



## Full wwPDB EM Validation Report ⓘ

Jun 21, 2026 – 12:14 pm BST

PDB ID : 8OZ0 / pdb\_00008oz0  
EMDB ID : EMD-17297  
Title : Structure of a human 48S translation initiation complex with eIF4F and eIF4A  
Authors : Brito Querido, J.; Sokabe, M.; Diaz-Lopez, I.; Gordiyenko, Y.; Fraser, C.S.;  
Ramakrishnan, V.  
Deposited on : 2023-05-06  
Resolution : 3.50 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

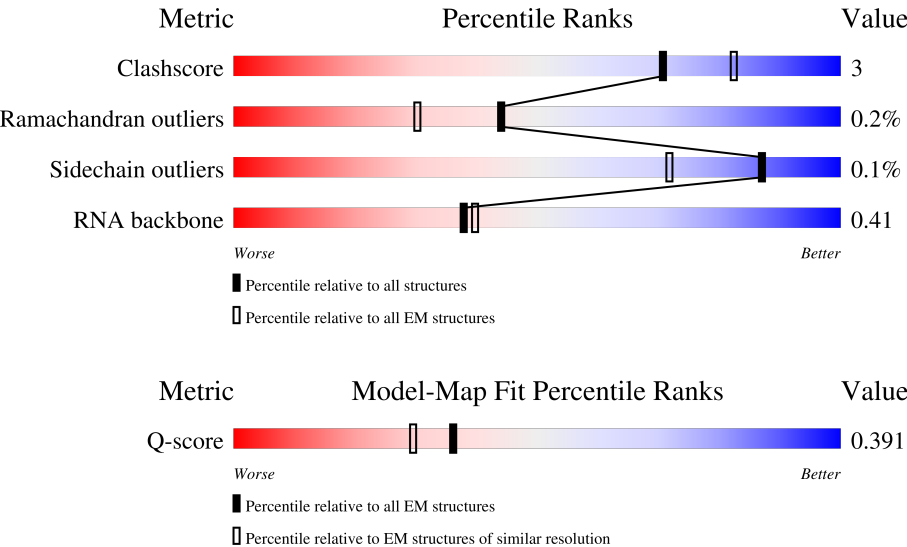
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 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 3.50 Å.

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



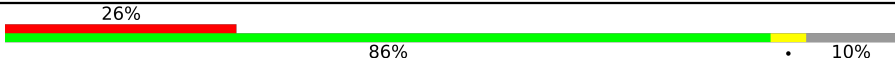
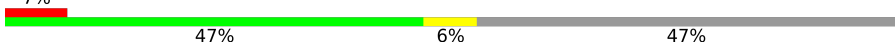
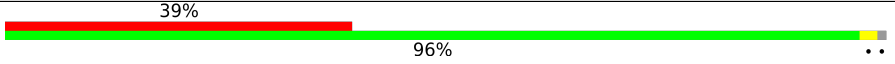
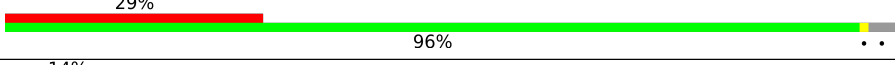
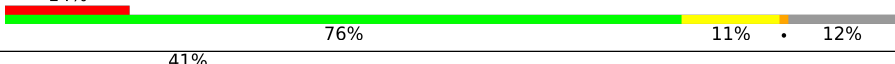
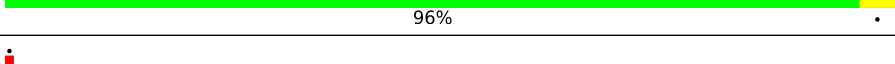
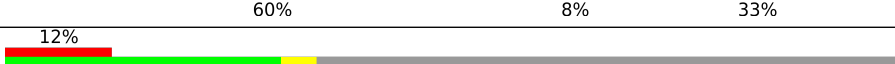
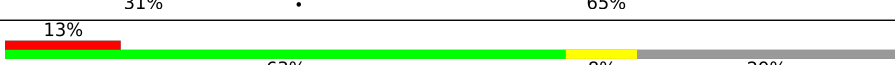
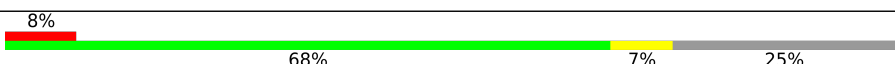
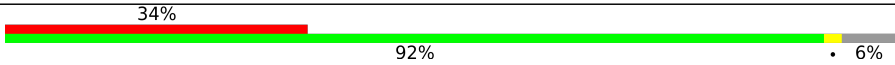
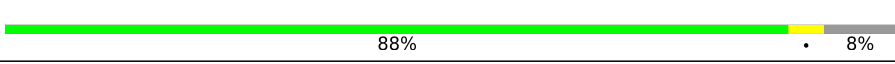
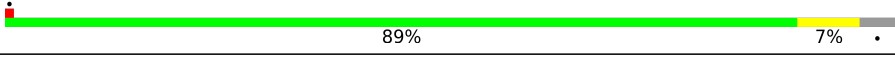
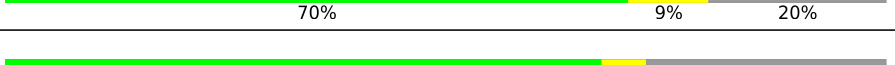
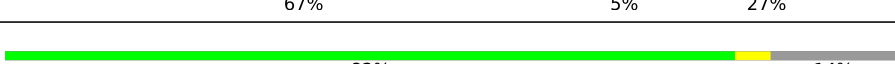
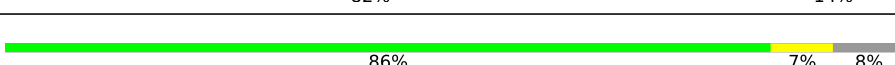
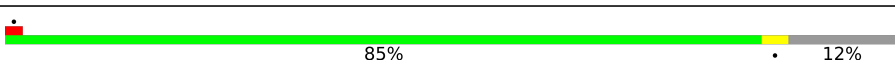
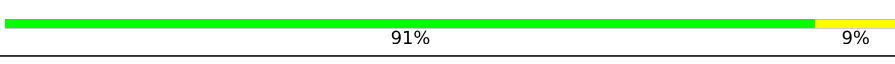
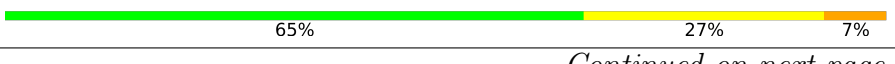
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 13950 ( 3.00 - 4.00 )                                    |

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   | 5     | 445    | <div> <div>19%</div> <div>95%</div> </div>                |
| 2   | 6     | 357    | <div> <div>24%</div> <div>74%</div> <div>25%</div> </div> |
| 3   | 7     | 320    | <div> <div>21%</div> <div>76%</div> </div>                |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | 8     | 352    |    |
| 5   | 9     | 25     |    |
| 6   | A     | 1382   |    |
| 7   | B     | 218    |    |
| 8   | C     | 374    |    |
| 9   | D     | 315    |    |
| 10  | E     | 472    |    |
| 11  | F     | 325    |    |
| 12  | G     | 144    |    |
| 13  | H     | 431    |    |
| 14  | I     | 814    |   |
| 15  | J     | 913    |  |
| 16  | K     | 564    |  |
| 17  | L     | 194    |  |
| 18  | M     | 84     |  |
| 19  | N     | 83     |  |
| 20  | O     | 293    |  |
| 21  | P     | 264    |  |
| 22  | Q     | 295    |  |
| 23  | R     | 115    |  |
| 24  | S     | 249    |  |
| 25  | T     | 151    |  |
| 26  | U     | 333    |  |
| 27  | V     | 151    |  |
| 28  | W     | 1719   |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 29  | X     | 158    |                  |
| 30  | Y     | 263    |                  |
| 31  | Z     | 194    |                  |
| 32  | a     | 143    |                  |
| 33  | b     | 59     |                  |
| 34  | c     | 130    |                  |
| 35  | d     | 208    |                  |
| 36  | e     | 133    |                  |
| 37  | f     | 204    |                  |
| 38  | g     | 146    |                  |
| 39  | h     | 243    |                  |
| 40  | i     | 165    |                  |
| 41  | j     | 145    |                  |
| 42  | k     | 317    |                  |
| 43  | l     | 145    |                  |
| 44  | m     | 125    |                  |
| 45  | n     | 151    |                  |
| 46  | o     | 56     |                  |
| 47  | p     | 156    |                  |
| 48  | q     | 132    |                  |
| 49  | s     | 69     |                  |
| 50  | v     | 135    |                  |
| 51  | w     | 119    |                  |
| 52  | x     | 548    |                  |
| 53  | y     | 75     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 54  | z     | 207    |                  |
| 55  | 1     | 406    |                  |
| 55  | 3     | 406    |                  |
| 56  | 2     | 1404   |                  |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 28  | JMH  | W     | 1219 | X         | -        | -       | -                |

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 121610 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Eukaryotic translation initiation factor 3 subunit E.

| Mol | Chain | Residues | Atoms |      |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 1   | 5     | 437      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 2175  | 1301 | 437 | 437 |         |       |

- Molecule 2 is a protein called Eukaryotic translation initiation factor 3 subunit F.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 2   | 6     | 269      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1330  | 791 | 269 | 270 |         |       |

- Molecule 3 is a protein called Eukaryotic translation initiation factor 3 subunit G.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 3   | 7     | 77       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 616   | 389 | 111 | 116 |         |       |

- Molecule 4 is a protein called Eukaryotic translation initiation factor 3 subunit H.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 4   | 8     | 316      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1569  | 936 | 316 | 317 |         |       |

- Molecule 5 is a protein called 60S ribosomal protein L41.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 5   | 9     | 24       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 230   | 139 | 62 | 26 | 3 |         |       |

- Molecule 6 is a protein called Eukaryotic translation initiation factor 3 subunit A.

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 6   | A     | 733      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5386  | 3376 | 979 | 1008 | 23 |         |       |

- Molecule 7 is a protein called Eukaryotic translation initiation factor 3 subunit K.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 7   | B     | 215      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1066  | 636 | 215 | 215 |         |       |

- Molecule 8 is a protein called Eukaryotic translation initiation factor 3 subunit M.

| Mol | Chain | Residues | Atoms |      |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 8   | C     | 364      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 1809  | 1080 | 364 | 365 |         |       |

- Molecule 9 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 9   | D     | 278      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2234  | 1410 | 390 | 421 | 13 |         |       |

- Molecule 10 is a protein called Eukaryotic translation initiation factor 2 subunit 3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 10  | E     | 464      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3540  | 2245 | 620 | 658 | 17 |         |       |

- Molecule 11 is a protein called Eukaryotic translation initiation factor 3 subunit I.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 11  | F     | 325      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1598  | 947 | 325 | 326 |         |       |

- Molecule 12 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | G     | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 789   | 492 | 147 | 146 | 4 |         |       |

- Molecule 13 is a protein called Eukaryotic translation initiation factor 5.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 13  | H     | 149      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1176  | 740 | 208 | 217 | 11 |         |       |

- Molecule 14 is a protein called Eukaryotic translation initiation factor 3 subunit B.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 14  | I     | 575      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4569  | 2935 | 788 | 828 | 18 |         |       |

- Molecule 15 is a protein called Eukaryotic translation initiation factor 3 subunit C.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 15  | J     | 687      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5207  | 3252 | 936 | 986 | 33 |         |       |

- Molecule 16 is a protein called Eukaryotic translation initiation factor 3 subunit L.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 16  | K     | 531      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2637  | 1574 | 531 | 532 |   |         |       |

- Molecule 17 is a protein called 40S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | L     | 178      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1439  | 923 | 262 | 253 | 1 |         |       |

- Molecule 18 is a protein called 40S ribosomal protein S27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | M     | 81       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 631   | 397 | 116 | 111 | 7 |         |       |

- Molecule 19 is a protein called 40S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | N     | 81       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 617   | 380 | 114 | 118 | 5 |         |       |

- Molecule 20 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 20  | O     | 220      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1707  | 1104 | 292 | 301 | 10 |         |       |

- Molecule 21 is a protein called 40S ribosomal protein S3a.



| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 21  | P     | 211      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1715  | 1088 | 307 | 306 | 14 |         |       |

- Molecule 22 is a protein called 40S ribosomal protein SA.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 22  | Q     | 214      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1695  | 1077 | 297 | 313 | 8 |         |       |

- Molecule 23 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | R     | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 792   | 492 | 165 | 130 | 5 |         |       |

- Molecule 24 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 24  | S     | 230      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1862  | 1164 | 371 | 320 | 7 |         |       |

- Molecule 25 is a protein called 40S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | T     | 133      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 997   | 610 | 196 | 185 | 6 |         |       |

- Molecule 26 is a protein called Eukaryotic translation initiation factor 2 subunit 2.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 26  | U     | 139      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 689   | 411 | 139 | 139 |         |       |

- Molecule 27 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | V     | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1208  | 773 | 229 | 205 | 1 |         |       |

- Molecule 28 is a RNA chain called 18S rRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 28  | W     | 1716     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 36639 | 16369 | 6570 | 11985 | 1715 |         |       |

- Molecule 29 is a protein called 40S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | X     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1166  | 743 | 218 | 199 | 6 |         |       |

- Molecule 30 is a protein called 40S ribosomal protein S4, X isoform.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 30  | Y     | 256      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2035  | 1302 | 378 | 347 | 8 |         |       |

- Molecule 31 is a protein called 40S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | Z     | 177      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1477  | 941 | 295 | 239 | 2 |         |       |

- Molecule 32 is a protein called 40S ribosomal protein S23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | a     | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1087  | 687 | 215 | 182 | 3 |         |       |

- Molecule 33 is a protein called 40S ribosomal protein S30.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 33  | b     | 47       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 378   | 231 | 85 | 61 | 1 |         |       |

- Molecule 34 is a protein called 40S ribosomal protein S15a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | c     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1034  | 659 | 193 | 176 | 6 |         |       |

- Molecule 35 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 35  | d     | 198      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1627  | 1021 | 322 | 279 | 5 |         |       |

- Molecule 36 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | e     | 125      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1015  | 642 | 199 | 169 | 5 |         |       |

- Molecule 37 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | f     | 184      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1461  | 914 | 276 | 264 | 7 |         |       |

- Molecule 38 is a protein called 40S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | g     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1124  | 715 | 212 | 194 | 3 |         |       |

- Molecule 39 is a protein called 40S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 39  | h     | 227      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1765  | 1125 | 317 | 315 | 8 |         |       |

- Molecule 40 is a protein called 40S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | i     | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 834   | 544 | 149 | 135 | 6 |         |       |

- Molecule 41 is a protein called 40S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | j     | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 913   | 580 | 168 | 158 | 7 |         |       |

- Molecule 42 is a protein called Receptor of activated protein C kinase 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 42  | k     | 313      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2436  | 1535 | 424 | 465 | 12 |         |       |

- Molecule 43 is a protein called 40S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | l     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1105  | 692 | 213 | 197 | 3 |         |       |

- Molecule 44 is a protein called 40S ribosomal protein S25.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 44  | m     | 66       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 523   | 338 | 93 | 91 | 1 |         |       |

- Molecule 45 is a protein called Small ribosomal subunit protein uS13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | n     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1176  | 737 | 239 | 199 | 1 |         |       |

- Molecule 46 is a protein called 40S ribosomal protein S29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 46  | o     | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 419   | 262 | 85 | 67 | 5 |         |       |

- Molecule 47 is a protein called Ubiquitin-40S ribosomal protein S27a.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 47  | p     | 53       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 435   | 276 | 82 | 70 | 7 |         |       |

- Molecule 48 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48  | q     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 950   | 596 | 168 | 177 | 9 |         |       |

- Molecule 49 is a protein called 40S ribosomal protein S28.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 49  | s     | 63       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 498   | 302 | 101 | 93 | 2 |         |       |

- Molecule 50 is a protein called 40S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50  | v     | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1064  | 668 | 198 | 194 | 4 |         |       |

- Molecule 51 is a protein called 40S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51  | w     | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 817   | 511 | 155 | 147 | 4 |         |       |

- Molecule 52 is a protein called Eukaryotic translation initiation factor 3 subunit D.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 52  | x     | 440      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2920  | 1798 | 539 | 574 | 9 |         |       |

- Molecule 53 is a RNA chain called tRNAiMet.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 53  | y     | 75       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1604  | 717 | 298 | 515 | 74 |         |       |

- Molecule 54 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 54  | z     | 50       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 853   | 373 | 104 | 326 | 50 |         |       |

- Molecule 55 is a protein called Eukaryotic initiation factor 4A-I.

| Mol | Chain | Residues | Atoms |      |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 55  | 3     | 378      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 1869  | 1113 | 378 | 378 |         |       |
| 55  | 1     | 371      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 1834  | 1092 | 371 | 371 |         |       |

- Molecule 56 is a protein called Eukaryotic translation initiation factor 4 gamma 1.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 56  | 2     | 237      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1178  | 704 | 237 | 237 |         |       |

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

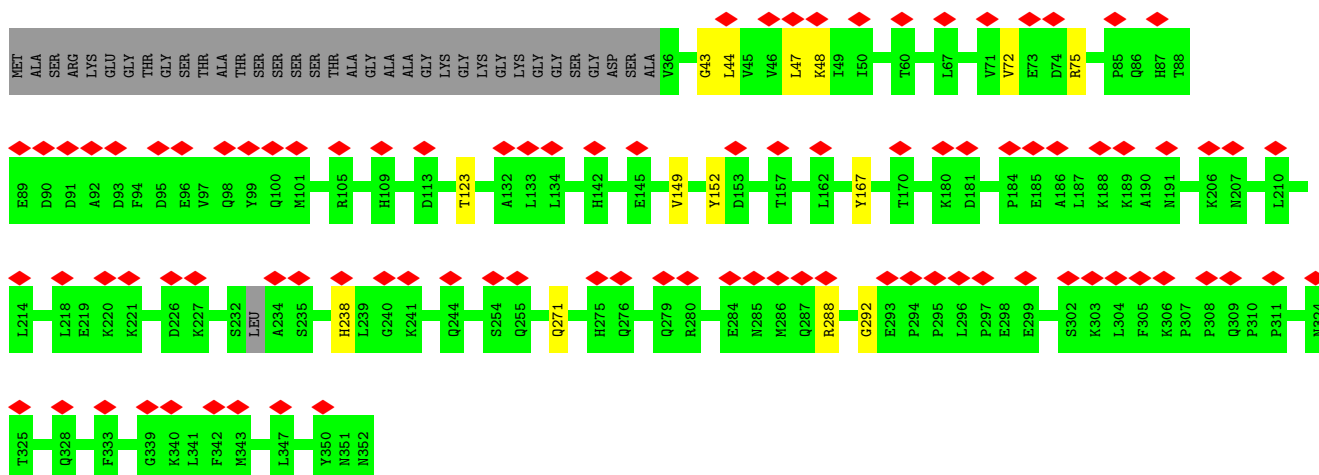
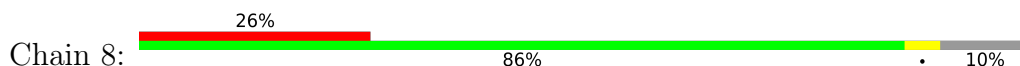
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 57  | R     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 57  | p     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

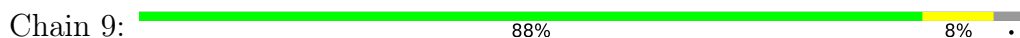
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 58  | T     | 2        | Total | Mg | 0       |
|     |       |          | 2     | 2  |         |
| 58  | W     | 86       | Total | Mg | 0       |
|     |       |          | 86    | 86 |         |
| 58  | f     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |



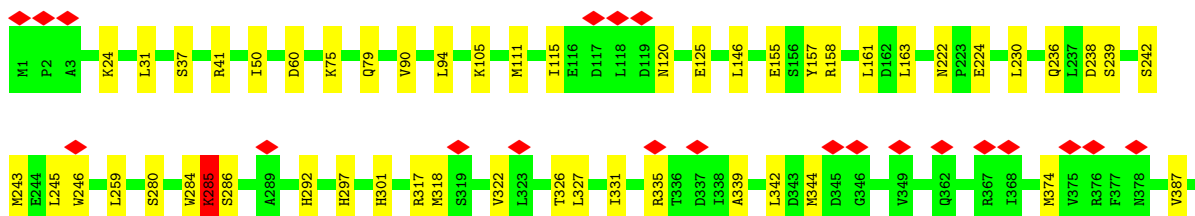
- Molecule 4: Eukaryotic translation initiation factor 3 subunit H



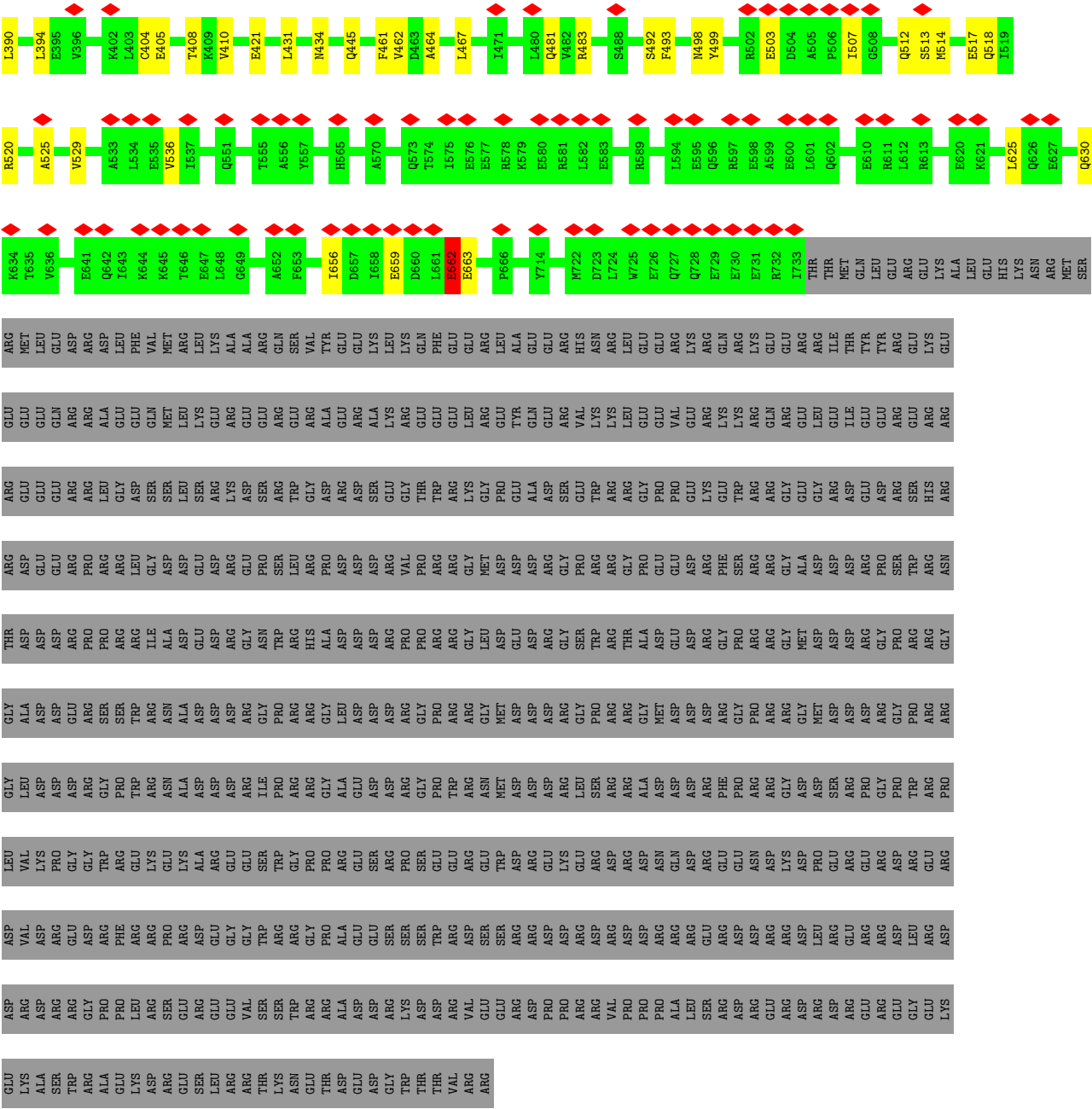
- Molecule 5: 60S ribosomal protein L41



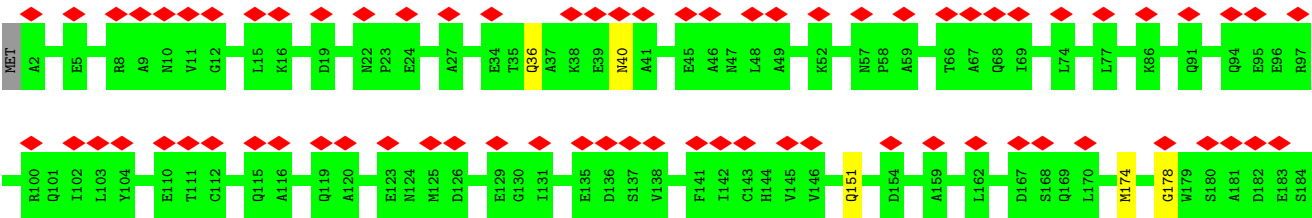
- Molecule 6: Eukaryotic translation initiation factor 3 subunit A

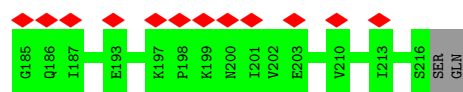




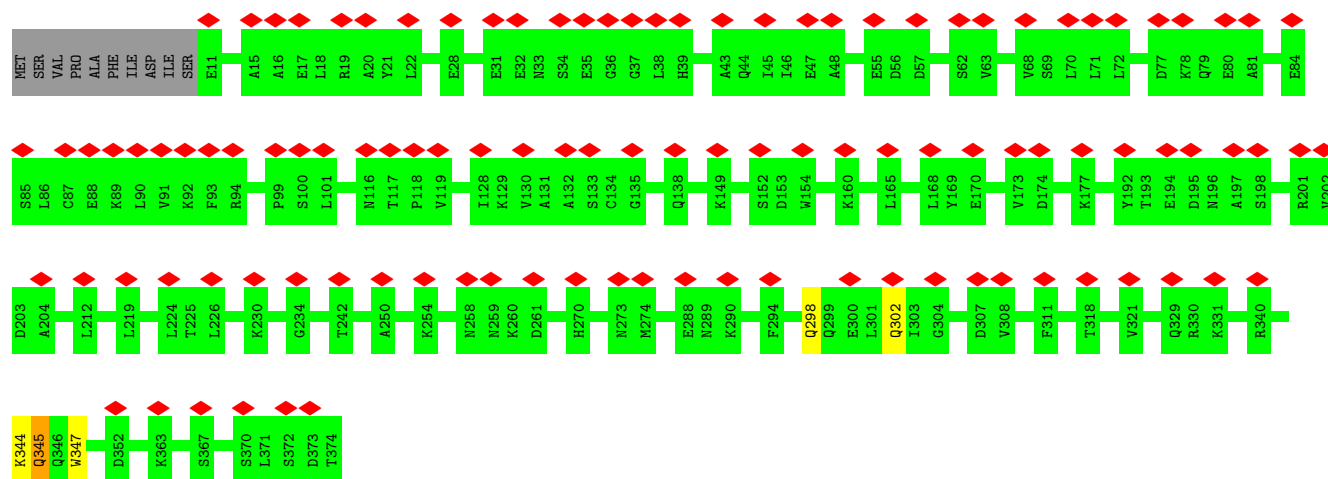


● Molecule 7: Eukaryotic translation initiation factor 3 subunit K

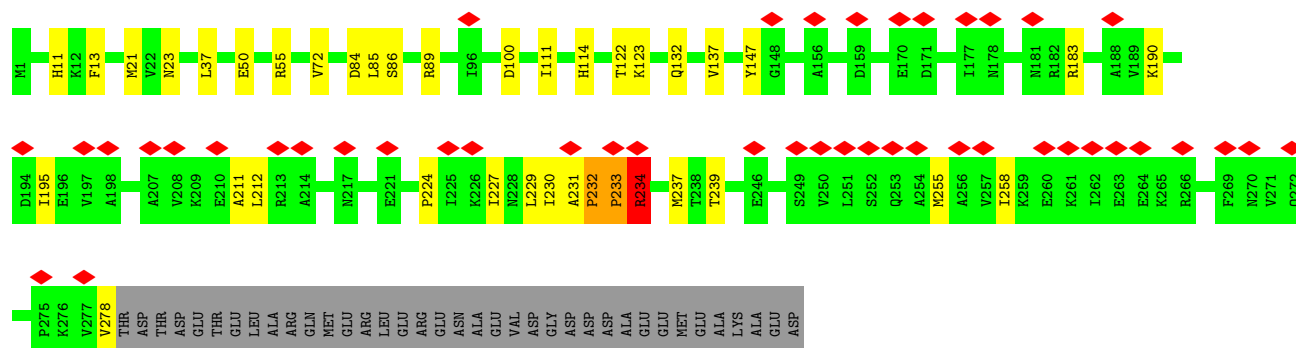
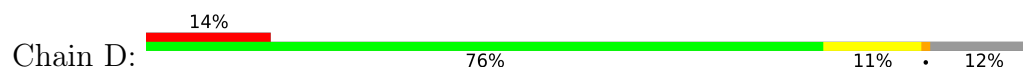




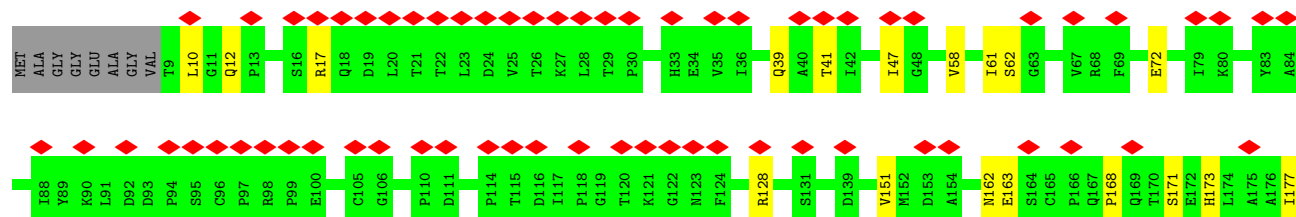
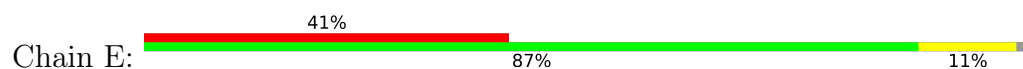
• Molecule 8: Eukaryotic translation initiation factor 3 subunit M

