



## Full wwPDB EM Validation Report ⓘ

Jun 25, 2026 – 02:02 AM EDT

PDB ID : 9ED0 / pdb\_00009ed0  
EMDB ID : EMD-47929  
Title : Human LARP1 bound to the 40S small ribosomal subunit  
Authors : Dong, W.; Kaufhold, R.; Brito Querido, J.  
Deposited on : 2024-11-15  
Resolution : 2.80 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:

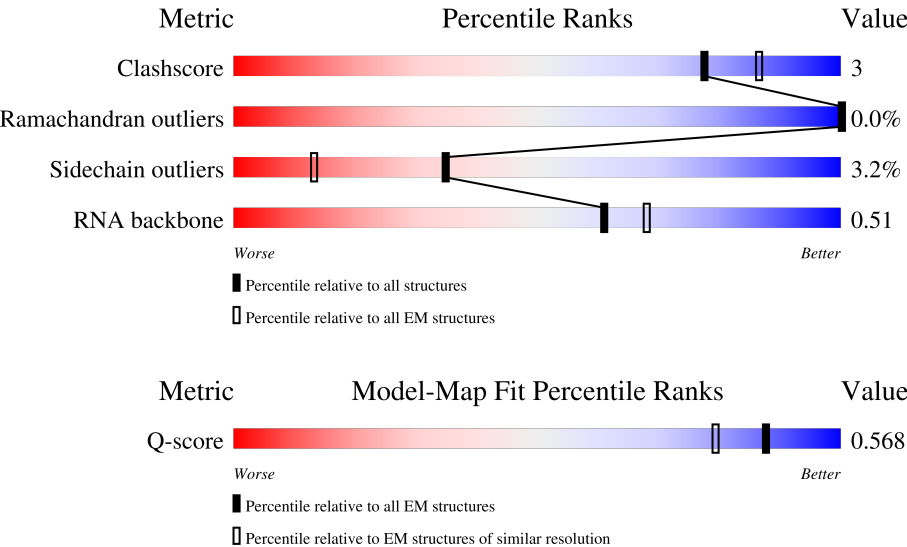
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 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 2.80 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 11806 ( 2.30 - 3.30 )                                    |

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

| Mol | Chain | Length | Quality of chain                                                        |
|-----|-------|--------|-------------------------------------------------------------------------|
| 1   | 2     | 1869   | <div> <div>7%</div> <div>64%</div> <div>20%</div> <div>13%</div> </div> |
| 2   | A     | 295    | <div> <div>7%</div> <div>59%</div> <div>11%</div> <div>30%</div> </div> |
| 3   | B     | 264    | <div> <div>16%</div> <div>71%</div> <div>8%</div> <div>20%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | C     | 293    |                  |
| 5   | D     | 243    |                  |
| 6   | E     | 263    |                  |
| 7   | F     | 204    |                  |
| 8   | G     | 249    |                  |
| 9   | H     | 194    |                  |
| 10  | I     | 208    |                  |
| 11  | J     | 194    |                  |
| 12  | K     | 165    |                  |
| 13  | L     | 158    |                  |
| 14  | M     | 132    |                  |
| 15  | N     | 151    |                  |
| 16  | O     | 151    |                  |
| 17  | P     | 145    |                  |
| 18  | Q     | 146    |                  |
| 19  | R     | 135    |                  |
| 20  | S     | 152    |                  |
| 21  | T     | 145    |                  |
| 22  | U     | 119    |                  |
| 23  | V     | 83     |                  |
| 24  | W     | 130    |                  |
| 25  | X     | 143    |                  |
| 26  | Y     | 133    |                  |
| 27  | Z     | 125    |                  |
| 28  | a     | 115    |                  |

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| Mol | Chain | Length | Quality of chain                                                                 |
|-----|-------|--------|----------------------------------------------------------------------------------|
| 29  | b     | 84     | <div><div><div></div><div></div><div></div></div><div>21%77%18%...</div></div>   |
| 30  | c     | 69     | <div><div><div></div><div></div><div></div></div><div>29%65%14%.•14%</div></div> |
| 31  | d     | 56     | <div><div><div></div><div></div><div></div></div><div>•88%11%.</div></div>       |
| 32  | e     | 59     | <div><div><div></div><div></div><div></div></div><div>15%78%15%7%</div></div>    |
| 33  | f     | 156    | <div><div><div></div><div></div><div></div></div><div>41%36%5%59%</div></div>    |
| 34  | g     | 317    | <div><div><div></div><div></div><div></div></div><div>79%76%21%..</div></div>    |
| 35  | h     | 1096   | <div><div><div></div><div></div><div></div></div><div>•96%</div></div>           |
| 36  | n     | 25     | <div><div><div></div><div></div><div></div></div><div>8%72%8%20%</div></div>     |

## 2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 73475 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called rRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 1   | 2     | 1617     | Total | C     | N    | O     | P    | 6       | 0     |
|     |       |          | 34700 | 15519 | 6236 | 11323 | 1622 |         |       |

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | A     | 206      | Total | C    | N   | O   | S | 1       | 0     |
|     |       |          | 1625  | 1040 | 287 | 290 | 8 |         |       |

- Molecule 3 is a protein called Small ribosomal subunit protein eS1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | B     | 210      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1711  | 1086 | 306 | 305 | 14 |         |       |

- Molecule 4 is a protein called Small ribosomal subunit protein uS5.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | C     | 219      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 1708  | 1105 | 295 | 298 | 10 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5   | D     | 224      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1745  | 1112 | 314 | 312 | 7 |         |       |

- Molecule 6 is a protein called Small ribosomal subunit protein eS4, X isoform.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6   | E     | 257      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2041  | 1305 | 379 | 349 | 8 |         |       |

- Molecule 7 is a protein called Small ribosomal subunit protein uS7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | F     | 182      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1445  | 906 | 271 | 261 | 7 |         |       |

- Molecule 8 is a protein called Small ribosomal subunit protein eS6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 8   | G     | 227      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1840  | 1149 | 367 | 317 | 7 |         |       |

- Molecule 9 is a protein called Small ribosomal subunit protein eS7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | H     | 184      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1477  | 942 | 271 | 263 | 1 |         |       |

- Molecule 10 is a protein called Small ribosomal subunit protein eS8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 10  | I     | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1682  | 1056 | 331 | 290 | 5 |         |       |

- Molecule 11 is a protein called Small ribosomal subunit protein uS4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | J     | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1525  | 969 | 306 | 248 | 2 |         |       |

- Molecule 12 is a protein called Small ribosomal subunit protein eS10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | K     | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 816   | 533 | 144 | 133 | 6 |         |       |

- Molecule 13 is a protein called Small ribosomal subunit protein uS17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | L     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1157  | 737 | 217 | 197 | 6 |         |       |

- Molecule 14 is a protein called Small ribosomal subunit protein eS12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | M     | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 790   | 494 | 138 | 151 | 7 |         |       |

- Molecule 15 is a protein called Small ribosomal subunit protein uS15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | N     | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1208  | 773 | 229 | 205 | 1 |         |       |

- Molecule 16 is a protein called Small ribosomal subunit protein uS11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | O     | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 957   | 585 | 189 | 177 | 6 |         |       |

- Molecule 17 is a protein called Small ribosomal subunit protein uS19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | P     | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 998   | 635 | 188 | 169 | 6 |         |       |

- Molecule 18 is a protein called Small ribosomal subunit protein uS9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | Q     | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1105  | 704 | 207 | 191 | 3 |         |       |

- Molecule 19 is a protein called Small ribosomal subunit protein eS17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | R     | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1064  | 668 | 198 | 194 | 4 |         |       |

- Molecule 20 is a protein called Small ribosomal subunit protein uS13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | S     | 143      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 1192  | 751 | 240 | 200 | 1 |         |       |

- Molecule 21 is a protein called Small ribosomal subunit protein eS19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | T     | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1112  | 697 | 214 | 198 | 3 |         |       |

- Molecule 22 is a protein called Small ribosomal subunit protein uS10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | U     | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 821   | 514 | 155 | 148 | 4 |         |       |

- Molecule 23 is a protein called Small ribosomal subunit protein eS21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | V     | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 636   | 393 | 117 | 121 | 5 |         |       |

- Molecule 24 is a protein called Small ribosomal subunit protein uS8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | W     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1034  | 659 | 193 | 176 | 6 |         |       |

- Molecule 25 is a protein called 40S ribosomal protein S23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | X     | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1087  | 687 | 215 | 182 | 3 |         |       |

- Molecule 26 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | Y     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1002  | 635 | 196 | 166 | 5 |         |       |

- Molecule 27 is a protein called Small ribosomal subunit protein eS25.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 27  | Z     | 72       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 570   | 366 | 104 | 99 | 1 |         |       |

- Molecule 28 is a protein called Small ribosomal subunit protein eS26.



| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | a     | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 792   | 492 | 165 | 130 | 5 |         |       |

- Molecule 29 is a protein called Small ribosomal subunit protein eS27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | b     | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 640   | 402 | 118 | 113 | 7 |         |       |

- Molecule 30 is a protein called Small ribosomal subunit protein eS28.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 30  | c     | 59       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 464   | 281 | 93 | 88 | 2 |         |       |

- Molecule 31 is a protein called Small ribosomal subunit protein uS14.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 31  | d     | 55       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 459   | 286 | 94 | 74 | 5 |         |       |

- Molecule 32 is a protein called Small ribosomal subunit protein eS30.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 32  | e     | 55       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 438   | 271 | 95 | 71 | 1 |         |       |

- Molecule 33 is a protein called Ubiquitin-ribosomal protein eS31 fusion protein.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 33  | f     | 64       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 522   | 329 | 99 | 87 | 7 |         |       |

- Molecule 34 is a protein called Receptor of activated protein C kinase 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 34  | g     | 312      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2408  | 1518 | 420 | 458 | 12 |         |       |

- Molecule 35 is a protein called La-related protein 1.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 35  | h     | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 345   | 214 | 63 | 67 | 1 |         |       |

- Molecule 36 is a protein called Small ribosomal subunit protein eS32.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 36  | n     | 20       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 193   | 119 | 51 | 20 | 3 |         |       |

- Molecule 37 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 37  | 2     | 68       | Total | K  | 0       |
|     |       |          | 68    | 68 |         |
| 37  | S     | 1        | Total | K  | 0       |
|     |       |          | 1     | 1  |         |
| 37  | X     | 1        | Total | K  | 0       |
|     |       |          | 1     | 1  |         |
| 37  | d     | 1        | Total | K  | 0       |
|     |       |          | 1     | 1  |         |

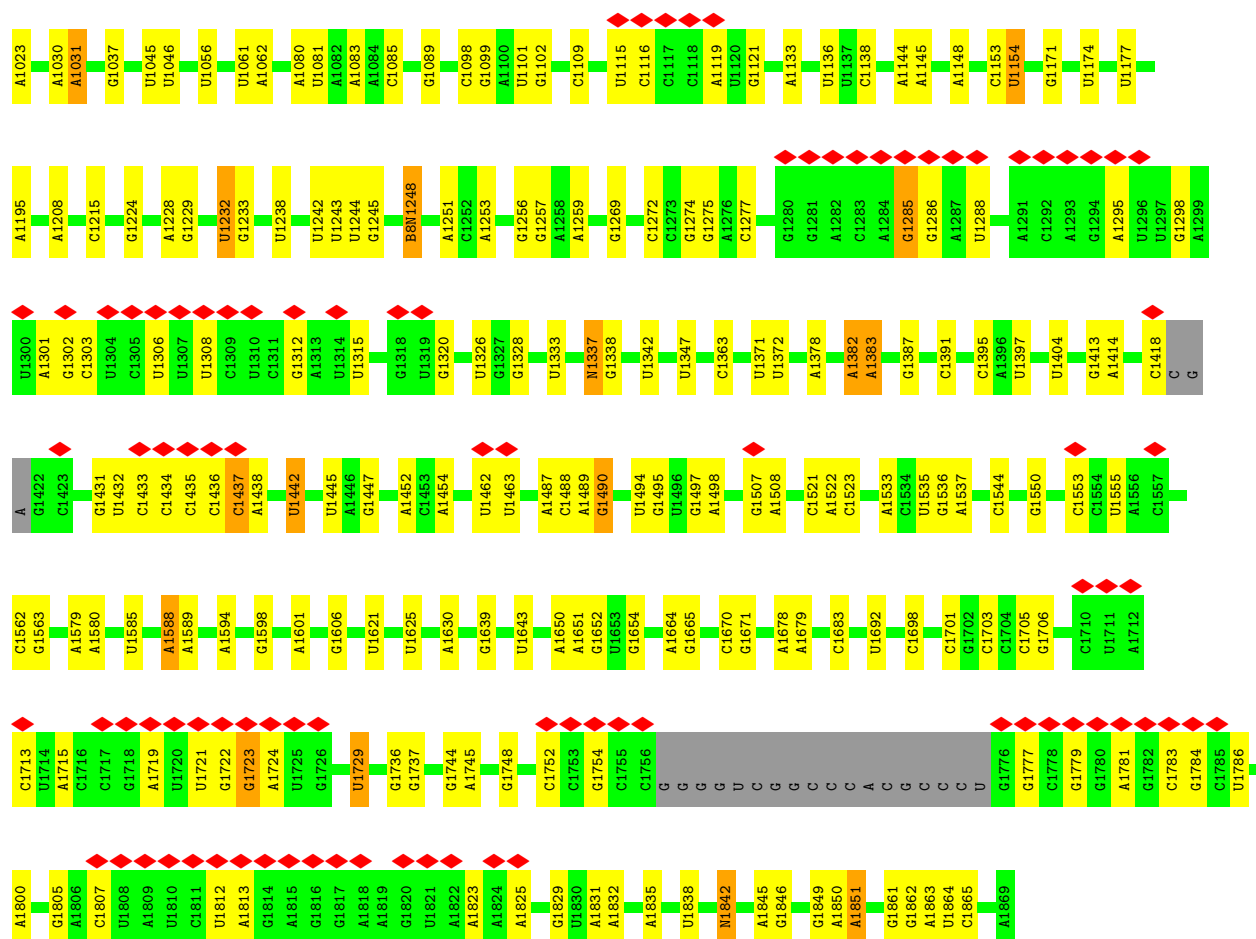
- Molecule 38 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 38  | 2     | 91       | Total | Mg | 0       |
|     |       |          | 91    | 91 |         |
| 38  | G     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

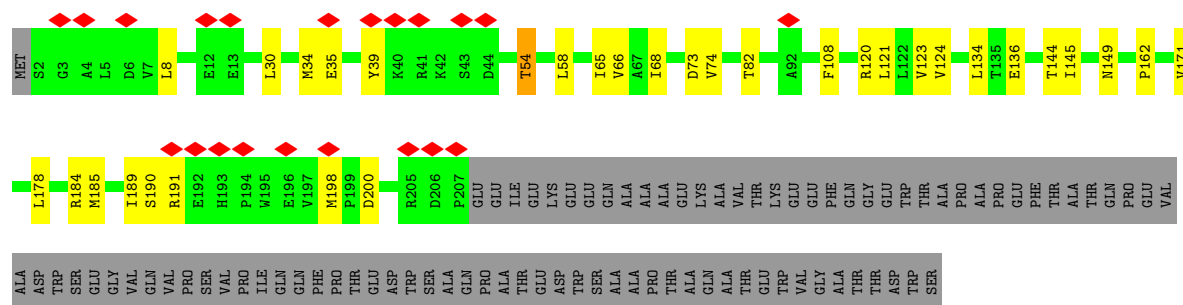
- Molecule 39 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 39  | a     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 39  | d     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 39  | f     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

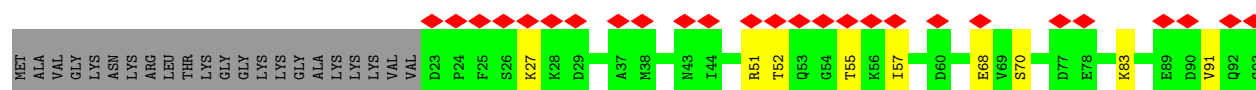




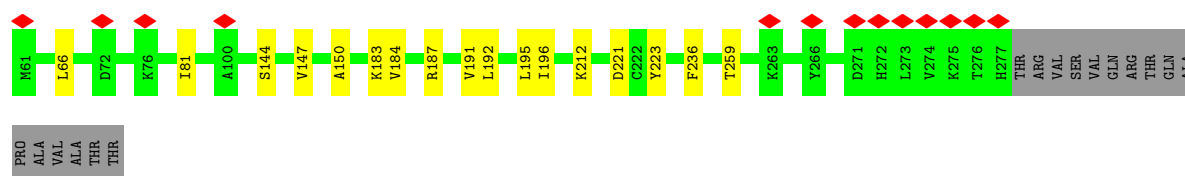
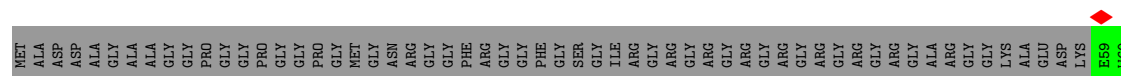
• Molecule 2: Small ribosomal subunit protein uS2



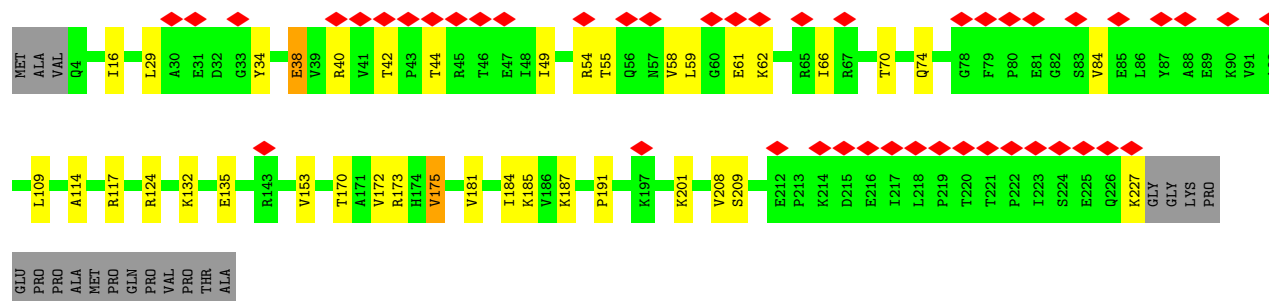
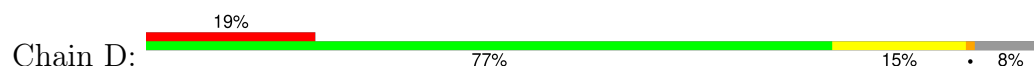
• Molecule 3: Small ribosomal subunit protein eS1



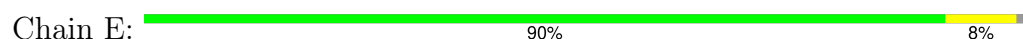
- Molecule 4: Small ribosomal subunit protein uS5



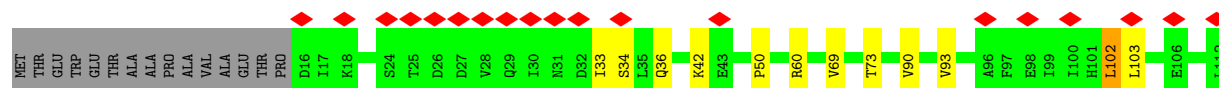
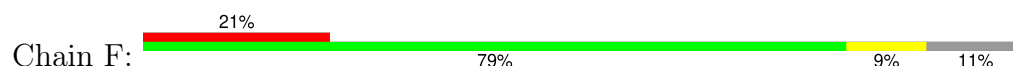
- Molecule 5: Small ribosomal subunit protein uS3

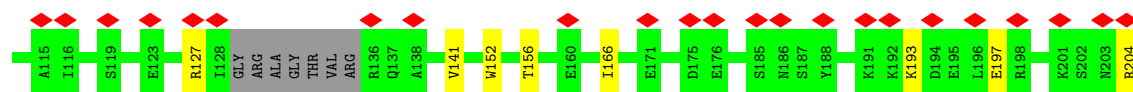


- Molecule 6: Small ribosomal subunit protein eS4, X isoform

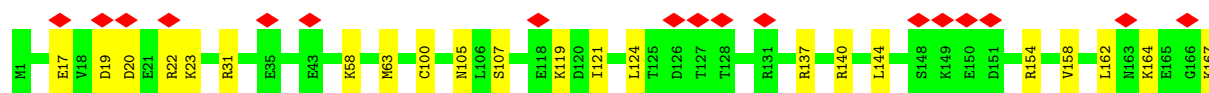
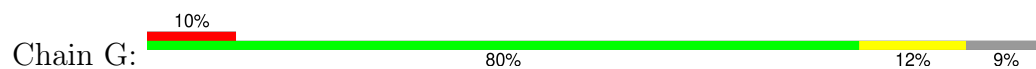


- Molecule 7: Small ribosomal subunit protein uS7

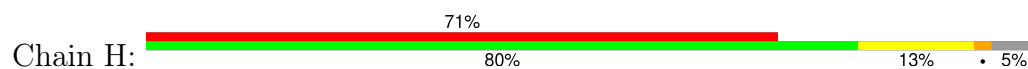




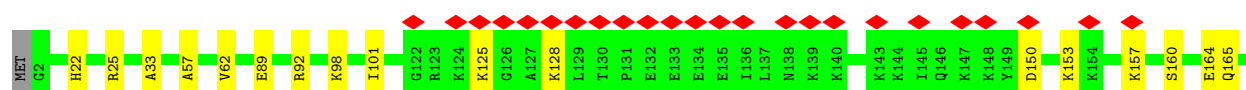
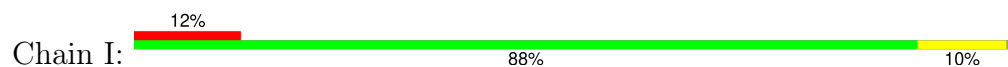
- Molecule 8: Small ribosomal subunit protein eS6



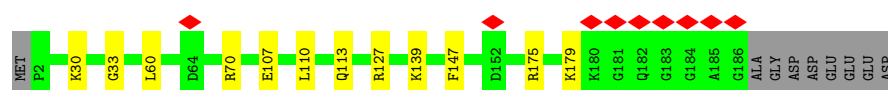
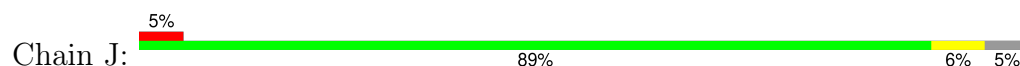
- Molecule 9: Small ribosomal subunit protein eS7



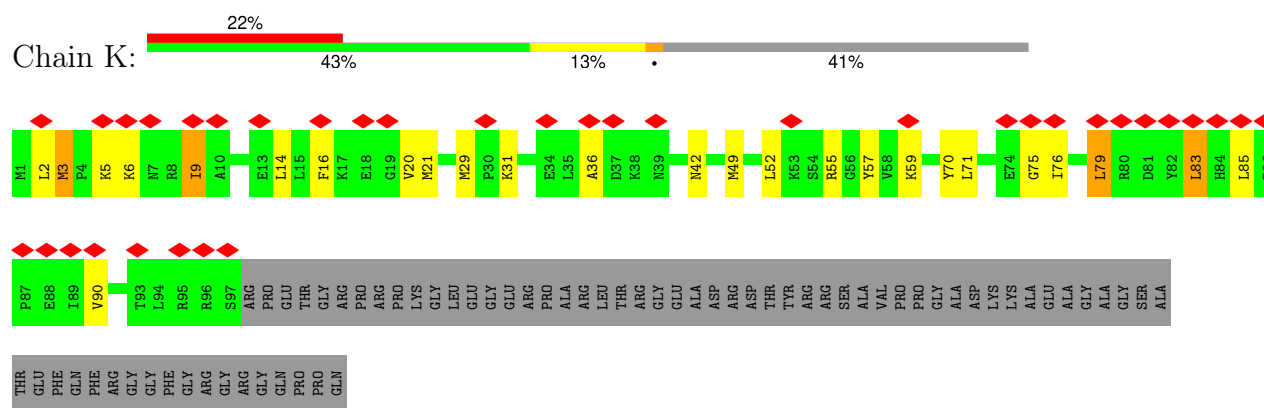
- Molecule 10: Small ribosomal subunit protein eS8



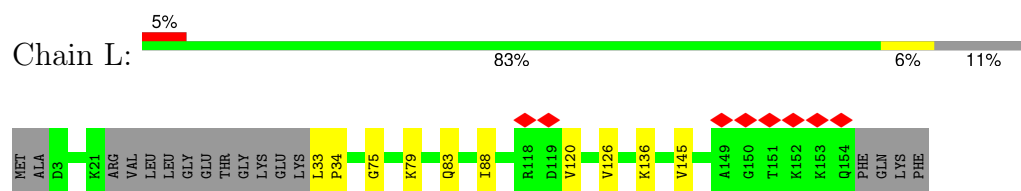
- Molecule 11: Small ribosomal subunit protein uS4



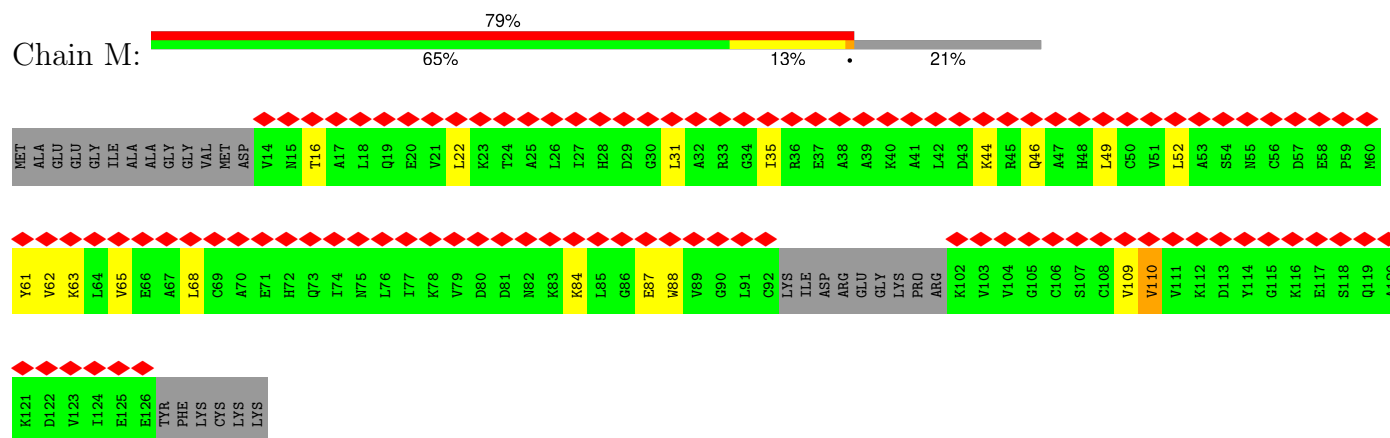
- Molecule 12: Small ribosomal subunit protein eS10



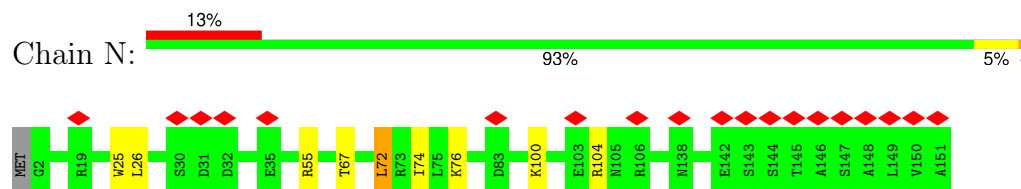
- Molecule 13: Small ribosomal subunit protein uS17



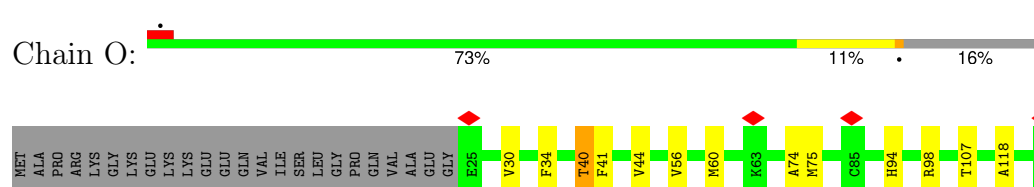
- Molecule 14: Small ribosomal subunit protein eS12



