



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:34 PM UTC

PDB ID : 7OHT / pdb\_00007oht  
EMDB ID : EMD-12908  
Title : Nog1-TAP associated immature ribosomal particles from *S. cerevisiae* after rpL2 expression shut down, population A  
Authors : Milkereit, P.; Poell, G.  
Deposited on : 2021-05-11  
Resolution : 4.70 Å(reported)  
Based on initial model : 3JCT

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:

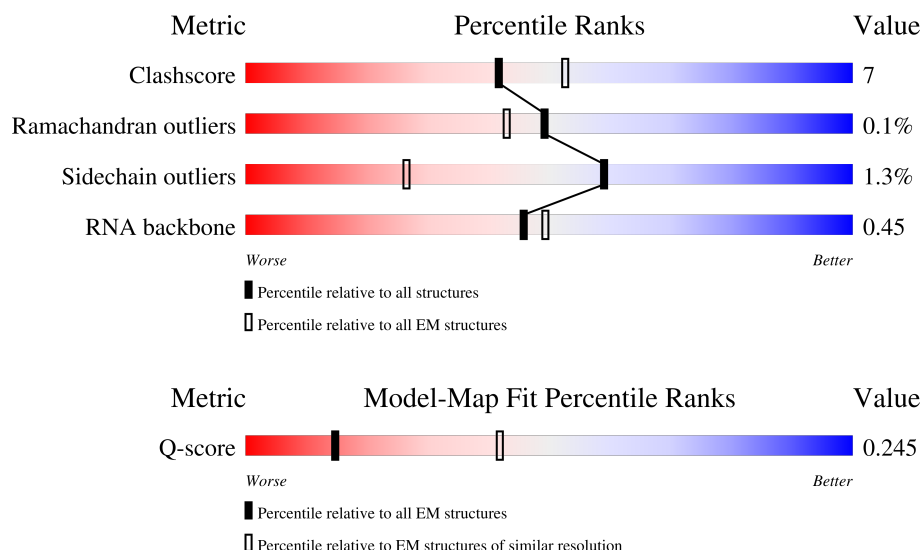
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 4.70 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.



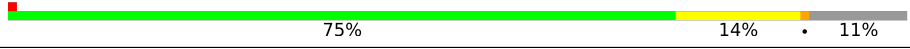
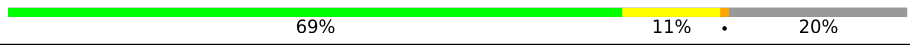
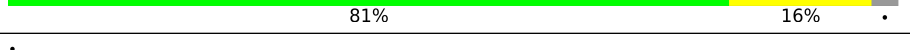
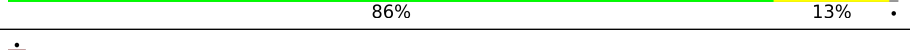
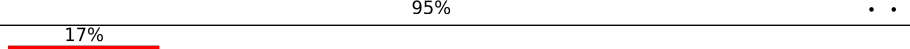
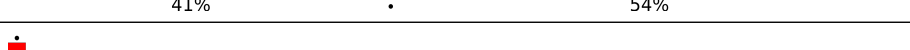
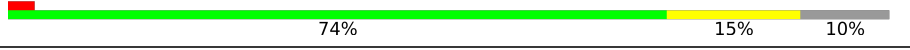
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 1989 ( 4.20 - 5.20 )                                     |

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   | 1     | 3396   |                  |
| 2   | 2     | 158    |                  |
| 3   | 3     | 121    |                  |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | B     | 387    |    |
| 5   | C     | 362    |    |
| 6   | D     | 297    |    |
| 7   | E     | 176    |    |
| 8   | F     | 244    |    |
| 9   | H     | 191    |    |
| 10  | J     | 174    |    |
| 11  | M     | 138    |    |
| 12  | O     | 199    |    |
| 13  | Q     | 186    |    |
| 14  | S     | 172    |    |
| 15  | T     | 160    |  |
| 16  | V     | 137    |  |
| 17  | W     | 236    |  |
| 18  | b     | 647    |  |
| 19  | e     | 130    |  |
| 20  | f     | 107    |  |
| 21  | m     | 486    |  |
| 22  | r     | 261    |  |
| 23  | u     | 199    |  |
| 24  | v     | 344    |  |
| 25  | w     | 203    |  |
| 26  | x     | 515    |  |
| 27  | y     | 245    |  |

## 2 Entry composition [i](#)

There are 29 unique types of molecules in this entry. The entry contains 135365 atoms, of which 59714 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 25S rRNA.

| Mol | Chain | Residues | Atoms |       |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|------|-------|------|---------|-------|
| 1   | 1     | 1485     | Total | C     | H     | N    | O     | P    | 0       | 0     |
|     |       |          | 47732 | 14188 | 15960 | 5725 | 10374 | 1485 |         |       |

- Molecule 2 is a RNA chain called 5.8S rRNA.

| Mol | Chain | Residues | Atoms |     |     |    |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|-----|----|---------|-------|
| 2   | 2     | 19       | Total | C   | H   | N  | O   | P  | 0       | 0     |
|     |       |          | 605   | 180 | 203 | 69 | 134 | 19 |         |       |

- Molecule 3 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|-----|---------|-------|
| 3   | 3     | 114      | Total | C    | H    | N   | O   | P   | 0       | 0     |
|     |       |          | 3661  | 1086 | 1229 | 436 | 796 | 114 |         |       |

- Molecule 4 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 4   | B     | 350      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 5624  | 1763 | 2849 | 516 | 489 | 7 |         |       |

- Molecule 5 is a protein called 60S ribosomal protein L4-A.

| Mol | Chain | Residues | Atoms |      |      |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|--|---------|-------|
| 5   | C     | 239      | Total | C    | H    | N   | O   |  | 0       | 0     |
|     |       |          | 3813  | 1178 | 1961 | 348 | 326 |  |         |       |

- Molecule 6 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 6   | D     | 265      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 4236  | 1352 | 2098 | 377 | 407 | 2 |         |       |

- Molecule 7 is a protein called 60S ribosomal protein L6-A.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 7   | E     | 141      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2338  | 724 | 1217 | 203 | 193 | 1 |         |       |

- Molecule 8 is a protein called 60S ribosomal protein L7-A.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 8   | F     | 222      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3647  | 1151 | 1863 | 324 | 308 | 1 |         |       |

- Molecule 9 is a protein called 60S ribosomal protein L9-A.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 9   | H     | 191      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3105  | 963 | 1587 | 274 | 277 | 4 |         |       |

- Molecule 10 is a protein called 60S ribosomal protein L11-A.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 10  | J     | 169      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2738  | 847 | 1385 | 253 | 249 | 4 |         |       |

- Molecule 11 is a protein called 60S ribosomal protein L14-A.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 11  | M     | 137      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2214  | 678 | 1155 | 200 | 179 | 2 |         |       |

- Molecule 12 is a protein called 60S ribosomal protein L16-A.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 12  | O     | 197      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3216  | 1003 | 1661 | 289 | 262 | 1 |         |       |

- Molecule 13 is a protein called 60S ribosomal protein L18-A.

| Mol | Chain | Residues | Atoms |     |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|--|---------|-------|
| 13  | Q     | 85       | Total | C   | H   | N   | O   |  | 0       | 0     |
|     |       |          | 1357  | 414 | 705 | 123 | 115 |  |         |       |

- Molecule 14 is a protein called 60S ribosomal protein L20-A.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 14  | S     | 171      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2913  | 925 | 1476 | 266 | 243 | 3 |         |       |

- Molecule 15 is a protein called 60S ribosomal protein L21-A.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 15  | T     | 116      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1899  | 583 | 976 | 176 | 161 | 3 |         |       |

- Molecule 16 is a protein called 60S ribosomal protein L23-A.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 16  | V     | 124      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1880  | 576 | 963 | 171 | 163 | 7 |         |       |

- Molecule 17 is a protein called Ribosome assembly factor MRT4.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 17  | W     | 234      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3806  | 1194 | 1921 | 323 | 362 | 6 |         |       |

- Molecule 18 is a protein called Nucleolar GTP-binding protein 1.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 18  | b     | 453      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 7406  | 2340 | 3727 | 635 | 686 | 18 |         |       |

- Molecule 19 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 19  | e     | 39       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 625   | 185 | 331 | 59 | 50 |   |         |       |

- Molecule 20 is a protein called 60S ribosomal protein L33-A.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 20  | f     | 106      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1731  | 540 | 881 | 165 | 144 | 1 |         |       |

- Molecule 21 is a protein called Nucleolar GTP-binding protein 2.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 21  | m     | 433      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 7069  | 2221 | 3565 | 633 | 641 | 9 |         |       |

- Molecule 22 is a protein called Ribosome biogenesis protein NSA2.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 22  | r     | 230      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3827  | 1177 | 1967 | 352 | 324 | 7 |         |       |

- Molecule 23 is a protein called Ribosome biogenesis protein RLP24.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 23  | u     | 94       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1633  | 504 | 833 | 164 | 123 | 9 |         |       |

- Molecule 24 is a protein called Ribosome biogenesis protein RPF2.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 24  | v     | 263      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4323  | 1365 | 2193 | 372 | 379 | 14 |         |       |

- Molecule 25 is a protein called Regulator of ribosome biosynthesis.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 25  | w     | 182      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2960  | 911 | 1512 | 261 | 271 | 5 |         |       |

- Molecule 26 is a protein called Ribosome assembly protein 4.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 26  | x     | 488      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 7606  | 2398 | 3799 | 677 | 711 | 21 |         |       |

- Molecule 27 is a protein called Eukaryotic translation initiation factor 6.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 27  | y     | 225      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3398  | 1056 | 1697 | 295 | 343 | 7 |         |       |

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

| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 28  | b     | 1        | Total<br>1 | Mg<br>1 | 0       |
| 28  | m     | 1        | Total<br>1 | Mg<br>1 | 0       |

- Molecule 29 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 29  | u     | 1        | Total<br>1 | Zn<br>1 | 0       |

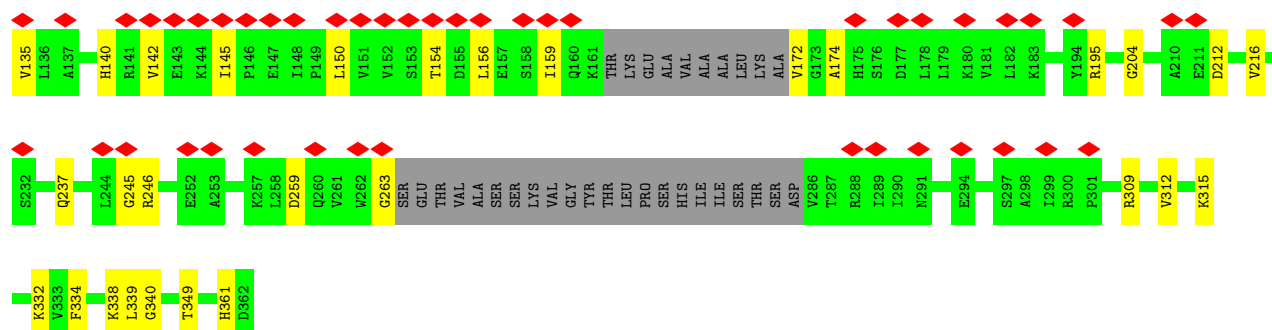




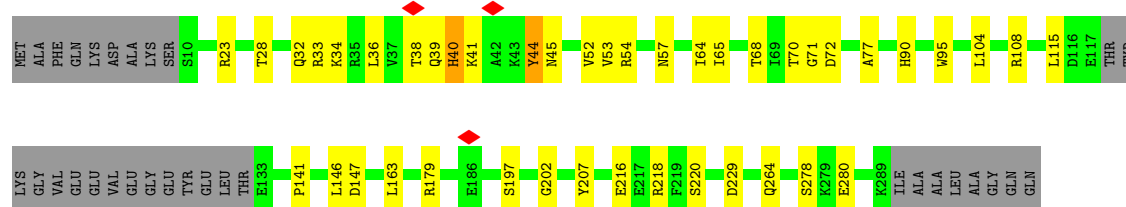




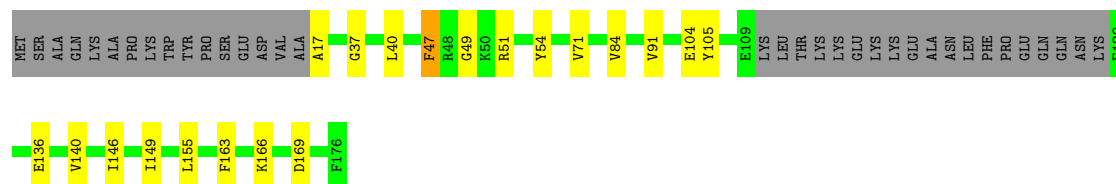




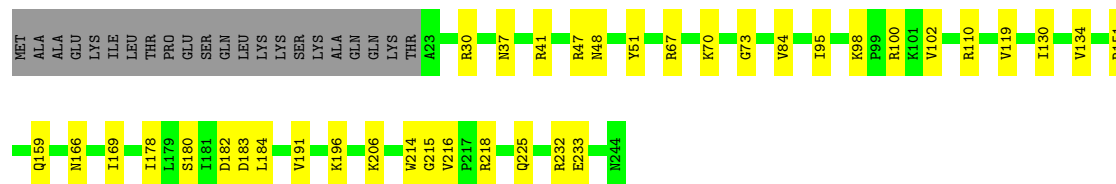
• Molecule 6: 60S ribosomal protein L5



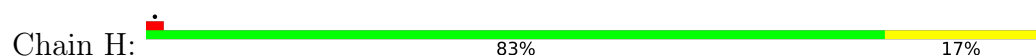
• Molecule 7: 60S ribosomal protein L6-A



• Molecule 8: 60S ribosomal protein L7-A

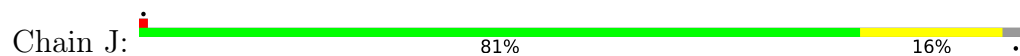


• Molecule 9: 60S ribosomal protein L9-A

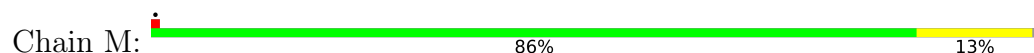




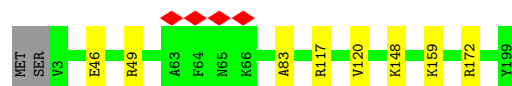
- Molecule 10: 60S ribosomal protein L11-A



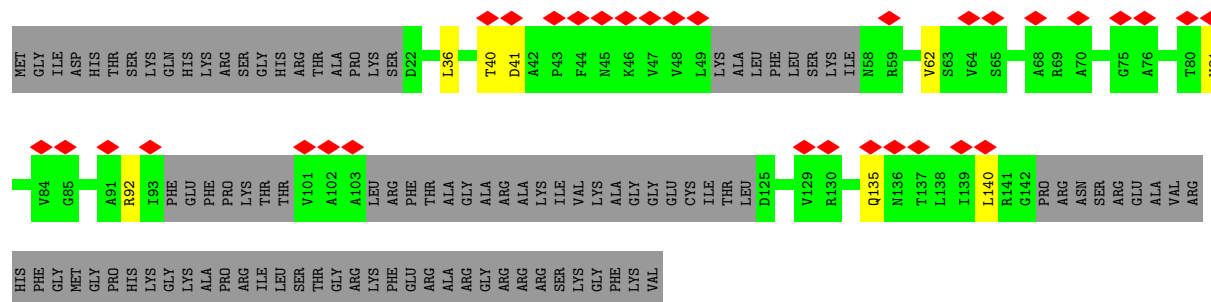
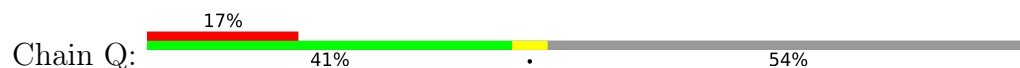
- Molecule 11: 60S ribosomal protein L14-A



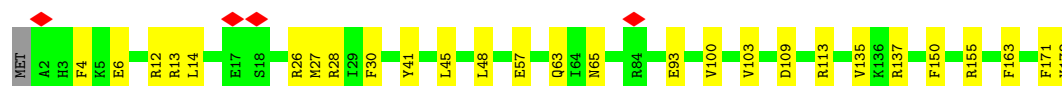
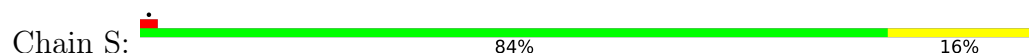
- Molecule 12: 60S ribosomal protein L16-A



- Molecule 13: 60S ribosomal protein L18-A



- Molecule 14: 60S ribosomal protein L20-A



- Molecule 15: 60S ribosomal protein L21-A



LYS  
ARG  
GLY  
VAL  
GLY  
LYS  
THR  
ASP  
PHE  
ARG

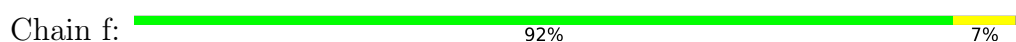
• Molecule 19: 60S ribosomal protein L32



MET  
ALA  
SER  
LEU  
PRO  
HIS  
PRO  
LYS  
ILE  
VAL  
LYS  
LYS  
HIS  
THR  
LYS  
LYS  
PHE  
LYS  
ARG  
HIS  
HIS  
HIS  
SER  
ASP  
ARG  
TVR  
HIS  
ARG  
VAL  
ALA  
GLU  
GLU  
ASN  
TRP  
ARG  
LYS  
GLN  
LYS  
GLY  
ILE  
ASP  
SER  
VAL  
VAL  
ARG  
ARG  
PHE  
ARG  
GLY  
ASN  
ILE  
SER  
GLN  
PRO  
LYS  
ILE  
GLY  
TYR  
GLY  
SER  
ASN

LYS  
LYS  
THR  
PHE  
LEU  
SER  
PRO  
SER  
PRO  
SER  
GLY  
HIS  
LYS  
THR  
PHE  
LEU  
VAL  
ALA  
N78  
N79  
K80  
D81  
L82  
E83  
T84  
LEU  
THR  
MET  
HIS  
THR  
LYS  
TYR  
ALA  
ALA  
GLY  
ILE  
A97  
H98  
V106  
V107  
I108  
L109  
A110  
R111  
A112  
K113  
A114  
L115  
G116  
I117  
K118  
V119  
L126  
A127  
L128  
GLU  
ALA

• Molecule 20: 60S ribosomal protein L33-A



MET  
K2  
V9  
D40  
A41  
Q42  
V59  
R60  
G61  
S62  
K63  
I100  
I107

• Molecule 21: Nucleolar GTP-binding protein 2



MET  
G2  
E7  
R10  
R11  
R12  
R13  
E14  
G15  
D16  
T17  
K18  
N21  
L22  
R23  
V24  
K25  
Y30  
R31  
D32  
S33  
K34  
R35  
V36  
K37  
F38  
L39  
N40  
M41  
Y42  
T43  
SER  
GLY  
LYS  
GLU  
ILE  
ARG  
ASN  
LYS  
GLY  
ASN  
ILE  
ALA  
ALA  
SER  
F61  
Q62  
D63  
S64  
T65  
I66  
P67  
D68

R76  
W77  
V83  
A85  
E98  
T99  
Q100  
K101  
R109  
R110  
E120  
K121  
D122  
A123  
D124  
E125  
S126  
R130  
S136  
D139  
K144  
R147  
K148  
R149  
P150  
R151  
L157  
E158  
D159  
L160  
V161  
T164  
N165  
E166  
Y171  
Q175  
VAL  
LEU  
ASP  
ALA  
THR  
GLY  
LEU  
MET

GLY  
ASN  
GLN  
GLU  
ASP  
LYS  
GLU  
ASN  
GLY  
W194  
S204  
S208  
K209  
R210  
I211  
W212  
N213  
E214  
L215  
V218  
S221  
S222  
D223  
V224  
V225  
I226  
H227  
V228  
D230  
A231  
R232  
D233  
P234  
L235  
G236  
T237  
R238  
K248  
K253  
H254  
Y257  
V258  
L259  
N260  
K261  
V269  
W273  
E280

T283  
F286  
H287  
A288  
S289  
I290  
T291  
N292  
S293  
F294  
L302  
Q308  
R313  
V318  
G319  
K328  
S329  
S330  
I331  
I332  
N333  
T334  
L335  
R336  
K337  
K338  
K339  
A344  
P345  
I346  
P347  
G348  
E349  
T350  
K351  
V352  
Q353  
Q354  
Y355  
L358  
M359  
K360  
R361  
I362  
D366  
C367  
I370  
S375  
K376

D377  
S378  
D381  
T382  
L383  
V390  
V393  
T394  
I400  
V403  
R406  
L412  
Y416  
I418  
S419  
G420  
D423  
A424  
T425  
E426  
A432  
K440  
G441  
G442  
E443  
V449  
M458  
R459  
G460  
K461  
I462  
V466  
L467  
P468  
P469  
GLU  
LYS  
GLY  
GLY  
PRO  
LYS  
LYS

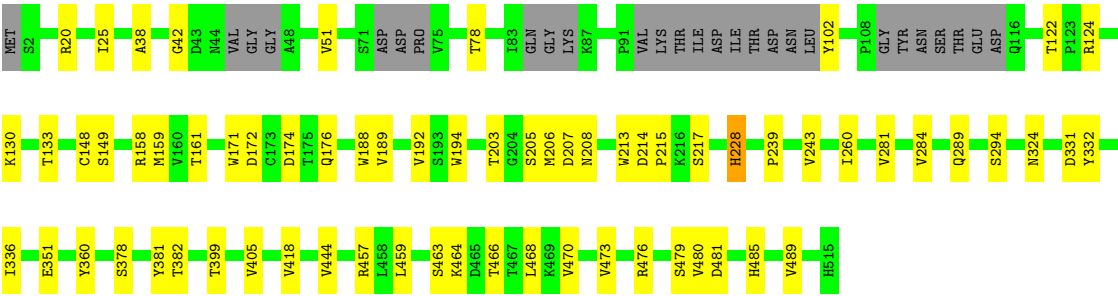
LYS  
GLU  
VAL  
GLU  
LYS  
THR  
ALA

• Molecule 22: Ribosome biogenesis protein NSA2

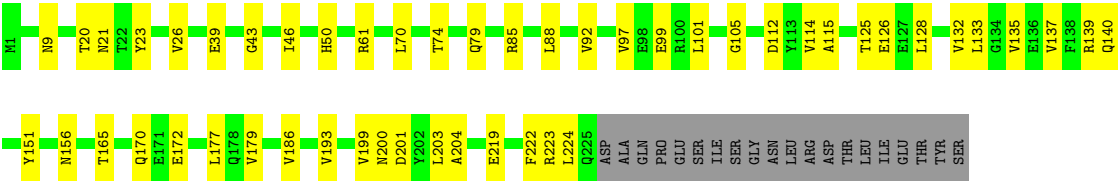








● Molecule 27: Eukaryotic translation initiation factor 6



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 21053                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 86.45                                   | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | FEI FALCON III (4k x 4k)                | Depositor |
| Maximum map value                    | 0.099                                   | Depositor |
| Minimum map value                    | -0.026                                  | Depositor |
| Average map value                    | -0.000                                  | Depositor |
| Map value standard deviation         | 0.005                                   | Depositor |
| Recommended contour level            | 0.018                                   | Depositor |
| Map size (Å)                         | 425.40002, 425.40002, 425.40002         | wwPDB     |
| Map dimensions                       | 400, 400, 400                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.0635, 1.0635, 1.0635                  | Depositor |