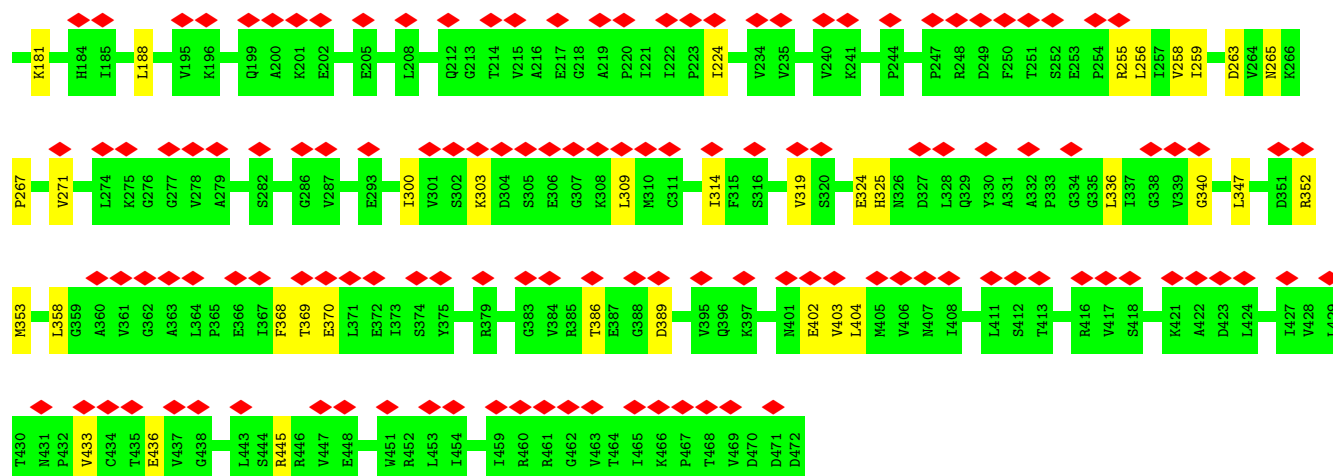


• Molecule 9: Eukaryotic translation initiation factor 2 subunit 1

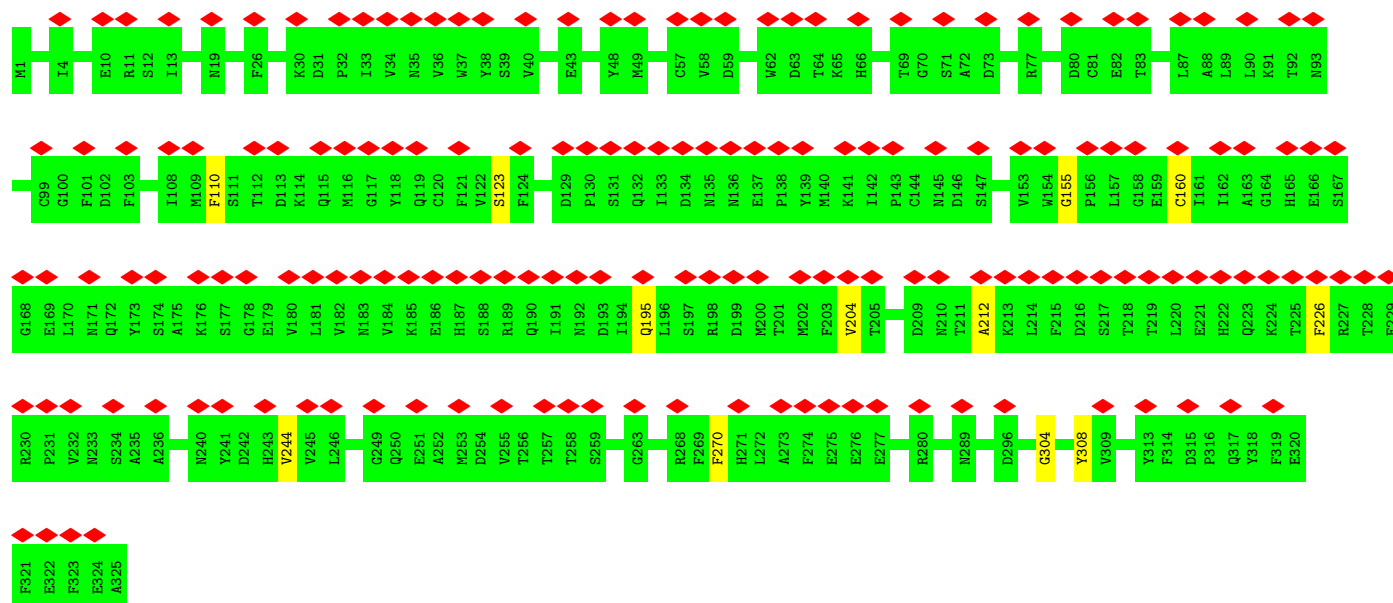


• Molecule 10: Eukaryotic translation initiation factor 2 subunit 3

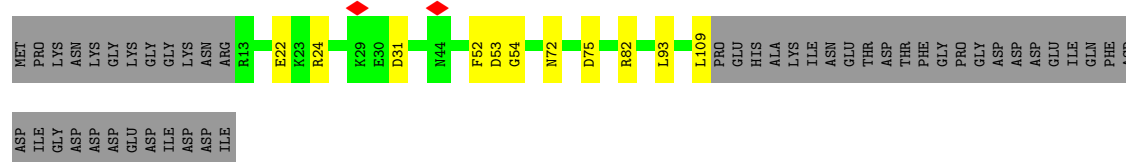




• Molecule 11: Eukaryotic translation initiation factor 3 subunit I

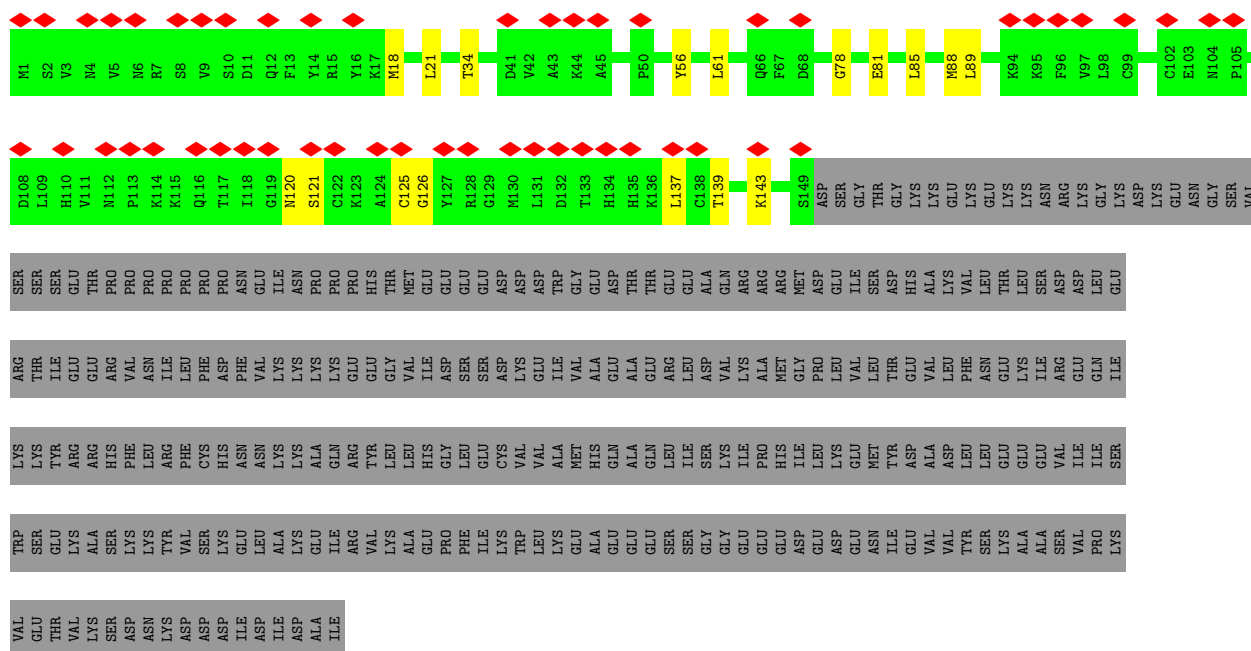


• Molecule 12: Eukaryotic translation initiation factor 1A, X-chromosomal

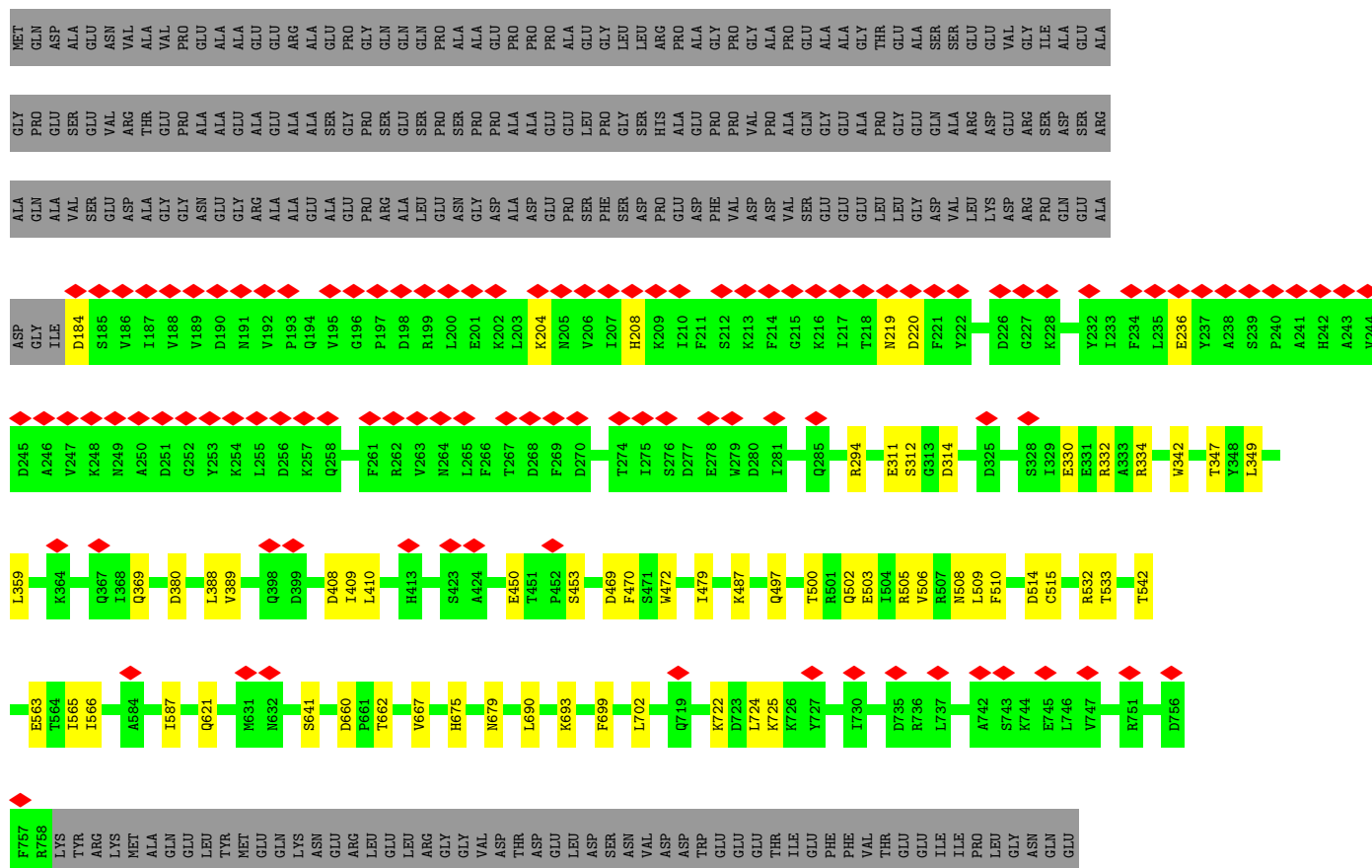


• Molecule 13: Eukaryotic translation initiation factor 5

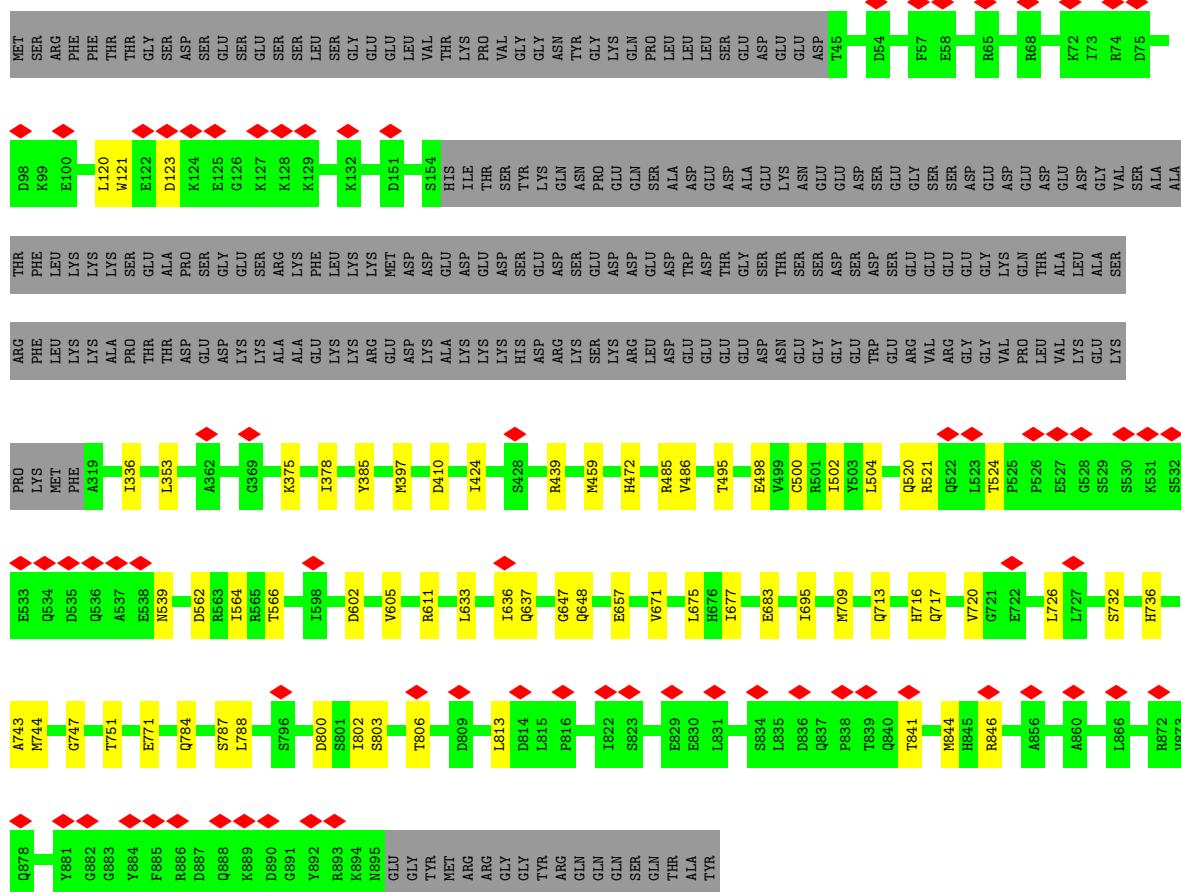




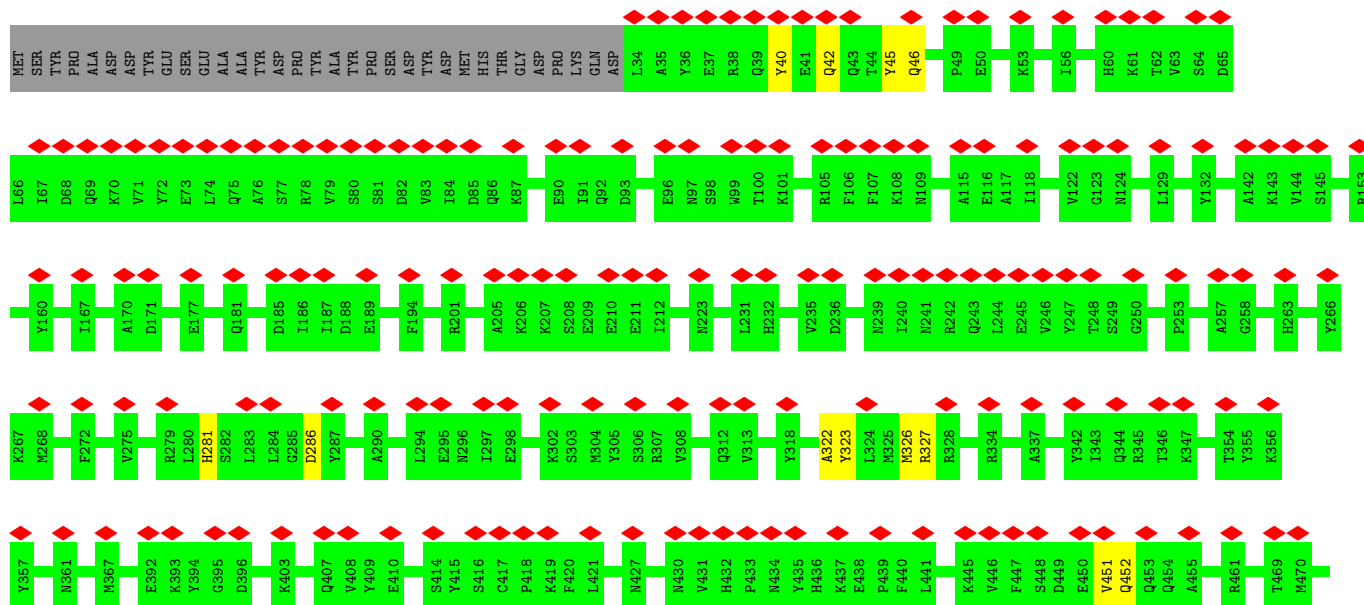
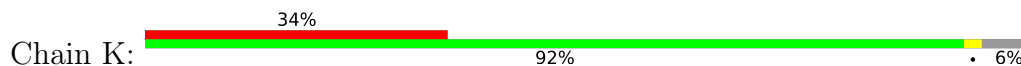
• Molecule 14: Eukaryotic translation initiation factor 3 subunit B

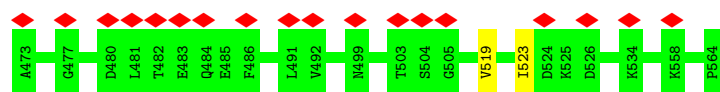


• Molecule 15: Eukaryotic translation initiation factor 3 subunit C



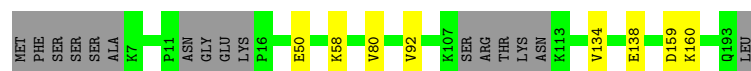
• Molecule 16: Eukaryotic translation initiation factor 3 subunit L





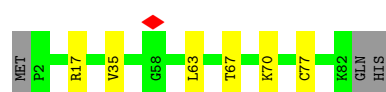
- Molecule 17: 40S ribosomal protein S7

Chain L: 88% 8%



- Molecule 18: 40S ribosomal protein S27

Chain M: 89% 7%



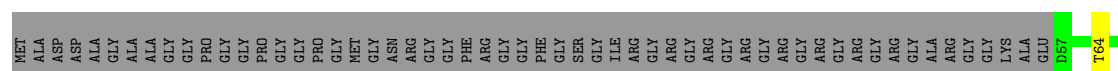
- Molecule 19: 40S ribosomal protein S21

Chain N: 84% 13%



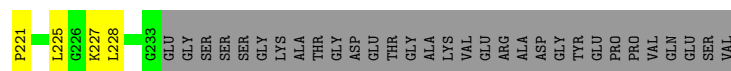
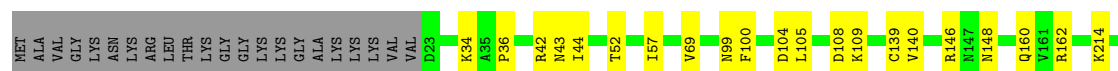
- Molecule 20: 40S ribosomal protein S2

Chain O: 68% 7% 25%



- Molecule 21: 40S ribosomal protein S3a

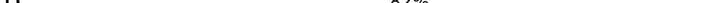
Chain P: 70% 9% 20%



- Molecule 22: 40S ribosomal protein SA

Chain Q: 67% 5% 27%

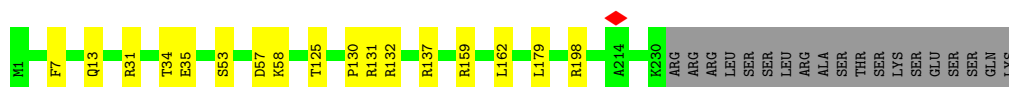
- Molecule 23: 40S ribosomal protein S26

Chain R:  82% 14%



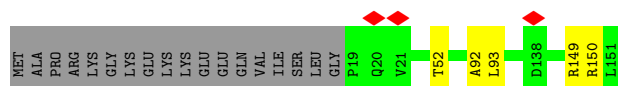
- Molecule 24: 40S ribosomal protein S6

Chain S:  86% 7% 8%

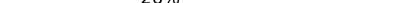


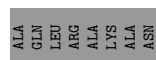
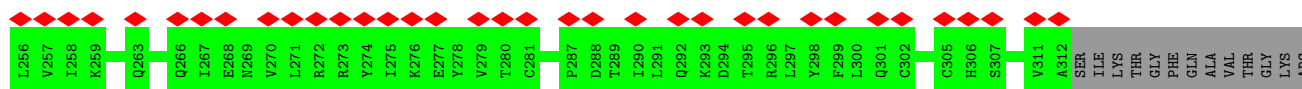
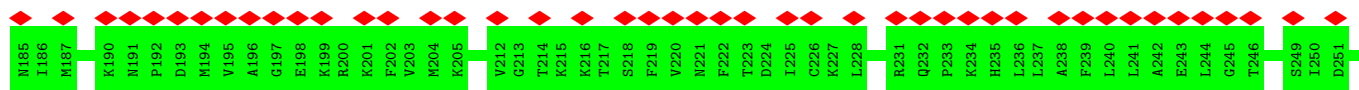
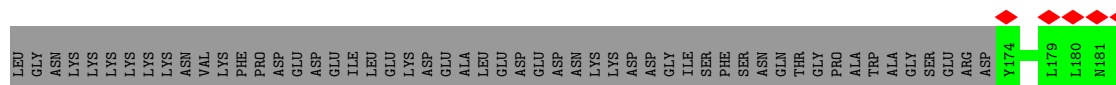
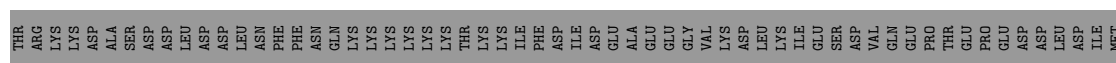
- Molecule 25: 40S ribosomal protein S14

Chain T:  85% 12%



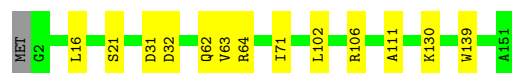
- Molecule 26: Eukaryotic translation initiation factor 2 subunit 2

Chain U: 



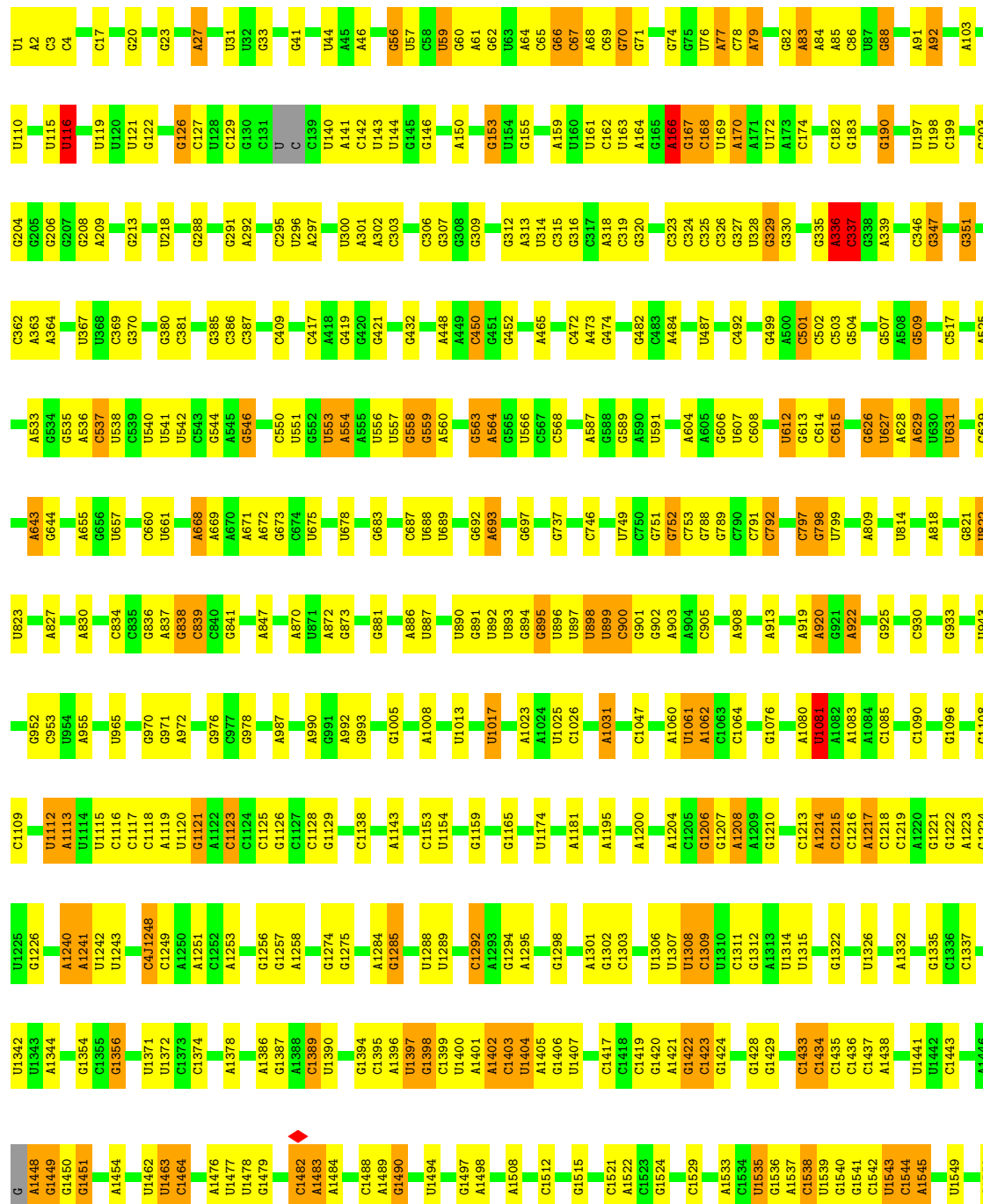
• Molecule 27: 40S ribosomal protein S13

Chain V:  91% 9%

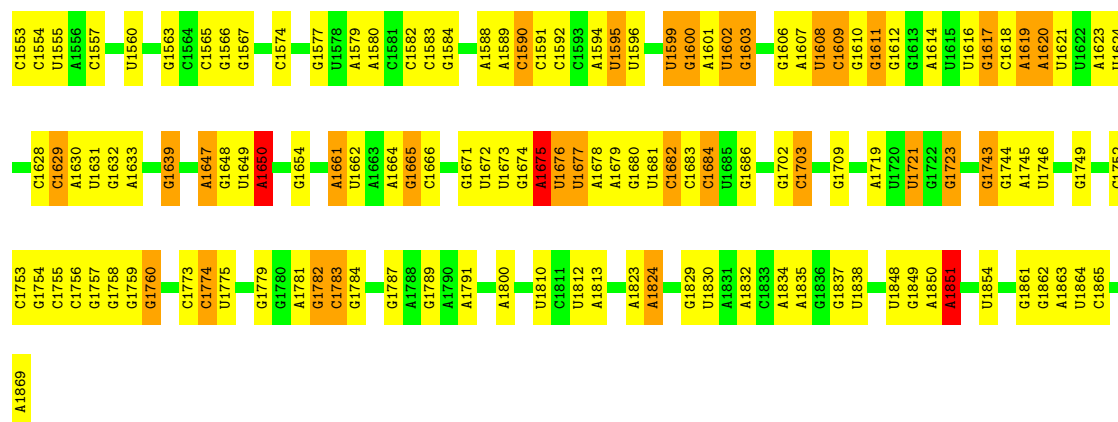


• Molecule 28: 18S rRNA

Chain W:  65% 27% 7%

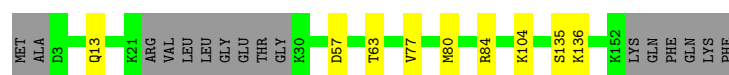






- Molecule 29: 40S ribosomal protein S11

Chain X: 84% 6% 10%



- Molecule 30: 40S ribosomal protein S4, X isoform

Chain Y: 90% 8% 2%



- Molecule 31: 40S ribosomal protein S9

Chain Z: 88% 9% 3%



- Molecule 32: 40S ribosomal protein S23

Chain a: 91% 7% 2%



- Molecule 33: 40S ribosomal protein S30

Chain b: 78% 20% 2%



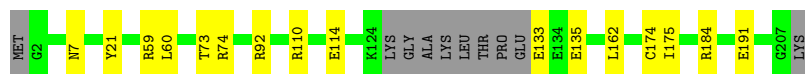
- Molecule 34: 40S ribosomal protein S15a

Chain c:  92% 7%



- Molecule 35: 40S ribosomal protein S8

Chain d:  88% 8% 5%



- Molecule 36: 40S ribosomal protein S24

Chain e:  86% 8% 6%



- Molecule 37: 40S ribosomal protein S5

Chain f:  83% 7% 10%



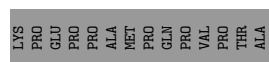
- Molecule 38: 40S ribosomal protein S16

Chain g:  84% 13%



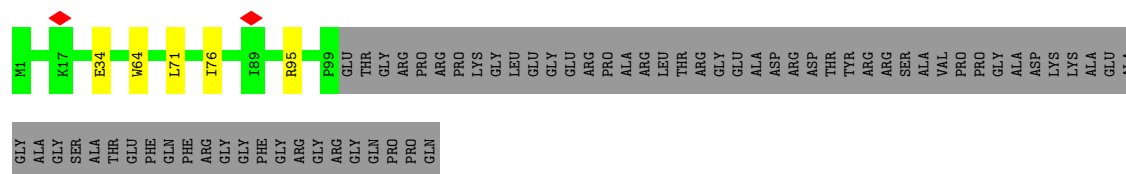
- Molecule 39: 40S ribosomal protein S3

Chain h:  81% 12% 7%



- Molecule 40: 40S ribosomal protein S10

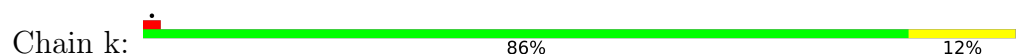
Chain i:  57% 40%



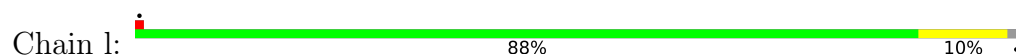
- Molecule 41: 40S ribosomal protein S15



- Molecule 42: Receptor of activated protein C kinase 1



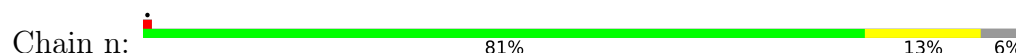
- Molecule 43: 40S ribosomal protein S19



- Molecule 44: 40S ribosomal protein S25



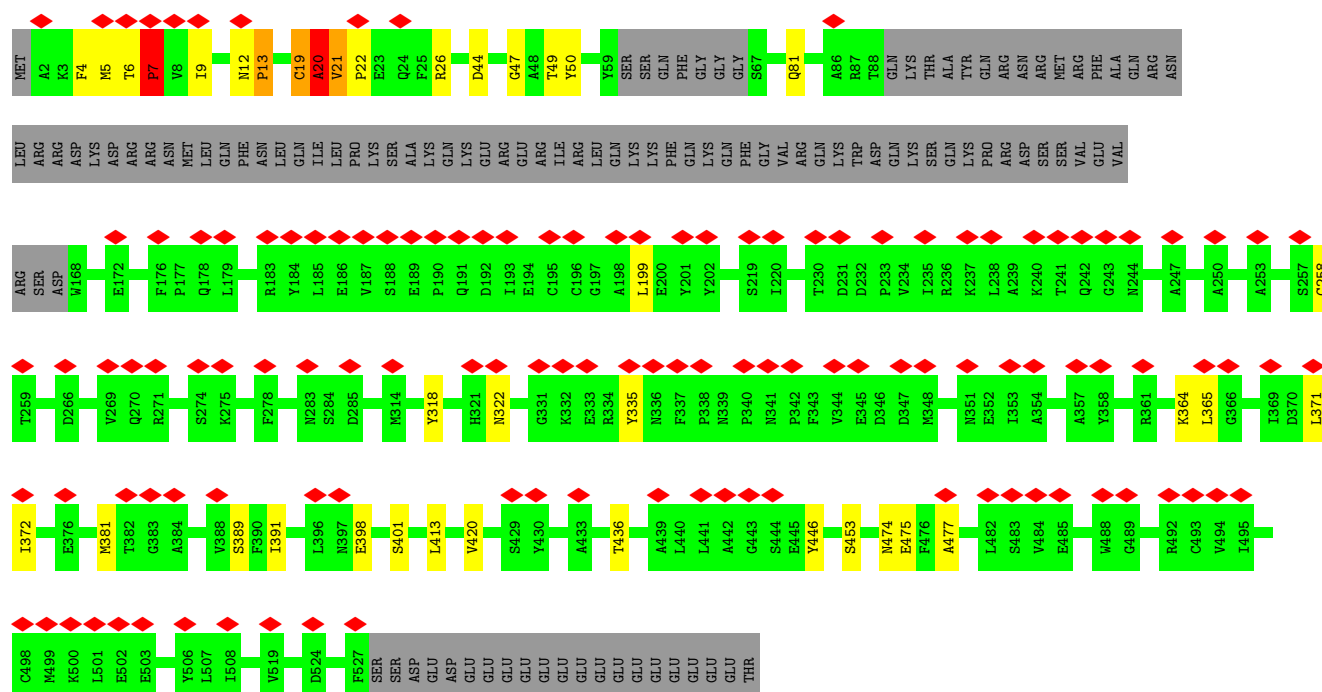
- Molecule 45: Small ribosomal subunit protein uS13





|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |      |      |      |      |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|
| Met | ALA | PHE | LYS | ASP | THR | GLY | LYS | THR | PRO | VAL | GLU | PRO | GLU | VAL | ALA | I17 | R21 | N28 | S31 | K34 | K46 | P53 | L88 | T101 | T102 | S103 | E107 | A119 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|

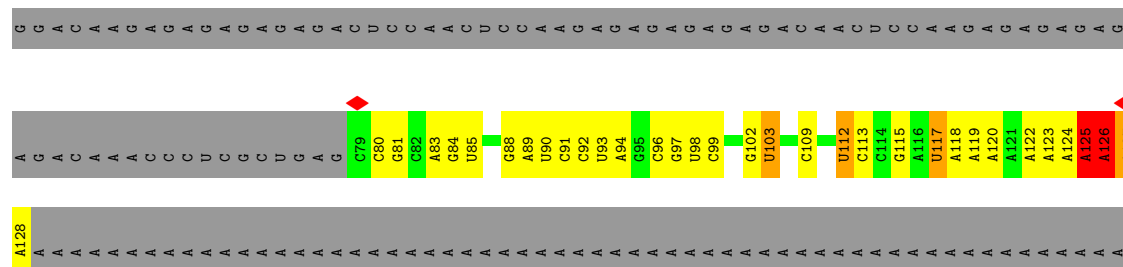
Chain x: 



Chain y: 

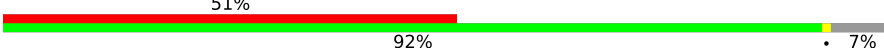


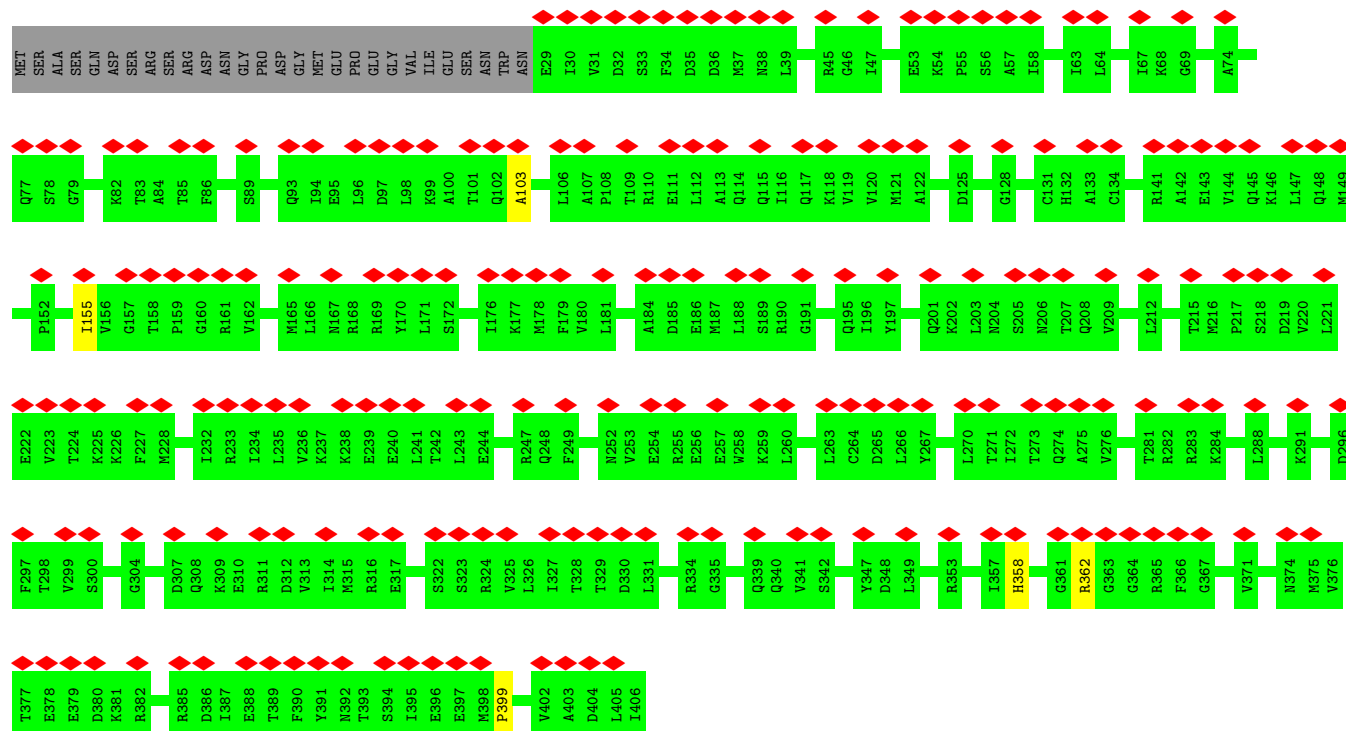
Chain z:  8% 13% .. 76%



A A A A A A A A A A A A A A A A A

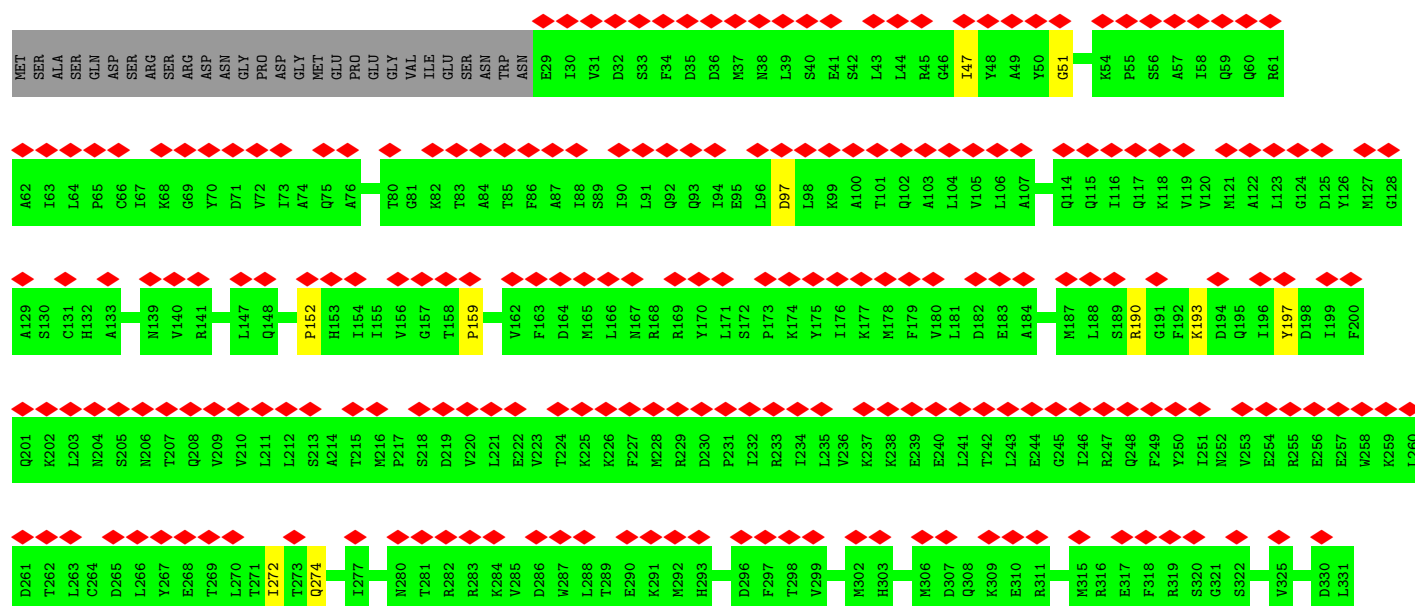
• Molecule 55: Eukaryotic initiation factor 4A-I

Chain 3: 

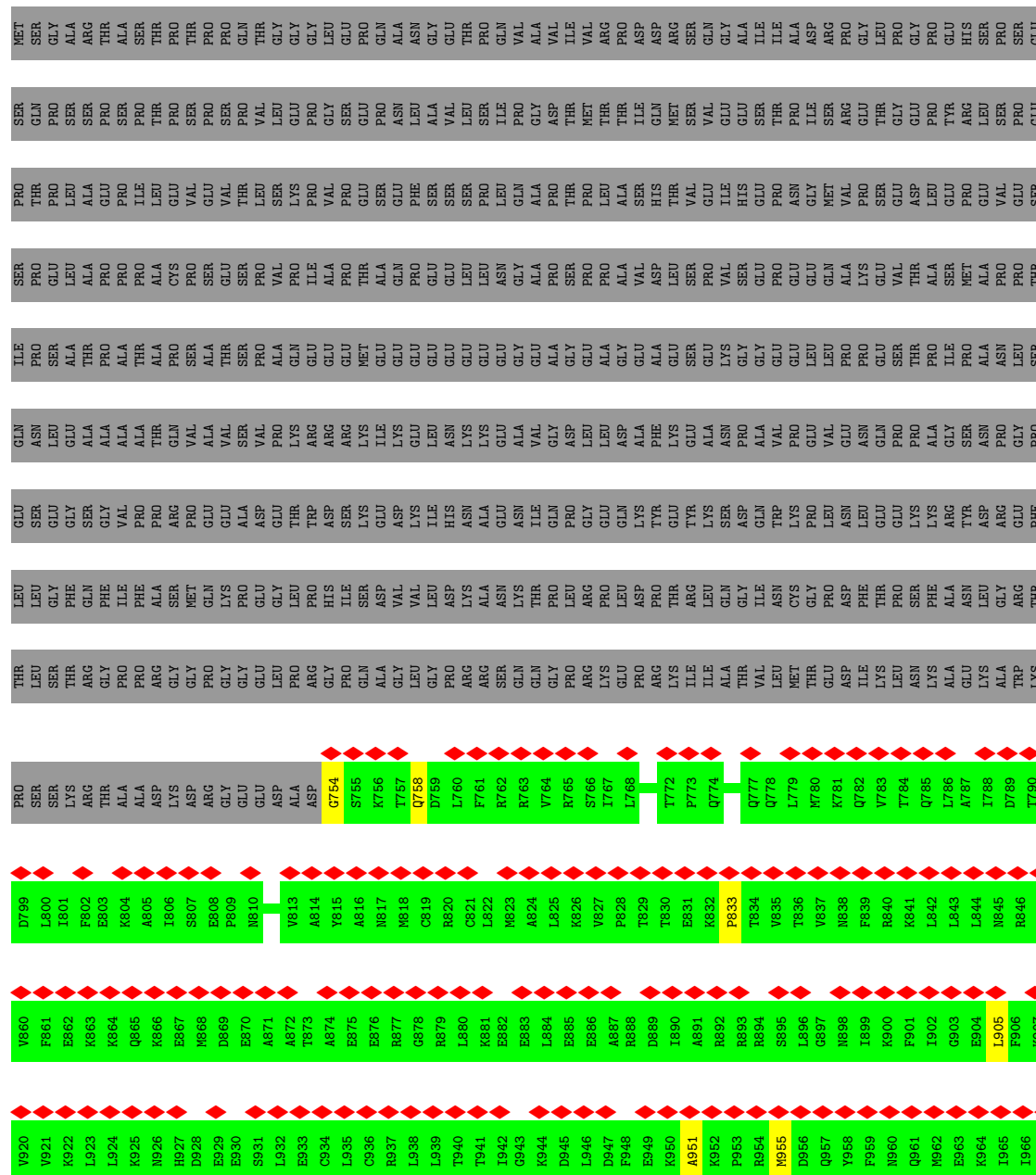


• Molecule 55: Eukaryotic initiation factor 4A-I

Chain 1: 



