47              |
| 10:J:37:PRO:HB2  | 10:J:70:ARG:NH1  | 2.27                     | 0.47              |
| 23:X:89:LYS:HG3  | 23:X:119:THR:HB  | 1.96                     | 0.47              |
| 1:A:25:C:H2'     | 1:A:26:A:H8      | 1.79                     | 0.47              |
| 1:A:240:C:H2'    | 1:A:241:C:H6     | 1.80                     | 0.47              |
| 1:A:548:G:C2     | 1:A:549:C:C2     | 3.03                     | 0.47              |
| 1:A:613:C:H2'    | 1:A:614:A:C8     | 2.49                     | 0.47              |
| 1:A:774:G:C2     | 1:A:806:C:C2     | 3.02                     | 0.47              |
| 1:A:823:G:N2     | 1:A:824:C:C2     | 2.82                     | 0.47              |
| 1:A:1255:G:O2'   | 1:A:1258:G:N3    | 2.46                     | 0.47              |
| 1:A:1373:G:H5''  | 7:G:36:LYS:HB3   | 1.96                     | 0.47              |
| 1:A:1444:C:H2'   | 1:A:1445:C:H6    | 1.80                     | 0.47              |
| 1:A:1526:G:C6    | 1:A:1527:C:N4    | 2.83                     | 0.47              |
| 2:B:146:GLN:HG2  | 2:B:153:ARG:HH21 | 1.79                     | 0.47              |
| 4:D:108:LEU:HB3  | 4:D:110:PHE:CE1  | 2.49                     | 0.47              |
| 16:P:11:SER:HB2  | 16:P:14:ASN:HD22 | 1.79                     | 0.47              |
| 1:A:542:G:C6     | 1:A:543:C:N4     | 2.82                     | 0.47              |
| 1:A:910:C:O2'    | 1:A:911:U:H5'    | 2.13                     | 0.47              |
| 1:A:1274:G:H2'   | 1:A:1275:A:H8    | 1.79                     | 0.47              |
| 2:B:25:ASN:HA    | 2:B:26:PRO:HD3   | 1.66                     | 0.47              |
| 4:D:133:VAL:HG13 | 4:D:135:LEU:HD12 | 1.96                     | 0.47              |
| 8:H:104:ARG:O    | 8:H:105:ARG:HB2  | 2.13                     | 0.47              |
| 11:K:54:ARG:H    | 11:K:54:ARG:CD   | 2.24                     | 0.47              |
| 1:A:17:U:H1'     | 1:A:1079:G:O2'   | 2.14                     | 0.47              |
| 1:A:18:C:H2'     | 1:A:19:C:H6      | 1.79                     | 0.47              |
| 1:A:63:C:H42     | 1:A:104:G:H1     | 1.62                     | 0.47              |
| 1:A:69:G:C2      | 1:A:101:A:N1     | 2.83                     | 0.47              |
| 1:A:246:A:C4     | 1:A:279:A:C6     | 3.03                     | 0.47              |
| 1:A:399:G:N2     | 1:A:400:C:C2     | 2.82                     | 0.47              |
| 1:A:1443:G:C2    | 1:A:1444:C:C4    | 3.02                     | 0.47              |
| 12:L:9:GLN:HG2   | 12:L:12:ARG:HH21 | 1.80                     | 0.47              |
| 1:A:73:G:H5''    | 1:A:76:C:OP2     | 2.15                     | 0.47              |
| 1:A:827:U:O3'    | 8:H:19:VAL:HG21  | 2.15                     | 0.47              |
| 1:A:975:A:H4'    | 1:A:976:G:H5'    | 1.97                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1089:G:N2    | 1:A:1097:C:C2    | 2.83                     | 0.47              |
| 1:A:1300:G:HO2'  | 1:A:1301:U:P     | 2.37                     | 0.47              |
| 1:A:1349:A:H5''  | 9:I:121:ARG:HB2  | 1.97                     | 0.47              |
| 1:A:1365:G:C5    | 1:A:1366:C:C4    | 3.03                     | 0.47              |
| 1:A:1418:A:H2'   | 1:A:1418:A:N3    | 2.29                     | 0.47              |
| 1:A:1497:G:H2'   | 1:A:1498:U:O4'   | 2.13                     | 0.47              |
| 3:C:140:ARG:O    | 3:C:143:GLU:HB2  | 2.14                     | 0.47              |
| 4:D:25:ARG:CZ    | 4:D:30:LYS:HB3   | 2.45                     | 0.47              |
| 4:D:64:LEU:HD12  | 4:D:203:VAL:HG21 | 1.95                     | 0.47              |
| 4:D:150:GLU:HA   | 4:D:153:ARG:HE   | 1.79                     | 0.47              |
| 11:K:84:VAL:HG21 | 11:K:91:ARG:NH2  | 2.30                     | 0.47              |
| 12:L:30:ALA:CB   | 12:L:33:ARG:HE   | 2.27                     | 0.47              |
| 13:M:23:TYR:HE1  | 13:M:70:LEU:HB3  | 1.80                     | 0.47              |
| 1:A:540:G:H2'    | 1:A:541:G:H8     | 1.77                     | 0.47              |
| 1:A:838:G:C2     | 1:A:849:C:C2     | 3.02                     | 0.47              |
| 1:A:944:G:H2'    | 1:A:945:G:H5'    | 1.97                     | 0.47              |
| 1:A:1008:C:N3    | 1:A:1022:G:N2    | 2.63                     | 0.47              |
| 1:A:1508:G:C2    | 1:A:1509:C:C2    | 3.03                     | 0.47              |
| 16:P:53:VAL:O    | 16:P:57:ARG:HD2  | 2.15                     | 0.47              |
| 1:A:1287:A:H5'   | 1:A:1287:A:H8    | 1.80                     | 0.47              |
| 2:B:98:LEU:H     | 2:B:101:MET:HE3  | 1.79                     | 0.47              |
| 7:G:125:MET:O    | 7:G:129:GLU:HG2  | 2.14                     | 0.47              |
| 10:J:6:ILE:HA    | 10:J:97:GLU:O    | 2.14                     | 0.47              |
| 1:A:25:C:H2'     | 1:A:26:A:C8      | 2.50                     | 0.47              |
| 1:A:67:C:O2'     | 1:A:68:G:O4'     | 2.30                     | 0.47              |
| 1:A:903:G:H2'    | 1:A:904:C:C6     | 2.50                     | 0.47              |
| 1:A:1106:G:N1    | 1:A:1107:C:C4    | 2.83                     | 0.47              |
| 1:A:1171:G:N2    | 1:A:1172:C:C2    | 2.83                     | 0.47              |
| 1:A:1246:C:H2'   | 1:A:1247:U:C6    | 2.49                     | 0.47              |
| 1:A:1445:C:N3    | 1:A:1458:G:C2    | 2.83                     | 0.47              |
| 1:A:1527:C:H2'   | 1:A:1528:U:C6    | 2.50                     | 0.47              |
| 11:K:100:ALA:O   | 11:K:102:GLY:N   | 2.47                     | 0.47              |
| 13:M:23:TYR:CE1  | 13:M:70:LEU:HB3  | 2.50                     | 0.47              |
| 1:A:115:G:O2'    | 1:A:289:G:H5''   | 2.15                     | 0.46              |
| 1:A:132:C:C2     | 1:A:231:G:N2     | 2.83                     | 0.46              |
| 1:A:172:A:H2'    | 1:A:174:C:C5     | 2.46                     | 0.46              |
| 1:A:321:A:H61    | 1:A:332:G:H1     | 1.63                     | 0.46              |
| 1:A:457:C:H2'    | 1:A:458:C:C6     | 2.50                     | 0.46              |
| 1:A:715:A:H2'    | 1:A:716:A:C8     | 2.50                     | 0.46              |
| 1:A:948:C:OP1    | 13:M:108:ARG:N   | 2.47                     | 0.46              |
| 1:A:1070:U:OP1   | 5:E:20:GLN:HG3   | 2.16                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1103:C:H5''  | 2:B:98:LEU:HD13   | 1.97                     | 0.46              |
| 1:A:1241:G:N1    | 1:A:1242:C:C4     | 2.83                     | 0.46              |
| 1:A:861:G:C2     | 1:A:862:C:C2      | 3.03                     | 0.46              |
| 1:A:881:G:C6     | 1:A:882:C:C4      | 3.03                     | 0.46              |
| 1:A:895:G:H1     | 1:A:904:C:N4      | 2.11                     | 0.46              |
| 1:A:1137:C:H4'   | 1:A:1138:G:C2     | 2.49                     | 0.46              |
| 4:D:140:VAL:HG11 | 4:D:146:ILE:HD11  | 1.98                     | 0.46              |
| 13:M:19:LEU:HB3  | 13:M:25:ILE:HG21  | 1.97                     | 0.46              |
| 23:X:16:VAL:HG12 | 23:X:55:PRO:HB2   | 1.96                     | 0.46              |
| 1:A:109:A:H5'    | 1:A:110:C:H5      | 1.79                     | 0.46              |
| 1:A:363:A:OP2    | 12:L:34:ARG:HG2   | 2.15                     | 0.46              |
| 1:A:443:C:C2     | 1:A:492:G:N2      | 2.84                     | 0.46              |
| 1:A:827:U:H5''   | 8:H:21:LYS:HE2    | 1.96                     | 0.46              |
| 4:D:9:CYS:SG     | 4:D:26:CYS:SG     | 3.13                     | 0.46              |
| 6:F:14:LEU:HD13  | 6:F:18:GLN:HB3    | 1.97                     | 0.46              |
| 7:G:12:LEU:H     | 7:G:12:LEU:HD12   | 1.80                     | 0.46              |
| 1:A:96:U:H2'     | 1:A:97:G:C8       | 2.50                     | 0.46              |
| 1:A:251:G:N1     | 1:A:266:G:C6      | 2.83                     | 0.46              |
| 1:A:377:G:H1     | 1:A:386:C:H42     | 1.62                     | 0.46              |
| 1:A:789:U:H2'    | 1:A:791:G:OP2     | 2.14                     | 0.46              |
| 1:A:868:C:H5'    | 1:A:873:A:N6      | 2.31                     | 0.46              |
| 1:A:1355:G:H1    | 1:A:1367:C:N4     | 2.12                     | 0.46              |
| 1:A:1384:C:H2'   | 1:A:1385:G:C8     | 2.50                     | 0.46              |
| 1:A:1432:G:O2'   | 1:A:1468:A:N6     | 2.49                     | 0.46              |
| 1:A:1464:G:C2    | 1:A:1465:C:C4     | 3.03                     | 0.46              |
| 9:I:71:SER:HA    | 9:I:74:ILE:HD12   | 1.96                     | 0.46              |
| 1:A:11:G:H2'     | 1:A:12:U:O4'      | 2.15                     | 0.46              |
| 1:A:334:C:H2'    | 1:A:335:C:H6      | 1.80                     | 0.46              |
| 1:A:369:C:H2'    | 1:A:370:C:C6      | 2.50                     | 0.46              |
| 1:A:1493:A:H4'   | 1:A:1494:G:OP1    | 2.15                     | 0.46              |
| 9:I:16:ARG:HH21  | 9:I:64:THR:HG21   | 1.81                     | 0.46              |
| 11:K:83:ILE:HG12 | 11:K:109:VAL:HG12 | 1.97                     | 0.46              |
| 1:A:778:G:C6     | 1:A:779:C:C4      | 3.04                     | 0.46              |
| 1:A:1127:G:H5''  | 1:A:1128:C:OP2    | 2.16                     | 0.46              |
| 9:I:26:VAL:HG13  | 9:I:63:ILE:HD12   | 1.97                     | 0.46              |
| 1:A:240:C:H2'    | 1:A:241:C:C6      | 2.50                     | 0.46              |
| 1:A:370:C:O2     | 1:A:482:A:O2'     | 2.34                     | 0.46              |
| 1:A:542:G:C2     | 1:A:543:C:C2      | 3.04                     | 0.46              |
| 1:A:564:C:O2     | 1:A:564:C:C2'     | 2.61                     | 0.46              |
| 1:A:577:G:C2     | 1:A:578:C:C2      | 3.03                     | 0.46              |
| 1:A:675:A:H2'    | 1:A:676:A:H8      | 1.81                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:814:A:H2'    | 1:A:816:A:H5''   | 1.98                     | 0.46              |
| 1:A:1077:G:N3    | 1:A:1079:G:H8    | 2.12                     | 0.46              |
| 1:A:1537:U:H6    | 1:A:1537:U:O5'   | 1.99                     | 0.46              |
| 5:E:127:ASN:HD21 | 5:E:129:ILE:H    | 1.63                     | 0.46              |
| 10:J:17:ASP:CG   | 10:J:70:ARG:HH22 | 2.06                     | 0.46              |
| 18:R:58:LEU:HB3  | 18:R:62:GLU:HB3  | 1.97                     | 0.46              |
| 1:A:17:U:C2      | 1:A:18:C:C4      | 3.04                     | 0.46              |
| 1:A:266:G:C3'    | 17:Q:67:LYS:HB2  | 2.34                     | 0.46              |
| 4:D:19:LEU:HD13  | 4:D:21:LEU:HD22  | 1.98                     | 0.46              |
| 4:D:69:GLY:C     | 4:D:70:ILE:HG13  | 2.41                     | 0.46              |
| 22:W:32:ILE:HD13 | 22:W:32:ILE:H    | 1.81                     | 0.46              |
| 1:A:244:U:O4     | 1:A:906:G:H1'    | 2.16                     | 0.46              |
| 1:A:378:G:C6     | 1:A:379:C:N4     | 2.83                     | 0.46              |
| 1:A:1445:C:C2    | 1:A:1458:G:N2    | 2.84                     | 0.46              |
| 1:A:1484:C:H2'   | 1:A:1485:U:O4'   | 2.16                     | 0.46              |
| 4:D:119:GLN:O    | 4:D:123:HIS:CD2  | 2.69                     | 0.46              |
| 11:K:18:ARG:HB2  | 11:K:33:THR:HG23 | 1.97                     | 0.46              |
| 16:P:59:TRP:C    | 16:P:62:VAL:HG22 | 2.39                     | 0.46              |
| 19:S:22:LEU:HD11 | 19:S:31:ILE:HD11 | 1.98                     | 0.46              |
| 19:S:40:ILE:HG21 | 19:S:62:ILE:HD11 | 1.98                     | 0.46              |
| 1:A:21:G:C2      | 1:A:22:G:C6      | 3.04                     | 0.46              |
| 1:A:39:G:C6      | 1:A:40:C:C4      | 3.04                     | 0.46              |
| 1:A:155:C:H42    | 1:A:166:G:H1     | 1.64                     | 0.46              |
| 1:A:246:A:O2'    | 17:Q:99:SER:HA   | 2.16                     | 0.46              |
| 1:A:614:A:H2'    | 1:A:615:C:C6     | 2.51                     | 0.46              |
| 1:A:938:A:H8     | 1:A:938:A:O5'    | 1.99                     | 0.46              |
| 1:A:1459:C:OP1   | 20:T:28:ALA:HA   | 2.16                     | 0.46              |
| 18:R:37:VAL:O    | 18:R:40:LEU:HB2  | 2.15                     | 0.46              |
| 1:A:132:C:N3     | 1:A:231:G:C2     | 2.84                     | 0.45              |
| 1:A:639:G:H2'    | 1:A:640:A:C8     | 2.51                     | 0.45              |
| 1:A:1074:G:H1'   | 1:A:1102:A:C2    | 2.51                     | 0.45              |
| 1:A:1315:U:O2'   | 1:A:1360:A:N3    | 2.48                     | 0.45              |
| 6:F:4:TYR:CZ     | 6:F:72:VAL:HG21  | 2.50                     | 0.45              |
| 13:M:3:ARG:H     | 13:M:57:ARG:HH22 | 1.63                     | 0.45              |
| 23:X:5:TYR:CE2   | 23:X:65:TRP:HH2  | 2.30                     | 0.45              |
| 1:A:289:G:C2     | 1:A:290:C:C2     | 3.04                     | 0.45              |
| 1:A:678:U:H2'    | 1:A:679:C:H6     | 1.76                     | 0.45              |
| 1:A:708:C:H2'    | 1:A:709:G:H8     | 1.82                     | 0.45              |
| 1:A:951:G:C6     | 1:A:1231:G:C6    | 3.04                     | 0.45              |
| 1:A:1102:A:H2'   | 1:A:1103:C:H6    | 1.76                     | 0.45              |
| 1:A:1386:G:H2'   | 1:A:1387:G:C8    | 2.41                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:64:LEU:HA    | 4:D:67:ILE:HD12  | 1.98                     | 0.45              |
| 5:E:10:MET:HA    | 5:E:32:VAL:HG23  | 1.97                     | 0.45              |
| 6:F:12:PRO:HD3   | 6:F:58:GLY:HA2   | 1.97                     | 0.45              |
| 6:F:33:TYR:HD1   | 6:F:71:ARG:HD2   | 1.81                     | 0.45              |
| 6:F:37:VAL:HA    | 6:F:65:VAL:HG12  | 1.98                     | 0.45              |
| 1:A:15:G:H2'     | 1:A:16:A:C8      | 2.32                     | 0.45              |
| 1:A:327:A:N3     | 1:A:329:A:H1'    | 2.31                     | 0.45              |
| 1:A:524:G:C2     | 1:A:525:C:C4     | 3.05                     | 0.45              |
| 1:A:974:A:OP2    | 14:N:32:SER:HB2  | 2.17                     | 0.45              |
| 1:A:1007:C:C2    | 1:A:1023:G:N1    | 2.84                     | 0.45              |
| 1:A:1220:G:H2'   | 1:A:1221:G:O4'   | 2.17                     | 0.45              |
| 1:A:1241:G:C6    | 1:A:1242:C:N4    | 2.84                     | 0.45              |
| 1:A:1493:A:C2    | 22:W:46:ARG:HA   | 2.52                     | 0.45              |
| 4:D:98:GLU:HA    | 4:D:103:ASN:HD22 | 1.80                     | 0.45              |
| 8:H:39:LEU:HD23  | 8:H:45:ILE:HG12  | 1.99                     | 0.45              |
| 11:K:18:ARG:HB2  | 11:K:33:THR:CG2  | 2.46                     | 0.45              |
| 11:K:43:SER:HB3  | 11:K:68:ALA:HB2  | 1.98                     | 0.45              |
| 16:P:12:LYS:C    | 16:P:14:ASN:H    | 2.24                     | 0.45              |
| 23:X:102:LYS:HD3 | 23:X:102:LYS:HA  | 1.78                     | 0.45              |
| 1:A:15:G:H21     | 5:E:19:MET:HB2   | 1.80                     | 0.45              |
| 1:A:79:G:H2'     | 1:A:80:G:C8      | 2.52                     | 0.45              |
| 1:A:1138:G:H2'   | 1:A:1140:C:H5''  | 1.98                     | 0.45              |
| 1:A:1162:C:N3    | 1:A:1175:G:C2    | 2.85                     | 0.45              |
| 14:N:6:LEU:C     | 14:N:8:GLU:H     | 2.23                     | 0.45              |
| 1:A:27:G:H2'     | 1:A:28:G:O4'     | 2.17                     | 0.45              |
| 1:A:317:G:C2     | 1:A:337:C:C2     | 3.04                     | 0.45              |
| 1:A:568:G:C6     | 1:A:569:C:N4     | 2.85                     | 0.45              |
| 1:A:823:G:C6     | 1:A:824:C:N4     | 2.84                     | 0.45              |
| 1:A:1050:G:C6    | 1:A:1051:C:N4    | 2.84                     | 0.45              |
| 1:A:1105:A:H2'   | 1:A:1106:G:C8    | 2.49                     | 0.45              |
| 1:A:1525:G:H2'   | 1:A:1526:G:C8    | 2.51                     | 0.45              |
| 2:B:131:PRO:HA   | 2:B:135:GLN:OE1  | 2.17                     | 0.45              |
| 1:A:284:G:H2'    | 1:A:285:G:H8     | 1.82                     | 0.45              |
| 1:A:501:C:H2'    | 1:A:502:G:C8     | 2.51                     | 0.45              |
| 1:A:524:G:H2'    | 1:A:525:C:C6     | 2.51                     | 0.45              |
| 1:A:639:G:H2'    | 1:A:640:A:H8     | 1.82                     | 0.45              |
| 1:A:1313:U:H2'   | 1:A:1314:C:H6    | 1.81                     | 0.45              |
| 1:A:1351:U:H2'   | 1:A:1352:C:H6    | 1.81                     | 0.45              |
| 1:A:1391:U:H2'   | 1:A:1392:G:C8    | 2.51                     | 0.45              |
| 1:A:1408:A:H2'   | 1:A:1409:C:C6    | 2.51                     | 0.45              |
| 14:N:37:PHE:HB3  | 14:N:39:LEU:HG   | 1.98                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 23:X:102:LYS:O   | 23:X:106:ILE:HG13 | 2.17                     | 0.45              |
| 1:A:287:U:C2'    | 1:A:288:A:H5'     | 2.47                     | 0.45              |
| 1:A:895:G:C2     | 1:A:896:C:C2      | 3.05                     | 0.45              |
| 1:A:931:C:H2'    | 1:A:932:C:O4'     | 2.17                     | 0.45              |
| 1:A:1422:G:H1    | 1:A:1478:C:H42    | 1.63                     | 0.45              |
| 3:C:29:TYR:CE1   | 14:N:37:PHE:CD1   | 3.04                     | 0.45              |
| 14:N:49:HIS:HE1  | 14:N:58:LYS:HE2   | 1.81                     | 0.45              |
| 15:O:7:GLU:O     | 15:O:11:VAL:HG23  | 2.16                     | 0.45              |
| 20:T:42:GLN:O    | 20:T:45:GLN:HB2   | 2.17                     | 0.45              |
| 1:A:202:U:OP2    | 1:A:203:U:H5      | 2.00                     | 0.45              |
| 1:A:285:G:H2'    | 1:A:286:G:O4'     | 2.16                     | 0.45              |
| 1:A:391:G:H2'    | 1:A:392:G:O4'     | 2.17                     | 0.45              |
| 1:A:439:A:H3'    | 1:A:441:A:H5''    | 1.98                     | 0.45              |
| 1:A:544:G:OP1    | 4:D:62:GLN:HG3    | 2.17                     | 0.45              |
| 1:A:573:A:H2'    | 1:A:574:A:O4'     | 2.17                     | 0.45              |
| 1:A:916:G:H2'    | 1:A:917:G:C8      | 2.52                     | 0.45              |
| 1:A:1116:C:H2'   | 1:A:1117:G:O4'    | 2.17                     | 0.45              |
| 1:A:1420:C:H2'   | 1:A:1421:G:H8     | 1.81                     | 0.45              |
| 3:C:6:HIS:HD2    | 3:C:9:GLY:H       | 1.65                     | 0.45              |
| 4:D:138:TYR:CD1  | 4:D:138:TYR:C     | 2.95                     | 0.45              |
| 7:G:31:MET:HG3   | 7:G:35:LYS:C      | 2.42                     | 0.45              |
| 9:I:48:GLU:N     | 9:I:49:PRO:HD2    | 2.32                     | 0.45              |
| 19:S:49:ILE:HD12 | 19:S:62:ILE:HG21  | 1.98                     | 0.45              |
| 1:A:319:G:C2     | 1:A:320:C:C2      | 3.05                     | 0.45              |
| 1:A:335:C:H2'    | 1:A:336:C:H6      | 1.77                     | 0.45              |
| 1:A:613:C:C2     | 1:A:628:G:N2      | 2.85                     | 0.45              |
| 1:A:985:C:C2     | 1:A:1221:G:C2     | 3.05                     | 0.45              |
| 1:A:1046:A:H3'   | 1:A:1047:G:H8     | 1.82                     | 0.45              |
| 7:G:71:PRO:HD2   | 7:G:96:GLN:HB2    | 1.99                     | 0.45              |
| 10:J:37:PRO:CB   | 10:J:70:ARG:HH11  | 2.30                     | 0.45              |
| 1:A:233:C:H2'    | 1:A:234:C:C6      | 2.52                     | 0.45              |
| 1:A:370:C:H42    | 1:A:391:G:H1      | 1.65                     | 0.45              |