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: 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   | 1     | 0.08         | 0/35525 | 0.25        | 0/55297  |
| 2   | 2     | 0.08         | 0/447   | 0.28        | 0/691    |
| 3   | 3     | 0.07         | 0/2715  | 0.22        | 0/4220   |
| 4   | B     | 0.10         | 0/2833  | 0.26        | 0/3806   |
| 5   | C     | 0.10         | 0/1883  | 0.26        | 0/2544   |
| 6   | D     | 0.10         | 0/2184  | 0.25        | 0/2945   |
| 7   | E     | 0.12         | 0/1137  | 0.24        | 0/1525   |
| 8   | F     | 0.10         | 0/1821  | 0.25        | 0/2451   |
| 9   | H     | 0.09         | 0/1539  | 0.26        | 0/2073   |
| 10  | J     | 0.10         | 0/1374  | 0.25        | 0/1842   |
| 11  | M     | 0.10         | 0/1074  | 0.23        | 0/1446   |
| 12  | O     | 0.10         | 0/1585  | 0.21        | 0/2128   |
| 13  | Q     | 0.12         | 0/656   | 0.24        | 0/886    |
| 14  | S     | 0.12         | 0/1473  | 0.28        | 0/1980   |
| 15  | T     | 0.11         | 0/936   | 0.25        | 0/1255   |
| 16  | V     | 0.10         | 0/931   | 0.24        | 0/1254   |
| 17  | W     | 0.09         | 0/1918  | 0.24        | 0/2586   |
| 18  | b     | 0.10         | 0/3748  | 0.29        | 0/5056   |
| 19  | e     | 0.13         | 0/294   | 0.23        | 0/393    |
| 20  | f     | 0.11         | 0/868   | 0.25        | 0/1168   |
| 21  | m     | 0.10         | 0/3577  | 0.29        | 0/4820   |
| 22  | r     | 0.10         | 0/1892  | 0.29        | 0/2528   |
| 23  | u     | 0.11         | 0/816   | 0.30        | 0/1078   |
| 24  | v     | 0.09         | 0/2172  | 0.22        | 0/2908   |
| 25  | w     | 0.10         | 0/1471  | 0.23        | 0/1980   |
| 26  | x     | 0.09         | 0/3897  | 0.23        | 0/5282   |
| 27  | y     | 0.08         | 0/1722  | 0.22        | 0/2343   |
| All | All   | 0.09         | 0/80488 | 0.25        | 0/116485 |

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 |
|-----|-------|---------------------|---------------------|
| 9   | H     | 0                   | 1                   |
| 21  | m     | 0                   | 1                   |
| 22  | r     | 0                   | 1                   |
| All | All   | 0                   | 3                   |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 9   | H     | 22  | SER  | Peptide |
| 21  | m     | 77  | TRP  | Peptide |
| 22  | r     | 4   | ASN  | Peptide |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 1     | 31772 | 15960    | 15999    | 388     | 0            |
| 2   | 2     | 402   | 203      | 205      | 3       | 0            |
| 3   | 3     | 2432  | 1229     | 1233     | 25      | 0            |
| 4   | B     | 2775  | 2849     | 2846     | 43      | 0            |
| 5   | C     | 1852  | 1961     | 1958     | 32      | 0            |
| 6   | D     | 2138  | 2098     | 2096     | 35      | 0            |
| 7   | E     | 1121  | 1217     | 1215     | 13      | 0            |
| 8   | F     | 1784  | 1863     | 1862     | 28      | 0            |
| 9   | H     | 1518  | 1587     | 1587     | 22      | 0            |
| 10  | J     | 1353  | 1385     | 1383     | 16      | 0            |
| 11  | M     | 1059  | 1155     | 1154     | 16      | 0            |
| 12  | O     | 1555  | 1661     | 1659     | 7       | 0            |
| 13  | Q     | 652   | 705      | 701      | 8       | 0            |
| 14  | S     | 1437  | 1476     | 1475     | 20      | 0            |
| 15  | T     | 923   | 976      | 973      | 20      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 16  | V     | 917   | 963      | 962      | 11      | 0            |
| 17  | W     | 1885  | 1921     | 1921     | 23      | 0            |
| 18  | b     | 3679  | 3727     | 3725     | 65      | 0            |
| 19  | e     | 294   | 331      | 329      | 2       | 0            |
| 20  | f     | 850   | 881      | 880      | 7       | 0            |
| 21  | m     | 3504  | 3565     | 3562     | 71      | 0            |
| 22  | r     | 1860  | 1967     | 1965     | 45      | 0            |
| 23  | u     | 800   | 833      | 830      | 11      | 0            |
| 24  | v     | 2130  | 2193     | 2191     | 19      | 0            |
| 25  | w     | 1448  | 1512     | 1510     | 24      | 0            |
| 26  | x     | 3807  | 3799     | 3790     | 45      | 0            |
| 27  | y     | 1701  | 1697     | 1697     | 38      | 0            |
| 28  | b     | 1     | 0        | 0        | 0       | 0            |
| 28  | m     | 1     | 0        | 0        | 0       | 0            |
| 29  | u     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 75651 | 59714    | 59708    | 887     | 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 7.