- Molecule 56: Eukaryotic translation initiation factor 4 gamma 1



[illegible]



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 241389                                  | 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 ( $e^-/\text{\AA}^2$ ) | 47.88                                   | Depositor |
| Minimum defocus (nm)                 | 1200                                    | Depositor |
| Maximum defocus (nm)                 | 3000                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 0.065                                   | Depositor |
| Minimum map value                    | -0.023                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.002                                   | Depositor |
| Recommended contour level            | 0.006                                   | Depositor |
| Map size ( $\text{\AA}$ )            | 423.99997, 423.99997, 423.99997         | wwPDB     |
| Map dimensions                       | 400, 400, 400                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.06, 1.06, 1.06                        | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, OMU, C4J, MA6, PSU, 5MU, 6MZ, JMH, A2M, 5MC, OMC, ZN, UR3

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   | 5     | 0.15         | 0/2174          | 0.40        | 0/3036          |
| 2   | 6     | 0.16         | 0/1329          | 0.33        | 0/1848          |
| 3   | 7     | 0.25         | 0/628           | 0.50        | 0/846           |
| 4   | 8     | 0.16         | 0/1567          | 0.35        | 0/2182          |
| 5   | 9     | 0.24         | 0/231           | 0.47        | 0/294           |
| 6   | A     | 0.22         | 0/5470          | 0.47        | 3/7444 (0.0%)   |
| 7   | B     | 0.15         | 0/1065          | 0.37        | 0/1484          |
| 8   | C     | 0.22         | 0/1807          | 0.37        | 0/2518          |
| 9   | D     | 0.28         | 0/2267          | 0.51        | 0/3056          |
| 10  | E     | 0.20         | 0/3598          | 0.42        | 0/4868          |
| 11  | F     | 0.15         | 0/1597          | 0.37        | 0/2216          |
| 12  | G     | 0.24         | 0/797           | 0.52        | 0/1061          |
| 13  | H     | 0.19         | 0/1200          | 0.41        | 0/1618          |
| 14  | I     | 0.23         | 0/4695          | 0.44        | 0/6376          |
| 15  | J     | 0.24         | 0/5288          | 0.49        | 0/7159          |
| 16  | K     | 0.25         | 0/2636          | 0.39        | 0/3676          |
| 17  | L     | 0.22         | 0/1460          | 0.46        | 0/1953          |
| 18  | M     | 0.22         | 0/644           | 0.42        | 0/864           |
| 19  | N     | 0.23         | 0/623           | 0.43        | 0/833           |
| 20  | O     | 0.24         | 0/1743          | 0.44        | 0/2354          |
| 21  | P     | 0.23         | 0/1742          | 0.44        | 0/2330          |
| 22  | Q     | 0.23         | 0/1732          | 0.42        | 0/2353          |
| 23  | R     | 0.24         | 0/805           | 0.44        | 0/1079          |
| 24  | S     | 0.22         | 0/1885          | 0.47        | 0/2510          |
| 25  | T     | 0.21         | 0/1010          | 0.45        | 0/1353          |
| 26  | U     | 0.16         | 0/688           | 0.39        | 0/958           |
| 27  | V     | 0.22         | 0/1232          | 0.41        | 0/1656          |
| 28  | W     | 0.78         | 17/40246 (0.0%) | 0.45        | 18/62715 (0.0%) |
| 29  | X     | 0.22         | 0/1186          | 0.40        | 0/1585          |
| 30  | Y     | 0.22         | 0/2077          | 0.39        | 0/2796          |
| 31  | Z     | 0.22         | 0/1502          | 0.42        | 0/2008          |
| 32  | a     | 0.23         | 0/1105          | 0.39        | 0/1476          |

| Mol | Chain | Bond lengths |                  | Bond angles |                  |
|-----|-------|--------------|------------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5          |
| 33  | b     | 0.21         | 0/380            | 0.37        | 0/496            |
| 34  | c     | 0.23         | 0/1051           | 0.40        | 0/1406           |
| 35  | d     | 0.21         | 0/1654           | 0.41        | 0/2203           |
| 36  | e     | 0.22         | 0/1032           | 0.42        | 0/1371           |
| 37  | f     | 0.20         | 0/1481           | 0.46        | 0/1988           |
| 38  | g     | 0.20         | 0/1142           | 0.45        | 0/1528           |
| 39  | h     | 0.22         | 0/1793           | 0.45        | 0/2414           |
| 40  | i     | 0.26         | 0/859            | 0.53        | 0/1159           |
| 41  | j     | 0.21         | 0/929            | 0.44        | 0/1241           |
| 42  | k     | 0.20         | 0/2493           | 0.44        | 0/3394           |
| 43  | l     | 0.20         | 0/1123           | 0.44        | 0/1504           |
| 44  | m     | 0.24         | 0/529            | 0.51        | 0/712            |
| 45  | n     | 0.21         | 0/1194           | 0.49        | 0/1599           |
| 46  | o     | 0.20         | 0/429            | 0.41        | 0/568            |
| 47  | p     | 0.24         | 0/444            | 0.45        | 0/588            |
| 48  | q     | 0.22         | 0/960            | 0.49        | 0/1286           |
| 49  | s     | 0.21         | 0/500            | 0.47        | 0/669            |
| 50  | v     | 0.23         | 0/1077           | 0.48        | 0/1444           |
| 51  | w     | 0.19         | 0/827            | 0.46        | 0/1110           |
| 52  | x     | 0.39         | 1/2963 (0.0%)    | 1.78        | 4/4050 (0.1%)    |
| 53  | y     | 0.18         | 0/1795           | 0.39        | 0/2798           |
| 54  | z     | 0.28         | 0/944            | 0.53        | 3/1463 (0.2%)    |
| 55  | 1     | 0.17         | 0/1833           | 0.39        | 0/2552           |
| 55  | 3     | 0.15         | 0/1868           | 0.37        | 0/2601           |
| 56  | 2     | 0.16         | 0/1177           | 0.32        | 0/1642           |
| All | All   | 0.47         | 18/126506 (0.0%) | 0.51        | 28/180291 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 6   | A     | 0                   | 1                   |
| 9   | D     | 0                   | 1                   |
| 28  | W     | 1                   | 0                   |
| 32  | a     | 0                   | 1                   |
| 39  | h     | 0                   | 1                   |
| 42  | k     | 0                   | 1                   |
| 52  | x     | 0                   | 1                   |
| All | All   | 1                   | 6                   |

All (18) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 28  | W     | 1675 | A    | C6-N1  | 56.51  | 2.48        | 1.35     |
| 28  | W     | 1675 | A    | C2-N3  | 56.33  | 2.46        | 1.33     |
| 28  | W     | 1675 | A    | N3-C4  | 54.78  | 2.44        | 1.34     |
| 28  | W     | 1675 | A    | N1-C2  | 54.24  | 2.42        | 1.34     |
| 28  | W     | 1675 | A    | C5-C6  | 49.15  | 2.39        | 1.41     |
| 28  | W     | 1650 | A    | N9-C4  | 45.36  | 2.28        | 1.37     |
| 28  | W     | 1675 | A    | C5-C4  | 44.35  | 2.27        | 1.38     |
| 28  | W     | 1650 | A    | C8-N7  | 36.92  | 2.05        | 1.31     |
| 28  | W     | 1650 | A    | N9-C8  | -24.46 | 0.88        | 1.37     |
| 52  | x     | 20   | ALA  | C-N    | 14.26  | 1.49        | 1.33     |
| 28  | W     | 1650 | A    | N7-C5  | 13.77  | 1.66        | 1.39     |
| 28  | W     | 1650 | A    | C1'-N9 | 12.46  | 1.66        | 1.48     |
| 28  | W     | 1650 | A    | C5-C4  | -10.53 | 1.17        | 1.38     |
| 28  | W     | 1678 | A2M  | O3'-P  | 6.06   | 1.62        | 1.56     |
| 28  | W     | 484  | A2M  | O3'-P  | 5.53   | 1.61        | 1.56     |
| 28  | W     | 668  | A2M  | O3'-P  | 5.30   | 1.61        | 1.56     |
| 28  | W     | 27   | A2M  | O3'-P  | 5.10   | 1.61        | 1.56     |
| 28  | W     | 159  | A2M  | O3'-P  | 5.02   | 1.61        | 1.56     |

All (28) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 52  | x     | 20   | ALA  | O-C-N     | -66.50 | 23.96       | 122.39   |
| 52  | x     | 20   | ALA  | CA-C-N    | -60.76 | 9.73        | 122.13   |
| 52  | x     | 20   | ALA  | C-N-CA    | -60.76 | 9.73        | 122.13   |
| 28  | W     | 1650 | A    | N7-C8-N9  | -25.84 | 36.27       | 113.80   |
| 28  | W     | 1650 | A    | C4-C5-N7  | -25.75 | 33.45       | 110.70   |
| 28  | W     | 1650 | A    | C8-N9-C1' | -19.70 | 68.59       | 127.70   |
| 28  | W     | 1650 | A    | C5-N7-C8  | 14.99  | 148.88      | 103.90   |
| 28  | W     | 337  | C    | P-O3'-C3' | -10.43 | 104.56      | 120.20   |
| 28  | W     | 1650 | A    | C8-N9-C4  | 9.90   | 135.49      | 105.80   |
| 28  | W     | 1650 | A    | C4-N9-C1' | 9.83   | 155.79      | 126.30   |
| 28  | W     | 1650 | A    | C6-C5-N7  | 8.94   | 159.11      | 132.30   |
| 28  | W     | 1449 | G    | P-O3'-C3' | -8.90  | 106.86      | 120.20   |
| 28  | W     | 1448 | A    | P-O3'-C3' | -8.53  | 107.41      | 120.20   |
| 54  | z     | 127  | A    | P-O3'-C3' | -7.74  | 108.58      | 120.20   |
| 54  | z     | 126  | A    | P-O3'-C3' | -7.23  | 109.35      | 120.20   |
| 28  | W     | 336  | A    | P-O3'-C3' | -7.01  | 109.69      | 120.20   |
| 28  | W     | 1650 | A    | N3-C4-C5  | -6.39  | 107.63      | 126.80   |
| 54  | z     | 125  | A    | P-O3'-C3' | -6.38  | 110.63      | 120.20   |
| 28  | W     | 1675 | A    | N3-C4-N9  | 5.94   | 145.23      | 127.40   |
| 28  | W     | 1650 | A    | N9-C4-C5  | 5.86   | 123.37      | 105.80   |
| 28  | W     | 1650 | A    | C2-N3-C4  | 5.82   | 128.07      | 110.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 28  | W     | 1451 | G    | P-O3'-C3'  | -5.68 | 111.69      | 120.20   |
| 6   | A     | 284  | TRP  | N-CA-C     | -5.41 | 106.81      | 113.41   |
| 6   | A     | 285  | LYS  | N-CA-C     | -5.33 | 106.61      | 113.01   |
| 28  | W     | 1650 | A    | N9-C1'-C2' | 5.21  | 119.81      | 112.00   |
| 28  | W     | 1675 | A    | N1-C2-N3   | -5.19 | 113.74      | 129.30   |
| 6   | A     | 662  | GLU  | N-CA-C     | -5.12 | 99.90       | 110.80   |
| 52  | x     | 7    | PRO  | N-CA-CB    | -5.04 | 97.96       | 103.25   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 28  | W     | 1219 | JMH  | C2'  |

All (6) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 6   | A     | 662 | GLU  | Peptide   |
| 9   | D     | 234 | ARG  | Sidechain |
| 32  | a     | 60  | LYS  | Peptide   |
| 39  | h     | 161 | GLY  | Peptide   |
| 42  | k     | 4   | GLN  | Peptide   |
| 52  | x     | 20  | ALA  | Peptide   |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 5     | 2175  | 0        | 954      | 9       | 0            |
| 2   | 6     | 1330  | 0        | 591      | 2       | 0            |
| 3   | 7     | 616   | 0        | 600      | 5       | 0            |
| 4   | 8     | 1569  | 0        | 674      | 7       | 0            |
| 5   | 9     | 230   | 0        | 276      | 2       | 0            |
| 6   | A     | 5386  | 0        | 4899     | 52      | 0            |
| 7   | B     | 1066  | 0        | 481      | 3       | 0            |
| 8   | C     | 1809  | 0        | 810      | 3       | 0            |
| 9   | D     | 2234  | 0        | 2288     | 29      | 0            |
| 10  | E     | 3540  | 0        | 3690     | 35      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 11  | F     | 1598  | 0        | 723      | 6       | 0            |
| 12  | G     | 789   | 0        | 806      | 8       | 0            |
| 13  | H     | 1176  | 0        | 1182     | 10      | 0            |
| 14  | I     | 4569  | 0        | 4316     | 35      | 0            |
| 15  | J     | 5207  | 0        | 4893     | 39      | 0            |
| 16  | K     | 2637  | 0        | 1135     | 7       | 0            |
| 17  | L     | 1439  | 0        | 1533     | 5       | 0            |
| 18  | M     | 631   | 0        | 657      | 5       | 0            |
| 19  | N     | 617   | 0        | 622      | 7       | 0            |
| 20  | O     | 1707  | 0        | 1794     | 13      | 0            |
| 21  | P     | 1715  | 0        | 1785     | 17      | 0            |
| 22  | Q     | 1695  | 0        | 1696     | 9       | 0            |
| 23  | R     | 792   | 0        | 843      | 4       | 0            |
| 24  | S     | 1862  | 0        | 2018     | 15      | 0            |
| 25  | T     | 997   | 0        | 1021     | 4       | 0            |
| 26  | U     | 689   | 0        | 290      | 0       | 0            |
| 27  | V     | 1208  | 0        | 1294     | 9       | 0            |
| 28  | W     | 36639 | 0        | 18516    | 237     | 0            |
| 29  | X     | 1166  | 0        | 1233     | 5       | 0            |
| 30  | Y     | 2035  | 0        | 2138     | 15      | 0            |
| 31  | Z     | 1477  | 0        | 1589     | 5       | 0            |
| 32  | a     | 1087  | 0        | 1154     | 7       | 0            |
| 33  | b     | 378   | 0        | 417      | 1       | 0            |
| 34  | c     | 1034  | 0        | 1080     | 6       | 0            |
| 35  | d     | 1627  | 0        | 1706     | 15      | 0            |
| 36  | e     | 1015  | 0        | 1086     | 6       | 0            |
| 37  | f     | 1461  | 0        | 1511     | 10      | 0            |
| 38  | g     | 1124  | 0        | 1193     | 13      | 0            |
| 39  | h     | 1765  | 0        | 1865     | 20      | 0            |
| 40  | i     | 834   | 0        | 861      | 4       | 0            |
| 41  | j     | 913   | 0        | 952      | 9       | 0            |
| 42  | k     | 2436  | 0        | 2393     | 27      | 0            |
| 43  | l     | 1105  | 0        | 1138     | 9       | 0            |
| 44  | m     | 523   | 0        | 573      | 7       | 0            |
| 45  | n     | 1176  | 0        | 1233     | 15      | 0            |
| 46  | o     | 419   | 0        | 415      | 6       | 0            |
| 47  | p     | 435   | 0        | 434      | 5       | 0            |
| 48  | q     | 950   | 0        | 987      | 7       | 0            |
| 49  | s     | 498   | 0        | 525      | 3       | 0            |
| 50  | v     | 1064  | 0        | 1117     | 8       | 0            |
| 51  | w     | 817   | 0        | 882      | 6       | 0            |
| 52  | x     | 2920  | 0        | 2231     | 30      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 53  | y     | 1604   | 0        | 816      | 15      | 0            |
| 54  | z     | 853    | 0        | 429      | 5       | 0            |
| 55  | 1     | 1834   | 0        | 821      | 5       | 0            |
| 55  | 3     | 1869   | 0        | 838      | 2       | 0            |
| 56  | 2     | 1178   | 0        | 511      | 3       | 0            |
| 57  | R     | 1      | 0        | 0        | 0       | 0            |
| 57  | p     | 1      | 0        | 0        | 0       | 0            |
| 58  | T     | 2      | 0        | 0        | 0       | 0            |
| 58  | W     | 86     | 0        | 0        | 0       | 0            |
| 58  | f     | 1      | 0        | 0        | 0       | 0            |
| All | All   | 121610 | 0        | 92515    | 727     | 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 3.