- Molecule 15: Small ribosomal subunit protein uS15

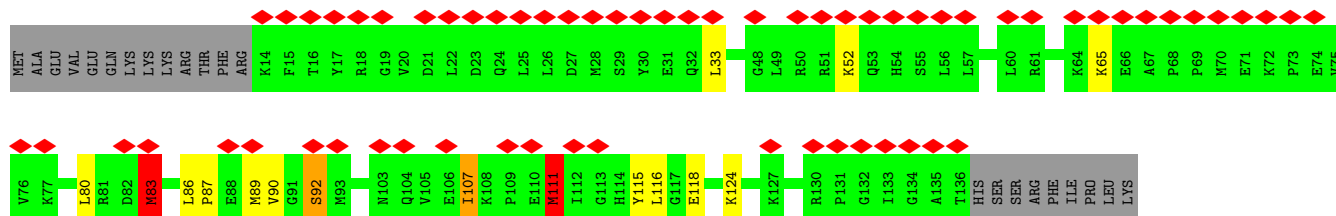
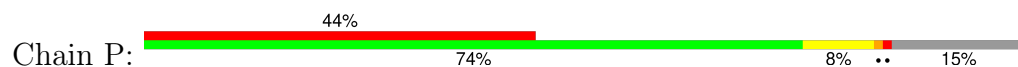


- Molecule 16: Small ribosomal subunit protein uS11

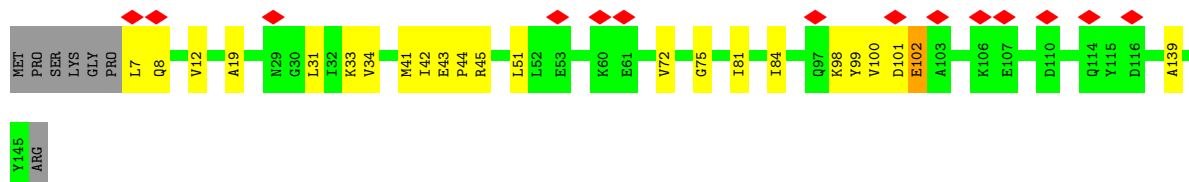
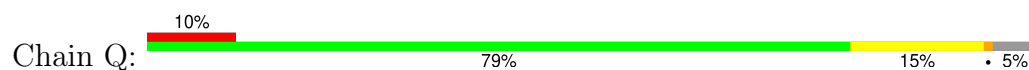




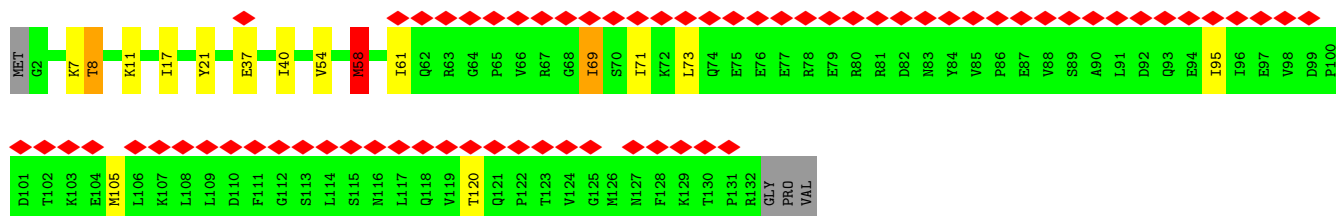
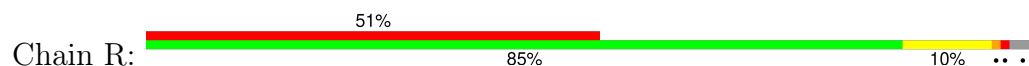
- Molecule 17: Small ribosomal subunit protein uS19



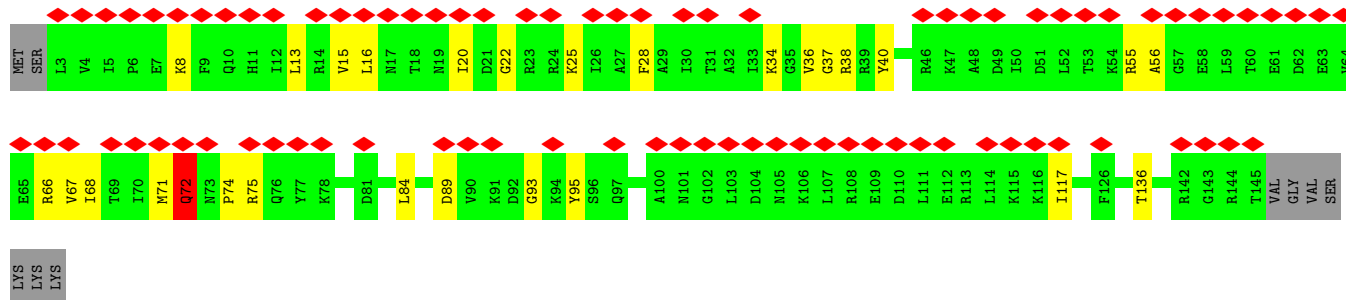
- Molecule 18: Small ribosomal subunit protein uS9



- Molecule 19: Small ribosomal subunit protein eS17

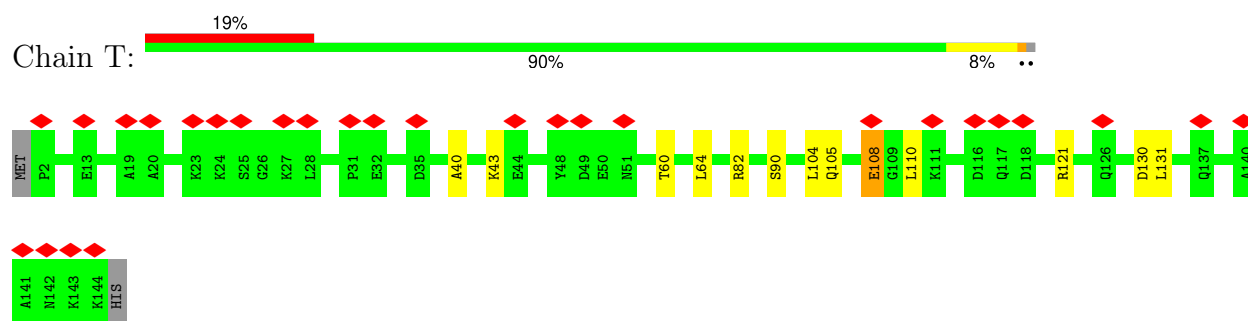


- Molecule 20: Small ribosomal subunit protein uS13

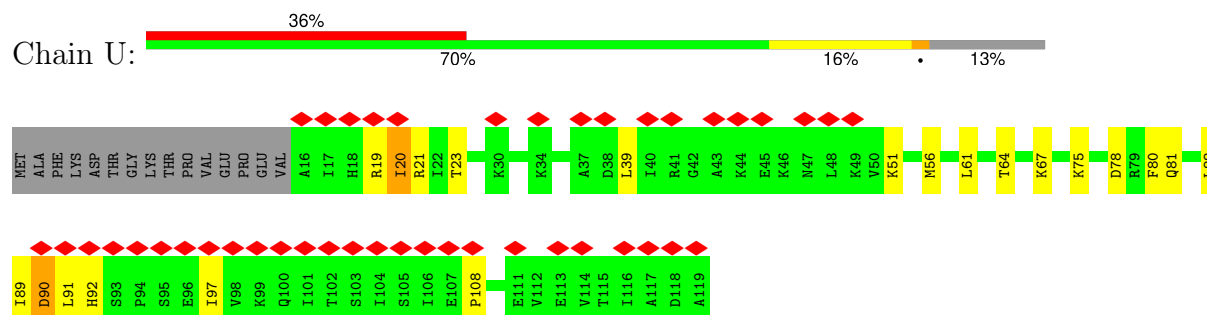


- Molecule 21: Small ribosomal subunit protein eS19

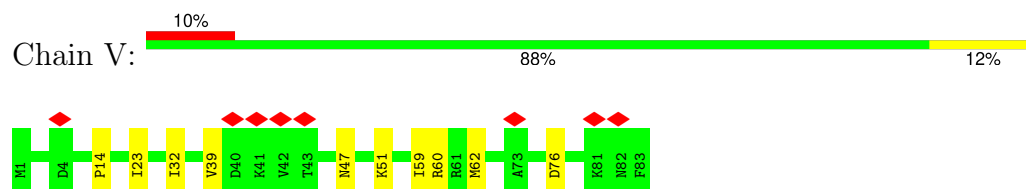




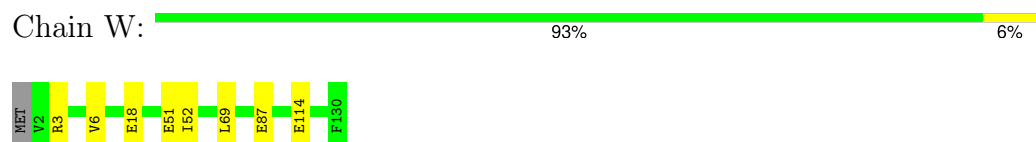
- Molecule 22: Small ribosomal subunit protein uS10



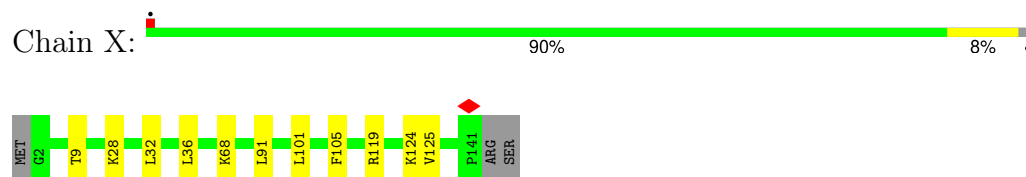
- Molecule 23: Small ribosomal subunit protein eS21



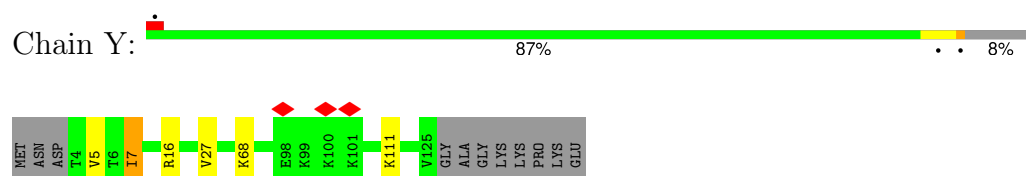
- Molecule 24: Small ribosomal subunit protein uS8



- Molecule 25: 40S ribosomal protein S23

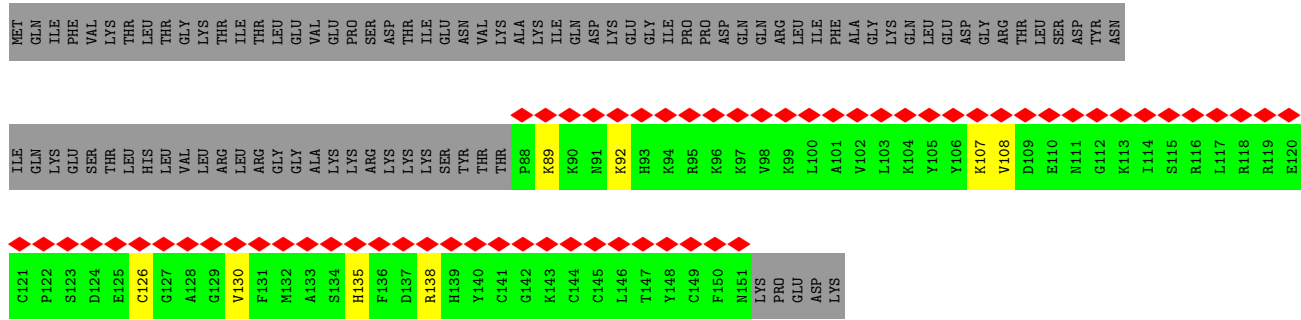


- Molecule 26: 40S ribosomal protein S24

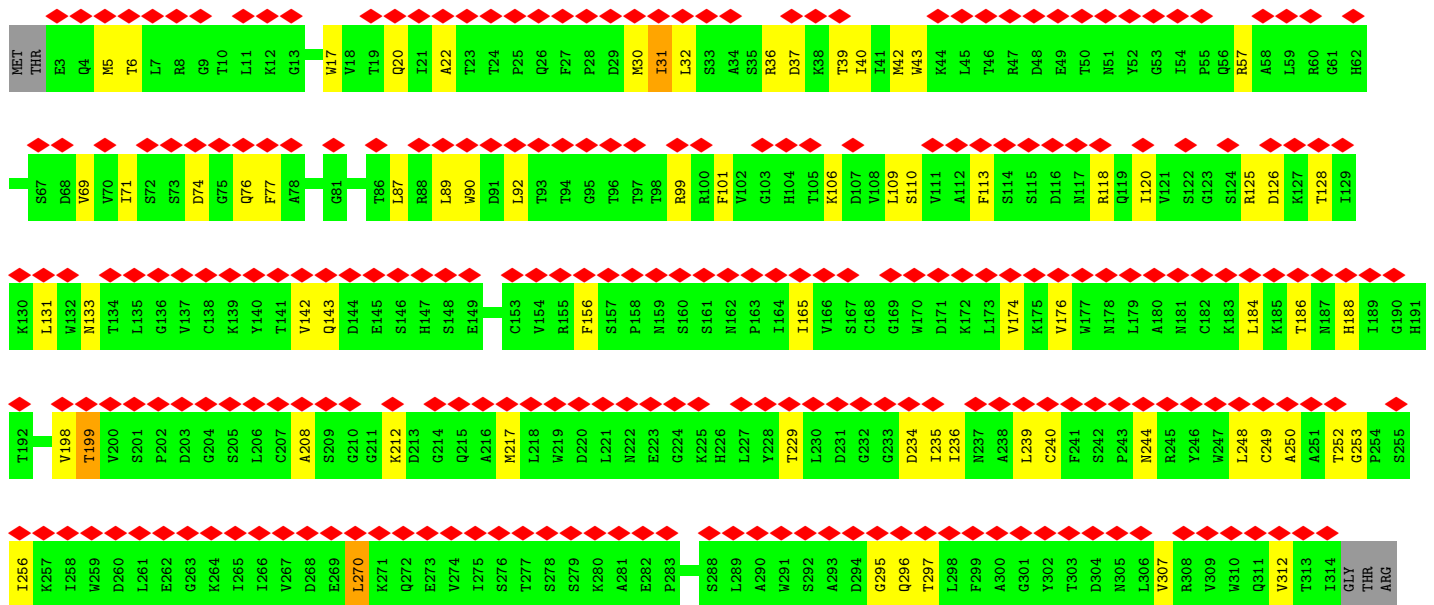


Chain Z: 

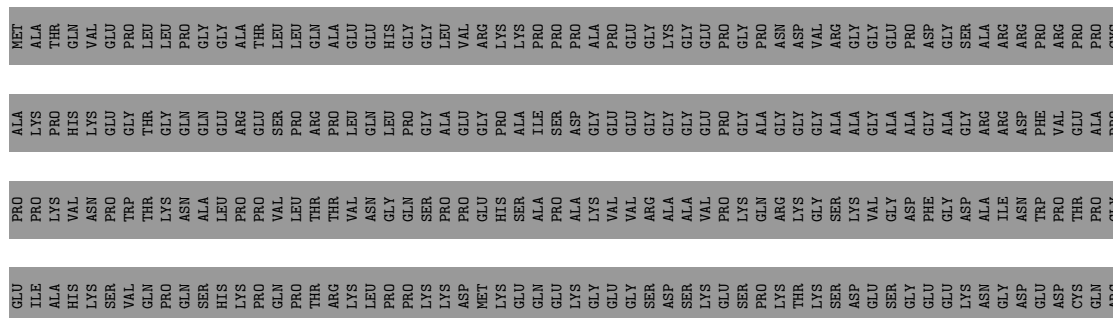
Chain f: 



Chain g:  79% 76% 21%



Chain h:  96%





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 124913                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 1                                       | Depositor |
| Minimum defocus (nm)                 | 1200                                    | Depositor |
| Maximum defocus (nm)                 | 3500                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 0.099                                   | Depositor |
| Minimum map value                    | -0.047                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.002                                   | Depositor |
| Recommended contour level            | 0.012                                   | Depositor |
| Map size ( $\text{\AA}$ )            | 411.5, 411.5, 411.5                     | wwPDB     |
| Map dimensions                       | 500, 500, 500                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 0.823, 0.823, 0.823                     | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, MG, OMG, B8N, K, OMC, MA6, 6MZ, OMU, A2M, 7MG, 4AC, ZN

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

| Mol | Chain | Bond lengths |                | Bond angles |                |
|-----|-------|--------------|----------------|-------------|----------------|
|     |       | RMSZ         | $\# Z  > 5$    | RMSZ        | $\# Z  > 5$    |
| 1   | 2     | 0.27         | 1/37048 (0.0%) | 0.39        | 1/57731 (0.0%) |
| 2   | A     | 0.33         | 0/1665         | 0.56        | 0/2262         |
| 3   | B     | 0.25         | 0/1738         | 0.50        | 1/2325 (0.0%)  |
| 4   | C     | 0.28         | 0/1748         | 0.49        | 0/2361         |
| 5   | D     | 0.25         | 0/1773         | 0.48        | 0/2387         |
| 6   | E     | 0.28         | 0/2083         | 0.50        | 0/2805         |
| 7   | F     | 0.37         | 1/1465 (0.1%)  | 0.58        | 0/1969         |
| 8   | G     | 0.39         | 2/1863 (0.1%)  | 0.57        | 1/2481 (0.0%)  |
| 9   | H     | 0.27         | 0/1498         | 0.63        | 0/2005         |
| 10  | I     | 0.36         | 1/1711 (0.1%)  | 0.52        | 0/2282         |
| 11  | J     | 0.29         | 0/1550         | 0.45        | 0/2069         |
| 12  | K     | 0.60         | 0/840          | 0.71        | 0/1133         |
| 13  | L     | 0.31         | 0/1177         | 0.47        | 0/1574         |
| 14  | M     | 0.63         | 1/796 (0.1%)   | 0.66        | 0/1072         |
| 15  | N     | 0.23         | 0/1232         | 0.45        | 0/1656         |
| 16  | O     | 0.32         | 0/969          | 0.51        | 0/1298         |
| 17  | P     | 0.39         | 2/1017 (0.2%)  | 0.61        | 1/1361 (0.1%)  |
| 18  | Q     | 0.65         | 6/1122 (0.5%)  | 0.62        | 2/1503 (0.1%)  |
| 19  | R     | 0.43         | 1/1078 (0.1%)  | 0.55        | 1/1447 (0.1%)  |
| 20  | S     | 0.65         | 3/1214 (0.2%)  | 1.22        | 4/1626 (0.2%)  |
| 21  | T     | 0.33         | 1/1131 (0.1%)  | 0.56        | 1/1515 (0.1%)  |
| 22  | U     | 0.29         | 0/831          | 0.60        | 0/1115         |
| 23  | V     | 0.46         | 1/643 (0.2%)   | 0.49        | 0/860          |
| 24  | W     | 0.30         | 0/1051         | 0.51        | 0/1406         |
| 25  | X     | 0.26         | 0/1105         | 0.52        | 0/1476         |
| 26  | Y     | 0.26         | 0/1019         | 0.42        | 0/1354         |
| 27  | Z     | 0.36         | 1/576 (0.2%)   | 0.54        | 0/774          |
| 28  | a     | 0.32         | 0/805          | 0.53        | 1/1079 (0.1%)  |
| 29  | b     | 0.45         | 2/653 (0.3%)   | 0.54        | 1/876 (0.1%)   |
| 30  | c     | 0.85         | 3/465 (0.6%)   | 0.81        | 1/621 (0.2%)   |
| 31  | d     | 0.27         | 0/470          | 0.48        | 0/623          |
| 32  | e     | 0.19         | 0/443          | 0.46        | 0/582          |

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5          |
| 33  | f     | 0.18         | 0/533           | 0.47        | 0/706            |
| 34  | g     | 0.43         | 2/2465 (0.1%)   | 0.66        | 1/3359 (0.0%)    |
| 35  | h     | 0.45         | 1/352 (0.3%)    | 0.70        | 0/475            |
| 36  | n     | 0.30         | 0/194           | 0.57        | 0/246            |
| All | All   | 0.33         | 29/76323 (0.0%) | 0.49        | 16/110414 (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 |
|-----|-------|---------------------|---------------------|
| 9   | H     | 0                   | 1                   |
| 20  | S     | 0                   | 1                   |
| All | All   | 0                   | 2                   |

All (29) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 20  | S     | 72  | GLN  | CD-NE2 | 14.96  | 1.64        | 1.33     |
| 14  | M     | 110 | VAL  | CB-CG1 | -11.73 | 1.13        | 1.52     |
| 30  | c     | 58  | LEU  | CG-CD2 | -11.33 | 1.15        | 1.52     |
| 18  | Q     | 102 | GLU  | CD-OE1 | -10.08 | 1.06        | 1.25     |
| 23  | V     | 47  | ASN  | CG-OD1 | -8.91  | 1.06        | 1.23     |
| 20  | S     | 72  | GLN  | CD-OE1 | -8.91  | 1.06        | 1.23     |
| 18  | Q     | 102 | GLU  | CA-C   | -8.84  | 1.41        | 1.52     |
| 30  | c     | 14  | VAL  | CB-CG1 | -8.70  | 1.23        | 1.52     |
| 20  | S     | 72  | GLN  | CA-CB  | -8.66  | 1.40        | 1.53     |
| 7   | F     | 36  | GLN  | CD-OE1 | -8.58  | 1.07        | 1.23     |
| 8   | G     | 17  | GLU  | CD-OE1 | -7.69  | 1.10        | 1.25     |
| 29  | b     | 57  | VAL  | CB-CG1 | -7.39  | 1.28        | 1.52     |
| 34  | g     | 76  | GLN  | CD-OE1 | -7.38  | 1.09        | 1.23     |
| 18  | Q     | 102 | GLU  | CG-CD  | -6.96  | 1.34        | 1.52     |
| 18  | Q     | 102 | GLU  | CA-CB  | 6.68   | 1.64        | 1.54     |
| 10  | I     | 168 | GLN  | CD-OE1 | -6.41  | 1.11        | 1.23     |
| 18  | Q     | 102 | GLU  | CD-OE2 | -6.28  | 1.13        | 1.25     |
| 19  | R     | 58  | MET  | SD-CE  | -6.12  | 1.64        | 1.79     |
| 8   | G     | 19  | ASP  | CG-OD2 | -5.89  | 1.14        | 1.25     |
| 17  | P     | 83  | MET  | SD-CE  | -5.86  | 1.65        | 1.79     |
| 34  | g     | 253 | GLY  | CA-C   | -5.85  | 1.43        | 1.51     |
| 30  | c     | 44  | ARG  | CG-CD  | -5.41  | 1.36        | 1.52     |
| 27  | Z     | 62  | VAL  | C-N    | 5.37   | 1.38        | 1.33     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 21  | T     | 130 | ASP  | CG-OD2 | -5.35 | 1.15        | 1.25     |
| 17  | P     | 111 | MET  | SD-CE  | -5.24 | 1.66        | 1.79     |
| 18  | Q     | 101 | ASP  | C-O    | -5.11 | 1.18        | 1.23     |
| 35  | h     | 666 | THR  | CB-CG2 | -5.09 | 1.35        | 1.52     |
| 29  | b     | 42  | LYS  | CD-CE  | -5.08 | 1.37        | 1.52     |
| 1   | 2     | 484 | A2M  | O3'-P  | 5.05  | 1.61        | 1.56     |

All (16) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 20  | S     | 72  | GLN  | CA-CB-CG   | 32.95  | 179.99      | 114.10   |
| 20  | S     | 72  | GLN  | OE1-CD-NE2 | -25.78 | 96.82       | 122.60   |
| 20  | S     | 72  | GLN  | N-CA-CB    | -6.61  | 100.49      | 110.73   |
| 20  | S     | 72  | GLN  | N-CA-C     | 6.40   | 121.14      | 112.88   |
| 30  | c     | 44  | ARG  | CG-CD-NE   | 6.16   | 125.54      | 112.00   |
| 1   | 2     | 627 | U    | P-O3'-C3'  | 5.90   | 129.05      | 120.20   |
| 17  | P     | 83  | MET  | CG-SD-CE   | 5.79   | 113.63      | 100.90   |
| 18  | Q     | 102 | GLU  | OE1-CD-OE2 | -5.72  | 109.16      | 122.90   |
| 8   | G     | 17  | GLU  | CG-CD-OE1  | -5.71  | 105.26      | 118.40   |
| 34  | g     | 253 | GLY  | CA-C-O     | -5.65  | 113.43      | 121.52   |
| 29  | b     | 42  | LYS  | CD-CE-NZ   | 5.65   | 129.98      | 111.90   |
| 3   | B     | 172 | MET  | CG-SD-CE   | -5.57  | 88.64       | 100.90   |
| 21  | T     | 108 | GLU  | CA-CB-CG   | 5.51   | 125.11      | 114.10   |
| 19  | R     | 37  | GLU  | OE1-CD-OE2 | -5.50  | 109.69      | 122.90   |
| 18  | Q     | 102 | GLU  | N-CA-C     | -5.44  | 106.64      | 113.72   |
| 28  | a     | 98  | PRO  | O-C-N      | 5.12   | 123.56      | 121.15   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 9   | H     | 15  | LYS  | Peptide   |
| 20  | S     | 72  | GLN  | Sidechain |