All (887) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:y:186:VAL:HG12 | 27:y:193:VAL:HG12 | 1.51                     | 0.92              |
| 1:1:1200:A:O2'    | 1:1:1201:C:O5'    | 1.85                     | 0.92              |
| 1:1:3366:G:OP1    | 23:u:111:ARG:NH2  | 2.03                     | 0.91              |
| 1:1:3072:C:OP2    | 1:1:3073:A:N6     | 2.02                     | 0.90              |
| 1:1:2764:C:O2'    | 1:1:2765:C:OP2    | 1.89                     | 0.89              |
| 1:1:1355:A:O2'    | 1:1:1356:U:OP2    | 1.91                     | 0.88              |
| 1:1:494:G:O2'     | 1:1:495:G:O5'     | 1.91                     | 0.87              |
| 1:1:988:U:O4      | 1:1:989:A:N6      | 2.08                     | 0.87              |
| 1:1:2655:U:O2'    | 1:1:2657:A:N6     | 2.08                     | 0.85              |
| 1:1:3018:C:OP1    | 27:y:9:ASN:ND2    | 2.08                     | 0.85              |
| 1:1:3343:G:O2'    | 1:1:3362:A:N6     | 2.10                     | 0.85              |
| 1:1:397:A:O2'     | 1:1:400:G:OP2     | 1.95                     | 0.84              |
| 21:m:83:VAL:HG22  | 22:r:238:VAL:HG22 | 1.59                     | 0.84              |
| 1:1:374:A:O2'     | 1:1:375:A:O5'     | 1.96                     | 0.83              |
| 1:1:2673:A:OP1    | 10:J:95:ASN:ND2   | 2.11                     | 0.83              |
| 5:C:126:ILE:O     | 5:C:129:THR:OG1   | 1.95                     | 0.83              |
| 1:1:3228:C:O2'    | 1:1:3229:G:OP2    | 1.97                     | 0.83              |
| 3:3:115:G:N2      | 6:D:71:GLY:O      | 2.12                     | 0.83              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:x:466:THR:OG1  | 26:x:485:HIS:O    | 1.97                     | 0.83              |
| 1:1:3195:U:O2'    | 1:1:3196:U:OP1    | 1.96                     | 0.82              |
| 1:1:2390:A:O2'    | 1:1:3307:A:N6     | 2.14                     | 0.81              |
| 4:B:301:THR:OG1   | 4:B:303:LYS:NZ    | 2.14                     | 0.81              |
| 1:1:960:U:O2      | 1:1:2615:G:O3'    | 1.98                     | 0.81              |
| 21:m:204:SER:HG   | 21:m:208:SER:HG   | 1.15                     | 0.81              |
| 1:1:1238:C:O2'    | 1:1:1239:C:OP1    | 1.97                     | 0.80              |
| 1:1:952:A:N3      | 1:1:1114:U:O2'    | 2.13                     | 0.80              |
| 1:1:203:G:O2'     | 1:1:204:A:O4'     | 2.00                     | 0.80              |
| 1:1:1176:C:OP2    | 1:1:1177:G:O2'    | 2.00                     | 0.80              |
| 1:1:984:G:N2      | 1:1:1138:U:OP1    | 2.15                     | 0.80              |
| 1:1:2646:C:OP1    | 25:w:185:LYS:NZ   | 2.14                     | 0.80              |
| 1:1:2890:A:O2'    | 1:1:2933:A:N3     | 2.13                     | 0.80              |
| 1:1:2752:U:O2'    | 1:1:2753:G:O4'    | 2.00                     | 0.79              |
| 26:x:214:ASP:OD1  | 26:x:217:SER:N    | 2.15                     | 0.79              |
| 1:1:437:G:O2'     | 1:1:438:A:O5'     | 1.99                     | 0.79              |
| 1:1:2690:G:O2'    | 1:1:2691:A:O5'    | 2.00                     | 0.79              |
| 1:1:2860:U:O2'    | 1:1:2861:U:OP1    | 2.00                     | 0.79              |
| 1:1:198:A:N3      | 1:1:218:G:O2'     | 2.16                     | 0.79              |
| 1:1:1329:U:O2'    | 1:1:1330:A:OP1    | 1.99                     | 0.79              |
| 22:r:231:VAL:HG22 | 22:r:237:VAL:HG23 | 1.64                     | 0.79              |
| 4:B:290:ASP:O     | 4:B:293:ASN:ND2   | 2.16                     | 0.78              |
| 1:1:2868:U:O2'    | 1:1:2869:U:OP2    | 2.01                     | 0.78              |
| 1:1:2964:G:N2     | 1:1:2967:A:OP2    | 2.15                     | 0.78              |
| 1:1:1245:A:N7     | 1:1:1271:A:O2'    | 2.15                     | 0.78              |
| 1:1:1129:A:O2'    | 1:1:1130:A:OP1    | 2.01                     | 0.78              |
| 1:1:1188:U:OP1    | 1:1:1210:U:O2'    | 1.99                     | 0.78              |
| 1:1:3190:C:OP1    | 12:O:172:ARG:NH1  | 2.16                     | 0.78              |
| 3:3:26:C:O2       | 3:3:57:G:N2       | 2.17                     | 0.78              |
| 1:1:1207:G:O2'    | 1:1:1209:G:OP1    | 2.01                     | 0.77              |
| 1:1:3151:U:OP1    | 1:1:3292:A:O2'    | 2.01                     | 0.77              |
| 1:1:1144:U:OP1    | 1:1:1367:G:O2'    | 2.03                     | 0.77              |
| 26:x:473:VAL:O    | 26:x:476:ARG:NH1  | 2.17                     | 0.77              |
| 21:m:209:LYS:O    | 21:m:212:TRP:N    | 2.17                     | 0.77              |
| 18:b:420:TYR:O    | 18:b:428:LYS:NZ   | 2.16                     | 0.77              |
| 1:1:971:G:O6      | 1:1:1111:U:O2     | 2.02                     | 0.77              |
| 1:1:3079:U:O2'    | 1:1:3080:G:OP1    | 2.02                     | 0.77              |
| 1:1:3084:C:O2'    | 1:1:3332:U:OP1    | 2.02                     | 0.77              |
| 1:1:679:U:O2'     | 1:1:788:C:O2      | 2.03                     | 0.76              |
| 21:m:7:GLU:OE2    | 21:m:10:ARG:NH2   | 2.18                     | 0.76              |
| 1:1:518:G:OP2     | 1:1:518:G:N2      | 2.19                     | 0.76              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:b:241:TYR:O    | 18:b:245:HIS:ND1  | 2.17                     | 0.76              |
| 3:3:27:A:O3'      | 10:J:141:ARG:NH1  | 2.19                     | 0.76              |
| 1:1:3110:C:O2'    | 9:H:155:SER:OG    | 2.02                     | 0.75              |
| 1:1:1101:G:OP2    | 8:F:196:LYS:NZ    | 2.19                     | 0.75              |
| 1:1:2612:U:O2'    | 1:1:2613:U:O4'    | 2.04                     | 0.75              |
| 1:1:1065:A:O2'    | 1:1:1066:G:N7     | 2.16                     | 0.75              |
| 1:1:1394:A:OP1    | 19:e:98:HIS:NE2   | 2.20                     | 0.75              |
| 1:1:2624:G:O2'    | 1:1:2625:C:OP1    | 2.05                     | 0.74              |
| 4:B:348:ARG:NH1   | 18:b:410:GLY:O    | 2.20                     | 0.74              |
| 6:D:36:LEU:O      | 6:D:39:GLN:NE2    | 2.20                     | 0.74              |
| 1:1:2702:A:O2'    | 1:1:2703:A:O5'    | 2.02                     | 0.74              |
| 1:1:1071:U:O2'    | 1:1:1072:G:N7     | 2.21                     | 0.74              |
| 21:m:289:SER:O    | 21:m:334:THR:OG1  | 2.06                     | 0.74              |
| 7:E:51:ARG:NH1    | 11:M:114:ASP:OD2  | 2.21                     | 0.73              |
| 26:x:78:THR:N     | 26:x:122:THR:O    | 2.20                     | 0.73              |
| 1:1:688:G:O2'     | 1:1:689:U:O5'     | 2.06                     | 0.73              |
| 1:1:1230:G:OP1    | 17:W:49:ARG:NH2   | 2.21                     | 0.73              |
| 1:1:784:A:O2'     | 13:Q:92:ARG:NH1   | 2.20                     | 0.73              |
| 14:S:63:GLN:NE2   | 14:S:65:ASN:OD1   | 2.22                     | 0.73              |
| 25:w:83:GLN:NE2   | 25:w:84:SER:O     | 2.21                     | 0.73              |
| 1:1:3112:G:OP1    | 9:H:77:ASN:ND2    | 2.22                     | 0.73              |
| 1:1:1157:G:O2'    | 1:1:1169:A:N3     | 2.20                     | 0.73              |
| 1:1:3109:G:N2     | 9:H:156:GLN:OE1   | 2.21                     | 0.72              |
| 3:3:23:A:N3       | 3:3:121:U:O2'     | 2.21                     | 0.72              |
| 1:1:991:G:N2      | 15:T:59:GLY:O     | 2.21                     | 0.72              |
| 1:1:990:U:N3      | 1:1:991:G:O6      | 2.21                     | 0.72              |
| 18:b:234:ASN:ND2  | 21:m:147:ARG:O    | 2.22                     | 0.72              |
| 1:1:2728:G:O2'    | 21:m:313:ARG:O    | 2.02                     | 0.72              |
| 1:1:1230:G:O2'    | 17:W:50:THR:OG1   | 2.06                     | 0.72              |
| 18:b:312:VAL:HG13 | 18:b:315:VAL:HG11 | 1.70                     | 0.72              |
| 3:3:82:G:O2'      | 3:3:83:U:O5'      | 2.05                     | 0.72              |
| 1:1:3164:C:O2'    | 1:1:3165:A:O5'    | 2.05                     | 0.72              |
| 1:1:2871:G:N2     | 22:r:169:GLU:OE1  | 2.23                     | 0.72              |
| 1:1:1192:C:O2'    | 1:1:1193:A:OP2    | 2.08                     | 0.71              |
| 1:1:2872:A:O2'    | 1:1:2874:G:N2     | 2.23                     | 0.71              |
| 22:r:4:ASN:O      | 22:r:6:TYR:N      | 2.23                     | 0.71              |
| 1:1:3026:G:N2     | 1:1:3029:A:OP2    | 2.24                     | 0.70              |
| 27:y:74:THR:OG1   | 27:y:97:VAL:O     | 2.09                     | 0.70              |
| 18:b:228:PRO:O    | 18:b:229:THR:OG1  | 2.09                     | 0.70              |
| 1:1:2819:A:O2'    | 1:1:2820:A:OP1    | 2.09                     | 0.70              |
| 1:1:1093:A:O2'    | 1:1:1094:U:O4'    | 2.09                     | 0.70              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:3086:A:O2'    | 1:1:3375:A:N6     | 2.25                     | 0.70              |
| 10:J:88:GLU:OE2   | 10:J:90:GLN:NE2   | 2.24                     | 0.70              |
| 22:r:203:ASN:OD1  | 22:r:216:THR:OG1  | 2.10                     | 0.70              |
| 1:1:681:U:OP1     | 5:C:115:HIS:N     | 2.25                     | 0.69              |
| 6:D:32:GLN:NE2    | 6:D:147:ASP:OD1   | 2.25                     | 0.69              |
| 1:1:2691:A:O2'    | 1:1:2692:A:O4'    | 2.09                     | 0.69              |
| 1:1:3195:U:O2'    | 1:1:3197:G:N2     | 2.25                     | 0.69              |
| 18:b:441:VAL:O    | 18:b:445:LEU:N    | 2.26                     | 0.69              |
| 1:1:1243:G:O2'    | 1:1:1244:A:O5'    | 2.09                     | 0.69              |
| 6:D:197:SER:O     | 6:D:202:GLY:N     | 2.25                     | 0.69              |
| 8:F:95:ILE:O      | 8:F:100:ARG:NH2   | 2.26                     | 0.69              |
| 1:1:3070:A:O2'    | 1:1:3071:U:OP1    | 2.11                     | 0.69              |
| 1:1:2954:U:O2'    | 1:1:2955:U:OP2    | 2.10                     | 0.69              |
| 21:m:344:ALA:N    | 21:m:349:GLU:OE2  | 2.25                     | 0.69              |
| 22:r:184:VAL:HG21 | 22:r:223:VAL:HG11 | 1.73                     | 0.69              |
| 1:1:1152:G:OP2    | 1:1:1152:G:N2     | 2.25                     | 0.69              |
| 1:1:550:A:O2'     | 1:1:551:A:O4'     | 2.08                     | 0.69              |
| 21:m:171:TYR:O    | 21:m:175:GLN:NE2  | 2.26                     | 0.69              |
| 21:m:226:ILE:HD11 | 21:m:258:VAL:HG21 | 1.74                     | 0.68              |
| 1:1:202:G:N2      | 1:1:203:G:O4'     | 2.26                     | 0.68              |
| 1:1:2969:A:O2'    | 1:1:2970:C:O5'    | 2.11                     | 0.68              |
| 24:v:181:VAL:HG11 | 25:w:58:VAL:HG21  | 1.75                     | 0.68              |
| 1:1:3030:G:O2'    | 1:1:3031:G:OP1    | 2.11                     | 0.68              |
| 1:1:974:G:O2'     | 1:1:975:C:OP1     | 2.10                     | 0.68              |
| 6:D:45:ASN:ND2    | 24:v:173:GLN:OE1  | 2.25                     | 0.68              |
| 1:1:3109:G:OP1    | 22:r:23:ARG:NE    | 2.26                     | 0.68              |
| 1:1:2831:G:N2     | 22:r:256:ASN:OD1  | 2.26                     | 0.68              |
| 1:1:370:U:O2      | 1:1:374:A:N7      | 2.27                     | 0.68              |
| 1:1:2692:A:O2'    | 1:1:2693:C:OP2    | 2.12                     | 0.68              |
| 1:1:3060:C:O3'    | 1:1:3371:G:N2     | 2.26                     | 0.68              |
| 18:b:43:ARG:NH2   | 18:b:117:LYS:O    | 2.26                     | 0.68              |
| 24:v:220:ARG:NH1  | 25:w:10:PRO:O     | 2.27                     | 0.68              |
| 1:1:3284:G:O2'    | 1:1:3285:C:O4'    | 2.06                     | 0.68              |
| 6:D:23:ARG:O      | 6:D:23:ARG:NH1    | 2.26                     | 0.68              |
| 1:1:1201:C:O2'    | 1:1:1202:A:OP2    | 2.11                     | 0.68              |
| 18:b:326:GLU:N    | 18:b:326:GLU:OE1  | 2.27                     | 0.68              |
| 21:m:204:SER:O    | 21:m:208:SER:OG   | 2.12                     | 0.67              |
| 1:1:1222:G:O2'    | 1:1:1223:A:OP2    | 2.10                     | 0.67              |
| 14:S:109:ASP:OD2  | 14:S:113:ARG:NH1  | 2.28                     | 0.67              |
| 26:x:208:ASN:ND2  | 26:x:228:HIS:O    | 2.28                     | 0.67              |
| 1:1:595:G:OP1     | 8:F:30:ARG:NH2    | 2.28                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:v:39:ASN:OD1   | 24:v:40:LYS:N     | 2.27                     | 0.67              |
| 26:x:38:ALA:N     | 26:x:42:GLY:O     | 2.27                     | 0.67              |
| 1:1:3135:U:OP1    | 12:O:148:LYS:NZ   | 2.25                     | 0.67              |
| 14:S:57:GLU:OE2   | 15:T:136:ARG:NE   | 2.27                     | 0.67              |
| 1:1:408:A:OP2     | 2:2:15:G:N2       | 2.28                     | 0.67              |
| 1:1:2745:G:N2     | 1:1:2748:A:OP2    | 2.26                     | 0.67              |
| 18:b:278:PHE:CD2  | 18:b:283:VAL:HG21 | 2.30                     | 0.66              |
| 3:3:7:G:O2'       | 6:D:72:ASP:OD2    | 2.09                     | 0.66              |
| 27:y:20:THR:OG1   | 27:y:23:TYR:O     | 2.13                     | 0.66              |
| 1:1:1097:G:O2'    | 15:T:108:ARG:NH2  | 2.29                     | 0.66              |
| 6:D:146:LEU:HD22  | 6:D:163:LEU:HD13  | 1.77                     | 0.66              |
| 18:b:180:LYS:NZ   | 18:b:221:THR:O    | 2.28                     | 0.66              |
| 21:m:328:LYS:NZ   | 21:m:367:CYS:O    | 2.28                     | 0.66              |
| 5:C:135:VAL:HG22  | 5:C:245:GLY:CA    | 2.26                     | 0.66              |
| 16:V:102:ILE:O    | 16:V:102:ILE:HD12 | 1.96                     | 0.66              |
| 18:b:220:ASP:OD1  | 18:b:221:THR:N    | 2.29                     | 0.66              |
| 1:1:1047:A:O2'    | 1:1:1048:A:OP1    | 2.12                     | 0.66              |
| 1:1:1312:C:O2'    | 12:O:83:ALA:O     | 2.14                     | 0.66              |
| 9:H:80:THR:O      | 9:H:84:LYS:N      | 2.29                     | 0.66              |
| 1:1:3314:A:OP2    | 4:B:175:LYS:NZ    | 2.28                     | 0.65              |
| 21:m:136:SER:N    | 21:m:139:ASP:OD2  | 2.28                     | 0.65              |
| 4:B:35:ASP:OD2    | 4:B:37:ARG:NH1    | 2.29                     | 0.65              |
| 22:r:6:TYR:O      | 22:r:9:ARG:N      | 2.29                     | 0.65              |
| 1:1:338:A:O2'     | 1:1:1380:G:O2'    | 1.94                     | 0.65              |
| 8:F:73:GLY:O      | 15:T:143:THR:OG1  | 2.13                     | 0.65              |
| 15:T:151:LEU:HD23 | 15:T:151:LEU:H    | 1.61                     | 0.65              |
| 22:r:148:LYS:NZ   | 22:r:169:GLU:OE2  | 2.21                     | 0.65              |
| 1:1:1364:C:OP1    | 8:F:110:ARG:NH1   | 2.30                     | 0.65              |
| 1:1:3060:C:N4     | 1:1:3061:G:O6     | 2.29                     | 0.65              |
| 1:1:3307:A:OP2    | 4:B:226:PHE:N     | 2.30                     | 0.65              |
| 1:1:2729:U:O4'    | 22:r:164:ARG:NH2  | 2.30                     | 0.65              |
| 1:1:2966:G:O2'    | 1:1:2967:A:O4'    | 2.10                     | 0.65              |
| 25:w:43:ASN:OD1   | 25:w:45:ARG:N     | 2.30                     | 0.65              |
| 1:1:2830:G:N2     | 22:r:254:CYS:SG   | 2.70                     | 0.64              |
| 1:1:943:U:O2'     | 1:1:1431:G:O2'    | 2.15                     | 0.64              |
| 1:1:3116:G:N2     | 1:1:3116:G:OP1    | 2.27                     | 0.64              |
| 26:x:468:LEU:HD21 | 26:x:489:VAL:HG11 | 1.80                     | 0.64              |
| 13:Q:81:VAL:HG21  | 13:Q:140:LEU:HD13 | 1.79                     | 0.64              |
| 21:m:222:SER:O    | 21:m:253:LYS:NZ   | 2.31                     | 0.64              |
| 27:y:39:GLU:O     | 27:y:43:GLY:N     | 2.31                     | 0.64              |
| 3:3:84:A:O2'      | 3:3:85:G:O4'      | 2.14                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:b:440:ASN:ND2  | 23:u:1:MET:O      | 2.31                     | 0.63              |
| 8:F:48:ASN:ND2    | 8:F:182:ASP:OD2   | 2.32                     | 0.63              |
| 14:S:27:MET:HG2   | 15:T:151:LEU:HD21 | 1.80                     | 0.63              |
| 27:y:165:THR:O    | 27:y:170:GLN:NE2  | 2.31                     | 0.63              |
| 1:1:1307:G:O2'    | 1:1:1308:A:O4'    | 2.17                     | 0.63              |
| 1:1:2955:U:OP2    | 1:1:2977:G:N2     | 2.32                     | 0.63              |
| 3:3:7:G:OP2       | 6:D:28:THR:OG1    | 2.13                     | 0.63              |
| 1:1:3343:G:N2     | 1:1:3362:A:OP2    | 2.32                     | 0.63              |
| 1:1:3180:A:O2'    | 12:O:117:ARG:NH1  | 2.32                     | 0.63              |
| 1:1:3368:U:OP1    | 4:B:384:LYS:NZ    | 2.24                     | 0.62              |
| 1:1:1240:A:N6     | 1:1:1244:A:OP1    | 2.31                     | 0.62              |
| 27:y:156:ASN:ND2  | 27:y:201:ASP:OD2  | 2.32                     | 0.62              |
| 20:f:60:ARG:O     | 20:f:60:ARG:NE    | 2.30                     | 0.62              |
| 22:r:237:VAL:HG21 | 26:x:444:VAL:HG21 | 1.80                     | 0.62              |
| 1:1:3242:G:OP1    | 12:O:159:LYS:NZ   | 2.29                     | 0.62              |
| 9:H:50:ASN:ND2    | 11:M:4:ASP:OD1    | 2.32                     | 0.62              |
| 1:1:1205:A:O2'    | 1:1:1206:G:OP1    | 2.16                     | 0.62              |
| 5:C:334:PHE:O     | 5:C:338:LYS:N     | 2.30                     | 0.62              |
| 10:J:172:LEU:HD23 | 10:J:172:LEU:O    | 1.99                     | 0.62              |
| 1:1:337:G:O2'     | 1:1:338:A:OP1     | 2.12                     | 0.62              |
| 1:1:2746:A:OP1    | 6:D:179:ARG:NE    | 2.31                     | 0.62              |
| 1:1:1394:A:N7     | 1:1:1417:G:N2     | 2.48                     | 0.62              |
| 18:b:210:ASP:OD2  | 18:b:215:ARG:NH1  | 2.32                     | 0.62              |
| 4:B:287:LYS:O     | 4:B:293:ASN:ND2   | 2.32                     | 0.61              |
| 3:3:12:U:OP2      | 3:3:68:C:O2'      | 2.16                     | 0.61              |
| 1:1:1303:A:O2'    | 1:1:1304:A:O4'    | 2.11                     | 0.61              |
| 1:1:1411:C:OP1    | 19:e:98:HIS:ND1   | 2.33                     | 0.61              |
| 1:1:2746:A:N3     | 6:D:146:LEU:HD23  | 2.16                     | 0.61              |
| 16:V:64:LYS:NZ    | 21:m:443:GLU:OE1  | 2.33                     | 0.61              |
| 13:Q:62:VAL:HG11  | 13:Q:140:LEU:CD2  | 2.31                     | 0.61              |
| 1:1:993:G:C6      | 1:1:1056:U:N3     | 2.68                     | 0.61              |
| 3:3:37:G:O2'      | 3:3:38:U:O4'      | 2.16                     | 0.61              |
| 1:1:2817:A:O2'    | 1:1:2818:U:OP1    | 2.17                     | 0.61              |
| 1:1:3120:C:OP2    | 22:r:26:LYS:NZ    | 2.34                     | 0.61              |
| 1:1:2765:C:OP2    | 1:1:2798:C:N4     | 2.21                     | 0.60              |
| 17:W:1:MET:HE3    | 17:W:3:ARG:O      | 2.01                     | 0.60              |
| 1:1:688:G:HO2'    | 1:1:689:U:P       | 2.23                     | 0.60              |
| 26:x:239:PRO:O    | 26:x:243:VAL:HG23 | 2.01                     | 0.60              |
| 1:1:1129:A:HO2'   | 1:1:1130:A:P      | 2.25                     | 0.60              |
| 1:1:2418:G:OP2    | 1:1:2606:G:N2     | 2.34                     | 0.60              |
| 1:1:1145:G:N2     | 1:1:1331:U:O2'    | 2.34                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:2895:G:OP2    | 9:H:166:ARG:NH1   | 2.33                     | 0.60              |
| 21:m:218:VAL:HG11 | 21:m:367:CYS:HB3  | 1.83                     | 0.60              |
| 5:C:361:HIS:O     | 14:S:26:ARG:NH2   | 2.34                     | 0.60              |
| 1:1:1160:C:N3     | 1:1:1366:A:O2'    | 2.34                     | 0.60              |
| 1:1:2876:C:O2'    | 1:1:2877:G:O5'    | 2.20                     | 0.60              |
| 5:C:142:VAL:O     | 5:C:145:ILE:HG23  | 2.02                     | 0.60              |
| 14:S:6:GLU:OE1    | 14:S:28:ARG:NH1   | 2.34                     | 0.60              |
| 18:b:98:ILE:HG12  | 18:b:143:LEU:HD21 | 1.84                     | 0.60              |
| 21:m:419:SER:OG   | 21:m:420:GLY:N    | 2.35                     | 0.60              |
| 17:W:162:GLU:OE1  | 17:W:166:ARG:NH2  | 2.35                     | 0.59              |
| 1:1:2875:U:O2'    | 1:1:2876:C:O5'    | 2.15                     | 0.59              |
| 3:3:7:G:OP1       | 6:D:33:ARG:NH1    | 2.36                     | 0.59              |
| 26:x:133:THR:HG22 | 26:x:480:VAL:HG11 | 1.84                     | 0.59              |
| 27:y:88:LEU:HD23  | 27:y:92:VAL:HG11  | 1.83                     | 0.59              |
| 1:1:3366:G:O2'    | 23:u:112:MET:O    | 2.21                     | 0.59              |
| 1:1:2814:G:O2'    | 1:1:2815:G:N7     | 2.36                     | 0.58              |
| 1:1:2818:U:O2'    | 1:1:2819:A:OP2    | 2.20                     | 0.58              |
| 1:1:695:C:OP2     | 5:C:115:HIS:NE2   | 2.34                     | 0.58              |
| 1:1:2764:C:HO2'   | 1:1:2765:C:P      | 2.23                     | 0.58              |
| 7:E:104:GLU:OE1   | 7:E:105:TYR:N     | 2.36                     | 0.58              |
| 21:m:412:LEU:O    | 21:m:416:TYR:N    | 2.36                     | 0.58              |
| 1:1:376:G:O2'     | 1:1:377:A:OP2     | 2.18                     | 0.58              |
| 22:r:206:SER:O    | 22:r:206:SER:OG   | 2.19                     | 0.58              |
| 25:w:161:GLU:O    | 25:w:162:VAL:HG13 | 2.04                     | 0.58              |
| 26:x:331:ASP:OD1  | 26:x:332:TYR:N    | 2.37                     | 0.58              |
| 1:1:2690:G:HO2'   | 1:1:2691:A:P      | 2.24                     | 0.58              |
| 1:1:3258:U:O2'    | 1:1:3260:G:OP1    | 2.22                     | 0.58              |
| 24:v:13:LYS:O     | 24:v:17:VAL:HG23  | 2.04                     | 0.58              |
| 1:1:3275:U:OP1    | 1:1:3276:G:N2     | 2.36                     | 0.57              |
| 16:V:81:GLN:O     | 16:V:98:ASN:ND2   | 2.37                     | 0.57              |
| 21:m:215:LEU:HD22 | 21:m:370:ILE:HG21 | 1.87                     | 0.57              |
| 17:W:70:ARG:NH1   | 17:W:98:GLY:O     | 2.37                     | 0.57              |
| 21:m:390:VAL:O    | 21:m:393:VAL:HG22 | 2.05                     | 0.57              |
| 26:x:25:ILE:O     | 26:x:25:ILE:HD12  | 2.05                     | 0.57              |
| 1:1:197:G:O6      | 1:1:395:A:N6      | 2.36                     | 0.57              |
| 1:1:700:C:O2'     | 1:1:701:G:O5'     | 2.22                     | 0.57              |
| 1:1:2892:A:HO2'   | 1:1:3129:A:HO2'   | 1.51                     | 0.57              |
| 4:B:56:ILE:HD12   | 4:B:76:VAL:HG21   | 1.86                     | 0.57              |
| 6:D:141:PRO:HD2   | 25:w:86:VAL:HG21  | 1.87                     | 0.57              |
| 1:1:209:A:O2'     | 1:1:211:A:OP2     | 2.14                     | 0.57              |
| 1:1:2791:G:O2'    | 1:1:2792:A:O4'    | 2.15                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:591:G:N2      | 1:1:612:U:OP1     | 2.37                     | 0.57              |
| 1:1:3120:C:OP1    | 22:r:30:ARG:NH2   | 2.37                     | 0.57              |
| 18:b:461:GLU:O    | 18:b:465:ASN:ND2  | 2.37                     | 0.57              |
| 15:T:129:LYS:O    | 15:T:131:GLN:NE2  | 2.37                     | 0.57              |
| 17:W:47:ASP:OD2   | 17:W:126:ARG:NE   | 2.38                     | 0.57              |
| 13:Q:36:LEU:O     | 13:Q:40:THR:OG1   | 2.15                     | 0.56              |
| 17:W:41:TRP:CZ2   | 17:W:109:VAL:HG23 | 2.40                     | 0.56              |
| 18:b:54:GLY:O     | 18:b:58:VAL:HG23  | 2.05                     | 0.56              |
| 24:v:22:LYS:O     | 25:w:101:ARG:NH1  | 2.38                     | 0.56              |
| 26:x:188:TRP:O    | 26:x:206:MET:N    | 2.35                     | 0.56              |
| 1:1:1101:G:O6     | 1:1:1102:A:N6     | 2.39                     | 0.56              |
| 21:m:400:ILE:O    | 21:m:403:VAL:HG22 | 2.06                     | 0.56              |
| 1:1:517:G:OP1     | 8:F:67:ARG:NH2    | 2.38                     | 0.56              |
| 3:3:47:C:OP1      | 6:D:95:TRP:N      | 2.36                     | 0.56              |
| 26:x:25:ILE:HD13  | 26:x:102:TYR:CD1  | 2.41                     | 0.56              |
| 26:x:174:ASP:O    | 26:x:176:GLN:NE2  | 2.39                     | 0.56              |
| 18:b:68:PHE:CZ    | 18:b:150:LEU:HD22 | 2.40                     | 0.56              |
| 1:1:3082:C:N4     | 1:1:3083:G:O6     | 2.38                     | 0.56              |
| 1:1:3184:A:N3     | 1:1:3187:A:O2'    | 2.35                     | 0.56              |
| 1:1:197:G:N3      | 1:1:218:G:N2      | 2.52                     | 0.55              |
| 6:D:34:LYS:O      | 6:D:38:THR:OG1    | 2.06                     | 0.55              |
| 1:1:394:G:N1      | 1:1:397:A:OP2     | 2.39                     | 0.55              |
| 1:1:2841:G:O2'    | 1:1:2847:A:N6     | 2.39                     | 0.55              |
| 22:r:214:VAL:HG12 | 22:r:216:THR:HG23 | 1.86                     | 0.55              |
| 1:1:2626:A:O2'    | 1:1:2627:C:O5'    | 2.25                     | 0.55              |
| 1:1:2878:G:O2'    | 1:1:2879:C:OP2    | 2.18                     | 0.55              |
| 1:1:3169:U:OP2    | 20:f:63:LYS:NZ    | 2.40                     | 0.55              |
| 9:H:22:SER:O      | 9:H:24:ILE:N      | 2.38                     | 0.55              |