| 1:A:674:G:H2'    | 1:A:675:A:H8      | 1.82                     | 0.45              |
| 1:A:928:G:H1     | 1:A:1389:C:N4     | 2.15                     | 0.45              |
| 1:A:1055:A:H2    | 3:C:194:GLY:HA2   | 1.81                     | 0.45              |
| 1:A:1246:C:H2'   | 1:A:1247:U:H6     | 1.82                     | 0.45              |
| 1:A:1526:G:C2    | 1:A:1527:C:C2     | 3.05                     | 0.45              |
| 16:P:67:THR:CG2  | 16:P:68:ASP:H     | 2.28                     | 0.45              |
| 23:X:117:LYS:HE2 | 23:X:162:ASN:HB2  | 1.99                     | 0.45              |
| 1:A:79:G:N1      | 1:A:91:C:C2       | 2.85                     | 0.44              |
| 1:A:189:G:H2'    | 1:A:189(A):C:C6   | 2.52                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:444:C:H42    | 1:A:490:G:H1     | 1.65                     | 0.44              |
| 1:A:502:G:OP1    | 12:L:118:SER:N   | 2.46                     | 0.44              |
| 1:A:516:U:H4'    | 22:W:2:LYS:HD2   | 1.99                     | 0.44              |
| 1:A:939:G:C2     | 1:A:940:C:N3     | 2.85                     | 0.44              |
| 2:B:211:ILE:H    | 2:B:211:ILE:HG13 | 1.58                     | 0.44              |
| 20:T:72:LEU:O    | 20:T:72:LEU:HG   | 2.15                     | 0.44              |
| 21:V:3:LYS:O     | 21:V:11:GLY:HA2  | 2.17                     | 0.44              |
| 1:A:33:A:H2'     | 1:A:34:C:C6      | 2.52                     | 0.44              |
| 1:A:279:A:N1     | 17:Q:98:LEU:HD23 | 2.30                     | 0.44              |
| 1:A:542:G:H2'    | 1:A:543:C:C6     | 2.52                     | 0.44              |
| 1:A:1015:A:H2'   | 1:A:1016:A:C8    | 2.52                     | 0.44              |
| 1:A:1101:A:H61   | 2:B:103:THR:HG21 | 1.82                     | 0.44              |
| 1:A:1430:C:C2    | 1:A:1471:G:N2    | 2.84                     | 0.44              |
| 1:A:1487:G:H5''  | 1:A:1488:G:OP1   | 2.17                     | 0.44              |
| 1:A:1509:C:H2'   | 1:A:1510:U:O4'   | 2.18                     | 0.44              |
| 3:C:29:TYR:CD1   | 14:N:36:PHE:CE2  | 3.06                     | 0.44              |
| 11:K:84:VAL:HG11 | 11:K:95:ILE:HD11 | 1.98                     | 0.44              |
| 1:A:551:U:H2'    | 1:A:552:U:C6     | 2.51                     | 0.44              |
| 1:A:763:G:C2     | 1:A:764:C:C2     | 3.06                     | 0.44              |
| 1:A:903:G:C2     | 1:A:904:C:C2     | 3.04                     | 0.44              |
| 1:A:1064:G:C8    | 1:A:1066:C:C2    | 3.06                     | 0.44              |
| 1:A:1251:A:H2'   | 1:A:1252:A:O4'   | 2.17                     | 0.44              |
| 1:A:1283:G:C6    | 1:A:1284:C:N4    | 2.85                     | 0.44              |
| 1:A:1329:A:H5''  | 13:M:26:GLY:N    | 2.31                     | 0.44              |
| 1:A:1391:U:H2'   | 1:A:1392:G:H8    | 1.81                     | 0.44              |
| 1:A:1541:U:O3'   | 18:R:19:LYS:HB3  | 2.16                     | 0.44              |
| 2:B:18:GLY:HA2   | 2:B:42:ILE:HD12  | 1.98                     | 0.44              |
| 4:D:13:ARG:HH12  | 4:D:40:PRO:HA    | 1.81                     | 0.44              |
| 4:D:43:HIS:CD2   | 4:D:43:HIS:H     | 2.36                     | 0.44              |
| 4:D:158:ILE:H    | 4:D:158:ILE:HG13 | 1.55                     | 0.44              |
| 19:S:30:LEU:H    | 19:S:48:THR:HB   | 1.82                     | 0.44              |
| 1:A:625:G:OP1    | 16:P:9:PHE:HB3   | 2.18                     | 0.44              |
| 1:A:1082:G:C8    | 1:A:1082:G:O5'   | 2.69                     | 0.44              |
| 1:A:1144:G:N2    | 1:A:1146:A:H62   | 2.15                     | 0.44              |
| 1:A:1151:A:H5'   | 10:J:41:PRO:HA   | 1.99                     | 0.44              |
| 3:C:24:ALA:HB2   | 3:C:32:LEU:HD12  | 2.00                     | 0.44              |
| 4:D:173:TRP:HB2  | 4:D:187:ARG:O    | 2.18                     | 0.44              |
| 7:G:24:THR:HA    | 7:G:27:ILE:HD12  | 1.99                     | 0.44              |
| 7:G:29:LYS:HB3   | 7:G:105:VAL:HG21 | 1.99                     | 0.44              |
| 1:A:51:A:C6      | 1:A:353:A:C2     | 3.05                     | 0.44              |
| 1:A:188:C:H5'    | 20:T:89:ARG:HD3  | 2.00                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:455:C:H2'    | 1:A:456:C:H6     | 1.81                     | 0.44              |
| 1:A:571:U:H5''   | 1:A:819:A:C5     | 2.53                     | 0.44              |
| 1:A:601:C:C2     | 1:A:638:G:N2     | 2.85                     | 0.44              |
| 1:A:604:G:H2'    | 1:A:605:U:O4'    | 2.17                     | 0.44              |
| 1:A:827:U:C4     | 1:A:872:A:N6     | 2.73                     | 0.44              |
| 1:A:942:G:C6     | 1:A:1342:C:N3    | 2.84                     | 0.44              |
| 1:A:1017:G:C6    | 1:A:1018:C:C4    | 3.06                     | 0.44              |
| 1:A:1106:G:H2'   | 1:A:1107:C:C6    | 2.53                     | 0.44              |
| 1:A:1163:C:H2'   | 1:A:1164:G:C8    | 2.45                     | 0.44              |
| 1:A:1304:G:H21   | 1:A:1333:A:H62   | 1.65                     | 0.44              |
| 1:A:1374:A:H1'   | 7:G:31:MET:HE1   | 1.99                     | 0.44              |
| 1:A:1438:G:N2    | 1:A:1439:C:C2    | 2.85                     | 0.44              |
| 3:C:14:ILE:H     | 3:C:14:ILE:HG12  | 1.40                     | 0.44              |
| 3:C:116:VAL:O    | 3:C:120:VAL:HG23 | 2.18                     | 0.44              |
| 4:D:108:LEU:HB3  | 4:D:110:PHE:HE1  | 1.83                     | 0.44              |
| 5:E:33:VAL:HG12  | 5:E:112:LEU:HD22 | 2.00                     | 0.44              |
| 1:A:344:A:H4'    | 1:A:345:C:OP2    | 2.18                     | 0.44              |
| 1:A:624:C:O3'    | 16:P:10:GLY:HA2  | 2.18                     | 0.44              |
| 1:A:751:U:C5     | 1:A:752:G:C5     | 3.05                     | 0.44              |
| 1:A:761:G:C5     | 1:A:762:C:C4     | 3.05                     | 0.44              |
| 1:A:864:A:O2'    | 1:A:865:A:O4'    | 2.35                     | 0.44              |
| 1:A:920:U:C2     | 1:A:921:U:C5     | 3.05                     | 0.44              |
| 1:A:1001(A):G:N2 | 1:A:1040:U:C2    | 2.86                     | 0.44              |
| 1:A:1007:C:N3    | 1:A:1023:G:C6    | 2.85                     | 0.44              |
| 3:C:50:ALA:HA    | 3:C:72:LYS:HB2   | 1.98                     | 0.44              |
| 3:C:153:VAL:HG22 | 3:C:198:VAL:HA   | 2.00                     | 0.44              |
| 8:H:4:ASP:CG     | 8:H:85:ARG:HH12  | 2.26                     | 0.44              |
| 15:O:54:ARG:HG3  | 15:O:55:GLY:N    | 2.32                     | 0.44              |
| 1:A:18:C:H4'     | 1:A:1078:U:H1'   | 1.99                     | 0.44              |
| 1:A:105:G:C2     | 1:A:106:C:C2     | 3.06                     | 0.44              |
| 1:A:1110:A:H2'   | 1:A:1111:A:O4'   | 2.18                     | 0.44              |
| 1:A:1276:G:H2'   | 1:A:1277:C:O4'   | 2.18                     | 0.44              |
| 10:J:7:LYS:HG2   | 10:J:71:LEU:CD2  | 2.48                     | 0.44              |
| 10:J:61:GLU:CD   | 10:J:61:GLU:C    | 2.85                     | 0.44              |
| 23:X:17:ARG:HB2  | 23:X:54:PRO:O    | 2.18                     | 0.44              |
| 1:A:291:C:O2     | 1:A:310:G:C2     | 2.71                     | 0.44              |
| 1:A:334:C:H2'    | 1:A:335:C:C6     | 2.52                     | 0.44              |
| 1:A:1419:G:C2    | 1:A:1420:C:C2    | 3.05                     | 0.44              |
| 2:B:132:LYS:HG2  | 2:B:135:GLN:CD   | 2.42                     | 0.44              |
| 11:K:50:TYR:CD2  | 11:K:54:ARG:HB2  | 2.52                     | 0.44              |
| 12:L:75:HIS:HB2  | 12:L:77:LEU:HD13 | 2.00                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:6:G:N2       | 5:E:98:THR:OG1    | 2.51                     | 0.44              |
| 1:A:236:G:C6     | 1:A:237:C:C4      | 3.06                     | 0.44              |
| 1:A:307:C:C6     | 1:A:308:C:C5      | 3.05                     | 0.44              |
| 1:A:926:G:C8     | 1:A:926:G:O5'     | 2.71                     | 0.44              |
| 1:A:1518:A:H2'   | 1:A:1519:A:H8     | 1.83                     | 0.44              |
| 12:L:60:LEU:HD11 | 12:L:85:ILE:HD13  | 2.00                     | 0.44              |
| 1:A:237:C:H2'    | 1:A:238:G:H8      | 1.83                     | 0.43              |
| 1:A:836:G:C6     | 1:A:851:G:C6      | 3.06                     | 0.43              |
| 1:A:1134:G:N2    | 1:A:1141:C:C2     | 2.85                     | 0.43              |
| 1:A:1401:G:O6    | 1:A:1504:G:N2     | 2.51                     | 0.43              |
| 1:A:1495:U:O2'   | 23:X:98:ASP:OD2   | 2.31                     | 0.43              |
| 3:C:55:VAL:HG22  | 3:C:68:VAL:HG13   | 1.98                     | 0.43              |
| 1:A:674:G:H2'    | 1:A:675:A:C8      | 2.53                     | 0.43              |
| 1:A:1081:G:C2'   | 1:A:1082:G:H8     | 2.00                     | 0.43              |
| 1:A:1253:G:C2    | 1:A:1254:C:C2     | 3.06                     | 0.43              |
| 3:C:91:LEU:HG    | 3:C:99:VAL:HG11   | 1.99                     | 0.43              |
| 10:J:38:ILE:HA   | 10:J:39:PRO:HD3   | 1.87                     | 0.43              |
| 16:P:21:VAL:HG12 | 16:P:34:GLU:HB3   | 2.00                     | 0.43              |
| 1:A:60:A:H8      | 1:A:60:A:OP1      | 2.01                     | 0.43              |
| 1:A:158:G:H8     | 1:A:158:G:O5'     | 2.01                     | 0.43              |
| 1:A:276:G:C2     | 1:A:277:C:C2      | 3.06                     | 0.43              |
| 1:A:792:A:H4'    | 1:A:793:U:C5'     | 2.49                     | 0.43              |
| 1:A:942:G:C2     | 1:A:1342:C:O2     | 2.71                     | 0.43              |
| 1:A:1098:C:C1'   | 1:A:1168:A:H2     | 2.31                     | 0.43              |
| 1:A:1241:G:C2    | 1:A:1242:C:C4     | 3.06                     | 0.43              |
| 1:A:1462:G:N2    | 1:A:1463:C:C2     | 2.87                     | 0.43              |
| 16:P:48:TRP:CD1  | 16:P:48:TRP:N     | 2.86                     | 0.43              |
| 17:Q:92:ARG:O    | 17:Q:95:TYR:HB2   | 2.18                     | 0.43              |
| 18:R:25:THR:HB   | 18:R:42:ARG:HH22  | 1.83                     | 0.43              |
| 1:A:767:A:H2'    | 1:A:768:A:O4'     | 2.17                     | 0.43              |
| 1:A:778:G:C2     | 1:A:779:C:C2      | 3.07                     | 0.43              |
| 1:A:1343:G:C6    | 1:A:1344:C:N3     | 2.87                     | 0.43              |
| 1:A:1381:U:H1'   | 7:G:78:ARG:HE     | 1.84                     | 0.43              |
| 3:C:36:ASP:HA    | 3:C:39:ILE:HD12   | 1.99                     | 0.43              |
| 4:D:119:GLN:HG2  | 4:D:120:LEU:N     | 2.33                     | 0.43              |
| 12:L:102:ARG:CZ  | 12:L:110:VAL:HG22 | 2.48                     | 0.43              |
| 18:R:31:LEU:C    | 18:R:33:ASP:H     | 2.27                     | 0.43              |
| 1:A:29:G:N2      | 1:A:555:C:C2      | 2.86                     | 0.43              |
| 1:A:70:G:C2      | 1:A:100:C:O2      | 2.71                     | 0.43              |
| 1:A:174:C:H2'    | 1:A:175:C:H6      | 1.83                     | 0.43              |
| 1:A:291:C:H2'    | 1:A:292:G:C8      | 2.53                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:321:A:H2'    | 1:A:322:C:C6     | 2.53                     | 0.43              |
| 1:A:457:C:H2'    | 1:A:458:C:H6     | 1.84                     | 0.43              |
| 1:A:602:A:H2'    | 1:A:603:U:O4'    | 2.17                     | 0.43              |
| 1:A:667:G:H2'    | 1:A:668:G:C8     | 2.51                     | 0.43              |
| 1:A:828:A:H2'    | 1:A:829:G:O4'    | 2.18                     | 0.43              |
| 1:A:886:G:N1     | 1:A:912:C:C2     | 2.86                     | 0.43              |
| 8:H:53:VAL:HG23  | 8:H:58:TYR:CD2   | 2.54                     | 0.43              |
| 11:K:84:VAL:CG2  | 11:K:91:ARG:HH22 | 2.30                     | 0.43              |
| 12:L:90:VAL:HG11 | 12:L:93:LEU:HD12 | 2.00                     | 0.43              |
| 1:A:245:C:C2     | 1:A:284:G:C2     | 3.06                     | 0.43              |
| 1:A:662:G:C2     | 1:A:744:C:O2     | 2.71                     | 0.43              |
| 1:A:734:G:C6     | 1:A:735:C:C4     | 3.07                     | 0.43              |
| 1:A:794:A:H2'    | 1:A:795:C:H6     | 1.84                     | 0.43              |
| 1:A:1081:G:OP1   | 5:E:18:ARG:HA    | 2.18                     | 0.43              |
| 1:A:1373:G:H5''  | 7:G:36:LYS:CB    | 2.49                     | 0.43              |
| 3:C:29:TYR:HE1   | 14:N:37:PHE:CD1  | 2.36                     | 0.43              |
| 3:C:30:ARG:HG2   | 14:N:37:PHE:O    | 2.17                     | 0.43              |
| 12:L:93:LEU:HA   | 12:L:94:PRO:HD3  | 1.68                     | 0.43              |
| 17:Q:51:TYR:HE2  | 17:Q:76:LEU:HB2  | 1.83                     | 0.43              |
| 1:A:115:G:C2     | 1:A:289:G:N7     | 2.87                     | 0.43              |
| 1:A:137:C:C2     | 1:A:227:G:C2     | 3.06                     | 0.43              |
| 1:A:166:G:H2'    | 1:A:167:G:H8     | 1.83                     | 0.43              |
| 1:A:407:G:H2'    | 1:A:408:A:C8     | 2.53                     | 0.43              |
| 1:A:677:U:H3     | 1:A:713:G:H1     | 1.66                     | 0.43              |
| 5:E:78:HIS:HB2   | 8:H:104:ARG:HD2  | 2.01                     | 0.43              |
| 5:E:88:LYS:HB3   | 5:E:123:LEU:HB2  | 2.00                     | 0.43              |
| 7:G:16:LEU:H     | 7:G:16:LEU:HG    | 1.54                     | 0.43              |
| 10:J:60:ARG:NH1  | 10:J:60:ARG:CB   | 2.81                     | 0.43              |
| 18:R:26:LEU:HD13 | 18:R:42:ARG:HE   | 1.84                     | 0.43              |
| 1:A:237:C:H2'    | 1:A:238:G:C8     | 2.54                     | 0.43              |
| 1:A:250:A:H1'    | 1:A:252:U:C4     | 2.54                     | 0.43              |
| 1:A:430:A:P      | 4:D:8:VAL:H      | 2.41                     | 0.43              |
| 1:A:529:G:H5'    | 1:A:530:G:OP2    | 2.19                     | 0.43              |
| 1:A:651:C:H2'    | 1:A:652:U:C6     | 2.53                     | 0.43              |
| 1:A:668:G:H2'    | 1:A:669:U:C6     | 2.54                     | 0.43              |
| 1:A:698:G:C6     | 1:A:699:C:N4     | 2.87                     | 0.43              |
| 1:A:861:G:C6     | 1:A:862:C:C4     | 3.07                     | 0.43              |
| 1:A:864:A:O2'    | 1:A:1078:U:O4    | 2.28                     | 0.43              |
| 1:A:922:G:C2     | 1:A:923:A:C4     | 3.06                     | 0.43              |
| 1:A:1081:G:P     | 5:E:18:ARG:HA    | 2.58                     | 0.43              |
| 8:H:89:PRO:HA    | 8:H:92:ARG:NH1   | 2.33                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:I:26:VAL:HB    | 9:I:33:PHE:HB2   | 2.01                     | 0.43              |
| 10:J:57:LYS:HA   | 10:J:60:ARG:HH22 | 1.84                     | 0.43              |
| 22:W:55:VAL:HG13 | 22:W:66:ARG:H    | 1.82                     | 0.43              |
| 1:A:39:G:C2      | 1:A:40:C:C2      | 3.07                     | 0.43              |
| 1:A:444:C:C2     | 1:A:491:G:N2     | 2.87                     | 0.43              |
| 1:A:502:G:H2'    | 1:A:503:C:O4'    | 2.19                     | 0.43              |
| 1:A:560:U:H2'    | 5:E:123:LEU:HD22 | 2.01                     | 0.43              |
| 1:A:740:U:H2'    | 1:A:741:G:H8     | 1.84                     | 0.43              |
| 1:A:1192:C:H2'   | 1:A:1193:G:O4'   | 2.18                     | 0.43              |
| 1:A:1419:G:C6    | 1:A:1420:C:C4    | 3.07                     | 0.43              |
| 1:A:1542:U:O2    | 1:A:1542:U:H2'   | 2.18                     | 0.43              |
| 14:N:15:LYS:HD3  | 14:N:19:ARG:HH12 | 1.83                     | 0.43              |
| 1:A:15:G:N1      | 1:A:921:U:C2     | 2.87                     | 0.43              |
| 1:A:73:G:N1      | 1:A:76:C:C2      | 2.87                     | 0.43              |
| 1:A:250:A:H4'    | 1:A:251:G:O5'    | 2.19                     | 0.43              |
| 1:A:276:G:O2'    | 17:Q:68:ARG:NH2  | 2.49                     | 0.43              |
| 1:A:442:C:H2'    | 1:A:443:C:H6     | 1.79                     | 0.43              |
| 1:A:476:G:H2'    | 1:A:477:A:C8     | 2.54                     | 0.43              |
| 1:A:769:G:C2     | 1:A:770:C:C4     | 3.07                     | 0.43              |
| 1:A:836:G:C6     | 1:A:837:G:C6     | 3.07                     | 0.43              |
| 1:A:1050:G:N2    | 1:A:1051:C:C2    | 2.87                     | 0.43              |
| 3:C:6:HIS:HA     | 3:C:7:PRO:HD3    | 1.85                     | 0.43              |
| 3:C:62:ASP:HA    | 3:C:97:LYS:HE3   | 2.00                     | 0.43              |
| 4:D:3:ARG:HD2    | 4:D:118:ARG:HD3  | 2.01                     | 0.43              |
| 5:E:15:ARG:HD3   | 5:E:28:PHE:CE1   | 2.54                     | 0.43              |
| 1:A:157:G:C6     | 1:A:165:C:N3     | 2.87                     | 0.42              |
| 1:A:399:G:H2'    | 1:A:400:C:C6     | 2.53                     | 0.42              |
| 1:A:416:G:C6     | 1:A:417:C:C4     | 3.07                     | 0.42              |
| 1:A:806:C:H2'    | 1:A:807:A:C8     | 2.54                     | 0.42              |
| 1:A:1141:C:H2'   | 1:A:1142:G:H8    | 1.84                     | 0.42              |
| 1:A:1256:A:C2'   | 3:C:27:LYS:HZ1   | 2.32                     | 0.42              |
| 1:A:1484:C:H6    | 1:A:1484:C:O5'   | 2.01                     | 0.42              |
| 1:A:1508:G:C6    | 1:A:1509:C:C4    | 3.07                     | 0.42              |
| 2:B:33:TYR:HB3   | 2:B:41:ILE:HG22  | 2.01                     | 0.42              |
| 8:H:25:ASP:OD2   | 8:H:53:VAL:HG21  | 2.18                     | 0.42              |
| 1:A:115:G:C2     | 1:A:289:G:C5     | 3.07                     | 0.42              |
| 1:A:621:A:H2'    | 1:A:622:A:H8     | 1.84                     | 0.42              |
| 1:A:1189:C:H5''  | 3:C:5:ILE:HG12   | 2.00                     | 0.42              |
| 1:A:1393:U:H2'   | 1:A:1395:C:H5    | 1.83                     | 0.42              |
| 2:B:55:PHE:HD1   | 2:B:55:PHE:HA    | 1.74                     | 0.42              |
| 8:H:6:ILE:HD12   | 8:H:35:ILE:HD12  | 2.00                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 12:L:79:GLU:C     | 12:L:81:SER:H    | 2.27                     | 0.42              |
| 1:A:258:G:H2'     | 1:A:259:G:H8     | 1.84                     | 0.42              |
| 1:A:456:C:C2      | 1:A:476:G:C2     | 3.07                     | 0.42              |
| 1:A:976:G:N2      | 1:A:1363:C:H5''  | 2.34                     | 0.42              |
| 1:A:1253:G:C6     | 1:A:1254:C:C4    | 3.07                     | 0.42              |
| 3:C:135:LYS:O     | 3:C:139:GLN:HG2  | 2.19                     | 0.42              |
| 4:D:150:GLU:O     | 4:D:153:ARG:HB2  | 2.19                     | 0.42              |
| 8:H:3:THR:HG23    | 8:H:4:ASP:H      | 1.83                     | 0.42              |
| 9:I:114:TYR:CD2   | 10:J:58:ASP:O    | 2.66                     | 0.42              |
| 11:K:21:ILE:HG23  | 11:K:30:VAL:HG22 | 2.01                     | 0.42              |
| 1:A:104:G:C2      | 1:A:105:G:C5     | 3.07                     | 0.42              |
| 1:A:333:G:C2      | 1:A:334:C:C2     | 3.08                     | 0.42              |
| 1:A:502:G:C2      | 1:A:503:C:C2     | 3.07                     | 0.42              |
| 1:A:786:G:N2      | 1:A:797:C:C2     | 2.88                     | 0.42              |
| 1:A:895:G:C6      | 1:A:896:C:C4     | 3.07                     | 0.42              |
| 1:A:1172:C:H2'    | 1:A:1173:G:C8    | 2.51                     | 0.42              |