## 5.2 Too-close contacts ⓘ

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



| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 2     | 34700 | 0        | 17574    | 84      | 0            |
| 2   | A     | 1625  | 0        | 1645     | 19      | 0            |
| 3   | B     | 1711  | 0        | 1782     | 9       | 0            |
| 4   | C     | 1708  | 0        | 1797     | 7       | 0            |
| 5   | D     | 1745  | 0        | 1839     | 18      | 0            |
| 6   | E     | 2041  | 0        | 2143     | 10      | 0            |
| 7   | F     | 1445  | 0        | 1495     | 11      | 0            |
| 8   | G     | 1840  | 0        | 1989     | 14      | 0            |
| 9   | H     | 1477  | 0        | 1573     | 16      | 0            |
| 10  | I     | 1682  | 0        | 1769     | 11      | 0            |
| 11  | J     | 1525  | 0        | 1640     | 9       | 0            |
| 12  | K     | 816   | 0        | 841      | 20      | 0            |
| 13  | L     | 1157  | 0        | 1222     | 5       | 0            |
| 14  | M     | 790   | 0        | 808      | 12      | 0            |
| 15  | N     | 1208  | 0        | 1293     | 5       | 0            |
| 16  | O     | 957   | 0        | 982      | 8       | 0            |
| 17  | P     | 998   | 0        | 1041     | 11      | 0            |
| 18  | Q     | 1105  | 0        | 1172     | 11      | 0            |
| 19  | R     | 1064  | 0        | 1118     | 8       | 0            |
| 20  | S     | 1192  | 0        | 1253     | 18      | 0            |
| 21  | T     | 1112  | 0        | 1146     | 4       | 0            |
| 22  | U     | 821   | 0        | 883      | 10      | 0            |
| 23  | V     | 636   | 0        | 637      | 5       | 0            |
| 24  | W     | 1034  | 0        | 1080     | 5       | 0            |
| 25  | X     | 1087  | 0        | 1154     | 6       | 0            |
| 26  | Y     | 1002  | 0        | 1075     | 2       | 0            |
| 27  | Z     | 570   | 0        | 626      | 6       | 0            |
| 28  | a     | 792   | 0        | 841      | 4       | 0            |
| 29  | b     | 640   | 0        | 665      | 9       | 0            |
| 30  | c     | 464   | 0        | 488      | 7       | 0            |
| 31  | d     | 459   | 0        | 448      | 3       | 0            |
| 32  | e     | 438   | 0        | 484      | 5       | 0            |
| 33  | f     | 522   | 0        | 529      | 6       | 0            |
| 34  | g     | 2408  | 0        | 2339     | 36      | 0            |
| 35  | h     | 345   | 0        | 303      | 1       | 0            |
| 36  | n     | 193   | 0        | 237      | 2       | 0            |
| 37  | 2     | 68    | 0        | 0        | 0       | 0            |
| 37  | S     | 1     | 0        | 0        | 0       | 0            |
| 37  | X     | 1     | 0        | 0        | 0       | 0            |
| 37  | d     | 1     | 0        | 0        | 0       | 0            |
| 38  | 2     | 91    | 0        | 0        | 0       | 0            |
| 38  | G     | 1     | 0        | 0        | 0       | 0            |
| 39  | a     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 39  | d     | 1     | 0        | 0        | 0       | 0            |
| 39  | f     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 73475 | 0        | 57911    | 372     | 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 (372) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 20:S:67:VAL:O    | 20:S:71:MET:HB2   | 1.62                     | 1.00              |
| 1:2:538:U:H3     | 1:2:549:C:H42     | 1.11                     | 0.97              |
| 2:A:58:LEU:HD12  | 2:A:178:LEU:HD23  | 1.74                     | 0.68              |
| 14:M:44:LYS:HG2  | 14:M:46:GLN:HG3   | 1.75                     | 0.68              |
| 34:g:87:LEU:HB2  | 34:g:101:PHE:HB2  | 1.76                     | 0.67              |
| 20:S:75:ARG:HE   | 20:S:95:TYR:HB2   | 1.60                     | 0.66              |
| 19:R:21:TYR:HD1  | 19:R:73:LEU:HD13  | 1.61                     | 0.66              |
| 34:g:212:LYS:HA  | 34:g:235:ILE:HG22 | 1.75                     | 0.66              |
| 17:P:115:TYR:H   | 17:P:118:GLU:HG3  | 1.61                     | 0.66              |
| 18:Q:102:GLU:OE2 | 34:g:57:ARG:HA    | 1.96                     | 0.65              |
| 1:2:538:U:O2     | 1:2:549:C:N3      | 2.29                     | 0.65              |
| 12:K:5:LYS:HE2   | 12:K:5:LYS:H      | 1.62                     | 0.65              |
| 20:S:16:LEU:HD11 | 20:S:72:GLN:NE2   | 2.12                     | 0.65              |
| 18:Q:51:LEU:HD21 | 18:Q:81:ILE:HG12  | 1.79                     | 0.65              |
| 1:2:940:U:H3     | 1:2:1002:U:H3     | 1.43                     | 0.64              |
| 34:g:106:LYS:HB2 | 34:g:126:ASP:HB3  | 1.80                     | 0.64              |
| 12:K:55:ARG:HE   | 12:K:57:TYR:HE1   | 1.45                     | 0.64              |
| 5:D:135:GLU:HG3  | 5:D:153:VAL:HG12  | 1.79                     | 0.64              |
| 2:A:66:VAL:HG21  | 2:A:185:MET:HB2   | 1.81                     | 0.63              |
| 1:2:1550:G:H3'   | 1:2:1579:A:H61    | 1.64                     | 0.61              |
| 34:g:234:ASP:HB3 | 34:g:252:THR:HG23 | 1.81                     | 0.61              |
| 22:U:80:PHE:HB3  | 31:d:52:PHE:HB3   | 1.83                     | 0.61              |
| 16:O:30:VAL:HG12 | 16:O:94:HIS:HB2   | 1.83                     | 0.61              |
| 34:g:128:THR:HA  | 34:g:142:VAL:O    | 2.01                     | 0.61              |
| 4:C:183:LYS:HA   | 4:C:195:LEU:O     | 2.01                     | 0.60              |
| 1:2:1729:U:H3    | 1:2:1805:G:H1     | 1.47                     | 0.60              |
| 21:T:105:GLN:HA  | 21:T:108:GLU:OE1  | 2.02                     | 0.59              |
| 5:D:124:ARG:HH21 | 35:h:685:TYR:HB3  | 1.66                     | 0.59              |
| 30:c:14:VAL:HG11 | 30:c:51:ARG:O     | 2.03                     | 0.59              |
| 34:g:198:VAL:HA  | 34:g:208:ALA:O    | 2.02                     | 0.58              |
| 2:A:198:MET:HG2  | 2:A:200:ASP:H     | 1.67                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:Q:41:MET:HA    | 18:Q:45:ARG:HH21  | 1.67                     | 0.58              |
| 1:2:536:A:H61     | 1:2:546:G:H1      | 1.50                     | 0.58              |
| 1:2:928:G:H1      | 1:2:1013:U:H3     | 1.51                     | 0.58              |
| 1:2:77:A:H5'      | 8:G:154:ARG:HB3   | 1.85                     | 0.58              |
| 11:J:127:ARG:HD3  | 32:e:31:ARG:HD3   | 1.85                     | 0.58              |
| 24:W:51:GLU:HG2   | 29:b:8:LEU:HD11   | 1.85                     | 0.58              |
| 24:W:3:ARG:HD3    | 24:W:6:VAL:HG12   | 1.86                     | 0.57              |
| 34:g:128:THR:HG22 | 34:g:143:GLN:HB3  | 1.87                     | 0.57              |
| 22:U:67:LYS:HG2   | 22:U:78:ASP:OD2   | 2.05                     | 0.57              |
| 18:Q:31:LEU:HD11  | 18:Q:33:LYS:HE3   | 1.87                     | 0.57              |
| 34:g:156:PHE:HA   | 34:g:165:ILE:HG22 | 1.86                     | 0.57              |
| 3:B:27:LYS:HA     | 3:B:51:ARG:HE     | 1.69                     | 0.57              |
| 1:2:1228:A:H2'    | 1:2:1229:G:C8     | 2.41                     | 0.56              |
| 9:H:69:LEU:HD13   | 9:H:96:ALA:HB2    | 1.86                     | 0.56              |
| 7:F:50:PRO:HG2    | 7:F:90:VAL:HG22   | 1.87                     | 0.56              |
| 20:S:16:LEU:HD21  | 20:S:72:GLN:HE22  | 1.70                     | 0.56              |
| 34:g:174:VAL:HB   | 34:g:188:HIS:HB2  | 1.87                     | 0.56              |
| 1:2:433:A:H5''    | 10:I:22:HIS:HB3   | 1.87                     | 0.56              |
| 1:2:1228:A:H2'    | 1:2:1229:G:H8     | 1.71                     | 0.56              |
| 2:A:184:ARG:HD2   | 2:A:191:ARG:HG2   | 1.86                     | 0.56              |
| 20:S:13:LEU:HB2   | 20:S:20:ILE:HB    | 1.87                     | 0.56              |
| 13:L:75:GLY:HA3   | 13:L:88:ILE:HD12  | 1.87                     | 0.56              |
| 8:G:181:THR:HG22  | 8:G:183:ARG:H     | 1.69                     | 0.55              |
| 6:E:11:ARG:HA     | 6:E:28:ALA:HB2    | 1.87                     | 0.55              |
| 17:P:52:LYS:HB3   | 17:P:80:LEU:HD11  | 1.89                     | 0.55              |
| 25:X:68:LYS:HB3   | 25:X:91:LEU:HD22  | 1.89                     | 0.55              |
| 3:B:146:ARG:HE    | 3:B:206:PRO:HG2   | 1.73                     | 0.54              |
| 23:V:32:ILE:HG12  | 23:V:60:ARG:HD2   | 1.89                     | 0.54              |
| 5:D:114:ALA:HB3   | 5:D:117:ARG:HG3   | 1.90                     | 0.54              |
| 17:P:86:LEU:H     | 17:P:89:MET:HE2   | 1.72                     | 0.54              |
| 2:A:68:ILE:HD11   | 2:A:74:VAL:HG23   | 1.88                     | 0.54              |
| 7:F:204:ARG:HG2   | 30:c:63:ARG:HH22  | 1.71                     | 0.54              |
| 7:F:73:THR:HG22   | 7:F:93:VAL:HG21   | 1.90                     | 0.54              |
| 34:g:199:THR:HG21 | 34:g:240:CYS:HA   | 1.89                     | 0.54              |
| 1:2:1017:U:H5'    | 15:N:55:ARG:HD3   | 1.90                     | 0.53              |
| 22:U:21:ARG:HD2   | 22:U:88:LEU:HD22  | 1.91                     | 0.53              |
| 1:2:874:G:H2'     | 1:2:875:A:H8      | 1.73                     | 0.53              |
| 2:A:54:THR:HG22   | 2:A:162:PRO:HG2   | 1.90                     | 0.53              |
| 5:D:16:ILE:HD11   | 31:d:36:LEU:HD23  | 1.89                     | 0.53              |
| 15:N:100:LYS:HE2  | 15:N:104:ARG:HH22 | 1.72                     | 0.53              |
| 29:b:34:ASP:O     | 29:b:79:PHE:HA    | 2.08                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:851:C:H5''    | 1:2:852:G:H5'     | 1.91                     | 0.53              |
| 3:B:52:THR:HG22   | 3:B:57:ILE:HA     | 1.90                     | 0.53              |
| 7:F:152:TRP:O     | 7:F:156:THR:HG23  | 2.08                     | 0.53              |
| 14:M:84:LYS:HA    | 14:M:87:GLU:HB2   | 1.91                     | 0.53              |
| 1:2:587:A:H5'     | 1:2:592:C:H41     | 1.74                     | 0.53              |
| 1:2:1748:G:H1     | 1:2:1786:U:H3     | 1.57                     | 0.53              |
| 12:K:71:LEU:HD11  | 12:K:79:LEU:HD12  | 1.91                     | 0.53              |
| 8:G:164:LYS:HD3   | 8:G:167:LYS:HG3   | 1.91                     | 0.52              |
| 27:Z:73:VAL:HG21  | 27:Z:88:LEU:HD11  | 1.91                     | 0.52              |
| 23:V:14:PRO:HG2   | 23:V:23:ILE:HD12  | 1.91                     | 0.52              |
| 5:D:172:VAL:HG22  | 5:D:185:LYS:HG2   | 1.91                     | 0.52              |
| 6:E:122:LYS:HD2   | 6:E:164:LEU:HD21  | 1.92                     | 0.52              |
| 22:U:39:LEU:HD13  | 22:U:89:ILE:HD12  | 1.90                     | 0.52              |
| 13:L:126:VAL:HG12 | 13:L:145:VAL:HG22 | 1.92                     | 0.52              |
| 10:I:89:GLU:CD    | 10:I:92:ARG:HE    | 2.18                     | 0.51              |
| 23:V:59:ILE:HD13  | 23:V:62:MET:HE3   | 1.91                     | 0.51              |
| 18:Q:19:ALA:HB2   | 18:Q:75:GLY:HA3   | 1.92                     | 0.51              |
| 34:g:239:LEU:HA   | 34:g:249:CYS:O    | 2.11                     | 0.51              |
| 9:H:74:LYS:HG3    | 9:H:75:ILE:HD13   | 1.91                     | 0.51              |
| 34:g:256:ILE:HB   | 34:g:270:LEU:HB2  | 1.92                     | 0.51              |
| 24:W:18:GLU:HG3   | 24:W:69:LEU:HB3   | 1.92                     | 0.51              |
| 8:G:20:ASP:HB3    | 8:G:23:LYS:HG3    | 1.92                     | 0.51              |
| 20:S:22:GLY:HA2   | 20:S:56:ALA:HB3   | 1.92                     | 0.51              |
| 1:2:377:G:H5'     | 10:I:98:LYS:HB3   | 1.92                     | 0.51              |
| 1:2:921:G:H5'     | 29:b:21:LYS:HE3   | 1.93                     | 0.51              |
| 15:N:67:THR:HG21  | 15:N:74:ILE:HD11  | 1.92                     | 0.51              |
| 9:H:30:LEU:HD22   | 9:H:82:GLU:HB3    | 1.92                     | 0.50              |
| 1:2:379:C:H5'     | 10:I:33:ALA:HA    | 1.93                     | 0.50              |
| 14:M:31:LEU:HD23  | 14:M:109:VAL:HG21 | 1.92                     | 0.50              |
| 22:U:20:ILE:HG12  | 22:U:91:LEU:HB2   | 1.93                     | 0.50              |
| 4:C:66:LEU:HD21   | 4:C:81:ILE:HG12   | 1.92                     | 0.50              |
| 11:J:30:LYS:HE2   | 32:e:42:PHE:CE1   | 2.46                     | 0.50              |
| 34:g:176:VAL:HB   | 34:g:186:THR:HG22 | 1.93                     | 0.50              |
| 6:E:100:ARG:HH21  | 6:E:118:GLU:HG2   | 1.75                     | 0.50              |
| 1:2:616:A:H1'     | 32:e:12:VAL:HG13  | 1.93                     | 0.50              |
| 3:B:124:HIS:HA    | 3:B:137:LEU:O     | 2.12                     | 0.50              |
| 1:2:1315:U:H4'    | 12:K:2:LEU:HD22   | 1.93                     | 0.50              |
| 5:D:61:GLU:HG2    | 5:D:62:LYS:HG3    | 1.93                     | 0.50              |
| 30:c:60:GLU:OE1   | 30:c:63:ARG:HG3   | 2.12                     | 0.50              |
| 11:J:175:ARG:O    | 11:J:179:LYS:HG3  | 2.11                     | 0.49              |
| 14:M:63:LYS:NZ    | 33:f:108:VAL:HG12 | 2.27                     | 0.49              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:U:23:THR:HG22   | 22:U:88:LEU:HD23  | 1.95                     | 0.49              |
| 14:M:110:VAL:O     | 14:M:110:VAL:HG13 | 2.11                     | 0.49              |
| 1:2:1337:4AC:H2'   | 1:2:1338:G:H8     | 1.78                     | 0.49              |
| 8:G:58:LYS:HE2     | 8:G:105:ASN:HA    | 1.94                     | 0.49              |
| 26:Y:7:ILE:HG22    | 26:Y:27:VAL:HG13  | 1.94                     | 0.49              |
| 10:I:101:ILE:HD12  | 10:I:190:LEU:HD11 | 1.93                     | 0.49              |
| 13:L:33:LEU:HD12   | 13:L:34:PRO:HD2   | 1.94                     | 0.49              |
| 28:a:11:ALA:HB3    | 28:a:33:ASP:HB2   | 1.94                     | 0.49              |
| 1:2:1723:G:H2'     | 1:2:1724:A:C8     | 2.47                     | 0.49              |
| 1:2:1706:G:H5'     | 36:n:1:MET:HB2    | 1.94                     | 0.49              |
| 9:H:144:ILE:HB     | 24:W:52:ILE:HB    | 1.93                     | 0.49              |
| 18:Q:34:VAL:HB     | 18:Q:42:ILE:HD11  | 1.93                     | 0.49              |
| 1:2:1650:A:H5''    | 18:Q:139:ALA:HB2  | 1.94                     | 0.49              |
| 12:K:59:LYS:HG3    | 12:K:70:TYR:HB2   | 1.93                     | 0.49              |
| 2:A:73:ASP:HB3     | 2:A:120:ARG:HB2   | 1.94                     | 0.49              |
| 22:U:64:THR:HA     | 22:U:78:ASP:O     | 2.13                     | 0.49              |
| 30:c:32:VAL:O      | 30:c:41:SER:HA    | 2.12                     | 0.48              |
| 34:g:20:GLN:HG2    | 34:g:69:VAL:H     | 1.77                     | 0.48              |
| 10:I:125:LYS:HE3   | 10:I:128:LYS:HD2  | 1.96                     | 0.48              |
| 1:2:1435:C:H4'     | 1:2:1437:C:H41    | 1.78                     | 0.48              |
| 17:P:111:MET:HG2   | 20:S:117:ILE:HB   | 1.95                     | 0.48              |
| 9:H:51:ILE:HD11    | 9:H:176:VAL:HG22  | 1.95                     | 0.48              |
| 20:S:28[A]:PHE:HE2 | 20:S:38:ARG:HE    | 1.61                     | 0.48              |
| 1:2:925:G:H1       | 1:2:1017:U:H3     | 1.60                     | 0.48              |
| 1:2:385:G:H3'      | 13:L:136:LYS:HB2  | 1.96                     | 0.48              |
| 1:2:535:G:H2'      | 1:2:536:A:C8      | 2.48                     | 0.48              |
| 16:O:40:THR:HG21   | 16:O:74:ALA:HB2   | 1.96                     | 0.48              |
| 17:P:33:LEU:HD21   | 17:P:87:PRO:HG2   | 1.95                     | 0.48              |
| 5:D:38:GLU:HG3     | 5:D:49:ILE:HB     | 1.96                     | 0.48              |
| 11:J:107:GLU:O     | 11:J:113:GLN:NE2  | 2.43                     | 0.48              |
| 15:N:72:LEU:HD13   | 15:N:76:LYS:HD2   | 1.96                     | 0.48              |
| 14:M:22:LEU:HD13   | 14:M:88:TRP:HB3   | 1.95                     | 0.48              |
| 18:Q:43:GLU:HG2    | 18:Q:44:PRO:HA    | 1.95                     | 0.48              |
| 1:2:543:C:H3'      | 1:2:544:G:H8      | 1.79                     | 0.47              |
| 4:C:187:ARG:HD3    | 4:C:192:LEU:HD12  | 1.96                     | 0.47              |
| 5:D:59:LEU:HD23    | 5:D:66:ILE:HG21   | 1.96                     | 0.47              |
| 19:R:17:ILE:HG22   | 19:R:69:ILE:HG21  | 1.95                     | 0.47              |
| 2:A:65:ILE:HG23    | 2:A:74:VAL:HG21   | 1.96                     | 0.47              |
| 2:A:108:PHE:HB2    | 2:A:136:GLU:HG2   | 1.95                     | 0.47              |
| 12:K:83:LEU:HB3    | 12:K:85:LEU:HG    | 1.97                     | 0.47              |
| 17:P:111:MET:HE2   | 20:S:117:ILE:HB   | 1.96                     | 0.47              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 4:C:196:ILE:HB      | 4:C:223:TYR:HB2   | 1.97                     | 0.47              |
| 6:E:20:LEU:HD21     | 6:E:46:ILE:HD12   | 1.97                     | 0.47              |
| 18:Q:72:VAL:HG11    | 18:Q:84:ILE:HD11  | 1.95                     | 0.47              |
| 1:2:1723:G:H2'      | 1:2:1724:A:H8     | 1.79                     | 0.47              |
| 34:g:31:ILE:HG13    | 34:g:43:TRP:HB2   | 1.96                     | 0.47              |
| 34:g:42:MET:HE3     | 34:g:57:ARG:HD2   | 1.96                     | 0.47              |
| 12:K:20:VAL:HG12    | 12:K:70:TYR:HA    | 1.96                     | 0.47              |
| 16:O:34:PHE:HB3     | 16:O:41:PHE:HB2   | 1.96                     | 0.47              |
| 5:D:227:LYS:HD2     | 34:g:184:LEU:HD11 | 1.97                     | 0.47              |
| 34:g:236:ILE:HG13   | 34:g:250:ALA:HB1  | 1.97                     | 0.47              |
| 7:F:34:SER:HB3      | 30:c:55:VAL:HG12  | 1.96                     | 0.46              |
| 20:S:36:VAL:HG22    | 20:S:40:TYR:HD2   | 1.79                     | 0.46              |
| 29:b:19:HIS:HB3     | 29:b:22:LYS:HG3   | 1.97                     | 0.46              |
| 1:2:1030:A:H2'      | 1:2:1031:A2M:H8   | 1.97                     | 0.46              |
| 14:M:52:LEU:HD21    | 14:M:62:VAL:HG13  | 1.97                     | 0.46              |
| 3:B:181:LEU:O       | 3:B:185:VAL:HG12  | 2.16                     | 0.46              |
| 2:A:30:LEU:HD21     | 2:A:35:GLU:HG2    | 1.97                     | 0.46              |
| 33:f:126:CYS:HB3    | 33:f:130:VAL:HG21 | 1.97                     | 0.46              |
| 11:J:60:LEU:HD22    | 11:J:70:ARG:HA    | 1.98                     | 0.46              |
| 25:X:28:LYS:HE2     | 25:X:32:LEU:HD11  | 1.98                     | 0.46              |
| 1:2:1630:A:H5''     | 20:S:37:GLY:H     | 1.81                     | 0.46              |
| 8:G:193:ALA:HA      | 8:G:196:LYS:HE3   | 1.98                     | 0.46              |
| 2:A:121[B]:LEU:HD11 | 2:A:145:ILE:HD12  | 1.98                     | 0.46              |
| 9:H:73:GLN:HA       | 9:H:76:GLN:HB2    | 1.98                     | 0.46              |
| 14:M:44:LYS:HB2     | 14:M:44:LYS:HE3   | 1.71                     | 0.46              |
| 1:2:165:G:H2'       | 1:2:166:A2M:H8    | 1.97                     | 0.46              |
| 1:2:1382:A:H2'      | 1:2:1383:A2M:H8   | 1.98                     | 0.46              |
| 1:2:1842:4AC:HM73   | 36:n:2:ARG:HH22   | 1.81                     | 0.46              |
| 5:D:170:THR:HG23    | 5:D:187:LYS:HG3   | 1.97                     | 0.46              |
| 9:H:58:LYS:HB2      | 9:H:90:LYS:HG3    | 1.98                     | 0.46              |
| 17:P:83:MET:HE2     | 17:P:83:MET:HA    | 1.97                     | 0.46              |
| 1:2:1037:G:H4'      | 1:2:1845:A:H4'    | 1.98                     | 0.45              |
| 5:D:132:LYS:HG3     | 5:D:191:PRO:HA    | 1.97                     | 0.45              |
| 12:K:16:PHE:CD2     | 12:K:79:LEU:HB3   | 2.50                     | 0.45              |
| 34:g:89:LEU:HB3     | 34:g:99:ARG:HB3   | 1.98                     | 0.45              |
| 3:B:139:CYS:HB2     | 3:B:172:MET:HE1   | 1.97                     | 0.45              |
| 8:G:31:ARG:HE       | 8:G:31:ARG:HB2    | 1.57                     | 0.45              |
| 21:T:104:LEU:HD13   | 21:T:121:ARG:HD3  | 1.98                     | 0.45              |
| 34:g:5:MET:HB2      | 34:g:270:LEU:HD11 | 1.96                     | 0.45              |
| 17:P:52:LYS:HD2     | 17:P:80:LEU:HD21  | 1.98                     | 0.45              |
| 1:2:382:C:H2'       | 1:2:383:G:H8      | 1.81                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 10:I:157:LYS:HD2 | 10:I:157:LYS:HA   | 1.65                     | 0.45              |
| 14:M:61:TYR:O    | 14:M:65:VAL:HG12  | 2.17                     | 0.45              |
| 16:O:98:ARG:HG3  | 16:O:132:VAL:HG23 | 1.98                     | 0.45              |
| 20:S:15:VAL:HG13 | 20:S:68:ILE:HD11  | 1.97                     | 0.45              |