| 20:f:9:VAL:N      | 20:f:100:ILE:O    | 2.38                     | 0.55              |
| 21:m:126:SER:O    | 21:m:126:SER:OG   | 2.23                     | 0.55              |
| 1:1:2626:A:O2'    | 1:1:2627:C:O4'    | 2.20                     | 0.55              |
| 3:3:37:G:O2'      | 3:3:38:U:O5'      | 2.25                     | 0.55              |
| 8:F:47:ARG:NH1    | 8:F:183:ASP:OD2   | 2.40                     | 0.55              |
| 7:E:47:PHE:N      | 7:E:47:PHE:CD1    | 2.75                     | 0.55              |
| 13:Q:62:VAL:HG11  | 13:Q:140:LEU:HD23 | 1.89                     | 0.55              |
| 1:1:406:G:O2'     | 1:1:407:A:OP2     | 2.24                     | 0.55              |
| 4:B:31:ALA:O      | 4:B:339:ARG:NH1   | 2.40                     | 0.55              |
| 4:B:160:VAL:N     | 4:B:181:ILE:O     | 2.39                     | 0.55              |
| 26:x:148:CYS:SG   | 26:x:192:VAL:HG22 | 2.46                     | 0.55              |
| 1:1:2893:C:H2'    | 1:1:2894:C:C1'    | 2.37                     | 0.55              |
| 8:F:51:TYR:OH     | 8:F:183:ASP:OD2   | 2.24                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:m:332:ILE:HD13 | 21:m:366:ASP:OD1  | 2.07                     | 0.55              |
| 11:M:20:VAL:HG13  | 11:M:66:THR:OG1   | 2.07                     | 0.54              |
| 21:m:346:ILE:HG22 | 21:m:347:PRO:HD2  | 1.89                     | 0.54              |
| 18:b:21:VAL:O     | 18:b:25:THR:HG23  | 2.07                     | 0.54              |
| 1:1:1238:C:H2'    | 1:1:1239:C:O4'    | 2.08                     | 0.54              |
| 9:H:137:SER:HB2   | 9:H:145:VAL:HG23  | 1.88                     | 0.54              |
| 1:1:412:G:O6      | 2:2:12:A:N6       | 2.41                     | 0.54              |
| 1:1:1135:A:C6     | 1:1:1136:A:N6     | 2.75                     | 0.54              |
| 1:1:1205:A:HO2'   | 1:1:1206:G:P      | 2.31                     | 0.54              |
| 1:1:3047:U:OP1    | 4:B:221:THR:OG1   | 2.25                     | 0.54              |
| 1:1:3057:U:OP2    | 1:1:3086:A:N6     | 2.39                     | 0.54              |
| 10:J:171:VAL:HG13 | 10:J:173:ASP:H    | 1.72                     | 0.54              |
| 18:b:25:THR:HG21  | 18:b:53:THR:HG23  | 1.89                     | 0.54              |
| 26:x:189:VAL:HG23 | 26:x:189:VAL:O    | 2.07                     | 0.54              |
| 1:1:2888:U:O4'    | 1:1:2911:A:N6     | 2.41                     | 0.54              |
| 10:J:15:GLU:HB3   | 10:J:130:VAL:HG13 | 1.90                     | 0.54              |
| 14:S:155:ARG:NE   | 14:S:171:PHE:O    | 2.38                     | 0.54              |
| 16:V:52:ALA:HB2   | 16:V:58:VAL:HG11  | 1.90                     | 0.54              |
| 18:b:1:MET:O      | 18:b:5:TRP:NE1    | 2.37                     | 0.54              |
| 27:y:85:ARG:O     | 27:y:85:ARG:NE    | 2.40                     | 0.54              |
| 1:1:3030:G:O2'    | 1:1:3031:G:P      | 2.65                     | 0.54              |
| 18:b:71:ILE:O     | 18:b:74:VAL:HG12  | 2.06                     | 0.54              |
| 21:m:31:ARG:O     | 21:m:36:VAL:HG23  | 2.08                     | 0.54              |
| 1:1:1205:A:O2'    | 1:1:1206:G:P      | 2.66                     | 0.54              |
| 1:1:2765:C:OP1    | 1:1:2794:G:N2     | 2.41                     | 0.54              |
| 17:W:41:TRP:HE3   | 17:W:217:VAL:HG21 | 1.72                     | 0.54              |
| 1:1:3306:U:O2'    | 1:1:3308:C:OP2    | 2.19                     | 0.54              |
| 1:1:2831:G:N3     | 22:r:256:ASN:ND2  | 2.54                     | 0.54              |
| 21:m:221:SER:OG   | 21:m:355:TYR:OH   | 2.24                     | 0.54              |
| 1:1:3113:A:OP1    | 9:H:69:ARG:NH1    | 2.41                     | 0.53              |
| 14:S:48:LEU:HD13  | 15:T:151:LEU:HD12 | 1.90                     | 0.53              |
| 18:b:324:LEU:HD23 | 18:b:324:LEU:H    | 1.73                     | 0.53              |
| 21:m:209:LYS:O    | 21:m:211:ILE:N    | 2.42                     | 0.53              |
| 6:D:77:ALA:O      | 6:D:108:ARG:NH1   | 2.39                     | 0.53              |
| 8:F:216:VAL:HG23  | 8:F:216:VAL:O     | 2.09                     | 0.53              |
| 9:H:41:ILE:CG2    | 9:H:43:VAL:HG22   | 2.39                     | 0.53              |
| 26:x:25:ILE:HD13  | 26:x:102:TYR:CG   | 2.43                     | 0.53              |
| 1:1:3389:U:O2'    | 1:1:3390:G:O5'    | 2.19                     | 0.53              |
| 1:1:3395:G:O2'    | 1:1:3396:U:OP2    | 2.21                     | 0.53              |
| 21:m:204:SER:OG   | 21:m:208:SER:OG   | 2.02                     | 0.53              |
| 25:w:54:THR:O     | 25:w:58:VAL:HG23  | 2.08                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:3210:A:OP1    | 11:M:109:ARG:NH1  | 2.41                     | 0.53              |
| 4:B:377:HIS:O     | 4:B:381:GLY:N     | 2.42                     | 0.53              |
| 10:J:138:VAL:HG22 | 10:J:141:ARG:NH1  | 2.24                     | 0.53              |
| 24:v:90:MET:SD    | 24:v:90:MET:N     | 2.79                     | 0.53              |
| 1:1:3295:A:OP1    | 4:B:126:LYS:N     | 2.41                     | 0.53              |
| 22:r:185:THR:HB   | 22:r:192:THR:HG22 | 1.90                     | 0.53              |
| 1:1:594:U:OP1     | 1:1:609:G:N1      | 2.35                     | 0.53              |
| 1:1:2876:C:HO2'   | 1:1:2877:G:C5'    | 2.21                     | 0.53              |
| 4:B:76:VAL:HG12   | 4:B:325:LYS:HA    | 1.90                     | 0.53              |
| 5:C:156:LEU:HD23  | 5:C:159:ILE:HD12  | 1.90                     | 0.53              |
| 25:w:35:ASP:OD1   | 25:w:49:LYS:NZ    | 2.37                     | 0.53              |
| 11:M:113:THR:HG22 | 11:M:114:ASP:H    | 1.73                     | 0.53              |
| 18:b:327:ASN:O    | 18:b:331:VAL:HG23 | 2.08                     | 0.53              |
| 6:D:207:TYR:OH    | 6:D:218:ARG:NH2   | 2.38                     | 0.53              |
| 17:W:166:ARG:NE   | 22:r:18:LEU:HD22  | 2.24                     | 0.53              |
| 26:x:260:ILE:HD11 | 26:x:281:VAL:HG11 | 1.91                     | 0.53              |
| 4:B:274:SER:O     | 4:B:275:ARG:NE    | 2.42                     | 0.53              |
| 17:W:81:ARG:NH2   | 17:W:84:GLU:OE2   | 2.42                     | 0.53              |
| 21:m:126:SER:OG   | 26:x:399:THR:OG1  | 2.25                     | 0.53              |
| 27:y:199:VAL:HG11 | 27:y:222:PHE:CZ   | 2.44                     | 0.53              |
| 8:F:178:ILE:HG22  | 8:F:178:ILE:O     | 2.07                     | 0.53              |
| 27:y:126:GLU:OE2  | 27:y:139:ARG:NH1  | 2.42                     | 0.53              |
| 22:r:133:MET:SD   | 22:r:134:PHE:N    | 2.82                     | 0.52              |
| 11:M:116:GLU:N    | 11:M:116:GLU:OE1  | 2.43                     | 0.52              |
| 1:1:1277:C:O2'    | 1:1:1278:A:O5'    | 2.27                     | 0.52              |
| 1:1:2624:G:O5'    | 25:w:151:ASN:ND2  | 2.42                     | 0.52              |
| 11:M:40:ASP:OD1   | 11:M:43:LYS:N     | 2.43                     | 0.52              |
| 17:W:148:GLN:O    | 17:W:149:ILE:HG23 | 2.08                     | 0.52              |
| 21:m:352:VAL:HG22 | 21:m:353:TRP:HD1  | 1.75                     | 0.52              |
| 1:1:2692:A:O2'    | 1:1:2693:C:P      | 2.67                     | 0.52              |
| 1:1:1057:A:O2'    | 1:1:1058:U:P      | 2.67                     | 0.52              |
| 1:1:1241:U:N3     | 1:1:1244:A:OP1    | 2.40                     | 0.52              |
| 17:W:166:ARG:CZ   | 22:r:18:LEU:HD22  | 2.40                     | 0.52              |
| 18:b:309:VAL:O    | 18:b:312:VAL:HG12 | 2.10                     | 0.52              |
| 21:m:269:VAL:HG22 | 21:m:467:LEU:HD21 | 1.91                     | 0.52              |
| 1:1:993:G:C5      | 1:1:1056:U:N3     | 2.78                     | 0.52              |
| 3:3:9:C:OP1       | 24:v:54:LYS:NZ    | 2.32                     | 0.52              |
| 4:B:375:GLU:OE1   | 4:B:375:GLU:N     | 2.43                     | 0.52              |
| 8:F:191:VAL:HG12  | 8:F:191:VAL:O     | 2.10                     | 0.52              |
| 1:1:608:A:OP1     | 5:C:315:LYS:NZ    | 2.44                     | 0.51              |
| 6:D:68:THR:HG22   | 6:D:70:THR:H      | 1.76                     | 0.51              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:y:140:GLN:NE2  | 27:y:172:GLU:OE1  | 2.43                     | 0.51              |
| 1:1:3030:G:HO2'   | 1:1:3031:G:P      | 2.32                     | 0.51              |
| 1:1:2896:A:OP1    | 22:r:27:ARG:NH1   | 2.42                     | 0.51              |
| 1:1:3305:A:OP1    | 4:B:223:GLY:N     | 2.39                     | 0.51              |
| 16:V:19:VAL:HG23  | 16:V:50:PRO:O     | 2.10                     | 0.51              |
| 1:1:2690:G:OP2    | 1:1:2692:A:N6     | 2.43                     | 0.51              |
| 1:1:3079:U:HO2'   | 1:1:3080:G:P      | 2.31                     | 0.51              |
| 21:m:126:SER:HG   | 26:x:399:THR:HG1  | 1.55                     | 0.51              |
| 1:1:499:G:O4'     | 1:1:3273:A:N6     | 2.43                     | 0.51              |
| 18:b:178:VAL:HG12 | 18:b:178:VAL:O    | 2.09                     | 0.51              |
| 1:1:3381:U:O2'    | 1:1:3383:G:N7     | 2.43                     | 0.51              |
| 21:m:233:ASP:OD1  | 21:m:233:ASP:N    | 2.43                     | 0.51              |
| 1:1:596:C:OP1     | 8:F:37:ASN:ND2    | 2.43                     | 0.51              |
| 1:1:1413:G:N1     | 1:1:1414:G:O6     | 2.44                     | 0.51              |
| 1:1:2828:G:N2     | 18:b:19:ASP:OD1   | 2.41                     | 0.51              |
| 1:1:3222:U:N3     | 1:1:3264:G:O6     | 2.44                     | 0.51              |
| 1:1:3344:A:OP2    | 1:1:3361:G:N2     | 2.44                     | 0.51              |
| 5:C:130:ALA:O     | 5:C:132:ALA:N     | 2.44                     | 0.51              |
| 18:b:4:SER:OG     | 18:b:4:SER:O      | 2.28                     | 0.51              |
| 1:1:3110:C:OP1    | 22:r:26:LYS:NZ    | 2.44                     | 0.51              |
| 15:T:126:VAL:HG22 | 15:T:127:GLN:H    | 1.75                     | 0.51              |
| 27:y:21:ASN:ND2   | 27:y:112:ASP:OD2  | 2.44                     | 0.51              |
| 27:y:219:GLU:OE1  | 27:y:224:LEU:N    | 2.44                     | 0.51              |
| 1:1:996:A:N6      | 1:1:999:G:O6      | 2.44                     | 0.50              |
| 1:1:1135:A:N6     | 1:1:1136:A:N6     | 2.58                     | 0.50              |
| 1:1:1201:C:O2'    | 1:1:1201:C:O2     | 2.29                     | 0.50              |
| 3:3:82:G:O2'      | 3:3:83:U:O4'      | 2.29                     | 0.50              |
| 9:H:61:GLY:O      | 9:H:65:VAL:HG23   | 2.10                     | 0.50              |
| 1:1:529:A:N6      | 1:1:564:G:O6      | 2.45                     | 0.50              |
| 8:F:98:LYS:O      | 8:F:102:VAL:HG23  | 2.10                     | 0.50              |
| 22:r:214:VAL:CG1  | 22:r:216:THR:HG23 | 2.41                     | 0.50              |
| 26:x:399:THR:HG23 | 26:x:399:THR:O    | 2.12                     | 0.50              |
| 1:1:494:G:HO2'    | 1:1:495:G:C5'     | 2.15                     | 0.50              |
| 1:1:2872:A:N6     | 1:1:2925:C:O2'    | 2.45                     | 0.50              |
| 27:y:97:VAL:HG11  | 27:y:125:THR:HG23 | 1.93                     | 0.50              |
| 27:y:126:GLU:CG   | 27:y:137:VAL:HG11 | 2.41                     | 0.50              |
| 1:1:3193:C:H2'    | 1:1:3194:C:C1'    | 2.42                     | 0.50              |
| 3:3:82:G:HO2'     | 3:3:83:U:C5'      | 2.20                     | 0.50              |
| 10:J:100:GLY:O    | 10:J:159:THR:HG21 | 2.11                     | 0.50              |
| 15:T:103:GLN:N    | 15:T:103:GLN:OE1  | 2.45                     | 0.50              |
| 18:b:46:TYR:HB3   | 18:b:116:LEU:HD21 | 1.93                     | 0.50              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:971:G:O6      | 1:1:1111:U:C2     | 2.64                     | 0.50              |
| 1:1:3046:A:N1     | 1:1:3096:C:N4     | 2.59                     | 0.50              |
| 8:F:180:SER:OG    | 8:F:183:ASP:OD1   | 2.30                     | 0.50              |
| 18:b:381:SER:O    | 18:b:385:LEU:HD13 | 2.12                     | 0.50              |
| 1:1:1137:C:OP1    | 15:T:81:GLY:N     | 2.38                     | 0.49              |
| 1:1:971:G:C6      | 1:1:1111:U:O2     | 2.65                     | 0.49              |
| 4:B:54:THR:HG23   | 4:B:76:VAL:HG23   | 1.95                     | 0.49              |
| 1:1:509:U:O2'     | 20:f:42:GLN:NE2   | 2.46                     | 0.49              |
| 1:1:2660:G:H21    | 1:1:2744:U:H4'    | 1.77                     | 0.49              |
| 14:S:4:PHE:O      | 14:S:100:VAL:HG21 | 2.12                     | 0.49              |
| 1:1:2715:A:O4'    | 25:w:128:ARG:NH2  | 2.46                     | 0.49              |
| 4:B:92:TYR:HB2    | 4:B:157:VAL:HG23  | 1.93                     | 0.49              |
| 1:1:195:U:H2'     | 1:1:196:G:O4'     | 2.12                     | 0.49              |
| 1:1:3389:U:HO2'   | 1:1:3390:G:P      | 2.35                     | 0.49              |
| 13:Q:135:GLN:N    | 13:Q:135:GLN:OE1  | 2.43                     | 0.49              |
| 21:m:210:ARG:HA   | 21:m:213:ASN:CG   | 2.38                     | 0.49              |
| 25:w:194:GLN:O    | 25:w:198:ASN:ND2  | 2.45                     | 0.49              |
| 1:1:406:G:N2      | 2:2:16:G:O2'      | 2.46                     | 0.49              |
| 17:W:41:TRP:CE3   | 17:W:217:VAL:HG21 | 2.47                     | 0.49              |
| 21:m:209:LYS:O    | 21:m:210:ARG:C    | 2.54                     | 0.49              |
| 1:1:2731:U:OP1    | 21:m:109:ARG:NH2  | 2.46                     | 0.49              |
| 18:b:323:GLN:OE1  | 18:b:323:GLN:N    | 2.46                     | 0.49              |
| 24:v:261:LYS:O    | 24:v:263:VAL:HG23 | 2.13                     | 0.49              |
| 1:1:990:U:O2'     | 1:1:991:G:P       | 2.70                     | 0.49              |
| 1:1:2798:C:OP1    | 21:m:18:LYS:NZ    | 2.44                     | 0.49              |
| 5:C:34:ILE:O      | 5:C:38:VAL:HG23   | 2.12                     | 0.49              |
| 24:v:67:HIS:O     | 24:v:71:ASP:N     | 2.46                     | 0.49              |
| 24:v:241:SER:OG   | 24:v:243:ASP:OD2  | 2.30                     | 0.49              |
| 18:b:188:THR:OG1  | 18:b:208:HIS:O    | 2.30                     | 0.49              |
| 21:m:95:ALA:O     | 21:m:99:THR:HG23  | 2.13                     | 0.49              |
| 21:m:462:ILE:HG23 | 21:m:462:ILE:O    | 2.13                     | 0.49              |
| 26:x:470:VAL:HG13 | 26:x:479:SER:HB3  | 1.94                     | 0.49              |
| 1:1:2386:A:N6     | 1:1:2993:G:O2'    | 2.45                     | 0.49              |
| 27:y:97:VAL:HG22  | 27:y:128:LEU:HD23 | 1.94                     | 0.49              |
| 1:1:3313:U:O4     | 1:1:3314:A:N6     | 2.46                     | 0.48              |
| 17:W:55:GLU:OE1   | 17:W:119:TYR:OH   | 2.14                     | 0.48              |
| 6:D:90:HIS:NE2    | 6:D:229:ASP:OD2   | 2.46                     | 0.48              |
| 27:y:46:ILE:HD12  | 27:y:46:ILE:O     | 2.14                     | 0.48              |
| 1:1:3241:G:OP2    | 4:B:153:LYS:NZ    | 2.46                     | 0.48              |
| 1:1:3369:G:OP2    | 23:u:111:ARG:NH1  | 2.39                     | 0.48              |
| 4:B:53:MET:SD     | 4:B:54:THR:N      | 2.87                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:71:GLU:OE1    | 27:y:79:GLN:NE2   | 2.43                     | 0.48              |
| 6:D:278:SER:OG    | 6:D:280:GLU:OE1   | 2.30                     | 0.48              |
| 24:v:100:MET:N    | 24:v:116:LEU:O    | 2.41                     | 0.48              |
| 25:w:159:LEU:HD12 | 25:w:159:LEU:O    | 2.14                     | 0.48              |
| 26:x:51:VAL:HG22  | 26:x:51:VAL:O     | 2.12                     | 0.48              |
| 26:x:207:ASP:OD2  | 26:x:208:ASN:N    | 2.40                     | 0.48              |
| 1:1:970:A:HO2'    | 1:1:971:G:H8      | 1.58                     | 0.48              |
| 1:1:1117:G:O6     | 1:1:1142:G:N2     | 2.47                     | 0.48              |
| 1:1:2691:A:HO2'   | 1:1:2692:A:C1'    | 2.25                     | 0.48              |
| 23:u:22:VAL:HG22  | 23:u:28:GLU:HA    | 1.94                     | 0.48              |
| 25:w:74:THR:O     | 26:x:481:ASP:N    | 2.47                     | 0.48              |
| 25:w:112:THR:HG22 | 25:w:198:ASN:HB3  | 1.96                     | 0.48              |
| 1:1:1093:A:O2'    | 1:1:1094:U:O5'    | 2.32                     | 0.48              |
| 21:m:224:VAL:HG13 | 21:m:318:VAL:HG23 | 1.95                     | 0.48              |
| 22:r:55:TYR:O     | 22:r:59:VAL:HG23  | 2.14                     | 0.48              |
| 1:1:1303:A:N7     | 18:b:32:VAL:HG21  | 2.29                     | 0.48              |
| 1:1:3141:A:OP1    | 1:1:3142:A:O2'    | 2.32                     | 0.48              |
| 1:1:3165:A:HO2'   | 1:1:3166:C:C5'    | 2.26                     | 0.48              |
| 1:1:3195:U:HO2'   | 1:1:3197:G:N2     | 2.12                     | 0.48              |
| 3:3:85:G:O2'      | 3:3:87:G:OP1      | 2.28                     | 0.48              |
| 4:B:46:PHE:HE2    | 4:B:208:VAL:HG21  | 1.79                     | 0.48              |
| 16:V:37:ILE:HD11  | 16:V:73:VAL:HG21  | 1.95                     | 0.48              |
| 16:V:39:VAL:HG13  | 16:V:58:VAL:HG12  | 1.96                     | 0.48              |
| 26:x:78:THR:N     | 26:x:124:ARG:HG3  | 2.28                     | 0.48              |
| 21:m:213:ASN:C    | 21:m:213:ASN:OD1  | 2.55                     | 0.48              |
| 1:1:1173:U:O4     | 1:1:1180:A:N6     | 2.47                     | 0.48              |
| 1:1:2386:A:OP2    | 1:1:2993:G:N2     | 2.45                     | 0.48              |
| 13:Q:41:ASP:OD1   | 13:Q:41:ASP:C     | 2.57                     | 0.48              |
| 15:T:91:LEU:CB    | 15:T:96:ILE:HD11  | 2.44                     | 0.48              |
| 17:W:187:LEU:O    | 17:W:187:LEU:HD12 | 2.13                     | 0.48              |
| 18:b:101:ALA:O    | 18:b:105:VAL:HG23 | 2.13                     | 0.48              |
| 21:m:432:ALA:HB2  | 21:m:449:VAL:HG21 | 1.96                     | 0.48              |
| 1:1:3143:C:O2'    | 1:1:3144:G:OP1    | 2.23                     | 0.48              |
| 7:E:71:VAL:HG23   | 7:E:146:ILE:HD12  | 1.96                     | 0.48              |
| 14:S:171:PHE:HA   | 14:S:172:TYR:HB2  | 1.96                     | 0.48              |
| 16:V:112:SER:O    | 27:y:151:TYR:OH   | 2.20                     | 0.48              |
| 5:C:135:VAL:HG22  | 5:C:245:GLY:HA2   | 1.95                     | 0.48              |
| 9:H:188:THR:HA    | 9:H:189:GLU:CB    | 2.43                     | 0.48              |
| 10:J:46:VAL:O     | 10:J:67:VAL:HG12  | 2.14                     | 0.48              |
| 11:M:19:ARG:NH2   | 11:M:66:THR:O     | 2.46                     | 0.48              |
| 21:m:76:ARG:O     | 21:m:77:TRP:C     | 2.57                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:C:145:ILE:HG22  | 5:C:150:LEU:CD1   | 2.44                     | 0.47              |
| 5:C:334:PHE:CD2   | 5:C:339:LEU:HD12  | 2.49                     | 0.47              |
| 7:E:166:LYS:N     | 7:E:169:ASP:OD2   | 2.46                     | 0.47              |
| 22:r:200:VAL:HG22 | 22:r:221:ILE:HG22 | 1.96                     | 0.47              |
| 1:1:2628:A:O2'    | 1:1:2629:U:O5'    | 2.31                     | 0.47              |
| 1:1:3069:G:N3     | 1:1:3069:G:H2'    | 2.28                     | 0.47              |
| 9:H:46:THR:N      | 9:H:54:LYS:O      | 2.46                     | 0.47              |
| 27:y:88:LEU:HD23  | 27:y:92:VAL:CG1   | 2.44                     | 0.47              |
| 1:1:518:G:O2'     | 1:1:521:A:O2'     | 2.24                     | 0.47              |
| 1:1:1268:G:H21    | 1:1:1273:A:H62    | 1.60                     | 0.47              |
| 1:1:3146:G:N3     | 4:B:101:SER:OG    | 2.46                     | 0.47              |
| 1:1:2828:G:OP2    | 18:b:129:LYS:NZ   | 2.46                     | 0.47              |
| 18:b:374:ARG:HH12 | 27:y:179:VAL:HG12 | 1.78                     | 0.47              |
| 18:b:398:LEU:O    | 18:b:400:ARG:N    | 2.47                     | 0.47              |
| 20:f:40:ASP:OD1   | 20:f:40:ASP:N     | 2.43                     | 0.47              |
| 23:u:42:GLN:OE1   | 23:u:44:ARG:NE    | 2.47                     | 0.47              |
| 1:1:688:G:O2'     | 1:1:689:U:P       | 2.71                     | 0.47              |
| 1:1:695:C:OP1     | 5:C:119:ARG:NE    | 2.40                     | 0.47              |
| 1:1:2834:G:O6     | 1:1:2854:U:O2     | 2.32                     | 0.47              |
| 1:1:3194:C:H2'    | 1:1:3195:U:H2'    | 1.96                     | 0.47              |
| 4:B:84:VAL:O      | 4:B:203:VAL:N     | 2.45                     | 0.47              |
| 26:x:378:SER:OG   | 26:x:382:THR:O    | 2.24                     | 0.47              |
| 8:F:214:TRP:O     | 8:F:216:VAL:HG22  | 2.15                     | 0.47              |
| 10:J:156:LYS:O    | 10:J:160:VAL:HG23 | 2.14                     | 0.47              |
| 3:3:57:G:OP1      | 10:J:149:GLY:N    | 2.48                     | 0.47              |
| 3:3:57:G:H4'      | 10:J:138:VAL:HG11 | 1.97                     | 0.47              |
| 26:x:214:ASP:OD1  | 26:x:214:ASP:C    | 2.57                     | 0.47              |
| 1:1:508:U:C2      | 1:1:584:G:N1      | 2.83                     | 0.47              |
| 1:1:2677:G:H2'    | 1:1:2677:G:N3     | 2.30                     | 0.47              |
| 1:1:2929:C:O2'    | 1:1:2930:A:OP2    | 2.28                     | 0.47              |
| 4:B:56:ILE:CD1    | 4:B:76:VAL:HG21   | 2.45                     | 0.47              |
| 18:b:154:ARG:HA   | 18:b:157:ILE:HG22 | 1.97                     | 0.47              |
| 21:m:423:ASP:O    | 21:m:425:THR:N    | 2.48                     | 0.47              |
| 16:V:52:ALA:CB    | 16:V:58:VAL:HG11  | 2.45                     | 0.46              |
| 1:1:374:A:HO2'    | 1:1:375:A:P       | 2.34                     | 0.46              |
| 8:F:84:VAL:HG13   | 8:F:119:VAL:CG2   | 2.45                     | 0.46              |
| 8:F:178:ILE:HG23  | 8:F:184:LEU:HA    | 1.97                     | 0.46              |
| 1:1:374:A:HO2'    | 1:1:375:A:C5'     | 2.19                     | 0.46              |
| 9:H:12:VAL:HG21   | 9:H:53:ILE:HD12   | 1.98                     | 0.46              |
| 14:S:14:LEU:HD22  | 15:T:136:ARG:NH2  | 2.30                     | 0.46              |
| 14:S:12:ARG:HD2   | 14:S:14:LEU:HD23  | 1.97                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:S:171:PHE:HA   | 14:S:172:TYR:C    | 2.40                     | 0.46              |
| 15:T:91:LEU:HB2   | 15:T:96:ILE:HD11  | 1.97                     | 0.46              |
| 18:b:87:GLU:O     | 18:b:87:GLU:HG3   | 2.14                     | 0.46              |
| 5:C:172:VAL:HG12  | 5:C:174:ALA:H     | 1.79                     | 0.46              |
| 7:E:40:LEU:HD13   | 7:E:84:VAL:HG11   | 1.97                     | 0.46              |
| 1:1:2743:A:H2'    | 1:1:2744:U:O4'    | 2.15                     | 0.46              |
| 1:1:3005:A:O2'    | 1:1:3140:G:N2     | 2.47                     | 0.46              |
| 18:b:74:VAL:HG13  | 18:b:75:HIS:N     | 2.31                     | 0.46              |
| 1:1:520:U:OP2     | 8:F:70:LYS:NZ     | 2.49                     | 0.46              |
| 18:b:163:ILE:HD12 | 18:b:163:ILE:O    | 2.16                     | 0.46              |
| 22:r:216:THR:O    | 22:r:217:LYS:C    | 2.59                     | 0.46              |
| 25:w:184:ARG:O    | 25:w:188:VAL:HG23 | 2.16                     | 0.46              |
| 26:x:466:THR:HG23 | 26:x:466:THR:O    | 2.16                     | 0.46              |
| 1:1:213:A:N6      | 1:1:228:U:O4'     | 2.49                     | 0.46              |
| 1:1:520:U:O4      | 5:C:349:THR:OG1   | 2.33                     | 0.46              |
| 11:M:15:VAL:HG22  | 14:S:150:PHE:O    | 2.16                     | 0.46              |
| 21:m:423:ASP:O    | 21:m:426:GLU:N    | 2.36                     | 0.46              |
| 1:1:340:C:OP2     | 5:C:195:ARG:NH1   | 2.48                     | 0.46              |
| 1:1:3341:U:H4'    | 1:1:3341:U:OP1    | 2.16                     | 0.46              |
| 4:B:161:LEU:HD22  | 4:B:178:LEU:HD11  | 1.97                     | 0.46              |
| 1:1:494:G:HO2'    | 1:1:495:G:P       | 2.31                     | 0.45              |
| 1:1:957:C:H3'     | 1:1:958:C:C5'     | 2.47                     | 0.45              |
| 4:B:61:ASP:OD2    | 18:b:413:ASN:ND2  | 2.50                     | 0.45              |
| 4:B:141:GLY:O     | 4:B:142:ALA:HB3   | 2.16                     | 0.45              |
| 7:E:40:LEU:HD12   | 7:E:54:TYR:HB2    | 1.98                     | 0.45              |
| 18:b:178:VAL:HG22 | 18:b:255:ASP:HB2  | 1.99                     | 0.45              |
| 24:v:211:SER:OG   | 24:v:215:GLY:O    | 2.21                     | 0.45              |
| 1:1:991:G:H21     | 15:T:59:GLY:C     | 2.24                     | 0.45              |
| 17:W:38:ARG:O     | 17:W:223:ASN:ND2  | 2.50                     | 0.45              |
| 18:b:153:VAL:O    | 18:b:157:ILE:N    | 2.41                     | 0.45              |
| 22:r:215:LEU:O    | 22:r:219:THR:OG1  | 2.27                     | 0.45              |
| 21:m:215:LEU:HD22 | 21:m:370:ILE:CG2  | 2.46                     | 0.45              |
| 4:B:47:LEU:H      | 4:B:47:LEU:HD23   | 1.82                     | 0.45              |
| 5:C:338:LYS:O     | 5:C:340:GLY:N     | 2.50                     | 0.45              |