| 1:A:1368:G:N1     | 1:A:1369:C:C4    | 2.88                     | 0.42              |
| 2:B:115:LEU:HD11  | 2:B:146:GLN:HG3  | 2.01                     | 0.42              |
| 8:H:134:ILE:H     | 8:H:134:ILE:HG13 | 1.62                     | 0.42              |
| 1:A:27:G:H2'      | 1:A:28:G:H8      | 1.83                     | 0.42              |
| 1:A:41:G:C6       | 1:A:402:G:C6     | 3.07                     | 0.42              |
| 1:A:293:G:C4      | 1:A:305:G:N2     | 2.88                     | 0.42              |
| 1:A:333:G:N1      | 1:A:334:C:C4     | 2.87                     | 0.42              |
| 1:A:357:G:OP1     | 1:A:367:U:H5''   | 2.20                     | 0.42              |
| 1:A:399:G:C2      | 1:A:400:C:C2     | 3.08                     | 0.42              |
| 1:A:402:G:OP1     | 4:D:74:GLN:HG3   | 2.19                     | 0.42              |
| 1:A:580:U:O4      | 1:A:581:G:C6     | 2.73                     | 0.42              |
| 1:A:810:C:H2'     | 1:A:811:C:O4'    | 2.19                     | 0.42              |
| 1:A:1119:C:C2     | 1:A:1155:G:N2    | 2.87                     | 0.42              |
| 20:T:61:SER:O     | 20:T:65:LYS:HG2  | 2.18                     | 0.42              |
| 1:A:112:G:C2      | 1:A:113:G:C8     | 3.08                     | 0.42              |
| 1:A:396:G:O2'     | 1:A:398:C:OP1    | 2.24                     | 0.42              |
| 1:A:577:G:N1      | 1:A:578:C:C4     | 2.87                     | 0.42              |
| 1:A:829:G:O4'     | 2:B:26:PRO:HG2   | 2.18                     | 0.42              |
| 1:A:874:G:C6      | 1:A:875:C:C4     | 3.07                     | 0.42              |
| 1:A:1030(C):G:H2' | 1:A:1030(D):A:C8 | 2.54                     | 0.42              |
| 4:D:36:ARG:HD3    | 4:D:38:TYR:CE2   | 2.49                     | 0.42              |
| 11:K:92:GLU:HA    | 11:K:95:ILE:HD12 | 2.01                     | 0.42              |
| 1:A:310:G:C6      | 1:A:311:C:C4     | 3.07                     | 0.42              |
| 1:A:617:G:C6      | 1:A:618:C:N4     | 2.87                     | 0.42              |
| 1:A:768:A:C5      | 1:A:769:G:C8     | 3.08                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:823:G:C2     | 1:A:824:C:C2     | 3.08                     | 0.42              |
| 1:A:939:G:H1'    | 1:A:1375:A:C2    | 2.54                     | 0.42              |
| 1:A:966:G:C6     | 1:A:967:C:C4     | 3.07                     | 0.42              |
| 1:A:998:G:N1     | 1:A:999:C:C4     | 2.88                     | 0.42              |
| 1:A:1081:G:OP1   | 5:E:18:ARG:CA    | 2.68                     | 0.42              |
| 1:A:1095:U:C4    | 1:A:1096:C:N4    | 2.87                     | 0.42              |
| 1:A:1270:C:H2'   | 1:A:1271:G:C8    | 2.54                     | 0.42              |
| 1:A:1286:A:H2'   | 1:A:1287:A:H4'   | 2.02                     | 0.42              |
| 1:A:1361:G:C6    | 1:A:1362:C:N3    | 2.87                     | 0.42              |
| 4:D:89:THR:HA    | 4:D:92:VAL:HG12  | 2.02                     | 0.42              |
| 7:G:26:PHE:O     | 7:G:30:ILE:HG13  | 2.20                     | 0.42              |
| 8:H:29:SER:HB3   | 8:H:32:LYS:CG    | 2.48                     | 0.42              |
| 1:A:374:A:C6     | 1:A:375:U:C4     | 3.08                     | 0.42              |
| 1:A:402:G:C2     | 1:A:403:C:C2     | 3.08                     | 0.42              |
| 1:A:590:C:N3     | 1:A:650:G:C2     | 2.87                     | 0.42              |
| 1:A:1123:A:H4'   | 10:J:36:GLY:HA3  | 2.02                     | 0.42              |
| 1:A:1158:C:O2    | 1:A:1158:C:H2'   | 2.20                     | 0.42              |
| 3:C:29:TYR:CE1   | 14:N:37:PHE:CE1  | 3.07                     | 0.42              |
| 3:C:34:LEU:HD11  | 14:N:25:VAL:HG21 | 2.01                     | 0.42              |
| 8:H:51:VAL:HB    | 8:H:52:ASP:H     | 1.73                     | 0.42              |
| 13:M:22:ILE:HG22 | 13:M:24:GLY:H    | 1.85                     | 0.42              |
| 1:A:187:C:N3     | 20:T:105:SER:HB2 | 2.35                     | 0.42              |
| 1:A:189(C):C:C2  | 1:A:189(I):G:C2  | 3.08                     | 0.42              |
| 1:A:200:G:C2     | 1:A:218:C:C2     | 3.08                     | 0.42              |
| 1:A:310:G:C2     | 1:A:311:C:C2     | 3.08                     | 0.42              |
| 1:A:402:G:C6     | 1:A:403:C:C4     | 3.08                     | 0.42              |
| 1:A:617:G:N1     | 1:A:618:C:C4     | 2.88                     | 0.42              |
| 1:A:1063:C:O5'   | 1:A:1064:G:H2'   | 2.19                     | 0.42              |
| 1:A:1356:G:N2    | 1:A:1367:C:C2    | 2.88                     | 0.42              |
| 3:C:113:ALA:N    | 3:C:114:PRO:CD   | 2.83                     | 0.42              |
| 5:E:41:VAL:HG23  | 5:E:67:VAL:HG12  | 2.02                     | 0.42              |
| 6:F:30:LEU:HD22  | 6:F:65:VAL:HG11  | 2.01                     | 0.42              |
| 16:P:67:THR:HG22 | 16:P:68:ASP:N    | 2.29                     | 0.42              |
| 1:A:17:U:H2'     | 1:A:18:C:C5      | 2.49                     | 0.42              |
| 1:A:35:G:C5      | 1:A:36:C:C4      | 3.07                     | 0.42              |
| 1:A:377:G:H1     | 1:A:386:C:N4     | 2.17                     | 0.42              |
| 1:A:495:A:H4'    | 1:A:496:A:OP1    | 2.19                     | 0.42              |
| 1:A:891:U:H2'    | 1:A:892:A:H8     | 1.84                     | 0.42              |
| 1:A:1405:G:H2'   | 1:A:1406:U:C6    | 2.55                     | 0.42              |
| 1:A:1411:C:H2'   | 1:A:1412:C:O4'   | 2.20                     | 0.42              |
| 1:A:1478:C:H2'   | 1:A:1479:C:C6    | 2.55                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:48:ALA:HB1   | 5:E:53:LEU:HD23  | 2.02                     | 0.42              |
| 8:H:96:GLY:HA2   | 8:H:130:GLY:HA3  | 2.01                     | 0.42              |
| 11:K:86:GLY:O    | 11:K:91:ARG:HD2  | 2.20                     | 0.42              |
| 18:R:51:LEU:HB3  | 18:R:55:ARG:HB2  | 2.02                     | 0.42              |
| 1:A:90:U:O2'     | 1:A:91:C:H5'     | 2.20                     | 0.41              |
| 1:A:178:C:H2'    | 1:A:179:A:H8     | 1.85                     | 0.41              |
| 1:A:306:G:C6     | 1:A:307:C:C4     | 3.08                     | 0.41              |
| 1:A:488:C:H2'    | 1:A:489:C:C6     | 2.55                     | 0.41              |
| 1:A:509:A:H4'    | 1:A:510:A:OP1    | 2.19                     | 0.41              |
| 1:A:942:G:N2     | 1:A:943:U:H1'    | 2.35                     | 0.41              |
| 1:A:947:G:C2     | 1:A:948:C:C2     | 3.08                     | 0.41              |
| 1:A:985:C:H2'    | 1:A:986:A:C8     | 2.55                     | 0.41              |
| 1:A:1050:G:C2    | 1:A:1051:C:C2    | 3.07                     | 0.41              |
| 1:A:1510:U:H2'   | 1:A:1511:G:C8    | 2.55                     | 0.41              |
| 1:A:1537:U:H3    | 24:Y:28:A:H61    | 1.68                     | 0.41              |
| 5:E:11:ILE:HB    | 5:E:31:LEU:HD12  | 2.02                     | 0.41              |
| 6:F:41:GLU:HB2   | 6:F:62:TRP:HE3   | 1.85                     | 0.41              |
| 1:A:289:G:C6     | 1:A:290:C:C4     | 3.08                     | 0.41              |
| 1:A:502:G:C6     | 1:A:503:C:C4     | 3.08                     | 0.41              |
| 1:A:1198:G:C5    | 1:A:1199:U:C4    | 3.08                     | 0.41              |
| 4:D:67:ILE:O     | 4:D:114:ARG:HD2  | 2.19                     | 0.41              |
| 1:A:241:C:C2     | 1:A:286:G:N2     | 2.89                     | 0.41              |
| 1:A:276:G:H2'    | 1:A:277:C:C6     | 2.55                     | 0.41              |
| 1:A:613:C:H42    | 1:A:627:G:H1     | 1.68                     | 0.41              |
| 1:A:673:G:H1     | 1:A:717:C:H42    | 1.68                     | 0.41              |
| 1:A:874:G:N2     | 1:A:875:C:C2     | 2.88                     | 0.41              |
| 1:A:942:G:N1     | 1:A:1342:C:C2    | 2.88                     | 0.41              |
| 1:A:966:G:C2     | 1:A:967:C:C2     | 3.08                     | 0.41              |
| 1:A:1106:G:C2    | 1:A:1107:C:C2    | 3.08                     | 0.41              |
| 1:A:1423:G:C2    | 1:A:1424:C:C2    | 3.09                     | 0.41              |
| 6:F:2:ARG:HB2    | 6:F:4:TYR:CE2    | 2.55                     | 0.41              |
| 11:K:27:ASN:HA   | 11:K:56:GLY:HA2  | 2.02                     | 0.41              |
| 15:O:9:GLN:HA    | 15:O:12:ILE:HD12 | 2.01                     | 0.41              |
| 18:R:25:THR:HB   | 18:R:42:ARG:NH2  | 2.35                     | 0.41              |
| 1:A:129(A):G:O2' | 1:A:189(F):U:H2' | 2.20                     | 0.41              |
| 1:A:324:G:H8     | 1:A:324:G:OP2    | 2.03                     | 0.41              |
| 1:A:352:C:N3     | 1:A:356:A:N6     | 2.67                     | 0.41              |
| 1:A:568:G:N1     | 1:A:883:C:C4     | 2.89                     | 0.41              |
| 1:A:590:C:C2     | 1:A:650:G:N2     | 2.88                     | 0.41              |
| 1:A:681:C:H42    | 1:A:709:G:H1     | 1.67                     | 0.41              |
| 1:A:725:G:C2     | 1:A:726:C:C2     | 3.09                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:1216:G:N2   | 1:A:1217:C:C2    | 2.88                     | 0.41              |
| 1:A:1526:G:C6   | 1:A:1527:C:C4    | 3.08                     | 0.41              |
| 2:B:105:PHE:HA  | 2:B:108:ILE:HG22 | 2.03                     | 0.41              |
| 3:C:148:GLY:HA3 | 3:C:172:ARG:O    | 2.20                     | 0.41              |
| 4:D:173:TRP:CD1 | 4:D:174:LEU:HG   | 2.56                     | 0.41              |
| 5:E:80:ILE:CD1  | 5:E:138:ALA:HB1  | 2.49                     | 0.41              |
| 7:G:71:PRO:HD3  | 7:G:103:TRP:HZ3  | 1.85                     | 0.41              |
| 10:J:20:ALA:HB1 | 10:J:37:PRO:HB3  | 2.02                     | 0.41              |
| 1:A:130:A:OP1   | 1:A:130:A:C8     | 2.72                     | 0.41              |
| 1:A:197:A:H4'   | 1:A:198:G:O5'    | 2.20                     | 0.41              |
| 1:A:333:G:C6    | 1:A:334:C:N4     | 2.88                     | 0.41              |
| 1:A:381:C:H2'   | 1:A:382:A:O4'    | 2.20                     | 0.41              |
| 1:A:841:U:H6    | 1:A:841:U:H5''   | 1.86                     | 0.41              |
| 1:A:886:G:C2    | 1:A:912:C:O2     | 2.73                     | 0.41              |
| 1:A:937:A:H1'   | 1:A:1379:G:N2    | 2.36                     | 0.41              |
| 1:A:1005:A:O4'  | 1:A:1036:G:N2    | 2.53                     | 0.41              |
| 1:A:1068:G:C2   | 1:A:1069:C:C2    | 3.09                     | 0.41              |
| 1:A:1171:G:C2   | 1:A:1172:C:C2    | 3.09                     | 0.41              |
| 1:A:1464:G:C2   | 1:A:1465:C:N3    | 2.88                     | 0.41              |
| 1:A:417:C:N4    | 1:A:418:C:N4     | 2.69                     | 0.41              |
| 1:A:521:G:C2    | 1:A:522:C:C4     | 3.08                     | 0.41              |
| 1:A:675:A:H2'   | 1:A:676:A:C8     | 2.56                     | 0.41              |
| 1:A:916:G:H2'   | 1:A:917:G:H8     | 1.83                     | 0.41              |
| 1:A:1158:C:O2   | 1:A:1158:C:C2'   | 2.68                     | 0.41              |
| 1:A:1458:G:OP1  | 20:T:32:ALA:HA   | 2.21                     | 0.41              |
| 1:A:1464:G:C6   | 1:A:1465:C:N4    | 2.88                     | 0.41              |
| 2:B:77:ALA:HB2  | 2:B:211:ILE:HG21 | 2.01                     | 0.41              |
| 5:E:79:GLU:HA   | 5:E:91:LEU:O     | 2.21                     | 0.41              |
| 8:H:36:LEU:HD12 | 8:H:59:LEU:HD22  | 2.02                     | 0.41              |
| 17:Q:29:HIS:CG  | 17:Q:30:PRO:HD2  | 2.55                     | 0.41              |
| 1:A:216:G:C2    | 1:A:217:C:N3     | 2.88                     | 0.41              |
| 1:A:306:G:C2    | 1:A:307:C:C2     | 3.08                     | 0.41              |
| 1:A:376:G:H2'   | 1:A:377:G:C8     | 2.52                     | 0.41              |
| 1:A:695:A:OP2   | 11:K:53:SER:N    | 2.53                     | 0.41              |
| 1:A:830:G:H2'   | 1:A:831:U:O4'    | 2.20                     | 0.41              |
| 1:A:1004:A:N7   | 1:A:1037:C:N3    | 2.68                     | 0.41              |
| 1:A:1096:C:C2   | 1:A:1097:C:C5    | 3.08                     | 0.41              |
| 1:A:1171:G:N1   | 1:A:1172:C:C4    | 2.89                     | 0.41              |
| 1:A:1413:A:H2'  | 1:A:1414:U:O4'   | 2.21                     | 0.41              |
| 1:A:1523:G:H2'  | 1:A:1524:C:C6    | 2.56                     | 0.41              |
| 12:L:93:LEU:O   | 12:L:96:VAL:HB   | 2.20                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 14:N:3:ARG:CZ    | 14:N:6:LEU:HD11  | 2.51                     | 0.41              |
| 19:S:17:GLU:HA   | 19:S:20:LEU:HG   | 2.02                     | 0.41              |
| 1:A:265:G:H2'    | 1:A:267:C:H5     | 1.85                     | 0.41              |
| 1:A:427:U:H4'    | 1:A:541:G:H5''   | 2.03                     | 0.41              |
| 1:A:691:G:C8     | 11:K:26:ASN:HB3  | 2.56                     | 0.41              |
| 1:A:769:G:N3     | 1:A:769:G:H2'    | 2.36                     | 0.41              |
| 1:A:903:G:C6     | 1:A:904:C:C4     | 3.09                     | 0.41              |
| 1:A:1398:A:H61   | 5:E:21:ALA:C     | 2.26                     | 0.41              |
| 1:A:1468:A:H2'   | 1:A:1469:G:O4'   | 2.21                     | 0.41              |
| 13:M:16:ASP:HB3  | 13:M:34:LEU:HD11 | 2.03                     | 0.41              |
| 1:A:197:A:N6     | 1:A:221:C:H4'    | 2.35                     | 0.41              |
| 1:A:299:G:C6     | 1:A:300:A:C6     | 3.09                     | 0.41              |
| 1:A:500:G:C2     | 1:A:501:C:C2     | 3.09                     | 0.41              |
| 1:A:563:A:N3     | 1:A:563:A:H2'    | 2.35                     | 0.41              |
| 1:A:577:G:C6     | 1:A:578:C:C4     | 3.08                     | 0.41              |
| 1:A:1048:G:C2    | 1:A:1210:C:C2    | 3.08                     | 0.41              |
| 1:A:1119:C:H2'   | 1:A:1120:G:O4'   | 2.21                     | 0.41              |
| 1:A:1283:G:N2    | 1:A:1284:C:C2    | 2.89                     | 0.41              |
| 1:A:1288:A:H2'   | 1:A:1289:A:H8    | 1.86                     | 0.41              |
| 1:A:1444:C:H6    | 1:A:1444:C:O5'   | 2.04                     | 0.41              |
| 2:B:54:THR:HG21  | 2:B:185:ILE:HG23 | 2.02                     | 0.41              |
| 2:B:215:LEU:O    | 2:B:219:VAL:HG23 | 2.21                     | 0.41              |
| 3:C:29:TYR:CD2   | 3:C:29:TYR:O     | 2.73                     | 0.41              |
| 3:C:65:ALA:HA    | 3:C:100:ALA:O    | 2.21                     | 0.41              |
| 5:E:127:ASN:HA   | 5:E:128:PRO:HD2  | 1.83                     | 0.41              |
| 10:J:60:ARG:CZ   | 10:J:60:ARG:CB   | 2.95                     | 0.41              |
| 20:T:43:LEU:HD11 | 20:T:55:ILE:HD13 | 2.03                     | 0.41              |
| 1:A:666:G:C6     | 1:A:741:G:C5     | 3.09                     | 0.41              |
| 1:A:716:A:C6     | 1:A:717:C:C4     | 3.10                     | 0.41              |
| 1:A:763:G:C6     | 1:A:764:C:C4     | 3.09                     | 0.41              |
| 1:A:794:A:H2'    | 1:A:795:C:C6     | 2.55                     | 0.41              |
| 1:A:861:G:H2'    | 1:A:862:C:C6     | 2.56                     | 0.41              |
| 1:A:1106:G:C2    | 1:A:1107:C:N3    | 2.89                     | 0.41              |
| 1:A:1323:G:H4'   | 1:A:1363:C:C2    | 2.56                     | 0.41              |
| 1:A:1341:U:H2'   | 1:A:1342:C:C6    | 2.55                     | 0.41              |
| 1:A:1374:A:O2'   | 7:G:28:ASN:HB3   | 2.21                     | 0.41              |
| 1:A:1514:C:H2'   | 1:A:1515:C:C6    | 2.56                     | 0.41              |
| 15:O:67:LEU:HD11 | 15:O:87:ILE:HG21 | 2.02                     | 0.41              |
| 1:A:673:G:H2'    | 1:A:674:G:C8     | 2.56                     | 0.40              |
| 1:A:749:C:H2'    | 1:A:750:G:H8     | 1.86                     | 0.40              |
| 1:A:784:C:C2     | 1:A:799:G:N2     | 2.89                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:886:G:C4     | 1:A:887:G:C8     | 3.08                     | 0.40              |
| 1:A:1423:G:C6    | 1:A:1424:C:C4    | 3.09                     | 0.40              |
| 1:A:1425:U:H2'   | 1:A:1426:C:C6    | 2.56                     | 0.40              |
| 1:A:1522:U:H2'   | 1:A:1523:G:H8    | 1.85                     | 0.40              |
| 1:A:1534:A:H2'   | 1:A:1535:C:C6    | 2.56                     | 0.40              |
| 3:C:13:GLY:HA2   | 14:N:57:ARG:HE   | 1.85                     | 0.40              |
| 7:G:39:ALA:HA    | 7:G:42:ILE:HD12  | 2.03                     | 0.40              |
| 8:H:55:GLY:C     | 8:H:56:LYS:HG3   | 2.45                     | 0.40              |
| 15:O:75:PRO:O    | 15:O:78:TYR:HB3  | 2.22                     | 0.40              |
| 1:A:977:A:H1'    | 1:A:982:U:O4     | 2.21                     | 0.40              |
| 1:A:1274:G:H2'   | 1:A:1275:A:C8    | 2.57                     | 0.40              |
| 4:D:61:LYS:HD2   | 4:D:207:TYR:HE1  | 1.86                     | 0.40              |
| 5:E:13:ILE:HA    | 5:E:29:GLY:O     | 2.22                     | 0.40              |
| 10:J:17:ASP:OD1  | 10:J:70:ARG:NH1  | 2.54                     | 0.40              |
| 18:R:61:LYS:HG2  | 18:R:62:GLU:N    | 2.37                     | 0.40              |
| 22:W:55:VAL:HA   | 22:W:66:ARG:O    | 2.19                     | 0.40              |
| 1:A:289:G:N1     | 1:A:290:C:C4     | 2.89                     | 0.40              |
| 1:A:394:G:C2     | 1:A:395:C:C2     | 3.10                     | 0.40              |
| 1:A:832:C:O2     | 1:A:855:G:C2     | 2.74                     | 0.40              |
| 1:A:1198:G:H2'   | 1:A:1199:U:C6    | 2.57                     | 0.40              |
| 1:A:1540:U:H3    | 24:Y:25:A:H61    | 1.67                     | 0.40              |
| 2:B:130:ARG:HD2  | 2:B:130:ARG:N    | 2.36                     | 0.40              |
| 3:C:30:ARG:NH1   | 3:C:30:ARG:CB    | 2.73                     | 0.40              |
| 5:E:127:ASN:O    | 5:E:131:ILE:HG12 | 2.20                     | 0.40              |
| 6:F:3:ARG:HB3    | 6:F:93:SER:HB2   | 2.04                     | 0.40              |
| 7:G:50:ILE:HD11  | 7:G:124:LEU:HB3  | 2.03                     | 0.40              |
| 10:J:17:ASP:CA   | 10:J:70:ARG:NH2  | 2.85                     | 0.40              |
| 10:J:90:LEU:HA   | 10:J:91:PRO:HD3  | 1.76                     | 0.40              |
| 13:M:16:ASP:HB3  | 13:M:34:LEU:CD1  | 2.52                     | 0.40              |
| 14:N:53:LEU:HA   | 14:N:54:PRO:HD2  | 1.85                     | 0.40              |
| 15:O:87:ILE:HG22 | 15:O:88:ARG:H    | 1.87                     | 0.40              |
| 16:P:70:ALA:O    | 16:P:74:LEU:HD12 | 2.21                     | 0.40              |
| 19:S:53:ASN:ND2  | 19:S:75:ALA:HB1  | 2.37                     | 0.40              |
| 20:T:43:LEU:HB3  | 20:T:52:ALA:HB2  | 2.03                     | 0.40              |
| 1:A:102:G:C2     | 1:A:103:C:C2     | 3.09                     | 0.40              |
| 1:A:319:G:C6     | 1:A:320:C:C4     | 3.09                     | 0.40              |
| 1:A:407:G:H1'    | 4:D:119:GLN:NE2  | 2.33                     | 0.40              |
| 1:A:926:G:O5'    | 1:A:926:G:H8     | 2.04                     | 0.40              |
| 1:A:975:A:H4'    | 1:A:976:G:C5'    | 2.51                     | 0.40              |
| 1:A:1099:G:C6    | 1:A:1100:C:C2    | 3.08                     | 0.40              |
| 1:A:1169:A:H2'   | 1:A:1170:A:O4'   | 2.21                     | 0.40              |