All (727) 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) |
|-----------------|------------------|--------------------------|-------------------|
| 28:W:1675:A:C5  | 28:W:1675:A:C4   | 2.27                     | 1.22              |
| 1:5:12:HIS:HA   | 52:x:9:ILE:HA    | 1.16                     | 1.11              |
| 28:W:1675:A:C5  | 28:W:1675:A:C6   | 2.39                     | 1.10              |
| 9:D:231:ALA:HA  | 10:E:267:PRO:HB3 | 1.40                     | 1.04              |
| 1:5:12:HIS:CA   | 52:x:9:ILE:HA    | 1.99                     | 0.93              |
| 1:5:12:HIS:HA   | 52:x:9:ILE:CA    | 2.03                     | 0.89              |
| 28:W:1650:A:N9  | 28:W:1675:A:C2   | 2.42                     | 0.88              |
| 28:W:1675:A:C2  | 28:W:1675:A:N1   | 2.42                     | 0.87              |
| 28:W:1675:A:C4  | 28:W:1675:A:N3   | 2.44                     | 0.86              |
| 28:W:288:G:C2   | 28:W:296:U:O2    | 2.28                     | 0.86              |
| 28:W:1650:A:C8  | 28:W:1675:A:C6   | 2.64                     | 0.85              |
| 28:W:1675:A:C2  | 28:W:1675:A:N3   | 2.46                     | 0.84              |
| 28:W:1650:A:N9  | 28:W:1675:A:N3   | 2.25                     | 0.84              |
| 28:W:92:A:OP2   | 30:Y:3:ARG:NH2   | 2.11                     | 0.84              |
| 28:W:1709:G:H1  | 28:W:1824:A:N6   | 1.77                     | 0.83              |
| 28:W:1404:U:O2' | 28:W:1405:A:O4'  | 1.96                     | 0.83              |
| 28:W:1675:A:C6  | 28:W:1675:A:N1   | 2.48                     | 0.82              |
| 9:D:230:ILE:HB  | 9:D:234:ARG:HB3  | 1.62                     | 0.81              |
| 28:W:56:G:H1    | 28:W:88:G:H22    | 1.26                     | 0.81              |
| 28:W:1387:G:OP2 | 28:W:1389:C:N4   | 2.13                     | 0.81              |
| 28:W:1650:A:N7  | 28:W:1675:A:N1   | 2.28                     | 0.80              |
| 28:W:1650:A:N7  | 28:W:1675:A:C2   | 2.49                     | 0.80              |
| 28:W:140:U:O2'  | 28:W:143:U:OP1   | 1.99                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 15:J:637:GLN:NE2 | 15:J:683:GLU:OE1 | 2.15                     | 0.80              |
| 28:W:1650:A:N9   | 28:W:1675:A:C4   | 2.50                     | 0.80              |
| 28:W:1650:A:N7   | 28:W:1675:A:C6   | 2.50                     | 0.79              |
| 28:W:1650:A:N7   | 28:W:1675:A:C5   | 2.51                     | 0.79              |
| 53:y:17:G:O2'    | 53:y:59:A:N1     | 2.16                     | 0.78              |
| 6:A:659:GLU:O    | 6:A:662:GLU:O    | 2.02                     | 0.77              |
| 21:P:148:ASN:O   | 28:W:1123:C:O2'  | 2.03                     | 0.77              |
| 39:h:196:GLY:O   | 39:h:201:LYS:NZ  | 2.18                     | 0.77              |
| 18:M:17:ARG:NH1  | 28:W:1128:C:OP1  | 2.18                     | 0.77              |
| 28:W:150:A:H62   | 28:W:168:C:N4    | 1.82                     | 0.77              |
| 15:J:521:ARG:NH2 | 15:J:539:ASN:O   | 2.18                     | 0.76              |
| 28:W:1650:A:C4   | 28:W:1675:A:C2   | 2.73                     | 0.76              |
| 52:x:20:ALA:HB3  | 52:x:22:PRO:HD3  | 1.67                     | 0.76              |
| 28:W:64:A:N6     | 28:W:84:A:N7     | 2.33                     | 0.76              |
| 15:J:495:THR:OG1 | 15:J:498:GLU:OE1 | 2.03                     | 0.76              |
| 28:W:1650:A:C8   | 28:W:1675:A:N1   | 2.54                     | 0.76              |
| 28:W:432:G:O2'   | 35:d:21:TYR:OH   | 2.03                     | 0.75              |
| 28:W:1650:A:C4   | 28:W:1675:A:C4   | 2.74                     | 0.75              |
| 28:W:1664:A:O2'  | 28:W:1666:C:N4   | 2.19                     | 0.75              |
| 28:W:1356:G:N2   | 28:W:1356:G:OP2  | 2.20                     | 0.75              |
| 28:W:1285:G:N7   | 48:q:107:SER:OG  | 2.20                     | 0.74              |
| 52:x:19:CYS:O    | 52:x:21:VAL:HB   | 1.86                     | 0.74              |
| 28:W:1488:C:O2'  | 28:W:1490:G:OP2  | 2.04                     | 0.74              |
| 14:I:660:ASP:OD2 | 14:I:662:THR:OG1 | 2.05                     | 0.74              |
| 28:W:1618:C:O2'  | 28:W:1619:A:O4'  | 2.05                     | 0.74              |
| 28:W:1650:A:C4   | 28:W:1675:A:N3   | 2.56                     | 0.74              |
| 6:A:297:HIS:O    | 6:A:301:HIS:ND1  | 2.20                     | 0.74              |
| 24:S:131:ARG:NH1 | 28:W:167:G:O2'   | 2.21                     | 0.74              |
| 52:x:20:ALA:HB3  | 52:x:22:PRO:CD   | 2.18                     | 0.74              |
| 21:P:221:PRO:O   | 21:P:227:LYS:NZ  | 2.20                     | 0.74              |
| 28:W:746:C:N4    | 28:W:797:C:O2    | 2.20                     | 0.74              |
| 28:W:1709:G:N1   | 28:W:1824:A:N6   | 2.36                     | 0.74              |
| 28:W:1221:G:O2'  | 28:W:1677:U:O4'  | 2.06                     | 0.73              |
| 28:W:1650:A:C5   | 28:W:1675:A:C6   | 2.75                     | 0.73              |
| 23:R:41:ILE:O    | 54:z:96:C:O2'    | 2.05                     | 0.73              |
| 14:I:497:GLN:OE1 | 14:I:500:THR:OG1 | 2.05                     | 0.73              |
| 28:W:1544:C:N3   | 28:W:1589:A:N7   | 2.36                     | 0.73              |
| 28:W:1650:A:N7   | 28:W:1675:A:C4   | 2.56                     | 0.73              |
| 49:s:37:ASP:OD2  | 49:s:40:ARG:NH1  | 2.22                     | 0.72              |
| 9:D:114:HIS:ND1  | 53:y:55:C:OP1    | 2.23                     | 0.72              |
| 28:W:895:G:N2    | 28:W:898:U:OP2   | 2.23                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:S:130:PRO:O    | 24:S:132:ARG:NH1  | 2.22                     | 0.72              |
| 28:W:1602:U:O2'   | 28:W:1603:G:N2    | 2.19                     | 0.71              |
| 28:W:920:A:O2'    | 28:W:922:A:OP1    | 2.08                     | 0.71              |
| 28:W:1512:C:O2'   | 46:o:7:TYR:O      | 2.08                     | 0.71              |
| 28:W:1617:G:OP1   | 28:W:1661:A:O2'   | 2.05                     | 0.71              |
| 28:W:64:A:N7      | 28:W:83:A:N6      | 2.37                     | 0.71              |
| 28:W:507:G:OP2    | 36:e:104:ARG:NH2  | 2.24                     | 0.71              |
| 28:W:1535:U:OP2   | 37:f:168:THR:OG1  | 2.06                     | 0.71              |
| 29:X:104:LYS:O    | 32:a:11:ARG:NH2   | 2.24                     | 0.71              |
| 3:7:241:ILE:HD12  | 3:7:297:ILE:HD11  | 1.73                     | 0.71              |
| 20:O:77:SER:N     | 20:O:80:GLU:OE2   | 2.23                     | 0.71              |
| 28:W:3:C:O2       | 31:Z:18:ARG:NH2   | 2.24                     | 0.71              |
| 28:W:1616:U:O2'   | 28:W:1617:G:O4'   | 2.09                     | 0.70              |
| 28:W:1673:U:O2'   | 37:f:84:GLY:O     | 2.05                     | 0.70              |
| 28:W:288:G:N2     | 28:W:296:U:O2     | 2.24                     | 0.70              |
| 41:j:103:ASN:OD1  | 41:j:120:SER:OG   | 2.05                     | 0.70              |
| 28:W:346:C:O2'    | 30:Y:6:LYS:N      | 2.23                     | 0.70              |
| 7:B:174:MET:O     | 7:B:178:GLY:N     | 2.25                     | 0.70              |
| 24:S:198:ARG:NH1  | 28:W:126:G:OP1    | 2.25                     | 0.70              |
| 20:O:200:ARG:O    | 31:Z:54:ARG:NH2   | 2.25                     | 0.70              |
| 28:W:1522:A:OP1   | 45:n:144:ARG:NH1  | 2.25                     | 0.70              |
| 24:S:53:SER:OG    | 28:W:166:A2M:OP1  | 2.10                     | 0.70              |
| 28:W:1538:C:N3    | 28:W:1595:U:O4    | 2.25                     | 0.70              |
| 10:E:256:LEU:HD23 | 10:E:358:LEU:HD22 | 1.74                     | 0.69              |
| 27:V:64:ARG:NH2   | 28:W:919:A:OP2    | 2.25                     | 0.69              |
| 28:W:150:A:N6     | 28:W:168:C:H42    | 1.90                     | 0.69              |
| 50:v:70:SER:OG    | 50:v:75:GLU:OE2   | 2.09                     | 0.69              |
| 14:I:219:ASN:ND2  | 14:I:236:GLU:OE1  | 2.24                     | 0.69              |
| 28:W:450:C:OP1    | 30:Y:3:ARG:NH2    | 2.26                     | 0.69              |
| 28:W:432:G:HO2'   | 35:d:21:TYR:HH    | 1.36                     | 0.69              |
| 28:W:1650:A:C8    | 28:W:1675:A:C5    | 2.80                     | 0.69              |
| 9:D:100:ASP:OD2   | 9:D:147:TYR:OH    | 2.10                     | 0.69              |
| 28:W:1647:A:OP1   | 38:g:138:ARG:NH1  | 2.25                     | 0.69              |
| 28:W:150:A:H62    | 28:W:168:C:H42    | 1.39                     | 0.69              |
| 38:g:9:SER:OG     | 38:g:25:CYS:O     | 2.09                     | 0.68              |
| 19:N:76:ASP:OD1   | 19:N:77:GLY:N     | 2.25                     | 0.68              |
| 28:W:1824:A:OP1   | 32:a:61:GLN:NE2   | 2.26                     | 0.68              |
| 28:W:1309:C:O2'   | 47:p:131:PHE:O    | 2.04                     | 0.68              |
| 50:v:76:GLU:OE1   | 50:v:80:ARG:NH2   | 2.26                     | 0.68              |
| 28:W:1214:A:N6    | 28:W:1682:C:O2    | 2.26                     | 0.68              |
| 12:G:72:ASN:ND2   | 12:G:75:ASP:OD2   | 2.26                     | 0.68              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 14:I:502:GLN:NE2 | 14:I:503:GLU:O    | 2.26                     | 0.68              |
| 28:W:1681:U:O2'  | 28:W:1682:C:O4'   | 2.05                     | 0.68              |
| 19:N:44:GLY:O    | 22:Q:191:ARG:NH2  | 2.27                     | 0.68              |
| 21:P:162:ARG:NH2 | 28:W:1005:G:OP2   | 2.27                     | 0.68              |
| 50:v:41:ILE:HG23 | 50:v:46:LEU:HD22  | 1.76                     | 0.68              |
| 28:W:1760:G:OP1  | 28:W:1774:C:O2'   | 2.10                     | 0.67              |
| 51:w:28:ASN:ND2  | 51:w:31:SER:OG    | 2.28                     | 0.67              |
| 15:J:732:SER:O   | 15:J:736:HIS:ND1  | 2.23                     | 0.67              |
| 30:Y:199:GLU:OE1 | 30:Y:201:HIS:NE2  | 2.26                     | 0.67              |
| 28:W:336:A:H2'   | 28:W:337:C:H5'    | 1.76                     | 0.67              |
| 9:D:11:HIS:ND1   | 9:D:13:PHE:O      | 2.27                     | 0.67              |
| 28:W:303:C:O2    | 35:d:184:ARG:NH2  | 2.27                     | 0.67              |
| 28:W:541:U:OP1   | 28:W:544:G:N1     | 2.28                     | 0.67              |
| 41:j:18:ARG:N    | 45:n:90:VAL:O     | 2.28                     | 0.67              |
| 28:W:1675:A:O2'  | 28:W:1676:U:OP1   | 2.12                     | 0.67              |
| 10:E:347:LEU:O   | 10:E:352:ARG:NH1  | 2.28                     | 0.66              |
| 28:W:788:G:N2    | 28:W:789:G:O6     | 2.29                     | 0.66              |
| 37:f:71:ARG:NH2  | 37:f:148:ASN:OD1  | 2.29                     | 0.66              |
| 6:A:155:GLU:OE1  | 6:A:158:ARG:NH2   | 2.29                     | 0.66              |
| 28:W:553:U:O4    | 28:W:554:A:N6     | 2.29                     | 0.66              |
| 9:D:229:LEU:HB2  | 10:E:271:VAL:HG22 | 1.77                     | 0.66              |
| 28:W:122:G:OP1   | 30:Y:75:LYS:NZ    | 2.27                     | 0.65              |
| 52:x:19:CYS:C    | 52:x:21:VAL:HB    | 2.05                     | 0.65              |
| 14:I:294:ARG:NH1 | 14:I:347:THR:OG1  | 2.29                     | 0.65              |
| 20:O:168:GLY:N   | 20:O:179:THR:O    | 2.28                     | 0.65              |
| 45:n:15:VAL:HG12 | 45:n:68:ILE:HD11  | 1.79                     | 0.65              |
| 20:O:146:GLU:OE1 | 39:h:120:TYR:OH   | 2.14                     | 0.65              |
| 28:W:1308:U:O2'  | 28:W:1309:C:OP2   | 2.15                     | 0.65              |
| 29:X:57:ASP:OD1  | 29:X:84:ARG:NH1   | 2.30                     | 0.65              |
| 9:D:234:ARG:HH12 | 53:y:73:C:H5'     | 1.62                     | 0.65              |
| 50:v:97:GLU:N    | 50:v:97:GLU:OE2   | 2.30                     | 0.64              |
| 28:W:1543:U:O2'  | 28:W:1545:A:OP1   | 2.13                     | 0.64              |
| 28:W:1294:G:N1   | 28:W:1306:U:O4    | 2.31                     | 0.64              |
| 55:1:193:LYS:O   | 55:1:197:TYR:CB   | 2.45                     | 0.64              |
| 28:W:613:G:N1    | 28:W:629:A:OP1    | 2.31                     | 0.64              |
| 39:h:66:ILE:HG23 | 39:h:86:LEU:HD22  | 1.78                     | 0.64              |
| 13:H:34:THR:OG1  | 13:H:78:GLY:O     | 2.10                     | 0.64              |
| 13:H:125:CYS:SG  | 13:H:126:GLY:N    | 2.71                     | 0.64              |
| 15:J:771:GLU:N   | 15:J:771:GLU:OE1  | 2.31                     | 0.63              |
| 28:W:1337:C:OP1  | 46:o:44:ARG:NH2   | 2.31                     | 0.63              |
| 28:W:60:G:O2'    | 28:W:61:A:O4'     | 2.15                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:W:1609:C:OP1   | 45:n:134:GLN:NE2  | 2.31                     | 0.63              |
| 32:a:95:GLU:OE1   | 32:a:140:ARG:NH1  | 2.31                     | 0.63              |
| 28:W:59:U:OP1     | 28:W:501:C:O2'    | 2.16                     | 0.63              |
| 6:A:513:SER:O     | 6:A:518:GLN:NE2   | 2.32                     | 0.63              |
| 28:W:643:A:OP1    | 31:Z:38:ARG:NH1   | 2.31                     | 0.63              |
| 28:W:1395:C:OP1   | 38:g:126:ARG:NH1  | 2.30                     | 0.63              |
| 30:Y:87:MET:HE1   | 30:Y:236:ILE:HD13 | 1.80                     | 0.63              |
| 4:8:238:HIS:N     | 6:A:503:GLU:OE2   | 2.32                     | 0.63              |
| 9:D:50:GLU:OE1    | 9:D:86:SER:OG     | 2.11                     | 0.63              |
| 40:i:95:ARG:O     | 40:i:95:ARG:NH1   | 2.32                     | 0.63              |
| 28:W:834:C:H42    | 28:W:839:C:H42    | 1.45                     | 0.63              |
| 28:W:1433:C:O2'   | 28:W:1434:C:OP2   | 2.17                     | 0.63              |
| 22:Q:122:LEU:HD23 | 22:Q:144:THR:HG22 | 1.81                     | 0.63              |
| 28:W:1618:C:O2'   | 28:W:1619:A:O5'   | 2.17                     | 0.63              |
| 15:J:520:GLN:O    | 15:J:524:THR:OG1  | 2.10                     | 0.62              |
| 28:W:1782:G:O2'   | 28:W:1783:C:O4'   | 2.17                     | 0.62              |
| 10:E:168:PRO:O    | 10:E:171:SER:OG   | 2.11                     | 0.62              |
| 28:W:218:U:O2     | 35:d:184:ARG:NH1  | 2.32                     | 0.62              |
| 28:W:1080:A:O2'   | 28:W:1081:PSU:OP2 | 2.12                     | 0.62              |
| 11:F:244:VAL:N    | 11:F:270:PHE:O    | 2.33                     | 0.62              |
| 27:V:106:ARG:NH2  | 28:W:1076:G:OP1   | 2.32                     | 0.62              |
| 45:n:15:VAL:CG1   | 45:n:68:ILE:HD11  | 2.29                     | 0.62              |
| 28:W:1159:G:OP1   | 34:c:76:SER:OG    | 2.17                     | 0.62              |
| 9:D:232:PRO:HD2   | 10:E:267:PRO:HA   | 1.81                     | 0.62              |
| 28:W:1617:G:N1    | 28:W:1620:A:OP2   | 2.32                     | 0.62              |
| 9:D:211:ALA:HB1   | 9:D:258:ILE:HG13  | 1.82                     | 0.62              |
| 15:J:611:ARG:NH2  | 15:J:675:LEU:O    | 2.33                     | 0.62              |
| 39:h:80:PRO:O     | 39:h:83:SER:OG    | 2.12                     | 0.62              |
| 53:y:46:U:O2'     | 53:y:48:G:OP1     | 2.16                     | 0.62              |
| 16:K:323:TYR:O    | 16:K:327:ARG:N    | 2.33                     | 0.61              |
| 28:W:1204:A:O2'   | 28:W:1206:G:O6    | 2.16                     | 0.61              |
| 4:8:44:LEU:O      | 4:8:48:LYS:N      | 2.34                     | 0.61              |
| 21:P:34:LYS:NZ    | 21:P:43:ASN:OD1   | 2.21                     | 0.61              |
| 53:y:7:G:OP1      | 53:y:47:C:O2'     | 2.14                     | 0.61              |
| 14:I:450:GLU:O    | 14:I:453:SER:OG   | 2.16                     | 0.61              |
| 28:W:83:A:N1      | 28:W:150:A:O2'    | 2.34                     | 0.61              |
| 38:g:101:ASP:OD1  | 38:g:103:ALA:N    | 2.34                     | 0.61              |
| 6:A:236:GLN:O     | 6:A:239:SER:OG    | 2.15                     | 0.60              |
| 22:Q:85:ARG:NH2   | 22:Q:201:LEU:O    | 2.34                     | 0.60              |
| 28:W:1335:G:OP1   | 39:h:185:LYS:NZ   | 2.34                     | 0.60              |
| 6:A:481:GLN:NE2   | 6:A:517:GLU:OE1   | 2.33                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:W:1650:A:N7    | 28:W:1675:A:N3    | 2.49                     | 0.60              |
| 21:P:214:LYS:NZ   | 28:W:943:U:OP1    | 2.34                     | 0.60              |
| 42:k:37:ASP:OD1   | 42:k:39:THR:OG1   | 2.18                     | 0.60              |
| 6:A:317:ARG:NH1   | 6:A:421:GLU:OE2   | 2.33                     | 0.60              |
| 28:W:1590:C:OP1   | 43:l:82:ARG:NE    | 2.30                     | 0.60              |
| 44:m:51:ASP:OD1   | 44:m:54:THR:OG1   | 2.08                     | 0.60              |
| 6:A:24:LYS:NZ     | 6:A:60:ASP:OD2    | 2.32                     | 0.60              |
| 6:A:238:ASP:O     | 6:A:242:SER:OG    | 2.13                     | 0.60              |
| 6:A:514:MET:O     | 6:A:518:GLN:N     | 2.34                     | 0.60              |
| 28:W:1544:C:N4    | 28:W:1589:A:C8    | 2.67                     | 0.60              |
| 10:E:188:LEU:HD21 | 10:E:224:ILE:HD11 | 1.82                     | 0.60              |
| 14:I:469:ASP:OD1  | 14:I:470:PHE:N    | 2.35                     | 0.60              |
| 42:k:201:SER:OG   | 42:k:203:ASP:OD1  | 2.09                     | 0.60              |
| 28:W:1292:C:O2'   | 47:p:138:ARG:NH2  | 2.34                     | 0.60              |
| 6:A:499:TYR:OH    | 15:J:846:ARG:NH1  | 2.35                     | 0.59              |
| 13:H:61:LEU:HD21  | 13:H:88:MET:HE1   | 1.83                     | 0.59              |
| 15:J:562:ASP:O    | 15:J:566:THR:OG1  | 2.15                     | 0.59              |
| 56:2:905:LEU:O    | 56:2:909:LYS:N    | 2.35                     | 0.59              |
| 28:W:789:G:OP2    | 28:W:789:G:N2     | 2.34                     | 0.59              |
| 14:I:314:ASP:O    | 14:I:334:ARG:N    | 2.35                     | 0.59              |
| 15:J:486:VAL:HG13 | 15:J:502:ILE:HD11 | 1.84                     | 0.59              |
| 28:W:537:C:H42    | 28:W:546:G:H22    | 1.51                     | 0.59              |
| 55:1:274:GLN:O    | 55:1:342:SER:N    | 2.34                     | 0.59              |
| 19:N:32:ILE:HD12  | 19:N:34:MET:HE3   | 1.85                     | 0.59              |
| 29:X:77:VAL:HG11  | 29:X:80:MET:HE3   | 1.85                     | 0.59              |
| 20:O:72:ASP:OD2   | 20:O:272:HIS:NE2  | 2.30                     | 0.59              |
| 52:x:391:ILE:HG22 | 52:x:446:TYR:HB2  | 1.84                     | 0.59              |
| 2:6:203:ASP:O     | 2:6:212:SER:N     | 2.36                     | 0.59              |
| 13:H:56:TYR:HB2   | 13:H:137:LEU:HD11 | 1.85                     | 0.59              |
| 28:W:604:A:N3     | 28:W:639:C:O2'    | 2.34                     | 0.59              |
| 36:e:86:GLU:OE2   | 36:e:90:ARG:NH1   | 2.35                     | 0.59              |
| 8:C:344:LYS:O     | 8:C:347:TRP:N     | 2.36                     | 0.59              |
| 10:E:256:LEU:N    | 10:E:358:LEU:O    | 2.36                     | 0.59              |
| 25:T:52:THR:HG21  | 28:W:952:G:H21    | 1.68                     | 0.58              |
| 46:o:21:CYS:SG    | 46:o:22:ARG:N     | 2.76                     | 0.58              |
| 52:x:474:ASN:OD1  | 52:x:475:GLU:N    | 2.36                     | 0.58              |
| 6:A:224:GLU:N     | 6:A:224:GLU:OE1   | 2.37                     | 0.58              |
| 6:A:445:GLN:O     | 6:A:512:GLN:NE2   | 2.36                     | 0.58              |
| 23:R:15:ARG:NH1   | 28:W:993:G:N7     | 2.51                     | 0.58              |
| 15:J:657:GLU:N    | 15:J:657:GLU:OE1  | 2.37                     | 0.58              |
| 28:W:1549:U:OP1   | 46:o:34:TYR:OH    | 2.21                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 55:3:103:ALA:O    | 55:3:155:ILE:N    | 2.36                     | 0.58              |
| 39:h:117:ARG:NH2  | 54:z:117:U:O3'    | 2.36                     | 0.58              |
| 42:k:94:THR:OG1   | 42:k:96:THR:OG1   | 2.21                     | 0.58              |
| 51:w:21:ARG:HH21  | 51:w:88:LEU:HD23  | 1.69                     | 0.58              |
| 28:W:558:G:O2'    | 28:W:559:G:OP2    | 2.18                     | 0.57              |
| 52:x:6:THR:O      | 52:x:7:PRO:C      | 2.47                     | 0.57              |
| 22:Q:77:ILE:HD12  | 22:Q:122:LEU:HD11 | 1.85                     | 0.57              |
| 16:K:281:HIS:O    | 16:K:286:ASP:N    | 2.37                     | 0.57              |
| 21:P:160:GLN:NE2  | 28:W:1121:G:OP1   | 2.37                     | 0.57              |
| 28:W:328:U:O2'    | 28:W:329:G:O5'    | 2.21                     | 0.57              |
| 36:e:103:SER:OG   | 36:e:106:GLN:OE1  | 2.22                     | 0.57              |
| 28:W:1608:U:O2'   | 45:n:130:ARG:NH1  | 2.37                     | 0.57              |
| 52:x:19:CYS:C     | 52:x:21:VAL:N     | 2.56                     | 0.57              |
| 30:Y:125:LYS:NZ   | 30:Y:225:ILE:O    | 2.30                     | 0.57              |
| 6:A:625:LEU:O     | 6:A:630:GLN:N     | 2.37                     | 0.56              |
| 15:J:633:LEU:HA   | 15:J:636:ILE:HD12 | 1.86                     | 0.56              |
| 2:6:121:LEU:N     | 2:6:133:ASN:O     | 2.37                     | 0.56              |
| 42:k:40:ILE:HD11  | 42:k:66:VAL:HG11  | 1.86                     | 0.56              |
| 6:A:243:MET:SD    | 6:A:245:LEU:HD13  | 2.46                     | 0.56              |
| 10:E:255:ARG:NH1  | 10:E:436:GLU:OE2  | 2.39                     | 0.56              |
| 25:T:150:ARG:NH1  | 28:W:1854:U:OP1   | 2.38                     | 0.56              |
| 28:W:1650:A:C4    | 28:W:1675:A:C5    | 2.93                     | 0.56              |
| 41:j:78:THR:HG22  | 41:j:80:LEU:H     | 1.71                     | 0.56              |
| 14:I:472:TRP:CZ2  | 14:I:479:ILE:HD11 | 2.41                     | 0.56              |
| 15:J:784:GLN:O    | 15:J:787:SER:OG   | 2.12                     | 0.56              |
| 28:W:693:A:H61    | 28:W:737:G:H1     | 1.53                     | 0.56              |
| 15:J:648:GLN:NE2  | 15:J:677:ILE:O    | 2.37                     | 0.56              |
| 43:l:11:GLN:OE1   | 43:l:62:ARG:NH1   | 2.38                     | 0.56              |
| 36:e:35:VAL:HG23  | 36:e:40:ILE:HD11  | 1.87                     | 0.56              |
| 14:I:408:ASP:OD1  | 14:I:409:ILE:N    | 2.39                     | 0.56              |
| 36:e:41:ARG:NH2   | 36:e:52:PRO:O     | 2.38                     | 0.56              |
| 6:A:331:ILE:HG23  | 6:A:507:ILE:HG21  | 1.89                     | 0.55              |
| 11:F:155:GLY:N    | 11:F:160:CYS:O    | 2.40                     | 0.55              |
| 22:Q:140:VAL:HG23 | 22:Q:142:LEU:CD1  | 2.37                     | 0.55              |
| 28:W:1721:U:O2'   | 28:W:1723:G:OP2   | 2.25                     | 0.55              |
| 28:W:1240:A:O2'   | 28:W:1241:A:OP1   | 2.24                     | 0.55              |
| 52:x:398:GLU:OE1  | 52:x:453:SER:OG   | 2.24                     | 0.55              |
| 16:K:322:ALA:O    | 16:K:326:MET:N    | 2.40                     | 0.54              |
| 49:s:61:SER:OG    | 49:s:62:GLU:N     | 2.41                     | 0.54              |
| 28:W:1650:A:N9    | 28:W:1675:A:N1    | 2.55                     | 0.54              |
| 15:J:521:ARG:NE   | 15:J:539:ASN:OD1  | 2.40                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:R:32:LYS:NZ    | 28:W:987:A:OP1    | 2.40                     | 0.54              |
| 28:W:1399:C:O2'   | 42:k:88:ARG:NH2   | 2.40                     | 0.54              |
| 41:j:111:MET:HG3  | 45:n:117:ILE:HD11 | 1.89                     | 0.54              |
| 52:x:5:MET:O      | 52:x:6:THR:C      | 2.49                     | 0.54              |
| 10:E:263:ASP:CB   | 53:y:75:A:H2'     | 2.38                     | 0.54              |
| 15:J:633:LEU:HD23 | 15:J:636:ILE:HD12 | 1.88                     | 0.54              |
| 39:h:75:LYS:NZ    | 40:i:34:GLU:OE2   | 2.26                     | 0.54              |
| 39:h:161:GLY:O    | 39:h:164:VAL:HG22 | 2.07                     | 0.54              |
| 6:A:31:LEU:HD12   | 6:A:50:ILE:HG23   | 1.89                     | 0.54              |
| 15:J:647:GLY:O    | 15:J:671:VAL:HG12 | 2.08                     | 0.54              |
| 27:V:63:VAL:HG21  | 27:V:71:ILE:HG13  | 1.90                     | 0.54              |
| 28:W:57:U:OP1     | 28:W:504:G:O2'    | 2.25                     | 0.54              |
| 28:W:1650:A:C5    | 28:W:1675:A:N1    | 2.76                     | 0.54              |
| 28:W:1650:A:N1    | 28:W:1674:G:O2'   | 2.36                     | 0.54              |
| 39:h:45:ARG:NH2   | 39:h:84:VAL:O     | 2.40                     | 0.54              |
| 12:G:52:PHE:CD1   | 12:G:109:LEU:HD21 | 2.42                     | 0.54              |
| 17:L:80:VAL:HG23  | 17:L:92:VAL:CG2   | 2.38                     | 0.54              |
| 28:W:1650:A:N9    | 28:W:1675:A:C5    | 2.76                     | 0.54              |
| 35:d:110:ARG:NH1  | 35:d:114:GLU:OE2  | 2.41                     | 0.54              |
| 43:l:35:ASP:OD1   | 43:l:36:THR:HG23  | 2.08                     | 0.54              |
| 10:E:151:VAL:HG21 | 10:E:259:ILE:HD11 | 1.89                     | 0.54              |
| 27:V:130:LYS:NZ   | 27:V:139:TRP:O    | 2.22                     | 0.54              |
| 28:W:550:C:O2'    | 28:W:551:U:O4'    | 2.10                     | 0.54              |
| 9:D:21:MET:HG3    | 9:D:37:LEU:HD12   | 1.90                     | 0.54              |
| 10:E:47:ILE:HD12  | 10:E:173:HIS:HB3  | 1.89                     | 0.54              |
| 14:I:369:GLN:NE2  | 14:I:410:LEU:O    | 2.41                     | 0.54              |
| 28:W:1535:U:O2'   | 37:f:82:ASN:OD1   | 2.25                     | 0.54              |
| 9:D:224:PRO:O     | 9:D:239:THR:OG1   | 2.20                     | 0.54              |
| 24:S:179:LEU:HD21 | 28:W:77:A:N6      | 2.23                     | 0.54              |
| 28:W:1650:A:N3    | 28:W:1675:A:N3    | 2.56                     | 0.53              |
| 13:H:21:LEU:HD11  | 13:H:89:LEU:HD22  | 1.91                     | 0.53              |
| 28:W:1215:C:H42   | 28:W:1221:G:H1    | 1.55                     | 0.53              |
| 14:I:342:TRP:CE2  | 14:I:349:LEU:HD13 | 2.43                     | 0.53              |
| 28:W:1664:A:HO2'  | 28:W:1666:C:H41   | 1.51                     | 0.53              |
| 41:j:52:LYS:O     | 41:j:55:SER:OG    | 2.17                     | 0.53              |
| 28:W:1332:A:O2'   | 39:h:145:GLN:O    | 2.16                     | 0.53              |
| 42:k:126:ASP:OD1  | 42:k:128:THR:OG1  | 2.23                     | 0.53              |
| 19:N:4:ASP:OD1    | 19:N:5:ALA:N      | 2.42                     | 0.53              |
| 15:J:385:TYR:CE2  | 15:J:397:MET:HE1  | 2.44                     | 0.53              |
| 15:J:713:GLN:OE1  | 15:J:717:GLN:NE2  | 2.41                     | 0.53              |
| 21:P:139:CYS:SG   | 21:P:140:VAL:N    | 2.82                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:y:18:G:N3      | 53:y:19:A:N6      | 2.55                     | 0.53              |
| 6:A:327:LEU:HB3   | 6:A:431:LEU:HD21  | 1.91                     | 0.53              |
| 10:E:386:THR:OG1  | 10:E:389:ASP:OD1  | 2.15                     | 0.53              |
| 47:p:129:GLY:O    | 48:q:36:ARG:NH2   | 2.42                     | 0.53              |
| 52:x:44:ASP:OD1   | 52:x:47:GLY:N     | 2.42                     | 0.53              |
| 15:J:375:LYS:HA   | 15:J:378:ILE:HD12 | 1.90                     | 0.53              |
| 28:W:56:G:OP2     | 36:e:115:LYS:NZ   | 2.32                     | 0.53              |
| 51:w:46:LYS:HE3   | 51:w:101:ILE:HD13 | 1.91                     | 0.53              |
| 10:E:39:GLN:NE2   | 10:E:336:LEU:O    | 2.41                     | 0.52              |
| 20:O:79:GLU:N     | 20:O:79:GLU:OE1   | 2.42                     | 0.52              |
| 28:W:1403:C:O2'   | 28:W:1404:U:OP2   | 2.21                     | 0.52              |
| 35:d:59:ARG:O     | 35:d:60:LEU:HD12  | 2.09                     | 0.52              |
| 45:n:82:TRP:O     | 45:n:87:GLN:NE2   | 2.41                     | 0.52              |
| 9:D:231:ALA:O     | 9:D:232:PRO:C     | 2.52                     | 0.52              |
| 20:O:174:ILE:O    | 20:O:200:ARG:NH2  | 2.41                     | 0.52              |
| 28:W:1544:C:H42   | 28:W:1589:A:H8    | 1.52                     | 0.52              |
| 28:W:153:G:H22    | 28:W:166:A2M:C2   | 2.23                     | 0.52              |
| 41:j:81:ARG:NH2   | 41:j:120:SER:O    | 2.41                     | 0.52              |
| 39:h:56:GLN:OE1   | 39:h:56:GLN:N     | 2.43                     | 0.52              |
| 53:y:10:G:OP1     | 53:y:45:G:N1      | 2.43                     | 0.52              |
| 28:W:1614:A:OP2   | 41:j:42:ARG:NH2   | 2.39                     | 0.52              |
| 28:W:1709:G:C6    | 28:W:1824:A:N6    | 2.78                     | 0.52              |
| 52:x:398:GLU:OE2  | 52:x:401:SER:OG   | 2.14                     | 0.52              |
| 20:O:102:LEU:HD22 | 20:O:130:ILE:HG12 | 1.92                     | 0.52              |
| 28:W:1577:G:O2'   | 28:W:1579:A:N3    | 2.36                     | 0.52              |
| 39:h:81:GLU:N     | 39:h:81:GLU:OE2   | 2.43                     | 0.52              |
| 10:E:177:ILE:O    | 10:E:181:LYS:N    | 2.42                     | 0.52              |
| 10:E:258:VAL:HG11 | 10:E:353:MET:HE1  | 1.92                     | 0.52              |
| 10:E:263:ASP:OD1  | 53:y:75:A:H2'     | 2.10                     | 0.52              |
| 1:5:304:ASP:O     | 1:5:308:ALA:N     | 2.41                     | 0.51              |
| 10:E:265:ASN:H    | 53:y:75:A:HO2'    | 1.59                     | 0.51              |
| 28:W:1214:A:N6    | 28:W:1682:C:C2    | 2.70                     | 0.51              |
| 15:J:336:ILE:HD12 | 15:J:353:LEU:HD13 | 1.93                     | 0.51              |
| 23:R:25:ASN:ND2   | 23:R:77:CYS:SG    | 2.83                     | 0.51              |
| 10:E:10:LEU:O     | 10:E:17:ARG:NH2   | 2.43                     | 0.51              |
| 28:W:1463:U:O2'   | 28:W:1464:C:O5'   | 2.26                     | 0.51              |
| 50:v:99:ASP:OD1   | 50:v:102:THR:HG22 | 2.10                     | 0.51              |
| 51:w:34:LYS:NZ    | 51:w:107:GLU:OE1  | 2.41                     | 0.51              |
| 6:A:461:PHE:CD2   | 6:A:462:VAL:HG23  | 2.45                     | 0.51              |
| 28:W:116:OMU:HN3  | 28:W:347:G:H1     | 1.57                     | 0.51              |
| 28:W:1400:U:H5    | 28:W:1448:A:N1    | 2.07                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:W:1403:C:H4'   | 28:W:1405:A:H62   | 1.76                     | 0.51              |
| 28:W:752:G:OP2    | 28:W:792:C:O2'    | 2.28                     | 0.51              |
| 10:E:368:PHE:N    | 10:E:433:VAL:O    | 2.43                     | 0.51              |
| 28:W:1448:A:H2'   | 28:W:1449:G:C8    | 2.45                     | 0.51              |
| 30:Y:208:VAL:HG21 | 30:Y:225:ILE:HG13 | 1.92                     | 0.51              |
| 14:I:563:GLU:N    | 14:I:563:GLU:OE1  | 2.44                     | 0.51              |
| 21:P:104:ASP:OD1  | 21:P:105:LEU:N    | 2.43                     | 0.51              |
| 15:J:788:LEU:HD22 | 15:J:813:LEU:HD13 | 1.91                     | 0.51              |
| 19:N:3:ASN:ND2    | 19:N:7:GLU:OE2    | 2.44                     | 0.51              |
| 28:W:1758:G:OP1   | 28:W:1774:C:N4    | 2.44                     | 0.51              |
| 9:D:72:VAL:HG21   | 9:D:89:ARG:HB2    | 1.92                     | 0.50              |
| 28:W:88:G:H21     | 28:W:499:G:H4'    | 1.76                     | 0.50              |
| 3:7:289:ARG:NH1   | 3:7:291:GLU:OE2   | 2.44                     | 0.50              |
| 15:J:716:HIS:O    | 15:J:720:VAL:HG22 | 2.12                     | 0.50              |
| 17:L:138:GLU:OE2  | 27:V:21:SER:OG    | 2.28                     | 0.50              |
| 28:W:1650:A:C1'   | 28:W:1675:A:N3    | 2.73                     | 0.50              |
| 20:O:64:THR:HG23  | 20:O:67:GLY:H     | 1.76                     | 0.50              |
| 14:I:514:ASP:OD1  | 14:I:515:CYS:N    | 2.44                     | 0.50              |
| 15:J:788:LEU:CD2  | 15:J:813:LEU:HD22 | 2.42                     | 0.50              |
| 17:L:159:ASP:OD1  | 17:L:160:LYS:N    | 2.44                     | 0.50              |
| 4:8:123:THR:N     | 4:8:152:TYR:O     | 2.43                     | 0.50              |
| 10:E:403:VAL:O    | 10:E:404:LEU:HD23 | 2.10                     | 0.50              |
| 24:S:31:ARG:NH1   | 28:W:1746:U:OP1   | 2.44                     | 0.50              |
| 6:A:404:CYS:SG    | 6:A:405:GLU:N     | 2.85                     | 0.50              |
| 56:2:754:GLY:O    | 56:2:758:GLN:N    | 2.41                     | 0.50              |
| 6:A:404:CYS:O     | 6:A:408:THR:OG1   | 2.18                     | 0.50              |
| 28:W:351:G:OP1    | 35:d:7:ASN:ND2    | 2.44                     | 0.50              |
| 38:g:98:LYS:O     | 42:k:57:ARG:NH1   | 2.43                     | 0.50              |
| 28:W:1524:G:OP2   | 45:n:141:ARG:NH1  | 2.43                     | 0.50              |
| 6:A:115:ILE:O     | 6:A:120:ASN:ND2   | 2.44                     | 0.49              |
| 24:S:13:GLN:OE1   | 28:W:153:G:N2     | 2.42                     | 0.49              |
| 42:k:306:LEU:HD23 | 42:k:307:VAL:N    | 2.26                     | 0.49              |
| 25:T:149:ARG:NH1  | 28:W:1064:C:O3'   | 2.45                     | 0.49              |
| 31:Z:113:GLN:O    | 31:Z:117:LEU:HD23 | 2.12                     | 0.49              |
| 14:I:690:LEU:HD21 | 14:I:693:LYS:CG   | 2.42                     | 0.49              |
| 28:W:70:G:H21     | 28:W:79:A:H62     | 1.60                     | 0.49              |
| 28:W:798:G:O2'    | 28:W:799:U:OP1    | 2.29                     | 0.49              |
| 52:x:21:VAL:O     | 52:x:26:ARG:NH2   | 2.46                     | 0.49              |
| 6:A:327:LEU:O     | 6:A:434:ASN:ND2   | 2.46                     | 0.49              |
| 42:k:247:TRP:CZ2  | 42:k:267:VAL:HG11 | 2.48                     | 0.49              |
| 50:v:18:GLU:HB3   | 50:v:69:ILE:HG23  | 1.95                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:I:675:HIS:O    | 14:I:679:ASN:ND2  | 2.41                     | 0.49              |
| 28:W:1745:A:N6    | 28:W:1789:G:O2'   | 2.46                     | 0.49              |
| 28:W:1743:G:H21   | 28:W:1791:A:H62   | 1.61                     | 0.49              |
| 43:l:44:GLU:O     | 43:l:45:LEU:HD22  | 2.13                     | 0.49              |
| 6:A:105:LYS:HA    | 6:A:146:LEU:HD21  | 1.95                     | 0.49              |
| 9:D:55:ARG:NH1    | 54:z:103:U:O2     | 2.46                     | 0.49              |
| 14:I:220:ASP:OD1  | 14:I:220:ASP:N    | 2.45                     | 0.49              |
| 15:J:695:ILE:HG21 | 15:J:744:MET:HG3  | 1.94                     | 0.49              |
| 21:P:225:LEU:HD12 | 21:P:228:LEU:HB2  | 1.95                     | 0.49              |
| 28:W:818:A:OP1    | 31:Z:80:ARG:NH2   | 2.44                     | 0.49              |
| 27:V:102:LEU:HD13 | 27:V:111:ALA:HB3  | 1.95                     | 0.49              |
| 22:Q:84:GLN:HG3   | 22:Q:100:ALA:HB1  | 1.95                     | 0.48              |
| 4:8:43:GLY:O      | 4:8:47:LEU:N      | 2.46                     | 0.48              |
| 24:S:159:ARG:NH2  | 28:W:76:U:O4      | 2.46                     | 0.48              |
| 28:W:346:C:O2'    | 30:Y:6:LYS:O      | 2.31                     | 0.48              |
| 4:8:288:ARG:O     | 4:8:292:GLY:N     | 2.47                     | 0.48              |
| 6:A:659:GLU:O     | 6:A:663:GLU:HA    | 2.12                     | 0.48              |
| 13:H:143:LYS:NZ   | 28:W:1061:U:O2    | 2.46                     | 0.48              |
| 18:M:35:VAL:CG1   | 18:M:63:LEU:HD11  | 2.44                     | 0.48              |
| 10:E:319:VAL:N    | 10:E:340:GLY:O    | 2.47                     | 0.48              |
| 28:W:925:G:H1     | 28:W:1017:U:H3    | 1.60                     | 0.48              |
| 28:W:1611:G:N1    | 28:W:1629:C:O2    | 2.47                     | 0.48              |
| 41:j:21:ASP:OD1   | 41:j:22:LEU:N     | 2.46                     | 0.48              |
| 56:2:951:ALA:O    | 56:2:955:MET:N    | 2.41                     | 0.48              |
| 11:F:195:GLN:O    | 11:F:204:VAL:N    | 2.46                     | 0.48              |
| 14:I:690:LEU:HD21 | 14:I:693:LYS:HG3  | 1.94                     | 0.48              |
| 6:A:517:GLU:OE1   | 6:A:517:GLU:N     | 2.47                     | 0.48              |
| 9:D:212:LEU:HD23  | 9:D:227:ILE:HD13  | 1.96                     | 0.48              |
| 37:f:32:ASP:OD1   | 37:f:33:ILE:N     | 2.47                     | 0.48              |
| 52:x:4:PHE:O      | 52:x:5:MET:C      | 2.56                     | 0.48              |
| 6:A:222:ASN:ND2   | 6:A:224:GLU:OE2   | 2.46                     | 0.47              |
| 50:v:58:MET:HE2   | 50:v:61:ILE:HD12  | 1.95                     | 0.47              |
| 1:5:353:ILE:N     | 1:5:389:GLY:O     | 2.47                     | 0.47              |
| 17:L:134:VAL:HG23 | 17:L:134:VAL:O    | 2.14                     | 0.47              |
| 24:S:13:GLN:CD    | 28:W:153:G:H21    | 2.22                     | 0.47              |
| 40:i:71:LEU:HD13  | 40:i:76:ILE:HD11  | 1.95                     | 0.47              |
| 6:A:75:LYS:O      | 6:A:79:GLN:NE2    | 2.47                     | 0.47              |
| 9:D:84:ASP:C      | 9:D:85:LEU:HD12   | 2.39                     | 0.47              |
| 12:G:22:GLU:N     | 12:G:22:GLU:OE1   | 2.48                     | 0.47              |
| 15:J:500:CYS:SG   | 15:J:564:ILE:HG21 | 2.54                     | 0.47              |
| 21:P:108:ASP:OD1  | 21:P:109:LYS:N    | 2.47                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:d:174:CYS:SG   | 35:d:175:ILE:N    | 2.86                     | 0.47              |
| 42:k:110:SER:O    | 42:k:122:SER:OG   | 2.17                     | 0.47              |
| 5:9:9:ARG:NH1     | 28:W:1851:MA6:OP1 | 2.47                     | 0.47              |
| 24:S:57:ASP:OD1   | 24:S:58:LYS:N     | 2.45                     | 0.47              |
| 9:D:190:LYS:O     | 9:D:278:VAL:HB    | 2.14                     | 0.47              |
| 6:A:335:ARG:NH1   | 6:A:339:ALA:HB3   | 2.30                     | 0.47              |
| 14:I:311:GLU:O    | 14:I:312:SER:OG   | 2.26                     | 0.47              |
| 24:S:31:ARG:O     | 24:S:34:THR:OG1   | 2.29                     | 0.47              |
| 48:q:48:HIS:ND1   | 48:q:112:LYS:O    | 2.33                     | 0.47              |
| 55:1:47:ILE:O     | 55:1:51:GLY:N     | 2.48                     | 0.47              |
| 55:1:339:GLN:O    | 55:1:341:VAL:N    | 2.48                     | 0.47              |
| 1:5:19:VAL:O      | 1:5:23:LEU:N      | 2.46                     | 0.47              |
| 28:W:419:G:N2     | 28:W:661:U:O2     | 2.48                     | 0.47              |
| 28:W:1284:A:C4    | 48:q:91:LEU:HD11  | 2.50                     | 0.47              |
| 38:g:67:ASP:OD2   | 38:g:69:ARG:NH2   | 2.48                     | 0.47              |
| 10:E:162:ASN:OD1  | 10:E:163:GLU:N    | 2.48                     | 0.47              |
| 47:p:120:GLU:OE1  | 47:p:120:GLU:N    | 2.46                     | 0.47              |
| 22:Q:128:ARG:NH2  | 22:Q:151:ASP:O    | 2.48                     | 0.47              |
| 28:W:1354:G:H2'   | 28:W:1356:G:H22   | 1.80                     | 0.47              |
| 28:W:1554:C:OP2   | 28:W:1555:U:O2'   | 2.26                     | 0.47              |
| 42:k:94:THR:HG1   | 42:k:96:THR:HG1   | 1.56                     | 0.47              |
| 28:W:1650:A:H61   | 28:W:1674:G:H1'   | 1.80                     | 0.46              |
| 39:h:39:VAL:HG12  | 39:h:48:ILE:HD13  | 1.98                     | 0.46              |
| 44:m:66:LYS:O     | 44:m:110:THR:HG23 | 2.15                     | 0.46              |
| 44:m:84:ALA:O     | 44:m:88:LEU:HD13  | 2.15                     | 0.46              |
| 6:A:37:SER:O      | 6:A:41:ARG:NH1    | 2.48                     | 0.46              |
| 28:W:1398:G:N1    | 38:g:11:GLN:O     | 2.49                     | 0.46              |
| 44:m:50:PHE:CZ    | 44:m:58:LEU:HD11  | 2.50                     | 0.46              |
| 6:A:498:ASN:OD1   | 6:A:520:ARG:NH2   | 2.49                     | 0.46              |
| 14:I:388:LEU:HD23 | 14:I:389:VAL:N    | 2.30                     | 0.46              |
| 24:S:137:ARG:N    | 28:W:170:A:OP2    | 2.42                     | 0.46              |
| 37:f:167:LYS:NZ   | 37:f:172:CYS:SG   | 2.82                     | 0.46              |
| 53:y:15:G:H1      | 53:y:58:A:H61     | 1.63                     | 0.46              |
| 27:V:31:ASP:OD1   | 27:V:32:ASP:N     | 2.48                     | 0.46              |
| 28:W:1650:A:C8    | 28:W:1675:A:C2    | 2.97                     | 0.46              |
| 39:h:177:LEU:HD12 | 39:h:182:LEU:HD23 | 1.98                     | 0.46              |
| 54:z:125:A:H5''   | 54:z:126:A:H5'    | 1.96                     | 0.46              |
| 3:7:287:PHE:O     | 3:7:288:HIS:ND1   | 2.49                     | 0.46              |
| 6:A:390:LEU:HD21  | 6:A:410:VAL:HG21  | 1.96                     | 0.46              |
| 14:I:510:PHE:O    | 14:I:532:ARG:NE   | 2.46                     | 0.46              |
| 15:J:424:ILE:HD13 | 15:J:439:ARG:HD3  | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:W:56:G:H22     | 28:W:88:G:N2      | 2.13                     | 0.46              |
| 48:q:17:ALA:O     | 48:q:21:VAL:HG12  | 2.16                     | 0.46              |
| 52:x:436:THR:CG2  | 52:x:477:ALA:HB2  | 2.46                     | 0.46              |
| 53:y:28:G:O2'     | 53:y:29:G:OP1     | 2.29                     | 0.46              |
| 10:E:41:THR:OG1   | 10:E:128:ARG:NH2  | 2.48                     | 0.46              |
| 10:E:300:ILE:HG13 | 10:E:314:ILE:HD11 | 1.97                     | 0.46              |
| 28:W:1208:A:O2'   | 28:W:1837:G:N2    | 2.48                     | 0.46              |
| 6:A:493:PHE:HB3   | 6:A:514:MET:HE1   | 1.97                     | 0.46              |
| 14:I:621:GLN:OE1  | 14:I:641:SER:OG   | 2.24                     | 0.46              |
| 28:W:1060:A:O2'   | 28:W:1062:A:N7    | 2.45                     | 0.46              |
| 28:W:1354:G:H2'   | 28:W:1356:G:H1    | 1.80                     | 0.46              |
| 55:3:358:HIS:O    | 55:3:362:ARG:N    | 2.48                     | 0.46              |
| 28:W:1217:A:H2    | 28:W:1684:C:H42   | 1.62                     | 0.46              |
| 9:D:84:ASP:OD1    | 37:f:198:ARG:NE   | 2.47                     | 0.46              |
| 16:K:40:TYR:C     | 16:K:42:GLN:N     | 2.72                     | 0.46              |
| 11:F:212:ALA:O    | 11:F:226:PHE:N    | 2.49                     | 0.46              |
| 28:W:56:G:H1      | 28:W:88:G:N2      | 2.04                     | 0.46              |
| 32:a:6:GLY:O      | 32:a:9:THR:HG22   | 2.15                     | 0.46              |
| 38:g:42:ILE:HG22  | 38:g:44:PRO:HD2   | 1.98                     | 0.46              |
| 28:W:1599:U:O2'   | 28:W:1600:G:O5'   | 2.33                     | 0.45              |
| 6:A:318:MET:O     | 6:A:322:VAL:HG23  | 2.17                     | 0.45              |
| 9:D:232:PRO:HA    | 9:D:233:PRO:HA    | 1.71                     | 0.45              |
| 21:P:146:ARG:CD   | 28:W:1121:G:H21   | 2.30                     | 0.45              |
| 28:W:1025:U:OP1   | 28:W:1090:C:O2'   | 2.33                     | 0.45              |
| 30:Y:252:ARG:NH2  | 30:Y:253:ASP:OD1  | 2.45                     | 0.45              |
| 12:G:31:ASP:OD1   | 12:G:31:ASP:N     | 2.50                     | 0.45              |
| 15:J:486:VAL:CG1  | 15:J:502:ILE:HD11 | 2.46                     | 0.45              |
| 16:K:451:VAL:O    | 16:K:452:GLN:C    | 2.59                     | 0.45              |
| 3:7:245:ASN:ND2   | 3:7:309:ILE:O     | 2.48                     | 0.45              |
| 4:8:149:VAL:O     | 4:8:167:TYR:N     | 2.49                     | 0.45              |
| 12:G:24:ARG:NH2   | 12:G:93:LEU:HD21  | 2.31                     | 0.45              |
| 28:W:1422:G:O2'   | 28:W:1423:C:OP1   | 2.28                     | 0.45              |
| 9:D:255:MET:HA    | 9:D:258:ILE:HG22  | 1.99                     | 0.45              |
| 27:V:16:LEU:HD21  | 27:V:62:GLN:OE1   | 2.17                     | 0.45              |
| 30:Y:143:ASP:OD1  | 30:Y:143:ASP:N    | 2.47                     | 0.45              |
| 50:v:46:LEU:HD23  | 50:v:50:ILE:HD12  | 1.99                     | 0.45              |
| 52:x:371:LEU:HA   | 52:x:372:ILE:HD12 | 1.99                     | 0.45              |
| 19:N:7:GLU:N      | 19:N:7:GLU:OE1    | 2.50                     | 0.45              |
| 21:P:99:ASN:OD1   | 21:P:100:PHE:N    | 2.50                     | 0.45              |
| 28:W:64:A:N6      | 28:W:84:A:H62     | 2.15                     | 0.45              |
| 28:W:190:G:H21    | 28:W:209:A:H62    | 1.64                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:W:693:A:N6     | 28:W:737:G:H1     | 2.14                     | 0.45              |
| 28:W:920:A:OP1    | 34:c:57:ARG:NH2   | 2.47                     | 0.45              |
| 9:D:132:GLN:O     | 9:D:137:VAL:HG23  | 2.17                     | 0.45              |
| 15:J:800:ASP:O    | 15:J:844:MET:N    | 2.48                     | 0.45              |
| 35:d:92:ARG:NH1   | 35:d:92:ARG:O     | 2.49                     | 0.45              |
| 45:n:103:LEU:O    | 45:n:107:LEU:HD23 | 2.16                     | 0.45              |
| 6:A:327:LEU:HD12  | 6:A:394:LEU:HD13  | 1.97                     | 0.45              |
| 8:C:298:GLN:O     | 8:C:302:GLN:N     | 2.49                     | 0.45              |
| 13:H:139:THR:HG23 | 28:W:1848:U:OP1   | 2.17                     | 0.45              |
| 6:A:285:LYS:HB3   | 6:A:285:LYS:HE3   | 1.46                     | 0.45              |
| 22:Q:81:ASN:OD1   | 22:Q:82:THR:HG23  | 2.16                     | 0.45              |
| 28:W:64:A:O2'     | 28:W:82:G:N1      | 2.50                     | 0.45              |
| 28:W:678:U:OP2    | 28:W:1026:C:N4    | 2.48                     | 0.45              |
| 28:W:1284:A:OP1   | 28:W:1285:G:O2'   | 2.31                     | 0.45              |
| 45:n:25:LYS:O     | 45:n:29:ALA:N     | 2.49                     | 0.45              |
| 6:A:125:GLU:OE1   | 6:A:125:GLU:N     | 2.50                     | 0.45              |
| 6:A:280:SER:OG    | 6:A:292:HIS:ND1   | 2.50                     | 0.45              |
| 10:E:263:ASP:CG   | 53:y:75:A:H2'     | 2.41                     | 0.45              |
| 17:L:50:GLU:OE1   | 17:L:58:LYS:NZ    | 2.37                     | 0.45              |
| 28:W:1482:C:H1'   | 28:W:1483:A:H5''  | 1.98                     | 0.45              |
| 42:k:65:PHE:C     | 42:k:82:SER:HG    | 2.17                     | 0.45              |
| 10:E:402:GLU:OE2  | 10:E:445:ARG:NE   | 2.49                     | 0.44              |
| 12:G:53:ASP:OD1   | 12:G:54:GLY:N     | 2.50                     | 0.44              |
| 44:m:48:VAL:HG21  | 45:n:23:ARG:HB2   | 1.98                     | 0.44              |
| 49:s:20:ARG:HD2   | 49:s:28:THR:HG22  | 1.98                     | 0.44              |
| 6:A:75:LYS:NZ     | 6:A:163:LEU:O     | 2.49                     | 0.44              |
| 35:d:162:LEU:HD11 | 35:d:191:GLU:HB3  | 2.00                     | 0.44              |
| 42:k:65:PHE:O     | 42:k:82:SER:OG    | 2.18                     | 0.44              |
| 1:5:432:SER:O     | 1:5:436:ASN:N     | 2.51                     | 0.44              |
| 28:W:626:G:O2'    | 28:W:627:U:OP2    | 2.27                     | 0.44              |
| 28:W:1112:U:O4    | 28:W:1113:A:N6    | 2.51                     | 0.44              |
| 35:d:73:THR:O     | 35:d:74:ARG:NH1   | 2.48                     | 0.44              |
| 6:A:157:TYR:O     | 6:A:161:LEU:HD23  | 2.18                     | 0.44              |
| 28:W:899:U:O2'    | 28:W:900:C:O5'    | 2.34                     | 0.44              |
| 35:d:59:ARG:C     | 35:d:60:LEU:HD12  | 2.41                     | 0.44              |
| 44:m:103:HIS:N    | 44:m:106:GLN:O    | 2.49                     | 0.44              |
| 14:I:699:PHE:HZ   | 14:I:702:LEU:HD22 | 1.83                     | 0.44              |
| 15:J:802:ILE:C    | 15:J:841:THR:HG23 | 2.43                     | 0.44              |
| 28:W:1214:A:N7    | 28:W:1682:C:N3    | 2.65                     | 0.44              |
| 37:f:116:ILE:HD11 | 37:f:151:ILE:CG1  | 2.47                     | 0.44              |
| 42:k:299:PHE:HE1  | 42:k:309:VAL:HG12 | 1.83                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 52:x:318:TYR:O    | 52:x:322:ASN:ND2  | 2.50                     | 0.44              |
| 12:G:52:PHE:CG    | 12:G:109:LEU:HD21 | 2.53                     | 0.44              |
| 20:O:116:THR:OG1  | 20:O:117:ARG:N    | 2.51                     | 0.44              |
| 25:T:92:ALA:C     | 25:T:93:LEU:HD22  | 2.43                     | 0.44              |
| 28:W:1402:A:O2'   | 51:w:53:PRO:O     | 2.33                     | 0.44              |
| 55:1:388:GLU:O    | 55:1:393:THR:N    | 2.48                     | 0.44              |
| 6:A:111:MET:HE3   | 6:A:111:MET:HA    | 1.99                     | 0.43              |
| 6:A:464:ALA:O     | 6:A:467:LEU:N     | 2.48                     | 0.43              |
| 9:D:111:ILE:HD13  | 9:D:183:ARG:HD2   | 1.99                     | 0.43              |
| 14:I:508:ASN:C    | 14:I:509:LEU:HD22 | 2.43                     | 0.43              |
| 28:W:1217:A:HO2'  | 28:W:1218:C:P     | 2.36                     | 0.43              |
| 28:W:1617:G:O6    | 41:j:43:ARG:NH1   | 2.51                     | 0.43              |
| 37:f:100:ILE:O    | 37:f:104:THR:HG22 | 2.17                     | 0.43              |
| 15:J:602:ASP:O    | 15:J:605:VAL:N    | 2.51                     | 0.43              |
| 28:W:615:C:OP2    | 32:a:64:SER:OG    | 2.32                     | 0.43              |
| 52:x:21:VAL:HG22  | 52:x:26:ARG:NH2   | 2.33                     | 0.43              |
| 20:O:187:ARG:NH2  | 28:W:1143:A:OP2   | 2.51                     | 0.43              |
| 24:S:7:PHE:CE2    | 24:S:125:THR:HG23 | 2.54                     | 0.43              |
| 28:W:629:A:O2'    | 28:W:631:U:OP1    | 2.36                     | 0.43              |
| 45:n:98:VAL:C     | 45:n:99:LEU:HD22  | 2.43                     | 0.43              |
| 1:5:135:ALA:HB2   | 1:5:150:TYR:CB    | 2.48                     | 0.43              |
| 14:I:542:THR:HG21 | 14:I:565:ILE:CD1  | 2.49                     | 0.43              |
| 34:c:96:SER:OG    | 34:c:97:ARG:N     | 2.51                     | 0.43              |
| 39:h:99:ILE:HG23  | 39:h:173:ARG:NH2  | 2.33                     | 0.43              |
| 42:k:187:ASN:OD1  | 42:k:188:HIS:N    | 2.51                     | 0.43              |
| 6:A:230:LEU:HD21  | 6:A:259:LEU:HD22  | 2.00                     | 0.43              |
| 28:W:1344:A:N6    | 28:W:1386:A:O4'   | 2.51                     | 0.43              |
| 9:D:195:ILE:HG12  | 9:D:237:MET:HE1   | 1.99                     | 0.43              |
| 28:W:1538:C:O2    | 28:W:1595:U:N3    | 2.44                     | 0.43              |
| 30:Y:163:ASP:O    | 30:Y:167:GLY:N    | 2.49                     | 0.43              |
| 37:f:116:ILE:HD11 | 37:f:151:ILE:HG13 | 1.99                     | 0.43              |
| 42:k:179:LEU:O    | 42:k:179:LEU:HD23 | 2.19                     | 0.43              |
| 28:W:1285:G:OP2   | 48:q:35:ILE:HD12  | 2.19                     | 0.43              |
| 29:X:135:SER:OG   | 29:X:136:LYS:N    | 2.51                     | 0.43              |
| 51:w:102:THR:HG22 | 51:w:103:SER:H    | 1.83                     | 0.43              |
| 10:E:12:GLN:NE2   | 10:E:325:HIS:O    | 2.50                     | 0.43              |
| 10:E:58:VAL:O     | 10:E:62:SER:OG    | 2.09                     | 0.43              |
| 28:W:336:A:H8     | 28:W:336:A:O5'    | 2.02                     | 0.43              |
| 42:k:299:PHE:CE1  | 42:k:309:VAL:HG12 | 2.53                     | 0.43              |
| 52:x:364:LYS:C    | 52:x:365:LEU:HD12 | 2.44                     | 0.43              |
| 11:F:304:GLY:N    | 11:F:308:TYR:O    | 2.49                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:I:204:LYS:O    | 14:I:208:HIS:ND1  | 2.51                     | 0.43              |
| 15:J:803:SER:OG   | 15:J:806:THR:OG1  | 2.35                     | 0.43              |
| 24:S:162:LEU:HD13 | 28:W:67:C:H5      | 1.83                     | 0.43              |
| 40:i:64:TRP:CD2   | 46:o:23:VAL:HG12  | 2.54                     | 0.43              |
| 45:n:81:ASP:OD1   | 45:n:82:TRP:N     | 2.52                     | 0.43              |
| 28:W:56:G:H22     | 28:W:88:G:H22     | 1.67                     | 0.42              |
| 39:h:146:ARG:NH1  | 54:z:112:U:O2'    | 2.47                     | 0.42              |
| 43:l:33:TRP:CZ3   | 43:l:37:VAL:HG22  | 2.53                     | 0.42              |
| 15:J:709:MET:SD   | 15:J:709:MET:N    | 2.87                     | 0.42              |
| 28:W:838:G:O2'    | 28:W:839:C:OP2    | 2.25                     | 0.42              |
| 8:C:344:LYS:O     | 8:C:345:GLN:C     | 2.61                     | 0.42              |
| 10:E:58:VAL:HA    | 10:E:61:ILE:HG22  | 2.02                     | 0.42              |
| 28:W:1482:C:O2'   | 28:W:1483:A:OP2   | 2.23                     | 0.42              |
| 28:W:1650:A:C8    | 28:W:1675:A:C4    | 3.03                     | 0.42              |
| 28:W:1709:G:N1    | 28:W:1824:A:C6    | 2.84                     | 0.42              |
| 35:d:133:GLU:N    | 35:d:133:GLU:OE1  | 2.52                     | 0.42              |
| 42:k:150:TRP:O    | 42:k:170:TRP:N    | 2.50                     | 0.42              |
| 10:E:72:GLU:OE1   | 10:E:72:GLU:N     | 2.51                     | 0.42              |
| 13:H:18:MET:SD    | 13:H:18:MET:N     | 2.92                     | 0.42              |
| 28:W:1403:C:OP2   | 28:W:1405:A:N6    | 2.50                     | 0.42              |
| 42:k:203:ASP:OD1  | 42:k:204:GLY:N    | 2.52                     | 0.42              |
| 7:B:151:GLN:N     | 16:K:523:ILE:O    | 2.53                     | 0.42              |
| 10:E:369:THR:HG23 | 10:E:370:GLU:HG3  | 2.02                     | 0.42              |
| 16:K:45:TYR:O     | 16:K:46:GLN:C     | 2.61                     | 0.42              |
| 28:W:1541:G:O2'   | 38:g:43:GLU:OE2   | 2.27                     | 0.42              |
| 28:W:1544:C:C4    | 28:W:1589:A:N7    | 2.86                     | 0.42              |
| 39:h:158:ILE:HD13 | 39:h:163:PRO:HB2  | 2.01                     | 0.42              |
| 44:m:65:TYR:HB2   | 44:m:68:ILE:HD11  | 2.00                     | 0.42              |
| 21:P:44:ILE:HD11  | 21:P:69:VAL:HG11  | 2.02                     | 0.42              |
| 22:Q:106:GLY:N    | 22:Q:136:GLU:OE1  | 2.53                     | 0.42              |
| 28:W:31:U:OP1     | 32:a:137:LYS:NZ   | 2.48                     | 0.42              |
| 28:W:563:G:O2'    | 28:W:564:A:O5'    | 2.37                     | 0.42              |
| 45:n:124:ARG:HB2  | 45:n:131:VAL:HG12 | 2.02                     | 0.42              |
| 52:x:49:THR:HG23  | 52:x:50:TYR:CD1   | 2.54                     | 0.42              |
| 21:P:36:PRO:O     | 21:P:42:ARG:NH2   | 2.49                     | 0.42              |
| 24:S:35:GLU:N     | 24:S:35:GLU:OE1   | 2.52                     | 0.42              |
| 42:k:48:ASP:OD1   | 42:k:48:ASP:N     | 2.51                     | 0.42              |
| 53:y:57:A:O2'     | 53:y:58:A:O3'     | 2.38                     | 0.42              |
| 1:5:44:LEU:O      | 1:5:48:THR:N      | 2.52                     | 0.42              |
| 6:A:246:TRP:NE1   | 15:J:726:LEU:O    | 2.53                     | 0.42              |
| 7:B:36:GLN:O      | 7:B:40:ASN:N      | 2.52                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:I:359:LEU:N    | 14:I:369:GLN:O    | 2.51                     | 0.42              |
| 21:P:146:ARG:HD3  | 28:W:1121:G:H21   | 1.85                     | 0.42              |
| 28:W:1226:G:N1    | 28:W:1639:G:OP2   | 2.45                     | 0.42              |
| 42:k:113:PHE:HA   | 42:k:120:ILE:HG22 | 2.01                     | 0.42              |
| 52:x:12:ASN:O     | 52:x:13:PRO:C     | 2.63                     | 0.42              |
| 28:W:301:A:O2'    | 35:d:73:THR:N     | 2.50                     | 0.42              |
| 38:g:43:GLU:O     | 38:g:45:ARG:N     | 2.53                     | 0.42              |
| 42:k:5:MET:HE3    | 42:k:6:THR:O      | 2.20                     | 0.42              |
| 47:p:124:ASP:OD1  | 47:p:124:ASP:N    | 2.49                     | 0.42              |
| 9:D:23:ASN:HB2    | 9:D:37:LEU:HD11   | 2.02                     | 0.42              |
| 15:J:504:LEU:HD22 | 15:J:564:ILE:HG23 | 2.00                     | 0.42              |
| 19:N:56:CYS:SG    | 19:N:57:GLY:N     | 2.93                     | 0.42              |
| 12:G:82:ARG:HA    | 33:b:81:ALA:HB3   | 2.02                     | 0.41              |
| 15:J:743:ALA:HB1  | 15:J:751:THR:OG1  | 2.20                     | 0.41              |
| 20:O:220:ASP:OD1  | 20:O:220:ASP:N    | 2.48                     | 0.41              |
| 13:H:81:GLU:O     | 13:H:85:LEU:HD13  | 2.20                     | 0.41              |
| 28:W:1665:G:C5    | 43:l:88:MET:HE1   | 2.56                     | 0.41              |
| 38:g:113:ILE:HD11 | 38:g:120:LEU:HB2  | 2.01                     | 0.41              |
| 39:h:193:ASP:OD1  | 39:h:193:ASP:N    | 2.53                     | 0.41              |
| 52:x:20:ALA:CB    | 52:x:22:PRO:N     | 2.83                     | 0.41              |
| 14:I:667:VAL:HG21 | 14:I:702:LEU:HD11 | 2.00                     | 0.41              |
| 27:V:32:ASP:N     | 27:V:32:ASP:OD1   | 2.53                     | 0.41              |
| 28:W:1583:C:OP2   | 28:W:1584:G:O2'   | 2.24                     | 0.41              |
| 4:8:72:VAL:N      | 4:8:75:ARG:O      | 2.46                     | 0.41              |
| 14:I:566:ILE:HD12 | 14:I:587:ILE:HD12 | 2.03                     | 0.41              |
| 28:W:1165:G:N1    | 32:a:20:GLN:OE1   | 2.46                     | 0.41              |
| 34:c:54:ASP:OD2   | 34:c:55:ASP:N     | 2.53                     | 0.41              |
| 39:h:16:ILE:HD12  | 46:o:50:ILE:HD11  | 2.02                     | 0.41              |
| 42:k:190:GLY:HA3  | 42:k:217:MET:HE1  | 2.02                     | 0.41              |
| 14:I:184:ASP:OD1  | 14:I:184:ASP:N    | 2.52                     | 0.41              |
| 14:I:330:GLU:OE1  | 14:I:332:ARG:NH2  | 2.53                     | 0.41              |
| 15:J:743:ALA:O    | 15:J:747:GLY:N    | 2.48                     | 0.41              |
| 18:M:67:THR:OG1   | 18:M:70:LYS:O     | 2.37                     | 0.41              |
| 28:W:172:U:OP1    | 28:W:314:U:O2'    | 2.39                     | 0.41              |
| 30:Y:43:PRO:HD2   | 30:Y:46:ILE:HD12  | 2.02                     | 0.41              |
| 42:k:189:ILE:HG22 | 42:k:189:ILE:O    | 2.20                     | 0.41              |
| 6:A:326:THR:HG21  | 6:A:374:MET:SD    | 2.60                     | 0.41              |
| 9:D:231:ALA:HA    | 10:E:267:PRO:CB   | 2.28                     | 0.41              |
| 15:J:410:ASP:OD1  | 15:J:485:ARG:NH2  | 2.52                     | 0.41              |
| 29:X:13:GLN:NE2   | 29:X:63:THR:OG1   | 2.54                     | 0.41              |
| 34:c:30:CYS:SG    | 34:c:31:SER:N     | 2.94                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 48:q:89:VAL:O     | 48:q:89:VAL:HG22  | 2.20                     | 0.41              |
| 52:x:199:LEU:O    | 52:x:335:TYR:N    | 2.53                     | 0.41              |
| 9:D:234:ARG:NH1   | 53:y:73:C:H5'     | 2.33                     | 0.41              |
| 11:F:110:PHE:O    | 11:F:123:SER:N    | 2.53                     | 0.41              |
| 14:I:724:LEU:O    | 14:I:725:LYS:C    | 2.64                     | 0.41              |
| 28:W:66:G:H8      | 28:W:82:G:H21     | 1.69                     | 0.41              |
| 43:l:73:GLY:O     | 43:l:76:THR:OG1   | 2.31                     | 0.41              |
| 28:W:1397:U:O2    | 28:W:1399:C:N4    | 2.53                     | 0.41              |
| 28:W:1529:C:O2'   | 43:l:87:VAL:O     | 2.35                     | 0.41              |
| 28:W:1650:A:H1'   | 28:W:1675:A:C4    | 2.56                     | 0.41              |
| 38:g:102:GLU:O    | 38:g:106:LYS:N    | 2.50                     | 0.41              |
| 5:9:17:ARG:NH2    | 28:W:1174:U:OP1   | 2.54                     | 0.41              |
| 6:A:342:LEU:HG    | 6:A:344:MET:HE2   | 2.03                     | 0.41              |
| 6:A:387:VAL:HA    | 6:A:390:LEU:HD23  | 2.03                     | 0.41              |
| 6:A:483:ARG:N     | 6:A:492:SER:O     | 2.48                     | 0.41              |
| 13:H:120:ASN:OD1  | 13:H:121:SER:N    | 2.53                     | 0.41              |
| 28:W:288:G:N1     | 28:W:296:U:C2     | 2.89                     | 0.41              |
| 43:l:6:VAL:HG21   | 43:l:65:TYR:CZ    | 2.55                     | 0.41              |
| 6:A:90:VAL:O      | 6:A:94:LEU:HD23   | 2.21                     | 0.41              |
| 18:M:77:CYS:O     | 52:x:81:GLN:NE2   | 2.49                     | 0.41              |
| 21:P:52:THR:HG23  | 21:P:57:ILE:HA    | 2.03                     | 0.41              |
| 30:Y:118:GLU:OE1  | 30:Y:118:GLU:N    | 2.46                     | 0.41              |
| 39:h:50:ILE:HD12  | 39:h:86:LEU:HD21  | 2.03                     | 0.41              |
| 42:k:145:GLU:OE1  | 42:k:184:LEU:HD23 | 2.21                     | 0.41              |
| 52:x:381:MET:N    | 52:x:389:SER:O    | 2.49                     | 0.41              |
| 6:A:327:LEU:HD12  | 6:A:394:LEU:CD1   | 2.51                     | 0.40              |
| 9:D:229:LEU:O     | 9:D:230:ILE:C     | 2.63                     | 0.40              |
| 10:E:303:LYS:HD3  | 10:E:309:LEU:HD23 | 2.02                     | 0.40              |
| 28:W:1215:C:N4    | 28:W:1221:G:H22   | 2.19                     | 0.40              |
| 14:I:505:ARG:NH1  | 14:I:506:VAL:O    | 2.54                     | 0.40              |
| 28:W:1096:G:OP1   | 34:c:20:ARG:NH1   | 2.54                     | 0.40              |
| 52:x:20:ALA:HB1   | 52:x:21:VAL:CG2   | 2.41                     | 0.40              |
| 3:7:305:TYR:CB    | 3:7:310:LEU:HD22  | 2.51                     | 0.40              |
| 9:D:232:PRO:HD2   | 10:E:267:PRO:CA   | 2.49                     | 0.40              |
| 18:M:35:VAL:HG11  | 18:M:63:LEU:HD11  | 2.03                     | 0.40              |
| 21:P:44:ILE:HD11  | 21:P:69:VAL:HG21  | 2.03                     | 0.40              |
| 35:d:133:GLU:N    | 35:d:135:GLU:OE1  | 2.54                     | 0.40              |
| 38:g:100:VAL:HG23 | 38:g:101:ASP:N    | 2.37                     | 0.40              |
| 6:A:525:ALA:O     | 6:A:529:VAL:HG23  | 2.22                     | 0.40              |
| 15:J:459:MET:HE1  | 15:J:472:HIS:HB3  | 2.02                     | 0.40              |
| 30:Y:100:ARG:HB2  | 30:Y:114:ILE:HD12 | 2.04                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:I:380:ASP:N    | 14:I:380:ASP:OD1  | 2.53                     | 0.40              |
| 14:I:533:THR:HG23 | 14:I:533:THR:O    | 2.22                     | 0.40              |
| 20:O:113:GLN:HG2  | 20:O:122:THR:HG22 | 2.02                     | 0.40              |
| 28:W:1013:U:OP1   | 28:W:1129:G:O2'   | 2.39                     | 0.40              |
| 42:k:4:GLN:N      | 42:k:4:GLN:OE1    | 2.54                     | 0.40              |
| 42:k:266:ILE:HG23 | 42:k:266:ILE:O    | 2.20                     | 0.40              |
| 52:x:413:LEU:HD22 | 52:x:420:VAL:HG21 | 2.03                     | 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 |     |
|-----|-------|----------------|-----------|----------|----------|-------------|-----|
| 1   | 5     | 435/445 (98%)  | 419 (96%) | 16 (4%)  | 0        | 100         | 100 |
| 2   | 6     | 267/357 (75%)  | 252 (94%) | 15 (6%)  | 0        | 100         | 100 |
| 3   | 7     | 75/320 (23%)   | 66 (88%)  | 9 (12%)  | 0        | 100         | 100 |
| 4   | 8     | 312/352 (89%)  | 294 (94%) | 17 (5%)  | 1 (0%)   | 36          | 67  |
| 5   | 9     | 22/25 (88%)    | 22 (100%) | 0        | 0        | 100         | 100 |
| 6   | A     | 731/1382 (53%) | 697 (95%) | 32 (4%)  | 2 (0%)   | 36          | 67  |
| 7   | B     | 213/218 (98%)  | 195 (92%) | 18 (8%)  | 0        | 100         | 100 |
| 8   | C     | 360/374 (96%)  | 340 (94%) | 19 (5%)  | 1 (0%)   | 36          | 67  |
| 9   | D     | 276/315 (88%)  | 257 (93%) | 17 (6%)  | 2 (1%)   | 18          | 51  |
| 10  | E     | 462/472 (98%)  | 442 (96%) | 19 (4%)  | 1 (0%)   | 43          | 74  |
| 11  | F     | 323/325 (99%)  | 290 (90%) | 33 (10%) | 0        | 100         | 100 |
| 12  | G     | 95/144 (66%)   | 87 (92%)  | 8 (8%)   | 0        | 100         | 100 |
| 13  | H     | 147/431 (34%)  | 139 (95%) | 8 (5%)   | 0        | 100         | 100 |
| 14  | I     | 571/814 (70%)  | 531 (93%) | 38 (7%)  | 2 (0%)   | 30          | 62  |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 15  | J     | 683/913 (75%) | 650 (95%) | 32 (5%) | 1 (0%)   | 48          | 79  |
| 16  | K     | 529/564 (94%) | 504 (95%) | 24 (4%) | 1 (0%)   | 43          | 74  |
| 17  | L     | 172/194 (89%) | 166 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 18  | M     | 79/84 (94%)   | 75 (95%)  | 4 (5%)  | 0        | 100         | 100 |
| 19  | N     | 79/83 (95%)   | 73 (92%)  | 6 (8%)  | 0        | 100         | 100 |
| 20  | O     | 218/293 (74%) | 212 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 21  | P     | 209/264 (79%) | 199 (95%) | 10 (5%) | 0        | 100         | 100 |
| 22  | Q     | 212/295 (72%) | 198 (93%) | 14 (7%) | 0        | 100         | 100 |
| 23  | R     | 97/115 (84%)  | 94 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 24  | S     | 228/249 (92%) | 219 (96%) | 9 (4%)  | 0        | 100         | 100 |
| 25  | T     | 131/151 (87%) | 123 (94%) | 8 (6%)  | 0        | 100         | 100 |
| 26  | U     | 137/333 (41%) | 126 (92%) | 11 (8%) | 0        | 100         | 100 |
| 27  | V     | 148/151 (98%) | 146 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 29  | X     | 138/158 (87%) | 135 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 30  | Y     | 254/263 (97%) | 245 (96%) | 9 (4%)  | 0        | 100         | 100 |
| 31  | Z     | 175/194 (90%) | 173 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 32  | a     | 138/143 (96%) | 135 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 33  | b     | 43/59 (73%)   | 41 (95%)  | 2 (5%)  | 0        | 100         | 100 |
| 34  | c     | 127/130 (98%) | 124 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 35  | d     | 194/208 (93%) | 190 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 36  | e     | 123/133 (92%) | 120 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 37  | f     | 180/204 (88%) | 167 (93%) | 13 (7%) | 0        | 100         | 100 |
| 38  | g     | 139/146 (95%) | 131 (94%) | 8 (6%)  | 0        | 100         | 100 |
| 39  | h     | 225/243 (93%) | 220 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 40  | i     | 97/165 (59%)  | 89 (92%)  | 8 (8%)  | 0        | 100         | 100 |
| 41  | j     | 108/145 (74%) | 103 (95%) | 5 (5%)  | 0        | 100         | 100 |
| 42  | k     | 311/317 (98%) | 293 (94%) | 18 (6%) | 0        | 100         | 100 |
| 43  | l     | 140/145 (97%) | 134 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 44  | m     | 64/125 (51%)  | 62 (97%)  | 2 (3%)  | 0        | 100         | 100 |
| 45  | n     | 140/151 (93%) | 129 (92%) | 11 (8%) | 0        | 100         | 100 |
| 46  | o     | 48/56 (86%)   | 47 (98%)  | 1 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 47  | p     | 49/156 (31%)      | 45 (92%)    | 4 (8%)   | 0        | 100         | 100 |
| 48  | q     | 120/132 (91%)     | 107 (89%)   | 13 (11%) | 0        | 100         | 100 |
| 49  | s     | 61/69 (88%)       | 52 (85%)    | 9 (15%)  | 0        | 100         | 100 |
| 50  | v     | 127/135 (94%)     | 117 (92%)   | 9 (7%)   | 1 (1%)   | 16          | 49  |
| 51  | w     | 101/119 (85%)     | 94 (93%)    | 7 (7%)   | 0        | 100         | 100 |
| 52  | x     | 434/548 (79%)     | 361 (83%)   | 68 (16%) | 5 (1%)   | 10          | 41  |
| 55  | 1     | 369/406 (91%)     | 304 (82%)   | 59 (16%) | 6 (2%)   | 7           | 36  |
| 55  | 3     | 376/406 (93%)     | 353 (94%)   | 22 (6%)  | 1 (0%)   | 36          | 67  |
| 56  | 2     | 235/1404 (17%)    | 216 (92%)   | 18 (8%)  | 1 (0%)   | 30          | 62  |
| All | All   | 11727/16023 (73%) | 11003 (94%) | 699 (6%) | 25 (0%)  | 44          | 74  |