| 23:u:111:ARG:HG2  | 23:u:112:MET:HE2  | 1.99                     | 0.45              |
| 6:D:40:HIS:N      | 6:D:41:LYS:HA     | 2.31                     | 0.45              |
| 22:r:157:VAL:HG22 | 22:r:173:ARG:HH21 | 1.82                     | 0.45              |
| 1:1:1241:U:O5'    | 21:m:149:ARG:NH1  | 2.47                     | 0.45              |
| 1:1:2900:A:N3     | 1:1:3025:C:O2'    | 2.35                     | 0.45              |
| 1:1:2964:G:OP1    | 21:m:35:ARG:NH2   | 2.46                     | 0.45              |
| 4:B:136:LYS:O     | 4:B:139:GLN:NE2   | 2.49                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:M:113:THR:HG22 | 11:M:114:ASP:N    | 2.31                     | 0.45              |
| 18:b:312:VAL:HG13 | 18:b:315:VAL:CG1  | 2.43                     | 0.45              |
| 21:m:287:HIS:NE2  | 21:m:289:SER:OG   | 2.50                     | 0.45              |
| 22:r:11:ILE:O     | 22:r:15:GLY:N     | 2.43                     | 0.45              |
| 1:1:792:G:N3      | 1:1:792:G:H2'     | 2.32                     | 0.45              |
| 1:1:2728:G:O2'    | 1:1:2729:U:OP2    | 2.35                     | 0.45              |
| 1:1:2800:G:O6     | 21:m:21:ASN:ND2   | 2.49                     | 0.45              |
| 1:1:2955:U:H3'    | 1:1:2956:A:H5''   | 1.99                     | 0.45              |
| 1:1:3211:C:C2     | 1:1:3212:C:C5     | 3.05                     | 0.45              |
| 16:V:35:TYR:O     | 16:V:61:THR:N     | 2.49                     | 0.45              |
| 26:x:203:THR:OG1  | 26:x:213:TRP:NE1  | 2.46                     | 0.45              |
| 1:1:598:A:OP1     | 8:F:41:ARG:NH1    | 2.50                     | 0.45              |
| 1:1:1355:A:HO2'   | 1:1:1356:U:P      | 2.29                     | 0.45              |
| 1:1:2752:U:H2'    | 1:1:2753:G:C8     | 2.52                     | 0.45              |
| 1:1:999:G:H4'     | 1:1:1000:C:O5'    | 2.17                     | 0.45              |
| 1:1:2418:G:N2     | 21:m:30:TYR:OH    | 2.49                     | 0.45              |
| 1:1:3340:G:H3'    | 1:1:3341:U:H5''   | 1.98                     | 0.45              |
| 18:b:150:LEU:HA   | 18:b:153:VAL:HG22 | 1.99                     | 0.45              |
| 18:b:193:ASP:N    | 18:b:193:ASP:OD1  | 2.48                     | 0.45              |
| 1:1:993:G:C5      | 1:1:1056:U:C2     | 3.05                     | 0.44              |
| 1:1:1152:G:H21    | 1:1:1152:G:P      | 2.38                     | 0.44              |
| 4:B:216:ASP:N     | 4:B:339:ARG:O     | 2.43                     | 0.44              |
| 14:S:48:LEU:CD1   | 15:T:151:LEU:HD12 | 2.46                     | 0.44              |
| 27:y:177:LEU:O    | 27:y:179:VAL:HG13 | 2.16                     | 0.44              |
| 27:y:199:VAL:HG23 | 27:y:204:ALA:HB2  | 1.99                     | 0.44              |
| 1:1:599:C:OP1     | 5:C:332:LYS:NZ    | 2.39                     | 0.44              |
| 1:1:1156:C:O2     | 1:1:1170:A:O2'    | 2.32                     | 0.44              |
| 1:1:2624:G:HO2'   | 1:1:2625:C:P      | 2.36                     | 0.44              |
| 1:1:2710:C:H2'    | 1:1:2711:C:C6     | 2.52                     | 0.44              |
| 1:1:2819:A:H3'    | 1:1:2820:A:H5''   | 1.97                     | 0.44              |
| 17:W:116:PHE:CD1  | 17:W:215:VAL:HG11 | 2.52                     | 0.44              |
| 25:w:30:ASP:OD1   | 25:w:32:ASN:ND2   | 2.46                     | 0.44              |
| 25:w:75:GLU:O     | 25:w:85:SER:OG    | 2.29                     | 0.44              |
| 26:x:324:ASN:ND2  | 26:x:405:VAL:O    | 2.50                     | 0.44              |
| 26:x:463:SER:HG   | 26:x:464:LYS:H    | 1.64                     | 0.44              |
| 10:J:43:GLN:NE2   | 10:J:70:THR:O     | 2.45                     | 0.44              |
| 22:r:161:PHE:O    | 22:r:164:ARG:NH1  | 2.50                     | 0.44              |
| 1:1:2648:G:H5'    | 25:w:178:THR:HG22 | 2.00                     | 0.44              |
| 1:1:3048:A:H2'    | 1:1:3048:A:N3     | 2.33                     | 0.44              |
| 14:S:41:TYR:O     | 14:S:45:LEU:HD23  | 2.17                     | 0.44              |
| 18:b:173:CYS:N    | 18:b:251:LEU:O    | 2.43                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 27:y:99:GLU:OE1  | 27:y:101:LEU:N    | 2.51                     | 0.44              |
| 1:1:1192:C:O2'   | 1:1:1193:A:P      | 2.75                     | 0.44              |
| 1:1:2712:U:O2'   | 1:1:2713:U:O2     | 2.25                     | 0.44              |
| 5:C:212:ASP:OD1  | 5:C:216:VAL:HG22  | 2.18                     | 0.44              |
| 8:F:151:ARG:NE   | 8:F:206:LYS:O     | 2.49                     | 0.44              |
| 11:M:127:LYS:O   | 11:M:131:VAL:HG23 | 2.17                     | 0.44              |
| 21:m:378:SER:O   | 21:m:381:ASP:N    | 2.49                     | 0.44              |
| 24:v:43:HIS:O    | 24:v:47:VAL:HG23  | 2.18                     | 0.44              |
| 1:1:3333:G:OP2   | 23:u:35:LYS:NZ    | 2.50                     | 0.44              |
| 9:H:71:VAL:O     | 9:H:75:VAL:HG23   | 2.18                     | 0.44              |
| 21:m:126:SER:CB  | 26:x:399:THR:HG1  | 2.31                     | 0.44              |
| 1:1:1299:U:O2    | 1:1:1299:U:O4'    | 2.36                     | 0.44              |
| 1:1:3278:C:H2'   | 1:1:3278:C:O2     | 2.18                     | 0.44              |
| 15:T:68:THR:OG1  | 15:T:69:LYS:N     | 2.48                     | 0.44              |
| 26:x:161:THR:OG1 | 26:x:171:TRP:NE1  | 2.50                     | 0.44              |
| 1:1:1249:G:C6    | 1:1:1250:G:C6     | 3.06                     | 0.44              |
| 1:1:2953:U:O2    | 1:1:2953:U:H2'    | 2.18                     | 0.44              |
| 1:1:3306:U:O2    | 1:1:3306:U:H2'    | 2.16                     | 0.44              |
| 3:3:121:U:O4     | 6:D:264:GLN:NE2   | 2.46                     | 0.44              |
| 4:B:121:ASN:O    | 4:B:125:SER:N     | 2.51                     | 0.44              |
| 6:D:40:HIS:HB2   | 6:D:41:LYS:C      | 2.42                     | 0.44              |
| 8:F:216:VAL:O    | 8:F:218:ARG:N     | 2.51                     | 0.44              |
| 8:F:225:GLN:N    | 8:F:225:GLN:OE1   | 2.51                     | 0.44              |
| 21:m:124:ASP:OD2 | 21:m:124:ASP:N    | 2.51                     | 0.44              |
| 26:x:159:MET:O   | 26:x:171:TRP:N    | 2.44                     | 0.44              |
| 1:1:1048:A:H2'   | 1:1:1048:A:N3     | 2.33                     | 0.44              |
| 1:1:1200:A:H4'   | 1:1:1201:C:OP1    | 2.17                     | 0.44              |
| 1:1:2655:U:O2'   | 1:1:2713:U:O4     | 2.35                     | 0.44              |
| 1:1:2724:U:O2    | 1:1:2724:U:O2'    | 2.34                     | 0.44              |
| 17:W:60:TRP:O    | 17:W:63:SER:N     | 2.51                     | 0.44              |
| 21:m:159:ASP:N   | 21:m:159:ASP:OD1  | 2.50                     | 0.44              |
| 24:v:36:GLN:N    | 24:v:64:ASN:O     | 2.51                     | 0.44              |
| 1:1:2728:G:O3'   | 22:r:164:ARG:NE   | 2.51                     | 0.43              |
| 1:1:2734:A:H2'   | 1:1:2735:U:O4'    | 2.17                     | 0.43              |
| 1:1:2872:A:O2'   | 1:1:2873:U:OP1    | 2.32                     | 0.43              |
| 3:3:83:U:O4      | 3:3:97:A:N6       | 2.50                     | 0.43              |
| 9:H:55:VAL:HG23  | 9:H:68:LEU:HD11   | 2.00                     | 0.43              |
| 14:S:93:GLU:OE1  | 14:S:135:VAL:HG13 | 2.18                     | 0.43              |
| 18:b:21:VAL:HG11 | 18:b:57:PHE:CE2   | 2.52                     | 0.43              |
| 22:r:231:VAL:CG2 | 22:r:237:VAL:HG23 | 2.43                     | 0.43              |
| 1:1:2796:G:H21   | 1:1:2797:C:H5''   | 1.83                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:2810:C:OP2    | 1:1:2955:U:O2'    | 2.37                     | 0.43              |
| 1:1:3189:G:O6     | 1:1:3204:C:N4     | 2.51                     | 0.43              |
| 6:D:34:LYS:O      | 6:D:38:THR:N      | 2.49                     | 0.43              |
| 10:J:37:LEU:HD11  | 10:J:67:VAL:HG23  | 2.01                     | 0.43              |
| 1:1:1048:A:O2'    | 1:1:1049:C:O4'    | 2.26                     | 0.43              |
| 1:1:3072:C:P      | 1:1:3073:A:H62    | 2.34                     | 0.43              |
| 1:1:3213:A:OP1    | 11:M:128:ARG:NE   | 2.51                     | 0.43              |
| 4:B:367:LYS:O     | 4:B:369:ARG:NH2   | 2.51                     | 0.43              |
| 9:H:36:LYS:NZ     | 9:H:152:GLU:OE2   | 2.35                     | 0.43              |
| 10:J:53:THR:OG1   | 10:J:61:ARG:N     | 2.51                     | 0.43              |
| 15:T:154:VAL:N    | 15:T:155:PRO:HA   | 2.33                     | 0.43              |
| 21:m:64:SER:N     | 22:r:130:GLU:O    | 2.49                     | 0.43              |
| 27:y:85:ARG:NH2   | 27:y:92:VAL:O     | 2.46                     | 0.43              |
| 1:1:591:G:O2'     | 7:E:17:ALA:O      | 2.30                     | 0.43              |
| 1:1:2393:G:N2     | 1:1:2394:G:O6     | 2.45                     | 0.43              |
| 1:1:2939:G:O2'    | 1:1:2940:A:O5'    | 2.37                     | 0.43              |
| 6:D:216:GLU:O     | 6:D:220:SER:N     | 2.51                     | 0.43              |
| 11:M:59:ASN:OD1   | 11:M:60:LEU:N     | 2.52                     | 0.43              |
| 1:1:3208:G:O4'    | 1:1:3210:A:C8     | 2.71                     | 0.43              |
| 1:1:3228:C:HO2'   | 1:1:3229:G:P      | 2.33                     | 0.43              |
| 1:1:3332:U:H2'    | 1:1:3333:G:O4'    | 2.18                     | 0.43              |
| 17:W:133:LEU:HD22 | 17:W:210:ALA:CB   | 2.48                     | 0.43              |
| 18:b:178:VAL:O    | 18:b:178:VAL:CG1  | 2.67                     | 0.43              |
| 1:1:1129:A:O2'    | 1:1:1130:A:P      | 2.73                     | 0.43              |
| 1:1:1222:G:HO2'   | 1:1:1223:A:P      | 2.38                     | 0.43              |
| 1:1:2818:U:O3'    | 1:1:2819:A:H4'    | 2.17                     | 0.43              |
| 6:D:44:TYR:CD1    | 6:D:44:TYR:N      | 2.87                     | 0.43              |
| 26:x:158:ARG:NH1  | 26:x:172:ASP:OD1  | 2.52                     | 0.43              |
| 26:x:457:ARG:O    | 26:x:473:VAL:HG12 | 2.18                     | 0.43              |
| 1:1:2722:U:O2     | 1:1:2722:U:O4'    | 2.35                     | 0.43              |
| 1:1:2862:U:O2     | 1:1:2862:U:O4'    | 2.36                     | 0.43              |
| 1:1:3040:A:C2     | 1:1:3041:U:C5     | 3.06                     | 0.43              |
| 1:1:1191:U:OP2    | 12:O:49:ARG:NH1   | 2.48                     | 0.43              |
| 1:1:1238:C:H2'    | 1:1:1239:C:C6     | 2.54                     | 0.43              |
| 1:1:1262:G:O6     | 1:1:1264:G:N2     | 2.52                     | 0.43              |
| 4:B:80:ASP:OD1    | 4:B:319:ASN:ND2   | 2.46                     | 0.43              |
| 9:H:21:LYS:O      | 9:H:22:SER:C      | 2.62                     | 0.43              |
| 14:S:13:ARG:O     | 14:S:14:LEU:C     | 2.61                     | 0.43              |
| 14:S:30:PHE:CE2   | 14:S:103:VAL:HG21 | 2.54                     | 0.43              |
| 16:V:58:VAL:O     | 16:V:76:ALA:N     | 2.40                     | 0.43              |
| 24:v:187:GLN:OE1  | 25:w:46:ARG:NH2   | 2.52                     | 0.43              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:E:71:VAL:HG21   | 7:E:149:ILE:HD13  | 2.00                     | 0.43              |
| 18:b:325:GLU:O    | 18:b:328:VAL:HG12 | 2.19                     | 0.43              |
| 1:1:1281:G:C2     | 1:1:1282:G:N7     | 2.86                     | 0.43              |
| 1:1:2711:C:H2'    | 1:1:2712:U:O4'    | 2.19                     | 0.43              |
| 1:1:2794:G:O2'    | 1:1:2795:U:OP2    | 2.33                     | 0.43              |
| 1:1:2822:U:HO2'   | 1:1:2823:G:P      | 2.42                     | 0.43              |
| 1:1:2861:U:H2'    | 1:1:2861:U:O2     | 2.19                     | 0.43              |
| 3:3:31:U:HO2'     | 6:D:218:ARG:HH12  | 1.66                     | 0.43              |
| 9:H:112:ILE:HD12  | 9:H:126:VAL:O     | 2.19                     | 0.43              |
| 18:b:109:ALA:O    | 18:b:113:VAL:HG23 | 2.19                     | 0.43              |
| 21:m:288:ALA:O    | 21:m:330:SER:OG   | 2.37                     | 0.43              |
| 1:1:2856:G:H21    | 22:r:192:THR:HG23 | 1.84                     | 0.42              |
| 1:1:3023:U:O2     | 1:1:3023:U:O4'    | 2.37                     | 0.42              |
| 7:E:136:GLU:O     | 7:E:140:VAL:HG23  | 2.19                     | 0.42              |
| 27:y:61:ARG:O     | 27:y:105:GLY:N    | 2.50                     | 0.42              |
| 27:y:133:LEU:HB2  | 27:y:135:VAL:HG22 | 2.01                     | 0.42              |
| 1:1:1241:U:C4'    | 1:1:1242:G:OP1    | 2.67                     | 0.42              |
| 1:1:2856:G:H2'    | 22:r:192:THR:OG1  | 2.18                     | 0.42              |
| 1:1:2923:U:OP2    | 21:m:211:ILE:HD12 | 2.18                     | 0.42              |
| 5:C:237:GLN:O     | 5:C:246:ARG:NH1   | 2.46                     | 0.42              |
| 15:T:52:MET:N     | 15:T:53:PRO:CD    | 2.82                     | 0.42              |
| 18:b:247:ARG:HG3  | 18:b:248:SER:H    | 1.83                     | 0.42              |
| 21:m:273:TRP:NE1  | 21:m:466:VAL:O    | 2.50                     | 0.42              |
| 22:r:16:LYS:O     | 22:r:17:ARG:C     | 2.62                     | 0.42              |
| 22:r:125:VAL:HG12 | 22:r:126:ARG:N    | 2.34                     | 0.42              |
| 24:v:220:ARG:HA   | 25:w:11:VAL:HG12  | 2.01                     | 0.42              |
| 1:1:374:A:O2'     | 1:1:375:A:H3'     | 2.19                     | 0.42              |
| 1:1:2767:U:H3'    | 1:1:2768:U:H5'    | 2.01                     | 0.42              |
| 5:C:38:VAL:HG21   | 5:C:121:ALA:HB2   | 2.01                     | 0.42              |
| 5:C:259:ASP:O     | 5:C:263:GLY:N     | 2.45                     | 0.42              |
| 13:Q:62:VAL:HG11  | 13:Q:140:LEU:HD21 | 2.02                     | 0.42              |
| 18:b:143:LEU:HD23 | 18:b:147:LEU:HD11 | 2.01                     | 0.42              |
| 21:m:287:HIS:CD2  | 21:m:289:SER:HG   | 2.36                     | 0.42              |
| 21:m:313:ARG:NH2  | 22:r:162:THR:OG1  | 2.52                     | 0.42              |
| 23:u:62:GLU:C     | 23:u:63:LEU:HD23  | 2.44                     | 0.42              |
| 27:y:219:GLU:O    | 27:y:223:ARG:N    | 2.49                     | 0.42              |
| 1:1:3085:G:OP1    | 23:u:34:SER:OG    | 2.35                     | 0.42              |
| 1:1:3214:U:OP2    | 11:M:128:ARG:NH2  | 2.45                     | 0.42              |
| 6:D:115:LEU:O     | 26:x:130:LYS:NZ   | 2.53                     | 0.42              |
| 18:b:104:LEU:O    | 18:b:108:VAL:HG23 | 2.20                     | 0.42              |
| 18:b:249:CYS:SG   | 18:b:284:MET:N    | 2.91                     | 0.42              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:1103:A:N3     | 1:1:1103:A:H2'    | 2.35                     | 0.42              |
| 5:C:132:ALA:HB1   | 5:C:135:VAL:HB    | 2.01                     | 0.42              |
| 17:W:175:ILE:HD13 | 22:r:14:HIS:O     | 2.20                     | 0.42              |
| 23:u:6:CYS:O      | 23:u:10:SER:N     | 2.45                     | 0.42              |
| 1:1:2657:A:N6     | 1:1:2713:U:O4     | 2.53                     | 0.42              |
| 1:1:2964:G:H4'    | 21:m:31:ARG:HD3   | 2.02                     | 0.42              |
| 3:3:12:U:O2'      | 3:3:112:G:O4'     | 2.38                     | 0.42              |
| 6:D:64:ILE:HG23   | 6:D:64:ILE:O      | 2.20                     | 0.42              |
| 7:E:71:VAL:HG23   | 7:E:146:ILE:CD1   | 2.49                     | 0.42              |
| 27:y:126:GLU:HG3  | 27:y:137:VAL:HG11 | 2.01                     | 0.42              |
| 1:1:1071:U:O2     | 1:1:1071:U:O4'    | 2.37                     | 0.42              |
| 1:1:2874:G:H22    | 1:1:2925:C:H41    | 1.67                     | 0.42              |
| 8:F:215:GLY:O     | 8:F:216:VAL:C     | 2.62                     | 0.42              |
| 8:F:232:ARG:O     | 8:F:233:GLU:C     | 2.62                     | 0.42              |
| 17:W:46:ASP:OD2   | 17:W:46:ASP:N     | 2.53                     | 0.42              |
| 1:1:992:A:N7      | 1:1:993:G:C6      | 2.88                     | 0.42              |
| 1:1:2409:G:O6     | 1:1:2813:A:N6     | 2.53                     | 0.42              |
| 1:1:3341:U:C2'    | 1:1:3342:A:OP2    | 2.68                     | 0.42              |
| 11:M:116:GLU:O    | 11:M:120:VAL:HG23 | 2.19                     | 0.42              |
| 21:m:61:PHE:N     | 22:r:130:GLU:OE1  | 2.52                     | 0.42              |
| 21:m:157:LEU:O    | 21:m:161:VAL:HG23 | 2.19                     | 0.42              |
| 1:1:1201:C:O2     | 1:1:1201:C:C2'    | 2.68                     | 0.42              |
| 1:1:1238:C:HO2'   | 1:1:1239:C:P      | 2.35                     | 0.42              |
| 3:3:5:G:O2'       | 6:D:52:VAL:HG11   | 2.20                     | 0.42              |
| 15:T:74:VAL:N     | 15:T:89:LEU:O     | 2.48                     | 0.42              |
| 27:y:61:ARG:NH2   | 27:y:105:GLY:O    | 2.53                     | 0.42              |
| 27:y:70:LEU:CD2   | 27:y:88:LEU:HD21  | 2.50                     | 0.42              |
| 7:E:49:GLY:O      | 7:E:163:PHE:N     | 2.51                     | 0.42              |
| 1:1:370:U:C2      | 1:1:374:A:N7      | 2.88                     | 0.41              |
| 1:1:1057:A:O2'    | 1:1:1058:U:OP2    | 2.29                     | 0.41              |
| 1:1:2794:G:OP2    | 25:w:193:LYS:NZ   | 2.49                     | 0.41              |
| 4:B:78:VAL:HG13   | 4:B:321:PHE:CD1   | 2.55                     | 0.41              |
| 18:b:118:PHE:O    | 18:b:120:GLN:NE2  | 2.53                     | 0.41              |
| 1:1:531:G:H2'     | 1:1:532:A:C8      | 2.55                     | 0.41              |
| 1:1:1361:U:O2     | 8:F:159:GLN:NE2   | 2.47                     | 0.41              |
| 6:D:53:VAL:O      | 6:D:54:ARG:NH1    | 2.49                     | 0.41              |
| 1:1:3164:C:O2'    | 1:1:3165:A:H8     | 2.04                     | 0.41              |
| 5:C:309:ARG:HB3   | 5:C:312:VAL:HG12  | 2.01                     | 0.41              |
| 18:b:422:LEU:HD23 | 18:b:422:LEU:HA   | 1.96                     | 0.41              |
| 21:m:208:SER:O    | 21:m:211:ILE:HG23 | 2.19                     | 0.41              |
| 1:1:1249:G:N1     | 1:1:1250:G:C6     | 2.88                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:3195:U:H1'    | 1:1:3196:U:P      | 2.61                     | 0.41              |
| 4:B:35:ASP:OD1    | 4:B:191:LYS:NZ    | 2.51                     | 0.41              |
| 22:r:6:TYR:O      | 22:r:7:ILE:C      | 2.62                     | 0.41              |
| 1:1:596:C:H3'     | 1:1:597:G:H5''    | 2.02                     | 0.41              |
| 1:1:2622:C:HO2'   | 1:1:2623:G:H8     | 1.65                     | 0.41              |
| 1:1:2726:C:H41    | 21:m:38:PHE:HB2   | 1.86                     | 0.41              |
| 1:1:2758:A:N3     | 1:1:2758:A:H2'    | 2.36                     | 0.41              |
| 26:x:418:VAL:HG21 | 26:x:459:LEU:HD22 | 2.02                     | 0.41              |
| 27:y:114:VAL:HG11 | 27:y:177:LEU:HD23 | 2.01                     | 0.41              |
| 5:C:38:VAL:O      | 5:C:42:VAL:HG23   | 2.21                     | 0.41              |
| 12:O:120:VAL:HG22 | 14:S:163:PHE:CE1  | 2.56                     | 0.41              |
| 1:1:1356:U:O2'    | 1:1:1357:G:OP1    | 2.31                     | 0.41              |
| 1:1:2764:C:O2     | 1:1:2764:C:H2'    | 2.20                     | 0.41              |
| 1:1:3008:A:N6     | 1:1:3139:A:N6     | 2.69                     | 0.41              |
| 1:1:3065:G:O6     | 1:1:3077:A:N6     | 2.54                     | 0.41              |
| 1:1:3155:U:O2     | 1:1:3155:U:H2'    | 2.20                     | 0.41              |
| 1:1:3267:A:OP1    | 1:1:3268:A:N6     | 2.54                     | 0.41              |
| 1:1:3341:U:O2'    | 1:1:3342:A:P      | 2.79                     | 0.41              |
| 6:D:207:TYR:HH    | 6:D:218:ARG:HH21  | 1.66                     | 0.41              |
| 11:M:6:ILE:O      | 11:M:6:ILE:HG22   | 2.20                     | 0.41              |
| 1:1:2731:U:O2     | 1:1:2731:U:O2'    | 2.34                     | 0.41              |
| 7:E:37:GLY:O      | 7:E:91:VAL:N      | 2.46                     | 0.41              |
| 18:b:173:CYS:O    | 18:b:253:PHE:N    | 2.49                     | 0.41              |
| 18:b:312:VAL:CG1  | 18:b:315:VAL:HG11 | 2.48                     | 0.41              |
| 22:r:146:SER:O    | 22:r:147:TRP:CG   | 2.73                     | 0.41              |
| 1:1:344:A:H2'     | 1:1:345:G:O4'     | 2.21                     | 0.41              |
| 1:1:720:A:C4'     | 1:1:721:G:OP2     | 2.69                     | 0.41              |
| 1:1:2390:A:H4'    | 1:1:3307:A:H61    | 1.86                     | 0.41              |
| 1:1:2657:A:H61    | 1:1:2713:U:H3     | 1.69                     | 0.41              |
| 1:1:3275:U:O4     | 20:f:62:SER:OG    | 2.33                     | 0.41              |
| 4:B:151:ILE:HG22  | 4:B:151:ILE:O     | 2.20                     | 0.41              |
| 5:C:135:VAL:HG12  | 5:C:140:HIS:HB2   | 2.02                     | 0.41              |
| 8:F:130:ILE:O     | 8:F:134:VAL:HG22  | 2.21                     | 0.41              |
| 17:W:42:VAL:O     | 17:W:217:VAL:HG23 | 2.20                     | 0.41              |
| 18:b:178:VAL:HG13 | 18:b:255:ASP:HB2  | 2.03                     | 0.41              |
| 20:f:59:VAL:HG22  | 20:f:62:SER:O     | 2.21                     | 0.41              |
| 26:x:214:ASP:HB2  | 26:x:215:PRO:HD2  | 2.03                     | 0.41              |
| 26:x:289:GLN:NE2  | 26:x:360:TYR:OH   | 2.53                     | 0.41              |
| 27:y:115:ALA:HB2  | 27:y:135:VAL:HG21 | 2.02                     | 0.41              |
| 27:y:128:LEU:O    | 27:y:132:VAL:HG23 | 2.21                     | 0.41              |
| 1:1:2699:G:O3'    | 24:v:61:ASN:ND2   | 2.54                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:3028:G:N1     | 18:b:162:SER:OG   | 2.54                     | 0.41              |
| 5:C:156:LEU:HA    | 5:C:159:ILE:HD12  | 2.02                     | 0.41              |
| 9:H:61:GLY:O      | 9:H:65:VAL:N      | 2.43                     | 0.41              |
| 9:H:137:SER:CB    | 9:H:145:VAL:HG23  | 2.51                     | 0.41              |
| 21:m:358:LEU:HD21 | 21:m:362:ILE:HG13 | 2.03                     | 0.41              |
| 1:1:547:G:H5''    | 1:1:548:G:P       | 2.61                     | 0.40              |
| 1:1:550:A:HO2'    | 1:1:551:A:C4'     | 2.31                     | 0.40              |
| 1:1:2733:A:N1     | 1:1:2734:A:N6     | 2.69                     | 0.40              |
| 1:1:2764:C:O2     | 1:1:2764:C:C2'    | 2.70                     | 0.40              |
| 1:1:2813:A:O2'    | 1:1:2814:G:O5'    | 2.34                     | 0.40              |
| 4:B:41:VAL:HG22   | 4:B:185:GLY:HA3   | 2.02                     | 0.40              |
| 5:C:130:ALA:C     | 5:C:132:ALA:N     | 2.79                     | 0.40              |
| 6:D:104:LEU:C     | 6:D:104:LEU:HD13  | 2.46                     | 0.40              |
| 8:F:166:ASN:HA    | 8:F:169:ILE:HD12  | 2.03                     | 0.40              |
| 18:b:194:VAL:HG12 | 18:b:194:VAL:O    | 2.20                     | 0.40              |
| 21:m:226:ILE:HG22 | 21:m:319:GLY:O    | 2.22                     | 0.40              |
| 27:y:26:VAL:HG23  | 27:y:50:HIS:ND1   | 2.35                     | 0.40              |
| 1:1:393:U:H2'     | 1:1:394:G:O4'     | 2.21                     | 0.40              |
| 1:1:952:A:H62     | 1:1:1142:G:H2'    | 1.86                     | 0.40              |
| 1:1:1240:A:H3'    | 1:1:1241:U:H5'    | 2.03                     | 0.40              |
| 1:1:1255:C:O5'    | 1:1:1255:C:O2     | 2.39                     | 0.40              |
| 1:1:2822:U:O2'    | 1:1:2823:G:OP1    | 2.38                     | 0.40              |
| 3:3:27:A:OP2      | 6:D:57:ASN:ND2    | 2.54                     | 0.40              |
| 4:B:59:ASP:O      | 4:B:355:SER:OG    | 2.39                     | 0.40              |
| 5:C:204:GLY:O     | 5:C:246:ARG:NH2   | 2.54                     | 0.40              |
| 5:C:154:THR:O     | 5:C:154:THR:HG22  | 2.20                     | 0.40              |
| 10:J:109:HIS:CE1  | 10:J:114:ILE:HD13 | 2.56                     | 0.40              |
| 17:W:134:THR:N    | 17:W:191:GLU:OE2  | 2.49                     | 0.40              |
| 18:b:398:LEU:C    | 18:b:400:ARG:N    | 2.79                     | 0.40              |
| 21:m:417:GLU:O    | 21:m:418:ILE:C    | 2.65                     | 0.40              |
| 24:v:143:PHE:O    | 25:w:30:ASP:N     | 2.49                     | 0.40              |
| 1:1:1108:U:O2     | 1:1:1108:U:H2'    | 2.21                     | 0.40              |
| 1:1:1135:A:H2'    | 1:1:1136:A:C8     | 2.56                     | 0.40              |
| 1:1:1204:A:O2'    | 1:1:1205:A:O4'    | 2.38                     | 0.40              |
| 1:1:2667:A:H2     | 1:1:2690:G:H21    | 1.69                     | 0.40              |
| 1:1:2687:G:H2'    | 1:1:2687:G:N3     | 2.37                     | 0.40              |
| 1:1:3278:C:H5''   | 1:1:3279:A:OP2    | 2.21                     | 0.40              |
| 4:B:93:VAL:HG22   | 4:B:155:ALA:H     | 1.87                     | 0.40              |
| 4:B:103:THR:HG22  | 4:B:104:THR:N     | 2.35                     | 0.40              |
| 6:D:65:ILE:HG22   | 6:D:72:ASP:HB3    | 2.02                     | 0.40              |
| 9:H:23:ARG:NH2    | 9:H:39:LYS:O      | 2.54                     | 0.40              |