| 2:A:8:LEU:HD11   | 23:V:39:VAL:HG21  | 1.98                     | 0.45              |
| 1:2:640:A:H2'    | 1:2:641:A:C8      | 2.52                     | 0.45              |
| 1:2:1845:A:H2'   | 1:2:1846:G:C8     | 2.52                     | 0.45              |
| 33:f:135:HIS:HB2 | 33:f:138:ARG:HG2  | 1.97                     | 0.45              |
| 9:H:10:LYS:HZ3   | 9:H:20:GLU:HG3    | 1.82                     | 0.45              |
| 34:g:40:ILE:HG21 | 34:g:69:VAL:HG21  | 1.99                     | 0.45              |
| 2:A:39:TYR:CG    | 19:R:105:MET:HG3  | 2.52                     | 0.45              |
| 7:F:193:LYS:O    | 7:F:197:GLU:HG2   | 2.17                     | 0.45              |
| 9:H:30:LEU:HD12  | 9:H:33:ASN:HD21   | 1.81                     | 0.45              |
| 16:O:75:MET:HG3  | 16:O:118:ALA:HB2  | 1.98                     | 0.45              |
| 34:g:42:MET:HE2  | 34:g:92:LEU:HB3   | 1.99                     | 0.45              |
| 1:2:28:U:H2'     | 1:2:29:G:H8       | 1.83                     | 0.44              |
| 12:K:31:LYS:HD2  | 12:K:36:ALA:HA    | 1.99                     | 0.44              |
| 22:U:61:LEU:O    | 22:U:81:GLN:HA    | 2.17                     | 0.44              |
| 1:2:448:A:H5''   | 10:I:25:ARG:HA    | 1.98                     | 0.44              |
| 1:2:484:A2M:H8   | 1:2:484:A2M:O5'   | 2.17                     | 0.44              |
| 1:2:1588:A:H2'   | 1:2:1589:A:C8     | 2.51                     | 0.44              |
| 20:S:25:LYS:HA   | 20:S:55:ARG:HA    | 1.99                     | 0.44              |
| 25:X:68:LYS:HE2  | 32:e:9:ALA:HB2    | 1.99                     | 0.44              |
| 27:Z:73:VAL:HG12 | 27:Z:79:ILE:HD11  | 2.00                     | 0.44              |
| 29:b:42:LYS:HE2  | 29:b:57:VAL:HG12  | 1.98                     | 0.44              |
| 1:2:5:U:H2'      | 1:2:6:G:H8        | 1.82                     | 0.44              |
| 8:G:137:ARG:HB3  | 8:G:140:ARG:HG3   | 2.00                     | 0.44              |
| 4:C:191:VAL:HG11 | 4:C:236:PHE:HA    | 1.98                     | 0.44              |
| 12:K:3:MET:HE3   | 12:K:3:MET:HB2    | 1.69                     | 0.44              |
| 28:a:64:LEU:HD12 | 28:a:64:LEU:HA    | 1.85                     | 0.44              |
| 34:g:120:ILE:O   | 34:g:131:LEU:HA   | 2.18                     | 0.44              |
| 34:g:296:GLN:HG2 | 34:g:312:VAL:HG12 | 1.98                     | 0.44              |
| 17:P:65:LYS:HE3  | 17:P:65:LYS:HB3   | 1.78                     | 0.44              |
| 1:2:1387:G:H21   | 19:R:8:THR:HG21   | 1.82                     | 0.44              |
| 1:2:1413:G:H2'   | 1:2:1414:A:H8     | 1.82                     | 0.44              |
| 12:K:52:LEU:HD22 | 12:K:57:TYR:HD1   | 1.83                     | 0.44              |
| 1:2:1562:C:H2'   | 1:2:1563:G:H8     | 1.83                     | 0.44              |
| 5:D:109:LEU:HD12 | 5:D:184:ILE:HD11  | 2.00                     | 0.44              |
| 20:S:36:VAL:HG22 | 20:S:40:TYR:CD2   | 2.53                     | 0.44              |
| 1:2:1010:G:H2'   | 1:2:1011:A:C8     | 2.53                     | 0.44              |
| 1:2:1679:A:H2'   | 7:F:60:ARG:HD2    | 2.00                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:D:201:LYS:HB2   | 5:D:201:LYS:HE3   | 1.73                     | 0.44              |
| 7:F:50:PRO:HB3    | 7:F:69:VAL:HG23   | 2.00                     | 0.44              |
| 29:b:34:ASP:HB3   | 29:b:43:ILE:HD11  | 1.99                     | 0.44              |
| 34:g:30:MET:HE2   | 34:g:30:MET:HB3   | 1.80                     | 0.44              |
| 12:K:49:MET:HE3   | 12:K:49:MET:HB3   | 1.83                     | 0.43              |
| 1:2:601:OMG:HM23  | 1:2:601:OMG:H1'   | 1.64                     | 0.43              |
| 1:2:981:A:H2'     | 1:2:982:G:C8      | 2.53                     | 0.43              |
| 1:2:1232:PSU:H2'  | 1:2:1233:G:H8     | 1.83                     | 0.43              |
| 7:F:69:VAL:O      | 7:F:73:THR:HG23   | 2.19                     | 0.43              |
| 9:H:135:PHE:CD2   | 9:H:136:PRO:HA    | 2.52                     | 0.43              |
| 14:M:63:LYS:HZ3   | 33:f:108:VAL:HG12 | 1.83                     | 0.43              |
| 34:g:37:ASP:OD1   | 34:g:39:THR:HG22  | 2.18                     | 0.43              |
| 2:A:34:MET:HE3    | 2:A:34:MET:HB3    | 1.63                     | 0.43              |
| 11:J:33:GLY:HA3   | 32:e:38:TYR:CG    | 2.53                     | 0.43              |
| 16:O:30:VAL:O     | 16:O:44:VAL:HA    | 2.19                     | 0.43              |
| 17:P:92:SER:O     | 17:P:107:ILE:HG12 | 2.18                     | 0.43              |
| 20:S:89:ASP:HB3   | 20:S:93:GLY:H     | 1.82                     | 0.43              |
| 1:2:681:PSU:H4'   | 25:X:9:THR:HG22   | 2.01                     | 0.43              |
| 8:G:58:LYS:HA     | 8:G:107:SER:HB3   | 1.99                     | 0.43              |
| 9:H:15:LYS:HA     | 9:H:15:LYS:HD2    | 1.92                     | 0.43              |
| 1:2:874:G:H2'     | 1:2:875:A:C8      | 2.53                     | 0.43              |
| 1:2:928:G:H2'     | 1:2:929:G:C8      | 2.52                     | 0.43              |
| 6:E:124:CYS:HB3   | 6:E:141:THR:HB    | 2.01                     | 0.43              |
| 14:M:84:LYS:HE2   | 14:M:88:TRP:CH2   | 2.54                     | 0.43              |
| 20:S:74:PRO:HG2   | 20:S:84:LEU:HD11  | 2.01                     | 0.43              |
| 25:X:101:LEU:HB3  | 25:X:124:LYS:HB2  | 2.01                     | 0.43              |
| 30:c:14:VAL:HG23  | 30:c:30:VAL:HB    | 1.99                     | 0.43              |
| 34:g:77:PHE:HA    | 34:g:90:TRP:O     | 2.18                     | 0.43              |
| 15:N:25:TRP:H     | 15:N:25:TRP:CD1   | 2.36                     | 0.43              |
| 17:P:83:MET:HB3   | 17:P:116:LEU:HD13 | 2.01                     | 0.43              |
| 27:Z:96:LEU:HD12  | 27:Z:97:ILE:HG23  | 2.01                     | 0.43              |
| 31:d:3:HIS:CE1    | 31:d:5:GLN:HB2    | 2.54                     | 0.43              |
| 34:g:244:ASN:HD21 | 34:g:295:GLY:HA3  | 1.83                     | 0.43              |
| 5:D:70:THR:HG23   | 5:D:84:VAL:HG12   | 2.00                     | 0.43              |
| 12:K:71:LEU:HD13  | 12:K:76:ILE:HG22  | 2.01                     | 0.43              |
| 29:b:33:MET:HE2   | 29:b:48:SER:HA    | 2.00                     | 0.43              |
| 25:X:28:LYS:HG2   | 25:X:32:LEU:HD12  | 2.01                     | 0.43              |
| 1:2:857:U:H2'     | 1:2:858:A:C8      | 2.54                     | 0.42              |
| 8:G:119:LYS:HE2   | 8:G:119:LYS:HB2   | 1.78                     | 0.42              |
| 33:f:107:LYS:HA   | 33:f:107:LYS:HD2  | 1.73                     | 0.42              |
| 11:J:30:LYS:HB2   | 11:J:30:LYS:HE3   | 1.63                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 29:b:67:THR:HG22  | 29:b:69:GLY:H    | 1.84                     | 0.42              |
| 1:2:528:A:H2'     | 1:2:529:A:H8     | 1.84                     | 0.42              |
| 1:2:1101:U:H2'    | 1:2:1102:G:C8    | 2.54                     | 0.42              |
| 1:2:1337:4AC:H2'  | 1:2:1338:G:C8    | 2.54                     | 0.42              |
| 19:R:54:VAL:O     | 19:R:58:MET:HB2  | 2.19                     | 0.42              |
| 34:g:109:LEU:HD11 | 34:g:125:ARG:HG2 | 2.00                     | 0.42              |
| 1:2:858:A:H2'     | 1:2:859:G:H8     | 1.84                     | 0.42              |
| 3:B:136:ARG:HB3   | 3:B:216:LYS:HB2  | 2.02                     | 0.42              |
| 6:E:129:ILE:HD13  | 6:E:139:LEU:HB3  | 2.02                     | 0.42              |
| 1:2:5:U:H2'       | 1:2:6:G:C8       | 2.54                     | 0.42              |
| 1:2:186:C:H2'     | 1:2:187:G:H8     | 1.84                     | 0.42              |
| 1:2:812:A:H5''    | 6:E:16:LYS:HD2   | 2.00                     | 0.42              |
| 13:L:79:LYS:HE3   | 13:L:79:LYS:HB2  | 1.74                     | 0.42              |
| 23:V:51:LYS:HZ3   | 23:V:76:ASP:CG   | 2.28                     | 0.42              |
| 12:K:16:PHE:CE2   | 12:K:79:LEU:HB3  | 2.55                     | 0.42              |
| 1:2:609:U:H2'     | 1:2:610:G:H8     | 1.85                     | 0.42              |
| 8:G:162:LEU:HD11  | 8:G:172:LYS:HD2  | 2.02                     | 0.42              |
| 19:R:7:LYS:HG3    | 19:R:11:LYS:HE2  | 2.01                     | 0.42              |
| 1:2:1154:U:H2'    | 4:C:192:LEU:HD11 | 2.02                     | 0.42              |
| 12:K:9:ILE:HD12   | 12:K:9:ILE:HA    | 1.82                     | 0.42              |
| 1:2:494:C:N4      | 1:2:509:OMG:HN22 | 2.17                     | 0.42              |
| 1:2:1098:C:H2'    | 1:2:1099:G:C8    | 2.55                     | 0.42              |
| 1:2:1705:C:H2'    | 1:2:1706:G:C8    | 2.55                     | 0.42              |
| 8:G:221:LYS:HE3   | 8:G:222:GLU:HG2  | 2.01                     | 0.42              |
| 7:F:102:LEU:HD11  | 27:Z:110:THR:HB  | 2.02                     | 0.41              |
| 12:K:14:LEU:HD12  | 12:K:14:LEU:HA   | 1.87                     | 0.41              |
| 20:S:8:LYS:HD2    | 20:S:8:LYS:HA    | 1.91                     | 0.41              |
| 24:W:87:GLU:OE2   | 24:W:87:GLU:HA   | 2.20                     | 0.41              |
| 34:g:22:ALA:HB3   | 34:g:32:LEU:HB2  | 2.02                     | 0.41              |
| 1:2:1277:C:H5''   | 12:K:55:ARG:HH11 | 1.85                     | 0.41              |
| 8:G:121:ILE:HG21  | 8:G:124:LEU:HD12 | 2.02                     | 0.41              |
| 30:c:44:ARG:HH11  | 30:c:58:LEU:HD23 | 1.85                     | 0.41              |
| 2:A:124:VAL:HG21  | 2:A:134:LEU:HD21 | 2.02                     | 0.41              |
| 5:D:173:ARG:HD3   | 5:D:173:ARG:HA   | 1.94                     | 0.41              |
| 20:S:34:LYS:HB2   | 20:S:34:LYS:HE2  | 1.65                     | 0.41              |
| 22:U:51:LYS:HB2   | 22:U:90:ASP:HB2  | 2.00                     | 0.41              |
| 28:a:18:VAL:HG21  | 28:a:33:ASP:OD1  | 2.20                     | 0.41              |
| 1:2:1736:G:H2'    | 1:2:1737:G:C8    | 2.56                     | 0.41              |
| 19:R:58:MET:HE3   | 19:R:58:MET:HA   | 2.02                     | 0.41              |
| 34:g:118:ARG:HH12 | 34:g:133:ASN:HB2 | 1.85                     | 0.41              |
| 34:g:217:MET:HB2  | 34:g:217:MET:HE3 | 1.73                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:2:1598:G:H3'   | 27:Z:80:ARG:HD2  | 2.01                     | 0.41              |
| 5:D:40:ARG:HD3   | 22:U:108:PRO:HG3 | 2.02                     | 0.41              |
| 6:E:175:PHE:HE2  | 6:E:198:ARG:HD2  | 1.84                     | 0.41              |
| 9:H:10:LYS:NZ    | 9:H:20:GLU:HG3   | 2.36                     | 0.41              |
| 11:J:110:LEU:HB2 | 11:J:147:PHE:HB3 | 2.02                     | 0.41              |
| 12:K:6:LYS:HB2   | 12:K:6:LYS:HE3   | 1.79                     | 0.41              |
| 1:2:944:A:H5''   | 16:O:134:PRO:HB3 | 2.02                     | 0.41              |
| 1:2:955:A:H4'    | 16:O:60:MET:HE3  | 2.01                     | 0.41              |
| 2:A:82:THR:HG22  | 2:A:171:VAL:HG11 | 2.03                     | 0.41              |
| 3:B:166:LYS:O    | 3:B:170:GLU:HG3  | 2.21                     | 0.41              |
| 4:C:144:SER:HB2  | 4:C:150:ALA:HB2  | 2.01                     | 0.41              |
| 9:H:30:LEU:HD21  | 9:H:83:LEU:HD22  | 2.02                     | 0.41              |
| 9:H:32:MET:HE2   | 9:H:32:MET:HB3   | 1.85                     | 0.41              |
| 10:I:57:ALA:HB2  | 10:I:183:GLY:HA2 | 2.03                     | 0.41              |
| 10:I:150:ASP:HA  | 10:I:153:LYS:HG2 | 2.02                     | 0.41              |
| 12:K:29:MET:HB3  | 12:K:42:ASN:HB2  | 2.02                     | 0.41              |
| 21:T:60:THR:O    | 21:T:64:LEU:HD22 | 2.21                     | 0.41              |
| 27:Z:72:VAL:O    | 27:Z:76:ARG:HB2  | 2.21                     | 0.41              |
| 5:D:29:LEU:HB2   | 5:D:34:TYR:HB2   | 2.01                     | 0.41              |
| 8:G:63:MET:HE3   | 8:G:100:CYS:HA   | 2.01                     | 0.41              |
| 28:a:70:LYS:HB3  | 28:a:70:LYS:HE3  | 1.85                     | 0.41              |
| 29:b:63:LEU:HD12 | 29:b:63:LEU:HA   | 1.95                     | 0.41              |
| 1:2:1285:G:H5'   | 14:M:35:ILE:HG13 | 2.02                     | 0.41              |
| 1:2:1651:A:H2'   | 1:2:1652:G:H8    | 1.86                     | 0.41              |
| 12:K:57:TYR:HB3  | 12:K:75:GLY:HA2  | 2.02                     | 0.41              |
| 1:2:35:C:H5''    | 1:2:579:C:H5''   | 2.03                     | 0.41              |
| 1:2:509:OMG:H1'  | 1:2:509:OMG:HM23 | 1.77                     | 0.41              |
| 2:A:134:LEU:HD22 | 2:A:144:THR:HG21 | 2.03                     | 0.41              |
| 9:H:7:LYS:HD3    | 9:H:7:LYS:HA     | 1.79                     | 0.41              |
| 9:H:63:PHE:HB3   | 9:H:97:GLN:HG2   | 2.03                     | 0.41              |
| 34:g:17:TRP:H    | 34:g:36:ARG:HB2  | 1.86                     | 0.41              |
| 1:2:1536:G:H2'   | 1:2:1537:A:C8    | 2.56                     | 0.41              |
| 2:A:184:ARG:HG2  | 2:A:189:ILE:HG13 | 2.02                     | 0.41              |
| 6:E:62:LYS:HE3   | 6:E:62:LYS:HB3   | 1.72                     | 0.41              |
| 2:A:34:MET:HE2   | 2:A:149:ASN:O    | 2.21                     | 0.40              |
| 18:Q:8:GLN:HG2   | 18:Q:99:TYR:CE1  | 2.56                     | 0.40              |
| 21:T:40:ALA:HB3  | 21:T:43:LYS:HG2  | 2.02                     | 0.40              |
| 26:Y:111:LYS:HE2 | 26:Y:111:LYS:HB3 | 1.97                     | 0.40              |
| 7:F:127:ARG:HA   | 7:F:127:ARG:HD2  | 1.83                     | 0.40              |
| 18:Q:98:LYS:HD3  | 18:Q:99:TYR:CE2  | 2.56                     | 0.40              |
| 1:2:1144:A:H2'   | 1:2:1145:A:C8    | 2.57                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:68:GLU:HB3   | 3:B:83:LYS:HD2   | 2.02                     | 0.40              |
| 6:E:160:ILE:HD12 | 6:E:162:ILE:HD11 | 2.03                     | 0.40              |
| 34:g:234:ASP:HB3 | 34:g:252:THR:CG2 | 2.49                     | 0.40              |
| 1:2:15:U:H2'     | 1:2:16:G:O4'     | 2.22                     | 0.40              |
| 1:2:191:A:H62    | 1:2:208:G:H21    | 1.70                     | 0.40              |
| 11:J:139:LYS:HB3 | 11:J:139:LYS:HE3 | 1.93                     | 0.40              |
| 19:R:95:ILE:HD13 | 19:R:95:ILE:HA   | 1.97                     | 0.40              |
| 34:g:22:ALA:HB1  | 34:g:71:ILE:HG22 | 2.03                     | 0.40              |
| 1:2:544:G:H3'    | 1:2:545:A:H8     | 1.85                     | 0.40              |
| 1:2:1670:C:H2'   | 1:2:1671:G:C8    | 2.56                     | 0.40              |
| 5:D:175:VAL:O    | 5:D:181:VAL:HA   | 2.21                     | 0.40              |
| 10:I:160:SER:O   | 10:I:164:GLU:HG2 | 2.20                     | 0.40              |
| 33:f:92:LYS:HD2  | 33:f:92:LYS:HA   | 1.85                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 2   | A     | 205/295 (70%) | 199 (97%)  | 6 (3%)  | 0        | 100         | 100 |
| 3   | B     | 208/264 (79%) | 207 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 4   | C     | 218/293 (74%) | 212 (97%)  | 6 (3%)  | 0        | 100         | 100 |
| 5   | D     | 222/243 (91%) | 222 (100%) | 0       | 0        | 100         | 100 |
| 6   | E     | 255/263 (97%) | 251 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 7   | F     | 178/204 (87%) | 171 (96%)  | 7 (4%)  | 0        | 100         | 100 |
| 8   | G     | 225/249 (90%) | 221 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 9   | H     | 180/194 (93%) | 166 (92%)  | 14 (8%) | 0        | 100         | 100 |
| 10  | I     | 203/208 (98%) | 194 (96%)  | 9 (4%)  | 0        | 100         | 100 |
| 11  | J     | 183/194 (94%) | 179 (98%)  | 4 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 12  | K     | 95/165 (58%)    | 94 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 13  | L     | 137/158 (87%)   | 132 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 14  | M     | 100/132 (76%)   | 92 (92%)   | 8 (8%)   | 0        | 100         | 100 |
| 15  | N     | 148/151 (98%)   | 146 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 16  | O     | 125/151 (83%)   | 119 (95%)  | 5 (4%)   | 1 (1%)   | 16          | 44  |
| 17  | P     | 121/145 (83%)   | 120 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 18  | Q     | 137/146 (94%)   | 134 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 19  | R     | 129/135 (96%)   | 125 (97%)  | 4 (3%)   | 0        | 100         | 100 |
| 20  | S     | 142/152 (93%)   | 137 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 21  | T     | 141/145 (97%)   | 139 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 22  | U     | 102/119 (86%)   | 96 (94%)   | 6 (6%)   | 0        | 100         | 100 |
| 23  | V     | 81/83 (98%)     | 80 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 24  | W     | 127/130 (98%)   | 125 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 25  | X     | 138/143 (96%)   | 135 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 26  | Y     | 120/133 (90%)   | 119 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 27  | Z     | 70/125 (56%)    | 67 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 28  | a     | 97/115 (84%)    | 96 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 29  | b     | 80/84 (95%)     | 77 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 30  | c     | 57/69 (83%)     | 55 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 31  | d     | 53/56 (95%)     | 52 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 32  | e     | 53/59 (90%)     | 52 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 33  | f     | 62/156 (40%)    | 56 (90%)   | 6 (10%)  | 0        | 100         | 100 |
| 34  | g     | 310/317 (98%)   | 297 (96%)  | 13 (4%)  | 0        | 100         | 100 |
| 35  | h     | 44/1096 (4%)    | 41 (93%)   | 3 (7%)   | 0        | 100         | 100 |
| 36  | n     | 18/25 (72%)     | 18 (100%)  | 0        | 0        | 100         | 100 |
| All | All   | 4764/6597 (72%) | 4626 (97%) | 137 (3%) | 1 (0%)   | 100         | 100 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16  | O     | 138 | ASP  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 2   | A     | 173/243 (71%) | 170 (98%)  | 3 (2%)   | 53          | 83  |
| 3   | B     | 192/231 (83%) | 187 (97%)  | 5 (3%)   | 40          | 75  |
| 4   | C     | 186/225 (83%) | 181 (97%)  | 5 (3%)   | 39          | 74  |
| 5   | D     | 188/202 (93%) | 178 (95%)  | 10 (5%)  | 20          | 52  |
| 6   | E     | 220/225 (98%) | 217 (99%)  | 3 (1%)   | 59          | 85  |
| 7   | F     | 155/170 (91%) | 149 (96%)  | 6 (4%)   | 28          | 64  |
| 8   | G     | 198/218 (91%) | 195 (98%)  | 3 (2%)   | 57          | 84  |
| 9   | H     | 164/174 (94%) | 157 (96%)  | 7 (4%)   | 26          | 60  |
| 10  | I     | 178/180 (99%) | 175 (98%)  | 3 (2%)   | 53          | 83  |
| 11  | J     | 161/168 (96%) | 161 (100%) | 0        | 100         | 100 |
| 12  | K     | 88/136 (65%)  | 82 (93%)   | 6 (7%)   | 14          | 42  |
| 13  | L     | 128/142 (90%) | 126 (98%)  | 2 (2%)   | 55          | 83  |
| 14  | M     | 86/108 (80%)  | 83 (96%)   | 3 (4%)   | 32          | 67  |
| 15  | N     | 130/131 (99%) | 128 (98%)  | 2 (2%)   | 57          | 84  |
| 16  | O     | 100/119 (84%) | 96 (96%)   | 4 (4%)   | 28          | 63  |
| 17  | P     | 106/130 (82%) | 100 (94%)  | 6 (6%)   | 18          | 49  |
| 18  | Q     | 115/121 (95%) | 112 (97%)  | 3 (3%)   | 40          | 75  |
| 19  | R     | 119/122 (98%) | 112 (94%)  | 7 (6%)   | 18          | 48  |
| 20  | S     | 125/132 (95%) | 123 (98%)  | 2 (2%)   | 55          | 83  |
| 21  | T     | 113/115 (98%) | 109 (96%)  | 4 (4%)   | 32          | 67  |
| 22  | U     | 94/107 (88%)  | 87 (93%)   | 7 (7%)   | 13          | 37  |
| 23  | V     | 67/67 (100%)  | 67 (100%)  | 0        | 100         | 100 |
| 24  | W     | 112/113 (99%) | 111 (99%)  | 1 (1%)   | 70          | 89  |
| 25  | X     | 112/115 (97%) | 108 (96%)  | 4 (4%)   | 31          | 66  |
| 26  | Y     | 107/115 (93%) | 103 (96%)  | 4 (4%)   | 30          | 65  |
| 27  | Z     | 63/103 (61%)  | 62 (98%)   | 1 (2%)   | 55          | 83  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 28  | a     | 86/98 (88%)     | 85 (99%)   | 1 (1%)   | 63          | 87  |
| 29  | b     | 74/76 (97%)     | 70 (95%)   | 4 (5%)   | 20          | 51  |
| 30  | c     | 52/62 (84%)     | 45 (86%)   | 7 (14%)  | 4           | 13  |
| 31  | d     | 48/49 (98%)     | 46 (96%)   | 2 (4%)   | 26          | 61  |
| 32  | e     | 45/48 (94%)     | 41 (91%)   | 4 (9%)   | 9           | 29  |
| 33  | f     | 57/140 (41%)    | 56 (98%)   | 1 (2%)   | 51          | 82  |
| 34  | g     | 264/275 (96%)   | 253 (96%)  | 11 (4%)  | 26          | 61  |
| 35  | h     | 31/948 (3%)     | 30 (97%)   | 1 (3%)   | 34          | 70  |
| 36  | n     | 19/24 (79%)     | 19 (100%)  | 0        | 100         | 100 |
| All | All   | 4156/5632 (74%) | 4024 (97%) | 132 (3%) | 35          | 70  |