*Continued on next page...*

Continued from previous page...

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1241:G:C2     | 1:A:1242:C:C2     | 3.09                     | 0.40              |
| 1:A:1342:C:H5''   | 9:I:125:TYR:CE1   | 2.57                     | 0.40              |
| 2:B:77:ALA:C      | 2:B:79:ASP:H      | 2.29                     | 0.40              |
| 2:B:201:ILE:HG21  | 2:B:214:ILE:HG21  | 2.02                     | 0.40              |
| 5:E:18:ARG:H      | 5:E:25:ARG:H      | 1.69                     | 0.40              |
| 10:J:47:PHE:CZ    | 14:N:37:PHE:HE2   | 2.40                     | 0.40              |
| 12:L:42:THR:CG2   | 12:L:52:LEU:HB3   | 2.51                     | 0.40              |
| 18:R:37:VAL:HG21  | 18:R:78:LEU:HB3   | 2.03                     | 0.40              |
| 23:X:90:PHE:HB2   | 23:X:120:ILE:HG12 | 2.03                     | 0.40              |
| 1:A:289:G:C6      | 1:A:290:C:N4      | 2.90                     | 0.40              |
| 1:A:434:U:H2'     | 1:A:435:C:H6      | 1.84                     | 0.40              |
| 1:A:725:G:C2      | 1:A:726:C:C4      | 3.10                     | 0.40              |
| 1:A:895:G:H2'     | 1:A:896:C:C6      | 2.55                     | 0.40              |
| 1:A:948:C:OP2     | 13:M:108:ARG:HG2  | 2.22                     | 0.40              |
| 1:A:1069:C:N4     | 1:A:1106:G:H1     | 2.18                     | 0.40              |
| 1:A:1113:C:O4'    | 3:C:14:ILE:CD1    | 2.68                     | 0.40              |
| 1:A:1356:G:N2     | 1:A:1357:A:C2     | 2.90                     | 0.40              |
| 1:A:1395:C:H2'    | 1:A:1396:A:C8     | 2.57                     | 0.40              |
| 4:D:42:GLN:C      | 4:D:44:GLY:N      | 2.80                     | 0.40              |
| 4:D:52:SER:O      | 4:D:55:ALA:HB3    | 2.21                     | 0.40              |
| 11:K:86:GLY:HA2   | 11:K:112:THR:HG23 | 2.04                     | 0.40              |
| 11:K:120:ARG:HH11 | 11:K:120:ARG:HG3  | 1.86                     | 0.40              |
| 16:P:19:ILE:H     | 16:P:19:ILE:HG13  | 1.72                     | 0.40              |
| 22:W:32:ILE:HD11  | 22:W:34:ALA:HB2   | 2.04                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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       |
|-----|-------|---------------|-----------|----------|----------|-------------------|
| 2   | B     | 232/256 (91%) | 186 (80%) | 26 (11%) | 20 (9%)  | <b>0</b> <b>9</b> |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 3   | C     | 204/239 (85%)   | 181 (89%)  | 17 (8%)   | 6 (3%)   | 3           | 23  |
| 4   | D     | 206/209 (99%)   | 181 (88%)  | 18 (9%)   | 7 (3%)   | 3           | 21  |
| 5   | E     | 148/162 (91%)   | 130 (88%)  | 13 (9%)   | 5 (3%)   | 3           | 21  |
| 6   | F     | 99/101 (98%)    | 90 (91%)   | 6 (6%)    | 3 (3%)   | 3           | 22  |
| 7   | G     | 153/156 (98%)   | 139 (91%)  | 10 (6%)   | 4 (3%)   | 4           | 25  |
| 8   | H     | 136/138 (99%)   | 124 (91%)  | 9 (7%)    | 3 (2%)   | 5           | 29  |
| 9   | I     | 125/128 (98%)   | 103 (82%)  | 17 (14%)  | 5 (4%)   | 2           | 18  |
| 10  | J     | 96/105 (91%)    | 81 (84%)   | 10 (10%)  | 5 (5%)   | 1           | 15  |
| 11  | K     | 117/129 (91%)   | 98 (84%)   | 14 (12%)  | 5 (4%)   | 2           | 17  |
| 12  | L     | 122/132 (92%)   | 93 (76%)   | 26 (21%)  | 3 (2%)   | 4           | 26  |
| 13  | M     | 115/126 (91%)   | 93 (81%)   | 20 (17%)  | 2 (2%)   | 7           | 35  |
| 14  | N     | 58/61 (95%)     | 45 (78%)   | 11 (19%)  | 2 (3%)   | 3           | 21  |
| 15  | O     | 86/89 (97%)     | 81 (94%)   | 5 (6%)    | 0        | 100         | 100 |
| 16  | P     | 81/88 (92%)     | 68 (84%)   | 13 (16%)  | 0        | 100         | 100 |
| 17  | Q     | 97/105 (92%)    | 82 (84%)   | 14 (14%)  | 1 (1%)   | 12          | 47  |
| 18  | R     | 71/88 (81%)     | 60 (84%)   | 7 (10%)   | 4 (6%)   | 1           | 15  |
| 19  | S     | 78/93 (84%)     | 64 (82%)   | 10 (13%)  | 4 (5%)   | 1           | 15  |
| 20  | T     | 97/106 (92%)    | 87 (90%)   | 5 (5%)    | 5 (5%)   | 1           | 15  |
| 21  | V     | 22/27 (82%)     | 19 (86%)   | 3 (14%)   | 0        | 100         | 100 |
| 22  | W     | 69/72 (96%)     | 63 (91%)   | 4 (6%)    | 2 (3%)   | 3           | 23  |
| 23  | X     | 162/171 (95%)   | 141 (87%)  | 14 (9%)   | 7 (4%)   | 2           | 17  |
| All | All   | 2574/2781 (93%) | 2209 (86%) | 272 (11%) | 93 (4%)  | 4           | 20  |

All (93) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 17  | PHE  |
| 2   | B     | 20  | GLU  |
| 2   | B     | 24  | TRP  |
| 2   | B     | 208 | ILE  |
| 4   | D     | 37  | PRO  |
| 5   | E     | 17  | ALA  |
| 5   | E     | 21  | ALA  |
| 9   | I     | 11  | LYS  |
| 12  | L     | 27  | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | L     | 45  | PRO  |
| 13  | M     | 113 | PRO  |
| 19  | S     | 71  | LEU  |
| 23  | X     | 54  | PRO  |
| 2   | B     | 16  | HIS  |
| 2   | B     | 21  | ARG  |
| 2   | B     | 204 | ASN  |
| 2   | B     | 228 | GLY  |
| 2   | B     | 229 | VAL  |
| 3   | C     | 13  | GLY  |
| 4   | D     | 5   | ILE  |
| 4   | D     | 42  | GLN  |
| 6   | F     | 96  | PRO  |
| 9   | I     | 56  | LEU  |
| 11  | K     | 101 | SER  |
| 17  | Q     | 67  | LYS  |
| 18  | R     | 18  | ARG  |
| 18  | R     | 20  | ALA  |
| 18  | R     | 32  | ARG  |
| 20  | T     | 49  | ALA  |
| 20  | T     | 95  | ALA  |
| 20  | T     | 98  | PRO  |
| 23  | X     | 83  | THR  |
| 23  | X     | 92  | VAL  |
| 3   | C     | 4   | LYS  |
| 4   | D     | 9   | CYS  |
| 4   | D     | 43  | HIS  |
| 7   | G     | 4   | ARG  |
| 7   | G     | 53  | LYS  |
| 10  | J     | 34  | VAL  |
| 10  | J     | 38  | ILE  |
| 10  | J     | 54  | PHE  |
| 10  | J     | 55  | LYS  |
| 11  | K     | 55  | LYS  |
| 13  | M     | 67  | GLU  |
| 19  | S     | 42  | PRO  |
| 2   | B     | 9   | GLU  |
| 2   | B     | 78  | GLN  |
| 2   | B     | 123 | ALA  |
| 3   | C     | 108 | ASN  |
| 4   | D     | 31  | CYS  |
| 7   | G     | 7   | ALA  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | G     | 55  | GLY  |
| 8   | H     | 5   | PRO  |
| 8   | H     | 102 | ARG  |
| 10  | J     | 56  | HIS  |
| 11  | K     | 14  | VAL  |
| 14  | N     | 23  | ARG  |
| 18  | R     | 17  | SER  |
| 19  | S     | 9   | VAL  |
| 20  | T     | 97  | ALA  |
| 22  | W     | 50  | GLY  |
| 23  | X     | 8   | ASN  |
| 23  | X     | 96  | GLU  |
| 23  | X     | 154 | PRO  |
| 2   | B     | 8   | LYS  |
| 2   | B     | 130 | ARG  |
| 2   | B     | 194 | PRO  |
| 2   | B     | 233 | SER  |
| 3   | C     | 156 | ARG  |
| 3   | C     | 179 | ARG  |
| 8   | H     | 75  | ARG  |
| 9   | I     | 54  | ASP  |
| 11  | K     | 74  | ALA  |
| 2   | B     | 75  | LYS  |
| 2   | B     | 125 | PRO  |
| 3   | C     | 3   | ASN  |
| 5   | E     | 85  | GLY  |
| 6   | F     | 15  | ASP  |
| 6   | F     | 35  | ALA  |
| 9   | I     | 24  | GLY  |
| 9   | I     | 119 | ALA  |
| 12  | L     | 79  | GLU  |
| 14  | N     | 7   | ILE  |
| 22  | W     | 2   | LYS  |
| 2   | B     | 167 | PRO  |
| 4   | D     | 69  | GLY  |
| 5   | E     | 77  | PRO  |
| 19  | S     | 8   | GLY  |
| 2   | B     | 131 | PRO  |
| 5   | E     | 105 | VAL  |
| 11  | K     | 48  | ILE  |
| 20  | T     | 96  | GLY  |
| 23  | X     | 55  | PRO  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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 |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 2   | B     | 202/220 (92%)   | 150 (74%)  | 52 (26%)  | 0           | 3  |
| 3   | C     | 160/188 (85%)   | 131 (82%)  | 29 (18%)  | 2           | 10 |
| 4   | D     | 180/181 (99%)   | 123 (68%)  | 57 (32%)  | 0           | 2  |
| 5   | E     | 115/123 (94%)   | 79 (69%)   | 36 (31%)  | 0           | 2  |
| 6   | F     | 90/90 (100%)    | 74 (82%)   | 16 (18%)  | 2           | 11 |
| 7   | G     | 126/127 (99%)   | 116 (92%)  | 10 (8%)   | 11          | 32 |
| 8   | H     | 119/119 (100%)  | 95 (80%)   | 24 (20%)  | 1           | 8  |
| 9   | I     | 98/99 (99%)     | 82 (84%)   | 16 (16%)  | 2           | 12 |
| 10  | J     | 87/92 (95%)     | 71 (82%)   | 16 (18%)  | 1           | 10 |
| 11  | K     | 90/99 (91%)     | 71 (79%)   | 19 (21%)  | 1           | 6  |
| 12  | L     | 104/109 (95%)   | 80 (77%)   | 24 (23%)  | 1           | 5  |
| 13  | M     | 94/101 (93%)    | 79 (84%)   | 15 (16%)  | 2           | 13 |
| 14  | N     | 49/50 (98%)     | 42 (86%)   | 7 (14%)   | 3           | 15 |
| 15  | O     | 79/80 (99%)     | 52 (66%)   | 27 (34%)  | 0           | 2  |
| 16  | P     | 72/74 (97%)     | 60 (83%)   | 12 (17%)  | 2           | 12 |
| 17  | Q     | 94/97 (97%)     | 81 (86%)   | 13 (14%)  | 3           | 15 |
| 18  | R     | 64/77 (83%)     | 47 (73%)   | 17 (27%)  | 0           | 3  |
| 19  | S     | 71/80 (89%)     | 59 (83%)   | 12 (17%)  | 2           | 12 |
| 20  | T     | 76/82 (93%)     | 60 (79%)   | 16 (21%)  | 1           | 6  |
| 21  | V     | 19/22 (86%)     | 17 (90%)   | 2 (10%)   | 6           | 23 |
| 22  | W     | 62/63 (98%)     | 54 (87%)   | 8 (13%)   | 4           | 17 |
| 23  | X     | 145/150 (97%)   | 125 (86%)  | 20 (14%)  | 3           | 15 |
| All | All   | 2196/2323 (94%) | 1748 (80%) | 448 (20%) | 3           | 8  |