*Continued on next page...*

Continued from previous page...

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:b:245:HIS:NE2  | 21:m:164:THR:HG22 | 2.35                     | 0.40              |
| 27:y:112:ASP:OD2  | 27:y:156:ASN:ND2  | 2.55                     | 0.40              |
| 1:l:2971:A:OP2    | 22:r:139:THR:OG1  | 2.28                     | 0.40              |
| 21:m:226:ILE:HG22 | 21:m:318:VAL:HG22 | 2.03                     | 0.40              |
| 26:x:149:SER:OG   | 26:x:159:MET:SD   | 2.79                     | 0.40              |
| 26:x:172:ASP:O    | 26:x:176:GLN:N    | 2.54                     | 0.40              |
| 26:x:284:VAL:HG23 | 26:x:294:SER:HB3  | 2.03                     | 0.40              |
| 27:y:200:ASN:OD1  | 27:y:203:LEU:N    | 2.42                     | 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 |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 4   | B     | 344/387 (89%) | 323 (94%) | 21 (6%) | 0        | 100         | 100 |
| 5   | C     | 231/362 (64%) | 209 (90%) | 21 (9%) | 1 (0%)   | 30          | 67  |
| 6   | D     | 261/297 (88%) | 249 (95%) | 12 (5%) | 0        | 100         | 100 |
| 7   | E     | 137/176 (78%) | 135 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 8   | F     | 220/244 (90%) | 211 (96%) | 9 (4%)  | 0        | 100         | 100 |
| 9   | H     | 189/191 (99%) | 180 (95%) | 9 (5%)  | 0        | 100         | 100 |
| 10  | J     | 167/174 (96%) | 160 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 11  | M     | 135/138 (98%) | 131 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 12  | O     | 195/199 (98%) | 193 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 13  | Q     | 77/186 (41%)  | 76 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 14  | S     | 169/172 (98%) | 159 (94%) | 10 (6%) | 0        | 100         | 100 |
| 15  | T     | 110/160 (69%) | 106 (96%) | 4 (4%)  | 0        | 100         | 100 |
| 16  | V     | 122/137 (89%) | 121 (99%) | 1 (1%)  | 0        | 100         | 100 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 17  | W     | 232/236 (98%)   | 224 (97%)  | 8 (3%)   | 0        | 100         | 100 |
| 18  | b     | 449/647 (69%)   | 413 (92%)  | 36 (8%)  | 0        | 100         | 100 |
| 19  | e     | 35/130 (27%)    | 35 (100%)  | 0        | 0        | 100         | 100 |
| 20  | f     | 104/107 (97%)   | 98 (94%)   | 6 (6%)   | 0        | 100         | 100 |
| 21  | m     | 427/486 (88%)   | 386 (90%)  | 39 (9%)  | 2 (0%)   | 24          | 63  |
| 22  | r     | 224/261 (86%)   | 193 (86%)  | 29 (13%) | 2 (1%)   | 14          | 49  |
| 23  | u     | 90/199 (45%)    | 89 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 24  | v     | 259/344 (75%)   | 255 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 25  | w     | 178/203 (88%)   | 171 (96%)  | 7 (4%)   | 0        | 100         | 100 |
| 26  | x     | 476/515 (92%)   | 449 (94%)  | 27 (6%)  | 0        | 100         | 100 |
| 27  | y     | 223/245 (91%)   | 215 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| All | All   | 5054/6196 (82%) | 4781 (95%) | 268 (5%) | 5 (0%)   | 49          | 83  |

All (5) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | m     | 209 | LYS  |
| 22  | r     | 4   | ASN  |
| 22  | r     | 5   | ASP  |
| 21  | m     | 210 | ARG  |
| 5   | C     | 131 | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 4   | B     | 291/323 (90%) | 285 (98%)  | 6 (2%)   | 47          | 65  |
| 5   | C     | 197/289 (68%) | 197 (100%) | 0        | 100         | 100 |
| 6   | D     | 221/245 (90%) | 219 (99%)  | 2 (1%)   | 70          | 77  |
| 7   | E     | 122/153 (80%) | 120 (98%)  | 2 (2%)   | 55          | 69  |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 8   | F     | 186/205 (91%)   | 186 (100%) | 0        | 100         | 100 |
| 9   | H     | 171/171 (100%)  | 171 (100%) | 0        | 100         | 100 |
| 10  | J     | 147/150 (98%)   | 143 (97%)  | 4 (3%)   | 39          | 60  |
| 11  | M     | 108/109 (99%)   | 108 (100%) | 0        | 100         | 100 |
| 12  | O     | 160/162 (99%)   | 159 (99%)  | 1 (1%)   | 78          | 81  |
| 13  | Q     | 70/151 (46%)    | 70 (100%)  | 0        | 100         | 100 |
| 14  | S     | 155/156 (99%)   | 154 (99%)  | 1 (1%)   | 78          | 81  |
| 15  | T     | 100/137 (73%)   | 97 (97%)   | 3 (3%)   | 36          | 57  |
| 16  | V     | 96/105 (91%)    | 96 (100%)  | 0        | 100         | 100 |
| 17  | W     | 211/213 (99%)   | 209 (99%)  | 2 (1%)   | 70          | 77  |
| 18  | b     | 408/573 (71%)   | 398 (98%)  | 10 (2%)  | 42          | 62  |
| 19  | e     | 31/111 (28%)    | 31 (100%)  | 0        | 100         | 100 |
| 20  | f     | 90/91 (99%)     | 90 (100%)  | 0        | 100         | 100 |
| 21  | m     | 385/428 (90%)   | 373 (97%)  | 12 (3%)  | 35          | 56  |
| 22  | r     | 203/229 (89%)   | 199 (98%)  | 4 (2%)   | 48          | 66  |
| 23  | u     | 82/180 (46%)    | 81 (99%)   | 1 (1%)   | 63          | 74  |
| 24  | v     | 238/309 (77%)   | 238 (100%) | 0        | 100         | 100 |
| 25  | w     | 161/179 (90%)   | 159 (99%)  | 2 (1%)   | 63          | 74  |
| 26  | x     | 428/451 (95%)   | 421 (98%)  | 7 (2%)   | 55          | 69  |
| 27  | y     | 193/211 (92%)   | 193 (100%) | 0        | 100         | 100 |
| All | All   | 4454/5331 (84%) | 4397 (99%) | 57 (1%)  | 59          | 72  |

All (57) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | B     | 14  | LEU  |
| 4   | B     | 46  | PHE  |
| 4   | B     | 108 | GLU  |
| 4   | B     | 128 | LYS  |
| 4   | B     | 346 | THR  |
| 4   | B     | 364 | LYS  |
| 6   | D     | 40  | HIS  |
| 6   | D     | 44  | TYR  |
| 7   | E     | 47  | PHE  |
| 7   | E     | 155 | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | J     | 30  | LEU  |
| 10  | J     | 94  | ARG  |
| 10  | J     | 112 | LEU  |
| 10  | J     | 166 | LYS  |
| 12  | O     | 46  | GLU  |
| 14  | S     | 137 | ARG  |
| 15  | T     | 89  | LEU  |
| 15  | T     | 96  | ILE  |
| 15  | T     | 139 | ARG  |
| 17  | W     | 47  | ASP  |
| 17  | W     | 149 | ILE  |
| 18  | b     | 17  | LEU  |
| 18  | b     | 171 | LEU  |
| 18  | b     | 250 | VAL  |
| 18  | b     | 271 | PHE  |
| 18  | b     | 328 | VAL  |
| 18  | b     | 339 | LEU  |
| 18  | b     | 367 | GLN  |
| 18  | b     | 374 | ARG  |
| 18  | b     | 435 | ILE  |
| 18  | b     | 468 | PHE  |
| 21  | m     | 77  | TRP  |
| 21  | m     | 99  | THR  |
| 21  | m     | 166 | GLU  |
| 21  | m     | 209 | LYS  |
| 21  | m     | 210 | ARG  |
| 21  | m     | 213 | ASN  |
| 21  | m     | 293 | SER  |
| 21  | m     | 302 | LEU  |
| 21  | m     | 346 | ILE  |
| 21  | m     | 362 | ILE  |
| 21  | m     | 366 | ASP  |
| 21  | m     | 383 | LEU  |
| 22  | r     | 171 | ILE  |
| 22  | r     | 203 | ASN  |
| 22  | r     | 210 | THR  |
| 22  | r     | 225 | VAL  |
| 23  | u     | 96  | ILE  |
| 25  | w     | 157 | GLN  |
| 25  | w     | 159 | LEU  |
| 26  | x     | 20  | ARG  |
| 26  | x     | 194 | TRP  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | x     | 205 | SER  |
| 26  | x     | 228 | HIS  |
| 26  | x     | 336 | ILE  |
| 26  | x     | 351 | GLU  |
| 26  | x     | 381 | TYR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | B     | 139 | GLN  |
| 4   | B     | 165 | GLN  |
| 4   | B     | 198 | HIS  |
| 5   | C     | 291 | ASN  |
| 5   | C     | 307 | GLN  |
| 6   | D     | 178 | ASN  |
| 9   | H     | 157 | ASN  |
| 9   | H     | 163 | GLN  |
| 10  | J     | 95  | ASN  |
| 10  | J     | 165 | GLN  |
| 11  | M     | 126 | GLN  |
| 12  | O     | 42  | ASN  |
| 14  | S     | 3   | HIS  |
| 14  | S     | 68  | HIS  |
| 14  | S     | 157 | GLN  |
| 15  | T     | 45  | ASN  |
| 15  | T     | 90  | ASN  |
| 15  | T     | 95  | HIS  |
| 16  | V     | 132 | ASN  |
| 17  | W     | 88  | ASN  |
| 17  | W     | 223 | ASN  |
| 18  | b     | 15  | ASN  |
| 18  | b     | 152 | GLN  |
| 20  | f     | 42  | GLN  |
| 21  | m     | 260 | ASN  |
| 22  | r     | 40  | GLN  |
| 23  | u     | 5   | GLN  |
| 24  | v     | 41  | ASN  |
| 24  | v     | 61  | ASN  |
| 24  | v     | 64  | ASN  |
| 24  | v     | 262 | ASN  |
| 26  | x     | 44  | ASN  |
| 26  | x     | 402 | GLN  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | y     | 21  | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | 1     | 1458/3396 (42%) | 375 (25%)         | 58 (3%)         |
| 2   | 2     | 17/158 (10%)    | 3 (17%)           | 0               |
| 3   | 3     | 109/121 (90%)   | 11 (10%)          | 1 (0%)          |
| All | All   | 1584/3675 (43%) | 389 (24%)         | 59 (3%)         |

All (389) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 187 | A    |
| 1   | 1     | 198 | A    |
| 1   | 1     | 200 | C    |
| 1   | 1     | 202 | G    |
| 1   | 1     | 203 | G    |
| 1   | 1     | 210 | U    |
| 1   | 1     | 218 | G    |
| 1   | 1     | 219 | A    |
| 1   | 1     | 221 | A    |
| 1   | 1     | 227 | G    |
| 1   | 1     | 338 | A    |
| 1   | 1     | 343 | U    |
| 1   | 1     | 375 | A    |
| 1   | 1     | 376 | G    |
| 1   | 1     | 377 | A    |
| 1   | 1     | 390 | G    |
| 1   | 1     | 398 | A    |
| 1   | 1     | 399 | A    |
| 1   | 1     | 401 | U    |
| 1   | 1     | 402 | A    |
| 1   | 1     | 403 | C    |
| 1   | 1     | 438 | A    |
| 1   | 1     | 439 | C    |
| 1   | 1     | 440 | A    |
| 1   | 1     | 495 | G    |
| 1   | 1     | 521 | A    |
| 1   | 1     | 535 | G    |
| 1   | 1     | 536 | U    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 543  | C    |
| 1   | 1     | 548  | G    |
| 1   | 1     | 552  | G    |
| 1   | 1     | 555  | U    |
| 1   | 1     | 557  | A    |
| 1   | 1     | 559  | A    |
| 1   | 1     | 578  | A    |
| 1   | 1     | 579  | G    |
| 1   | 1     | 589  | A    |
| 1   | 1     | 592  | A    |
| 1   | 1     | 597  | G    |
| 1   | 1     | 604  | G    |
| 1   | 1     | 611  | A    |
| 1   | 1     | 677  | A    |
| 1   | 1     | 681  | U    |
| 1   | 1     | 689  | U    |
| 1   | 1     | 701  | G    |
| 1   | 1     | 716  | A    |
| 1   | 1     | 720  | A    |
| 1   | 1     | 721  | G    |
| 1   | 1     | 722  | G    |
| 1   | 1     | 785  | G    |
| 1   | 1     | 944  | C    |
| 1   | 1     | 960  | U    |
| 1   | 1     | 961  | C    |
| 1   | 1     | 965  | A    |
| 1   | 1     | 966  | U    |
| 1   | 1     | 970  | A    |
| 1   | 1     | 975  | C    |
| 1   | 1     | 976  | U    |
| 1   | 1     | 980  | A    |
| 1   | 1     | 981  | U    |
| 1   | 1     | 989  | A    |
| 1   | 1     | 990  | U    |
| 1   | 1     | 991  | G    |
| 1   | 1     | 992  | A    |
| 1   | 1     | 994  | G    |
| 1   | 1     | 995  | U    |
| 1   | 1     | 996  | A    |
| 1   | 1     | 998  | A    |
| 1   | 1     | 999  | G    |
| 1   | 1     | 1000 | C    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 1048 | A    |
| 1   | 1     | 1049 | C    |
| 1   | 1     | 1056 | U    |
| 1   | 1     | 1058 | U    |
| 1   | 1     | 1063 | G    |
| 1   | 1     | 1064 | A    |
| 1   | 1     | 1065 | A    |
| 1   | 1     | 1066 | G    |
| 1   | 1     | 1071 | U    |
| 1   | 1     | 1072 | G    |
| 1   | 1     | 1087 | G    |
| 1   | 1     | 1093 | A    |
| 1   | 1     | 1094 | U    |
| 1   | 1     | 1095 | U    |
| 1   | 1     | 1097 | G    |
| 1   | 1     | 1098 | A    |
| 1   | 1     | 1103 | A    |
| 1   | 1     | 1104 | G    |
| 1   | 1     | 1108 | U    |
| 1   | 1     | 1111 | U    |
| 1   | 1     | 1116 | G    |
| 1   | 1     | 1117 | G    |
| 1   | 1     | 1118 | C    |
| 1   | 1     | 1123 | U    |
| 1   | 1     | 1124 | U    |
| 1   | 1     | 1128 | U    |
| 1   | 1     | 1129 | A    |
| 1   | 1     | 1130 | A    |
| 1   | 1     | 1153 | A    |
| 1   | 1     | 1155 | C    |
| 1   | 1     | 1172 | G    |
| 1   | 1     | 1180 | A    |
| 1   | 1     | 1181 | U    |
| 1   | 1     | 1189 | C    |
| 1   | 1     | 1192 | C    |
| 1   | 1     | 1193 | A    |
| 1   | 1     | 1194 | G    |
| 1   | 1     | 1196 | C    |
| 1   | 1     | 1197 | A    |
| 1   | 1     | 1198 | C    |
| 1   | 1     | 1201 | C    |
| 1   | 1     | 1202 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 1206 | G    |
| 1   | 1     | 1207 | G    |
| 1   | 1     | 1208 | U    |
| 1   | 1     | 1209 | G    |
| 1   | 1     | 1221 | A    |
| 1   | 1     | 1222 | G    |
| 1   | 1     | 1227 | C    |
| 1   | 1     | 1234 | G    |
| 1   | 1     | 1239 | C    |
| 1   | 1     | 1241 | U    |
| 1   | 1     | 1242 | G    |
| 1   | 1     | 1243 | G    |
| 1   | 1     | 1244 | A    |
| 1   | 1     | 1245 | A    |
| 1   | 1     | 1246 | G    |
| 1   | 1     | 1248 | C    |
| 1   | 1     | 1249 | G    |
| 1   | 1     | 1251 | A    |
| 1   | 1     | 1252 | A    |
| 1   | 1     | 1258 | U    |
| 1   | 1     | 1260 | A    |
| 1   | 1     | 1262 | G    |
| 1   | 1     | 1263 | A    |
| 1   | 1     | 1264 | G    |
| 1   | 1     | 1265 | U    |
| 1   | 1     | 1270 | A    |
| 1   | 1     | 1271 | A    |
| 1   | 1     | 1272 | C    |
| 1   | 1     | 1278 | A    |
| 1   | 1     | 1287 | A    |
| 1   | 1     | 1299 | U    |
| 1   | 1     | 1303 | A    |
| 1   | 1     | 1307 | G    |
| 1   | 1     | 1308 | A    |
| 1   | 1     | 1309 | U    |
| 1   | 1     | 1313 | G    |
| 1   | 1     | 1330 | A    |
| 1   | 1     | 1348 | U    |
| 1   | 1     | 1356 | U    |
| 1   | 1     | 1357 | G    |
| 1   | 1     | 1386 | A    |
| 1   | 1     | 1417 | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 1418 | A    |
| 1   | 1     | 1419 | A    |
| 1   | 1     | 2402 | A    |
| 1   | 1     | 2411 | U    |
| 1   | 1     | 2414 | G    |
| 1   | 1     | 2418 | G    |
| 1   | 1     | 2422 | C    |
| 1   | 1     | 2606 | G    |
| 1   | 1     | 2607 | G    |
| 1   | 1     | 2613 | U    |
| 1   | 1     | 2614 | G    |
| 1   | 1     | 2615 | G    |
| 1   | 1     | 2620 | G    |
| 1   | 1     | 2621 | G    |
| 1   | 1     | 2623 | G    |
| 1   | 1     | 2625 | C    |
| 1   | 1     | 2626 | A    |
| 1   | 1     | 2628 | A    |
| 1   | 1     | 2632 | G    |
| 1   | 1     | 2639 | G    |
| 1   | 1     | 2649 | A    |
| 1   | 1     | 2650 | U    |
| 1   | 1     | 2652 | U    |
| 1   | 1     | 2654 | C    |
| 1   | 1     | 2655 | U    |
| 1   | 1     | 2656 | A    |
| 1   | 1     | 2657 | A    |
| 1   | 1     | 2658 | G    |
| 1   | 1     | 2659 | G    |
| 1   | 1     | 2668 | U    |
| 1   | 1     | 2672 | G    |
| 1   | 1     | 2674 | A    |
| 1   | 1     | 2677 | G    |
| 1   | 1     | 2683 | U    |
| 1   | 1     | 2687 | G    |
| 1   | 1     | 2688 | U    |
| 1   | 1     | 2689 | A    |
| 1   | 1     | 2690 | G    |
| 1   | 1     | 2691 | A    |
| 1   | 1     | 2693 | C    |
| 1   | 1     | 2694 | A    |
| 1   | 1     | 2695 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 2698 | G    |
| 1   | 1     | 2699 | G    |
| 1   | 1     | 2703 | A    |
| 1   | 1     | 2704 | A    |
| 1   | 1     | 2713 | U    |
| 1   | 1     | 2714 | G    |
| 1   | 1     | 2715 | A    |
| 1   | 1     | 2716 | U    |
| 1   | 1     | 2724 | U    |
| 1   | 1     | 2725 | U    |
| 1   | 1     | 2726 | C    |
| 1   | 1     | 2727 | A    |
| 1   | 1     | 2728 | G    |
| 1   | 1     | 2729 | U    |
| 1   | 1     | 2730 | G    |
| 1   | 1     | 2731 | U    |
| 1   | 1     | 2732 | G    |
| 1   | 1     | 2734 | A    |
| 1   | 1     | 2752 | U    |
| 1   | 1     | 2754 | G    |
| 1   | 1     | 2758 | A    |
| 1   | 1     | 2759 | U    |
| 1   | 1     | 2760 | C    |
| 1   | 1     | 2762 | A    |
| 1   | 1     | 2763 | U    |
| 1   | 1     | 2764 | C    |
| 1   | 1     | 2765 | C    |
| 1   | 1     | 2766 | U    |
| 1   | 1     | 2768 | U    |
| 1   | 1     | 2795 | U    |
| 1   | 1     | 2797 | C    |
| 1   | 1     | 2798 | C    |
| 1   | 1     | 2800 | G    |
| 1   | 1     | 2801 | A    |
| 1   | 1     | 2802 | A    |
| 1   | 1     | 2803 | A    |
| 1   | 1     | 2807 | U    |
| 1   | 1     | 2808 | A    |
| 1   | 1     | 2809 | C    |
| 1   | 1     | 2810 | C    |
| 1   | 1     | 2815 | G    |
| 1   | 1     | 2818 | U    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 2819 | A    |
| 1   | 1     | 2820 | A    |
| 1   | 1     | 2821 | C    |
| 1   | 1     | 2822 | U    |
| 1   | 1     | 2823 | G    |
| 1   | 1     | 2824 | G    |
| 1   | 1     | 2825 | C    |
| 1   | 1     | 2834 | G    |
| 1   | 1     | 2841 | G    |
| 1   | 1     | 2842 | U    |
| 1   | 1     | 2843 | U    |
| 1   | 1     | 2857 | C    |
| 1   | 1     | 2861 | U    |
| 1   | 1     | 2863 | G    |
| 1   | 1     | 2867 | C    |
| 1   | 1     | 2868 | U    |
| 1   | 1     | 2869 | U    |
| 1   | 1     | 2870 | C    |
| 1   | 1     | 2872 | A    |
| 1   | 1     | 2873 | U    |
| 1   | 1     | 2875 | U    |
| 1   | 1     | 2876 | C    |
| 1   | 1     | 2877 | G    |
| 1   | 1     | 2878 | G    |
| 1   | 1     | 2879 | C    |
| 1   | 1     | 2887 | A    |
| 1   | 1     | 2889 | C    |
| 1   | 1     | 2894 | C    |
| 1   | 1     | 2898 | G    |
| 1   | 1     | 2901 | G    |
| 1   | 1     | 2918 | G    |
| 1   | 1     | 2920 | U    |
| 1   | 1     | 2921 | U    |
| 1   | 1     | 2923 | U    |
| 1   | 1     | 2925 | C    |
| 1   | 1     | 2926 | A    |
| 1   | 1     | 2929 | C    |
| 1   | 1     | 2930 | A    |
| 1   | 1     | 2935 | U    |
| 1   | 1     | 2936 | A    |
| 1   | 1     | 2940 | A    |
| 1   | 1     | 2952 | G    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 2953 | U    |
| 1   | 1     | 2954 | U    |
| 1   | 1     | 2955 | U    |
| 1   | 1     | 2968 | G    |
| 1   | 1     | 2970 | C    |
| 1   | 1     | 2971 | A    |
| 1   | 1     | 2972 | G    |
| 1   | 1     | 2979 | U    |
| 1   | 1     | 2988 | C    |
| 1   | 1     | 2996 | U    |
| 1   | 1     | 2997 | G    |
| 1   | 1     | 3003 | G    |
| 1   | 1     | 3012 | A    |
| 1   | 1     | 3017 | A    |
| 1   | 1     | 3021 | A    |
| 1   | 1     | 3022 | G    |
| 1   | 1     | 3023 | U    |
| 1   | 1     | 3026 | G    |
| 1   | 1     | 3028 | G    |
| 1   | 1     | 3029 | A    |
| 1   | 1     | 3031 | G    |
| 1   | 1     | 3034 | C    |
| 1   | 1     | 3047 | U    |
| 1   | 1     | 3054 | U    |
| 1   | 1     | 3055 | U    |
| 1   | 1     | 3058 | U    |
| 1   | 1     | 3071 | U    |
| 1   | 1     | 3073 | A    |
| 1   | 1     | 3080 | G    |
| 1   | 1     | 3086 | A    |
| 1   | 1     | 3092 | C    |
| 1   | 1     | 3093 | C    |
| 1   | 1     | 3099 | C    |
| 1   | 1     | 3100 | U    |
| 1   | 1     | 3129 | A    |
| 1   | 1     | 3130 | A    |
| 1   | 1     | 3131 | U    |
| 1   | 1     | 3142 | A    |
| 1   | 1     | 3143 | C    |
| 1   | 1     | 3155 | U    |
| 1   | 1     | 3158 | G    |
| 1   | 1     | 3163 | A    |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 3165 | A    |
| 1   | 1     | 3172 | A    |
| 1   | 1     | 3173 | G    |
| 1   | 1     | 3174 | A    |
| 1   | 1     | 3176 | G    |
| 1   | 1     | 3178 | A    |
| 1   | 1     | 3179 | U    |
| 1   | 1     | 3181 | C    |
| 1   | 1     | 3187 | A    |
| 1   | 1     | 3195 | U    |
| 1   | 1     | 3196 | U    |
| 1   | 1     | 3197 | G    |
| 1   | 1     | 3217 | C    |
| 1   | 1     | 3218 | A    |
| 1   | 1     | 3219 | G    |
| 1   | 1     | 3229 | G    |
| 1   | 1     | 3243 | A    |
| 1   | 1     | 3245 | A    |
| 1   | 1     | 3247 | G    |
| 1   | 1     | 3253 | G    |
| 1   | 1     | 3259 | U    |
| 1   | 1     | 3260 | G    |
| 1   | 1     | 3266 | G    |
| 1   | 1     | 3270 | U    |
| 1   | 1     | 3271 | G    |
| 1   | 1     | 3273 | A    |
| 1   | 1     | 3276 | G    |
| 1   | 1     | 3279 | A    |
| 1   | 1     | 3280 | U    |
| 1   | 1     | 3281 | U    |
| 1   | 1     | 3287 | U    |
| 1   | 1     | 3289 | G    |
| 1   | 1     | 3294 | A    |
| 1   | 1     | 3296 | A    |
| 1   | 1     | 3304 | U    |
| 1   | 1     | 3316 | A    |
| 1   | 1     | 3317 | U    |
| 1   | 1     | 3319 | U    |
| 1   | 1     | 3334 | U    |
| 1   | 1     | 3340 | G    |
| 1   | 1     | 3341 | U    |
| 1   | 1     | 3342 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 3350 | C    |
| 1   | 1     | 3359 | A    |
| 1   | 1     | 3363 | U    |
| 1   | 1     | 3368 | U    |
| 1   | 1     | 3369 | G    |
| 1   | 1     | 3374 | U    |
| 1   | 1     | 3375 | A    |
| 1   | 1     | 3376 | A    |
| 1   | 1     | 3383 | G    |
| 1   | 1     | 3389 | U    |
| 1   | 1     | 3390 | G    |
| 2   | 2     | 13   | A    |
| 2   | 2     | 16   | G    |
| 2   | 2     | 23   | U    |
| 3   | 3     | 13   | A    |
| 3   | 3     | 42   | A    |
| 3   | 3     | 76   | A    |
| 3   | 3     | 77   | G    |
| 3   | 3     | 83   | U    |
| 3   | 3     | 84   | A    |
| 3   | 3     | 95   | A    |
| 3   | 3     | 100  | C    |
| 3   | 3     | 102  | A    |
| 3   | 3     | 112  | G    |
| 3   | 3     | 121  | U    |