All (132) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | A     | 54  | THR  |
| 2   | A     | 123 | VAL  |
| 2   | A     | 190 | SER  |
| 3   | B     | 55  | THR  |
| 3   | B     | 70  | SER  |
| 3   | B     | 91  | VAL  |
| 3   | B     | 97  | LEU  |
| 3   | B     | 225 | LEU  |
| 4   | C     | 147 | VAL  |
| 4   | C     | 184 | VAL  |
| 4   | C     | 212 | LYS  |
| 4   | C     | 221 | ASP  |
| 4   | C     | 259 | THR  |
| 5   | D     | 38  | GLU  |
| 5   | D     | 42  | THR  |
| 5   | D     | 44  | THR  |
| 5   | D     | 54  | ARG  |
| 5   | D     | 55  | THR  |
| 5   | D     | 58  | VAL  |
| 5   | D     | 74  | GLN  |
| 5   | D     | 175 | VAL  |
| 5   | D     | 208 | VAL  |
| 5   | D     | 209 | SER  |
| 6   | E     | 105 | THR  |
| 6   | E     | 168 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | E     | 173 | ILE  |
| 7   | F     | 33  | ILE  |
| 7   | F     | 42  | LYS  |
| 7   | F     | 102 | LEU  |
| 7   | F     | 103 | LEU  |
| 7   | F     | 141 | VAL  |
| 7   | F     | 166 | ILE  |
| 8   | G     | 22  | ARG  |
| 8   | G     | 144 | LEU  |
| 8   | G     | 158 | VAL  |
| 9   | H     | 10  | LYS  |
| 9   | H     | 23  | ILE  |
| 9   | H     | 50  | GLU  |
| 9   | H     | 75  | ILE  |
| 9   | H     | 77  | VAL  |
| 9   | H     | 92  | VAL  |
| 9   | H     | 93  | VAL  |
| 10  | I     | 62  | VAL  |
| 10  | I     | 165 | GLN  |
| 10  | I     | 193 | LYS  |
| 12  | K     | 3   | MET  |
| 12  | K     | 9   | ILE  |
| 12  | K     | 21  | MET  |
| 12  | K     | 79  | LEU  |
| 12  | K     | 83  | LEU  |
| 12  | K     | 90  | VAL  |
| 13  | L     | 83  | GLN  |
| 13  | L     | 120 | VAL  |
| 14  | M     | 16  | THR  |
| 14  | M     | 49  | LEU  |
| 14  | M     | 68  | LEU  |
| 15  | N     | 26  | LEU  |
| 15  | N     | 72  | LEU  |
| 16  | O     | 40  | THR  |
| 16  | O     | 56  | VAL  |
| 16  | O     | 107 | THR  |
| 16  | O     | 130 | GLU  |
| 17  | P     | 83  | MET  |
| 17  | P     | 90  | VAL  |
| 17  | P     | 92  | SER  |
| 17  | P     | 107 | ILE  |
| 17  | P     | 111 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | P     | 124 | LYS  |
| 18  | Q     | 7   | LEU  |
| 18  | Q     | 12  | VAL  |
| 18  | Q     | 100 | VAL  |
| 19  | R     | 8   | THR  |
| 19  | R     | 40  | ILE  |
| 19  | R     | 58  | MET  |
| 19  | R     | 61  | ILE  |
| 19  | R     | 69  | ILE  |
| 19  | R     | 71  | ILE  |
| 19  | R     | 120 | THR  |
| 20  | S     | 66  | ARG  |
| 20  | S     | 136 | THR  |
| 21  | T     | 82  | ARG  |
| 21  | T     | 90  | SER  |
| 21  | T     | 110 | LEU  |
| 21  | T     | 131 | LEU  |
| 22  | U     | 19  | ARG  |
| 22  | U     | 20  | ILE  |
| 22  | U     | 56  | MET  |
| 22  | U     | 75  | LYS  |
| 22  | U     | 90  | ASP  |
| 22  | U     | 92  | HIS  |
| 22  | U     | 97  | ILE  |
| 24  | W     | 114 | GLU  |
| 25  | X     | 36  | LEU  |
| 25  | X     | 105 | PHE  |
| 25  | X     | 119 | ARG  |
| 25  | X     | 125 | VAL  |
| 26  | Y     | 5   | VAL  |
| 26  | Y     | 7   | ILE  |
| 26  | Y     | 16  | ARG  |
| 26  | Y     | 68  | LYS  |
| 27  | Z     | 92  | LEU  |
| 28  | a     | 64  | LEU  |
| 29  | b     | 37  | CYS  |
| 29  | b     | 44  | THR  |
| 29  | b     | 57  | VAL  |
| 29  | b     | 81  | ARG  |
| 30  | c     | 14  | VAL  |
| 30  | c     | 17  | VAL  |
| 30  | c     | 27  | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | c     | 28  | THR  |
| 30  | c     | 41  | SER  |
| 30  | c     | 56  | LEU  |
| 30  | c     | 58  | LEU  |
| 31  | d     | 6   | LEU  |
| 31  | d     | 30  | LEU  |
| 32  | e     | 16  | THR  |
| 32  | e     | 21  | LYS  |
| 32  | e     | 29  | THR  |
| 32  | e     | 46  | VAL  |
| 33  | f     | 89  | LYS  |
| 34  | g     | 6   | THR  |
| 34  | g     | 31  | ILE  |
| 34  | g     | 74  | ASP  |
| 34  | g     | 110 | SER  |
| 34  | g     | 113 | PHE  |
| 34  | g     | 199 | THR  |
| 34  | g     | 229 | THR  |
| 34  | g     | 248 | LEU  |
| 34  | g     | 270 | LEU  |
| 34  | g     | 297 | THR  |
| 34  | g     | 307 | VAL  |
| 35  | h     | 677 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | A     | 36  | GLN  |
| 3   | B     | 149 | GLN  |
| 6   | E     | 50  | ASN  |
| 9   | H     | 12  | ASN  |
| 9   | H     | 163 | GLN  |
| 10  | I     | 165 | GLN  |
| 12  | K     | 28  | HIS  |
| 12  | K     | 61  | GLN  |
| 13  | L     | 19  | ASN  |
| 15  | N     | 13  | GLN  |
| 17  | P     | 53  | GLN  |
| 18  | Q     | 29  | ASN  |
| 19  | R     | 121 | GLN  |
| 20  | S     | 72  | GLN  |
| 21  | T     | 63  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | T     | 117 | GLN  |
| 23  | V     | 35  | ASN  |
| 24  | W     | 24  | GLN  |
| 24  | W     | 64  | ASN  |
| 28  | a     | 86  | ASN  |
| 30  | c     | 45  | ASN  |
| 31  | d     | 26  | ASN  |
| 31  | d     | 37  | ASN  |
| 32  | e     | 44  | ASN  |
| 34  | g     | 15  | ASN  |
| 34  | g     | 178 | ASN  |
| 34  | g     | 188 | HIS  |
| 34  | g     | 215 | GLN  |
| 34  | g     | 226 | HIS  |
| 34  | g     | 285 | GLN  |
| 34  | g     | 305 | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | 2     | 1601/1869 (85%) | 261 (16%)         | 4 (0%)          |