All (448) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 8   | LYS  |
| 2   | B     | 10  | LEU  |
| 2   | B     | 15  | VAL  |
| 2   | B     | 16  | HIS  |
| 2   | B     | 21  | ARG  |
| 2   | B     | 23  | ARG  |
| 2   | B     | 28  | PHE  |
| 2   | B     | 30  | ARG  |
| 2   | B     | 40  | HIS  |
| 2   | B     | 44  | LEU  |
| 2   | B     | 45  | GLN  |
| 2   | B     | 61  | LEU  |
| 2   | B     | 64  | ARG  |
| 2   | B     | 73  | THR  |
| 2   | B     | 82  | ARG  |
| 2   | B     | 83  | MET  |
| 2   | B     | 87  | ARG  |
| 2   | B     | 95  | GLN  |
| 2   | B     | 96  | ARG  |
| 2   | B     | 102 | LEU  |
| 2   | B     | 107 | THR  |
| 2   | B     | 111 | ARG  |
| 2   | B     | 112 | VAL  |
| 2   | B     | 114 | ARG  |
| 2   | B     | 126 | GLU  |
| 2   | B     | 127 | ILE  |
| 2   | B     | 130 | ARG  |
| 2   | B     | 136 | VAL  |
| 2   | B     | 137 | ARG  |
| 2   | B     | 142 | LEU  |
| 2   | B     | 144 | ARG  |
| 2   | B     | 146 | GLN  |
| 2   | B     | 154 | LEU  |
| 2   | B     | 155 | LEU  |
| 2   | B     | 157 | ARG  |
| 2   | B     | 165 | VAL  |
| 2   | B     | 168 | THR  |
| 2   | B     | 169 | LYS  |
| 2   | B     | 172 | ILE  |
| 2   | B     | 178 | ARG  |
| 2   | B     | 180 | LEU  |
| 2   | B     | 187 | LEU  |
| 2   | B     | 190 | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 195 | ASP  |
| 2   | B     | 198 | ASP  |
| 2   | B     | 200 | ILE  |
| 2   | B     | 205 | ASP  |
| 2   | B     | 208 | ILE  |
| 2   | B     | 211 | ILE  |
| 2   | B     | 213 | LEU  |
| 2   | B     | 221 | LEU  |
| 2   | B     | 229 | VAL  |
| 3   | C     | 3   | ASN  |
| 3   | C     | 4   | LYS  |
| 3   | C     | 14  | ILE  |
| 3   | C     | 21  | ARG  |
| 3   | C     | 27  | LYS  |
| 3   | C     | 30  | ARG  |
| 3   | C     | 33  | LEU  |
| 3   | C     | 40  | ARG  |
| 3   | C     | 45  | LYS  |
| 3   | C     | 52  | LEU  |
| 3   | C     | 68  | VAL  |
| 3   | C     | 77  | ILE  |
| 3   | C     | 82  | GLU  |
| 3   | C     | 87  | LEU  |
| 3   | C     | 90  | GLU  |
| 3   | C     | 91  | LEU  |
| 3   | C     | 94  | LEU  |
| 3   | C     | 98  | ASN  |
| 3   | C     | 101 | LEU  |
| 3   | C     | 102 | ASN  |
| 3   | C     | 115 | LEU  |
| 3   | C     | 119 | ARG  |
| 3   | C     | 157 | ILE  |
| 3   | C     | 173 | VAL  |
| 3   | C     | 177 | THR  |
| 3   | C     | 188 | LEU  |
| 3   | C     | 190 | ARG  |
| 3   | C     | 191 | THR  |
| 3   | C     | 204 | LEU  |
| 4   | D     | 5   | ILE  |
| 4   | D     | 11  | LEU  |
| 4   | D     | 13  | ARG  |
| 4   | D     | 14  | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 15  | GLU  |
| 4   | D     | 21  | LEU  |
| 4   | D     | 22  | LYS  |
| 4   | D     | 25  | ARG  |
| 4   | D     | 27  | TYR  |
| 4   | D     | 30  | LYS  |
| 4   | D     | 35  | ARG  |
| 4   | D     | 43  | HIS  |
| 4   | D     | 45  | GLN  |
| 4   | D     | 46  | LYS  |
| 4   | D     | 49  | ARG  |
| 4   | D     | 53  | ASP  |
| 4   | D     | 59  | ARG  |
| 4   | D     | 64  | LEU  |
| 4   | D     | 65  | ARG  |
| 4   | D     | 70  | ILE  |
| 4   | D     | 74  | GLN  |
| 4   | D     | 76  | ARG  |
| 4   | D     | 78  | LEU  |
| 4   | D     | 83  | SER  |
| 4   | D     | 84  | LYS  |
| 4   | D     | 96  | LEU  |
| 4   | D     | 97  | LEU  |
| 4   | D     | 112 | VAL  |
| 4   | D     | 115 | ARG  |
| 4   | D     | 119 | GLN  |
| 4   | D     | 122 | ARG  |
| 4   | D     | 132 | ARG  |
| 4   | D     | 135 | LEU  |
| 4   | D     | 137 | SER  |
| 4   | D     | 139 | ARG  |
| 4   | D     | 140 | VAL  |
| 4   | D     | 141 | ARG  |
| 4   | D     | 144 | ASP  |
| 4   | D     | 154 | ASN  |
| 4   | D     | 155 | LEU  |
| 4   | D     | 157 | LEU  |
| 4   | D     | 158 | ILE  |
| 4   | D     | 162 | LEU  |
| 4   | D     | 163 | GLU  |
| 4   | D     | 168 | ARG  |
| 4   | D     | 174 | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 176 | LEU  |
| 4   | D     | 178 | VAL  |
| 4   | D     | 181 | MET  |
| 4   | D     | 186 | LEU  |
| 4   | D     | 187 | ARG  |
| 4   | D     | 190 | ASP  |
| 4   | D     | 192 | GLU  |
| 4   | D     | 193 | ASP  |
| 4   | D     | 196 | LEU  |
| 4   | D     | 200 | GLU  |
| 4   | D     | 209 | ARG  |
| 5   | E     | 7   | GLU  |
| 5   | E     | 11  | ILE  |
| 5   | E     | 12  | LEU  |
| 5   | E     | 13  | ILE  |
| 5   | E     | 14  | ARG  |
| 5   | E     | 19  | MET  |
| 5   | E     | 27  | ARG  |
| 5   | E     | 32  | VAL  |
| 5   | E     | 33  | VAL  |
| 5   | E     | 34  | VAL  |
| 5   | E     | 36  | ASP  |
| 5   | E     | 37  | ARG  |
| 5   | E     | 40  | ARG  |
| 5   | E     | 41  | VAL  |
| 5   | E     | 43  | LEU  |
| 5   | E     | 47  | LYS  |
| 5   | E     | 63  | ARG  |
| 5   | E     | 67  | VAL  |
| 5   | E     | 71  | LEU  |
| 5   | E     | 76  | ILE  |
| 5   | E     | 79  | GLU  |
| 5   | E     | 80  | ILE  |
| 5   | E     | 91  | LEU  |
| 5   | E     | 98  | THR  |
| 5   | E     | 107 | ARG  |
| 5   | E     | 111 | GLU  |
| 5   | E     | 115 | VAL  |
| 5   | E     | 116 | THR  |
| 5   | E     | 118 | ILE  |
| 5   | E     | 127 | ASN  |
| 5   | E     | 135 | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | E     | 136 | MET  |
| 5   | E     | 141 | GLN  |
| 5   | E     | 144 | THR  |
| 5   | E     | 147 | ASP  |
| 5   | E     | 148 | VAL  |
| 6   | F     | 3   | ARG  |
| 6   | F     | 5   | GLU  |
| 6   | F     | 10  | LEU  |
| 6   | F     | 18  | GLN  |
| 6   | F     | 19  | LEU  |
| 6   | F     | 27  | GLN  |
| 6   | F     | 28  | ARG  |
| 6   | F     | 31  | GLU  |
| 6   | F     | 40  | VAL  |
| 6   | F     | 61  | LEU  |
| 6   | F     | 69  | GLU  |
| 6   | F     | 75  | LEU  |
| 6   | F     | 77  | ARG  |
| 6   | F     | 82  | ARG  |
| 6   | F     | 86  | ARG  |
| 6   | F     | 91  | VAL  |
| 7   | G     | 16  | LEU  |
| 7   | G     | 24  | THR  |
| 7   | G     | 57  | GLU  |
| 7   | G     | 60  | LYS  |
| 7   | G     | 74  | GLU  |
| 7   | G     | 91  | VAL  |
| 7   | G     | 136 | LYS  |
| 7   | G     | 137 | LYS  |
| 7   | G     | 142 | GLU  |
| 7   | G     | 156 | TRP  |
| 8   | H     | 8   | ASP  |
| 8   | H     | 11  | THR  |
| 8   | H     | 18  | ARG  |
| 8   | H     | 21  | LYS  |
| 8   | H     | 26  | VAL  |
| 8   | H     | 38  | ILE  |
| 8   | H     | 39  | LEU  |
| 8   | H     | 45  | ILE  |
| 8   | H     | 50  | ARG  |
| 8   | H     | 53  | VAL  |
| 8   | H     | 59  | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | H     | 61  | VAL  |
| 8   | H     | 63  | LEU  |
| 8   | H     | 69  | ARG  |
| 8   | H     | 77  | GLU  |
| 8   | H     | 78  | GLN  |
| 8   | H     | 82  | HIS  |
| 8   | H     | 92  | ARG  |
| 8   | H     | 93  | VAL  |
| 8   | H     | 109 | ILE  |
| 8   | H     | 120 | THR  |
| 8   | H     | 127 | LEU  |
| 8   | H     | 134 | ILE  |
| 8   | H     | 135 | CYS  |
| 9   | I     | 3   | GLN  |
| 9   | I     | 12  | GLU  |
| 9   | I     | 38  | GLN  |
| 9   | I     | 56  | LEU  |
| 9   | I     | 65  | VAL  |
| 9   | I     | 78  | LYS  |
| 9   | I     | 79  | LEU  |
| 9   | I     | 85  | LEU  |
| 9   | I     | 87  | GLN  |
| 9   | I     | 95  | LYS  |
| 9   | I     | 102 | LEU  |
| 9   | I     | 109 | VAL  |
| 9   | I     | 111 | ARG  |
| 9   | I     | 112 | LYS  |
| 9   | I     | 113 | LYS  |
| 9   | I     | 127 | LYS  |
| 10  | J     | 4   | ILE  |
| 10  | J     | 8   | LEU  |
| 10  | J     | 16  | LEU  |
| 10  | J     | 23  | ILE  |
| 10  | J     | 44  | VAL  |
| 10  | J     | 46  | ARG  |
| 10  | J     | 49  | VAL  |
| 10  | J     | 61  | GLU  |
| 10  | J     | 62  | HIS  |
| 10  | J     | 66  | ARG  |
| 10  | J     | 71  | LEU  |
| 10  | J     | 74  | ILE  |
| 10  | J     | 82  | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | J     | 83  | GLU  |
| 10  | J     | 86  | MET  |
| 10  | J     | 87  | THR  |
| 11  | K     | 18  | ARG  |
| 11  | K     | 25  | TYR  |
| 11  | K     | 29  | ILE  |
| 11  | K     | 41  | THR  |
| 11  | K     | 47  | VAL  |
| 11  | K     | 48  | ILE  |
| 11  | K     | 54  | ARG  |
| 11  | K     | 57  | THR  |
| 11  | K     | 62  | GLN  |
| 11  | K     | 63  | LEU  |
| 11  | K     | 77  | MET  |
| 11  | K     | 85  | ARG  |
| 11  | K     | 92  | GLU  |
| 11  | K     | 93  | GLN  |
| 11  | K     | 98  | LEU  |
| 11  | K     | 103 | LEU  |
| 11  | K     | 109 | VAL  |
| 11  | K     | 116 | HIS  |
| 11  | K     | 123 | LYS  |
| 12  | L     | 6   | THR  |
| 12  | L     | 7   | ILE  |
| 12  | L     | 11  | VAL  |
| 12  | L     | 17  | LYS  |
| 12  | L     | 18  | VAL  |
| 12  | L     | 33  | ARG  |
| 12  | L     | 36  | VAL  |
| 12  | L     | 39  | VAL  |
| 12  | L     | 41  | ARG  |
| 12  | L     | 46  | LYS  |
| 12  | L     | 53  | ARG  |
| 12  | L     | 57  | LYS  |
| 12  | L     | 59  | ARG  |
| 12  | L     | 70  | ILE  |
| 12  | L     | 81  | SER  |
| 12  | L     | 83  | VAL  |
| 12  | L     | 85  | ILE  |
| 12  | L     | 89  | ARG  |
| 12  | L     | 90  | VAL  |
| 12  | L     | 96  | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | L     | 104 | VAL  |
| 12  | L     | 110 | VAL  |
| 12  | L     | 113 | ARG  |
| 12  | L     | 122 | THR  |
| 13  | M     | 8   | GLU  |
| 13  | M     | 12  | ASN  |
| 13  | M     | 15  | VAL  |
| 13  | M     | 17  | VAL  |
| 13  | M     | 32  | GLU  |
| 13  | M     | 37  | THR  |
| 13  | M     | 44  | ARG  |
| 13  | M     | 45  | VAL  |
| 13  | M     | 54  | VAL  |
| 13  | M     | 73  | GLU  |
| 13  | M     | 80  | ARG  |
| 13  | M     | 90  | LEU  |
| 13  | M     | 110 | ARG  |
| 13  | M     | 115 | LYS  |
| 13  | M     | 116 | THR  |
| 14  | N     | 7   | ILE  |
| 14  | N     | 12  | ARG  |
| 14  | N     | 17  | LYS  |
| 14  | N     | 33  | VAL  |
| 14  | N     | 41  | ARG  |
| 14  | N     | 44  | LEU  |
| 14  | N     | 56  | VAL  |
| 15  | O     | 10  | LYS  |
| 15  | O     | 17  | ARG  |
| 15  | O     | 21  | ASP  |
| 15  | O     | 22  | THR  |
| 15  | O     | 25  | THR  |
| 15  | O     | 27  | VAL  |
| 15  | O     | 28  | GLN  |
| 15  | O     | 29  | VAL  |
| 15  | O     | 39  | LEU  |
| 15  | O     | 40  | SER  |
| 15  | O     | 41  | GLU  |
| 15  | O     | 43  | LEU  |
| 15  | O     | 45  | VAL  |
| 15  | O     | 48  | LYS  |
| 15  | O     | 49  | ASP  |
| 15  | O     | 52  | SER  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | O     | 54  | ARG  |
| 15  | O     | 56  | LEU  |
| 15  | O     | 57  | LEU  |
| 15  | O     | 64  | ARG  |
| 15  | O     | 67  | LEU  |
| 15  | O     | 68  | ARG  |
| 15  | O     | 70  | LEU  |
| 15  | O     | 72  | ARG  |
| 15  | O     | 77  | ARG  |
| 15  | O     | 84  | LYS  |
| 15  | O     | 87  | ILE  |
| 16  | P     | 20  | VAL  |
| 16  | P     | 23  | ASP  |
| 16  | P     | 28  | ARG  |
| 16  | P     | 29  | ASP  |
| 16  | P     | 42  | ARG  |
| 16  | P     | 44  | THR  |
| 16  | P     | 45  | THR  |
| 16  | P     | 54  | GLU  |
| 16  | P     | 55  | ARG  |
| 16  | P     | 60  | LEU  |
| 16  | P     | 73  | LEU  |
| 16  | P     | 81  | ARG  |
| 17  | Q     | 5   | VAL  |
| 17  | Q     | 15  | MET  |
| 17  | Q     | 27  | PHE  |
| 17  | Q     | 36  | ILE  |
| 17  | Q     | 38  | ARG  |
| 17  | Q     | 52  | LYS  |
| 17  | Q     | 53  | LEU  |
| 17  | Q     | 63  | ARG  |
| 17  | Q     | 68  | ARG  |
| 17  | Q     | 81  | ARG  |
| 17  | Q     | 89  | LEU  |
| 17  | Q     | 93  | GLN  |
| 17  | Q     | 100 | LYS  |
| 18  | R     | 35  | ARG  |
| 18  | R     | 38  | GLU  |
| 18  | R     | 41  | LYS  |
| 18  | R     | 44  | LEU  |
| 18  | R     | 46  | GLU  |
| 18  | R     | 47  | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | R     | 53  | ARG  |
| 18  | R     | 54  | ARG  |
| 18  | R     | 56  | THR  |
| 18  | R     | 61  | LYS  |
| 18  | R     | 66  | LEU  |
| 18  | R     | 69  | THR  |
| 18  | R     | 75  | ILE  |
| 18  | R     | 76  | LEU  |
| 18  | R     | 82  | THR  |
| 18  | R     | 86  | VAL  |
| 18  | R     | 87  | ARG  |
| 19  | S     | 6   | LYS  |
| 19  | S     | 7   | LYS  |
| 19  | S     | 13  | ASP  |
| 19  | S     | 15  | LEU  |
| 19  | S     | 19  | VAL  |
| 19  | S     | 25  | LYS  |
| 19  | S     | 29  | ARG  |
| 19  | S     | 30  | LEU  |
| 19  | S     | 37  | ARG  |
| 19  | S     | 39  | THR  |
| 19  | S     | 41  | VAL  |
| 19  | S     | 63  | THR  |
| 20  | T     | 10  | LEU  |
| 20  | T     | 19  | SER  |
| 20  | T     | 22  | ARG  |
| 20  | T     | 23  | ARG  |
| 20  | T     | 24  | LEU  |
| 20  | T     | 38  | LYS  |
| 20  | T     | 46  | GLU  |
| 20  | T     | 55  | ILE  |
| 20  | T     | 56  | MET  |
| 20  | T     | 62  | LEU  |
| 20  | T     | 64  | ASP  |
| 20  | T     | 68  | LYS  |
| 20  | T     | 72  | LEU  |
| 20  | T     | 74  | LYS  |
| 20  | T     | 75  | ASN  |
| 20  | T     | 84  | LEU  |
| 21  | V     | 7   | ARG  |
| 21  | V     | 12  | LYS  |
| 22  | W     | 8   | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | W     | 12  | VAL  |
| 22  | W     | 19  | ASN  |
| 22  | W     | 23  | ARG  |
| 22  | W     | 32  | ILE  |
| 22  | W     | 33  | LEU  |
| 22  | W     | 47  | ILE  |
| 22  | W     | 48  | LEU  |
| 23  | X     | 31  | THR  |
| 23  | X     | 35  | LEU  |
| 23  | X     | 73  | GLU  |
| 23  | X     | 74  | LYS  |
| 23  | X     | 78  | LYS  |
| 23  | X     | 83  | THR  |
| 23  | X     | 98  | ASP  |
| 23  | X     | 118 | VAL  |
| 23  | X     | 121 | MET  |
| 23  | X     | 123 | ARG  |
| 23  | X     | 125 | ARG  |
| 23  | X     | 132 | LEU  |
| 23  | X     | 134 | GLU  |
| 23  | X     | 143 | ASP  |
| 23  | X     | 144 | LEU  |
| 23  | X     | 152 | MET  |
| 23  | X     | 161 | MET  |
| 23  | X     | 163 | MET  |
| 23  | X     | 164 | LEU  |
| 23  | X     | 170 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 16  | HIS  |
| 2   | B     | 19  | HIS  |
| 2   | B     | 25  | ASN  |
| 2   | B     | 95  | GLN  |
| 2   | B     | 146 | GLN  |
| 2   | B     | 204 | ASN  |
| 3   | C     | 3   | ASN  |
| 3   | C     | 6   | HIS  |
| 3   | C     | 28  | GLN  |
| 3   | C     | 63  | ASN  |
| 3   | C     | 107 | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 108 | ASN  |
| 3   | C     | 123 | GLN  |
| 3   | C     | 176 | HIS  |
| 4   | D     | 103 | ASN  |
| 4   | D     | 119 | GLN  |
| 4   | D     | 123 | HIS  |
| 4   | D     | 125 | HIS  |
| 4   | D     | 129 | ASN  |
| 6   | F     | 7   | ASN  |
| 6   | F     | 18  | GLN  |
| 6   | F     | 64  | GLN  |
| 6   | F     | 100 | ASN  |
| 7   | G     | 64  | GLN  |
| 7   | G     | 86  | GLN  |
| 7   | G     | 97  | GLN  |
| 9   | I     | 23  | ASN  |
| 10  | J     | 68  | HIS  |
| 10  | J     | 76  | ASN  |
| 12  | L     | 8   | ASN  |
| 12  | L     | 49  | ASN  |
| 12  | L     | 75  | HIS  |
| 12  | L     | 80  | HIS  |
| 13  | M     | 106 | ASN  |
| 15  | O     | 28  | GLN  |
| 15  | O     | 37  | ASN  |
| 15  | O     | 46  | HIS  |
| 15  | O     | 53  | HIS  |
| 15  | O     | 62  | GLN  |
| 16  | P     | 14  | ASN  |
| 16  | P     | 65  | GLN  |
| 17  | Q     | 93  | GLN  |
| 18  | R     | 36  | ASN  |
| 18  | R     | 63  | GLN  |
| 19  | S     | 14  | HIS  |
| 19  | S     | 53  | ASN  |
| 19  | S     | 65  | ASN  |
| 20  | T     | 73  | HIS  |
| 23  | X     | 97  | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | A     | 1507/1522 (99%) | 474 (31%)         | 114 (7%)        |
| 24  | Y     | 17/45 (37%)     | 8 (47%)           | 0               |
| All | All   | 1524/1567 (97%) | 482 (31%)         | 114 (7%)        |