All (25) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 8     | 271 | GLN  |
| 9   | D     | 232 | PRO  |
| 9   | D     | 233 | PRO  |
| 52  | x     | 13  | PRO  |
| 52  | x     | 21  | VAL  |
| 55  | 3     | 399 | PRO  |
| 55  | 1     | 152 | PRO  |
| 55  | 1     | 159 | PRO  |
| 56  | 2     | 833 | PRO  |
| 6   | A     | 536 | VAL  |
| 6   | A     | 656 | ILE  |
| 52  | x     | 7   | PRO  |
| 55  | 1     | 97  | ASP  |
| 55  | 1     | 340 | GLN  |
| 10  | E     | 324 | GLU  |
| 15  | J     | 121 | TRP  |
| 52  | x     | 19  | CYS  |
| 14  | I     | 487 | LYS  |
| 52  | x     | 258 | CYS  |
| 8   | C     | 345 | GLN  |
| 14  | I     | 722 | LYS  |
| 16  | K     | 519 | VAL  |
| 50  | v     | 96  | ILE  |
| 55  | 1     | 272 | ILE  |
| 55  | 1     | 190 | ARG  |

### 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 |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 3   | 7     | 64/277 (23%)   | 64 (100%)  | 0        | 100         | 100 |
| 5   | 9     | 23/24 (96%)    | 23 (100%)  | 0        | 100         | 100 |
| 6   | A     | 495/1259 (39%) | 493 (100%) | 2 (0%)   | 84          | 81  |
| 9   | D     | 249/280 (89%)  | 246 (99%)  | 3 (1%)   | 63          | 73  |
| 10  | E     | 394/397 (99%)  | 394 (100%) | 0        | 100         | 100 |
| 12  | G     | 83/123 (68%)   | 83 (100%)  | 0        | 100         | 100 |
| 13  | H     | 133/389 (34%)  | 133 (100%) | 0        | 100         | 100 |
| 14  | I     | 470/702 (67%)  | 470 (100%) | 0        | 100         | 100 |
| 15  | J     | 511/811 (63%)  | 509 (100%) | 2 (0%)   | 84          | 81  |
| 17  | L     | 160/174 (92%)  | 160 (100%) | 0        | 100         | 100 |
| 18  | M     | 73/76 (96%)    | 73 (100%)  | 0        | 100         | 100 |
| 19  | N     | 65/67 (97%)    | 65 (100%)  | 0        | 100         | 100 |
| 20  | O     | 186/225 (83%)  | 186 (100%) | 0        | 100         | 100 |
| 21  | P     | 192/231 (83%)  | 192 (100%) | 0        | 100         | 100 |
| 22  | Q     | 180/243 (74%)  | 180 (100%) | 0        | 100         | 100 |
| 23  | R     | 86/98 (88%)    | 86 (100%)  | 0        | 100         | 100 |
| 24  | S     | 200/218 (92%)  | 200 (100%) | 0        | 100         | 100 |
| 25  | T     | 104/119 (87%)  | 104 (100%) | 0        | 100         | 100 |
| 27  | V     | 130/131 (99%)  | 130 (100%) | 0        | 100         | 100 |
| 29  | X     | 129/142 (91%)  | 129 (100%) | 0        | 100         | 100 |
| 30  | Y     | 220/225 (98%)  | 220 (100%) | 0        | 100         | 100 |
| 31  | Z     | 158/168 (94%)  | 158 (100%) | 0        | 100         | 100 |
| 32  | a     | 112/115 (97%)  | 112 (100%) | 0        | 100         | 100 |
| 33  | b     | 38/48 (79%)    | 38 (100%)  | 0        | 100         | 100 |
| 34  | c     | 112/113 (99%)  | 112 (100%) | 0        | 100         | 100 |
| 35  | d     | 172/180 (96%)  | 172 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 36  | e     | 107/115 (93%)   | 107 (100%)  | 0        | 100         | 100 |
| 37  | f     | 156/170 (92%)   | 156 (100%)  | 0        | 100         | 100 |
| 38  | g     | 117/121 (97%)   | 117 (100%)  | 0        | 100         | 100 |
| 39  | h     | 190/202 (94%)   | 190 (100%)  | 0        | 100         | 100 |
| 40  | i     | 90/136 (66%)    | 90 (100%)   | 0        | 100         | 100 |
| 41  | j     | 100/130 (77%)   | 100 (100%)  | 0        | 100         | 100 |
| 42  | k     | 272/275 (99%)   | 272 (100%)  | 0        | 100         | 100 |
| 43  | l     | 112/115 (97%)   | 112 (100%)  | 0        | 100         | 100 |
| 44  | m     | 58/103 (56%)    | 58 (100%)   | 0        | 100         | 100 |
| 45  | n     | 123/131 (94%)   | 123 (100%)  | 0        | 100         | 100 |
| 46  | o     | 44/49 (90%)     | 44 (100%)   | 0        | 100         | 100 |
| 47  | p     | 47/140 (34%)    | 47 (100%)   | 0        | 100         | 100 |
| 48  | q     | 104/108 (96%)   | 104 (100%)  | 0        | 100         | 100 |
| 49  | s     | 56/62 (90%)     | 56 (100%)   | 0        | 100         | 100 |
| 50  | v     | 119/122 (98%)   | 119 (100%)  | 0        | 100         | 100 |
| 51  | w     | 94/107 (88%)    | 94 (100%)   | 0        | 100         | 100 |
| 52  | x     | 205/494 (42%)   | 205 (100%)  | 0        | 100         | 100 |
| All | All   | 6733/9415 (72%) | 6726 (100%) | 7 (0%)   | 87          | 87  |

All (7) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | A     | 285 | LYS  |
| 6   | A     | 286 | SER  |
| 9   | D     | 122 | THR  |
| 9   | D     | 123 | LYS  |
| 9   | D     | 234 | ARG  |
| 15  | J     | 120 | LEU  |
| 15  | J     | 123 | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | A     | 47  | HIS  |
| 6   | A     | 466 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | D     | 228 | ASN  |
| 10  | E     | 65  | HIS  |
| 10  | E     | 190 | ASN  |
| 13  | H     | 144 | ASN  |
| 15  | J     | 355 | GLN  |
| 15  | J     | 377 | ASN  |
| 15  | J     | 600 | HIS  |
| 15  | J     | 630 | HIS  |
| 15  | J     | 753 | HIS  |
| 17  | L     | 126 | HIS  |
| 17  | L     | 193 | GLN  |
| 18  | M     | 51  | GLN  |
| 21  | P     | 124 | HIS  |
| 21  | P     | 186 | ASN  |
| 21  | P     | 208 | HIS  |
| 22  | Q     | 132 | GLN  |
| 23  | R     | 17  | HIS  |
| 25  | T     | 113 | GLN  |
| 30  | Y     | 17  | HIS  |
| 30  | Y     | 36  | HIS  |
| 30  | Y     | 216 | ASN  |
| 31  | Z     | 113 | GLN  |
| 32  | a     | 61  | GLN  |
| 34  | c     | 56  | HIS  |
| 36  | e     | 85  | ASN  |
| 37  | f     | 95  | HIS  |
| 42  | k     | 104 | HIS  |
| 44  | m     | 106 | GLN  |
| 45  | n     | 72  | GLN  |
| 45  | n     | 73  | ASN  |
| 45  | n     | 135 | HIS  |
| 50  | v     | 118 | GLN  |
| 52  | x     | 31  | GLN  |
| 52  | x     | 326 | GLN  |
| 52  | x     | 392 | ASN  |
| 52  | x     | 456 | HIS  |
| 52  | x     | 481 | ASN  |

### 5.3.3 RNA ⓘ

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| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 28  | W     | 1706/1719 (99%) | 467 (27%)         | 13 (0%)         |
| 53  | y     | 74/75 (98%)     | 33 (44%)          | 0               |
| 54  | z     | 49/207 (23%)    | 32 (65%)          | 0               |
| All | All   | 1829/2001 (91%) | 532 (29%)         | 13 (0%)         |