All (261) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 17  | C    |
| 1   | 2     | 25  | A    |
| 1   | 2     | 33  | G    |
| 1   | 2     | 41  | G    |
| 1   | 2     | 45  | A    |
| 1   | 2     | 46  | A    |
| 1   | 2     | 56  | G    |
| 1   | 2     | 65  | C    |
| 1   | 2     | 67  | C    |
| 1   | 2     | 68  | A    |
| 1   | 2     | 72  | C    |
| 1   | 2     | 73  | C    |
| 1   | 2     | 74  | G    |
| 1   | 2     | 75  | G    |
| 1   | 2     | 77  | A    |
| 1   | 2     | 99  | A2M  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 103 | A    |
| 1   | 2     | 113 | G    |
| 1   | 2     | 114 | G    |
| 1   | 2     | 115 | U    |
| 1   | 2     | 126 | G    |
| 1   | 2     | 130 | G    |
| 1   | 2     | 142 | C    |
| 1   | 2     | 143 | U    |
| 1   | 2     | 155 | G    |
| 1   | 2     | 160 | U    |
| 1   | 2     | 168 | C    |
| 1   | 2     | 175 | A    |
| 1   | 2     | 178 | C    |
| 1   | 2     | 182 | C    |
| 1   | 2     | 191 | A    |
| 1   | 2     | 212 | C    |
| 1   | 2     | 302 | A    |
| 1   | 2     | 306 | C    |
| 1   | 2     | 309 | G    |
| 1   | 2     | 319 | C    |
| 1   | 2     | 320 | G    |
| 1   | 2     | 330 | G    |
| 1   | 2     | 332 | G    |
| 1   | 2     | 339 | A    |
| 1   | 2     | 340 | C    |
| 1   | 2     | 362 | C    |
| 1   | 2     | 364 | A    |
| 1   | 2     | 369 | C    |
| 1   | 2     | 370 | G    |
| 1   | 2     | 385 | G    |
| 1   | 2     | 386 | C    |
| 1   | 2     | 400 | C    |
| 1   | 2     | 409 | C    |
| 1   | 2     | 448 | A    |
| 1   | 2     | 449 | A    |
| 1   | 2     | 450 | C    |
| 1   | 2     | 464 | A    |
| 1   | 2     | 465 | A    |
| 1   | 2     | 471 | G    |
| 1   | 2     | 472 | C    |
| 1   | 2     | 474 | G    |
| 1   | 2     | 482 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 487 | U    |
| 1   | 2     | 492 | C    |
| 1   | 2     | 508 | A    |
| 1   | 2     | 512 | A2M  |
| 1   | 2     | 516 | A    |
| 1   | 2     | 525 | A    |
| 1   | 2     | 532 | C    |
| 1   | 2     | 537 | C    |
| 1   | 2     | 538 | U    |
| 1   | 2     | 539 | C    |
| 1   | 2     | 540 | U    |
| 1   | 2     | 541 | U    |
| 1   | 2     | 544 | G    |
| 1   | 2     | 546 | G    |
| 1   | 2     | 547 | G    |
| 1   | 2     | 548 | C    |
| 1   | 2     | 549 | C    |
| 1   | 2     | 550 | C    |
| 1   | 2     | 554 | A    |
| 1   | 2     | 555 | A    |
| 1   | 2     | 559 | G    |
| 1   | 2     | 563 | G    |
| 1   | 2     | 564 | A    |
| 1   | 2     | 576 | A2M  |
| 1   | 2     | 583 | C    |
| 1   | 2     | 587 | A    |
| 1   | 2     | 589 | G    |
| 1   | 2     | 591 | U    |
| 1   | 2     | 593 | C    |
| 1   | 2     | 604 | A    |
| 1   | 2     | 608 | C    |
| 1   | 2     | 614 | C    |
| 1   | 2     | 617 | G    |
| 1   | 2     | 626 | G    |
| 1   | 2     | 627 | U    |
| 1   | 2     | 628 | A    |
| 1   | 2     | 629 | A    |
| 1   | 2     | 630 | U    |
| 1   | 2     | 632 | C    |
| 1   | 2     | 643 | A    |
| 1   | 2     | 655 | A    |
| 1   | 2     | 660 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2     | 663  | C    |
| 1   | 2     | 668  | A2M  |
| 1   | 2     | 669  | A    |
| 1   | 2     | 671  | A    |
| 1   | 2     | 672  | A    |
| 1   | 2     | 673  | G    |
| 1   | 2     | 687  | C    |
| 1   | 2     | 688  | U    |
| 1   | 2     | 689  | U    |
| 1   | 2     | 821  | G    |
| 1   | 2     | 822  | PSU  |
| 1   | 2     | 834  | C    |
| 1   | 2     | 847  | A    |
| 1   | 2     | 870  | A    |
| 1   | 2     | 871  | U    |
| 1   | 2     | 872  | A    |
| 1   | 2     | 913  | A    |
| 1   | 2     | 914  | U    |
| 1   | 2     | 920  | A    |
| 1   | 2     | 922  | A    |
| 1   | 2     | 933  | G    |
| 1   | 2     | 943  | U    |
| 1   | 2     | 950  | C    |
| 1   | 2     | 955  | A    |
| 1   | 2     | 970  | G    |
| 1   | 2     | 971  | G    |
| 1   | 2     | 990  | A    |
| 1   | 2     | 992  | A    |
| 1   | 2     | 1017 | U    |
| 1   | 2     | 1023 | A    |
| 1   | 2     | 1061 | U    |
| 1   | 2     | 1062 | A    |
| 1   | 2     | 1080 | A    |
| 1   | 2     | 1083 | A    |
| 1   | 2     | 1085 | C    |
| 1   | 2     | 1089 | G    |
| 1   | 2     | 1109 | C    |
| 1   | 2     | 1115 | U    |
| 1   | 2     | 1116 | C    |
| 1   | 2     | 1119 | A    |
| 1   | 2     | 1121 | G    |
| 1   | 2     | 1133 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2     | 1138 | C    |
| 1   | 2     | 1148 | A    |
| 1   | 2     | 1153 | C    |
| 1   | 2     | 1154 | U    |
| 1   | 2     | 1171 | G    |
| 1   | 2     | 1195 | A    |
| 1   | 2     | 1208 | A    |
| 1   | 2     | 1215 | C    |
| 1   | 2     | 1224 | G    |
| 1   | 2     | 1242 | U    |
| 1   | 2     | 1243 | U    |
| 1   | 2     | 1245 | G    |
| 1   | 2     | 1248 | B8N  |
| 1   | 2     | 1251 | A    |
| 1   | 2     | 1253 | A    |
| 1   | 2     | 1256 | G    |
| 1   | 2     | 1257 | G    |
| 1   | 2     | 1259 | A    |
| 1   | 2     | 1269 | G    |
| 1   | 2     | 1274 | G    |
| 1   | 2     | 1275 | G    |
| 1   | 2     | 1285 | G    |
| 1   | 2     | 1286 | G    |
| 1   | 2     | 1295 | A    |
| 1   | 2     | 1298 | G    |
| 1   | 2     | 1301 | A    |
| 1   | 2     | 1302 | G    |
| 1   | 2     | 1303 | C    |
| 1   | 2     | 1306 | U    |
| 1   | 2     | 1308 | U    |
| 1   | 2     | 1312 | G    |
| 1   | 2     | 1320 | G    |
| 1   | 2     | 1333 | U    |
| 1   | 2     | 1342 | U    |
| 1   | 2     | 1363 | C    |
| 1   | 2     | 1371 | U    |
| 1   | 2     | 1372 | U    |
| 1   | 2     | 1378 | A    |
| 1   | 2     | 1382 | A    |
| 1   | 2     | 1395 | C    |
| 1   | 2     | 1397 | U    |
| 1   | 2     | 1404 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2     | 1418 | C    |
| 1   | 2     | 1431 | G    |
| 1   | 2     | 1432 | U    |
| 1   | 2     | 1433 | C    |
| 1   | 2     | 1434 | C    |
| 1   | 2     | 1436 | C    |
| 1   | 2     | 1437 | C    |
| 1   | 2     | 1438 | A    |
| 1   | 2     | 1442 | OMU  |
| 1   | 2     | 1452 | A    |
| 1   | 2     | 1454 | A    |
| 1   | 2     | 1462 | U    |
| 1   | 2     | 1463 | U    |
| 1   | 2     | 1487 | A    |
| 1   | 2     | 1488 | C    |
| 1   | 2     | 1489 | A    |
| 1   | 2     | 1490 | OMG  |
| 1   | 2     | 1494 | U    |
| 1   | 2     | 1495 | G    |
| 1   | 2     | 1497 | G    |
| 1   | 2     | 1498 | A    |
| 1   | 2     | 1507 | G    |
| 1   | 2     | 1508 | A    |
| 1   | 2     | 1521 | C    |
| 1   | 2     | 1522 | A    |
| 1   | 2     | 1523 | C    |
| 1   | 2     | 1533 | A    |
| 1   | 2     | 1535 | U    |
| 1   | 2     | 1544 | C    |
| 1   | 2     | 1553 | C    |
| 1   | 2     | 1555 | U    |
| 1   | 2     | 1580 | A    |
| 1   | 2     | 1585 | U    |
| 1   | 2     | 1588 | A    |
| 1   | 2     | 1594 | A    |
| 1   | 2     | 1601 | A    |
| 1   | 2     | 1606 | G    |
| 1   | 2     | 1621 | U    |
| 1   | 2     | 1654 | G    |
| 1   | 2     | 1664 | A    |
| 1   | 2     | 1665 | G    |
| 1   | 2     | 1683 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2     | 1698 | C    |
| 1   | 2     | 1701 | C    |
| 1   | 2     | 1713 | C    |
| 1   | 2     | 1715 | A    |
| 1   | 2     | 1719 | A    |
| 1   | 2     | 1721 | U    |
| 1   | 2     | 1722 | G    |
| 1   | 2     | 1723 | G    |
| 1   | 2     | 1729 | U    |
| 1   | 2     | 1744 | G    |
| 1   | 2     | 1745 | A    |
| 1   | 2     | 1752 | C    |
| 1   | 2     | 1754 | G    |
| 1   | 2     | 1777 | G    |
| 1   | 2     | 1779 | G    |
| 1   | 2     | 1781 | A    |
| 1   | 2     | 1783 | C    |
| 1   | 2     | 1784 | G    |
| 1   | 2     | 1800 | A    |
| 1   | 2     | 1807 | C    |
| 1   | 2     | 1812 | U    |
| 1   | 2     | 1813 | A    |
| 1   | 2     | 1823 | A    |
| 1   | 2     | 1825 | A    |
| 1   | 2     | 1829 | G    |
| 1   | 2     | 1831 | A    |
| 1   | 2     | 1835 | A    |
| 1   | 2     | 1838 | U    |
| 1   | 2     | 1849 | G    |
| 1   | 2     | 1851 | MA6  |
| 1   | 2     | 1861 | G    |
| 1   | 2     | 1862 | G    |
| 1   | 2     | 1863 | A    |
| 1   | 2     | 1864 | U    |
| 1   | 2     | 1865 | C    |

All (4) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 331 | C    |
| 1   | 2     | 531 | A    |
| 1   | 2     | 627 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 871 | U    |

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

73 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 |
| 1   | PSU  | 2     | 1046 | 1    | 18,21,22     | 2.48 | 8 (44%)  | 21,30,33    | 2.04 | 3 (14%)  |
| 1   | PSU  | 2     | 1174 | 1,37 | 18,21,22     | 2.47 | 7 (38%)  | 21,30,33    | 2.08 | 4 (19%)  |
| 1   | A2M  | 2     | 668  | 1,38 | 22,25,26     | 3.45 | 7 (31%)  | 30,36,39    | 2.11 | 9 (30%)  |
| 1   | A2M  | 2     | 590  | 1    | 22,25,26     | 3.44 | 7 (31%)  | 30,36,39    | 2.39 | 11 (36%) |
| 1   | OMU  | 2     | 121  | 1    | 19,22,23     | 2.80 | 7 (36%)  | 25,31,34    | 1.75 | 5 (20%)  |
| 1   | OMG  | 2     | 683  | 1    | 23,26,27     | 2.50 | 3 (13%)  | 32,38,41    | 1.94 | 9 (28%)  |
| 1   | PSU  | 2     | 1045 | 1    | 18,21,22     | 2.42 | 7 (38%)  | 21,30,33    | 2.02 | 4 (19%)  |
| 1   | PSU  | 2     | 1136 | 1    | 18,21,22     | 2.46 | 7 (38%)  | 21,30,33    | 2.09 | 4 (19%)  |
| 1   | PSU  | 2     | 1692 | 1,37 | 18,21,22     | 2.47 | 7 (38%)  | 21,30,33    | 2.01 | 4 (19%)  |
| 1   | 4AC  | 2     | 1842 | 1    | 21,24,25     | 1.92 | 7 (33%)  | 28,34,37    | 2.00 | 8 (28%)  |
| 1   | OMU  | 2     | 1288 | 1    | 19,22,23     | 2.70 | 6 (31%)  | 25,31,34    | 1.91 | 7 (28%)  |
| 1   | PSU  | 2     | 1081 | 1    | 18,21,22     | 2.58 | 8 (44%)  | 21,30,33    | 2.06 | 5 (23%)  |
| 1   | PSU  | 2     | 572  | 1,37 | 18,21,22     | 2.47 | 7 (38%)  | 21,30,33    | 2.08 | 4 (19%)  |
| 1   | OMG  | 2     | 644  | 1    | 23,26,27     | 2.47 | 4 (17%)  | 32,38,41    | 1.93 | 9 (28%)  |
| 1   | PSU  | 2     | 93   | 1    | 18,21,22     | 2.48 | 7 (38%)  | 21,30,33    | 2.00 | 4 (19%)  |
| 1   | B8N  | 2     | 1248 | 1    | 25,29,30     | 2.56 | 8 (32%)  | 28,42,45    | 1.54 | 5 (17%)  |
| 1   | PSU  | 2     | 119  | 1    | 18,21,22     | 2.56 | 7 (38%)  | 21,30,33    | 2.03 | 4 (19%)  |
| 1   | OMU  | 2     | 428  | 1    | 19,22,23     | 2.75 | 7 (36%)  | 25,31,34    | 1.96 | 6 (24%)  |
| 1   | A2M  | 2     | 484  | 1    | 22,25,26     | 3.45 | 7 (31%)  | 30,36,39    | 2.13 | 8 (26%)  |
| 1   | PSU  | 2     | 1232 | 1    | 18,21,22     | 2.48 | 7 (38%)  | 21,30,33    | 2.17 | 4 (19%)  |
| 1   | PSU  | 2     | 814  | 1    | 18,21,22     | 2.50 | 8 (44%)  | 21,30,33    | 2.02 | 3 (14%)  |
| 1   | 4AC  | 2     | 1337 | 1    | 21,24,25     | 1.97 | 7 (33%)  | 28,34,37    | 1.76 | 5 (17%)  |

| Mol | Type | Chain | Res  | Link    | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|---------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |         | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | PSU  | 2     | 1347 | 1       | 18,21,22     | 2.47 | 7 (38%)  | 21,30,33    | 2.04 | 4 (19%)  |
| 1   | MA6  | 2     | 1850 | 1       | 23,26,27     | 1.32 | 3 (13%)  | 33,38,41    | 2.38 | 10 (30%) |
| 1   | PSU  | 2     | 863  | 1       | 18,21,22     | 2.50 | 7 (38%)  | 21,30,33    | 2.04 | 4 (19%)  |
| 1   | PSU  | 2     | 296  | 1       | 18,21,22     | 2.46 | 7 (38%)  | 21,30,33    | 2.15 | 4 (19%)  |
| 1   | OMU  | 2     | 354  | 1       | 19,22,23     | 2.76 | 7 (36%)  | 25,31,34    | 1.81 | 5 (20%)  |
| 1   | PSU  | 2     | 1056 | 1       | 18,21,22     | 2.41 | 7 (38%)  | 21,30,33    | 1.98 | 4 (19%)  |
| 1   | A2M  | 2     | 468  | 1       | 22,25,26     | 3.46 | 7 (31%)  | 30,36,39    | 2.12 | 8 (26%)  |
| 1   | A2M  | 2     | 27   | 1,38    | 22,25,26     | 3.46 | 6 (27%)  | 30,36,39    | 2.19 | 10 (33%) |
| 1   | A2M  | 2     | 1031 | 1       | 22,25,26     | 3.47 | 7 (31%)  | 30,36,39    | 2.04 | 8 (26%)  |
| 1   | PSU  | 2     | 105  | 1,37    | 18,21,22     | 2.48 | 7 (38%)  | 21,30,33    | 2.11 | 4 (19%)  |
| 1   | OMU  | 2     | 1326 | 1,38    | 19,22,23     | 2.74 | 7 (36%)  | 25,31,34    | 2.03 | 6 (24%)  |
| 1   | PSU  | 2     | 1643 | 1,38    | 18,21,22     | 2.44 | 7 (38%)  | 21,30,33    | 2.07 | 5 (23%)  |
| 1   | 6MZ  | 2     | 1832 | 1,37,38 | 22,25,26     | 2.49 | 3 (13%)  | 29,36,39    | 2.54 | 11 (37%) |
| 1   | A2M  | 2     | 576  | 1,37    | 22,25,26     | 3.46 | 7 (31%)  | 30,36,39    | 2.08 | 9 (30%)  |
| 1   | OMG  | 2     | 1328 | 1,37    | 23,26,27     | 2.49 | 3 (13%)  | 32,38,41    | 1.93 | 9 (28%)  |
| 1   | OMG  | 2     | 601  | 1       | 23,26,27     | 2.47 | 4 (17%)  | 32,38,41    | 1.92 | 9 (28%)  |
| 1   | PSU  | 2     | 651  | 1       | 18,21,22     | 2.48 | 7 (38%)  | 21,30,33    | 2.08 | 4 (19%)  |
| 1   | PSU  | 2     | 1238 | 1       | 18,21,22     | 2.42 | 7 (38%)  | 21,30,33    | 2.00 | 4 (19%)  |
| 1   | PSU  | 2     | 1445 | 1       | 18,21,22     | 2.41 | 7 (38%)  | 21,30,33    | 2.08 | 5 (23%)  |
| 1   | OMG  | 2     | 1490 | 1,38    | 23,26,27     | 2.45 | 4 (17%)  | 32,38,41    | 1.89 | 9 (28%)  |
| 1   | 7MG  | 2     | 1639 | 1       | 23,26,27     | 3.55 | 6 (26%)  | 27,39,42    | 2.12 | 8 (29%)  |
| 1   | OMC  | 2     | 1703 | 1       | 19,22,23     | 1.77 | 5 (26%)  | 25,31,34    | 1.04 | 1 (4%)   |
| 1   | PSU  | 2     | 36   | 1       | 18,21,22     | 2.52 | 7 (38%)  | 21,30,33    | 1.93 | 4 (19%)  |
| 1   | A2M  | 2     | 99   | 1,38    | 22,25,26     | 3.49 | 7 (31%)  | 30,36,39    | 2.12 | 8 (26%)  |
| 1   | PSU  | 2     | 815  | 1       | 18,21,22     | 2.45 | 7 (38%)  | 21,30,33    | 2.10 | 4 (19%)  |
| 1   | PSU  | 2     | 686  | 1       | 18,21,22     | 2.39 | 7 (38%)  | 21,30,33    | 2.05 | 4 (19%)  |
| 1   | OMC  | 2     | 517  | 1       | 19,22,23     | 1.76 | 5 (26%)  | 25,31,34    | 1.11 | 1 (4%)   |
| 1   | PSU  | 2     | 649  | 1       | 18,21,22     | 2.50 | 7 (38%)  | 21,30,33    | 2.10 | 4 (19%)  |
| 1   | A2M  | 2     | 512  | 1       | 22,25,26     | 3.47 | 7 (31%)  | 30,36,39    | 2.17 | 10 (33%) |
| 1   | OMC  | 2     | 1272 | 1       | 19,22,23     | 1.74 | 4 (21%)  | 25,31,34    | 1.08 | 1 (4%)   |
| 1   | OMC  | 2     | 1391 | 1       | 19,22,23     | 1.78 | 5 (26%)  | 25,31,34    | 1.03 | 1 (4%)   |
| 1   | OMG  | 2     | 436  | 1       | 23,26,27     | 2.48 | 4 (17%)  | 32,38,41    | 1.96 | 9 (28%)  |
| 1   | OMG  | 2     | 509  | 1,38    | 23,26,27     | 2.43 | 5 (21%)  | 32,38,41    | 1.93 | 9 (28%)  |
| 1   | PSU  | 2     | 109  | 1,37    | 18,21,22     | 2.46 | 7 (38%)  | 21,30,33    | 2.12 | 4 (19%)  |
| 1   | PSU  | 2     | 681  | 1       | 18,21,22     | 2.47 | 8 (44%)  | 21,30,33    | 1.99 | 4 (19%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | OMU  | 2     | 172  | 1    | 19,22,23     | 2.77 | 7 (36%)  | 25,31,34    | 1.96 | 5 (20%)  |
| 1   | PSU  | 2     | 1625 | 1    | 18,21,22     | 2.43 | 7 (38%)  | 21,30,33    | 1.96 | 4 (19%)  |
| 1   | PSU  | 2     | 822  | 1    | 18,21,22     | 2.53 | 8 (44%)  | 21,30,33    | 2.11 | 5 (23%)  |
| 1   | A2M  | 2     | 1678 | 1    | 22,25,26     | 3.53 | 6 (27%)  | 30,36,39    | 2.17 | 8 (26%)  |
| 1   | OMC  | 2     | 462  | 1    | 19,22,23     | 1.79 | 5 (26%)  | 25,31,34    | 1.06 | 1 (4%)   |
| 1   | A2M  | 2     | 159  | 1    | 22,25,26     | 3.48 | 7 (31%)  | 30,36,39    | 2.10 | 8 (26%)  |
| 1   | A2M  | 2     | 166  | 1    | 22,25,26     | 3.49 | 7 (31%)  | 30,36,39    | 2.20 | 8 (26%)  |
| 1   | OMC  | 2     | 174  | 1,38 | 19,22,23     | 1.77 | 5 (26%)  | 25,31,34    | 1.01 | 1 (4%)   |
| 1   | PSU  | 2     | 406  | 1    | 18,21,22     | 2.49 | 7 (38%)  | 21,30,33    | 2.05 | 4 (19%)  |
| 1   | PSU  | 2     | 1177 | 1    | 18,21,22     | 2.45 | 7 (38%)  | 21,30,33    | 2.04 | 4 (19%)  |
| 1   | A2M  | 2     | 1383 | 1    | 22,25,26     | 3.48 | 7 (31%)  | 30,36,39    | 2.09 | 8 (26%)  |
| 1   | OMU  | 2     | 1442 | 1,38 | 19,22,23     | 2.73 | 7 (36%)  | 25,31,34    | 1.90 | 5 (20%)  |
| 1   | OMG  | 2     | 1447 | 1    | 23,26,27     | 2.49 | 3 (13%)  | 32,38,41    | 1.92 | 9 (28%)  |
| 1   | MA6  | 2     | 1851 | 1    | 23,26,27     | 1.35 | 3 (13%)  | 33,38,41    | 2.39 | 11 (33%) |
| 1   | OMU  | 2     | 116  | 1    | 19,22,23     | 2.76 | 8 (42%)  | 25,31,34    | 1.82 | 4 (16%)  |
| 1   | PSU  | 2     | 1244 | 1    | 18,21,22     | 2.42 | 7 (38%)  | 21,30,33    | 2.06 | 4 (19%)  |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 1   | PSU  | 2     | 1046 | 1    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 2     | 1174 | 1,37 | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | A2M  | 2     | 668  | 1,38 | -       | 3/9/27/28  | 0/3/3/3 |
| 1   | A2M  | 2     | 590  | 1    | -       | 1/9/27/28  | 0/3/3/3 |
| 1   | OMU  | 2     | 121  | 1    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | OMG  | 2     | 683  | 1    | -       | 2/9/27/28  | 0/3/3/3 |
| 1   | PSU  | 2     | 1045 | 1    | -       | 2/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 2     | 1136 | 1    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 2     | 1692 | 1,37 | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 4AC  | 2     | 1842 | 1    | -       | 2/11/29/30 | 0/2/2/2 |
| 1   | OMU  | 2     | 1288 | 1    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | PSU  | 2     | 1081 | 1    | -       | 1/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 2     | 572  | 1,37 | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMG  | 2     | 644  | 1    | -       | 1/9/27/28  | 0/3/3/3 |
| 1   | PSU  | 2     | 93   | 1    | -       | 0/7/25/26  | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link    | Chirals | Torsions   | Rings   |
|-----|------|-------|------|---------|---------|------------|---------|
| 1   | B8N  | 2     | 1248 | 1       | -       | 6/16/34/35 | 0/2/2/2 |
| 1   | PSU  | 2     | 119  | 1       | -       | 1/7/25/26  | 0/2/2/2 |
| 1   | OMU  | 2     | 428  | 1       | -       | 4/9/27/28  | 0/2/2/2 |
| 1   | A2M  | 2     | 484  | 1       | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | PSU  | 2     | 1232 | 1       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 2     | 814  | 1       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 4AC  | 2     | 1337 | 1       | -       | 4/11/29/30 | 0/2/2/2 |
| 1   | PSU  | 2     | 1347 | 1       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | MA6  | 2     | 1850 | 1       | -       | 3/11/29/30 | 0/3/3/3 |
| 1   | PSU  | 2     | 863  | 1       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 2     | 296  | 1       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMU  | 2     | 354  | 1       | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | PSU  | 2     | 1056 | 1       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | A2M  | 2     | 468  | 1       | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | A2M  | 2     | 27   | 1,38    | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | A2M  | 2     | 1031 | 1       | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | PSU  | 2     | 105  | 1,37    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMU  | 2     | 1326 | 1,38    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | PSU  | 2     | 1643 | 1,38    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 6MZ  | 2     | 1832 | 1,37,38 | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | A2M  | 2     | 576  | 1,37    | -       | 2/9/27/28  | 0/3/3/3 |
| 1   | OMG  | 2     | 1328 | 1,37    | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | OMG  | 2     | 601  | 1       | -       | 1/9/27/28  | 0/3/3/3 |
| 1   | PSU  | 2     | 651  | 1       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 2     | 1238 | 1       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 2     | 1445 | 1       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMG  | 2     | 1490 | 1,38    | -       | 1/9/27/28  | 0/3/3/3 |
| 1   | 7MG  | 2     | 1639 | 1       | -       | 1/7/37/38  | 0/3/3/3 |
| 1   | OMC  | 2     | 1703 | 1       | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | PSU  | 2     | 36   | 1       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | A2M  | 2     | 99   | 1,38    | -       | 2/9/27/28  | 0/3/3/3 |
| 1   | PSU  | 2     | 815  | 1       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 2     | 686  | 1       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMC  | 2     | 517  | 1       | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | PSU  | 2     | 649  | 1       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | A2M  | 2     | 512  | 1       | -       | 2/9/27/28  | 0/3/3/3 |
| 1   | OMC  | 2     | 1272 | 1       | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | OMC  | 2     | 1391 | 1       | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | OMG  | 2     | 436  | 1       | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | OMG  | 2     | 509  | 1,38    | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | PSU  | 2     | 109  | 1,37    | -       | 0/7/25/26  | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 1   | PSU  | 2     | 681  | 1    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMU  | 2     | 172  | 1    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | PSU  | 2     | 1625 | 1    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 2     | 822  | 1    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | A2M  | 2     | 1678 | 1    | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | OMC  | 2     | 462  | 1    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | A2M  | 2     | 159  | 1    | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | A2M  | 2     | 166  | 1    | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | OMC  | 2     | 174  | 1,38 | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | PSU  | 2     | 406  | 1    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 2     | 1177 | 1    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | A2M  | 2     | 1383 | 1    | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | OMU  | 2     | 1442 | 1,38 | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | OMG  | 2     | 1447 | 1    | -       | 2/9/27/28  | 0/3/3/3 |
| 1   | MA6  | 2     | 1851 | 1    | -       | 5/11/29/30 | 0/3/3/3 |
| 1   | OMU  | 2     | 116  | 1    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | PSU  | 2     | 1244 | 1    | -       | 0/7/25/26  | 0/2/2/2 |