All (482) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 8   | A    |
| 1   | A     | 9   | G    |
| 1   | A     | 13  | U    |
| 1   | A     | 14  | U    |
| 1   | A     | 18  | C    |
| 1   | A     | 19  | C    |
| 1   | A     | 22  | G    |
| 1   | A     | 29  | G    |
| 1   | A     | 30  | U    |
| 1   | A     | 31  | G    |
| 1   | A     | 32  | A    |
| 1   | A     | 35  | G    |
| 1   | A     | 39  | G    |
| 1   | A     | 43  | C    |
| 1   | A     | 44  | G    |
| 1   | A     | 47  | C    |
| 1   | A     | 48  | C    |
| 1   | A     | 49  | U    |
| 1   | A     | 50  | A    |
| 1   | A     | 51  | A    |
| 1   | A     | 52  | G    |
| 1   | A     | 54  | C    |
| 1   | A     | 59  | A    |
| 1   | A     | 60  | A    |
| 1   | A     | 61  | G    |
| 1   | A     | 62  | U    |
| 1   | A     | 66  | G    |
| 1   | A     | 68  | G    |
| 1   | A     | 73  | G    |
| 1   | A     | 76  | C    |
| 1   | A     | 77  | G    |
| 1   | A     | 79  | G    |
| 1   | A     | 81  | U    |
| 1   | A     | 83  | U    |
| 1   | A     | 91  | C    |
| 1   | A     | 97  | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 101    | A    |
| 1   | A     | 108    | G    |
| 1   | A     | 115    | G    |
| 1   | A     | 116    | A    |
| 1   | A     | 120    | A    |
| 1   | A     | 121    | C    |
| 1   | A     | 122    | G    |
| 1   | A     | 129(A) | G    |
| 1   | A     | 130    | A    |
| 1   | A     | 131    | C    |
| 1   | A     | 142    | G    |
| 1   | A     | 144    | G    |
| 1   | A     | 151    | A    |
| 1   | A     | 153    | C    |
| 1   | A     | 157    | G    |
| 1   | A     | 163    | C    |
| 1   | A     | 167    | G    |
| 1   | A     | 173    | U    |
| 1   | A     | 174    | C    |
| 1   | A     | 175    | C    |
| 1   | A     | 181    | G    |
| 1   | A     | 182    | U    |
| 1   | A     | 189(E) | U    |
| 1   | A     | 189(F) | U    |
| 1   | A     | 189(G) | G    |
| 1   | A     | 189(H) | G    |
| 1   | A     | 195    | A    |
| 1   | A     | 196    | A    |
| 1   | A     | 197    | A    |
| 1   | A     | 198    | G    |
| 1   | A     | 199    | G    |
| 1   | A     | 201    | C    |
| 1   | A     | 203    | U    |
| 1   | A     | 204    | U    |
| 1   | A     | 217    | C    |
| 1   | A     | 220    | G    |
| 1   | A     | 243    | A    |
| 1   | A     | 244    | U    |
| 1   | A     | 245    | C    |
| 1   | A     | 247    | G    |
| 1   | A     | 251    | G    |
| 1   | A     | 252    | U    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 253 | U    |
| 1   | A     | 266 | G    |
| 1   | A     | 267 | C    |
| 1   | A     | 279 | A    |
| 1   | A     | 280 | C    |
| 1   | A     | 281 | G    |
| 1   | A     | 282 | A    |
| 1   | A     | 283 | C    |
| 1   | A     | 288 | A    |
| 1   | A     | 289 | G    |
| 1   | A     | 290 | C    |
| 1   | A     | 291 | C    |
| 1   | A     | 298 | A    |
| 1   | A     | 299 | G    |
| 1   | A     | 300 | A    |
| 1   | A     | 301 | G    |
| 1   | A     | 306 | G    |
| 1   | A     | 309 | G    |
| 1   | A     | 315 | A    |
| 1   | A     | 316 | G    |
| 1   | A     | 321 | A    |
| 1   | A     | 324 | G    |
| 1   | A     | 325 | A    |
| 1   | A     | 327 | A    |
| 1   | A     | 328 | C    |
| 1   | A     | 329 | A    |
| 1   | A     | 330 | C    |
| 1   | A     | 332 | G    |
| 1   | A     | 339 | C    |
| 1   | A     | 340 | U    |
| 1   | A     | 342 | C    |
| 1   | A     | 344 | A    |
| 1   | A     | 345 | C    |
| 1   | A     | 350 | G    |
| 1   | A     | 351 | G    |
| 1   | A     | 352 | C    |
| 1   | A     | 353 | A    |
| 1   | A     | 357 | G    |
| 1   | A     | 366 | C    |
| 1   | A     | 367 | U    |
| 1   | A     | 368 | U    |
| 1   | A     | 372 | C    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 373 | A    |
| 1   | A     | 375 | U    |
| 1   | A     | 378 | G    |
| 1   | A     | 384 | G    |
| 1   | A     | 388 | G    |
| 1   | A     | 389 | A    |
| 1   | A     | 390 | C    |
| 1   | A     | 392 | G    |
| 1   | A     | 393 | A    |
| 1   | A     | 395 | C    |
| 1   | A     | 397 | A    |
| 1   | A     | 398 | C    |
| 1   | A     | 406 | G    |
| 1   | A     | 409 | G    |
| 1   | A     | 412 | A    |
| 1   | A     | 413 | G    |
| 1   | A     | 414 | A    |
| 1   | A     | 419 | C    |
| 1   | A     | 421 | U    |
| 1   | A     | 422 | C    |
| 1   | A     | 423 | G    |
| 1   | A     | 428 | G    |
| 1   | A     | 429 | U    |
| 1   | A     | 438 | G    |
| 1   | A     | 439 | A    |
| 1   | A     | 441 | A    |
| 1   | A     | 444 | C    |
| 1   | A     | 446 | G    |
| 1   | A     | 450 | G    |
| 1   | A     | 451 | A    |
| 1   | A     | 452 | A    |
| 1   | A     | 470 | C    |
| 1   | A     | 484 | G    |
| 1   | A     | 485 | G    |
| 1   | A     | 492 | G    |
| 1   | A     | 495 | A    |
| 1   | A     | 496 | A    |
| 1   | A     | 498 | U    |
| 1   | A     | 510 | A    |
| 1   | A     | 511 | C    |
| 1   | A     | 517 | G    |
| 1   | A     | 518 | C    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 519 | C    |
| 1   | A     | 521 | G    |
| 1   | A     | 524 | G    |
| 1   | A     | 527 | G    |
| 1   | A     | 528 | C    |
| 1   | A     | 529 | G    |
| 1   | A     | 531 | U    |
| 1   | A     | 532 | A    |
| 1   | A     | 534 | U    |
| 1   | A     | 535 | A    |
| 1   | A     | 540 | G    |
| 1   | A     | 545 | C    |
| 1   | A     | 547 | A    |
| 1   | A     | 548 | G    |
| 1   | A     | 550 | G    |
| 1   | A     | 559 | A    |
| 1   | A     | 560 | U    |
| 1   | A     | 561 | U    |
| 1   | A     | 562 | C    |
| 1   | A     | 564 | C    |
| 1   | A     | 565 | U    |
| 1   | A     | 568 | G    |
| 1   | A     | 572 | A    |
| 1   | A     | 573 | A    |
| 1   | A     | 576 | G    |
| 1   | A     | 577 | G    |
| 1   | A     | 578 | C    |
| 1   | A     | 587 | G    |
| 1   | A     | 588 | G    |
| 1   | A     | 595 | G    |
| 1   | A     | 596 | C    |
| 1   | A     | 597 | G    |
| 1   | A     | 607 | A    |
| 1   | A     | 619 | U    |
| 1   | A     | 620 | C    |
| 1   | A     | 641 | U    |
| 1   | A     | 642 | A    |
| 1   | A     | 644 | G    |
| 1   | A     | 650 | G    |
| 1   | A     | 652 | U    |
| 1   | A     | 653 | A    |
| 1   | A     | 654 | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 665 | A    |
| 1   | A     | 666 | G    |
| 1   | A     | 671 | G    |
| 1   | A     | 672 | U    |
| 1   | A     | 677 | U    |
| 1   | A     | 687 | A    |
| 1   | A     | 688 | G    |
| 1   | A     | 697 | U    |
| 1   | A     | 701 | C    |
| 1   | A     | 702 | A    |
| 1   | A     | 703 | G    |
| 1   | A     | 713 | G    |
| 1   | A     | 716 | A    |
| 1   | A     | 717 | C    |
| 1   | A     | 721 | G    |
| 1   | A     | 723 | U    |
| 1   | A     | 724 | G    |
| 1   | A     | 731 | G    |
| 1   | A     | 737 | A    |
| 1   | A     | 740 | U    |
| 1   | A     | 748 | C    |
| 1   | A     | 749 | C    |
| 1   | A     | 755 | G    |
| 1   | A     | 760 | G    |
| 1   | A     | 764 | C    |
| 1   | A     | 777 | A    |
| 1   | A     | 784 | C    |
| 1   | A     | 785 | G    |
| 1   | A     | 787 | A    |
| 1   | A     | 792 | A    |
| 1   | A     | 793 | U    |
| 1   | A     | 794 | A    |
| 1   | A     | 802 | A    |
| 1   | A     | 812 | C    |
| 1   | A     | 815 | A    |
| 1   | A     | 817 | C    |
| 1   | A     | 819 | A    |
| 1   | A     | 821 | G    |
| 1   | A     | 828 | A    |
| 1   | A     | 835 | U    |
| 1   | A     | 839 | U    |
| 1   | A     | 840 | C    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 841 | U    |
| 1   | A     | 851 | G    |
| 1   | A     | 853 | G    |
| 1   | A     | 855 | G    |
| 1   | A     | 859 | A    |
| 1   | A     | 864 | A    |
| 1   | A     | 865 | A    |
| 1   | A     | 866 | C    |
| 1   | A     | 869 | G    |
| 1   | A     | 871 | U    |
| 1   | A     | 872 | A    |
| 1   | A     | 873 | A    |
| 1   | A     | 874 | G    |
| 1   | A     | 876 | G    |
| 1   | A     | 882 | C    |
| 1   | A     | 885 | G    |
| 1   | A     | 889 | A    |
| 1   | A     | 900 | A    |
| 1   | A     | 902 | G    |
| 1   | A     | 911 | U    |
| 1   | A     | 920 | U    |
| 1   | A     | 922 | G    |
| 1   | A     | 927 | G    |
| 1   | A     | 930 | C    |
| 1   | A     | 932 | C    |
| 1   | A     | 933 | G    |
| 1   | A     | 934 | C    |
| 1   | A     | 935 | A    |
| 1   | A     | 937 | A    |
| 1   | A     | 942 | G    |
| 1   | A     | 943 | U    |
| 1   | A     | 945 | G    |
| 1   | A     | 950 | U    |
| 1   | A     | 960 | U    |
| 1   | A     | 961 | U    |
| 1   | A     | 965 | A    |
| 1   | A     | 966 | G    |
| 1   | A     | 968 | A    |
| 1   | A     | 969 | A    |
| 1   | A     | 971 | G    |
| 1   | A     | 972 | C    |
| 1   | A     | 974 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | A     | 975     | A    |
| 1   | A     | 976     | G    |
| 1   | A     | 977     | A    |
| 1   | A     | 989     | C    |
| 1   | A     | 991     | U    |
| 1   | A     | 992     | U    |
| 1   | A     | 993     | G    |
| 1   | A     | 994     | A    |
| 1   | A     | 998     | G    |
| 1   | A     | 1000    | U    |
| 1   | A     | 1001    | A    |
| 1   | A     | 1005    | A    |
| 1   | A     | 1007    | C    |
| 1   | A     | 1023    | G    |
| 1   | A     | 1024    | G    |
| 1   | A     | 1025    | U    |
| 1   | A     | 1026    | G    |
| 1   | A     | 1028    | C    |
| 1   | A     | 1029    | C    |
| 1   | A     | 1030(C) | G    |
| 1   | A     | 1031    | G    |
| 1   | A     | 1045    | C    |
| 1   | A     | 1046    | A    |
| 1   | A     | 1049    | U    |
| 1   | A     | 1050    | G    |
| 1   | A     | 1051    | C    |
| 1   | A     | 1053    | G    |
| 1   | A     | 1054    | C    |
| 1   | A     | 1055    | A    |
| 1   | A     | 1060    | C    |
| 1   | A     | 1065    | U    |
| 1   | A     | 1066    | C    |
| 1   | A     | 1067    | A    |
| 1   | A     | 1070    | U    |
| 1   | A     | 1074    | G    |
| 1   | A     | 1078    | U    |
| 1   | A     | 1079    | G    |
| 1   | A     | 1081    | G    |
| 1   | A     | 1085    | U    |
| 1   | A     | 1086    | U    |
| 1   | A     | 1092    | A    |
| 1   | A     | 1093    | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1094 | G    |
| 1   | A     | 1095 | U    |
| 1   | A     | 1097 | C    |
| 1   | A     | 1098 | C    |
| 1   | A     | 1100 | C    |
| 1   | A     | 1101 | A    |
| 1   | A     | 1102 | A    |
| 1   | A     | 1104 | G    |
| 1   | A     | 1117 | G    |
| 1   | A     | 1118 | C    |
| 1   | A     | 1124 | G    |
| 1   | A     | 1125 | U    |
| 1   | A     | 1126 | U    |
| 1   | A     | 1127 | G    |
| 1   | A     | 1128 | C    |
| 1   | A     | 1129 | C    |
| 1   | A     | 1130 | A    |
| 1   | A     | 1131 | G    |
| 1   | A     | 1135 | U    |
| 1   | A     | 1136 | U    |
| 1   | A     | 1137 | C    |
| 1   | A     | 1138 | G    |
| 1   | A     | 1139 | G    |
| 1   | A     | 1145 | C    |
| 1   | A     | 1146 | A    |
| 1   | A     | 1150 | U    |
| 1   | A     | 1151 | A    |
| 1   | A     | 1152 | A    |
| 1   | A     | 1157 | A    |
| 1   | A     | 1158 | C    |
| 1   | A     | 1159 | U    |
| 1   | A     | 1170 | A    |
| 1   | A     | 1171 | G    |
| 1   | A     | 1183 | A    |
| 1   | A     | 1184 | G    |
| 1   | A     | 1187 | G    |
| 1   | A     | 1190 | G    |
| 1   | A     | 1191 | A    |
| 1   | A     | 1195 | C    |
| 1   | A     | 1196 | U    |
| 1   | A     | 1197 | G    |
| 1   | A     | 1200 | C    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1201 | A    |
| 1   | A     | 1202 | G    |
| 1   | A     | 1205 | U    |
| 1   | A     | 1212 | U    |
| 1   | A     | 1213 | A    |
| 1   | A     | 1215 | G    |
| 1   | A     | 1224 | G    |
| 1   | A     | 1225 | A    |
| 1   | A     | 1226 | C    |
| 1   | A     | 1227 | A    |
| 1   | A     | 1238 | A    |
| 1   | A     | 1239 | A    |
| 1   | A     | 1240 | U    |
| 1   | A     | 1249 | C    |
| 1   | A     | 1250 | A    |
| 1   | A     | 1256 | A    |
| 1   | A     | 1257 | U    |
| 1   | A     | 1258 | G    |
| 1   | A     | 1260 | C    |
| 1   | A     | 1266 | G    |
| 1   | A     | 1270 | C    |
| 1   | A     | 1278 | U    |
| 1   | A     | 1279 | A    |
| 1   | A     | 1280 | A    |
| 1   | A     | 1281 | U    |
| 1   | A     | 1282 | C    |
| 1   | A     | 1285 | A    |
| 1   | A     | 1286 | A    |
| 1   | A     | 1287 | A    |
| 1   | A     | 1295 | G    |
| 1   | A     | 1297 | C    |
| 1   | A     | 1300 | G    |
| 1   | A     | 1301 | U    |
| 1   | A     | 1302 | U    |
| 1   | A     | 1303 | C    |
| 1   | A     | 1305 | G    |
| 1   | A     | 1306 | A    |
| 1   | A     | 1312 | G    |
| 1   | A     | 1317 | C    |
| 1   | A     | 1318 | A    |
| 1   | A     | 1319 | A    |
| 1   | A     | 1321 | C    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | A     | 1322    | C    |
| 1   | A     | 1323    | G    |
| 1   | A     | 1331    | G    |
| 1   | A     | 1332    | A    |
| 1   | A     | 1336    | C    |
| 1   | A     | 1338    | G    |
| 1   | A     | 1342    | C    |
| 1   | A     | 1346    | A    |
| 1   | A     | 1347    | G    |
| 1   | A     | 1351    | U    |
| 1   | A     | 1353    | G    |
| 1   | A     | 1357    | A    |
| 1   | A     | 1362    | C    |
| 1   | A     | 1363    | C    |
| 1   | A     | 1363(A) | A    |
| 1   | A     | 1364    | U    |
| 1   | A     | 1365    | G    |
| 1   | A     | 1370    | G    |
| 1   | A     | 1379    | G    |
| 1   | A     | 1380    | U    |
| 1   | A     | 1381    | U    |
| 1   | A     | 1394    | A    |
| 1   | A     | 1398    | A    |
| 1   | A     | 1409    | C    |
| 1   | A     | 1412    | C    |
| 1   | A     | 1418    | A    |
| 1   | A     | 1419    | G    |
| 1   | A     | 1433    | A    |
| 1   | A     | 1440    | C    |
| 1   | A     | 1442    | G    |
| 1   | A     | 1442(A) | G    |
| 1   | A     | 1443    | G    |
| 1   | A     | 1447    | A    |
| 1   | A     | 1452    | C    |
| 1   | A     | 1456    | G    |
| 1   | A     | 1457    | G    |
| 1   | A     | 1485    | U    |
| 1   | A     | 1486    | G    |
| 1   | A     | 1488    | G    |
| 1   | A     | 1492    | A    |
| 1   | A     | 1494    | G    |
| 1   | A     | 1497    | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1499 | A    |
| 1   | A     | 1503 | A    |
| 1   | A     | 1504 | G    |
| 1   | A     | 1505 | G    |
| 1   | A     | 1506 | U    |
| 1   | A     | 1507 | A    |
| 1   | A     | 1517 | G    |
| 1   | A     | 1519 | A    |
| 1   | A     | 1520 | G    |
| 1   | A     | 1528 | U    |
| 1   | A     | 1529 | G    |
| 1   | A     | 1530 | G    |
| 1   | A     | 1531 | A    |
| 1   | A     | 1535 | C    |
| 1   | A     | 1536 | C    |
| 1   | A     | 1539 | C    |
| 1   | A     | 1541 | U    |
| 1   | A     | 1542 | U    |
| 24  | Y     | 28   | A    |
| 24  | Y     | 30   | G    |
| 24  | Y     | 31   | U    |
| 24  | Y     | 32   | A    |
| 24  | Y     | 35   | A    |
| 24  | Y     | 36   | A    |
| 24  | Y     | 37   | U    |
| 24  | Y     | 39   | U    |

All (114) RNA pucker outliers are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 7      | G    |
| 1   | A     | 8      | A    |
| 1   | A     | 13     | U    |
| 1   | A     | 30     | U    |
| 1   | A     | 31     | G    |
| 1   | A     | 48     | C    |
| 1   | A     | 49     | U    |
| 1   | A     | 51     | A    |
| 1   | A     | 60     | A    |
| 1   | A     | 115    | G    |
| 1   | A     | 119    | A    |
| 1   | A     | 129(A) | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 145 | G    |
| 1   | A     | 156 | G    |
| 1   | A     | 173 | U    |
| 1   | A     | 181 | G    |
| 1   | A     | 195 | A    |
| 1   | A     | 197 | A    |
| 1   | A     | 202 | U    |
| 1   | A     | 243 | A    |
| 1   | A     | 250 | A    |
| 1   | A     | 251 | G    |
| 1   | A     | 266 | G    |
| 1   | A     | 274 | A    |
| 1   | A     | 279 | A    |
| 1   | A     | 281 | G    |
| 1   | A     | 289 | G    |
| 1   | A     | 327 | A    |
| 1   | A     | 328 | C    |
| 1   | A     | 329 | A    |
| 1   | A     | 344 | A    |
| 1   | A     | 350 | G    |
| 1   | A     | 351 | G    |
| 1   | A     | 366 | C    |
| 1   | A     | 372 | C    |
| 1   | A     | 389 | A    |
| 1   | A     | 421 | U    |
| 1   | A     | 428 | G    |
| 1   | A     | 484 | G    |
| 1   | A     | 495 | A    |
| 1   | A     | 496 | A    |
| 1   | A     | 509 | A    |
| 1   | A     | 518 | C    |
| 1   | A     | 535 | A    |
| 1   | A     | 559 | A    |
| 1   | A     | 560 | U    |
| 1   | A     | 561 | U    |
| 1   | A     | 576 | G    |
| 1   | A     | 577 | G    |
| 1   | A     | 595 | G    |
| 1   | A     | 641 | U    |
| 1   | A     | 653 | A    |
| 1   | A     | 687 | A    |
| 1   | A     | 701 | C    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 702  | A    |
| 1   | A     | 748  | C    |
| 1   | A     | 777  | A    |
| 1   | A     | 792  | A    |
| 1   | A     | 840  | C    |
| 1   | A     | 864  | A    |
| 1   | A     | 872  | A    |
| 1   | A     | 884  | U    |
| 1   | A     | 932  | C    |
| 1   | A     | 933  | G    |
| 1   | A     | 960  | U    |
| 1   | A     | 965  | A    |
| 1   | A     | 975  | A    |
| 1   | A     | 992  | U    |
| 1   | A     | 993  | G    |
| 1   | A     | 1000 | U    |
| 1   | A     | 1050 | G    |
| 1   | A     | 1065 | U    |
| 1   | A     | 1077 | G    |
| 1   | A     | 1078 | U    |
| 1   | A     | 1082 | G    |
| 1   | A     | 1092 | A    |
| 1   | A     | 1101 | A    |
| 1   | A     | 1145 | C    |
| 1   | A     | 1151 | A    |
| 1   | A     | 1182 | G    |
| 1   | A     | 1187 | G    |
| 1   | A     | 1190 | G    |
| 1   | A     | 1196 | U    |
| 1   | A     | 1200 | C    |
| 1   | A     | 1201 | A    |
| 1   | A     | 1212 | U    |
| 1   | A     | 1214 | C    |
| 1   | A     | 1224 | G    |
| 1   | A     | 1226 | C    |
| 1   | A     | 1239 | A    |
| 1   | A     | 1257 | U    |
| 1   | A     | 1278 | U    |
| 1   | A     | 1279 | A    |
| 1   | A     | 1285 | A    |
| 1   | A     | 1299 | A    |
| 1   | A     | 1300 | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | A     | 1301    | U    |
| 1   | A     | 1322    | C    |
| 1   | A     | 1331    | G    |
| 1   | A     | 1335    | C    |
| 1   | A     | 1337    | G    |
| 1   | A     | 1346    | A    |
| 1   | A     | 1364    | U    |
| 1   | A     | 1380    | U    |
| 1   | A     | 1398    | A    |
| 1   | A     | 1442(B) | A    |
| 1   | A     | 1447    | A    |
| 1   | A     | 1452    | C    |
| 1   | A     | 1493    | A    |
| 1   | A     | 1498    | U    |
| 1   | A     | 1503    | A    |
| 1   | A     | 1504    | G    |
| 1   | A     | 1529    | G    |
| 1   | A     | 1534    | A    |

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 110 ligands modelled in this entry, 110 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1   | A     | 7                |
| 23  | X     | 2                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | A     | 84:U      | O3'    | 88:A      | P      | 5.27         |
| 1     | A     | 93:G      | O3'    | 96:U      | P      | 4.63         |
| 1     | A     | 204:U     | O3'    | 216:G     | P      | 4.48         |
| 1     | A     | 841:U     | O3'    | 848:C     | P      | 4.32         |
| 1     | A     | 1442(A):G | O3'    | 1442(B):A | P      | 3.82         |
| 1     | X     | 81:LYS    | C      | 82:ARG    | N      | 3.73         |
| 1     | X     | 79:LYS    | C      | 80:ALA    | N      | 3.54         |
| 1     | A     | 1387:G    | O3'    | 1388:C    | P      | 3.33         |
| 1     | A     | 927:G     | O3'    | 928:G     | P      | 2.65         |

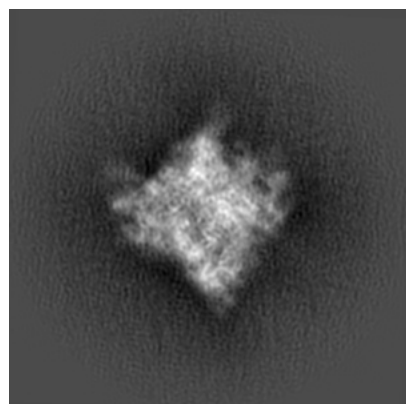
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4074. These allow visual inspection of the internal detail of the map and identification of artifacts.