All (532) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | W     | 2   | A    |
| 28  | W     | 4   | C    |
| 28  | W     | 17  | C    |
| 28  | W     | 20  | G    |
| 28  | W     | 23  | G    |
| 28  | W     | 27  | A2M  |
| 28  | W     | 33  | G    |
| 28  | W     | 41  | G    |
| 28  | W     | 44  | U    |
| 28  | W     | 46  | A    |
| 28  | W     | 56  | G    |
| 28  | W     | 59  | U    |
| 28  | W     | 62  | G    |
| 28  | W     | 65  | C    |
| 28  | W     | 66  | G    |
| 28  | W     | 67  | C    |
| 28  | W     | 68  | A    |
| 28  | W     | 69  | C    |
| 28  | W     | 70  | G    |
| 28  | W     | 71  | G    |
| 28  | W     | 74  | G    |
| 28  | W     | 77  | A    |
| 28  | W     | 78  | C    |
| 28  | W     | 79  | A    |
| 28  | W     | 83  | A    |
| 28  | W     | 85  | A    |
| 28  | W     | 86  | C    |
| 28  | W     | 88  | G    |
| 28  | W     | 91  | A    |
| 28  | W     | 92  | A    |
| 28  | W     | 103 | A    |
| 28  | W     | 110 | U    |
| 28  | W     | 115 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | W     | 116 | OMU  |
| 28  | W     | 126 | G    |
| 28  | W     | 127 | C    |
| 28  | W     | 129 | C    |
| 28  | W     | 141 | A    |
| 28  | W     | 142 | C    |
| 28  | W     | 144 | U    |
| 28  | W     | 146 | G    |
| 28  | W     | 153 | G    |
| 28  | W     | 155 | G    |
| 28  | W     | 161 | U    |
| 28  | W     | 162 | C    |
| 28  | W     | 163 | U    |
| 28  | W     | 164 | A    |
| 28  | W     | 166 | A2M  |
| 28  | W     | 167 | G    |
| 28  | W     | 168 | C    |
| 28  | W     | 169 | U    |
| 28  | W     | 170 | A    |
| 28  | W     | 182 | C    |
| 28  | W     | 183 | G    |
| 28  | W     | 190 | G    |
| 28  | W     | 197 | U    |
| 28  | W     | 198 | U    |
| 28  | W     | 199 | C    |
| 28  | W     | 203 | G    |
| 28  | W     | 204 | G    |
| 28  | W     | 206 | G    |
| 28  | W     | 208 | G    |
| 28  | W     | 213 | G    |
| 28  | W     | 291 | G    |
| 28  | W     | 292 | A    |
| 28  | W     | 295 | C    |
| 28  | W     | 297 | A    |
| 28  | W     | 300 | U    |
| 28  | W     | 302 | A    |
| 28  | W     | 306 | C    |
| 28  | W     | 307 | G    |
| 28  | W     | 309 | G    |
| 28  | W     | 312 | G    |
| 28  | W     | 313 | A    |
| 28  | W     | 315 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | W     | 316 | G    |
| 28  | W     | 318 | A    |
| 28  | W     | 319 | C    |
| 28  | W     | 320 | G    |
| 28  | W     | 323 | C    |
| 28  | W     | 324 | C    |
| 28  | W     | 325 | C    |
| 28  | W     | 326 | C    |
| 28  | W     | 327 | G    |
| 28  | W     | 329 | G    |
| 28  | W     | 330 | G    |
| 28  | W     | 335 | G    |
| 28  | W     | 336 | A    |
| 28  | W     | 337 | C    |
| 28  | W     | 339 | A    |
| 28  | W     | 347 | G    |
| 28  | W     | 351 | G    |
| 28  | W     | 362 | C    |
| 28  | W     | 363 | A    |
| 28  | W     | 364 | A    |
| 28  | W     | 367 | U    |
| 28  | W     | 369 | C    |
| 28  | W     | 370 | G    |
| 28  | W     | 380 | G    |
| 28  | W     | 381 | C    |
| 28  | W     | 385 | G    |
| 28  | W     | 386 | C    |
| 28  | W     | 387 | C    |
| 28  | W     | 409 | C    |
| 28  | W     | 417 | C    |
| 28  | W     | 421 | G    |
| 28  | W     | 448 | A    |
| 28  | W     | 450 | C    |
| 28  | W     | 452 | G    |
| 28  | W     | 465 | A    |
| 28  | W     | 472 | C    |
| 28  | W     | 473 | A    |
| 28  | W     | 474 | G    |
| 28  | W     | 482 | G    |
| 28  | W     | 487 | U    |
| 28  | W     | 492 | C    |
| 28  | W     | 501 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | W     | 502 | C    |
| 28  | W     | 503 | C    |
| 28  | W     | 509 | OMG  |
| 28  | W     | 525 | A    |
| 28  | W     | 533 | A    |
| 28  | W     | 535 | G    |
| 28  | W     | 536 | A    |
| 28  | W     | 537 | C    |
| 28  | W     | 538 | U    |
| 28  | W     | 540 | U    |
| 28  | W     | 542 | U    |
| 28  | W     | 546 | G    |
| 28  | W     | 553 | U    |
| 28  | W     | 554 | A    |
| 28  | W     | 556 | U    |
| 28  | W     | 557 | U    |
| 28  | W     | 558 | G    |
| 28  | W     | 559 | G    |
| 28  | W     | 560 | A    |
| 28  | W     | 563 | G    |
| 28  | W     | 564 | A    |
| 28  | W     | 566 | U    |
| 28  | W     | 568 | C    |
| 28  | W     | 587 | A    |
| 28  | W     | 589 | G    |
| 28  | W     | 591 | U    |
| 28  | W     | 606 | G    |
| 28  | W     | 607 | U    |
| 28  | W     | 608 | C    |
| 28  | W     | 612 | PSU  |
| 28  | W     | 614 | C    |
| 28  | W     | 615 | C    |
| 28  | W     | 626 | G    |
| 28  | W     | 627 | U    |
| 28  | W     | 628 | A    |
| 28  | W     | 629 | A    |
| 28  | W     | 631 | U    |
| 28  | W     | 643 | A    |
| 28  | W     | 655 | A    |
| 28  | W     | 657 | U    |
| 28  | W     | 660 | C    |
| 28  | W     | 668 | A2M  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | W     | 669 | A    |
| 28  | W     | 671 | A    |
| 28  | W     | 672 | A    |
| 28  | W     | 673 | G    |
| 28  | W     | 675 | U    |
| 28  | W     | 687 | C    |
| 28  | W     | 688 | U    |
| 28  | W     | 689 | U    |
| 28  | W     | 692 | G    |
| 28  | W     | 693 | A    |
| 28  | W     | 697 | G    |
| 28  | W     | 749 | U    |
| 28  | W     | 751 | G    |
| 28  | W     | 752 | G    |
| 28  | W     | 753 | C    |
| 28  | W     | 791 | C    |
| 28  | W     | 792 | C    |
| 28  | W     | 797 | C    |
| 28  | W     | 798 | G    |
| 28  | W     | 809 | A    |
| 28  | W     | 821 | G    |
| 28  | W     | 822 | PSU  |
| 28  | W     | 827 | A    |
| 28  | W     | 830 | A    |
| 28  | W     | 836 | G    |
| 28  | W     | 837 | A    |
| 28  | W     | 838 | G    |
| 28  | W     | 839 | C    |
| 28  | W     | 841 | G    |
| 28  | W     | 847 | A    |
| 28  | W     | 870 | A    |
| 28  | W     | 872 | A    |
| 28  | W     | 873 | G    |
| 28  | W     | 881 | G    |
| 28  | W     | 886 | A    |
| 28  | W     | 887 | U    |
| 28  | W     | 890 | U    |
| 28  | W     | 891 | G    |
| 28  | W     | 892 | U    |
| 28  | W     | 893 | U    |
| 28  | W     | 894 | G    |
| 28  | W     | 895 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 28  | W     | 896  | U    |
| 28  | W     | 897  | U    |
| 28  | W     | 898  | U    |
| 28  | W     | 899  | U    |
| 28  | W     | 900  | C    |
| 28  | W     | 901  | G    |
| 28  | W     | 902  | G    |
| 28  | W     | 903  | A    |
| 28  | W     | 905  | C    |
| 28  | W     | 908  | A    |
| 28  | W     | 913  | A    |
| 28  | W     | 920  | A    |
| 28  | W     | 922  | A    |
| 28  | W     | 930  | C    |
| 28  | W     | 933  | G    |
| 28  | W     | 953  | C    |
| 28  | W     | 955  | A    |
| 28  | W     | 965  | U    |
| 28  | W     | 970  | G    |
| 28  | W     | 971  | G    |
| 28  | W     | 972  | A    |
| 28  | W     | 976  | G    |
| 28  | W     | 978  | G    |
| 28  | W     | 990  | A    |
| 28  | W     | 992  | A    |
| 28  | W     | 1008 | A    |
| 28  | W     | 1017 | U    |
| 28  | W     | 1023 | A    |
| 28  | W     | 1031 | A2M  |
| 28  | W     | 1047 | C    |
| 28  | W     | 1061 | U    |
| 28  | W     | 1062 | A    |
| 28  | W     | 1081 | PSU  |
| 28  | W     | 1083 | A    |
| 28  | W     | 1085 | C    |
| 28  | W     | 1108 | G    |
| 28  | W     | 1109 | C    |
| 28  | W     | 1112 | U    |
| 28  | W     | 1113 | A    |
| 28  | W     | 1115 | U    |
| 28  | W     | 1116 | C    |
| 28  | W     | 1117 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 28  | W     | 1118 | C    |
| 28  | W     | 1119 | A    |
| 28  | W     | 1120 | U    |
| 28  | W     | 1121 | G    |
| 28  | W     | 1123 | C    |
| 28  | W     | 1125 | C    |
| 28  | W     | 1126 | G    |
| 28  | W     | 1138 | C    |
| 28  | W     | 1153 | C    |
| 28  | W     | 1154 | U    |
| 28  | W     | 1181 | A    |
| 28  | W     | 1195 | A    |
| 28  | W     | 1200 | A    |
| 28  | W     | 1206 | G    |
| 28  | W     | 1207 | G    |
| 28  | W     | 1208 | A    |
| 28  | W     | 1210 | G    |
| 28  | W     | 1213 | C    |
| 28  | W     | 1214 | A    |
| 28  | W     | 1215 | C    |
| 28  | W     | 1216 | C    |
| 28  | W     | 1217 | A    |
| 28  | W     | 1222 | G    |
| 28  | W     | 1223 | A    |
| 28  | W     | 1224 | G    |
| 28  | W     | 1241 | A    |
| 28  | W     | 1242 | U    |
| 28  | W     | 1248 | C4J  |
| 28  | W     | 1249 | C    |
| 28  | W     | 1251 | A    |
| 28  | W     | 1253 | A    |
| 28  | W     | 1256 | G    |
| 28  | W     | 1257 | G    |
| 28  | W     | 1258 | A    |
| 28  | W     | 1274 | G    |
| 28  | W     | 1275 | G    |
| 28  | W     | 1285 | G    |
| 28  | W     | 1288 | U    |
| 28  | W     | 1289 | U    |
| 28  | W     | 1292 | C    |
| 28  | W     | 1295 | A    |
| 28  | W     | 1298 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 28  | W     | 1301 | A    |
| 28  | W     | 1302 | G    |
| 28  | W     | 1303 | C    |
| 28  | W     | 1307 | U    |
| 28  | W     | 1308 | U    |
| 28  | W     | 1309 | C    |
| 28  | W     | 1311 | C    |
| 28  | W     | 1312 | G    |
| 28  | W     | 1314 | U    |
| 28  | W     | 1315 | U    |
| 28  | W     | 1322 | G    |
| 28  | W     | 1326 | U    |
| 28  | W     | 1342 | U    |
| 28  | W     | 1356 | G    |
| 28  | W     | 1371 | U    |
| 28  | W     | 1372 | U    |
| 28  | W     | 1378 | A    |
| 28  | W     | 1389 | C    |
| 28  | W     | 1390 | U    |
| 28  | W     | 1394 | G    |
| 28  | W     | 1396 | A    |
| 28  | W     | 1397 | U    |
| 28  | W     | 1398 | G    |
| 28  | W     | 1401 | A    |
| 28  | W     | 1402 | A    |
| 28  | W     | 1403 | C    |
| 28  | W     | 1404 | U    |
| 28  | W     | 1406 | G    |
| 28  | W     | 1407 | U    |
| 28  | W     | 1417 | C    |
| 28  | W     | 1419 | C    |
| 28  | W     | 1420 | G    |
| 28  | W     | 1421 | A    |
| 28  | W     | 1422 | G    |
| 28  | W     | 1423 | C    |
| 28  | W     | 1424 | G    |
| 28  | W     | 1428 | G    |
| 28  | W     | 1429 | G    |
| 28  | W     | 1433 | C    |
| 28  | W     | 1434 | C    |
| 28  | W     | 1435 | C    |
| 28  | W     | 1436 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 28  | W     | 1437 | C    |
| 28  | W     | 1438 | A    |
| 28  | W     | 1441 | U    |
| 28  | W     | 1443 | C    |
| 28  | W     | 1450 | G    |
| 28  | W     | 1451 | G    |
| 28  | W     | 1454 | A    |
| 28  | W     | 1462 | U    |
| 28  | W     | 1463 | U    |
| 28  | W     | 1464 | C    |
| 28  | W     | 1476 | A    |
| 28  | W     | 1477 | U    |
| 28  | W     | 1478 | U    |
| 28  | W     | 1479 | G    |
| 28  | W     | 1482 | C    |
| 28  | W     | 1483 | A    |
| 28  | W     | 1484 | A    |
| 28  | W     | 1489 | A    |
| 28  | W     | 1490 | G    |
| 28  | W     | 1494 | U    |
| 28  | W     | 1497 | G    |
| 28  | W     | 1498 | A    |
| 28  | W     | 1508 | A    |
| 28  | W     | 1515 | G    |
| 28  | W     | 1521 | C    |
| 28  | W     | 1533 | A    |
| 28  | W     | 1535 | U    |
| 28  | W     | 1536 | G    |
| 28  | W     | 1537 | A    |
| 28  | W     | 1538 | C    |
| 28  | W     | 1539 | U    |
| 28  | W     | 1540 | G    |
| 28  | W     | 1542 | C    |
| 28  | W     | 1543 | U    |
| 28  | W     | 1544 | C    |
| 28  | W     | 1545 | A    |
| 28  | W     | 1552 | G    |
| 28  | W     | 1553 | C    |
| 28  | W     | 1557 | C    |
| 28  | W     | 1560 | U    |
| 28  | W     | 1563 | G    |
| 28  | W     | 1565 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 28  | W     | 1566 | G    |
| 28  | W     | 1567 | G    |
| 28  | W     | 1574 | C    |
| 28  | W     | 1580 | A    |
| 28  | W     | 1582 | C    |
| 28  | W     | 1588 | A    |
| 28  | W     | 1590 | C    |
| 28  | W     | 1591 | C    |
| 28  | W     | 1592 | C    |
| 28  | W     | 1594 | A    |
| 28  | W     | 1595 | U    |
| 28  | W     | 1596 | U    |
| 28  | W     | 1599 | U    |
| 28  | W     | 1600 | G    |
| 28  | W     | 1601 | A    |
| 28  | W     | 1602 | U    |
| 28  | W     | 1603 | G    |
| 28  | W     | 1607 | A    |
| 28  | W     | 1608 | U    |
| 28  | W     | 1609 | C    |
| 28  | W     | 1610 | G    |
| 28  | W     | 1611 | G    |
| 28  | W     | 1612 | G    |
| 28  | W     | 1617 | G    |
| 28  | W     | 1619 | A    |
| 28  | W     | 1620 | A    |
| 28  | W     | 1621 | U    |
| 28  | W     | 1623 | A    |
| 28  | W     | 1624 | U    |
| 28  | W     | 1628 | C    |
| 28  | W     | 1629 | C    |
| 28  | W     | 1630 | A    |
| 28  | W     | 1631 | U    |
| 28  | W     | 1632 | G    |
| 28  | W     | 1633 | A    |
| 28  | W     | 1639 | G    |
| 28  | W     | 1647 | A    |
| 28  | W     | 1648 | G    |
| 28  | W     | 1649 | U    |
| 28  | W     | 1650 | A    |
| 28  | W     | 1654 | G    |
| 28  | W     | 1661 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 28  | W     | 1662 | U    |
| 28  | W     | 1665 | G    |
| 28  | W     | 1671 | G    |
| 28  | W     | 1672 | U    |
| 28  | W     | 1675 | A    |
| 28  | W     | 1676 | U    |
| 28  | W     | 1677 | U    |
| 28  | W     | 1679 | A    |
| 28  | W     | 1680 | G    |
| 28  | W     | 1682 | C    |
| 28  | W     | 1683 | C    |
| 28  | W     | 1684 | C    |
| 28  | W     | 1686 | G    |
| 28  | W     | 1702 | G    |
| 28  | W     | 1703 | OMC  |
| 28  | W     | 1719 | A    |
| 28  | W     | 1721 | U    |
| 28  | W     | 1723 | G    |
| 28  | W     | 1743 | G    |
| 28  | W     | 1744 | G    |
| 28  | W     | 1749 | G    |
| 28  | W     | 1752 | C    |
| 28  | W     | 1753 | C    |
| 28  | W     | 1754 | G    |
| 28  | W     | 1755 | C    |
| 28  | W     | 1756 | C    |
| 28  | W     | 1757 | G    |
| 28  | W     | 1759 | G    |
| 28  | W     | 1760 | G    |
| 28  | W     | 1773 | C    |
| 28  | W     | 1774 | C    |
| 28  | W     | 1775 | U    |
| 28  | W     | 1779 | G    |
| 28  | W     | 1781 | A    |
| 28  | W     | 1782 | G    |
| 28  | W     | 1783 | C    |
| 28  | W     | 1784 | G    |
| 28  | W     | 1787 | G    |
| 28  | W     | 1800 | A    |
| 28  | W     | 1810 | U    |
| 28  | W     | 1812 | U    |
| 28  | W     | 1813 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 28  | W     | 1823 | A    |
| 28  | W     | 1824 | A    |
| 28  | W     | 1829 | G    |
| 28  | W     | 1834 | A    |
| 28  | W     | 1835 | A    |
| 28  | W     | 1838 | U    |
| 28  | W     | 1849 | G    |
| 28  | W     | 1851 | MA6  |
| 28  | W     | 1861 | G    |
| 28  | W     | 1862 | G    |
| 28  | W     | 1863 | A    |
| 28  | W     | 1864 | U    |
| 28  | W     | 1865 | C    |
| 28  | W     | 1869 | A    |
| 53  | y     | 2    | G    |
| 53  | y     | 4    | A    |
| 53  | y     | 6    | A    |
| 53  | y     | 8    | U    |
| 53  | y     | 9    | G    |
| 53  | y     | 11   | C    |
| 53  | y     | 12   | G    |
| 53  | y     | 14   | A    |
| 53  | y     | 15   | G    |
| 53  | y     | 17   | G    |
| 53  | y     | 18   | G    |
| 53  | y     | 19   | A    |
| 53  | y     | 20   | A    |
| 53  | y     | 21   | G    |
| 53  | y     | 29   | G    |
| 53  | y     | 42   | G    |
| 53  | y     | 43   | A    |
| 53  | y     | 45   | G    |
| 53  | y     | 46   | U    |
| 53  | y     | 47   | C    |
| 53  | y     | 48   | G    |
| 53  | y     | 50   | U    |
| 53  | y     | 51   | G    |
| 53  | y     | 55   | C    |
| 53  | y     | 56   | G    |
| 53  | y     | 57   | A    |
| 53  | y     | 58   | A    |
| 53  | y     | 59   | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | y     | 60  | C    |
| 53  | y     | 62  | A    |
| 53  | y     | 71  | U    |
| 53  | y     | 72  | A    |
| 53  | y     | 75  | A    |
| 54  | z     | 80  | C    |
| 54  | z     | 81  | G    |
| 54  | z     | 83  | A    |
| 54  | z     | 84  | G    |
| 54  | z     | 85  | U    |
| 54  | z     | 88  | G    |
| 54  | z     | 89  | A    |
| 54  | z     | 90  | U    |
| 54  | z     | 91  | C    |
| 54  | z     | 92  | C    |
| 54  | z     | 93  | U    |
| 54  | z     | 94  | A    |
| 54  | z     | 97  | G    |
| 54  | z     | 98  | U    |
| 54  | z     | 99  | C    |
| 54  | z     | 102 | G    |
| 54  | z     | 103 | U    |
| 54  | z     | 109 | C    |
| 54  | z     | 112 | U    |
| 54  | z     | 113 | C    |
| 54  | z     | 115 | G    |
| 54  | z     | 117 | U    |
| 54  | z     | 118 | A    |
| 54  | z     | 119 | A    |
| 54  | z     | 120 | A    |
| 54  | z     | 122 | A    |
| 54  | z     | 123 | A    |
| 54  | z     | 124 | A    |
| 54  | z     | 125 | A    |
| 54  | z     | 126 | A    |
| 54  | z     | 127 | A    |
| 54  | z     | 128 | A    |

All (13) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | W     | 1   | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 28  | W     | 163  | U    |
| 28  | W     | 291  | G    |
| 28  | W     | 688  | U    |
| 28  | W     | 1240 | A    |
| 28  | W     | 1437 | C    |
| 28  | W     | 1450 | G    |
| 28  | W     | 1463 | U    |
| 28  | W     | 1599 | U    |
| 28  | W     | 1606 | G    |
| 28  | W     | 1631 | U    |
| 28  | W     | 1675 | A    |
| 28  | W     | 1782 | G    |

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

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

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

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 28  | OMC  | W     | 517  | 28    | 19,22,23     | 2.54 | 3 (15%)  | 26,31,34    | 0.80 | 0        |
| 28  | PSU  | W     | 1243 | 28    | 18,21,22     | 3.82 | 5 (27%)  | 22,30,33    | 1.87 | 5 (22%)  |
| 28  | A2M  | W     | 166  | 28    | 22,25,26     | 2.93 | 8 (36%)  | 31,36,39    | 2.52 | 9 (29%)  |
| 28  | PSU  | W     | 1081 | 28    | 18,21,22     | 3.71 | 6 (33%)  | 22,30,33    | 1.77 | 4 (18%)  |
| 28  | OMC  | W     | 174  | 28    | 19,22,23     | 2.52 | 3 (15%)  | 26,31,34    | 0.77 | 0        |
| 28  | A2M  | W     | 27   | 28    | 22,25,26     | 2.94 | 9 (40%)  | 31,36,39    | 2.67 | 7 (22%)  |
| 28  | C4J  | W     | 1248 | 28    | 24,29,30     | 1.54 | 5 (20%)  | 29,42,45    | 1.50 | 4 (13%)  |
| 28  | JMH  | W     | 1219 | 58,28 | 18,22,23     | 2.89 | 6 (33%)  | 21,32,35    | 3.44 | 5 (23%)  |
| 28  | OMU  | W     | 116  | 28    | 19,22,23     | 2.78 | 5 (26%)  | 26,31,34    | 3.31 | 8 (30%)  |
| 28  | MA6  | W     | 1851 | 28    | 23,26,27     | 1.69 | 6 (26%)  | 34,38,41    | 2.69 | 10 (29%) |
| 28  | PSU  | W     | 822  | 28    | 18,21,22     | 3.79 | 6 (33%)  | 22,30,33    | 1.80 | 4 (18%)  |
| 28  | 5MC  | W     | 1374 | 28    | 18,22,23     | 2.73 | 4 (22%)  | 26,32,35    | 1.08 | 2 (7%)   |
| 28  | A2M  | W     | 484  | 28    | 22,25,26     | 2.80 | 8 (36%)  | 31,36,39    | 2.60 | 9 (29%)  |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 28  | OMG  | W     | 509  | 58,28 | 23,26,27     | 2.45 | 6 (26%)  | 33,38,41    | 2.02 | 10 (30%) |
| 28  | A2M  | W     | 668  | 58,28 | 22,25,26     | 2.86 | 7 (31%)  | 31,36,39    | 2.78 | 12 (38%) |
| 28  | PSU  | W     | 612  | 28    | 18,21,22     | 3.72 | 6 (33%)  | 22,30,33    | 1.71 | 5 (22%)  |
| 28  | PSU  | W     | 823  | 28    | 18,21,22     | 3.72 | 5 (27%)  | 22,30,33    | 1.84 | 5 (22%)  |
| 28  | A2M  | W     | 159  | 28    | 22,25,26     | 2.94 | 8 (36%)  | 31,36,39    | 2.76 | 10 (32%) |
| 28  | 5MU  | W     | 814  | 28    | 19,22,23     | 2.92 | 6 (31%)  | 28,32,35    | 2.28 | 8 (28%)  |
| 28  | OMC  | W     | 1703 | 28    | 19,22,23     | 2.52 | 3 (15%)  | 26,31,34    | 0.78 | 1 (3%)   |
| 28  | A2M  | W     | 1678 | 28    | 22,25,26     | 2.79 | 5 (22%)  | 31,36,39    | 2.74 | 10 (32%) |
| 28  | 6MZ  | W     | 1832 | 58,28 | 22,25,26     | 2.56 | 6 (27%)  | 30,36,39    | 2.85 | 11 (36%) |
| 28  | A2M  | W     | 1031 | 28    | 22,25,26     | 2.97 | 9 (40%)  | 31,36,39    | 2.74 | 10 (32%) |
| 28  | OMU  | W     | 121  | 28    | 19,22,23     | 2.78 | 5 (26%)  | 26,31,34    | 3.36 | 8 (30%)  |
| 28  | OMG  | W     | 644  | 28    | 23,26,27     | 2.46 | 6 (26%)  | 33,38,41    | 2.04 | 10 (30%) |
| 28  | MA6  | W     | 1850 | 28    | 23,26,27     | 1.64 | 6 (26%)  | 34,38,41    | 2.64 | 10 (29%) |
| 28  | PSU  | W     | 119  | 28    | 18,21,22     | 3.79 | 5 (27%)  | 22,30,33    | 1.58 | 3 (13%)  |
| 28  | UR3  | W     | 1830 | 28    | 19,22,23     | 1.94 | 5 (26%)  | 26,32,35    | 1.59 | 4 (15%)  |
| 28  | OMG  | W     | 683  | 28    | 23,26,27     | 2.47 | 5 (21%)  | 33,38,41    | 2.01 | 9 (27%)  |

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

| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 28  | OMC  | W     | 517  | 28    | -       | 0/9/27/28  | 0/2/2/2 |
| 28  | PSU  | W     | 1243 | 28    | -       | 1/7/25/26  | 0/2/2/2 |
| 28  | A2M  | W     | 166  | 28    | -       | 7/9/27/28  | 0/3/3/3 |
| 28  | PSU  | W     | 1081 | 28    | -       | 3/7/25/26  | 0/2/2/2 |
| 28  | OMC  | W     | 174  | 28    | -       | 0/9/27/28  | 0/2/2/2 |
| 28  | A2M  | W     | 27   | 28    | -       | 2/9/27/28  | 0/3/3/3 |
| 28  | C4J  | W     | 1248 | 28    | -       | 2/16/34/35 | 0/2/2/2 |
| 28  | JMH  | W     | 1219 | 58,28 | 1/1/5/5 | 6/7/25/26  | 0/2/2/2 |
| 28  | OMU  | W     | 116  | 28    | -       | 2/9/27/28  | 0/2/2/2 |
| 28  | MA6  | W     | 1851 | 28    | -       | 3/11/29/30 | 0/3/3/3 |
| 28  | PSU  | W     | 822  | 28    | -       | 1/7/25/26  | 0/2/2/2 |
| 28  | 5MC  | W     | 1374 | 28    | -       | 0/7/25/26  | 0/2/2/2 |
| 28  | A2M  | W     | 484  | 28    | -       | 0/9/27/28  | 0/3/3/3 |
| 28  | OMG  | W     | 509  | 58,28 | -       | 2/9/27/28  | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 28  | A2M  | W     | 668  | 58,28 | -       | 2/9/27/28  | 0/3/3/3 |
| 28  | PSU  | W     | 612  | 28    | -       | 2/7/25/26  | 0/2/2/2 |
| 28  | PSU  | W     | 823  | 28    | -       | 0/7/25/26  | 0/2/2/2 |
| 28  | A2M  | W     | 159  | 28    | -       | 0/9/27/28  | 0/3/3/3 |
| 28  | 5MU  | W     | 814  | 28    | -       | 0/7/25/26  | 0/2/2/2 |
| 28  | OMC  | W     | 1703 | 28    | -       | 2/9/27/28  | 0/2/2/2 |
| 28  | A2M  | W     | 1678 | 28    | -       | 2/9/27/28  | 0/3/3/3 |
| 28  | 6MZ  | W     | 1832 | 58,28 | -       | 2/9/27/28  | 0/3/3/3 |
| 28  | A2M  | W     | 1031 | 28    | -       | 2/9/27/28  | 0/3/3/3 |
| 28  | OMU  | W     | 121  | 28    | -       | 0/9/27/28  | 0/2/2/2 |
| 28  | OMG  | W     | 644  | 28    | -       | 1/9/27/28  | 0/3/3/3 |
| 28  | MA6  | W     | 1850 | 28    | -       | 2/11/29/30 | 0/3/3/3 |
| 28  | PSU  | W     | 119  | 28    | -       | 0/7/25/26  | 0/2/2/2 |
| 28  | UR3  | W     | 1830 | 28    | -       | 2/7/25/26  | 0/2/2/2 |
| 28  | OMG  | W     | 683  | 28    | -       | 0/9/27/28  | 0/3/3/3 |

All (167) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 28  | W     | 166  | A2M  | O3'-C3' | -10.28 | 1.18        | 1.43     |
| 28  | W     | 1031 | A2M  | O3'-C3' | -10.20 | 1.19        | 1.43     |
| 28  | W     | 159  | A2M  | O3'-C3' | -10.10 | 1.19        | 1.43     |
| 28  | W     | 668  | A2M  | O3'-C3' | -10.02 | 1.19        | 1.43     |
| 28  | W     | 27   | A2M  | O3'-C3' | -10.01 | 1.19        | 1.43     |
| 28  | W     | 1832 | 6MZ  | C6-N6   | 9.92   | 1.44        | 1.34     |
| 28  | W     | 484  | A2M  | O3'-C3' | -9.63  | 1.20        | 1.43     |
| 28  | W     | 1678 | A2M  | O3'-C3' | -9.60  | 1.20        | 1.43     |
| 28  | W     | 1219 | JMH  | O2-C2   | 9.18   | 1.39        | 1.22     |
| 28  | W     | 1243 | PSU  | C2-N1   | 8.91   | 1.48        | 1.36     |
| 28  | W     | 1703 | OMC  | O2-C2   | 8.72   | 1.39        | 1.23     |
| 28  | W     | 823  | PSU  | C2-N1   | 8.69   | 1.48        | 1.36     |
| 28  | W     | 517  | OMC  | O2-C2   | 8.67   | 1.39        | 1.23     |
| 28  | W     | 174  | OMC  | O2-C2   | 8.65   | 1.39        | 1.23     |
| 28  | W     | 822  | PSU  | C2-N1   | 8.63   | 1.48        | 1.36     |
| 28  | W     | 814  | 5MU  | O4-C4   | 8.62   | 1.40        | 1.23     |
| 28  | W     | 119  | PSU  | C2-N1   | 8.58   | 1.48        | 1.36     |
| 28  | W     | 1081 | PSU  | O4-C4   | 8.58   | 1.39        | 1.23     |
| 28  | W     | 119  | PSU  | O4-C4   | 8.56   | 1.39        | 1.23     |
| 28  | W     | 683  | OMG  | O6-C6   | 8.56   | 1.39        | 1.23     |
| 28  | W     | 1243 | PSU  | O4-C4   | 8.53   | 1.39        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 28  | W     | 509  | OMG  | O6-C6 | 8.51 | 1.39        | 1.23     |
| 28  | W     | 644  | OMG  | O6-C6 | 8.50 | 1.39        | 1.23     |
| 28  | W     | 612  | PSU  | O4-C4 | 8.50 | 1.39        | 1.23     |
| 28  | W     | 822  | PSU  | O4-C4 | 8.48 | 1.39        | 1.23     |
| 28  | W     | 1374 | 5MC  | O2-C2 | 8.42 | 1.39        | 1.23     |
| 28  | W     | 1081 | PSU  | C2-N1 | 8.31 | 1.48        | 1.36     |
| 28  | W     | 823  | PSU  | O4-C4 | 8.18 | 1.39        | 1.23     |
| 28  | W     | 612  | PSU  | C2-N1 | 8.16 | 1.47        | 1.36     |
| 28  | W     | 1243 | PSU  | O2-C2 | 8.05 | 1.40        | 1.23     |
| 28  | W     | 823  | PSU  | O2-C2 | 7.97 | 1.40        | 1.23     |
| 28  | W     | 119  | PSU  | O2-C2 | 7.93 | 1.40        | 1.23     |
| 28  | W     | 116  | OMU  | O4-C4 | 7.87 | 1.39        | 1.24     |
| 28  | W     | 121  | OMU  | O4-C4 | 7.86 | 1.39        | 1.24     |
| 28  | W     | 822  | PSU  | O2-C2 | 7.84 | 1.39        | 1.23     |
| 28  | W     | 612  | PSU  | O2-C2 | 7.79 | 1.39        | 1.23     |
| 28  | W     | 1081 | PSU  | O2-C2 | 7.74 | 1.39        | 1.23     |
| 28  | W     | 814  | 5MU  | C6-N1 | 6.04 | 1.48        | 1.38     |
| 28  | W     | 121  | OMU  | C2-N1 | 5.69 | 1.47        | 1.38     |
| 28  | W     | 116  | OMU  | C2-N1 | 5.63 | 1.47        | 1.38     |
| 28  | W     | 119  | PSU  | C6-C5 | 5.60 | 1.41        | 1.35     |
| 28  | W     | 612  | PSU  | C6-C5 | 5.58 | 1.41        | 1.35     |
| 28  | W     | 116  | OMU  | C6-N1 | 5.41 | 1.51        | 1.38     |
| 28  | W     | 822  | PSU  | C6-C5 | 5.40 | 1.41        | 1.35     |
| 28  | W     | 121  | OMU  | C6-N1 | 5.26 | 1.50        | 1.38     |
| 28  | W     | 823  | PSU  | C6-C5 | 5.26 | 1.41        | 1.35     |
| 28  | W     | 1243 | PSU  | C6-C5 | 5.20 | 1.41        | 1.35     |
| 28  | W     | 1081 | PSU  | C6-C5 | 5.02 | 1.41        | 1.35     |
| 28  | W     | 1830 | UR3  | C2-N1 | 4.92 | 1.45        | 1.38     |
| 28  | W     | 517  | OMC  | C4-N4 | 4.91 | 1.45        | 1.33     |
| 28  | W     | 1219 | JMH  | C2-N1 | 4.82 | 1.45        | 1.38     |
| 28  | W     | 1703 | OMC  | C4-N4 | 4.81 | 1.45        | 1.33     |
| 28  | W     | 174  | OMC  | C4-N4 | 4.79 | 1.45        | 1.33     |
| 28  | W     | 1248 | C4J  | C6-N1 | 4.59 | 1.48        | 1.36     |
| 28  | W     | 683  | OMG  | C2-N2 | 4.58 | 1.45        | 1.34     |
| 28  | W     | 1851 | MA6  | C5-N7 | 4.55 | 1.47        | 1.39     |
| 28  | W     | 644  | OMG  | C2-N2 | 4.55 | 1.45        | 1.34     |
| 28  | W     | 166  | A2M  | C6-N6 | 4.51 | 1.45        | 1.34     |
| 28  | W     | 509  | OMG  | C2-N2 | 4.50 | 1.44        | 1.34     |
| 28  | W     | 159  | A2M  | C6-N6 | 4.50 | 1.45        | 1.34     |
| 28  | W     | 1678 | A2M  | C6-N6 | 4.45 | 1.45        | 1.34     |
| 28  | W     | 1374 | 5MC  | C4-N4 | 4.42 | 1.45        | 1.34     |
| 28  | W     | 1830 | UR3  | C6-N1 | 4.40 | 1.48        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 28  | W     | 1374 | 5MC  | C2-N3   | 4.39  | 1.45        | 1.36     |
| 28  | W     | 668  | A2M  | C6-N6   | 4.38  | 1.45        | 1.34     |
| 28  | W     | 1374 | 5MC  | C6-C5   | 4.37  | 1.41        | 1.34     |
| 28  | W     | 1850 | MA6  | C5-N7   | 4.32  | 1.47        | 1.39     |
| 28  | W     | 27   | A2M  | C6-N6   | 4.31  | 1.45        | 1.34     |
| 28  | W     | 1031 | A2M  | C6-N6   | 4.29  | 1.44        | 1.34     |
| 28  | W     | 484  | A2M  | C6-N6   | 4.27  | 1.44        | 1.34     |
| 28  | W     | 814  | 5MU  | C4-C5   | 4.26  | 1.51        | 1.44     |
| 28  | W     | 814  | 5MU  | C2-N1   | 4.15  | 1.45        | 1.38     |
| 28  | W     | 644  | OMG  | C5-N7   | 4.06  | 1.47        | 1.39     |
| 28  | W     | 1219 | JMH  | C4-N4   | 4.00  | 1.45        | 1.28     |
| 28  | W     | 683  | OMG  | C5-N7   | 3.93  | 1.46        | 1.39     |
| 28  | W     | 509  | OMG  | C5-N7   | 3.90  | 1.46        | 1.39     |
| 28  | W     | 174  | OMC  | C2-N3   | 3.85  | 1.44        | 1.36     |
| 28  | W     | 517  | OMC  | C2-N3   | 3.83  | 1.44        | 1.36     |
| 28  | W     | 1703 | OMC  | C2-N3   | 3.69  | 1.43        | 1.36     |
| 28  | W     | 1832 | 6MZ  | C5-N7   | 3.67  | 1.45        | 1.39     |
| 28  | W     | 159  | A2M  | C5-N7   | 3.64  | 1.45        | 1.39     |
| 28  | W     | 683  | OMG  | C2-N3   | 3.63  | 1.41        | 1.33     |
| 28  | W     | 1031 | A2M  | C5-N7   | 3.61  | 1.45        | 1.39     |
| 28  | W     | 509  | OMG  | C2-N3   | 3.55  | 1.41        | 1.33     |
| 28  | W     | 116  | OMU  | C2-N3   | 3.53  | 1.44        | 1.38     |
| 28  | W     | 644  | OMG  | C2-N3   | 3.52  | 1.41        | 1.33     |
| 28  | W     | 1678 | A2M  | C5-N7   | 3.51  | 1.45        | 1.39     |
| 28  | W     | 27   | A2M  | C3'-C2' | -3.49 | 1.45        | 1.52     |
| 28  | W     | 668  | A2M  | C5-N7   | 3.45  | 1.45        | 1.39     |
| 28  | W     | 27   | A2M  | C5-N7   | 3.45  | 1.45        | 1.39     |
| 28  | W     | 166  | A2M  | C5-N7   | 3.41  | 1.45        | 1.39     |
| 28  | W     | 1031 | A2M  | C3'-C2' | -3.41 | 1.45        | 1.52     |
| 28  | W     | 121  | OMU  | C2-N3   | 3.38  | 1.44        | 1.38     |
| 28  | W     | 166  | A2M  | C3'-C2' | -3.33 | 1.45        | 1.52     |
| 28  | W     | 1219 | JMH  | C6-N1   | 3.28  | 1.45        | 1.38     |
| 28  | W     | 1830 | UR3  | C5-C4   | 3.25  | 1.52        | 1.43     |
| 28  | W     | 484  | A2M  | C5-N7   | 3.18  | 1.45        | 1.39     |
| 28  | W     | 1248 | C4J  | O4'-C1' | -3.11 | 1.39        | 1.43     |
| 28  | W     | 159  | A2M  | C3'-C2' | -3.11 | 1.46        | 1.52     |
| 28  | W     | 1851 | MA6  | C6-N6   | 3.10  | 1.46        | 1.36     |
| 28  | W     | 484  | A2M  | C3'-C2' | -3.04 | 1.46        | 1.52     |
| 28  | W     | 668  | A2M  | C3'-C2' | -3.01 | 1.46        | 1.52     |
| 28  | W     | 1850 | MA6  | C6-N6   | 3.00  | 1.45        | 1.36     |
| 28  | W     | 1031 | A2M  | C8-N7   | 2.93  | 1.37        | 1.31     |
| 28  | W     | 668  | A2M  | C8-N7   | 2.91  | 1.37        | 1.31     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 28  | W     | 1678 | A2M  | C8-N7   | 2.90  | 1.37        | 1.31     |
| 28  | W     | 27   | A2M  | C8-N7   | 2.88  | 1.37        | 1.31     |
| 28  | W     | 1851 | MA6  | C8-N7   | 2.85  | 1.37        | 1.31     |
| 28  | W     | 159  | A2M  | C8-N7   | 2.83  | 1.36        | 1.31     |
| 28  | W     | 1243 | PSU  | C2-N3   | 2.83  | 1.42        | 1.37     |
| 28  | W     | 1851 | MA6  | C8-N9   | -2.78 | 1.32        | 1.37     |
| 28  | W     | 1832 | 6MZ  | C8-N7   | 2.78  | 1.36        | 1.31     |
| 28  | W     | 822  | PSU  | C2-N3   | 2.76  | 1.42        | 1.37     |
| 28  | W     | 166  | A2M  | C8-N7   | 2.75  | 1.36        | 1.31     |
| 28  | W     | 1850 | MA6  | C8-N9   | -2.74 | 1.32        | 1.37     |
| 28  | W     | 1850 | MA6  | C4-N9   | -2.70 | 1.31        | 1.37     |
| 28  | W     | 1851 | MA6  | C4-N9   | -2.69 | 1.31        | 1.37     |
| 28  | W     | 121  | OMU  | O2-C2   | -2.67 | 1.18        | 1.23     |
| 28  | W     | 1219 | JMH  | C6-C5   | 2.64  | 1.41        | 1.35     |
| 28  | W     | 1850 | MA6  | C8-N7   | 2.64  | 1.36        | 1.31     |
| 28  | W     | 814  | 5MU  | O2-C2   | -2.63 | 1.18        | 1.23     |
| 28  | W     | 1081 | PSU  | O4'-C1' | -2.63 | 1.40        | 1.43     |
| 28  | W     | 484  | A2M  | C8-N7   | 2.63  | 1.36        | 1.31     |
| 28  | W     | 116  | OMU  | O2-C2   | -2.56 | 1.18        | 1.23     |
| 28  | W     | 1830 | UR3  | O2-C2   | -2.54 | 1.17        | 1.22     |
| 28  | W     | 1832 | 6MZ  | C5-C6   | -2.52 | 1.35        | 1.41     |
| 28  | W     | 612  | PSU  | C2-N3   | 2.51  | 1.41        | 1.37     |
| 28  | W     | 119  | PSU  | C2-N3   | 2.43  | 1.41        | 1.37     |
| 28  | W     | 823  | PSU  | C2-N3   | 2.42  | 1.41        | 1.37     |
| 28  | W     | 644  | OMG  | C4-N9   | -2.40 | 1.31        | 1.38     |
| 28  | W     | 27   | A2M  | C4-N9   | -2.38 | 1.32        | 1.37     |
| 28  | W     | 159  | A2M  | C4-N9   | -2.38 | 1.32        | 1.37     |
| 28  | W     | 509  | OMG  | C4-N9   | -2.38 | 1.31        | 1.38     |
| 28  | W     | 683  | OMG  | C4-N9   | -2.36 | 1.31        | 1.38     |
| 28  | W     | 1678 | A2M  | C3'-C2' | -2.33 | 1.47        | 1.52     |
| 28  | W     | 1830 | UR3  | O4-C4   | -2.31 | 1.18        | 1.23     |
| 28  | W     | 1081 | PSU  | C2-N3   | 2.31  | 1.41        | 1.37     |
| 28  | W     | 484  | A2M  | O5'-C5' | -2.31 | 1.39        | 1.44     |
| 28  | W     | 668  | A2M  | O5'-C5' | -2.30 | 1.39        | 1.44     |
| 28  | W     | 822  | PSU  | O4'-C1' | -2.29 | 1.40        | 1.43     |
| 28  | W     | 1832 | 6MZ  | C4-N9   | -2.25 | 1.32        | 1.37     |
| 28  | W     | 612  | PSU  | O4'-C1' | -2.25 | 1.40        | 1.43     |
| 28  | W     | 1031 | A2M  | C4-N9   | -2.23 | 1.32        | 1.37     |
| 28  | W     | 27   | A2M  | C5-C6   | -2.20 | 1.35        | 1.41     |
| 28  | W     | 1850 | MA6  | C5-C6   | -2.19 | 1.35        | 1.41     |
| 28  | W     | 814  | 5MU  | C2-N3   | 2.17  | 1.41        | 1.38     |
| 28  | W     | 1031 | A2M  | C5-C6   | -2.13 | 1.35        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 28  | W     | 1248 | C4J  | O2-C2   | -2.12 | 1.18        | 1.22     |
| 28  | W     | 1248 | C4J  | O4-C4   | -2.12 | 1.18        | 1.23     |
| 28  | W     | 1031 | A2M  | C8-N9   | -2.11 | 1.33        | 1.37     |
| 28  | W     | 509  | OMG  | C8-N9   | -2.11 | 1.32        | 1.37     |
| 28  | W     | 668  | A2M  | C4-N9   | -2.10 | 1.33        | 1.37     |
| 28  | W     | 484  | A2M  | C5-C6   | -2.09 | 1.35        | 1.41     |
| 28  | W     | 159  | A2M  | C8-N9   | -2.09 | 1.33        | 1.37     |
| 28  | W     | 27   | A2M  | O5'-C5' | -2.08 | 1.39        | 1.44     |
| 28  | W     | 1219 | JMH  | C2-N3   | 2.08  | 1.43        | 1.39     |
| 28  | W     | 27   | A2M  | C8-N9   | -2.07 | 1.33        | 1.37     |
| 28  | W     | 644  | OMG  | C8-N9   | -2.07 | 1.32        | 1.37     |
| 28  | W     | 1851 | MA6  | C5-C6   | -2.06 | 1.36        | 1.41     |
| 28  | W     | 159  | A2M  | C5-C6   | -2.05 | 1.35        | 1.41     |
| 28  | W     | 166  | A2M  | C8-N9   | -2.05 | 1.33        | 1.37     |
| 28  | W     | 1031 | A2M  | O5'-C5' | -2.04 | 1.39        | 1.44     |
| 28  | W     | 166  | A2M  | C5-C6   | -2.04 | 1.35        | 1.41     |
| 28  | W     | 1248 | C4J  | C2-N1   | 2.03  | 1.45        | 1.39     |
| 28  | W     | 166  | A2M  | C4-N9   | -2.03 | 1.33        | 1.37     |
| 28  | W     | 1832 | 6MZ  | C8-N9   | -2.01 | 1.33        | 1.37     |
| 28  | W     | 484  | A2M  | C4-N9   | -2.01 | 1.33        | 1.37     |