All (59) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 337  | G    |
| 1   | 1     | 374  | A    |
| 1   | 1     | 375  | A    |
| 1   | 1     | 437  | G    |
| 1   | 1     | 494  | G    |
| 1   | 1     | 547  | G    |
| 1   | 1     | 688  | G    |
| 1   | 1     | 720  | A    |
| 1   | 1     | 974  | G    |
| 1   | 1     | 990  | U    |
| 1   | 1     | 999  | G    |
| 1   | 1     | 1047 | A    |
| 1   | 1     | 1064 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 1093 | A    |
| 1   | 1     | 1097 | G    |
| 1   | 1     | 1102 | A    |
| 1   | 1     | 1103 | A    |
| 1   | 1     | 1128 | U    |
| 1   | 1     | 1129 | A    |
| 1   | 1     | 1192 | C    |
| 1   | 1     | 1200 | A    |
| 1   | 1     | 1205 | A    |
| 1   | 1     | 1238 | C    |
| 1   | 1     | 1241 | U    |
| 1   | 1     | 1243 | G    |
| 1   | 1     | 1244 | A    |
| 1   | 1     | 1259 | A    |
| 1   | 1     | 1302 | A    |
| 1   | 1     | 1306 | G    |
| 1   | 1     | 1329 | U    |
| 1   | 1     | 1355 | A    |
| 1   | 1     | 1416 | C    |
| 1   | 1     | 2624 | G    |
| 1   | 1     | 2625 | C    |
| 1   | 1     | 2651 | G    |
| 1   | 1     | 2658 | G    |
| 1   | 1     | 2667 | A    |
| 1   | 1     | 2690 | G    |
| 1   | 1     | 2702 | A    |
| 1   | 1     | 2725 | U    |
| 1   | 1     | 2728 | G    |
| 1   | 1     | 2764 | C    |
| 1   | 1     | 2817 | A    |
| 1   | 1     | 2822 | U    |
| 1   | 1     | 2840 | C    |
| 1   | 1     | 2860 | U    |
| 1   | 1     | 2868 | U    |
| 1   | 1     | 2875 | U    |
| 1   | 1     | 2967 | A    |
| 1   | 1     | 3030 | G    |
| 1   | 1     | 3070 | A    |
| 1   | 1     | 3079 | U    |
| 1   | 1     | 3157 | U    |
| 1   | 1     | 3195 | U    |
| 1   | 1     | 3228 | C    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 3269 | U    |
| 1   | 1     | 3316 | A    |
| 1   | 1     | 3341 | U    |
| 3   | 3     | 82   | G    |

## 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 3 ligands modelled in this entry, 3 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](#)

There are no chain breaks in this entry.

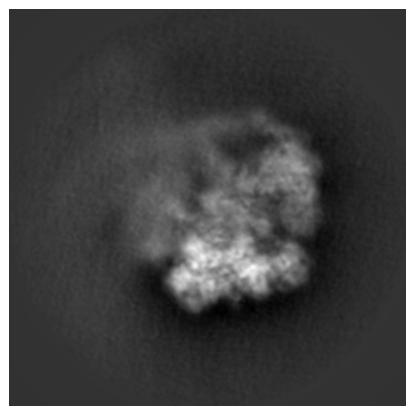
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12908. These allow visual inspection of the internal detail of the map and identification of artifacts.

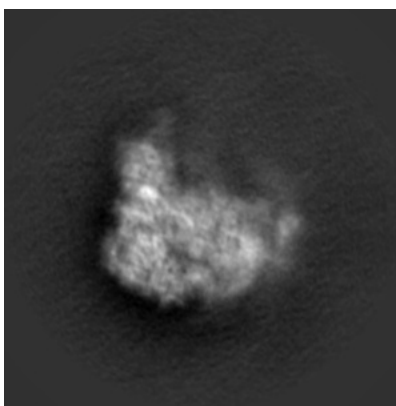
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

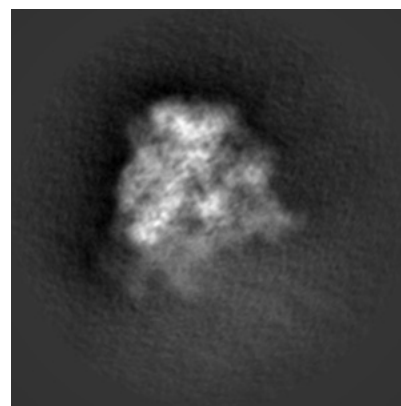
#### 6.1.1 Primary map



X

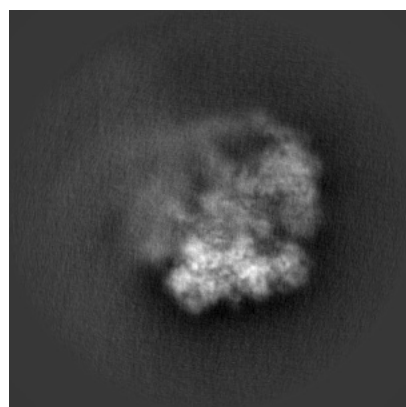


Y

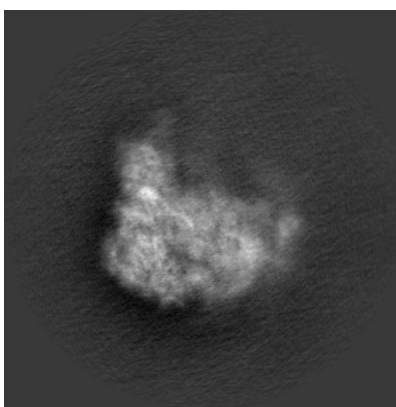


Z

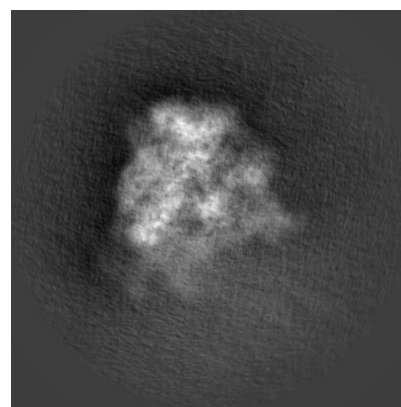
#### 6.1.2 Raw map



X



Y

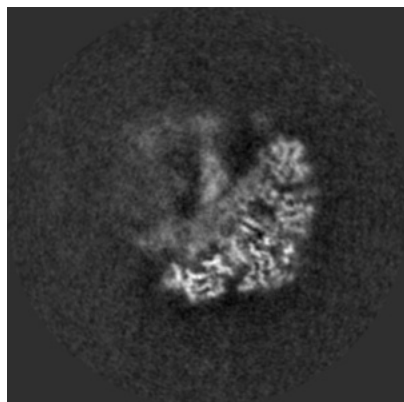


Z

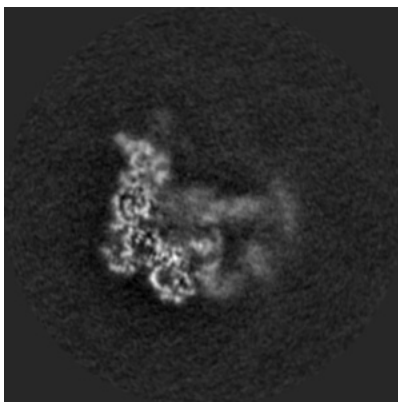
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

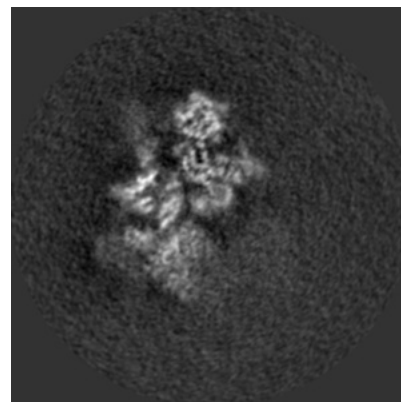
### 6.2.1 Primary map



X Index: 200

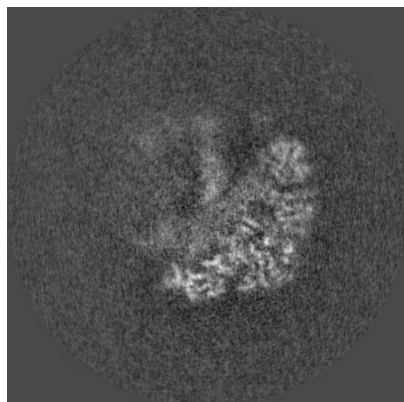


Y Index: 200

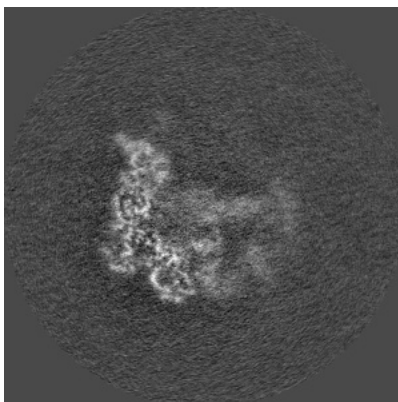


Z Index: 200

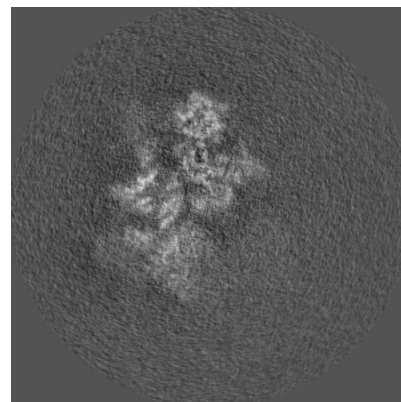
### 6.2.2 Raw map



X Index: 200



Y Index: 200

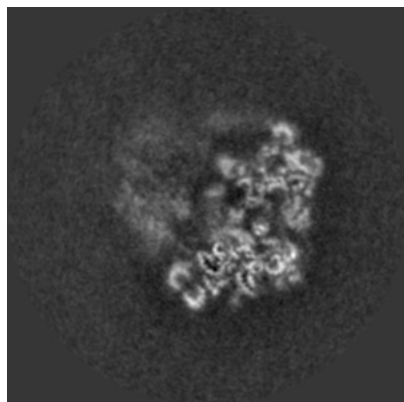


Z Index: 200

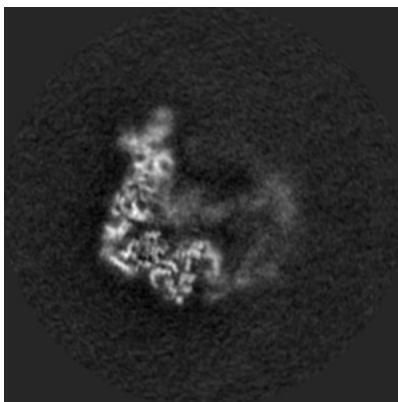
The images above show central slices of the map in three orthogonal directions.

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

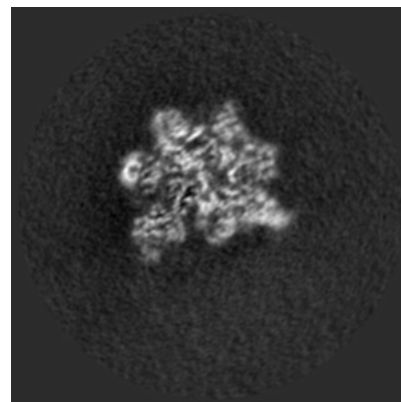
### 6.3.1 Primary map



X Index: 171

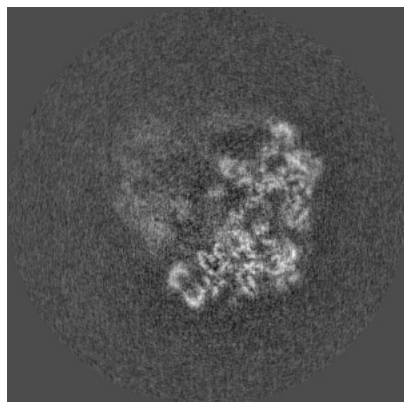


Y Index: 193

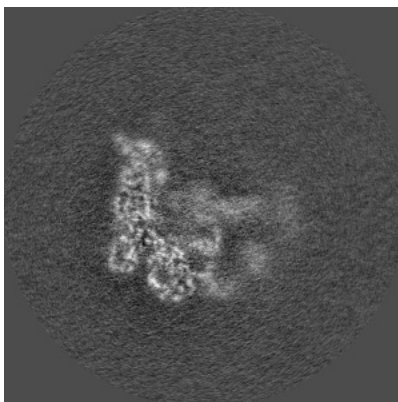


Z Index: 142

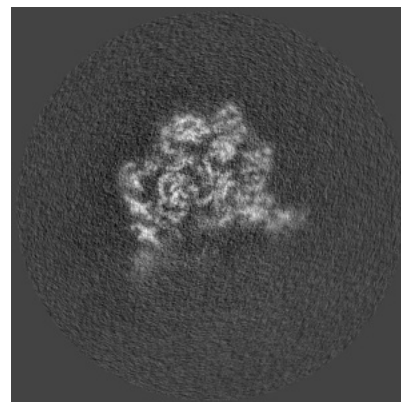
### 6.3.2 Raw map



X Index: 172



Y Index: 203



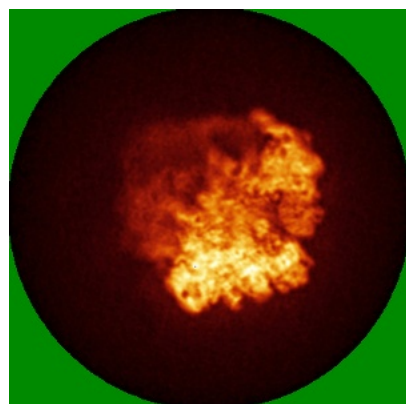
Z Index: 150

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

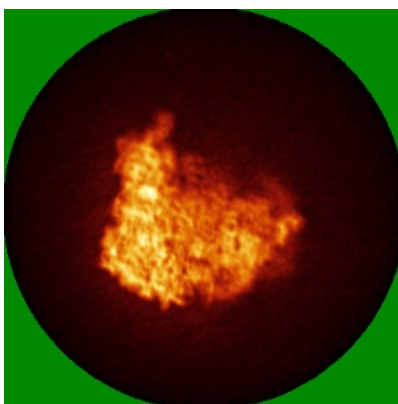


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

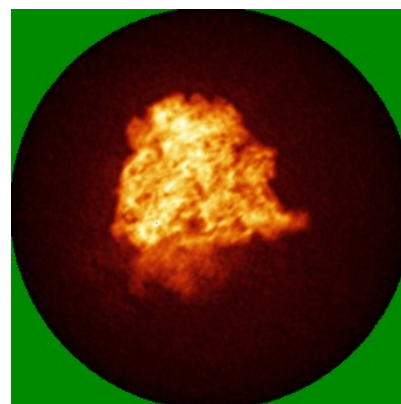
### 6.4.1 Primary map



X

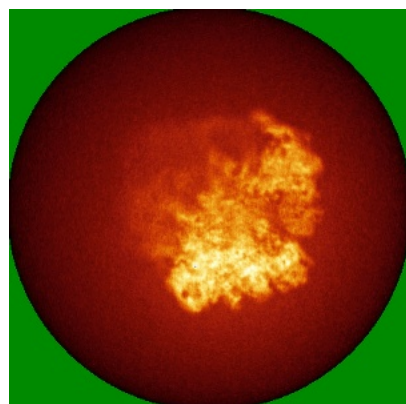


Y

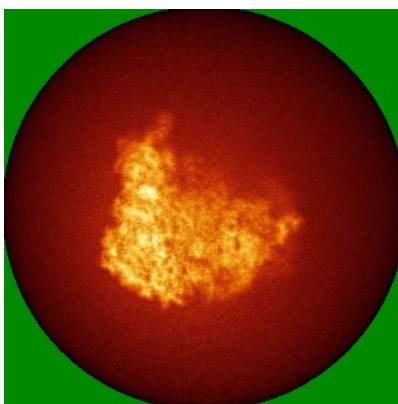


Z

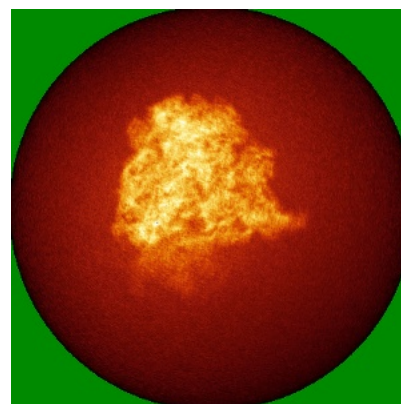
### 6.4.2 Raw map



X



Y



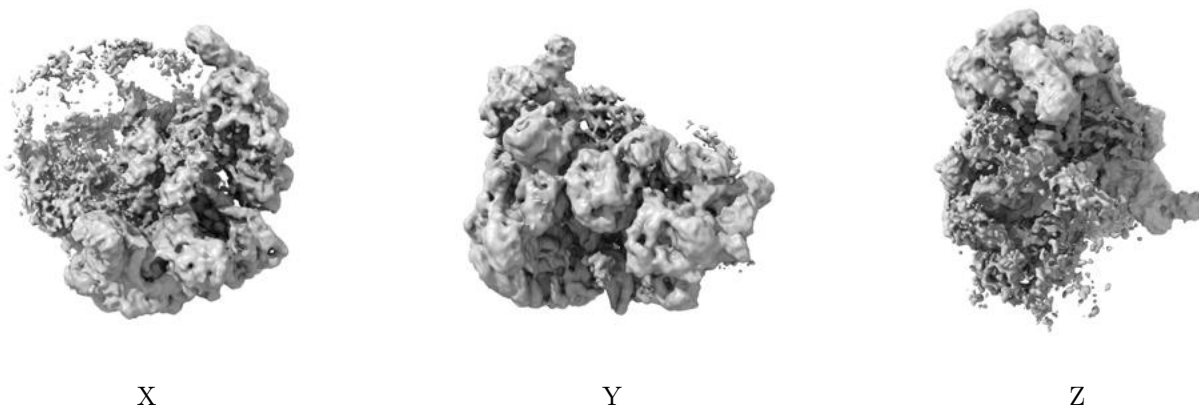
Z

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.



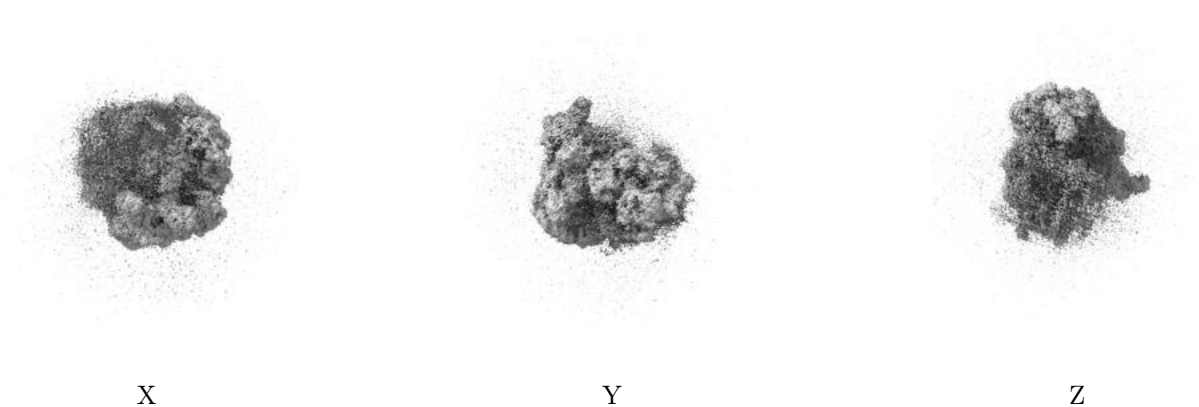
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.018. 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.