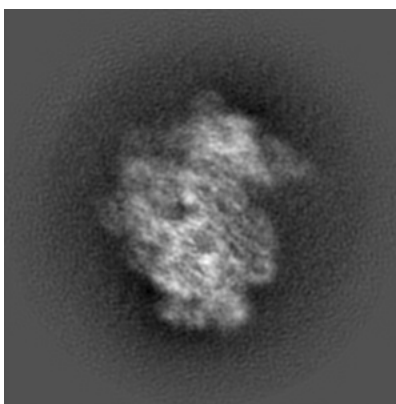
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

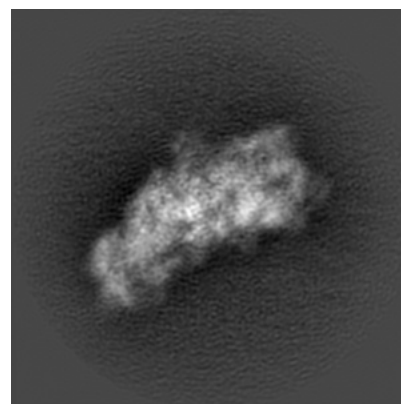
#### 6.1.1 Primary map



X

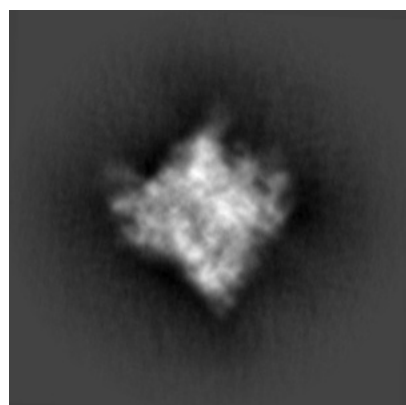


Y

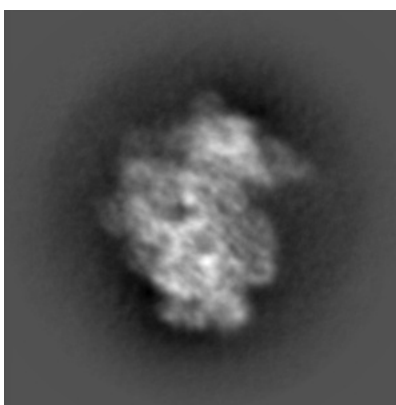


Z

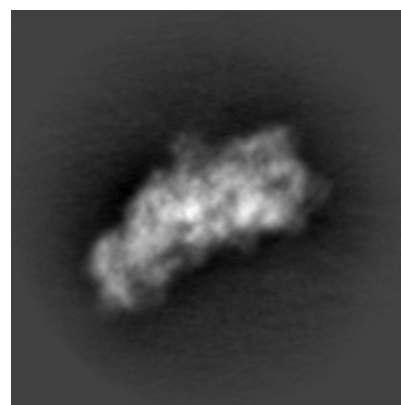
#### 6.1.2 Raw map



X



Y

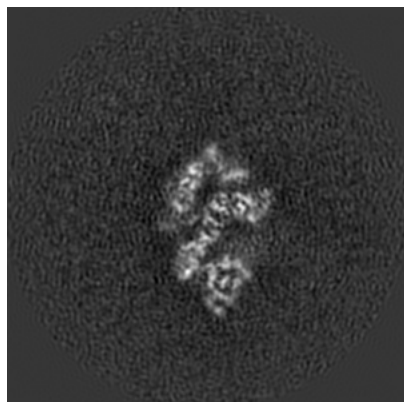


Z

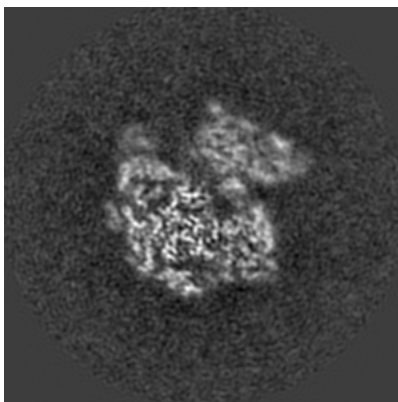
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

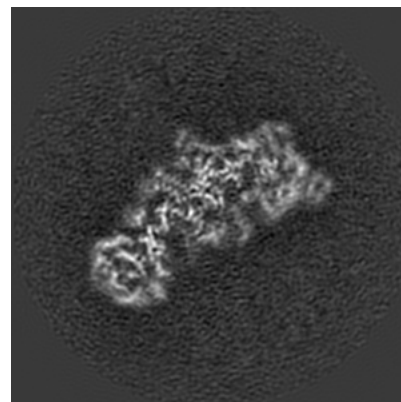
### 6.2.1 Primary map



X Index: 130

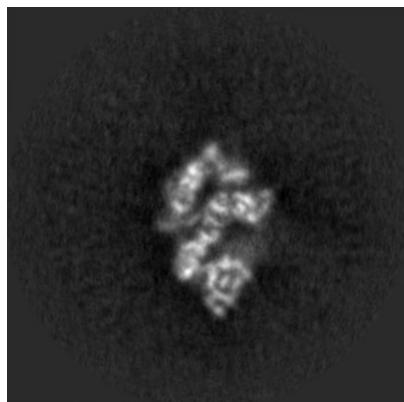


Y Index: 130

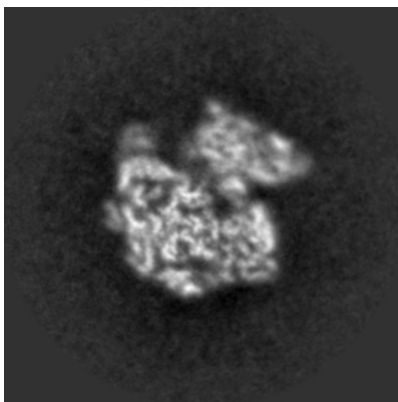


Z Index: 130

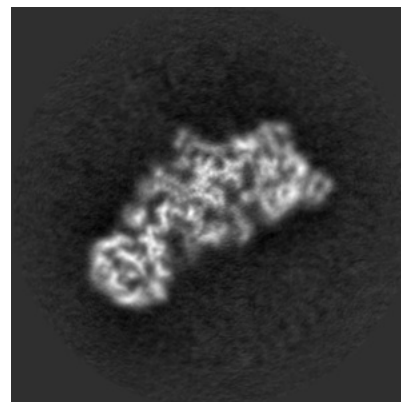
### 6.2.2 Raw map



X Index: 130



Y Index: 130

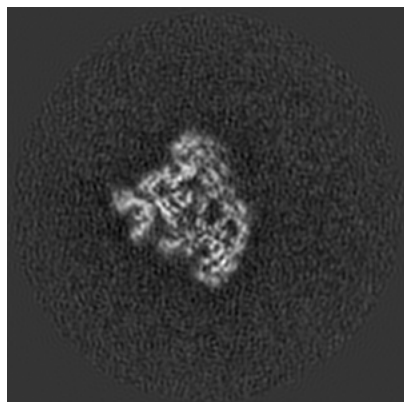


Z Index: 130

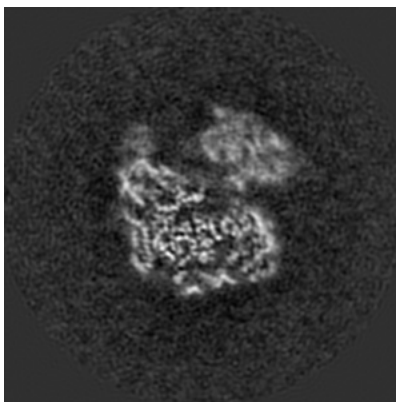
The images above show central slices of the map in three orthogonal directions.

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

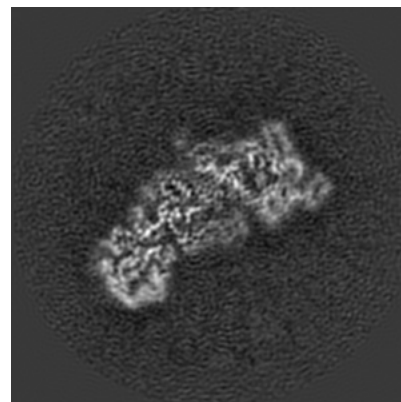
### 6.3.1 Primary map



X Index: 95

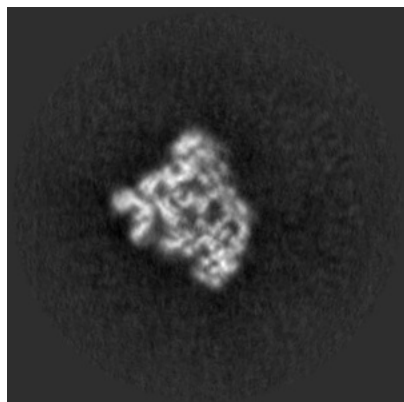


Y Index: 127

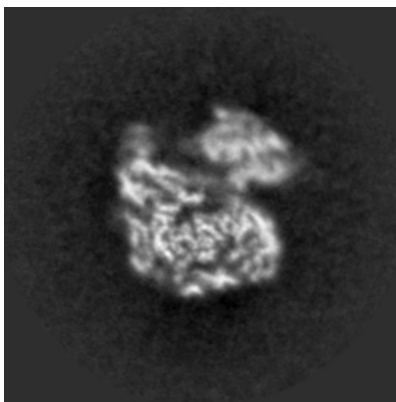


Z Index: 134

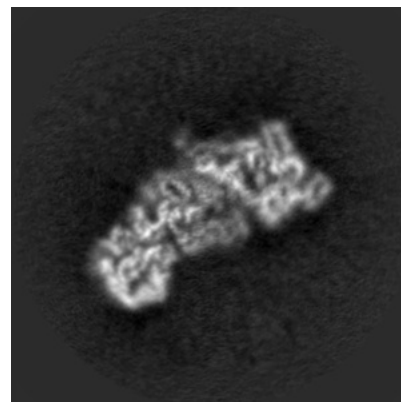
### 6.3.2 Raw map



X Index: 96



Y Index: 126

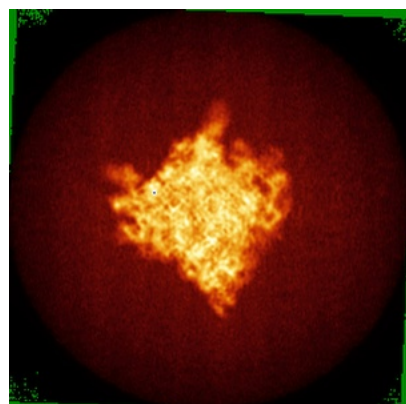


Z Index: 134

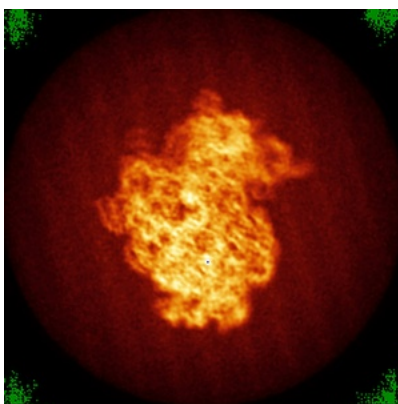
The images above show the largest variance slices of the map in three orthogonal directions.

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

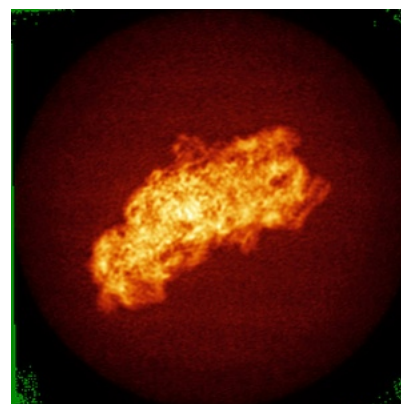
### 6.4.1 Primary map



X

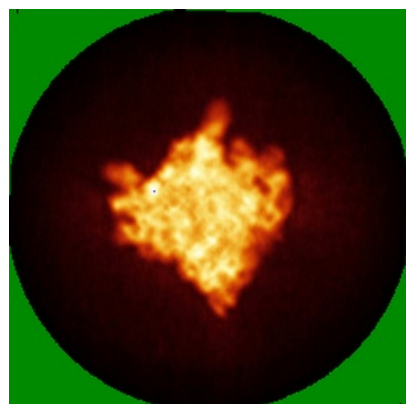


Y

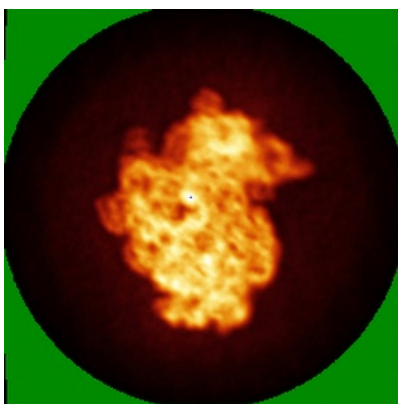


Z

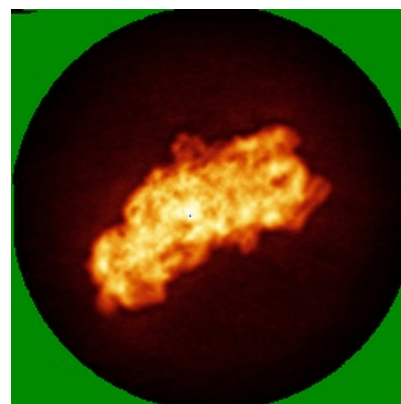
### 6.4.2 Raw map



X



Y

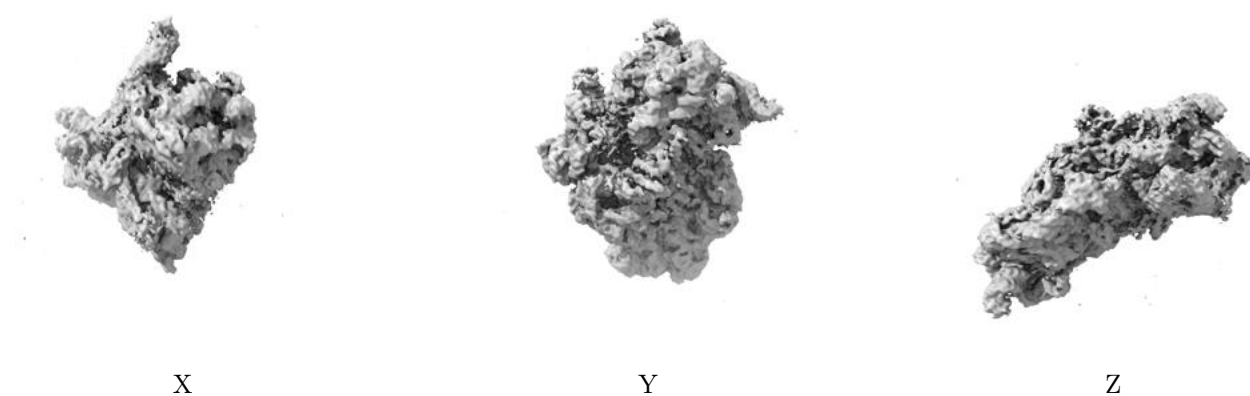


Z

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.

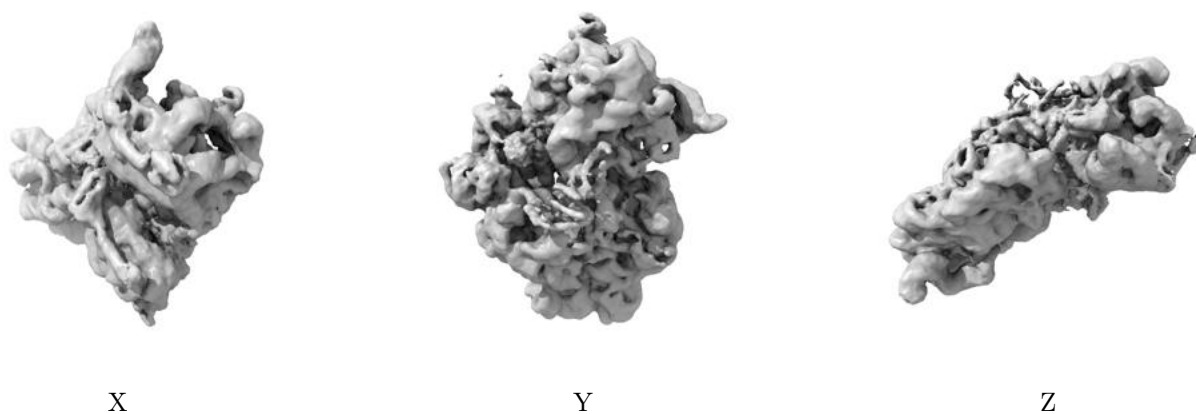
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. 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



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.

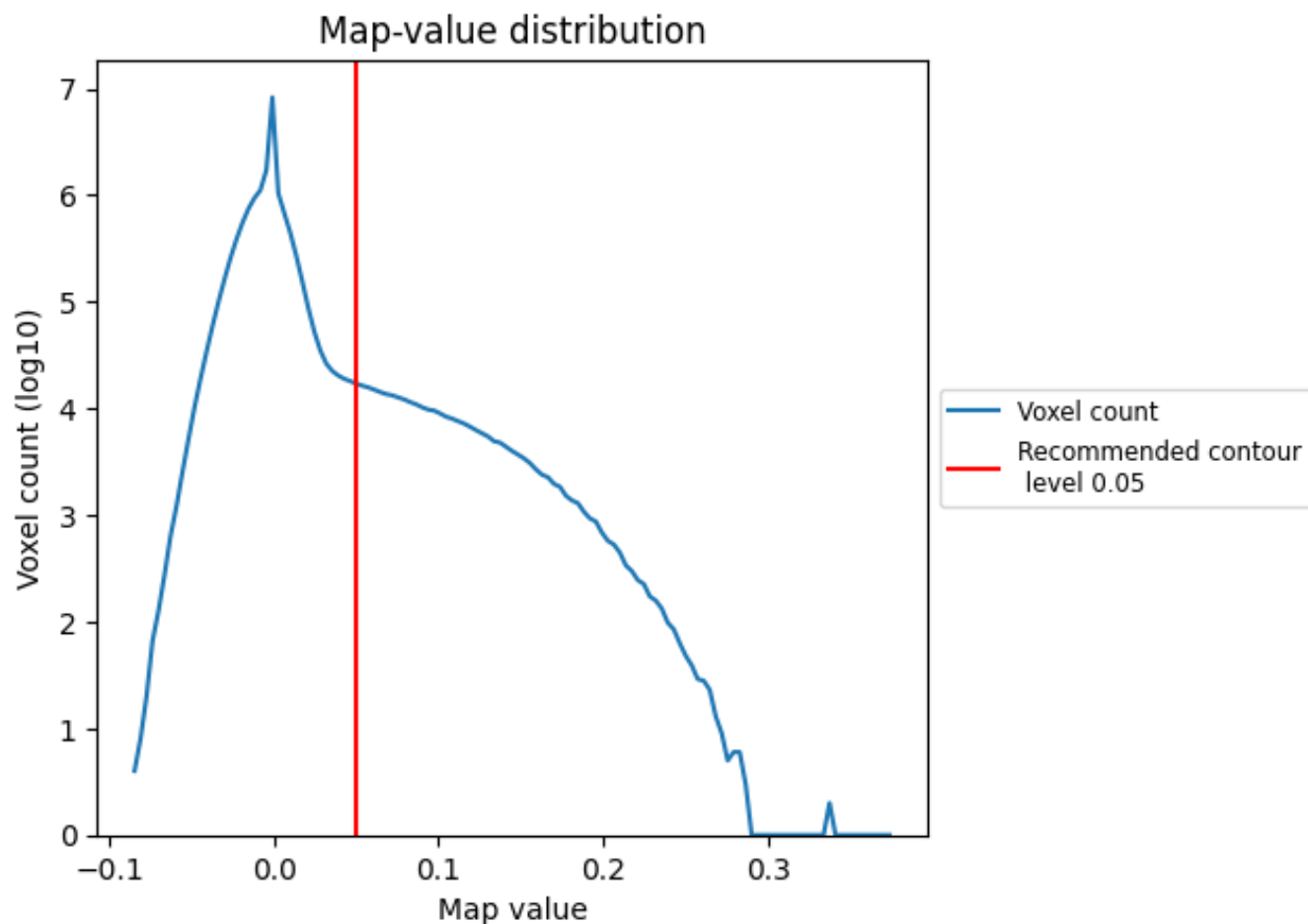
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