All (193) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 28  | W     | 1219 | JMH  | C1'-N1-C2 | 11.47 | 136.35      | 116.99   |
| 28  | W     | 121  | OMU  | N3-C2-N1  | 8.98  | 126.81      | 114.89   |
| 28  | W     | 121  | OMU  | C4-N3-C2  | -8.67 | 115.14      | 126.58   |
| 28  | W     | 116  | OMU  | N3-C2-N1  | 8.61  | 126.32      | 114.89   |
| 28  | W     | 159  | A2M  | C4-N9-C8  | 8.48  | 114.92      | 105.73   |
| 28  | W     | 1832 | 6MZ  | C4-N9-C8  | 8.42  | 114.86      | 105.73   |
| 28  | W     | 116  | OMU  | C4-N3-C2  | -8.38 | 115.52      | 126.58   |
| 28  | W     | 1031 | A2M  | C4-N9-C8  | 8.35  | 114.78      | 105.73   |
| 28  | W     | 1851 | MA6  | C4-N9-C8  | 8.08  | 114.49      | 105.73   |
| 28  | W     | 1850 | MA6  | C4-N9-C8  | 8.06  | 114.46      | 105.73   |
| 28  | W     | 27   | A2M  | C4-N9-C8  | 7.98  | 114.38      | 105.73   |
| 28  | W     | 668  | A2M  | C4-N9-C8  | 7.43  | 113.78      | 105.73   |
| 28  | W     | 116  | OMU  | C6-N1-C2  | -7.20 | 111.78      | 120.99   |
| 28  | W     | 1678 | A2M  | C4-N9-C8  | 7.15  | 113.47      | 105.73   |
| 28  | W     | 121  | OMU  | C6-N1-C2  | -7.12 | 111.88      | 120.99   |
| 28  | W     | 166  | A2M  | C4-N9-C8  | 6.97  | 113.28      | 105.73   |
| 28  | W     | 484  | A2M  | C4-N9-C8  | 6.87  | 113.17      | 105.73   |
| 28  | W     | 814  | 5MU  | C4-N3-C2  | -6.21 | 119.31      | 127.35   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 28  | W     | 1219 | JMH  | C6-N1-C2  | -6.21 | 116.22      | 121.79   |
| 28  | W     | 1219 | JMH  | C1'-N1-C6 | -6.16 | 107.42      | 120.84   |
| 28  | W     | 27   | A2M  | N3-C2-N1  | -6.07 | 119.11      | 128.60   |
| 28  | W     | 1851 | MA6  | N1-C2-N3  | -6.04 | 119.16      | 128.60   |
| 28  | W     | 1832 | 6MZ  | N9-C8-N7  | -5.98 | 105.73      | 113.91   |
| 28  | W     | 1031 | A2M  | N3-C2-N1  | -5.86 | 119.44      | 128.60   |
| 28  | W     | 166  | A2M  | N3-C2-N1  | -5.85 | 119.45      | 128.60   |
| 28  | W     | 159  | A2M  | N9-C8-N7  | -5.82 | 105.96      | 113.91   |
| 28  | W     | 159  | A2M  | N3-C2-N1  | -5.78 | 119.56      | 128.60   |
| 28  | W     | 668  | A2M  | N3-C2-N1  | -5.77 | 119.58      | 128.60   |
| 28  | W     | 1031 | A2M  | N9-C8-N7  | -5.76 | 106.04      | 113.91   |
| 28  | W     | 484  | A2M  | C5-C4-N3  | -5.68 | 119.35      | 126.75   |
| 28  | W     | 1832 | 6MZ  | N1-C2-N3  | -5.60 | 119.84      | 128.60   |
| 28  | W     | 484  | A2M  | N3-C2-N1  | -5.60 | 119.84      | 128.60   |
| 28  | W     | 668  | A2M  | C5-C4-N3  | -5.58 | 119.48      | 126.75   |
| 28  | W     | 1850 | MA6  | N1-C2-N3  | -5.54 | 119.93      | 128.60   |
| 28  | W     | 27   | A2M  | N9-C8-N7  | -5.50 | 106.40      | 113.91   |
| 28  | W     | 1678 | A2M  | N3-C2-N1  | -5.48 | 120.02      | 128.60   |
| 28  | W     | 814  | 5MU  | C5-C4-N3  | 5.40  | 119.92      | 115.31   |
| 28  | W     | 668  | A2M  | N9-C8-N7  | -5.38 | 106.55      | 113.91   |
| 28  | W     | 1678 | A2M  | C5-C4-N3  | -5.33 | 119.79      | 126.75   |
| 28  | W     | 1851 | MA6  | N9-C8-N7  | -5.32 | 106.64      | 113.91   |
| 28  | W     | 1830 | UR3  | C4-N3-C2  | -5.20 | 119.67      | 124.56   |
| 28  | W     | 166  | A2M  | C5-C4-N3  | -5.19 | 119.98      | 126.75   |
| 28  | W     | 509  | OMG  | C5-C4-N3  | -5.19 | 120.04      | 128.46   |
| 28  | W     | 1850 | MA6  | C5-C4-N3  | -5.13 | 120.05      | 126.75   |
| 28  | W     | 683  | OMG  | C5-C4-N3  | -5.06 | 120.25      | 128.46   |
| 28  | W     | 116  | OMU  | C5-C4-N3  | 5.01  | 122.33      | 114.84   |
| 28  | W     | 1850 | MA6  | N9-C8-N7  | -4.99 | 107.09      | 113.91   |
| 28  | W     | 1031 | A2M  | C5-C4-N3  | -4.95 | 120.29      | 126.75   |
| 28  | W     | 1832 | 6MZ  | C5-C4-N3  | -4.95 | 120.30      | 126.75   |
| 28  | W     | 121  | OMU  | C5-C4-N3  | 4.94  | 122.23      | 114.84   |
| 28  | W     | 644  | OMG  | C5-C4-N3  | -4.94 | 120.45      | 128.46   |
| 28  | W     | 1219 | JMH  | O2-C2-N3  | -4.90 | 114.44      | 121.34   |
| 28  | W     | 27   | A2M  | C5-C4-N3  | -4.82 | 120.46      | 126.75   |
| 28  | W     | 1248 | C4J  | C4-N3-C2  | -4.81 | 119.37      | 125.46   |
| 28  | W     | 823  | PSU  | C4-N3-C2  | -4.81 | 119.41      | 126.34   |
| 28  | W     | 121  | OMU  | O2-C2-N1  | -4.80 | 116.41      | 122.79   |
| 28  | W     | 484  | A2M  | N9-C8-N7  | -4.76 | 107.40      | 113.91   |
| 28  | W     | 116  | OMU  | O2-C2-N1  | -4.76 | 116.46      | 122.79   |
| 28  | W     | 1678 | A2M  | N9-C8-N7  | -4.75 | 107.41      | 113.91   |
| 28  | W     | 159  | A2M  | C5-C4-N3  | -4.72 | 120.59      | 126.75   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 28  | W     | 1851 | MA6  | C5-C4-N3  | -4.70 | 120.62      | 126.75   |
| 28  | W     | 1243 | PSU  | C4-N3-C2  | -4.70 | 119.57      | 126.34   |
| 28  | W     | 814  | 5MU  | N3-C2-N1  | 4.68  | 121.10      | 114.89   |
| 28  | W     | 1851 | MA6  | C4-C5-N7  | -4.65 | 104.95      | 110.62   |
| 28  | W     | 822  | PSU  | C4-N3-C2  | -4.61 | 119.69      | 126.34   |
| 28  | W     | 644  | OMG  | C8-N9-C4  | 4.59  | 114.78      | 106.05   |
| 28  | W     | 1081 | PSU  | C4-N3-C2  | -4.57 | 119.75      | 126.34   |
| 28  | W     | 166  | A2M  | N9-C8-N7  | -4.48 | 107.78      | 113.91   |
| 28  | W     | 1243 | PSU  | N1-C2-N3  | 4.43  | 120.15      | 115.13   |
| 28  | W     | 644  | OMG  | C2-N3-C4  | 4.42  | 120.18      | 112.30   |
| 28  | W     | 683  | OMG  | C2-N3-C4  | 4.41  | 120.15      | 112.30   |
| 28  | W     | 509  | OMG  | C2-N3-C4  | 4.40  | 120.13      | 112.30   |
| 28  | W     | 484  | A2M  | N3-C4-N9  | 4.38  | 134.30      | 127.08   |
| 28  | W     | 814  | 5MU  | O4-C4-C5  | -4.34 | 119.87      | 124.90   |
| 28  | W     | 823  | PSU  | N1-C2-N3  | 4.33  | 120.04      | 115.13   |
| 28  | W     | 683  | OMG  | C8-N9-C4  | 4.33  | 114.29      | 106.05   |
| 28  | W     | 822  | PSU  | N1-C2-N3  | 4.32  | 120.03      | 115.13   |
| 28  | W     | 1851 | MA6  | C2-N1-C6  | 4.32  | 121.95      | 111.75   |
| 28  | W     | 509  | OMG  | C8-N9-C4  | 4.29  | 114.22      | 106.05   |
| 28  | W     | 1081 | PSU  | N1-C2-N3  | 4.29  | 119.98      | 115.13   |
| 28  | W     | 1678 | A2M  | N3-C4-N9  | 4.22  | 134.03      | 127.08   |
| 28  | W     | 119  | PSU  | C4-N3-C2  | -4.21 | 120.27      | 126.34   |
| 28  | W     | 668  | A2M  | N3-C4-N9  | 4.16  | 133.94      | 127.08   |
| 28  | W     | 1850 | MA6  | C4-C5-N7  | -4.13 | 105.59      | 110.62   |
| 28  | W     | 166  | A2M  | N3-C4-N9  | 4.10  | 133.83      | 127.08   |
| 28  | W     | 612  | PSU  | N1-C2-N3  | 4.07  | 119.74      | 115.13   |
| 28  | W     | 1031 | A2M  | N3-C4-N9  | 4.07  | 133.78      | 127.08   |
| 28  | W     | 668  | A2M  | C2-N3-C4  | 4.03  | 121.28      | 111.75   |
| 28  | W     | 1832 | 6MZ  | N3-C4-N9  | 3.96  | 133.61      | 127.08   |
| 28  | W     | 1850 | MA6  | C2-N1-C6  | 3.95  | 121.09      | 111.75   |
| 28  | W     | 612  | PSU  | C4-N3-C2  | -3.94 | 120.66      | 126.34   |
| 28  | W     | 159  | A2M  | N3-C4-N9  | 3.90  | 133.50      | 127.08   |
| 28  | W     | 116  | OMU  | O4-C4-C5  | -3.89 | 118.33      | 125.16   |
| 28  | W     | 119  | PSU  | N1-C2-N3  | 3.85  | 119.49      | 115.13   |
| 28  | W     | 116  | OMU  | C1'-N1-C2 | 3.85  | 124.53      | 117.57   |
| 28  | W     | 166  | A2M  | C2-N3-C4  | 3.83  | 120.80      | 111.75   |
| 28  | W     | 484  | A2M  | C2-N3-C4  | 3.83  | 120.80      | 111.75   |
| 28  | W     | 27   | A2M  | N3-C4-N9  | 3.83  | 133.39      | 127.08   |
| 28  | W     | 509  | OMG  | N9-C4-N3  | 3.79  | 133.54      | 125.94   |
| 28  | W     | 1031 | A2M  | C2-N3-C4  | 3.78  | 120.67      | 111.75   |
| 28  | W     | 1678 | A2M  | C2-N3-C4  | 3.75  | 120.60      | 111.75   |
| 28  | W     | 27   | A2M  | C2-N3-C4  | 3.74  | 120.58      | 111.75   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 28  | W     | 121  | OMU  | O4-C4-C5    | -3.71 | 118.64      | 125.16   |
| 28  | W     | 121  | OMU  | C1'-N1-C2   | 3.70  | 124.27      | 117.57   |
| 28  | W     | 1678 | A2M  | CM'-O2'-C2' | 3.70  | 124.22      | 114.52   |
| 28  | W     | 1850 | MA6  | N3-C4-N9    | 3.69  | 133.16      | 127.08   |
| 28  | W     | 159  | A2M  | C2-N3-C4    | 3.68  | 120.44      | 111.75   |
| 28  | W     | 1850 | MA6  | C4-C5-C6    | 3.64  | 119.95      | 115.88   |
| 28  | W     | 683  | OMG  | N9-C4-N3    | 3.63  | 133.22      | 125.94   |
| 28  | W     | 1851 | MA6  | C2-N3-C4    | 3.60  | 120.26      | 111.75   |
| 28  | W     | 1832 | 6MZ  | C2-N3-C4    | 3.60  | 120.25      | 111.75   |
| 28  | W     | 644  | OMG  | N9-C4-N3    | 3.59  | 133.14      | 125.94   |
| 28  | W     | 644  | OMG  | N9-C8-N7    | -3.58 | 106.64      | 113.39   |
| 28  | W     | 1850 | MA6  | C2-N3-C4    | 3.52  | 120.08      | 111.75   |
| 28  | W     | 1830 | UR3  | C1'-N1-C2   | 3.47  | 122.84      | 116.99   |
| 28  | W     | 1832 | 6MZ  | C4-C5-N7    | -3.46 | 106.41      | 110.62   |
| 28  | W     | 1832 | 6MZ  | C4-C5-C6    | 3.40  | 119.44      | 116.81   |
| 28  | W     | 814  | 5MU  | C5-C6-N1    | -3.37 | 119.87      | 123.34   |
| 28  | W     | 683  | OMG  | N9-C8-N7    | -3.37 | 107.05      | 113.39   |
| 28  | W     | 668  | A2M  | C4-C5-N7    | -3.33 | 106.56      | 110.62   |
| 28  | W     | 668  | A2M  | C3'-C2'-C1' | 3.28  | 109.05      | 102.89   |
| 28  | W     | 1678 | A2M  | O2'-C2'-C1' | 3.25  | 115.41      | 109.08   |
| 28  | W     | 509  | OMG  | N9-C8-N7    | -3.17 | 107.42      | 113.39   |
| 28  | W     | 159  | A2M  | C4-C5-N7    | -3.16 | 106.77      | 110.62   |
| 28  | W     | 1851 | MA6  | C4-C5-C6    | 3.15  | 119.41      | 115.88   |
| 28  | W     | 1374 | 5MC  | CM5-C5-C6   | -3.12 | 118.68      | 122.85   |
| 28  | W     | 612  | PSU  | C6-N1-C2    | -3.11 | 119.50      | 122.68   |
| 28  | W     | 1031 | A2M  | C4-C5-N7    | -3.11 | 106.83      | 110.62   |
| 28  | W     | 27   | A2M  | C4-C5-N7    | -3.07 | 106.88      | 110.62   |
| 28  | W     | 683  | OMG  | C2-N1-C6    | -3.05 | 119.55      | 125.10   |
| 28  | W     | 814  | 5MU  | C6-C5-C4    | 3.04  | 120.57      | 118.03   |
| 28  | W     | 509  | OMG  | C2-N1-C6    | -3.03 | 119.57      | 125.10   |
| 28  | W     | 1374 | 5MC  | C5-C6-N1    | -3.02 | 120.24      | 123.34   |
| 28  | W     | 1851 | MA6  | N3-C4-N9    | 2.97  | 131.97      | 127.08   |
| 28  | W     | 1219 | JMH  | C2'-C1'-N1  | 2.95  | 121.57      | 113.22   |
| 28  | W     | 484  | A2M  | C4-C5-N7    | -2.91 | 107.08      | 110.62   |
| 28  | W     | 644  | OMG  | C2-N1-C6    | -2.90 | 119.81      | 125.10   |
| 28  | W     | 1678 | A2M  | C4-C5-N7    | -2.84 | 107.16      | 110.62   |
| 28  | W     | 1830 | UR3  | C3U-N3-C2   | 2.78  | 122.19      | 117.31   |
| 28  | W     | 166  | A2M  | C4-C5-N7    | -2.77 | 107.24      | 110.62   |
| 28  | W     | 1678 | A2M  | C3'-C2'-C1' | 2.77  | 108.09      | 102.89   |
| 28  | W     | 1248 | C4J  | C3-N3-C4    | 2.73  | 121.33      | 117.31   |
| 28  | W     | 484  | A2M  | C3'-C2'-C1' | 2.73  | 108.01      | 102.89   |
| 28  | W     | 644  | OMG  | C4-C5-N7    | -2.70 | 106.45      | 110.72   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 28  | W     | 1830 | UR3  | C6-N1-C2    | -2.69 | 119.38      | 121.79   |
| 28  | W     | 668  | A2M  | C2'-C1'-N9  | 2.69  | 118.06      | 113.53   |
| 28  | W     | 1243 | PSU  | O2-C2-N1    | -2.68 | 119.84      | 122.79   |
| 28  | W     | 683  | OMG  | C5-C6-N1    | 2.64  | 119.89      | 113.19   |
| 28  | W     | 509  | OMG  | C5-C6-N1    | 2.63  | 119.86      | 113.19   |
| 28  | W     | 1243 | PSU  | C6-N1-C2    | -2.63 | 120.00      | 122.68   |
| 28  | W     | 1832 | 6MZ  | C9-N6-C6    | -2.61 | 120.62      | 122.87   |
| 28  | W     | 644  | OMG  | C5-C6-N1    | 2.61  | 119.81      | 113.19   |
| 28  | W     | 822  | PSU  | O2-C2-N1    | -2.60 | 119.92      | 122.79   |
| 28  | W     | 644  | OMG  | O6-C6-C5    | -2.56 | 119.80      | 126.60   |
| 28  | W     | 612  | PSU  | O2-C2-N1    | -2.56 | 119.97      | 122.79   |
| 28  | W     | 683  | OMG  | C4-C5-N7    | -2.54 | 106.69      | 110.72   |
| 28  | W     | 121  | OMU  | O2-C2-N3    | -2.54 | 116.78      | 121.50   |
| 28  | W     | 822  | PSU  | C6-N1-C2    | -2.54 | 120.09      | 122.68   |
| 28  | W     | 509  | OMG  | O6-C6-C5    | -2.50 | 119.96      | 126.60   |
| 28  | W     | 683  | OMG  | O6-C6-C5    | -2.50 | 119.96      | 126.60   |
| 28  | W     | 1243 | PSU  | C6-C5-C4    | 2.50  | 119.94      | 118.20   |
| 28  | W     | 509  | OMG  | C4-C5-N7    | -2.48 | 106.80      | 110.72   |
| 28  | W     | 1248 | C4J  | N3-C2-N1    | 2.42  | 120.17      | 116.76   |
| 28  | W     | 1081 | PSU  | O2-C2-N1    | -2.41 | 120.13      | 122.79   |
| 28  | W     | 814  | 5MU  | O2-C2-N1    | -2.40 | 119.59      | 122.79   |
| 28  | W     | 1832 | 6MZ  | C5-N7-C8    | 2.40  | 106.91      | 103.51   |
| 28  | W     | 1081 | PSU  | C6-N1-C2    | -2.36 | 120.27      | 122.68   |
| 28  | W     | 823  | PSU  | O2-C2-N1    | -2.35 | 120.20      | 122.79   |
| 28  | W     | 1248 | C4J  | C5-C4-N3    | 2.35  | 120.52      | 116.17   |
| 28  | W     | 119  | PSU  | C6-N1-C2    | -2.34 | 120.29      | 122.68   |
| 28  | W     | 1850 | MA6  | C1'-N9-C8   | -2.34 | 121.86      | 127.14   |
| 28  | W     | 823  | PSU  | C6-N1-C2    | -2.31 | 120.32      | 122.68   |
| 28  | W     | 116  | OMU  | O2-C2-N3    | -2.30 | 117.22      | 121.50   |
| 28  | W     | 1832 | 6MZ  | C1'-N9-C8   | -2.23 | 122.11      | 127.14   |
| 28  | W     | 612  | PSU  | O4'-C1'-C2' | 2.22  | 108.28      | 105.14   |
| 28  | W     | 1031 | A2M  | C1'-N9-C8   | -2.20 | 122.16      | 127.14   |
| 28  | W     | 166  | A2M  | C4-N9-C1'   | -2.18 | 121.39      | 126.59   |
| 28  | W     | 823  | PSU  | C6-C5-C4    | 2.16  | 119.71      | 118.20   |
| 28  | W     | 1851 | MA6  | C5-N7-C8    | 2.12  | 106.52      | 103.51   |
| 28  | W     | 484  | A2M  | C6-C5-C4    | 2.12  | 120.03      | 117.18   |
| 28  | W     | 668  | A2M  | C5-N7-C8    | 2.11  | 106.51      | 103.51   |
| 28  | W     | 509  | OMG  | C1'-N9-C8   | -2.08 | 120.77      | 126.70   |
| 28  | W     | 159  | A2M  | C5-N7-C8    | 2.07  | 106.45      | 103.51   |
| 28  | W     | 159  | A2M  | C2'-C1'-N9  | -2.06 | 110.06      | 113.53   |
| 28  | W     | 644  | OMG  | C6-C5-N7    | 2.06  | 134.08      | 130.25   |
| 28  | W     | 1031 | A2M  | C5-N7-C8    | 2.05  | 106.43      | 103.51   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 28  | W     | 166  | A2M  | C2'-C1'-N9  | 2.05  | 116.99      | 113.53   |
| 28  | W     | 668  | A2M  | C4-N9-C1'   | -2.05 | 121.72      | 126.59   |
| 28  | W     | 668  | A2M  | C4'-O4'-C1' | -2.04 | 104.97      | 109.47   |
| 28  | W     | 1703 | OMC  | O2-C2-N3    | -2.04 | 119.01      | 122.33   |
| 28  | W     | 814  | 5MU  | C6-N1-C2    | -2.04 | 119.23      | 121.30   |
| 28  | W     | 1031 | A2M  | C4'-O4'-C1' | -2.02 | 105.00      | 109.47   |
| 28  | W     | 159  | A2M  | C4-N9-C1'   | -2.02 | 121.77      | 126.59   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 28  | W     | 1219 | JMH  | C2'  |

All (46) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 28  | W     | 166  | A2M  | C3'-C4'-C5'-O5' |
| 28  | W     | 509  | OMG  | O4'-C4'-C5'-O5' |
| 28  | W     | 509  | OMG  | C3'-C4'-C5'-O5' |
| 28  | W     | 668  | A2M  | O4'-C4'-C5'-O5' |
| 28  | W     | 668  | A2M  | C3'-C4'-C5'-O5' |
| 28  | W     | 1219 | JMH  | C2'-C1'-N1-C2   |
| 28  | W     | 1219 | JMH  | C3'-C4'-C5'-O5' |
| 28  | W     | 1219 | JMH  | O4'-C4'-C5'-O5' |
| 28  | W     | 1678 | A2M  | C1'-C2'-O2'-CM' |
| 28  | W     | 1703 | OMC  | C3'-C4'-C5'-O5' |
| 28  | W     | 1703 | OMC  | O4'-C4'-C5'-O5' |
| 28  | W     | 1830 | UR3  | O4'-C1'-N1-C6   |
| 28  | W     | 1830 | UR3  | O4'-C1'-N1-C2   |
| 28  | W     | 1832 | 6MZ  | C5-C6-N6-C9     |
| 28  | W     | 1832 | 6MZ  | N1-C6-N6-C9     |
| 28  | W     | 1850 | MA6  | C5-C6-N6-C10    |
| 28  | W     | 1851 | MA6  | O4'-C4'-C5'-O5' |
| 28  | W     | 1851 | MA6  | C3'-C4'-C5'-O5' |
| 28  | W     | 27   | A2M  | O4'-C4'-C5'-O5' |
| 28  | W     | 116  | OMU  | C3'-C4'-C5'-O5' |
| 28  | W     | 116  | OMU  | O4'-C4'-C5'-O5' |
| 28  | W     | 1081 | PSU  | O4'-C4'-C5'-O5' |
| 28  | W     | 1219 | JMH  | C2'-C1'-N1-C6   |
| 28  | W     | 27   | A2M  | C3'-C4'-C5'-O5' |
| 28  | W     | 166  | A2M  | O4'-C4'-C5'-O5' |
| 28  | W     | 612  | PSU  | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 28  | W     | 1081 | PSU  | C3'-C4'-C5'-O5' |
| 28  | W     | 166  | A2M  | C2'-C1'-N9-C8   |
| 28  | W     | 1031 | A2M  | O4'-C4'-C5'-O5' |
| 28  | W     | 166  | A2M  | C2'-C1'-N9-C4   |
| 28  | W     | 1851 | MA6  | C5-C6-N6-C10    |
| 28  | W     | 1248 | C4J  | C4'-C5'-O5'-P   |
| 28  | W     | 1219 | JMH  | C4'-C5'-O5'-P   |
| 28  | W     | 1850 | MA6  | C5-C6-N6-C9     |
| 28  | W     | 822  | PSU  | C3'-C4'-C5'-O5' |
| 28  | W     | 166  | A2M  | C4'-C5'-O5'-P   |
| 28  | W     | 1243 | PSU  | C4'-C5'-O5'-P   |
| 28  | W     | 612  | PSU  | C3'-C4'-C5'-O5' |
| 28  | W     | 166  | A2M  | C3'-C2'-O2'-CM' |
| 28  | W     | 1678 | A2M  | C3'-C4'-C5'-O5' |
| 28  | W     | 166  | A2M  | O4'-C1'-N9-C8   |
| 28  | W     | 1031 | A2M  | C3'-C4'-C5'-O5' |
| 28  | W     | 1219 | JMH  | O4'-C1'-N1-C6   |
| 28  | W     | 1248 | C4J  | C3-C31-C32-N33  |
| 28  | W     | 644  | OMG  | C4'-C5'-O5'-P   |
| 28  | W     | 1081 | PSU  | C4'-C5'-O5'-P   |

There are no ring outliers.

4 monomers are involved in 5 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 28  | W     | 166  | A2M  | 2       | 0            |
| 28  | W     | 1081 | PSU  | 1       | 0            |
| 28  | W     | 116  | OMU  | 1       | 0            |
| 28  | W     | 1851 | MA6  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 91 ligands modelled in this entry, 91 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.



There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 28  | W     | 7                |
| 8   | C     | 1                |
| 14  | I     | 1                |
| 50  | v     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | W     | 753:C     | O3'    | 788:G     | P      | 16.10        |
| 1     | W     | 1760:G    | O3'    | 1771:G    | P      | 15.61        |
| 1     | W     | 697:G     | O3'    | 733:C     | P      | 15.25        |
| 1     | W     | 225:G     | O3'    | 287:U     | P      | 11.87        |
| 1     | W     | 740:C     | O3'    | 746:C     | P      | 6.05         |
| 1     | C     | 155:ASN   | C      | 156:LEU   | N      | 5.87         |
| 1     | W     | 1219:JMH  | O3'    | 1220:A    | P      | 5.81         |
| 1     | I     | 713:SER   | C      | 714:GLN   | N      | 3.71         |
| 1     | v     | 93:GLN    | C      | 94:GLU    | N      | 3.41         |
| 1     | W     | 1310:U    | O3'    | 1311:C    | P      | 3.02         |

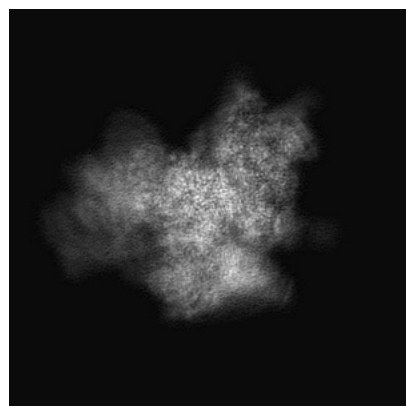
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17297. These allow visual inspection of the internal detail of the map and identification of artifacts.

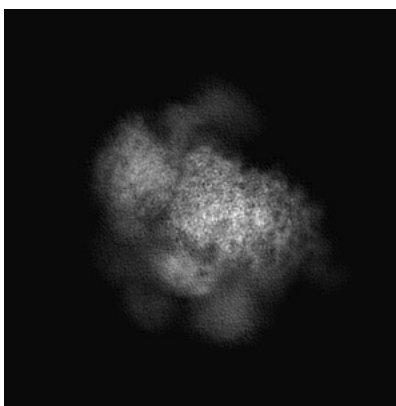
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

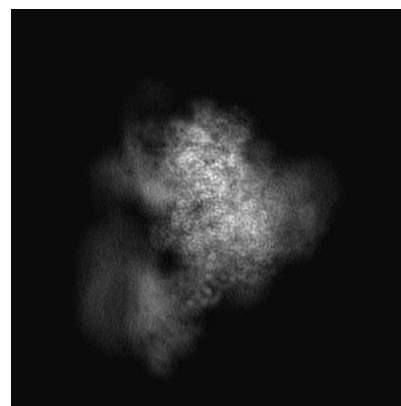
#### 6.1.1 Primary map



X

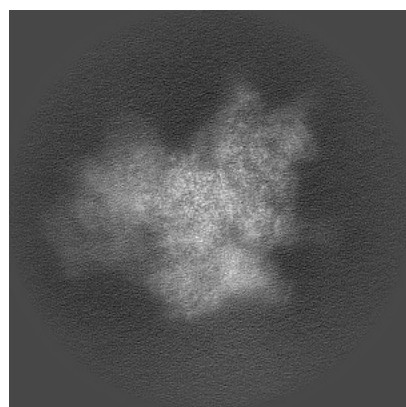


Y

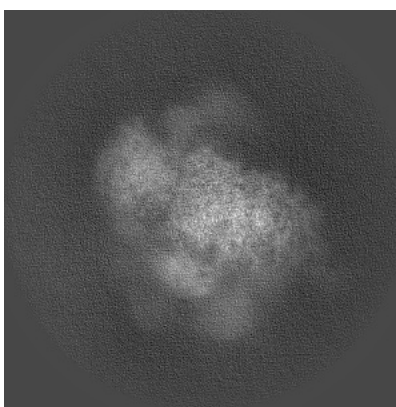


Z

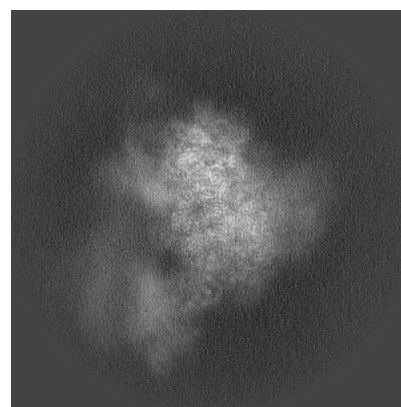
#### 6.1.2 Raw map



X



Y

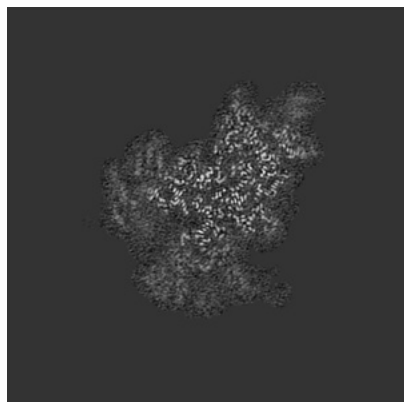


Z

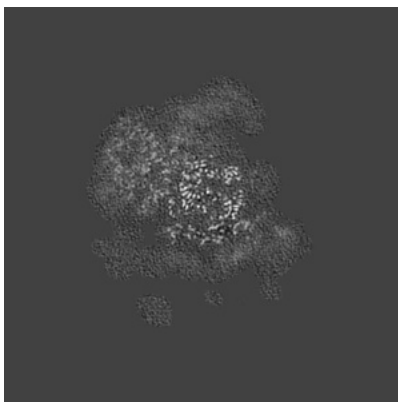
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

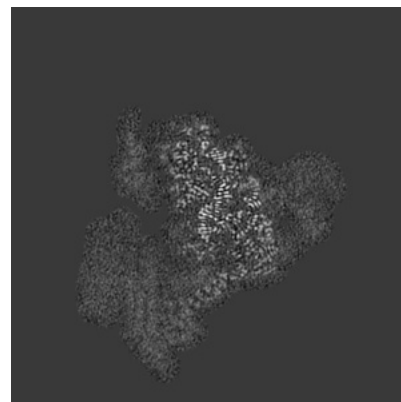
### 6.2.1 Primary map



X Index: 200

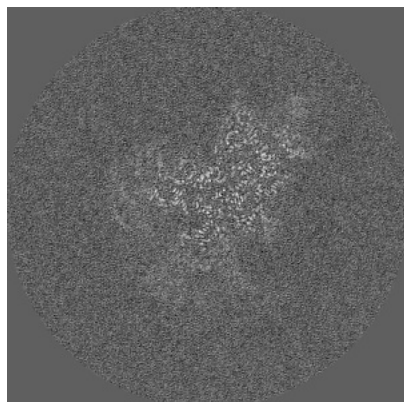


Y Index: 200

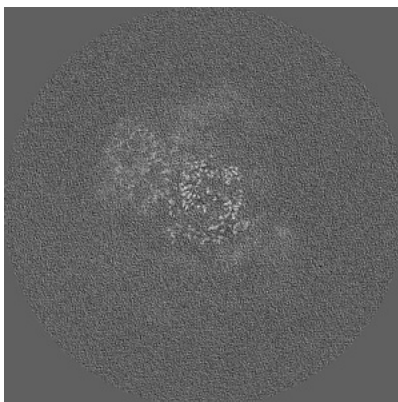


Z Index: 200

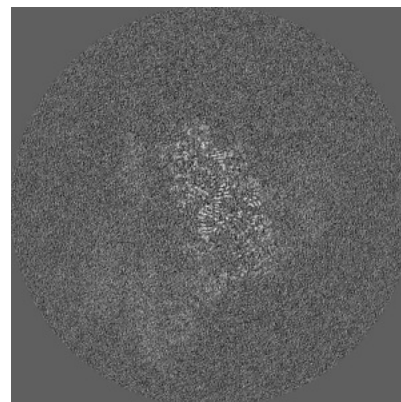
### 6.2.2 Raw map



X Index: 200



Y Index: 200

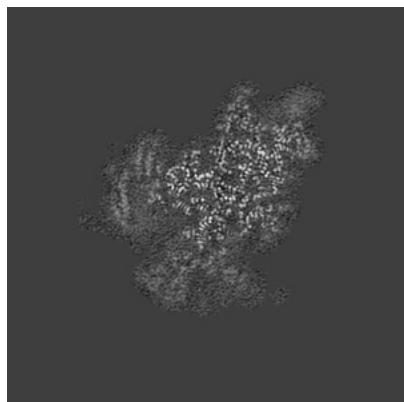


Z Index: 200

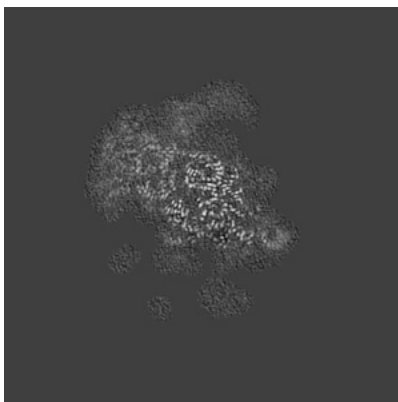
The images above show central slices of the map in three orthogonal directions.