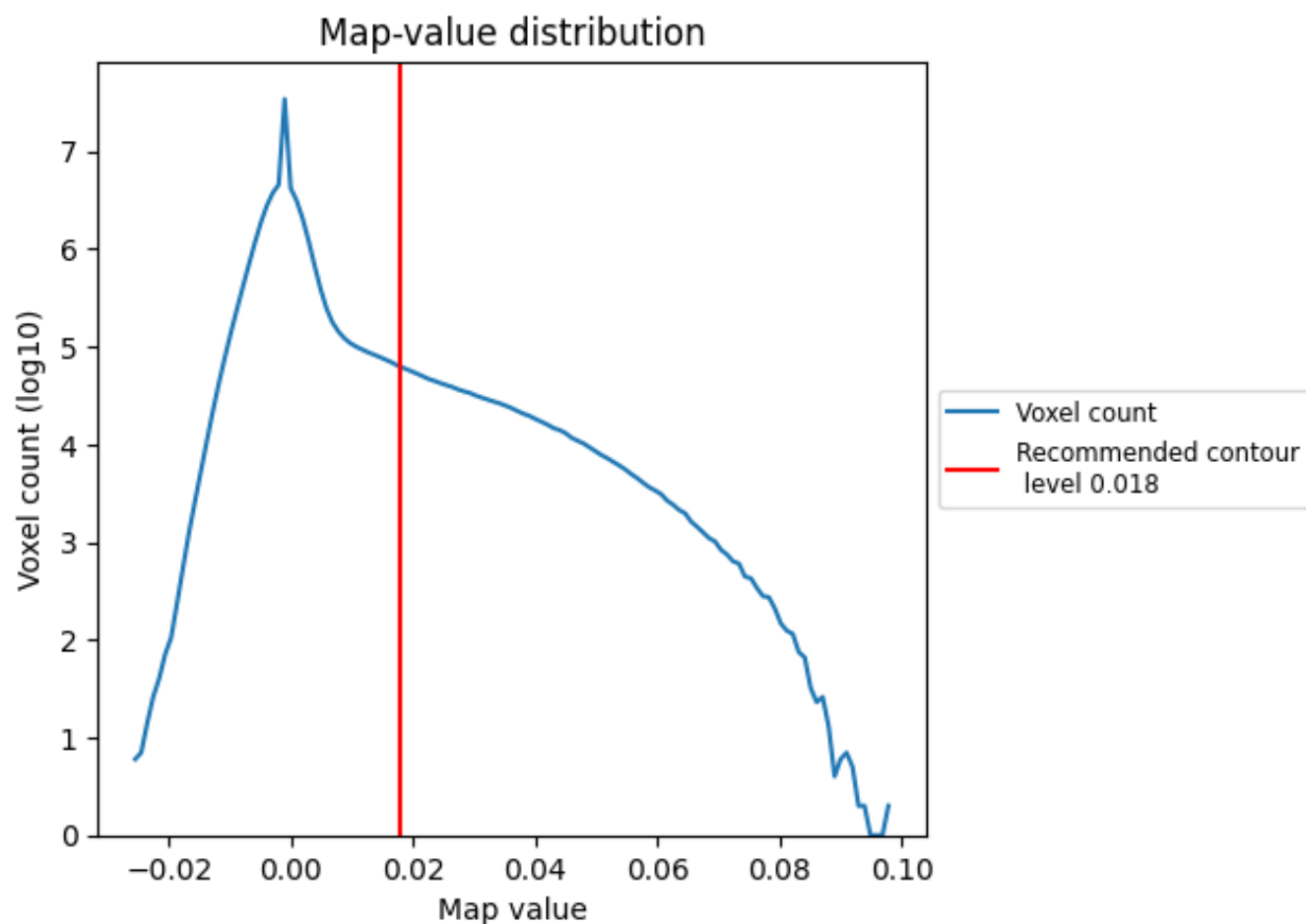
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

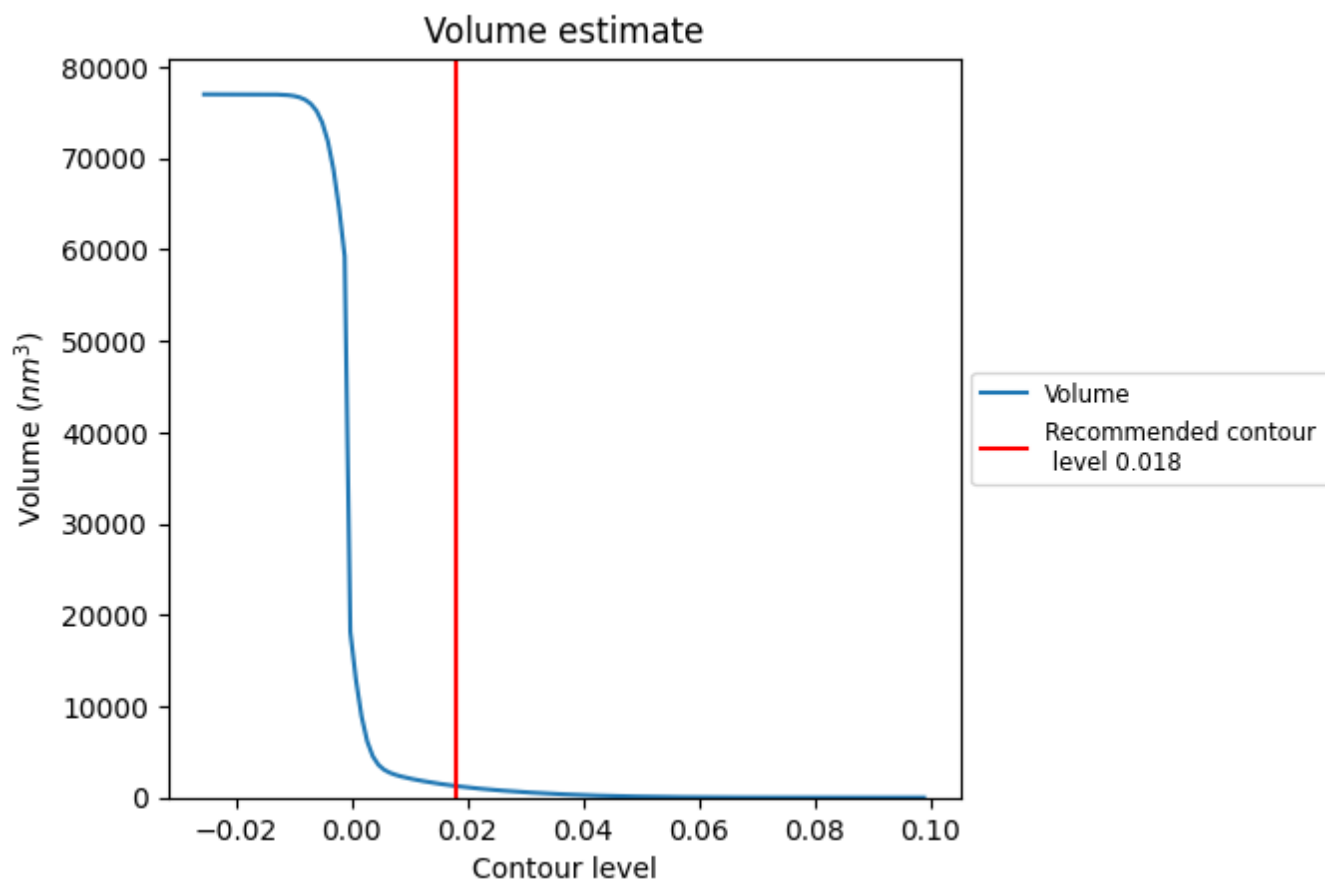
This section contains the results of statistical analysis of the map.

### 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.

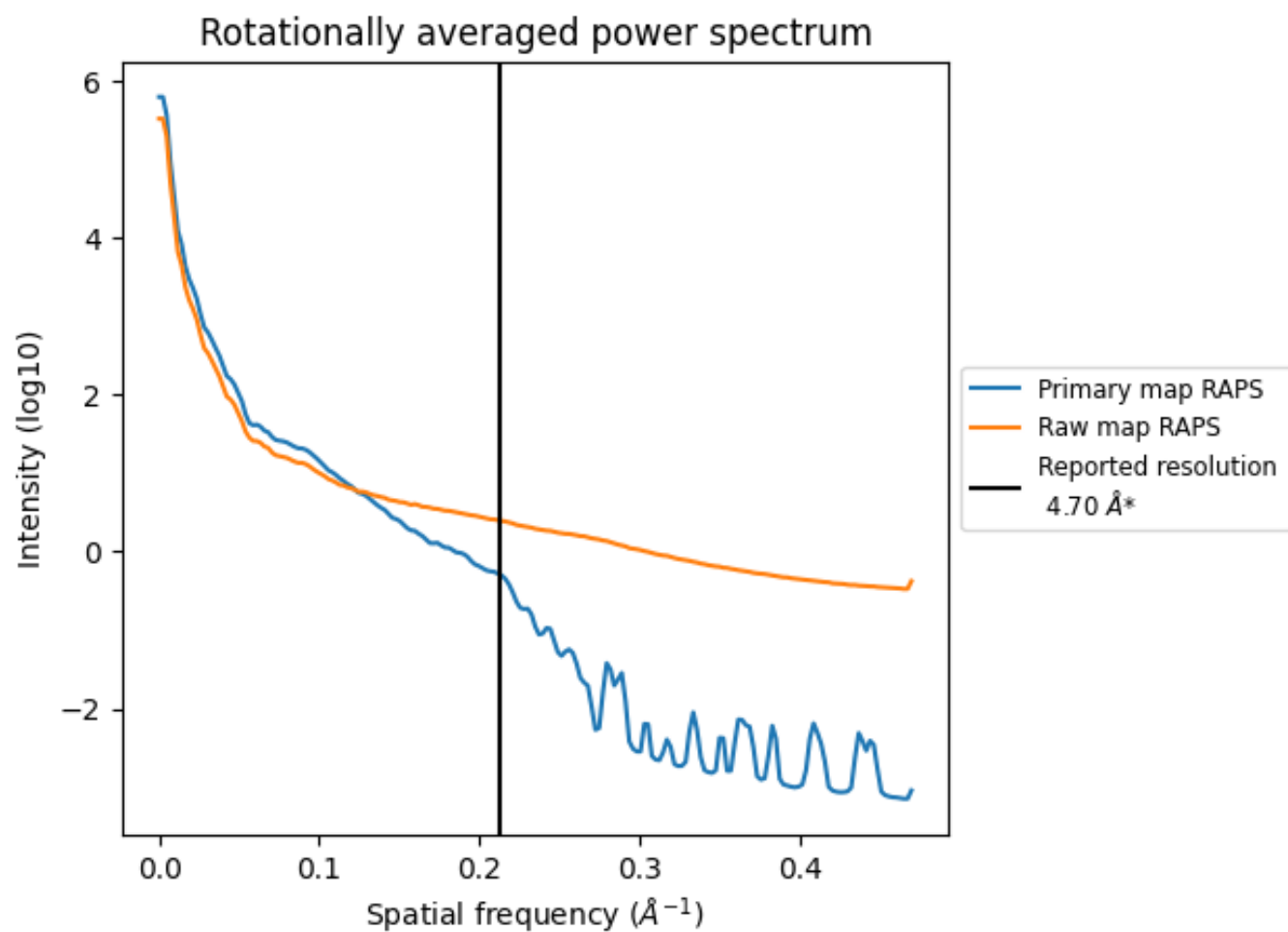
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1261 nm<sup>3</sup>; this corresponds to an approximate mass of 1139 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 ⓘ

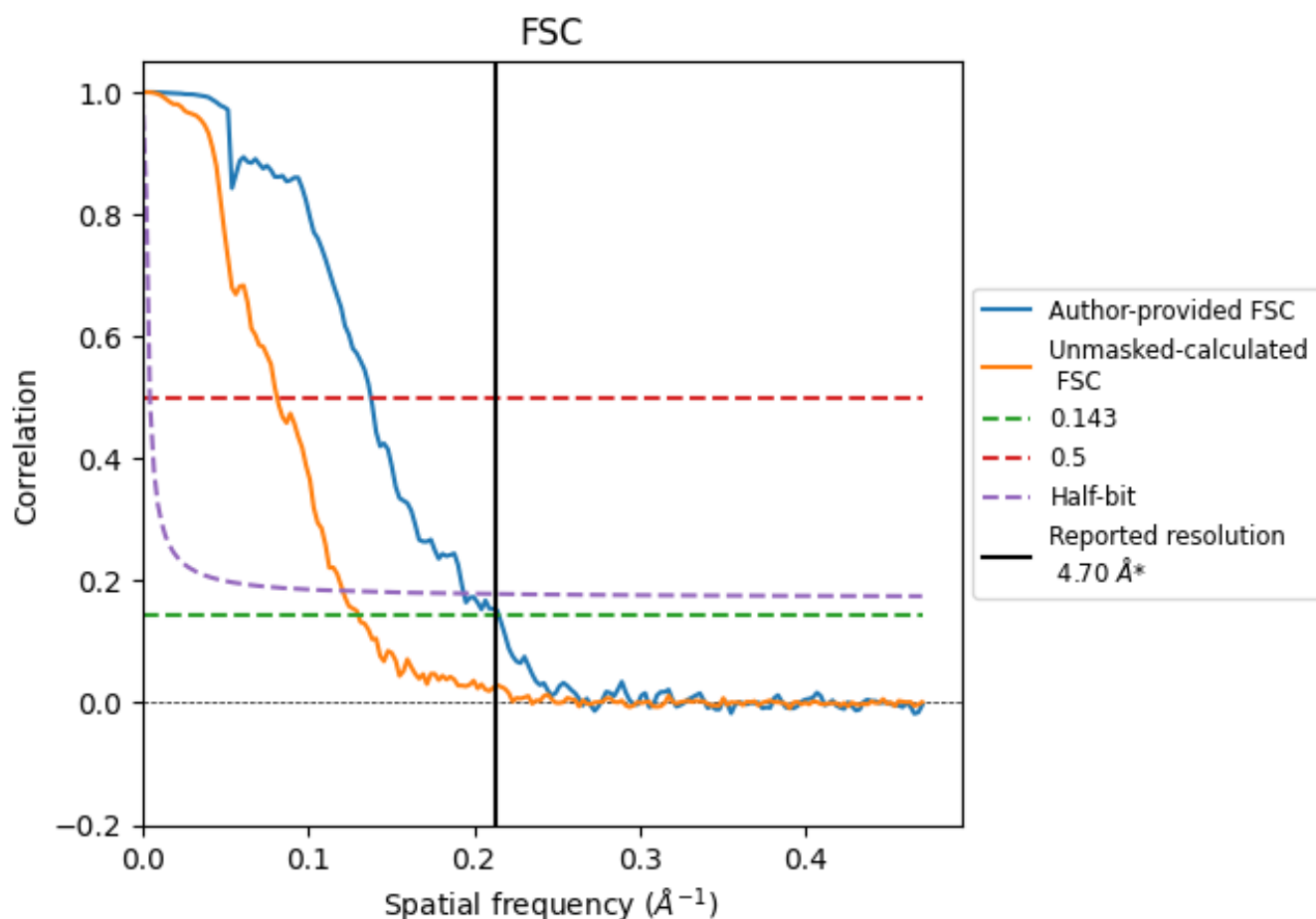


\*Reported resolution corresponds to spatial frequency of 0.213  $\text{\AA}^{-1}$

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

## 8.2 Resolution estimates [i](#)

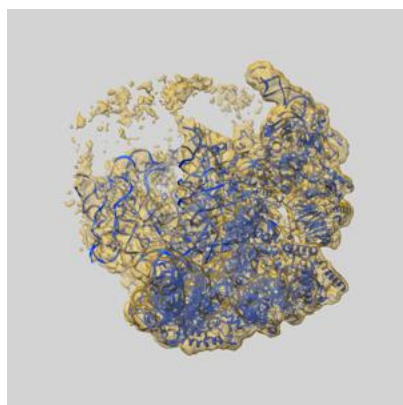
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |       |          |
|---------------------------|------------------------------------|-------|----------|
|                           | 0.143                              | 0.5   | Half-bit |
| Reported by author        | 4.70                               | -     | -        |
| Author-provided FSC curve | 4.65                               | 7.26  | 5.16     |
| Unmasked-calculated*      | 7.68                               | 12.30 | 8.27     |

\*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 7.68 differs from the reported value 4.7 by more than 10 %

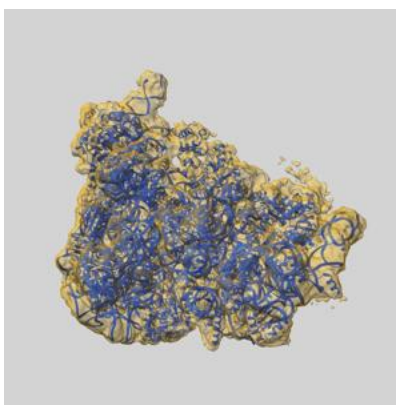
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12908 and PDB model 7OHT. Per-residue inclusion information can be found in section [3](#) on page [9](#).

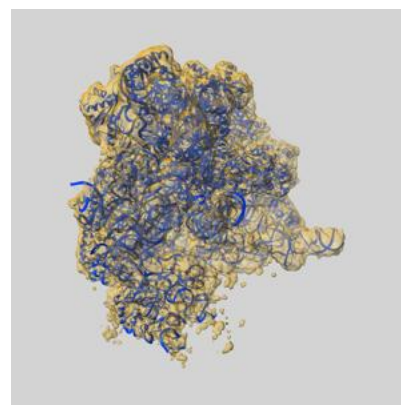
### 9.1 Map-model overlay [i](#)



X



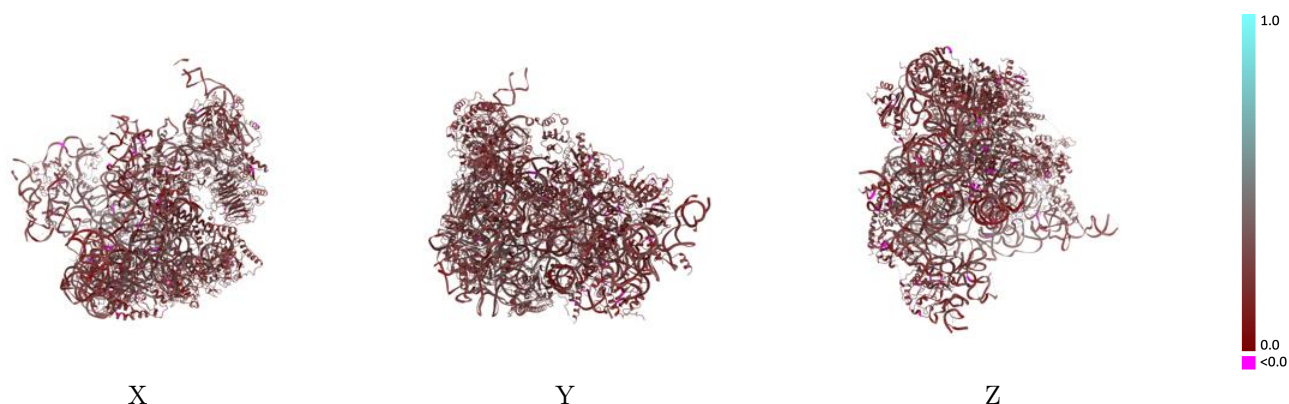
Y



Z

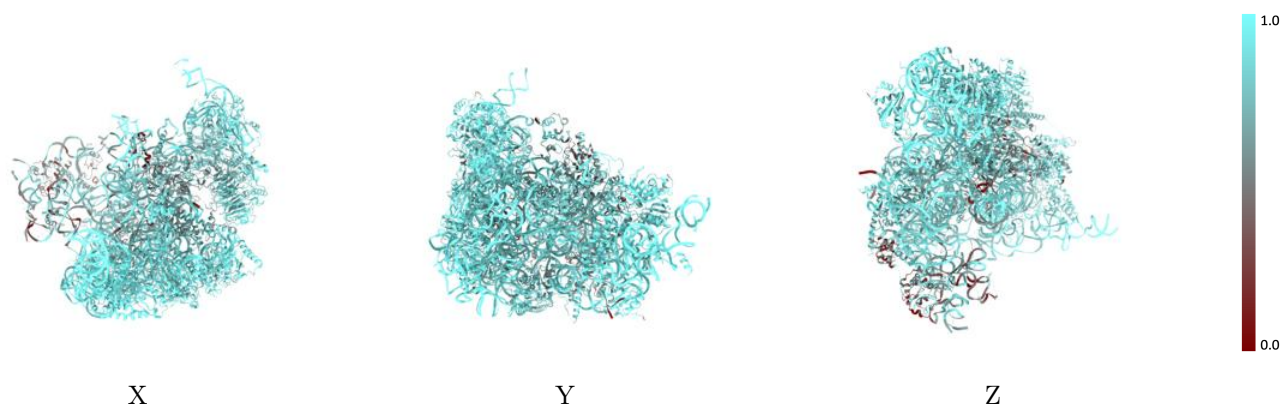
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

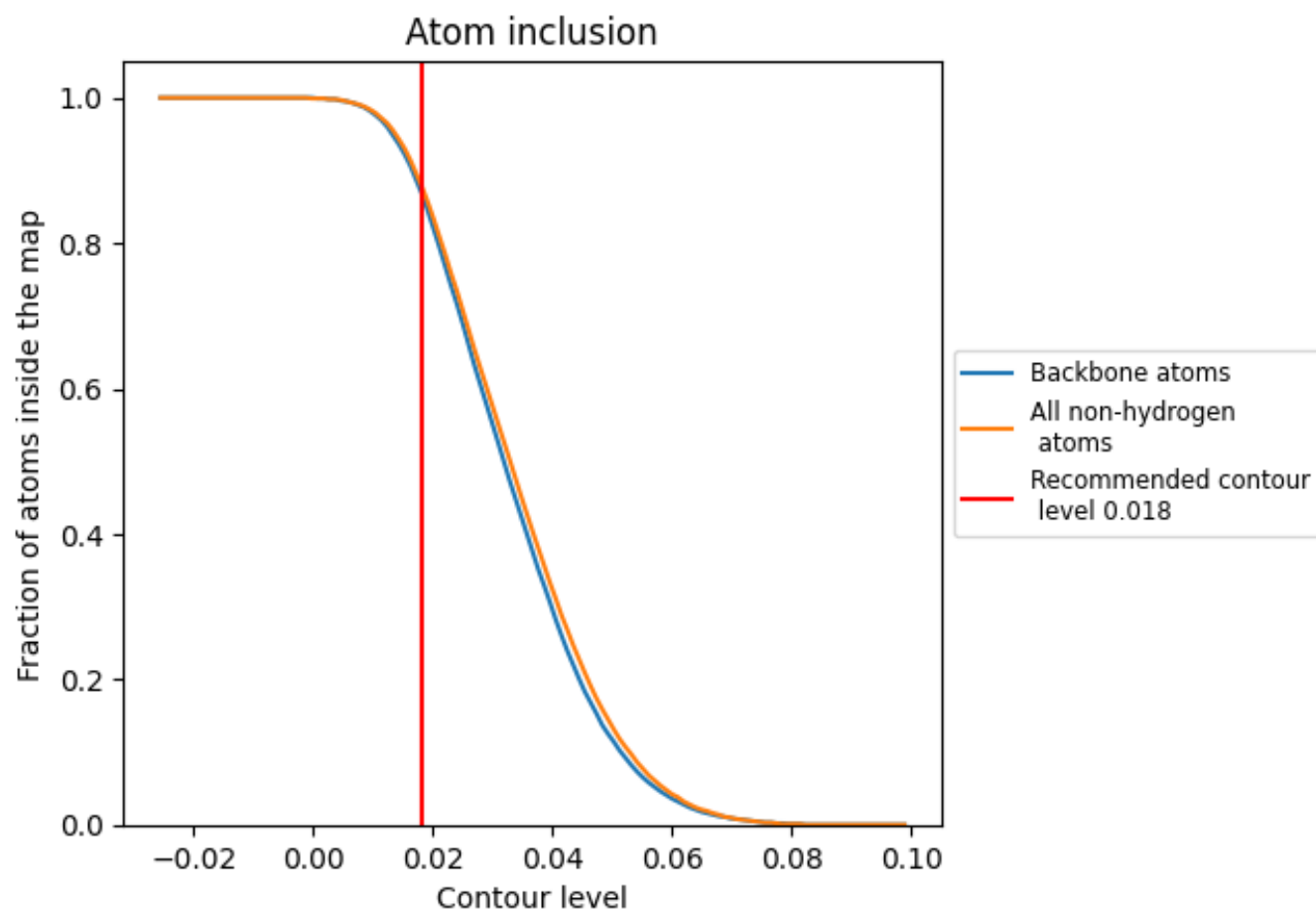
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.018).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 88% 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 (0.018) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8810   |  0.2450   |
| 1     |  0.9150   |  0.2400   |
| 2     |  0.5550   |  0.2080   |
| 3     |  0.9990   |  0.2450   |
| B     |  0.9260   |  0.2660   |
| C     |  0.6310   |  0.2350   |
| D     |  0.9040   |  0.2240   |
| E     |  0.9200   |  0.2720   |
| F     |  0.8660   |  0.2730   |
| H     |  0.8860   |  0.2880   |
| J     |  0.9340   |  0.2000   |
| M     |  0.8890   |  0.2870   |
| O     |  0.8480   |  0.2890   |
| Q     |  0.4970   |  0.2190   |
| S     |  0.8720  |  0.2880  |
| T     |  0.7790 |  0.2650 |
| V     |  0.9030 |  0.2320 |
| W     |  0.9320 |  0.2480 |
| b     |  0.8810 |  0.2300 |
| e     |  0.3990 |  0.2760 |
| f     |  0.8650 |  0.3130 |
| m     |  0.6400 |  0.2240 |
| r     |  0.7660 |  0.2480 |
| u     |  0.9690 |  0.2030 |
| v     |  0.8910 |  0.2470 |
| w     |  0.8270 |  0.2340 |
| x     |  0.8830 |  0.2520 |
| y     |  0.9470 |  0.2340 |