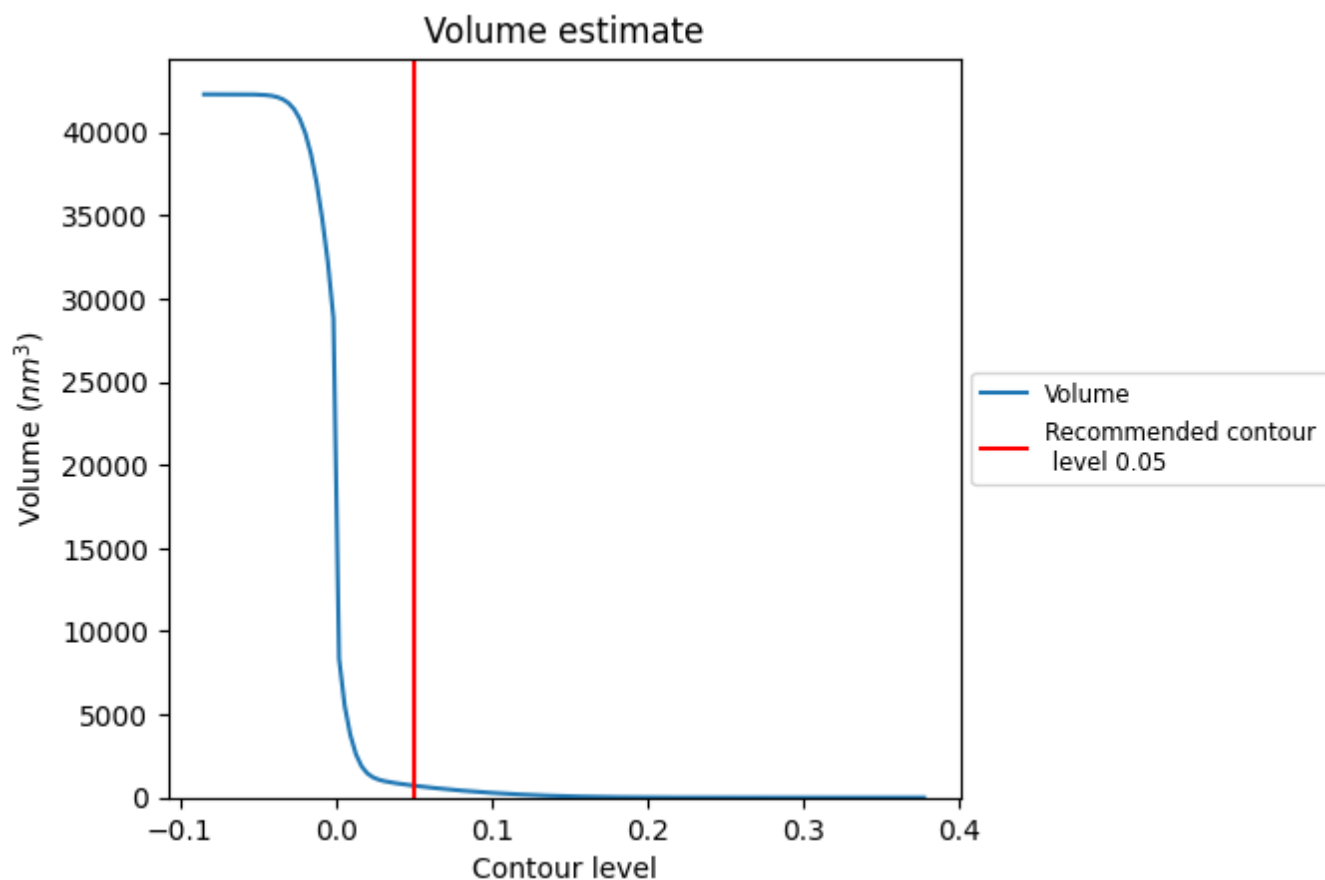
This section contains the results of statistical analysis of the map.

### 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.

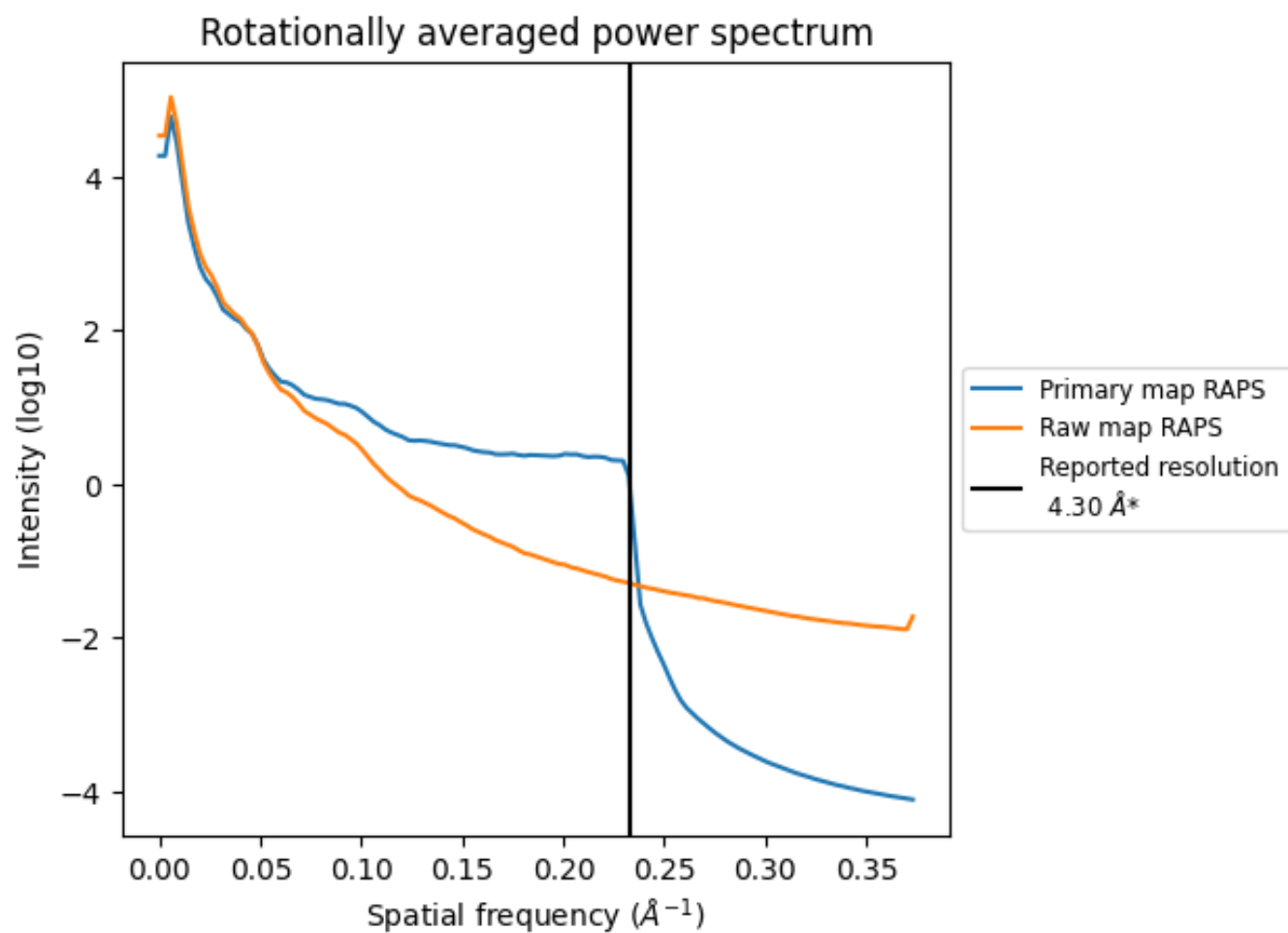
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 718  $\text{nm}^3$ ; this corresponds to an approximate mass of 649 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 ⓘ

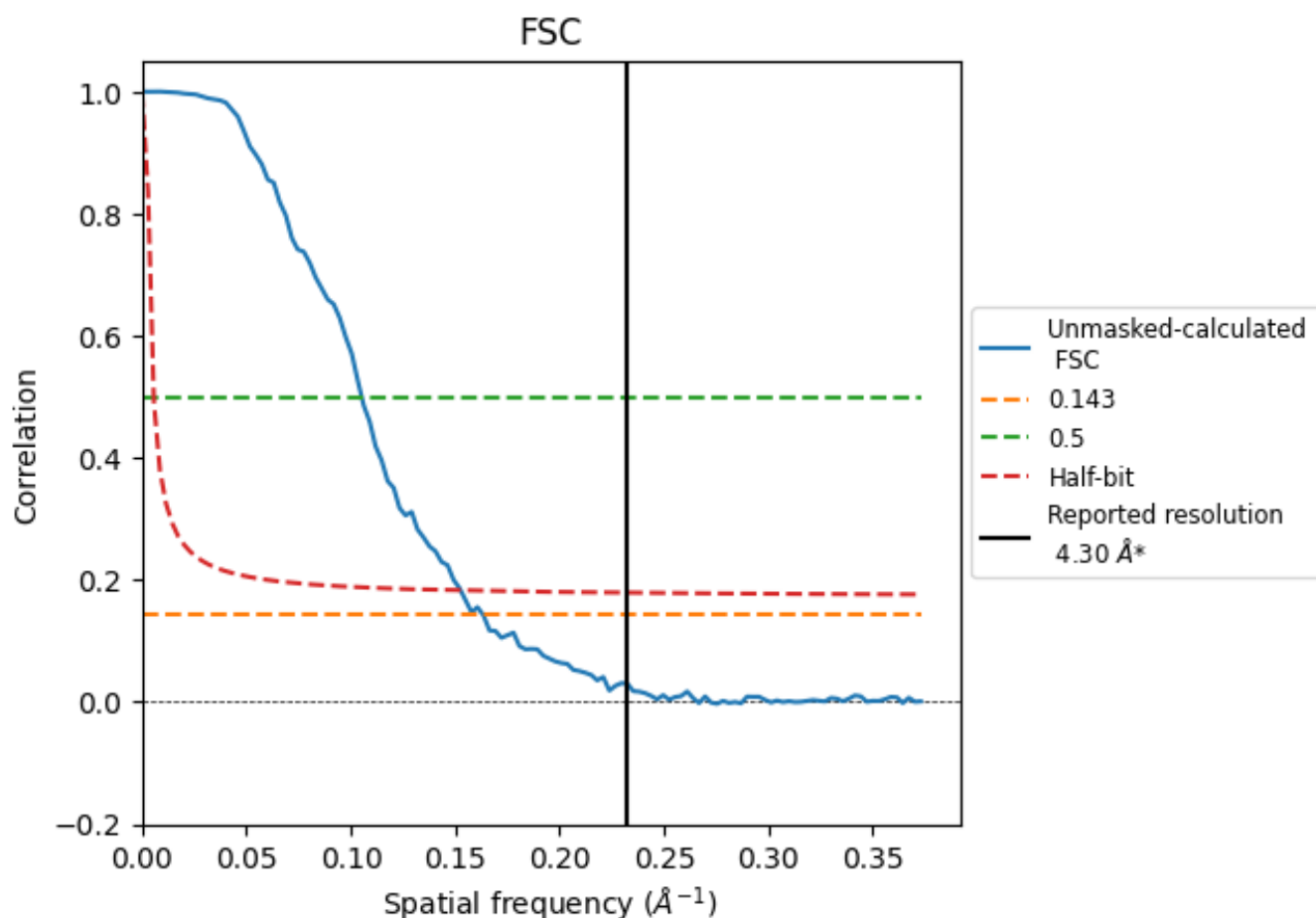


\*Reported resolution corresponds to spatial frequency of 0.233 Å<sup>-1</sup>

## 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 0.233  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

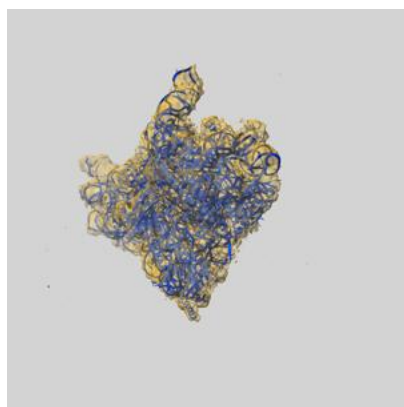
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 4.30                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 6.12                               | 9.51 | 6.55     |

\*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 6.12 differs from the reported value 4.3 by more than 10 %

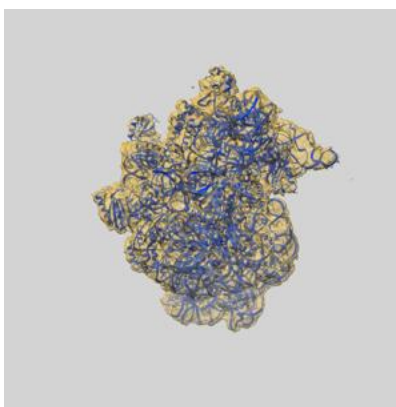
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4074 and PDB model 5LMO. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

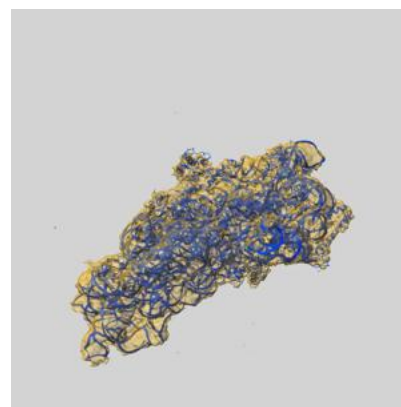
### 9.1 Map-model overlay [i](#)



X



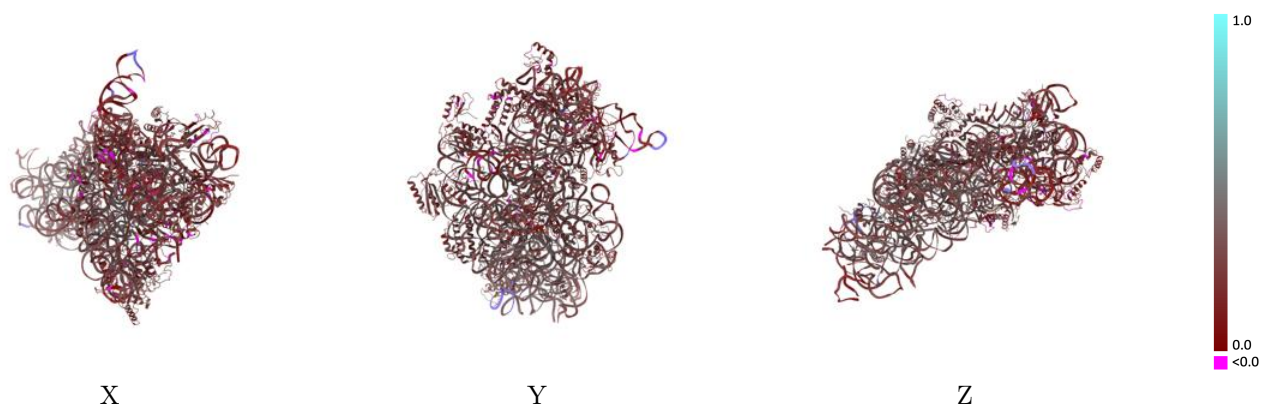
Y



Z

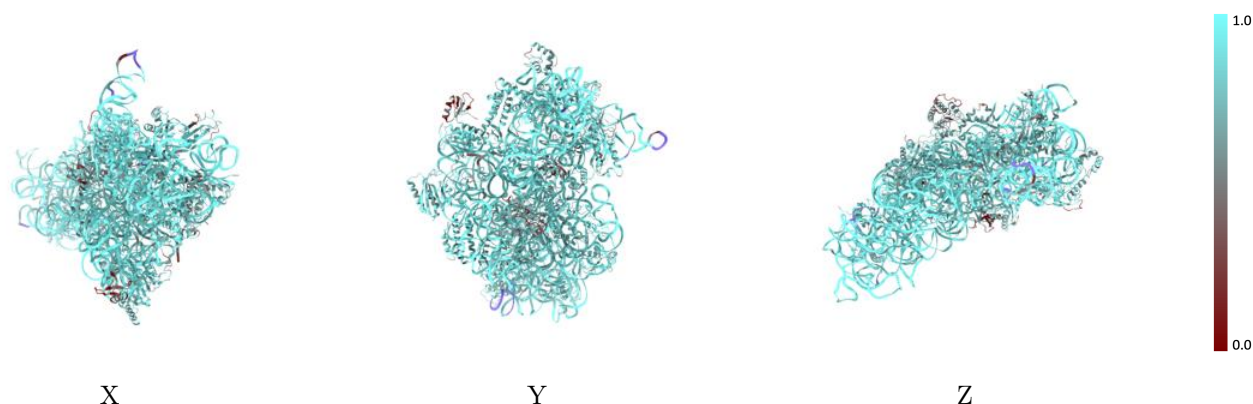
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



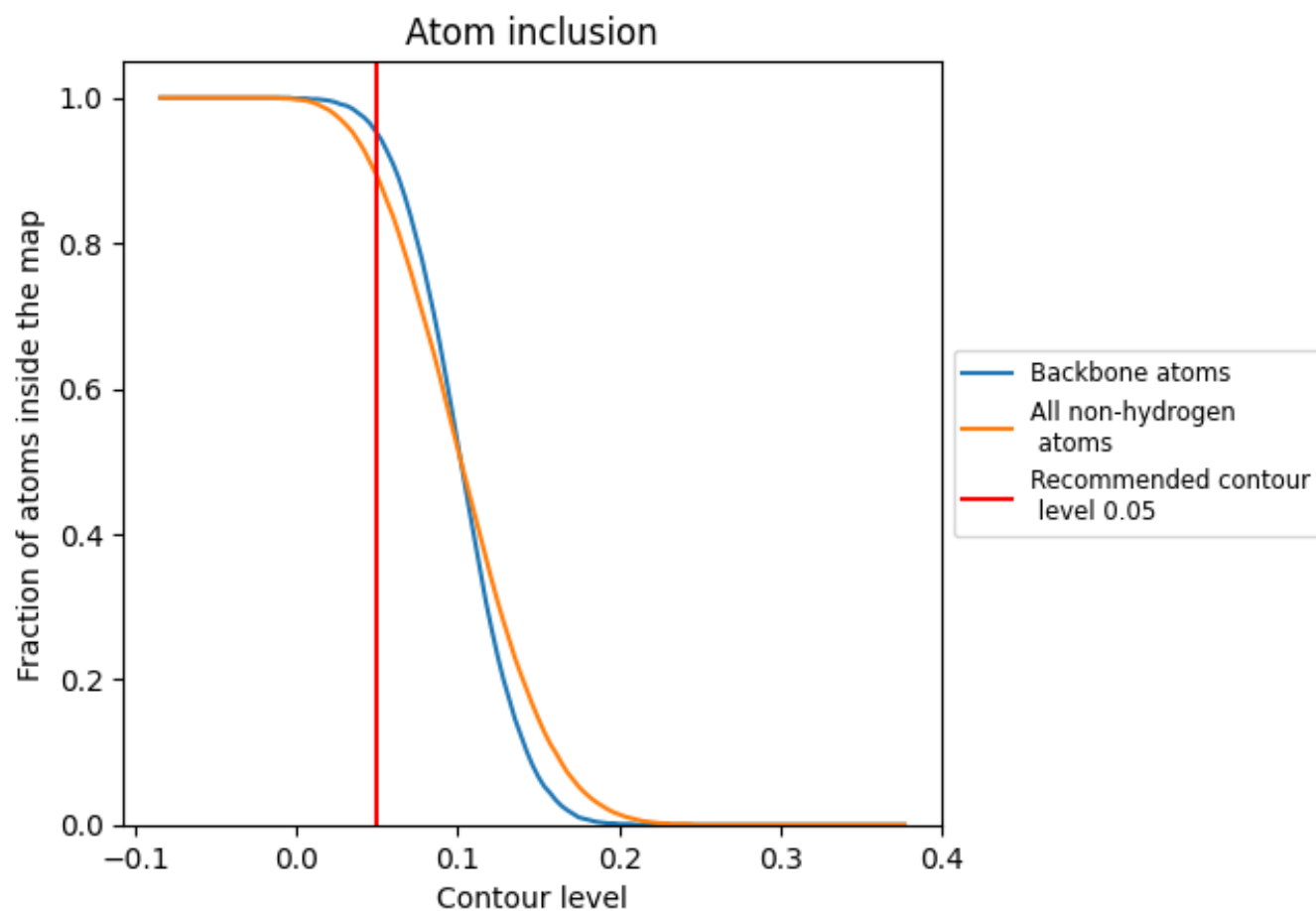
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 95% of all backbone atoms, 89% 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 (0.05) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8920   |  0.2810   |
| A     |  0.9700   |  0.2960   |
| B     |  0.5990   |  0.2470   |
| C     |  0.8220   |  0.2530   |
| D     |  0.8110   |  0.2790   |
| E     |  0.8230   |  0.3090   |
| F     |  0.8070   |  0.2710   |
| G     |  0.8110   |  0.2100   |
| H     |  0.8620   |  0.3350   |
| I     |  0.7850   |  0.2350   |
| J     |  0.7340   |  0.2470   |
| K     |  0.8390   |  0.2620   |
| L     |  0.8260   |  0.3450   |
| M     |  0.7700   |  0.1780   |
| N     |  0.7930  |  0.2400  |
| O     |  0.8390 |  0.2900 |
| P     |  0.8740 |  0.3290 |
| Q     |  0.8580 |  0.3270 |
| R     |  0.7720 |  0.2370 |
| S     |  0.7320 |  0.1660 |
| T     |  0.8300 |  0.2720 |
| V     |  0.8530 |  0.2280 |
| W     |  0.4250 |  0.2150 |
| X     |  0.6320 |  0.2290 |
| Y     |  0.6980 |  0.1540 |