All (463) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | 2     | 1832 | 6MZ  | C6-N6   | 10.52 | 1.46        | 1.34     |
| 1   | 2     | 1288 | OMU  | O4-C4   | 9.92  | 1.43        | 1.24     |
| 1   | 2     | 172  | OMU  | O4-C4   | 9.79  | 1.43        | 1.24     |
| 1   | 2     | 116  | OMU  | O4-C4   | 9.76  | 1.43        | 1.24     |
| 1   | 2     | 121  | OMU  | O4-C4   | 9.73  | 1.43        | 1.24     |
| 1   | 2     | 428  | OMU  | O4-C4   | 9.66  | 1.43        | 1.24     |
| 1   | 2     | 1326 | OMU  | O4-C4   | 9.66  | 1.43        | 1.24     |
| 1   | 2     | 1442 | OMU  | O4-C4   | 9.62  | 1.43        | 1.24     |
| 1   | 2     | 354  | OMU  | O4-C4   | 9.56  | 1.43        | 1.24     |
| 1   | 2     | 1678 | A2M  | C2'-C1' | -9.24 | 1.30        | 1.53     |
| 1   | 2     | 99   | A2M  | C2'-C1' | -9.14 | 1.30        | 1.53     |
| 1   | 2     | 1639 | 7MG  | C5-N7   | 9.11  | 1.47        | 1.35     |
| 1   | 2     | 1639 | 7MG  | O6-C6   | 9.09  | 1.40        | 1.23     |
| 1   | 2     | 27   | A2M  | C2'-C1' | -9.04 | 1.30        | 1.53     |
| 1   | 2     | 1031 | A2M  | C2'-C1' | -9.02 | 1.30        | 1.53     |
| 1   | 2     | 468  | A2M  | C2'-C1' | -9.00 | 1.31        | 1.53     |
| 1   | 2     | 1383 | A2M  | C2'-C1' | -8.96 | 1.31        | 1.53     |
| 1   | 2     | 576  | A2M  | C2'-C1' | -8.96 | 1.31        | 1.53     |
| 1   | 2     | 166  | A2M  | C2'-C1' | -8.95 | 1.31        | 1.53     |
| 1   | 2     | 159  | A2M  | C2'-C1' | -8.95 | 1.31        | 1.53     |
| 1   | 2     | 512  | A2M  | C2'-C1' | -8.93 | 1.31        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | 2     | 166  | A2M  | O4'-C1' | 8.81  | 1.62        | 1.42     |
| 1   | 2     | 484  | A2M  | C2'-C1' | -8.80 | 1.31        | 1.53     |
| 1   | 2     | 1383 | A2M  | O4'-C1' | 8.76  | 1.62        | 1.42     |
| 1   | 2     | 668  | A2M  | C2'-C1' | -8.75 | 1.31        | 1.53     |
| 1   | 2     | 1678 | A2M  | O4'-C1' | 8.71  | 1.62        | 1.42     |
| 1   | 2     | 99   | A2M  | O4'-C1' | 8.67  | 1.62        | 1.42     |
| 1   | 2     | 512  | A2M  | O4'-C1' | 8.65  | 1.62        | 1.42     |
| 1   | 2     | 1031 | A2M  | O4'-C1' | 8.63  | 1.61        | 1.42     |
| 1   | 2     | 159  | A2M  | O4'-C1' | 8.60  | 1.61        | 1.42     |
| 1   | 2     | 590  | A2M  | O4'-C1' | 8.55  | 1.61        | 1.42     |
| 1   | 2     | 27   | A2M  | O4'-C1' | 8.52  | 1.61        | 1.42     |
| 1   | 2     | 468  | A2M  | O4'-C1' | 8.51  | 1.61        | 1.42     |
| 1   | 2     | 590  | A2M  | C2'-C1' | -8.50 | 1.32        | 1.53     |
| 1   | 2     | 484  | A2M  | O4'-C1' | 8.48  | 1.61        | 1.42     |
| 1   | 2     | 1248 | B8N  | O4-C4   | 8.40  | 1.40        | 1.23     |
| 1   | 2     | 576  | A2M  | O4'-C1' | 8.36  | 1.61        | 1.42     |
| 1   | 2     | 1639 | 7MG  | C4-N9   | 8.30  | 1.48        | 1.37     |
| 1   | 2     | 1447 | OMG  | C2-N2   | 8.17  | 1.53        | 1.34     |
| 1   | 2     | 668  | A2M  | O4'-C1' | 8.15  | 1.60        | 1.42     |
| 1   | 2     | 683  | OMG  | C2-N2   | 8.12  | 1.53        | 1.34     |
| 1   | 2     | 1328 | OMG  | C2-N2   | 8.09  | 1.53        | 1.34     |
| 1   | 2     | 436  | OMG  | C2-N2   | 7.98  | 1.52        | 1.34     |
| 1   | 2     | 644  | OMG  | C2-N2   | 7.93  | 1.52        | 1.34     |
| 1   | 2     | 601  | OMG  | C2-N2   | 7.91  | 1.52        | 1.34     |
| 1   | 2     | 1490 | OMG  | C2-N2   | 7.71  | 1.52        | 1.34     |
| 1   | 2     | 509  | OMG  | C2-N2   | 7.59  | 1.51        | 1.34     |
| 1   | 2     | 1328 | OMG  | O6-C6   | 7.40  | 1.37        | 1.23     |
| 1   | 2     | 1447 | OMG  | O6-C6   | 7.38  | 1.37        | 1.23     |
| 1   | 2     | 1490 | OMG  | O6-C6   | 7.35  | 1.37        | 1.23     |
| 1   | 2     | 683  | OMG  | O6-C6   | 7.35  | 1.37        | 1.23     |
| 1   | 2     | 644  | OMG  | O6-C6   | 7.32  | 1.37        | 1.23     |
| 1   | 2     | 601  | OMG  | O6-C6   | 7.32  | 1.37        | 1.23     |
| 1   | 2     | 436  | OMG  | O6-C6   | 7.25  | 1.37        | 1.23     |
| 1   | 2     | 509  | OMG  | O6-C6   | 7.11  | 1.37        | 1.23     |
| 1   | 2     | 159  | A2M  | C6-N6   | 7.08  | 1.52        | 1.34     |
| 1   | 2     | 1678 | A2M  | C6-N6   | 7.07  | 1.52        | 1.34     |
| 1   | 2     | 576  | A2M  | C6-N6   | 7.07  | 1.52        | 1.34     |
| 1   | 2     | 166  | A2M  | C6-N6   | 7.06  | 1.52        | 1.34     |
| 1   | 2     | 468  | A2M  | C6-N6   | 7.04  | 1.52        | 1.34     |
| 1   | 2     | 484  | A2M  | C6-N6   | 7.02  | 1.52        | 1.34     |
| 1   | 2     | 512  | A2M  | C6-N6   | 7.02  | 1.52        | 1.34     |
| 1   | 2     | 1031 | A2M  | C6-N6   | 7.01  | 1.52        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | 2     | 1383 | A2M  | C6-N6   | 7.00  | 1.52        | 1.34     |
| 1   | 2     | 27   | A2M  | C6-N6   | 6.99  | 1.52        | 1.34     |
| 1   | 2     | 590  | A2M  | C6-N6   | 6.99  | 1.52        | 1.34     |
| 1   | 2     | 668  | A2M  | C6-N6   | 6.98  | 1.52        | 1.34     |
| 1   | 2     | 99   | A2M  | C6-N6   | 6.90  | 1.51        | 1.34     |
| 1   | 2     | 668  | A2M  | O4'-C4' | -6.13 | 1.31        | 1.45     |
| 1   | 2     | 590  | A2M  | O4'-C4' | -5.86 | 1.32        | 1.45     |
| 1   | 2     | 119  | PSU  | O4-C4   | -5.85 | 1.12        | 1.23     |
| 1   | 2     | 1678 | A2M  | O4'-C4' | -5.67 | 1.32        | 1.45     |
| 1   | 2     | 863  | PSU  | O4-C4   | -5.64 | 1.12        | 1.23     |
| 1   | 2     | 822  | PSU  | O4-C4   | -5.62 | 1.12        | 1.23     |
| 1   | 2     | 1136 | PSU  | O4-C4   | -5.62 | 1.12        | 1.23     |
| 1   | 2     | 576  | A2M  | O4'-C4' | -5.62 | 1.32        | 1.45     |
| 1   | 2     | 484  | A2M  | O4'-C4' | -5.61 | 1.32        | 1.45     |
| 1   | 2     | 468  | A2M  | O4'-C4' | -5.59 | 1.32        | 1.45     |
| 1   | 2     | 27   | A2M  | O4'-C4' | -5.58 | 1.32        | 1.45     |
| 1   | 2     | 572  | PSU  | O4-C4   | -5.57 | 1.13        | 1.23     |
| 1   | 2     | 1177 | PSU  | O4-C4   | -5.53 | 1.13        | 1.23     |
| 1   | 2     | 651  | PSU  | O4-C4   | -5.53 | 1.13        | 1.23     |
| 1   | 2     | 99   | A2M  | O4'-C4' | -5.53 | 1.32        | 1.45     |
| 1   | 2     | 1081 | PSU  | O4-C4   | -5.52 | 1.13        | 1.23     |
| 1   | 2     | 159  | A2M  | O4'-C4' | -5.51 | 1.32        | 1.45     |
| 1   | 2     | 36   | PSU  | O4-C4   | -5.51 | 1.13        | 1.23     |
| 1   | 2     | 1031 | A2M  | O4'-C4' | -5.51 | 1.32        | 1.45     |
| 1   | 2     | 1232 | PSU  | O4-C4   | -5.51 | 1.13        | 1.23     |
| 1   | 2     | 814  | PSU  | O4-C4   | -5.50 | 1.13        | 1.23     |
| 1   | 2     | 681  | PSU  | O4-C4   | -5.50 | 1.13        | 1.23     |
| 1   | 2     | 1692 | PSU  | O4-C4   | -5.49 | 1.13        | 1.23     |
| 1   | 2     | 1046 | PSU  | O4-C4   | -5.47 | 1.13        | 1.23     |
| 1   | 2     | 109  | PSU  | O4-C4   | -5.47 | 1.13        | 1.23     |
| 1   | 2     | 1383 | A2M  | O4'-C4' | -5.47 | 1.32        | 1.45     |
| 1   | 2     | 649  | PSU  | O4-C4   | -5.47 | 1.13        | 1.23     |
| 1   | 2     | 815  | PSU  | O4-C4   | -5.47 | 1.13        | 1.23     |
| 1   | 2     | 166  | A2M  | O4'-C4' | -5.46 | 1.32        | 1.45     |
| 1   | 2     | 686  | PSU  | O4-C4   | -5.46 | 1.13        | 1.23     |
| 1   | 2     | 1347 | PSU  | O4-C4   | -5.45 | 1.13        | 1.23     |
| 1   | 2     | 105  | PSU  | O4-C4   | -5.42 | 1.13        | 1.23     |
| 1   | 2     | 406  | PSU  | O4-C4   | -5.41 | 1.13        | 1.23     |
| 1   | 2     | 512  | A2M  | O4'-C4' | -5.41 | 1.33        | 1.45     |
| 1   | 2     | 296  | PSU  | O4-C4   | -5.41 | 1.13        | 1.23     |
| 1   | 2     | 1643 | PSU  | O4-C4   | -5.41 | 1.13        | 1.23     |
| 1   | 2     | 1174 | PSU  | O4-C4   | -5.40 | 1.13        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | 2     | 93   | PSU  | O4-C4  | -5.40 | 1.13        | 1.23     |
| 1   | 2     | 1445 | PSU  | O4-C4  | -5.40 | 1.13        | 1.23     |
| 1   | 2     | 1244 | PSU  | O4-C4  | -5.38 | 1.13        | 1.23     |
| 1   | 2     | 1639 | 7MG  | C2-N2  | 5.38  | 1.46        | 1.34     |
| 1   | 2     | 1056 | PSU  | O4-C4  | -5.38 | 1.13        | 1.23     |
| 1   | 2     | 1045 | PSU  | O4-C4  | -5.36 | 1.13        | 1.23     |
| 1   | 2     | 1238 | PSU  | O4-C4  | -5.33 | 1.13        | 1.23     |
| 1   | 2     | 1625 | PSU  | O4-C4  | -5.28 | 1.13        | 1.23     |
| 1   | 2     | 1081 | PSU  | C1'-C5 | 5.08  | 1.61        | 1.50     |
| 1   | 2     | 119  | PSU  | C1'-C5 | 4.92  | 1.61        | 1.50     |
| 1   | 2     | 1272 | OMC  | C4-N4  | 4.73  | 1.45        | 1.33     |
| 1   | 2     | 1046 | PSU  | C1'-C5 | 4.71  | 1.60        | 1.50     |
| 1   | 2     | 1045 | PSU  | C1'-C5 | 4.71  | 1.60        | 1.50     |
| 1   | 2     | 1703 | OMC  | C4-N4  | 4.68  | 1.45        | 1.33     |
| 1   | 2     | 93   | PSU  | C1'-C5 | 4.67  | 1.60        | 1.50     |
| 1   | 2     | 462  | OMC  | C4-N4  | 4.66  | 1.45        | 1.33     |
| 1   | 2     | 1625 | PSU  | C1'-C5 | 4.65  | 1.60        | 1.50     |
| 1   | 2     | 174  | OMC  | C4-N4  | 4.62  | 1.45        | 1.33     |
| 1   | 2     | 1391 | OMC  | C4-N4  | 4.61  | 1.45        | 1.33     |
| 1   | 2     | 822  | PSU  | C1'-C5 | 4.59  | 1.60        | 1.50     |
| 1   | 2     | 1238 | PSU  | C1'-C5 | 4.55  | 1.60        | 1.50     |
| 1   | 2     | 1177 | PSU  | C1'-C5 | 4.55  | 1.60        | 1.50     |
| 1   | 2     | 863  | PSU  | C1'-C5 | 4.55  | 1.60        | 1.50     |
| 1   | 2     | 814  | PSU  | C1'-C5 | 4.54  | 1.60        | 1.50     |
| 1   | 2     | 1244 | PSU  | C1'-C5 | 4.54  | 1.60        | 1.50     |
| 1   | 2     | 1174 | PSU  | C1'-C5 | 4.54  | 1.60        | 1.50     |
| 1   | 2     | 649  | PSU  | C1'-C5 | 4.54  | 1.60        | 1.50     |
| 1   | 2     | 1056 | PSU  | C1'-C5 | 4.50  | 1.60        | 1.50     |
| 1   | 2     | 105  | PSU  | C1'-C5 | 4.46  | 1.60        | 1.50     |
| 1   | 2     | 517  | OMC  | C4-N4  | 4.45  | 1.44        | 1.33     |
| 1   | 2     | 1136 | PSU  | C1'-C5 | 4.44  | 1.60        | 1.50     |
| 1   | 2     | 1347 | PSU  | C1'-C5 | 4.43  | 1.60        | 1.50     |
| 1   | 2     | 1445 | PSU  | C1'-C5 | 4.41  | 1.60        | 1.50     |
| 1   | 2     | 815  | PSU  | C1'-C5 | 4.40  | 1.60        | 1.50     |
| 1   | 2     | 1232 | PSU  | C1'-C5 | 4.39  | 1.60        | 1.50     |
| 1   | 2     | 681  | PSU  | C1'-C5 | 4.39  | 1.60        | 1.50     |
| 1   | 2     | 572  | PSU  | C1'-C5 | 4.39  | 1.60        | 1.50     |
| 1   | 2     | 1692 | PSU  | C1'-C5 | 4.37  | 1.60        | 1.50     |
| 1   | 2     | 406  | PSU  | C1'-C5 | 4.37  | 1.60        | 1.50     |
| 1   | 2     | 1248 | B8N  | C4-N3  | -4.36 | 1.32        | 1.40     |
| 1   | 2     | 109  | PSU  | C1'-C5 | 4.35  | 1.60        | 1.50     |
| 1   | 2     | 686  | PSU  | C1'-C5 | 4.35  | 1.60        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | 2     | 1643 | PSU  | C1'-C5 | 4.35  | 1.60        | 1.50     |
| 1   | 2     | 36   | PSU  | C1'-C5 | 4.32  | 1.60        | 1.50     |
| 1   | 2     | 296  | PSU  | C1'-C5 | 4.31  | 1.60        | 1.50     |
| 1   | 2     | 1850 | MA6  | C6-N6  | 4.28  | 1.48        | 1.36     |
| 1   | 2     | 651  | PSU  | C1'-C5 | 4.26  | 1.59        | 1.50     |
| 1   | 2     | 1851 | MA6  | C6-N6  | 4.07  | 1.48        | 1.36     |
| 1   | 2     | 1248 | B8N  | C1'-C5 | -3.97 | 1.41        | 1.50     |
| 1   | 2     | 354  | OMU  | C4-N3  | -3.85 | 1.32        | 1.38     |
| 1   | 2     | 1081 | PSU  | C2-N3  | -3.84 | 1.31        | 1.37     |
| 1   | 2     | 36   | PSU  | C2-N3  | -3.83 | 1.31        | 1.37     |
| 1   | 2     | 1248 | B8N  | C2-N3  | -3.81 | 1.32        | 1.38     |
| 1   | 2     | 1337 | 4AC  | C4-N4  | 3.81  | 1.45        | 1.39     |
| 1   | 2     | 1337 | 4AC  | C2-N1  | -3.79 | 1.32        | 1.40     |
| 1   | 2     | 119  | PSU  | C2-N3  | -3.78 | 1.31        | 1.37     |
| 1   | 2     | 1842 | 4AC  | C4-N4  | 3.76  | 1.45        | 1.39     |
| 1   | 2     | 296  | PSU  | C2-N1  | -3.74 | 1.31        | 1.36     |
| 1   | 2     | 1337 | 4AC  | C7-N4  | 3.74  | 1.44        | 1.37     |
| 1   | 2     | 1842 | 4AC  | C7-N4  | 3.74  | 1.44        | 1.37     |
| 1   | 2     | 121  | OMU  | C4-N3  | -3.73 | 1.32        | 1.38     |
| 1   | 2     | 406  | PSU  | C2-N3  | -3.72 | 1.31        | 1.37     |
| 1   | 2     | 1842 | 4AC  | C2-N1  | -3.72 | 1.32        | 1.40     |
| 1   | 2     | 1347 | PSU  | C2-N3  | -3.72 | 1.31        | 1.37     |
| 1   | 2     | 1248 | B8N  | C4-C5  | -3.71 | 1.39        | 1.47     |
| 1   | 2     | 814  | PSU  | C2-N1  | -3.71 | 1.31        | 1.36     |
| 1   | 2     | 651  | PSU  | C2-N3  | -3.71 | 1.31        | 1.37     |
| 1   | 2     | 1692 | PSU  | C2-N3  | -3.70 | 1.31        | 1.37     |
| 1   | 2     | 814  | PSU  | C2-N3  | -3.69 | 1.31        | 1.37     |
| 1   | 2     | 93   | PSU  | C2-N3  | -3.68 | 1.31        | 1.37     |
| 1   | 2     | 649  | PSU  | C2-N3  | -3.67 | 1.31        | 1.37     |
| 1   | 2     | 681  | PSU  | C2-N3  | -3.66 | 1.31        | 1.37     |
| 1   | 2     | 1081 | PSU  | C2-N1  | -3.65 | 1.31        | 1.36     |
| 1   | 2     | 822  | PSU  | C2-N3  | -3.64 | 1.31        | 1.37     |
| 1   | 2     | 406  | PSU  | C2-N1  | -3.63 | 1.31        | 1.36     |
| 1   | 2     | 1046 | PSU  | C2-N1  | -3.63 | 1.31        | 1.36     |
| 1   | 2     | 36   | PSU  | C2-N1  | -3.62 | 1.31        | 1.36     |
| 1   | 2     | 36   | PSU  | C4-N3  | -3.62 | 1.32        | 1.38     |
| 1   | 2     | 105  | PSU  | C2-N3  | -3.61 | 1.31        | 1.37     |
| 1   | 2     | 572  | PSU  | C2-N3  | -3.60 | 1.31        | 1.37     |
| 1   | 2     | 1136 | PSU  | C2-N3  | -3.59 | 1.31        | 1.37     |
| 1   | 2     | 1174 | PSU  | C2-N1  | -3.59 | 1.32        | 1.36     |
| 1   | 2     | 1232 | PSU  | C2-N3  | -3.58 | 1.31        | 1.37     |
| 1   | 2     | 863  | PSU  | C2-N3  | -3.57 | 1.31        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | 2     | 109  | PSU  | C2-N3 | -3.57 | 1.31        | 1.37     |
| 1   | 2     | 1174 | PSU  | C2-N3 | -3.56 | 1.31        | 1.37     |
| 1   | 2     | 815  | PSU  | C2-N3 | -3.56 | 1.31        | 1.37     |
| 1   | 2     | 1643 | PSU  | C2-N3 | -3.54 | 1.31        | 1.37     |
| 1   | 2     | 119  | PSU  | C2-N1 | -3.54 | 1.32        | 1.36     |
| 1   | 2     | 1442 | OMU  | C4-N3 | -3.54 | 1.32        | 1.38     |
| 1   | 2     | 109  | PSU  | C2-N1 | -3.53 | 1.32        | 1.36     |
| 1   | 2     | 1326 | OMU  | C2-N1 | -3.53 | 1.32        | 1.38     |
| 1   | 2     | 822  | PSU  | C2-N1 | -3.52 | 1.32        | 1.36     |
| 1   | 2     | 651  | PSU  | C4-N3 | -3.52 | 1.32        | 1.38     |
| 1   | 2     | 1045 | PSU  | C2-N3 | -3.51 | 1.31        | 1.37     |
| 1   | 2     | 1177 | PSU  | C2-N3 | -3.51 | 1.31        | 1.37     |
| 1   | 2     | 649  | PSU  | C2-N1 | -3.51 | 1.32        | 1.36     |
| 1   | 2     | 121  | OMU  | C2-N1 | -3.51 | 1.33        | 1.38     |
| 1   | 2     | 105  | PSU  | C4-N3 | -3.51 | 1.32        | 1.38     |
| 1   | 2     | 863  | PSU  | C2-N1 | -3.50 | 1.32        | 1.36     |
| 1   | 2     | 1692 | PSU  | C4-N3 | -3.50 | 1.32        | 1.38     |
| 1   | 2     | 651  | PSU  | C2-N1 | -3.50 | 1.32        | 1.36     |
| 1   | 2     | 1347 | PSU  | C4-N3 | -3.50 | 1.32        | 1.38     |
| 1   | 2     | 1244 | PSU  | C2-N3 | -3.50 | 1.31        | 1.37     |
| 1   | 2     | 1238 | PSU  | C2-N3 | -3.49 | 1.31        | 1.37     |
| 1   | 2     | 815  | PSU  | C2-N1 | -3.49 | 1.32        | 1.36     |
| 1   | 2     | 1056 | PSU  | C2-N3 | -3.48 | 1.31        | 1.37     |
| 1   | 2     | 406  | PSU  | C4-N3 | -3.48 | 1.32        | 1.38     |
| 1   | 2     | 296  | PSU  | C2-N3 | -3.48 | 1.31        | 1.37     |
| 1   | 2     | 681  | PSU  | C2-N1 | -3.48 | 1.32        | 1.36     |
| 1   | 2     | 105  | PSU  | C2-N1 | -3.46 | 1.32        | 1.36     |
| 1   | 2     | 822  | PSU  | C4-N3 | -3.45 | 1.32        | 1.38     |
| 1   | 2     | 428  | OMU  | C4-N3 | -3.45 | 1.32        | 1.38     |
| 1   | 2     | 1232 | PSU  | C4-N3 | -3.45 | 1.32        | 1.38     |
| 1   | 2     | 93   | PSU  | C2-N1 | -3.44 | 1.32        | 1.36     |
| 1   | 2     | 1625 | PSU  | C2-N3 | -3.44 | 1.31        | 1.37     |
| 1   | 2     | 1347 | PSU  | C2-N1 | -3.44 | 1.32        | 1.36     |
| 1   | 2     | 116  | OMU  | C4-N3 | -3.43 | 1.32        | 1.38     |
| 1   | 2     | 172  | OMU  | C4-N3 | -3.42 | 1.32        | 1.38     |
| 1   | 2     | 1288 | OMU  | C4-N3 | -3.42 | 1.32        | 1.38     |
| 1   | 2     | 814  | PSU  | C4-N3 | -3.42 | 1.32        | 1.38     |
| 1   | 2     | 119  | PSU  | C4-N3 | -3.41 | 1.32        | 1.38     |
| 1   | 2     | 109  | PSU  | C4-N3 | -3.41 | 1.32        | 1.38     |
| 1   | 2     | 462  | OMC  | C2-N1 | -3.41 | 1.32        | 1.40     |
| 1   | 2     | 1692 | PSU  | C2-N1 | -3.40 | 1.32        | 1.36     |
| 1   | 2     | 686  | PSU  | C2-N3 | -3.40 | 1.31        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | 2     | 1445 | PSU  | C2-N3 | -3.40 | 1.31        | 1.37     |
| 1   | 2     | 572  | PSU  | C4-N3 | -3.40 | 1.32        | 1.38     |
| 1   | 2     | 1391 | OMC  | C2-N1 | -3.39 | 1.33        | 1.40     |
| 1   | 2     | 1136 | PSU  | C4-N3 | -3.39 | 1.32        | 1.38     |
| 1   | 2     | 681  | PSU  | C4-N3 | -3.39 | 1.32        | 1.38     |
| 1   | 2     | 649  | PSU  | C4-N3 | -3.39 | 1.32        | 1.38     |
| 1   | 2     | 863  | PSU  | C4-N3 | -3.39 | 1.32        | 1.38     |
| 1   | 2     | 1625 | PSU  | C2-N1 | -3.39 | 1.32        | 1.36     |
| 1   | 2     | 172  | OMU  | C2-N1 | -3.38 | 1.33        | 1.38     |
| 1   | 2     | 1046 | PSU  | C2-N3 | -3.38 | 1.31        | 1.37     |
| 1   | 2     | 572  | PSU  | C2-N1 | -3.37 | 1.32        | 1.36     |
| 1   | 2     | 174  | OMC  | C2-N1 | -3.37 | 1.33        | 1.40     |
| 1   | 2     | 1643 | PSU  | C2-N1 | -3.37 | 1.32        | 1.36     |
| 1   | 2     | 815  | PSU  | C4-N3 | -3.37 | 1.32        | 1.38     |
| 1   | 2     | 1703 | OMC  | C2-N1 | -3.36 | 1.33        | 1.40     |
| 1   | 2     | 428  | OMU  | C2-N1 | -3.36 | 1.33        | 1.38     |
| 1   | 2     | 1081 | PSU  | C4-N3 | -3.36 | 1.32        | 1.38     |
| 1   | 2     | 1326 | OMU  | C4-N3 | -3.35 | 1.32        | 1.38     |
| 1   | 2     | 1056 | PSU  | C4-N3 | -3.34 | 1.32        | 1.38     |
| 1   | 2     | 296  | PSU  | C4-N3 | -3.34 | 1.32        | 1.38     |
| 1   | 2     | 93   | PSU  | C4-N3 | -3.33 | 1.32        | 1.38     |
| 1   | 2     | 517  | OMC  | C2-N1 | -3.33 | 1.33        | 1.40     |
| 1   | 2     | 1643 | PSU  | C4-N3 | -3.33 | 1.32        | 1.38     |
| 1   | 2     | 1238 | PSU  | C2-N1 | -3.32 | 1.32        | 1.36     |
| 1   | 2     | 1177 | PSU  | C2-N1 | -3.32 | 1.32        | 1.36     |
| 1   | 2     | 1174 | PSU  | C4-N3 | -3.31 | 1.32        | 1.38     |
| 1   | 2     | 1232 | PSU  | C2-N1 | -3.29 | 1.32        | 1.36     |
| 1   | 2     | 1045 | PSU  | C2-N1 | -3.29 | 1.32        | 1.36     |
| 1   | 2     | 116  | OMU  | C2-N1 | -3.28 | 1.33        | 1.38     |
| 1   | 2     | 1056 | PSU  | C2-N1 | -3.28 | 1.32        | 1.36     |
| 1   | 2     | 1136 | PSU  | C2-N1 | -3.28 | 1.32        | 1.36     |
| 1   | 2     | 1177 | PSU  | C4-N3 | -3.28 | 1.32        | 1.38     |
| 1   | 2     | 1244 | PSU  | C2-N1 | -3.27 | 1.32        | 1.36     |
| 1   | 2     | 1272 | OMC  | C2-N1 | -3.26 | 1.33        | 1.40     |
| 1   | 2     | 1832 | 6MZ  | C8-N9 | -3.26 | 1.32        | 1.37     |
| 1   | 2     | 1244 | PSU  | C4-N3 | -3.26 | 1.32        | 1.38     |
| 1   | 2     | 1445 | PSU  | C4-N3 | -3.25 | 1.32        | 1.38     |
| 1   | 2     | 686  | PSU  | C4-N3 | -3.25 | 1.32        | 1.38     |
| 1   | 2     | 1045 | PSU  | C4-N3 | -3.25 | 1.32        | 1.38     |
| 1   | 2     | 1238 | PSU  | C4-N3 | -3.24 | 1.32        | 1.38     |
| 1   | 2     | 1625 | PSU  | C4-N3 | -3.23 | 1.32        | 1.38     |
| 1   | 2     | 1445 | PSU  | C2-N1 | -3.22 | 1.32        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | 2     | 686  | PSU  | C2-N1   | -3.21 | 1.32        | 1.36     |
| 1   | 2     | 1639 | 7MG  | C8-N9   | 3.20  | 1.47        | 1.45     |
| 1   | 2     | 1046 | PSU  | C4-N3   | -3.20 | 1.32        | 1.38     |
| 1   | 2     | 1639 | 7MG  | C6-N1   | -3.11 | 1.33        | 1.38     |
| 1   | 2     | 159  | A2M  | O2'-C2' | 3.09  | 1.50        | 1.42     |
| 1   | 2     | 354  | OMU  | C2-N1   | -3.09 | 1.33        | 1.38     |
| 1   | 2     | 1851 | MA6  | C8-N9   | -3.09 | 1.32        | 1.37     |
| 1   | 2     | 296  | PSU  | O2-C2   | -3.07 | 1.16        | 1.23     |
| 1   | 2     | 1678 | A2M  | O2'-C2' | 3.05  | 1.50        | 1.42     |
| 1   | 2     | 354  | OMU  | C2-N3   | -3.05 | 1.32        | 1.38     |
| 1   | 2     | 105  | PSU  | O2-C2   | -3.02 | 1.16        | 1.23     |
| 1   | 2     | 166  | A2M  | O2'-C2' | 3.00  | 1.50        | 1.42     |
| 1   | 2     | 1442 | OMU  | C2-N1   | -3.00 | 1.33        | 1.38     |
| 1   | 2     | 1383 | A2M  | O2'-C2' | 2.99  | 1.50        | 1.42     |
| 1   | 2     | 484  | A2M  | O2'-C2' | 2.98  | 1.50        | 1.42     |
| 1   | 2     | 576  | A2M  | O2'-C2' | 2.97  | 1.50        | 1.42     |
| 1   | 2     | 590  | A2M  | O2'-C2' | 2.97  | 1.49        | 1.42     |
| 1   | 2     | 36   | PSU  | O2-C2   | -2.95 | 1.17        | 1.23     |
| 1   | 2     | 121  | OMU  | C2-N3   | -2.95 | 1.32        | 1.38     |
| 1   | 2     | 668  | A2M  | O2'-C2' | 2.94  | 1.49        | 1.42     |
| 1   | 2     | 814  | PSU  | O2-C2   | -2.93 | 1.17        | 1.23     |
| 1   | 2     | 406  | PSU  | O2-C2   | -2.93 | 1.17        | 1.23     |
| 1   | 2     | 512  | A2M  | O2'-C2' | 2.93  | 1.49        | 1.42     |
| 1   | 2     | 509  | OMG  | C6-N1   | -2.92 | 1.33        | 1.38     |
| 1   | 2     | 1643 | PSU  | O2-C2   | -2.91 | 1.17        | 1.23     |
| 1   | 2     | 649  | PSU  | O2-C2   | -2.91 | 1.17        | 1.23     |
| 1   | 2     | 1031 | A2M  | O2'-C2' | 2.91  | 1.49        | 1.42     |
| 1   | 2     | 1692 | PSU  | O2-C2   | -2.90 | 1.17        | 1.23     |
| 1   | 2     | 468  | A2M  | O2'-C2' | 2.90  | 1.49        | 1.42     |
| 1   | 2     | 1232 | PSU  | O2-C2   | -2.90 | 1.17        | 1.23     |
| 1   | 2     | 651  | PSU  | O2-C2   | -2.90 | 1.17        | 1.23     |
| 1   | 2     | 1850 | MA6  | C8-N9   | -2.90 | 1.32        | 1.37     |
| 1   | 2     | 99   | A2M  | O2'-C2' | 2.90  | 1.49        | 1.42     |
| 1   | 2     | 815  | PSU  | O2-C2   | -2.89 | 1.17        | 1.23     |
| 1   | 2     | 572  | PSU  | O2-C2   | -2.89 | 1.17        | 1.23     |
| 1   | 2     | 109  | PSU  | O2-C2   | -2.89 | 1.17        | 1.23     |
| 1   | 2     | 681  | PSU  | O2-C2   | -2.88 | 1.17        | 1.23     |
| 1   | 2     | 1347 | PSU  | O2-C2   | -2.88 | 1.17        | 1.23     |
| 1   | 2     | 822  | PSU  | O2-C2   | -2.88 | 1.17        | 1.23     |
| 1   | 2     | 1174 | PSU  | O2-C2   | -2.87 | 1.17        | 1.23     |
| 1   | 2     | 1391 | OMC  | O2-C2   | -2.87 | 1.18        | 1.23     |
| 1   | 2     | 1081 | PSU  | O2-C2   | -2.86 | 1.17        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | 2     | 1046 | PSU  | O2-C2   | -2.86 | 1.17        | 1.23     |
| 1   | 2     | 93   | PSU  | O2-C2   | -2.85 | 1.17        | 1.23     |
| 1   | 2     | 863  | PSU  | O2-C2   | -2.84 | 1.17        | 1.23     |
| 1   | 2     | 1136 | PSU  | O2-C2   | -2.84 | 1.17        | 1.23     |
| 1   | 2     | 1248 | B8N  | C6-C5   | 2.83  | 1.39        | 1.35     |
| 1   | 2     | 1244 | PSU  | O2-C2   | -2.83 | 1.17        | 1.23     |
| 1   | 2     | 119  | PSU  | O2-C2   | -2.83 | 1.17        | 1.23     |
| 1   | 2     | 1056 | PSU  | O2-C2   | -2.82 | 1.17        | 1.23     |
| 1   | 2     | 1177 | PSU  | O2-C2   | -2.81 | 1.17        | 1.23     |
| 1   | 2     | 1445 | PSU  | O2-C2   | -2.80 | 1.17        | 1.23     |
| 1   | 2     | 462  | OMC  | O2-C2   | -2.80 | 1.18        | 1.23     |
| 1   | 2     | 1337 | 4AC  | CM7-C7  | 2.80  | 1.56        | 1.50     |
| 1   | 2     | 1045 | PSU  | O2-C2   | -2.77 | 1.17        | 1.23     |
| 1   | 2     | 1337 | 4AC  | C6-N1   | -2.76 | 1.31        | 1.38     |
| 1   | 2     | 174  | OMC  | O2-C2   | -2.76 | 1.18        | 1.23     |
| 1   | 2     | 1703 | OMC  | O2-C2   | -2.75 | 1.18        | 1.23     |
| 1   | 2     | 1238 | PSU  | O2-C2   | -2.75 | 1.17        | 1.23     |
| 1   | 2     | 686  | PSU  | O2-C2   | -2.74 | 1.17        | 1.23     |
| 1   | 2     | 517  | OMC  | O2-C2   | -2.74 | 1.18        | 1.23     |
| 1   | 2     | 1625 | PSU  | O2-C2   | -2.73 | 1.17        | 1.23     |
| 1   | 2     | 1337 | 4AC  | O2-C2   | -2.72 | 1.18        | 1.23     |
| 1   | 2     | 27   | A2M  | O2'-C2' | 2.71  | 1.49        | 1.42     |
| 1   | 2     | 1232 | PSU  | C6-C5   | 2.69  | 1.38        | 1.35     |
| 1   | 2     | 1442 | OMU  | C2-N3   | -2.69 | 1.33        | 1.38     |
| 1   | 2     | 1272 | OMC  | O2-C2   | -2.68 | 1.18        | 1.23     |
| 1   | 2     | 428  | OMU  | C2-N3   | -2.67 | 1.33        | 1.38     |
| 1   | 2     | 172  | OMU  | C2-N3   | -2.65 | 1.33        | 1.38     |
| 1   | 2     | 1326 | OMU  | C2-N3   | -2.63 | 1.33        | 1.38     |
| 1   | 2     | 1625 | PSU  | C6-C5   | 2.63  | 1.38        | 1.35     |
| 1   | 2     | 1238 | PSU  | C6-C5   | 2.62  | 1.38        | 1.35     |
| 1   | 2     | 601  | OMG  | C6-N1   | -2.61 | 1.34        | 1.38     |
| 1   | 2     | 668  | A2M  | C8-N9   | -2.60 | 1.33        | 1.37     |
| 1   | 2     | 1842 | 4AC  | C6-N1   | -2.60 | 1.31        | 1.38     |
| 1   | 2     | 116  | OMU  | C2-N3   | -2.59 | 1.33        | 1.38     |
| 1   | 2     | 436  | OMG  | C6-N1   | -2.59 | 1.34        | 1.38     |
| 1   | 2     | 1842 | 4AC  | O2-C2   | -2.58 | 1.18        | 1.23     |
| 1   | 2     | 649  | PSU  | C6-C5   | 2.57  | 1.38        | 1.35     |
| 1   | 2     | 1490 | OMG  | C6-N1   | -2.57 | 1.34        | 1.38     |
| 1   | 2     | 590  | A2M  | C8-N9   | -2.57 | 1.33        | 1.37     |
| 1   | 2     | 576  | A2M  | C8-N9   | -2.57 | 1.33        | 1.37     |
| 1   | 2     | 1678 | A2M  | C8-N9   | -2.56 | 1.33        | 1.37     |
| 1   | 2     | 406  | PSU  | C6-C5   | 2.56  | 1.38        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | 2     | 644  | OMG  | C6-N1 | -2.55 | 1.34        | 1.38     |
| 1   | 2     | 1174 | PSU  | C6-C5 | 2.54  | 1.38        | 1.35     |
| 1   | 2     | 484  | A2M  | C8-N9 | -2.54 | 1.33        | 1.37     |
| 1   | 2     | 683  | OMG  | C6-N1 | -2.52 | 1.34        | 1.38     |
| 1   | 2     | 166  | A2M  | C8-N9 | -2.48 | 1.33        | 1.37     |
| 1   | 2     | 27   | A2M  | C8-N9 | -2.48 | 1.33        | 1.37     |
| 1   | 2     | 1832 | 6MZ  | C5-N7 | -2.48 | 1.34        | 1.39     |
| 1   | 2     | 1244 | PSU  | C6-C5 | 2.47  | 1.38        | 1.35     |
| 1   | 2     | 93   | PSU  | C6-C5 | 2.47  | 1.38        | 1.35     |
| 1   | 2     | 1383 | A2M  | C8-N9 | -2.46 | 1.33        | 1.37     |
| 1   | 2     | 1081 | PSU  | C6-C5 | 2.45  | 1.38        | 1.35     |
| 1   | 2     | 99   | A2M  | C8-N9 | -2.44 | 1.33        | 1.37     |
| 1   | 2     | 1447 | OMG  | C6-N1 | -2.44 | 1.34        | 1.38     |
| 1   | 2     | 159  | A2M  | C8-N9 | -2.43 | 1.33        | 1.37     |
| 1   | 2     | 1442 | OMU  | O2-C2 | -2.42 | 1.18        | 1.23     |
| 1   | 2     | 512  | A2M  | C8-N9 | -2.42 | 1.33        | 1.37     |
| 1   | 2     | 1045 | PSU  | C6-C5 | 2.41  | 1.38        | 1.35     |
| 1   | 2     | 815  | PSU  | C6-C5 | 2.41  | 1.38        | 1.35     |
| 1   | 2     | 863  | PSU  | C6-C5 | 2.41  | 1.38        | 1.35     |
| 1   | 2     | 1850 | MA6  | C5-N7 | -2.41 | 1.34        | 1.39     |
| 1   | 2     | 686  | PSU  | C6-C5 | 2.40  | 1.38        | 1.35     |
| 1   | 2     | 1177 | PSU  | C6-C5 | 2.40  | 1.37        | 1.35     |
| 1   | 2     | 1288 | OMU  | C2-N3 | -2.40 | 1.33        | 1.38     |
| 1   | 2     | 116  | OMU  | O2-C2 | -2.39 | 1.18        | 1.23     |
| 1   | 2     | 121  | OMU  | O2-C2 | -2.39 | 1.18        | 1.23     |
| 1   | 2     | 517  | OMC  | C2-N3 | -2.39 | 1.31        | 1.36     |
| 1   | 2     | 428  | OMU  | O2-C2 | -2.39 | 1.18        | 1.23     |
| 1   | 2     | 1328 | OMG  | C6-N1 | -2.38 | 1.34        | 1.38     |
| 1   | 2     | 172  | OMU  | O2-C2 | -2.38 | 1.18        | 1.23     |
| 1   | 2     | 428  | OMU  | C6-C5 | 2.37  | 1.40        | 1.35     |
| 1   | 2     | 1326 | OMU  | O2-C2 | -2.35 | 1.18        | 1.23     |
| 1   | 2     | 1031 | A2M  | C8-N9 | -2.34 | 1.33        | 1.37     |
| 1   | 2     | 468  | A2M  | C8-N9 | -2.33 | 1.33        | 1.37     |
| 1   | 2     | 572  | PSU  | C6-C5 | 2.33  | 1.37        | 1.35     |
| 1   | 2     | 462  | OMC  | C6-N1 | -2.33 | 1.32        | 1.38     |
| 1   | 2     | 651  | PSU  | C6-C5 | 2.32  | 1.37        | 1.35     |
| 1   | 2     | 1692 | PSU  | C6-C5 | 2.32  | 1.37        | 1.35     |
| 1   | 2     | 1288 | OMU  | C6-C5 | 2.32  | 1.40        | 1.35     |
| 1   | 2     | 1442 | OMU  | C6-C5 | 2.31  | 1.40        | 1.35     |
| 1   | 2     | 172  | OMU  | C6-C5 | 2.31  | 1.40        | 1.35     |
| 1   | 2     | 172  | OMU  | C6-N1 | -2.30 | 1.32        | 1.38     |
| 1   | 2     | 354  | OMU  | O2-C2 | -2.30 | 1.19        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | 2     | 1391 | OMC  | C6-N1   | -2.30 | 1.32        | 1.38     |
| 1   | 2     | 1445 | PSU  | C6-C5   | 2.30  | 1.37        | 1.35     |
| 1   | 2     | 36   | PSU  | C6-C5   | 2.29  | 1.37        | 1.35     |
| 1   | 2     | 1851 | MA6  | C5-N7   | -2.29 | 1.34        | 1.39     |
| 1   | 2     | 1347 | PSU  | C6-C5   | 2.27  | 1.37        | 1.35     |
| 1   | 2     | 1248 | B8N  | C2-N1   | -2.27 | 1.32        | 1.39     |
| 1   | 2     | 1326 | OMU  | C6-C5   | 2.26  | 1.40        | 1.35     |
| 1   | 2     | 1643 | PSU  | C6-C5   | 2.25  | 1.37        | 1.35     |
| 1   | 2     | 822  | PSU  | C6-C5   | 2.25  | 1.37        | 1.35     |
| 1   | 2     | 99   | A2M  | C5-N7   | -2.25 | 1.35        | 1.39     |
| 1   | 2     | 105  | PSU  | C6-C5   | 2.24  | 1.37        | 1.35     |
| 1   | 2     | 296  | PSU  | C6-N1   | -2.23 | 1.32        | 1.36     |
| 1   | 2     | 1490 | OMG  | C5-N7   | -2.22 | 1.34        | 1.39     |
| 1   | 2     | 174  | OMC  | C6-N1   | -2.22 | 1.32        | 1.38     |
| 1   | 2     | 1383 | A2M  | C5-N7   | -2.22 | 1.35        | 1.39     |
| 1   | 2     | 1136 | PSU  | C6-C5   | 2.22  | 1.37        | 1.35     |
| 1   | 2     | 512  | A2M  | C5-N7   | -2.22 | 1.35        | 1.39     |
| 1   | 2     | 121  | OMU  | C6-C5   | 2.22  | 1.40        | 1.35     |
| 1   | 2     | 1272 | OMC  | C6-N1   | -2.21 | 1.32        | 1.38     |
| 1   | 2     | 354  | OMU  | C6-C5   | 2.21  | 1.40        | 1.35     |
| 1   | 2     | 484  | A2M  | C5-N7   | -2.21 | 1.35        | 1.39     |
| 1   | 2     | 1046 | PSU  | C6-C5   | 2.20  | 1.37        | 1.35     |
| 1   | 2     | 1842 | 4AC  | CM7-C7  | 2.20  | 1.55        | 1.50     |
| 1   | 2     | 509  | OMG  | C2-N1   | -2.20 | 1.32        | 1.37     |
| 1   | 2     | 509  | OMG  | C5-N7   | -2.19 | 1.34        | 1.39     |
| 1   | 2     | 1326 | OMU  | C6-N1   | -2.19 | 1.32        | 1.38     |
| 1   | 2     | 1703 | OMC  | C6-N1   | -2.18 | 1.32        | 1.38     |
| 1   | 2     | 428  | OMU  | C6-N1   | -2.18 | 1.32        | 1.38     |
| 1   | 2     | 174  | OMC  | C2-N3   | -2.17 | 1.32        | 1.36     |
| 1   | 2     | 116  | OMU  | C6-C5   | 2.17  | 1.40        | 1.35     |
| 1   | 2     | 1288 | OMU  | C2-N1   | -2.17 | 1.35        | 1.38     |
| 1   | 2     | 1391 | OMC  | C2-N3   | -2.16 | 1.32        | 1.36     |
| 1   | 2     | 822  | PSU  | O4'-C1' | -2.15 | 1.40        | 1.43     |
| 1   | 2     | 462  | OMC  | C2-N3   | -2.15 | 1.32        | 1.36     |
| 1   | 2     | 116  | OMU  | C6-N1   | -2.14 | 1.33        | 1.38     |
| 1   | 2     | 1703 | OMC  | C2-N3   | -2.14 | 1.32        | 1.36     |
| 1   | 2     | 1842 | 4AC  | C2-N3   | -2.13 | 1.32        | 1.36     |
| 1   | 2     | 576  | A2M  | C5-N7   | -2.12 | 1.35        | 1.39     |
| 1   | 2     | 109  | PSU  | C6-C5   | 2.12  | 1.37        | 1.35     |
| 1   | 2     | 1056 | PSU  | C6-C5   | 2.12  | 1.37        | 1.35     |
| 1   | 2     | 814  | PSU  | C6-C5   | 2.11  | 1.37        | 1.35     |
| 1   | 2     | 119  | PSU  | C6-C5   | 2.11  | 1.37        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | 2     | 116  | OMU  | C5-C4   | -2.10 | 1.39        | 1.43     |
| 1   | 2     | 517  | OMC  | C6-N1   | -2.10 | 1.33        | 1.38     |
| 1   | 2     | 590  | A2M  | C5-N7   | -2.09 | 1.35        | 1.39     |
| 1   | 2     | 1031 | A2M  | C5-N7   | -2.09 | 1.35        | 1.39     |
| 1   | 2     | 1337 | 4AC  | C2-N3   | -2.08 | 1.32        | 1.36     |
| 1   | 2     | 436  | OMG  | C5-N7   | -2.08 | 1.34        | 1.39     |
| 1   | 2     | 121  | OMU  | C5-C4   | -2.07 | 1.39        | 1.43     |
| 1   | 2     | 681  | PSU  | C6-C5   | 2.06  | 1.37        | 1.35     |
| 1   | 2     | 601  | OMG  | C5-N7   | -2.05 | 1.35        | 1.39     |
| 1   | 2     | 1288 | OMU  | O2-C2   | -2.05 | 1.19        | 1.23     |
| 1   | 2     | 468  | A2M  | C5-N7   | -2.05 | 1.35        | 1.39     |
| 1   | 2     | 814  | PSU  | C6-N1   | -2.04 | 1.33        | 1.36     |
| 1   | 2     | 668  | A2M  | C5-N7   | -2.04 | 1.35        | 1.39     |
| 1   | 2     | 681  | PSU  | C6-N1   | -2.04 | 1.33        | 1.36     |
| 1   | 2     | 1442 | OMU  | C6-N1   | -2.04 | 1.33        | 1.38     |
| 1   | 2     | 1081 | PSU  | O4'-C1' | -2.03 | 1.41        | 1.43     |
| 1   | 2     | 166  | A2M  | C5-N7   | -2.03 | 1.35        | 1.39     |
| 1   | 2     | 159  | A2M  | C5-N7   | -2.02 | 1.35        | 1.39     |
| 1   | 2     | 354  | OMU  | C5-C4   | -2.02 | 1.39        | 1.43     |
| 1   | 2     | 644  | OMG  | C5-N7   | -2.00 | 1.35        | 1.39     |
| 1   | 2     | 1046 | PSU  | C6-N1   | -2.00 | 1.33        | 1.36     |
| 1   | 2     | 1248 | B8N  | C6-N1   | -2.00 | 1.32        | 1.36     |