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

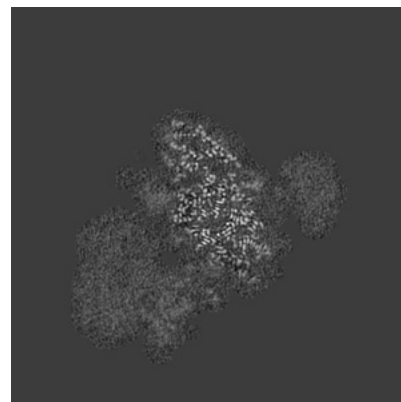
### 6.3.1 Primary map



X Index: 197

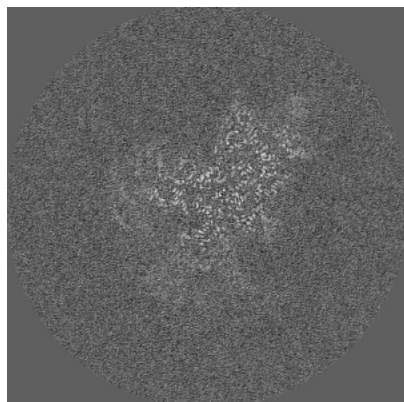


Y Index: 192

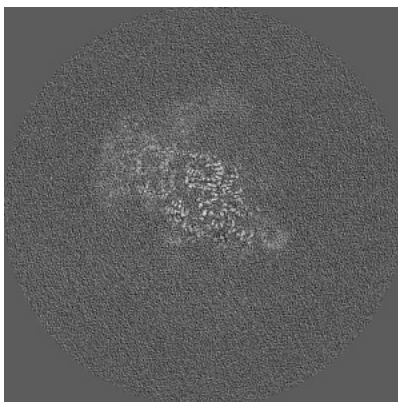


Z Index: 218

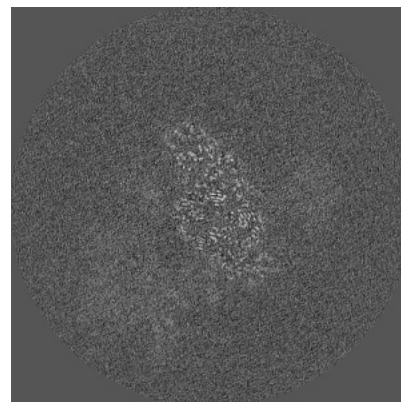
### 6.3.2 Raw map



X Index: 200



Y Index: 192

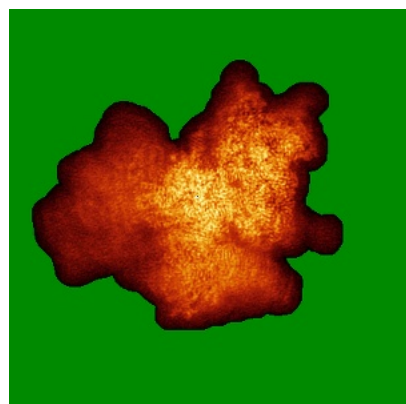


Z Index: 213

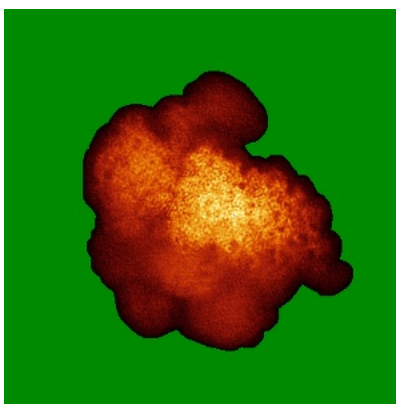
The images above show the largest variance slices of the map in three orthogonal directions.

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

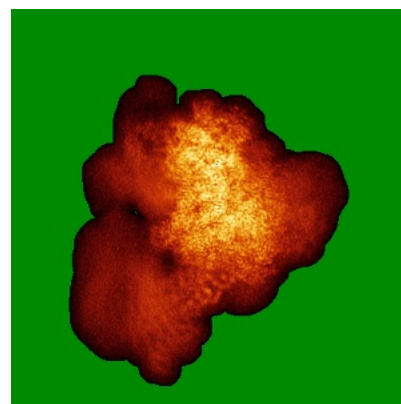
### 6.4.1 Primary map



X

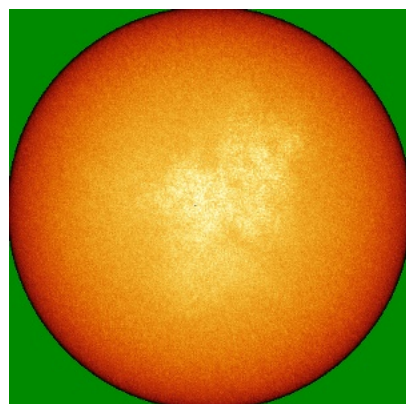


Y

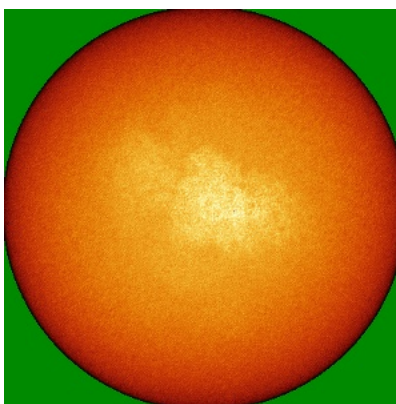


Z

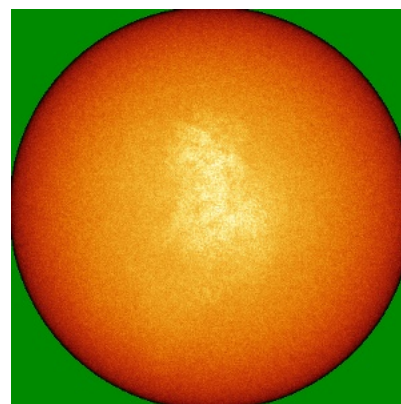
### 6.4.2 Raw map



X



Y



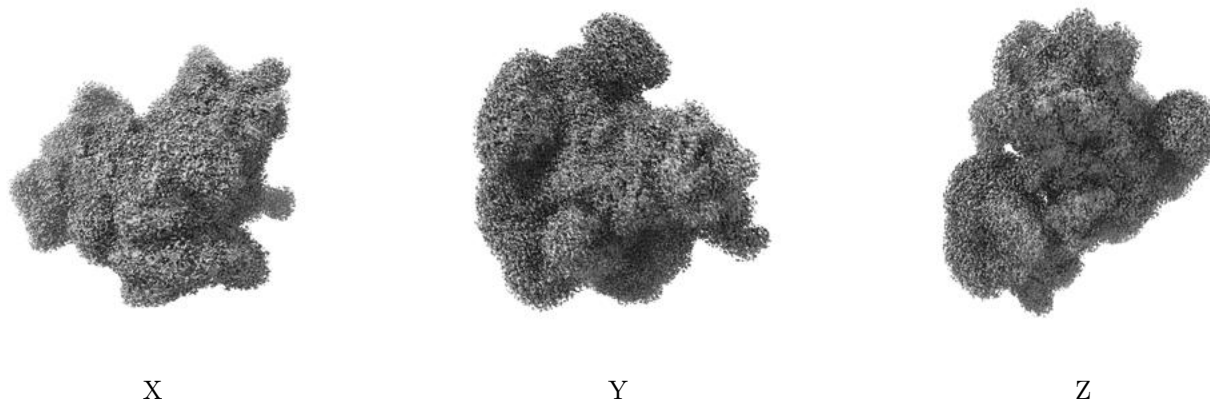
Z

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.



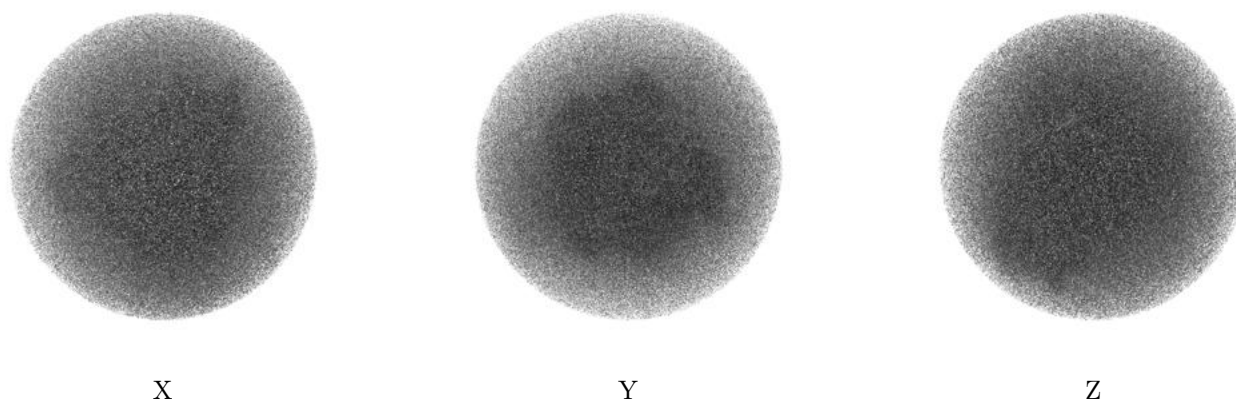
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. 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.

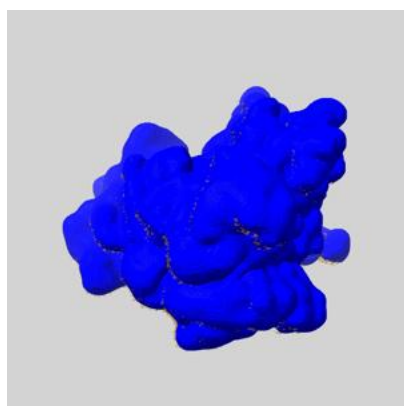
## 6.6 Mask visualisation [i](#)

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

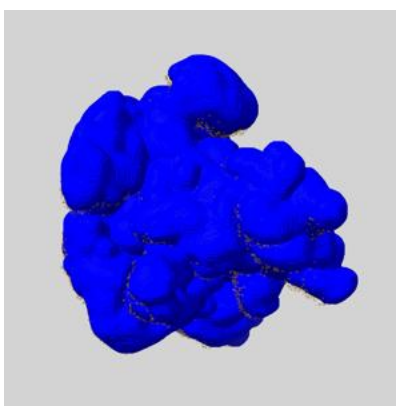
A mask typically either:

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

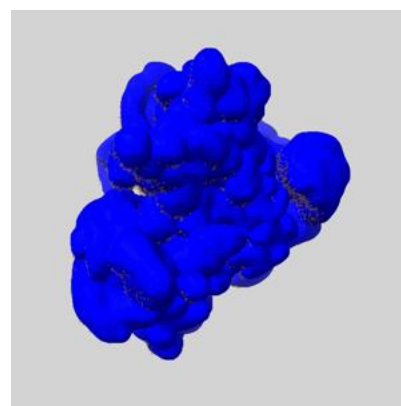
### 6.6.1 emd\_17297\_msk\_1.map [i](#)



X



Y

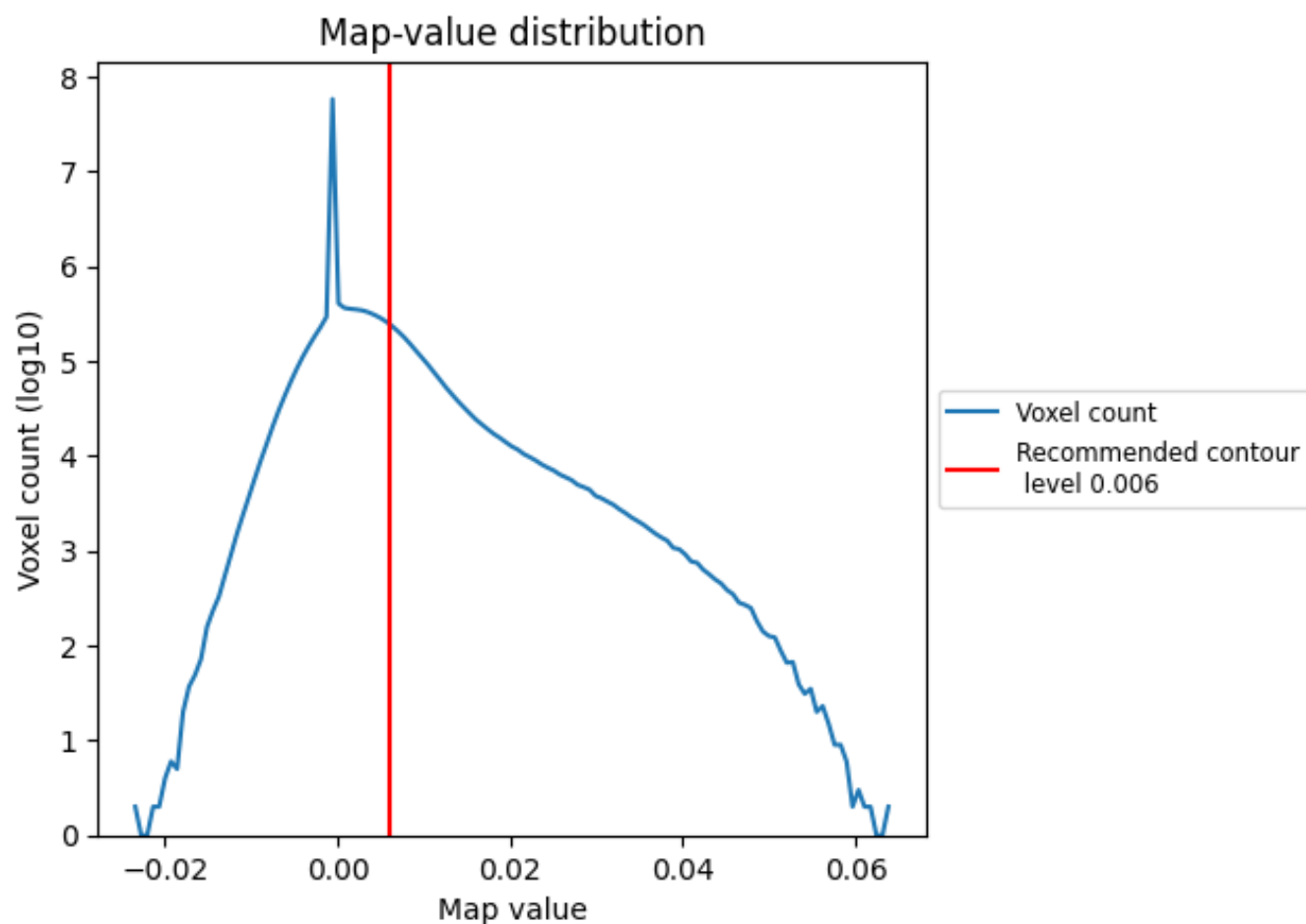


Z

## 7 Map analysis [i](#)

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

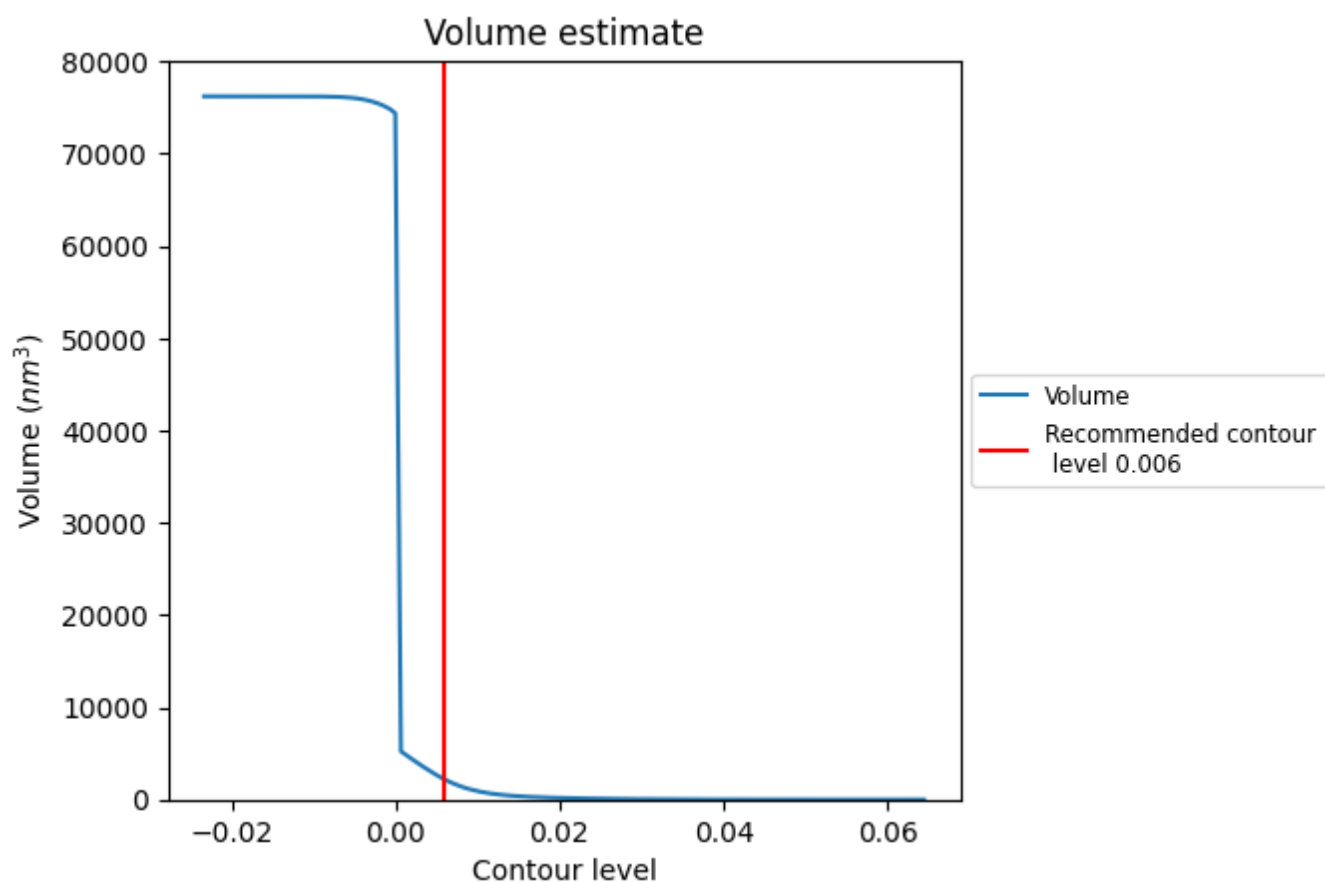
### 7.1 Map-value distribution [i](#)



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



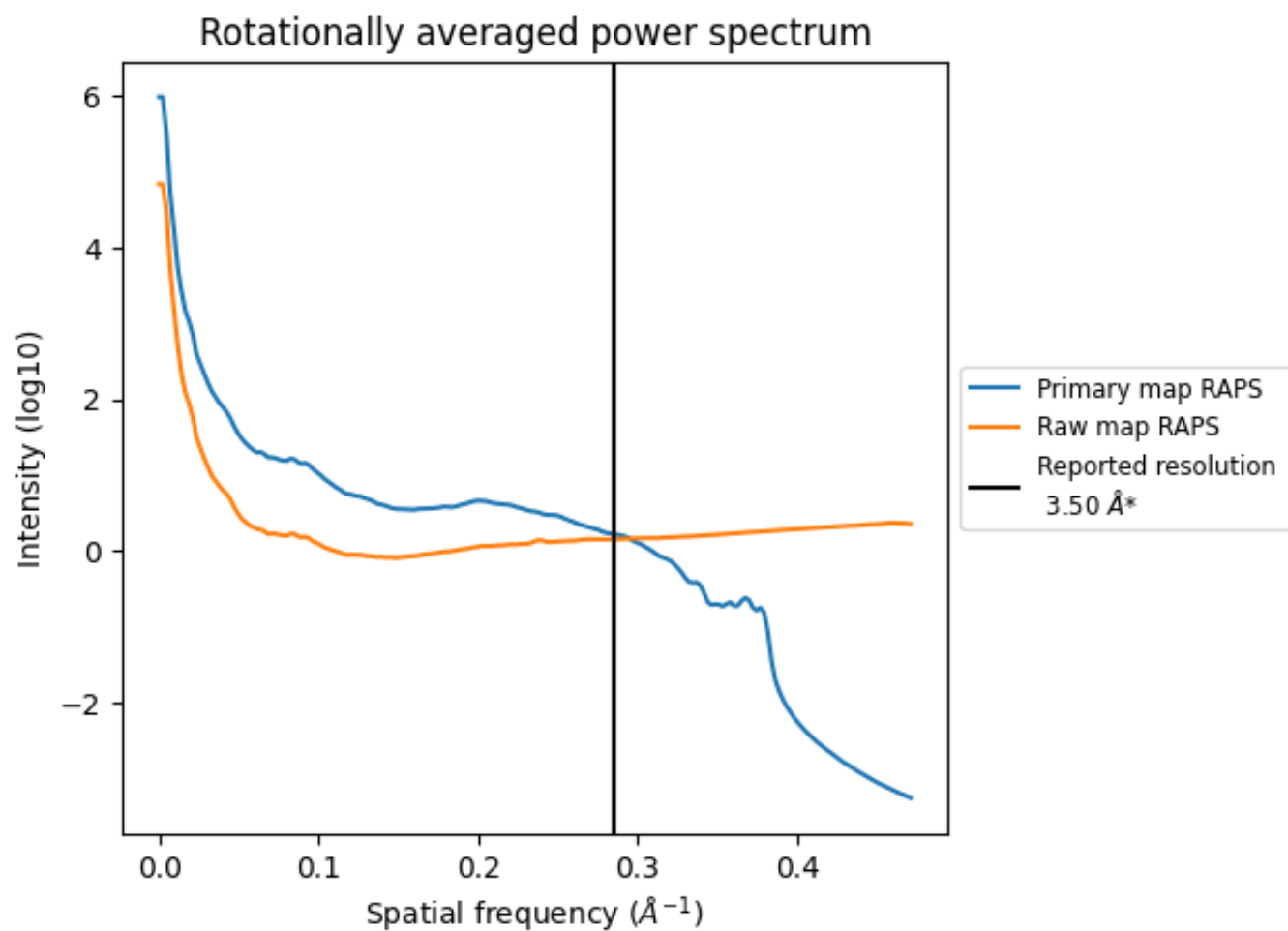
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2177  $\text{nm}^3$ ; this corresponds to an approximate mass of 1966 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 ⓘ

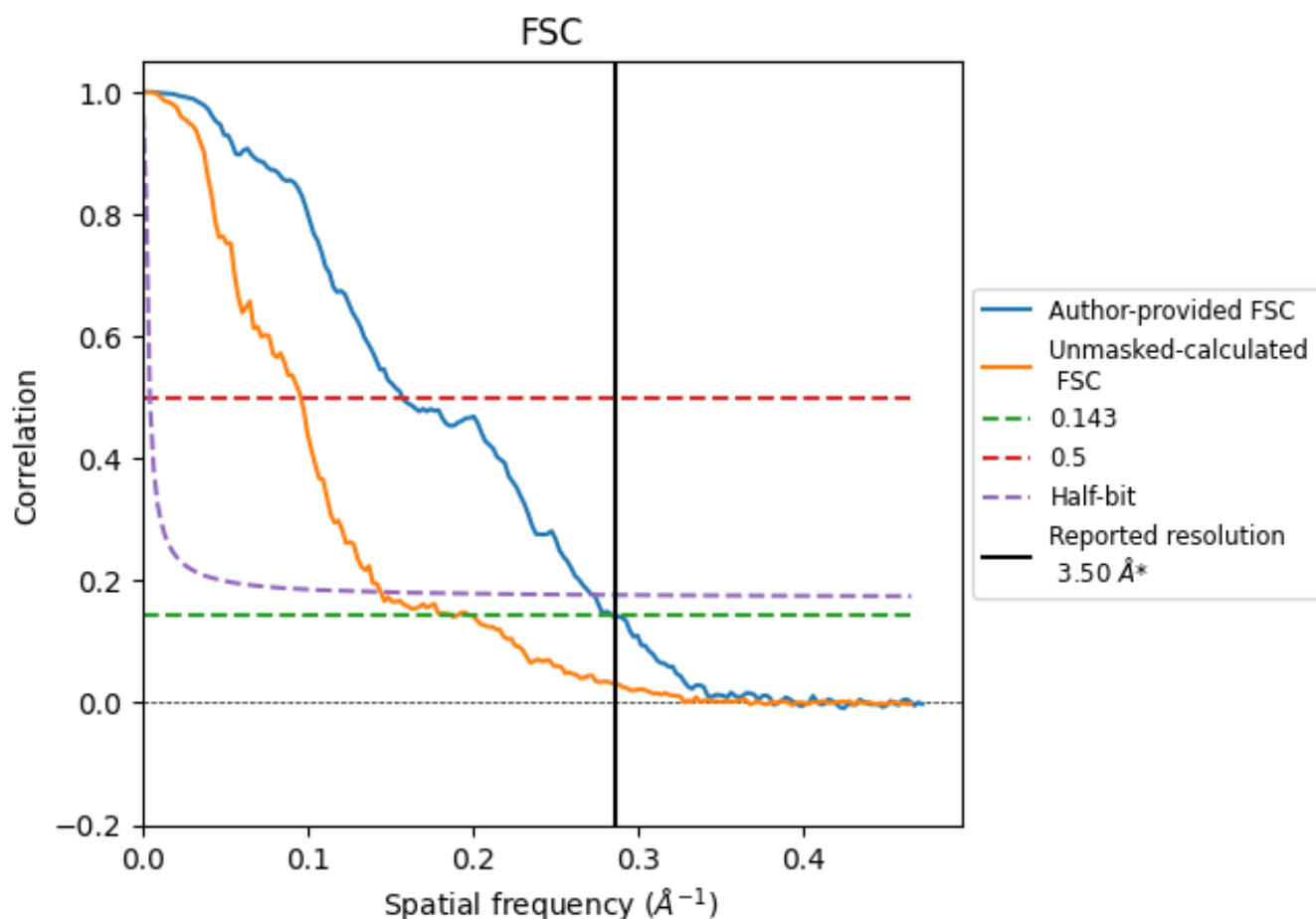


\*Reported resolution corresponds to spatial frequency of 0.286  $\text{\AA}^{-1}$

## 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  $0.286 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

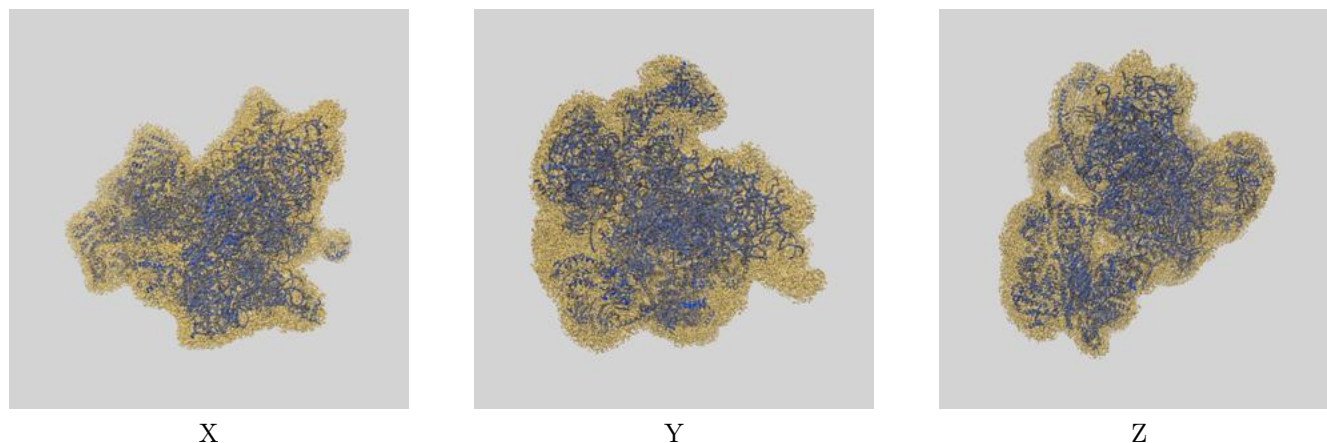
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |       |          |
|---------------------------|------------------------------------|-------|----------|
|                           | 0.143                              | 0.5   | Half-bit |
| Reported by author        | 3.50                               | -     | -        |
| Author-provided FSC curve | 3.52                               | 6.36  | 3.66     |
| Unmasked-calculated*      | 5.35                               | 10.43 | 6.93     |

\*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 5.35 differs from the reported value 3.5 by more than 10 %

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

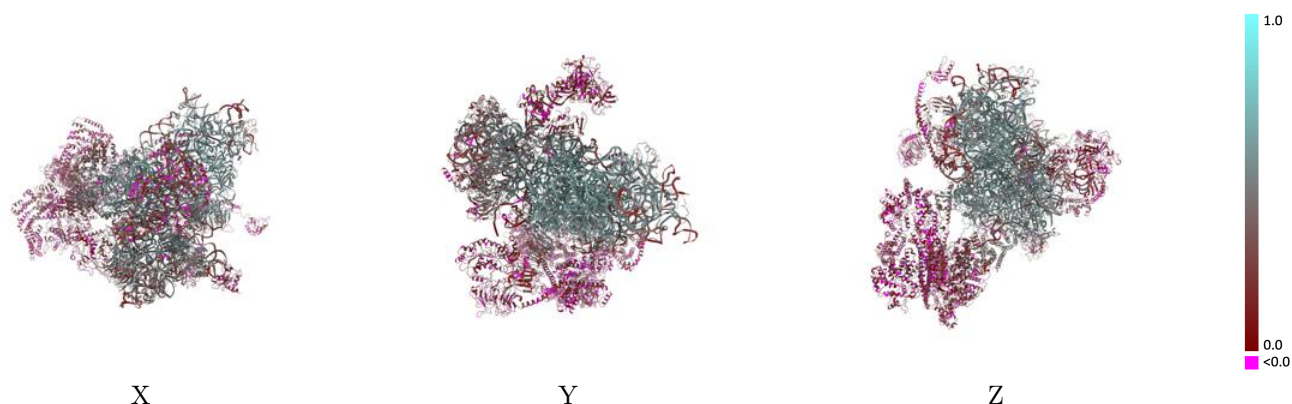
This section contains information regarding the fit between EMDB map EMD-17297 and PDB model 8OZ0. Per-residue inclusion information can be found in section [3](#) on page [15](#).

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



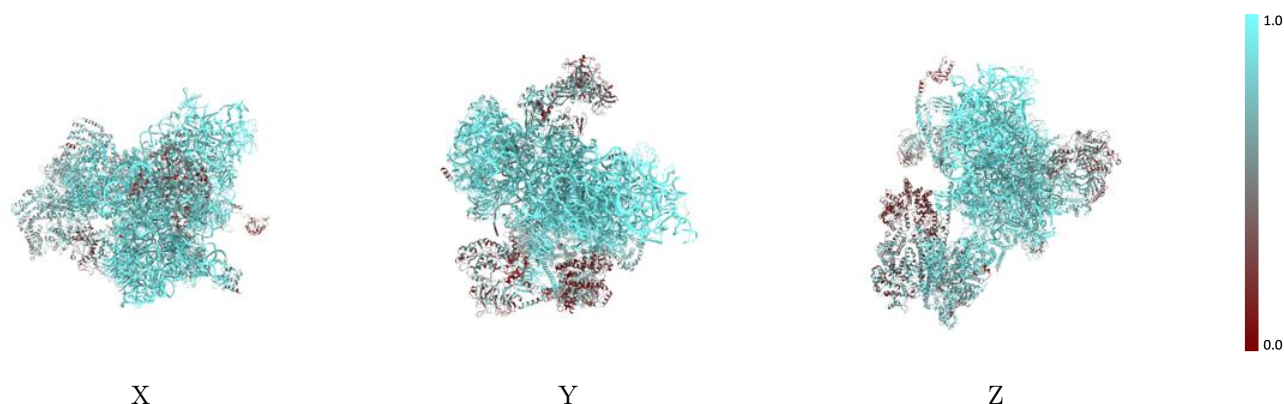
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



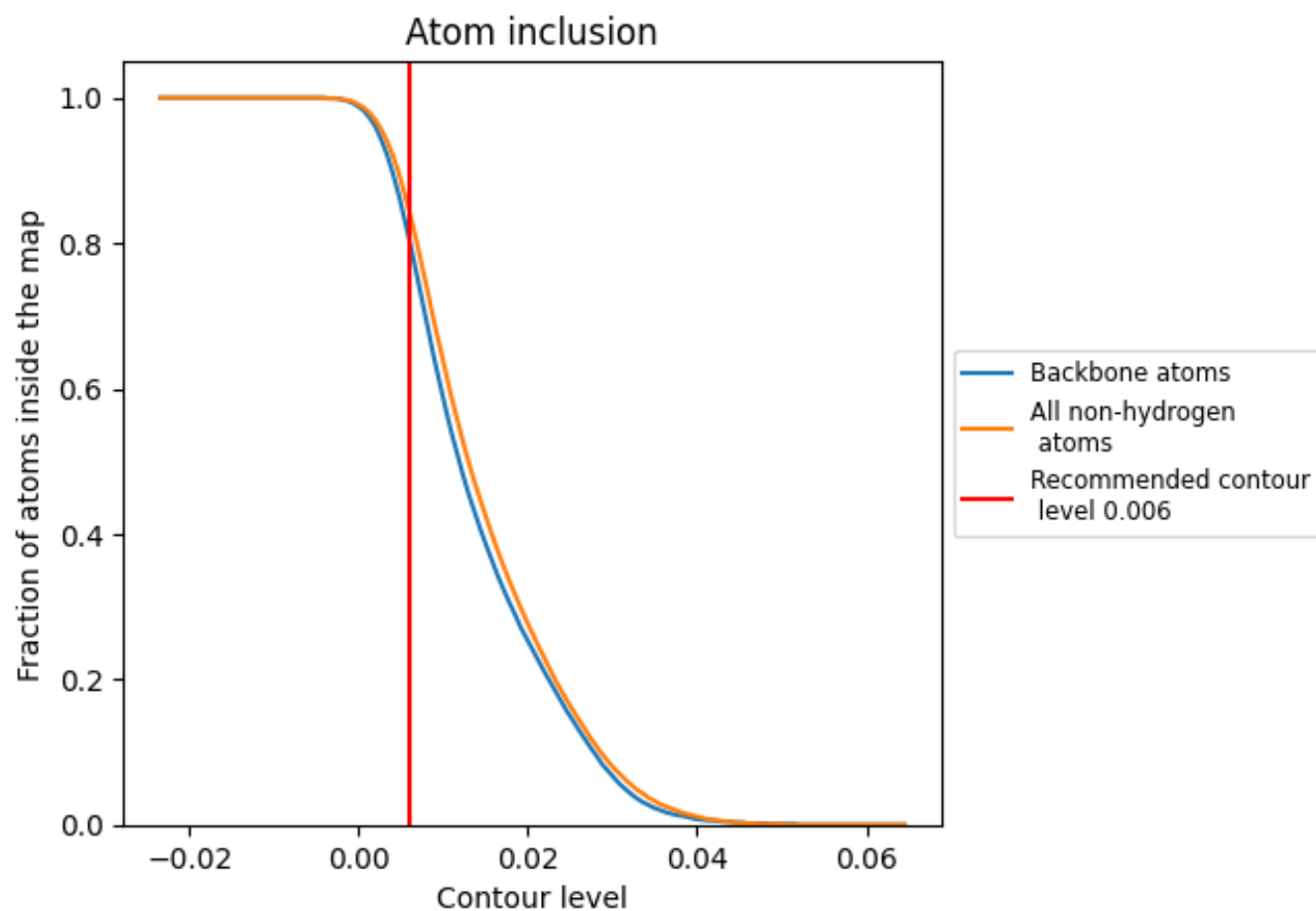
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 84% 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 (0.006) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8440   |  0.3910   |
| 1     |  0.3550   |  0.1560   |
| 2     |  0.2350   |  0.1320   |
| 3     |  0.4650   |  0.1990   |
| 5     |  0.7240   |  0.1690   |
| 6     |  0.6350   |  0.1830   |
| 7     |  0.7650   |  0.2560   |
| 8     |  0.6560   |  0.1800   |
| 9     |  0.9760   |  0.5390   |
| A     |  0.7770   |  0.2550   |
| B     |  0.5570   |  0.1480   |
| C     |  0.6220   |  0.1600   |
| D     |  0.7210   |  0.2600   |
| E     |  0.4530   |  0.1810   |
| F     |  0.4770  |  0.1950  |
| G     |  0.8750 |  0.3700 |
| H     |  0.5600 |  0.2520 |
| I     |  0.7370 |  0.2770 |
| J     |  0.8020 |  0.2830 |
| K     |  0.5950 |  0.1740 |
| L     |  0.9570 |  0.4930 |
| M     |  0.9870 |  0.5550 |
| N     |  0.9770 |  0.5480 |
| O     |  0.9890 |  0.5750 |
| P     |  0.9780 |  0.5390 |
| Q     |  0.9840 |  0.5580 |
| R     |  0.9910 |  0.5650 |
| S     |  0.9490 |  0.4490 |
| T     |  0.9620 |  0.5230 |
| U     |  0.4310 |  0.1720 |
| V     |  0.9860 |  0.5450 |
| W     |  0.9780 |  0.4960 |
| X     |  0.9850 |  0.5730 |
| Y     |  0.9950 |  0.5760 |
| Z     |  0.9890 |  0.5690 |



*Continued on next page...*



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| a     |  0.9940   |  0.5880   |
| b     |  0.9950   |  0.5600   |
| c     |  0.9890   |  0.5880   |
| d     |  0.9840   |  0.5310   |
| e     |  0.9840   |  0.5450   |
| f     |  0.9670   |  0.4750   |
| g     |  0.9590   |  0.4650   |
| h     |  0.9580   |  0.4450   |
| i     |  0.9290   |  0.4260   |
| j     |  0.8950   |  0.4160   |
| k     |  0.9030   |  0.3770   |
| l     |  0.9530   |  0.4250   |
| m     |  0.8930   |  0.3980   |
| n     |  0.9040   |  0.3970   |
| o     |  0.9900   |  0.5110   |
| p     |  0.7610   |  0.1950   |
| q     |  0.6560   |  0.2460   |
| s     |  0.9310   |  0.4720   |
| v     |  0.9640   |  0.4920   |
| w     |  0.9440  |  0.4450  |
| x     |  0.6540 |  0.2610 |
| y     |  0.8600 |  0.2650 |
| z     |  0.7990 |  0.2440 |