All (418) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | 2     | 1842 | 4AC  | CM7-C7-N4 | 7.29  | 127.03      | 115.27   |
| 1   | 2     | 590  | A2M  | C5-C4-N3  | -6.63 | 117.59      | 126.72   |
| 1   | 2     | 1232 | PSU  | N1-C2-N3  | 6.44  | 121.96      | 115.17   |
| 1   | 2     | 105  | PSU  | N1-C2-N3  | 6.35  | 121.87      | 115.17   |
| 1   | 2     | 1337 | 4AC  | CM7-C7-N4 | 6.32  | 125.47      | 115.27   |
| 1   | 2     | 296  | PSU  | N1-C2-N3  | 6.31  | 121.83      | 115.17   |
| 1   | 2     | 815  | PSU  | N1-C2-N3  | 6.24  | 121.75      | 115.17   |
| 1   | 2     | 1850 | MA6  | C5-C4-N3  | -6.21 | 118.16      | 126.72   |
| 1   | 2     | 406  | PSU  | N1-C2-N3  | 6.20  | 121.71      | 115.17   |
| 1   | 2     | 651  | PSU  | N1-C2-N3  | 6.20  | 121.70      | 115.17   |
| 1   | 2     | 649  | PSU  | N1-C2-N3  | 6.19  | 121.69      | 115.17   |
| 1   | 2     | 109  | PSU  | N1-C2-N3  | 6.14  | 121.64      | 115.17   |
| 1   | 2     | 572  | PSU  | N1-C2-N3  | 6.10  | 121.60      | 115.17   |
| 1   | 2     | 1643 | PSU  | N1-C2-N3  | 6.09  | 121.59      | 115.17   |
| 1   | 2     | 1445 | PSU  | N1-C2-N3  | 6.07  | 121.58      | 115.17   |
| 1   | 2     | 1174 | PSU  | N1-C2-N3  | 6.06  | 121.56      | 115.17   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | 2     | 1347 | PSU  | N1-C2-N3 | 6.05  | 121.55      | 115.17   |
| 1   | 2     | 686  | PSU  | N1-C2-N3 | 6.04  | 121.54      | 115.17   |
| 1   | 2     | 166  | A2M  | C5-C4-N3 | -6.04 | 118.41      | 126.72   |
| 1   | 2     | 1238 | PSU  | N1-C2-N3 | 6.03  | 121.53      | 115.17   |
| 1   | 2     | 1692 | PSU  | N1-C2-N3 | 6.02  | 121.51      | 115.17   |
| 1   | 2     | 822  | PSU  | N1-C2-N3 | 5.99  | 121.49      | 115.17   |
| 1   | 2     | 484  | A2M  | C5-C4-N3 | -5.98 | 118.49      | 126.72   |
| 1   | 2     | 1244 | PSU  | N1-C2-N3 | 5.98  | 121.47      | 115.17   |
| 1   | 2     | 512  | A2M  | C5-C4-N3 | -5.97 | 118.49      | 126.72   |
| 1   | 2     | 1046 | PSU  | N1-C2-N3 | 5.97  | 121.47      | 115.17   |
| 1   | 2     | 863  | PSU  | N1-C2-N3 | 5.96  | 121.45      | 115.17   |
| 1   | 2     | 814  | PSU  | N1-C2-N3 | 5.93  | 121.42      | 115.17   |
| 1   | 2     | 1136 | PSU  | N1-C2-N3 | 5.93  | 121.42      | 115.17   |
| 1   | 2     | 93   | PSU  | N1-C2-N3 | 5.89  | 121.39      | 115.17   |
| 1   | 2     | 681  | PSU  | N1-C2-N3 | 5.87  | 121.36      | 115.17   |
| 1   | 2     | 1177 | PSU  | N1-C2-N3 | 5.86  | 121.35      | 115.17   |
| 1   | 2     | 1625 | PSU  | N1-C2-N3 | 5.86  | 121.35      | 115.17   |
| 1   | 2     | 1045 | PSU  | N1-C2-N3 | 5.84  | 121.33      | 115.17   |
| 1   | 2     | 1056 | PSU  | N1-C2-N3 | 5.84  | 121.33      | 115.17   |
| 1   | 2     | 36   | PSU  | N1-C2-N3 | 5.83  | 121.31      | 115.17   |
| 1   | 2     | 1383 | A2M  | C5-C4-N3 | -5.78 | 118.76      | 126.72   |
| 1   | 2     | 159  | A2M  | C5-C4-N3 | -5.78 | 118.77      | 126.72   |
| 1   | 2     | 99   | A2M  | C5-C4-N3 | -5.74 | 118.82      | 126.72   |
| 1   | 2     | 509  | OMG  | C5-C4-N3 | -5.73 | 119.27      | 128.39   |
| 1   | 2     | 27   | A2M  | C5-C4-N3 | -5.72 | 118.84      | 126.72   |
| 1   | 2     | 1081 | PSU  | N1-C2-N3 | 5.69  | 121.17      | 115.17   |
| 1   | 2     | 1851 | MA6  | C5-C4-N3 | -5.68 | 118.89      | 126.72   |
| 1   | 2     | 1678 | A2M  | C5-C4-N3 | -5.62 | 118.98      | 126.72   |
| 1   | 2     | 119  | PSU  | N1-C2-N3 | 5.57  | 121.04      | 115.17   |
| 1   | 2     | 576  | A2M  | C5-C4-N3 | -5.57 | 119.05      | 126.72   |
| 1   | 2     | 1490 | OMG  | C5-C4-N3 | -5.52 | 119.61      | 128.39   |
| 1   | 2     | 1442 | OMU  | N3-C2-N1 | 5.51  | 122.06      | 114.89   |
| 1   | 2     | 601  | OMG  | C5-C4-N3 | -5.50 | 119.64      | 128.39   |
| 1   | 2     | 1447 | OMG  | C5-C4-N3 | -5.49 | 119.65      | 128.39   |
| 1   | 2     | 468  | A2M  | C5-C4-N3 | -5.42 | 119.25      | 126.72   |
| 1   | 2     | 1328 | OMG  | C5-C4-N3 | -5.39 | 119.81      | 128.39   |
| 1   | 2     | 1031 | A2M  | C5-C4-N3 | -5.39 | 119.30      | 126.72   |
| 1   | 2     | 116  | OMU  | N3-C2-N1 | 5.35  | 121.85      | 114.89   |
| 1   | 2     | 172  | OMU  | N3-C2-N1 | 5.34  | 121.84      | 114.89   |
| 1   | 2     | 428  | OMU  | N3-C2-N1 | 5.32  | 121.81      | 114.89   |
| 1   | 2     | 590  | A2M  | N3-C4-N9 | 5.31  | 136.20      | 127.17   |
| 1   | 2     | 354  | OMU  | N3-C2-N1 | 5.31  | 121.81      | 114.89   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | 2     | 121  | OMU  | N3-C2-N1 | 5.31  | 121.80      | 114.89   |
| 1   | 2     | 436  | OMG  | C5-C4-N3 | -5.30 | 119.96      | 128.39   |
| 1   | 2     | 644  | OMG  | C5-C4-N3 | -5.29 | 119.98      | 128.39   |
| 1   | 2     | 1326 | OMU  | C4-N3-C2 | -5.22 | 120.13      | 126.61   |
| 1   | 2     | 1851 | MA6  | N1-C2-N3 | -5.22 | 120.67      | 128.58   |
| 1   | 2     | 683  | OMG  | C5-C4-N3 | -5.20 | 120.12      | 128.39   |
| 1   | 2     | 1326 | OMU  | N3-C2-N1 | 5.18  | 121.64      | 114.89   |
| 1   | 2     | 668  | A2M  | C5-C4-N3 | -5.12 | 119.67      | 126.72   |
| 1   | 2     | 1832 | 6MZ  | C5-C4-N3 | -5.06 | 119.75      | 126.72   |
| 1   | 2     | 428  | OMU  | C4-N3-C2 | -5.06 | 120.33      | 126.61   |
| 1   | 2     | 1850 | MA6  | N1-C2-N3 | -5.01 | 121.00      | 128.58   |
| 1   | 2     | 1832 | 6MZ  | N1-C2-N3 | -5.00 | 121.02      | 128.58   |
| 1   | 2     | 1639 | 7MG  | C2-N3-C4 | 4.98  | 120.88      | 112.30   |
| 1   | 2     | 1639 | 7MG  | N9-C4-N3 | 4.98  | 132.75      | 125.46   |
| 1   | 2     | 172  | OMU  | C4-N3-C2 | -4.88 | 120.55      | 126.61   |
| 1   | 2     | 1288 | OMU  | N3-C2-N1 | 4.87  | 121.23      | 114.89   |
| 1   | 2     | 1639 | 7MG  | C5-C4-N3 | -4.85 | 119.02      | 128.13   |
| 1   | 2     | 1851 | MA6  | C4-C5-N7 | -4.84 | 105.05      | 110.58   |
| 1   | 2     | 512  | A2M  | N3-C4-N9 | 4.82  | 135.37      | 127.17   |
| 1   | 2     | 1832 | 6MZ  | C6-C5-N7 | 4.76  | 137.62      | 132.43   |
| 1   | 2     | 1328 | OMG  | C2-N3-C4 | 4.76  | 120.49      | 112.30   |
| 1   | 2     | 1447 | OMG  | C2-N3-C4 | 4.74  | 120.46      | 112.30   |
| 1   | 2     | 1232 | PSU  | C4-N3-C2 | -4.73 | 119.85      | 126.37   |
| 1   | 2     | 601  | OMG  | C2-N3-C4 | 4.73  | 120.45      | 112.30   |
| 1   | 2     | 1442 | OMU  | C4-N3-C2 | -4.73 | 120.74      | 126.61   |
| 1   | 2     | 1832 | 6MZ  | C4-C5-N7 | -4.72 | 105.19      | 110.58   |
| 1   | 2     | 512  | A2M  | N3-C2-N1 | -4.70 | 121.46      | 128.58   |
| 1   | 2     | 166  | A2M  | N3-C4-N9 | 4.69  | 135.15      | 127.17   |
| 1   | 2     | 1136 | PSU  | C4-N3-C2 | -4.69 | 119.91      | 126.37   |
| 1   | 2     | 436  | OMG  | C2-N3-C4 | 4.69  | 120.37      | 112.30   |
| 1   | 2     | 683  | OMG  | C2-N3-C4 | 4.68  | 120.37      | 112.30   |
| 1   | 2     | 644  | OMG  | C2-N3-C4 | 4.66  | 120.33      | 112.30   |
| 1   | 2     | 99   | A2M  | N3-C4-N9 | 4.64  | 135.06      | 127.17   |
| 1   | 2     | 1490 | OMG  | C2-N3-C4 | 4.62  | 120.26      | 112.30   |
| 1   | 2     | 109  | PSU  | C4-N3-C2 | -4.59 | 120.05      | 126.37   |
| 1   | 2     | 509  | OMG  | C2-N3-C4 | 4.56  | 120.16      | 112.30   |
| 1   | 2     | 1832 | 6MZ  | C9-N6-C6 | 4.56  | 127.08      | 122.85   |
| 1   | 2     | 572  | PSU  | C4-N3-C2 | -4.54 | 120.11      | 126.37   |
| 1   | 2     | 1445 | PSU  | C4-N3-C2 | -4.54 | 120.12      | 126.37   |
| 1   | 2     | 822  | PSU  | C4-N3-C2 | -4.53 | 120.13      | 126.37   |
| 1   | 2     | 1177 | PSU  | C4-N3-C2 | -4.51 | 120.16      | 126.37   |
| 1   | 2     | 815  | PSU  | C4-N3-C2 | -4.50 | 120.17      | 126.37   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | 2     | 1244 | PSU  | C4-N3-C2  | -4.50 | 120.17      | 126.37   |
| 1   | 2     | 1383 | A2M  | N3-C4-N9  | 4.49  | 134.80      | 127.17   |
| 1   | 2     | 105  | PSU  | C4-N3-C2  | -4.47 | 120.21      | 126.37   |
| 1   | 2     | 651  | PSU  | C4-N3-C2  | -4.44 | 120.25      | 126.37   |
| 1   | 2     | 686  | PSU  | C4-N3-C2  | -4.44 | 120.25      | 126.37   |
| 1   | 2     | 649  | PSU  | C4-N3-C2  | -4.43 | 120.26      | 126.37   |
| 1   | 2     | 1850 | MA6  | C4-C5-N7  | -4.43 | 105.52      | 110.58   |
| 1   | 2     | 484  | A2M  | N3-C4-N9  | 4.41  | 134.67      | 127.17   |
| 1   | 2     | 1643 | PSU  | C4-N3-C2  | -4.40 | 120.31      | 126.37   |
| 1   | 2     | 296  | PSU  | C4-N3-C2  | -4.40 | 120.32      | 126.37   |
| 1   | 2     | 863  | PSU  | C4-N3-C2  | -4.39 | 120.32      | 126.37   |
| 1   | 2     | 1045 | PSU  | C4-N3-C2  | -4.39 | 120.33      | 126.37   |
| 1   | 2     | 1174 | PSU  | C4-N3-C2  | -4.38 | 120.33      | 126.37   |
| 1   | 2     | 119  | PSU  | C4-N3-C2  | -4.35 | 120.38      | 126.37   |
| 1   | 2     | 27   | A2M  | N3-C2-N1  | -4.34 | 122.00      | 128.58   |
| 1   | 2     | 1347 | PSU  | C4-N3-C2  | -4.34 | 120.39      | 126.37   |
| 1   | 2     | 576  | A2M  | N3-C4-N9  | 4.34  | 134.55      | 127.17   |
| 1   | 2     | 1678 | A2M  | N3-C4-N9  | 4.33  | 134.53      | 127.17   |
| 1   | 2     | 166  | A2M  | N3-C2-N1  | -4.33 | 122.03      | 128.58   |
| 1   | 2     | 1851 | MA6  | C2-N3-C4  | 4.31  | 122.35      | 111.83   |
| 1   | 2     | 296  | PSU  | O2-C2-N1  | -4.30 | 118.35      | 122.79   |
| 1   | 2     | 27   | A2M  | N3-C4-N9  | 4.30  | 134.48      | 127.17   |
| 1   | 2     | 468  | A2M  | N3-C2-N1  | -4.28 | 122.10      | 128.58   |
| 1   | 2     | 1031 | A2M  | N3-C2-N1  | -4.27 | 122.12      | 128.58   |
| 1   | 2     | 1046 | PSU  | C4-N3-C2  | -4.27 | 120.49      | 126.37   |
| 1   | 2     | 93   | PSU  | C4-N3-C2  | -4.26 | 120.50      | 126.37   |
| 1   | 2     | 590  | A2M  | N3-C2-N1  | -4.26 | 122.14      | 128.58   |
| 1   | 2     | 1383 | A2M  | N3-C2-N1  | -4.25 | 122.16      | 128.58   |
| 1   | 2     | 668  | A2M  | N3-C2-N1  | -4.24 | 122.17      | 128.58   |
| 1   | 2     | 814  | PSU  | C4-N3-C2  | -4.24 | 120.54      | 126.37   |
| 1   | 2     | 1639 | 7MG  | C5-C6-N1  | 4.22  | 118.37      | 110.94   |
| 1   | 2     | 1692 | PSU  | C4-N3-C2  | -4.22 | 120.56      | 126.37   |
| 1   | 2     | 159  | A2M  | N3-C4-N9  | 4.22  | 134.34      | 127.17   |
| 1   | 2     | 1031 | A2M  | N3-C4-N9  | 4.21  | 134.33      | 127.17   |
| 1   | 2     | 1288 | OMU  | C1'-N1-C2 | 4.21  | 125.15      | 117.59   |
| 1   | 2     | 1850 | MA6  | C2-N3-C4  | 4.20  | 122.10      | 111.83   |
| 1   | 2     | 1678 | A2M  | N3-C2-N1  | -4.20 | 122.23      | 128.58   |
| 1   | 2     | 681  | PSU  | C4-N3-C2  | -4.18 | 120.61      | 126.37   |
| 1   | 2     | 1056 | PSU  | C4-N3-C2  | -4.17 | 120.63      | 126.37   |
| 1   | 2     | 1238 | PSU  | C4-N3-C2  | -4.16 | 120.64      | 126.37   |
| 1   | 2     | 99   | A2M  | N3-C2-N1  | -4.15 | 122.30      | 128.58   |
| 1   | 2     | 468  | A2M  | N3-C4-N9  | 4.15  | 134.22      | 127.17   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | 2     | 1248 | B8N  | C4-N3-C2 | -4.15 | 120.52      | 125.62   |
| 1   | 2     | 354  | OMU  | C4-N3-C2 | -4.13 | 121.49      | 126.61   |
| 1   | 2     | 1832 | 6MZ  | C5-N7-C8 | 4.12  | 109.92      | 103.45   |
| 1   | 2     | 406  | PSU  | C4-N3-C2 | -4.11 | 120.70      | 126.37   |
| 1   | 2     | 1850 | MA6  | N3-C4-N9 | 4.07  | 134.08      | 127.17   |
| 1   | 2     | 1625 | PSU  | C4-N3-C2 | -4.06 | 120.77      | 126.37   |
| 1   | 2     | 1081 | PSU  | C4-N3-C2 | -4.06 | 120.78      | 126.37   |
| 1   | 2     | 484  | A2M  | N3-C2-N1 | -4.04 | 122.47      | 128.58   |
| 1   | 2     | 1851 | MA6  | C2-N1-C6 | 4.00  | 121.60      | 111.83   |
| 1   | 2     | 1850 | MA6  | C2-N1-C6 | 3.99  | 121.57      | 111.83   |
| 1   | 2     | 116  | OMU  | C4-N3-C2 | -3.94 | 121.72      | 126.61   |
| 1   | 2     | 1851 | MA6  | C5-N7-C8 | 3.94  | 109.64      | 103.45   |
| 1   | 2     | 576  | A2M  | N3-C2-N1 | -3.93 | 122.63      | 128.58   |
| 1   | 2     | 517  | OMC  | O2-C2-N3 | -3.93 | 116.13      | 122.33   |
| 1   | 2     | 36   | PSU  | C4-N3-C2 | -3.93 | 120.96      | 126.37   |
| 1   | 2     | 159  | A2M  | N3-C2-N1 | -3.88 | 122.71      | 128.58   |
| 1   | 2     | 1850 | MA6  | C5-N7-C8 | 3.86  | 109.51      | 103.45   |
| 1   | 2     | 590  | A2M  | C2-N3-C4 | 3.86  | 121.25      | 111.83   |
| 1   | 2     | 1832 | 6MZ  | C2-N3-C4 | 3.82  | 121.16      | 111.83   |
| 1   | 2     | 1851 | MA6  | N9-C8-N7 | -3.82 | 108.52      | 113.94   |
| 1   | 2     | 668  | A2M  | N3-C4-N9 | 3.82  | 133.66      | 127.17   |
| 1   | 2     | 1248 | B8N  | N3-C2-N1 | 3.80  | 121.36      | 116.72   |
| 1   | 2     | 1046 | PSU  | O2-C2-N1 | -3.79 | 118.88      | 122.79   |
| 1   | 2     | 1174 | PSU  | O2-C2-N1 | -3.77 | 118.90      | 122.79   |
| 1   | 2     | 109  | PSU  | O2-C2-N1 | -3.71 | 118.96      | 122.79   |
| 1   | 2     | 121  | OMU  | C4-N3-C2 | -3.71 | 122.00      | 126.61   |
| 1   | 2     | 1678 | A2M  | N9-C8-N7 | -3.63 | 108.79      | 113.94   |
| 1   | 2     | 166  | A2M  | C2-N3-C4 | 3.62  | 120.66      | 111.83   |
| 1   | 2     | 512  | A2M  | C2-N3-C4 | 3.60  | 120.63      | 111.83   |
| 1   | 2     | 1703 | OMC  | O2-C2-N3 | -3.59 | 116.66      | 122.33   |
| 1   | 2     | 815  | PSU  | O2-C2-N1 | -3.57 | 119.10      | 122.79   |
| 1   | 2     | 1447 | OMG  | N9-C4-N3 | 3.57  | 133.09      | 125.95   |
| 1   | 2     | 509  | OMG  | N9-C4-N3 | 3.55  | 133.05      | 125.95   |
| 1   | 2     | 1643 | PSU  | O2-C2-N1 | -3.54 | 119.13      | 122.79   |
| 1   | 2     | 27   | A2M  | C2-N3-C4 | 3.53  | 120.45      | 111.83   |
| 1   | 2     | 1326 | OMU  | C5-C4-N3 | 3.51  | 119.72      | 114.80   |
| 1   | 2     | 484  | A2M  | C2-N3-C4 | 3.51  | 120.40      | 111.83   |
| 1   | 2     | 1832 | 6MZ  | N9-C8-N7 | -3.51 | 108.96      | 113.94   |
| 1   | 2     | 105  | PSU  | O2-C2-N1 | -3.48 | 119.20      | 122.79   |
| 1   | 2     | 668  | A2M  | N9-C8-N7 | -3.46 | 109.03      | 113.94   |
| 1   | 2     | 1288 | OMU  | C4-N3-C2 | -3.46 | 122.32      | 126.61   |
| 1   | 2     | 601  | OMG  | N9-C4-N3 | 3.46  | 132.87      | 125.95   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | 2     | 649  | PSU  | O2-C2-N1  | -3.46 | 119.22      | 122.79   |
| 1   | 2     | 1383 | A2M  | C2-N3-C4  | 3.44  | 120.23      | 111.83   |
| 1   | 2     | 1850 | MA6  | N9-C8-N7  | -3.44 | 109.06      | 113.94   |
| 1   | 2     | 1238 | PSU  | O2-C2-N1  | -3.44 | 119.25      | 122.79   |
| 1   | 2     | 1445 | PSU  | O2-C2-N1  | -3.43 | 119.25      | 122.79   |
| 1   | 2     | 1678 | A2M  | C2-N3-C4  | 3.43  | 120.21      | 111.83   |
| 1   | 2     | 1490 | OMG  | N9-C4-N3  | 3.42  | 132.79      | 125.95   |
| 1   | 2     | 1678 | A2M  | C5-N7-C8  | 3.41  | 108.82      | 103.45   |
| 1   | 2     | 462  | OMC  | O2-C2-N3  | -3.41 | 116.96      | 122.33   |
| 1   | 2     | 1842 | 4AC  | O7-C7-CM7 | -3.40 | 116.00      | 122.05   |
| 1   | 2     | 428  | OMU  | C5-C4-N3  | 3.39  | 119.55      | 114.80   |
| 1   | 2     | 436  | OMG  | N9-C4-N3  | 3.39  | 132.74      | 125.95   |
| 1   | 2     | 686  | PSU  | O2-C2-N1  | -3.39 | 119.30      | 122.79   |
| 1   | 2     | 159  | A2M  | C2-N3-C4  | 3.39  | 120.10      | 111.83   |
| 1   | 2     | 1391 | OMC  | O2-C2-N3  | -3.38 | 117.00      | 122.33   |
| 1   | 2     | 822  | PSU  | O2-C2-N1  | -3.38 | 119.30      | 122.79   |
| 1   | 2     | 572  | PSU  | O2-C2-N1  | -3.37 | 119.31      | 122.79   |
| 1   | 2     | 99   | A2M  | C2-N3-C4  | 3.37  | 120.05      | 111.83   |
| 1   | 2     | 1625 | PSU  | O2-C2-N1  | -3.36 | 119.33      | 122.79   |
| 1   | 2     | 1045 | PSU  | O2-C2-N1  | -3.35 | 119.33      | 122.79   |
| 1   | 2     | 683  | OMG  | N9-C4-N3  | 3.34  | 132.63      | 125.95   |
| 1   | 2     | 1337 | 4AC  | O7-C7-N4  | -3.34 | 116.64      | 121.90   |
| 1   | 2     | 814  | PSU  | O2-C2-N1  | -3.34 | 119.34      | 122.79   |
| 1   | 2     | 1244 | PSU  | O2-C2-N1  | -3.34 | 119.35      | 122.79   |
| 1   | 2     | 406  | PSU  | O2-C2-N1  | -3.32 | 119.36      | 122.79   |
| 1   | 2     | 1136 | PSU  | O2-C2-N1  | -3.32 | 119.36      | 122.79   |
| 1   | 2     | 651  | PSU  | O2-C2-N1  | -3.32 | 119.36      | 122.79   |
| 1   | 2     | 1056 | PSU  | O2-C2-N1  | -3.32 | 119.36      | 122.79   |
| 1   | 2     | 174  | OMC  | O2-C2-N3  | -3.32 | 117.10      | 122.33   |
| 1   | 2     | 1288 | OMU  | O2-C2-N3  | -3.31 | 115.39      | 121.49   |
| 1   | 2     | 468  | A2M  | C2-N3-C4  | 3.31  | 119.91      | 111.83   |
| 1   | 2     | 863  | PSU  | O2-C2-N1  | -3.29 | 119.39      | 122.79   |
| 1   | 2     | 1851 | MA6  | N3-C4-N9  | 3.29  | 132.76      | 127.17   |
| 1   | 2     | 159  | A2M  | C5-N7-C8  | 3.29  | 108.61      | 103.45   |
| 1   | 2     | 1177 | PSU  | O2-C2-N1  | -3.28 | 119.40      | 122.79   |
| 1   | 2     | 159  | A2M  | C4-C5-N7  | -3.28 | 106.83      | 110.58   |
| 1   | 2     | 1031 | A2M  | C2-N3-C4  | 3.27  | 119.82      | 111.83   |
| 1   | 2     | 1232 | PSU  | O2-C2-N1  | -3.27 | 119.42      | 122.79   |
| 1   | 2     | 576  | A2M  | C2-N3-C4  | 3.27  | 119.81      | 111.83   |
| 1   | 2     | 1347 | PSU  | O2-C2-N1  | -3.26 | 119.42      | 122.79   |
| 1   | 2     | 166  | A2M  | C5-N7-C8  | 3.26  | 108.57      | 103.45   |
| 1   | 2     | 468  | A2M  | N9-C8-N7  | -3.26 | 109.31      | 113.94   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | 2     | 644  | OMG  | N9-C4-N3    | 3.25  | 132.46      | 125.95   |
| 1   | 2     | 27   | A2M  | N9-C8-N7    | -3.25 | 109.32      | 113.94   |
| 1   | 2     | 1442 | OMU  | C5-C4-N3    | 3.25  | 119.35      | 114.80   |
| 1   | 2     | 354  | OMU  | C5-C4-N3    | 3.23  | 119.33      | 114.80   |
| 1   | 2     | 668  | A2M  | C2-N3-C4    | 3.22  | 119.70      | 111.83   |
| 1   | 2     | 1031 | A2M  | N9-C8-N7    | -3.22 | 109.37      | 113.94   |
| 1   | 2     | 99   | A2M  | N9-C8-N7    | -3.22 | 109.37      | 113.94   |
| 1   | 2     | 1678 | A2M  | C4-C5-N7    | -3.22 | 106.90      | 110.58   |
| 1   | 2     | 1328 | OMG  | N9-C4-N3    | 3.22  | 132.38      | 125.95   |
| 1   | 2     | 1272 | OMC  | O2-C2-N3    | -3.21 | 117.26      | 122.33   |
| 1   | 2     | 166  | A2M  | N9-C8-N7    | -3.20 | 109.40      | 113.94   |
| 1   | 2     | 576  | A2M  | N9-C8-N7    | -3.19 | 109.41      | 113.94   |
| 1   | 2     | 590  | A2M  | C5-N7-C8    | 3.19  | 108.46      | 103.45   |
| 1   | 2     | 668  | A2M  | C5-N7-C8    | 3.18  | 108.44      | 103.45   |
| 1   | 2     | 27   | A2M  | C5-N7-C8    | 3.17  | 108.43      | 103.45   |
| 1   | 2     | 683  | OMG  | C6-C5-N7    | 3.17  | 136.05      | 130.29   |
| 1   | 2     | 1692 | PSU  | O2-C2-N1    | -3.17 | 119.52      | 122.79   |
| 1   | 2     | 159  | A2M  | N9-C8-N7    | -3.16 | 109.45      | 113.94   |
| 1   | 2     | 644  | OMG  | C6-C5-N7    | 3.16  | 136.05      | 130.29   |
| 1   | 2     | 484  | A2M  | C5-N7-C8    | 3.16  | 108.41      | 103.45   |
| 1   | 2     | 1832 | 6MZ  | N3-C4-N9    | 3.16  | 132.53      | 127.17   |
| 1   | 2     | 681  | PSU  | O2-C2-N1    | -3.15 | 119.54      | 122.79   |
| 1   | 2     | 1842 | 4AC  | O2-C2-N3    | -3.14 | 117.37      | 122.33   |
| 1   | 2     | 1326 | OMU  | O4-C4-C5    | -3.14 | 119.74      | 125.16   |
| 1   | 2     | 172  | OMU  | C5-C4-N3    | 3.14  | 119.20      | 114.80   |
| 1   | 2     | 484  | A2M  | C4-C5-N7    | -3.14 | 106.99      | 110.58   |
| 1   | 2     | 1328 | OMG  | C6-C5-N7    | 3.13  | 135.99      | 130.29   |
| 1   | 2     | 1842 | 4AC  | O7-C7-N4    | -3.13 | 116.97      | 121.90   |
| 1   | 2     | 1081 | PSU  | O2-C2-N1    | -3.13 | 119.56      | 122.79   |
| 1   | 2     | 436  | OMG  | C6-C5-N7    | 3.13  | 135.98      | 130.29   |
| 1   | 2     | 668  | A2M  | C4-C5-N7    | -3.12 | 107.02      | 110.58   |
| 1   | 2     | 1678 | A2M  | C4-N9-C8    | 3.10  | 108.99      | 105.74   |
| 1   | 2     | 93   | PSU  | O2-C2-N1    | -3.09 | 119.60      | 122.79   |
| 1   | 2     | 468  | A2M  | C5-N7-C8    | 3.08  | 108.30      | 103.45   |
| 1   | 2     | 27   | A2M  | C4-C5-N7    | -3.08 | 107.07      | 110.58   |
| 1   | 2     | 576  | A2M  | C5-N7-C8    | 3.05  | 108.25      | 103.45   |
| 1   | 2     | 99   | A2M  | C5-N7-C8    | 3.05  | 108.25      | 103.45   |
| 1   | 2     | 1328 | OMG  | C4-C5-N7    | -3.04 | 105.85      | 110.67   |
| 1   | 2     | 601  | OMG  | C6-C5-N7    | 3.04  | 135.82      | 130.29   |
| 1   | 2     | 590  | A2M  | C4'-O4'-C1' | -3.02 | 102.80      | 109.47   |
| 1   | 2     | 166  | A2M  | C4-C5-N7    | -3.02 | 107.13      | 110.58   |
| 1   | 2     | 1383 | A2M  | N9-C8-N7    | -3.01 | 109.67      | 113.94   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | 2     | 1383 | A2M  | C5-N7-C8 | 3.00  | 108.17      | 103.45   |
| 1   | 2     | 1031 | A2M  | C5-N7-C8 | 3.00  | 108.16      | 103.45   |
| 1   | 2     | 119  | PSU  | C6-C5-C4 | -2.99 | 116.16      | 118.17   |
| 1   | 2     | 119  | PSU  | O2-C2-N1 | -2.98 | 119.72      | 122.79   |
| 1   | 2     | 428  | OMU  | O4-C4-C5 | -2.97 | 120.04      | 125.16   |
| 1   | 2     | 509  | OMG  | C4-C5-N7 | -2.96 | 105.98      | 110.67   |
| 1   | 2     | 644  | OMG  | C4-C5-N7 | -2.96 | 105.98      | 110.67   |
| 1   | 2     | 668  | A2M  | C4-N9-C8 | 2.95  | 108.84      | 105.74   |
| 1   | 2     | 601  | OMG  | C4-C5-N7 | -2.95 | 106.00      | 110.67   |
| 1   | 2     | 509  | OMG  | C6-C5-N7 | 2.93  | 135.62      | 130.29   |
| 1   | 2     | 436  | OMG  | C4-C5-N7 | -2.93 | 106.03      | 110.67   |
| 1   | 2     | 1490 | OMG  | C4-C5-N7 | -2.93 | 106.03      | 110.67   |
| 1   | 2     | 1447 | OMG  | C6-C5-N7 | 2.92  | 135.60      | 130.29   |
| 1   | 2     | 116  | OMU  | O4-C4-C5 | -2.91 | 120.14      | 125.16   |
| 1   | 2     | 683  | OMG  | C4-C5-N7 | -2.90 | 106.07      | 110.67   |
| 1   | 2     | 590  | A2M  | N9-C8-N7 | -2.90 | 109.82      | 113.94   |
| 1   | 2     | 1490 | OMG  | C6-C5-N7 | 2.89  | 135.56      | 130.29   |
| 1   | 2     | 484  | A2M  | N9-C8-N7 | -2.89 | 109.83      | 113.94   |
| 1   | 2     | 512  | A2M  | C5-N7-C8 | 2.89  | 107.99      | 103.45   |
| 1   | 2     | 1337 | 4AC  | O2-C2-N3 | -2.88 | 117.78      | 122.33   |
| 1   | 2     | 468  | A2M  | C4-C5-N7 | -2.88 | 107.29      | 110.58   |
| 1   | 2     | 1639 | 7MG  | C4-C5-N7 | 2.88  | 108.78      | 105.38   |
| 1   | 2     | 121  | OMU  | C5-C4-N3 | 2.88  | 118.83      | 114.80   |
| 1   | 2     | 36   | PSU  | O2-C2-N1 | -2.87 | 119.83      | 122.79   |
| 1   | 2     | 590  | A2M  | C4-C5-N7 | -2.86 | 107.31      | 110.58   |
| 1   | 2     | 576  | A2M  | C4-C5-N7 | -2.86 | 107.31      | 110.58   |
| 1   | 2     | 1447 | OMG  | C4-C5-N7 | -2.85 | 106.15      | 110.67   |
| 1   | 2     | 512  | A2M  | N9-C8-N7 | -2.83 | 109.92      | 113.94   |
| 1   | 2     | 1081 | PSU  | C6-C5-C4 | -2.83 | 116.26      | 118.17   |
| 1   | 2     | 172  | OMU  | O4-C4-C5 | -2.83 | 120.28      | 125.16   |
| 1   | 2     | 116  | OMU  | C5-C4-N3 | 2.82  | 118.75      | 114.80   |
| 1   | 2     | 436  | OMG  | C8-N7-C5 | 2.82  | 109.28      | 104.26   |
| 1   | 2     | 683  | OMG  | C8-N7-C5 | 2.81  | 109.27      | 104.26   |
| 1   | 2     | 1328 | OMG  | C8-N7-C5 | 2.76  | 109.18      | 104.26   |
| 1   | 2     | 99   | A2M  | C4-N9-C8 | 2.76  | 108.63      | 105.74   |
| 1   | 2     | 644  | OMG  | C8-N7-C5 | 2.76  | 109.17      | 104.26   |
| 1   | 2     | 1326 | OMU  | O2-C2-N1 | -2.75 | 119.21      | 122.80   |
| 1   | 2     | 576  | A2M  | C4-N9-C8 | 2.75  | 108.63      | 105.74   |
| 1   | 2     | 601  | OMG  | C8-N7-C5 | 2.75  | 109.16      | 104.26   |
| 1   | 2     | 1850 | MA6  | C4-C5-C6 | 2.75  | 118.75      | 115.91   |
| 1   | 2     | 1383 | A2M  | C4-C5-N7 | -2.74 | 107.44      | 110.58   |
| 1   | 2     | 1031 | A2M  | C4-N9-C8 | 2.72  | 108.60      | 105.74   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | 2     | 683  | OMG  | N9-C8-N7    | -2.71 | 108.38      | 113.40   |
| 1   | 2     | 1031 | A2M  | C4-C5-N7    | -2.70 | 107.50      | 110.58   |
| 1   | 2     | 468  | A2M  | C4-N9-C8    | 2.70  | 108.57      | 105.74   |
| 1   | 2     | 436  | OMG  | N9-C8-N7    | -2.69 | 108.41      | 113.40   |
| 1   | 2     | 121  | OMU  | O4-C4-C5    | -2.68 | 120.53      | 125.16   |
| 1   | 2     | 1490 | OMG  | C8-N7-C5    | 2.67  | 109.02      | 104.26   |
| 1   | 2     | 1447 | OMG  | C8-N7-C5    | 2.67  | 109.02      | 104.26   |
| 1   | 2     | 1442 | OMU  | O4-C4-C5    | -2.66 | 120.58      | 125.16   |
| 1   | 2     | 1136 | PSU  | C5-C6-N1    | -2.64 | 118.48      | 122.14   |
| 1   | 2     | 509  | OMG  | C8-N7-C5    | 2.64  | 108.95      | 104.26   |
| 1   | 2     | 27   | A2M  | C4-N9-C8    | 2.63  | 108.50      | 105.74   |
| 1   | 2     | 1288 | OMU  | C5-C4-N3    | 2.61  | 118.46      | 114.80   |
| 1   | 2     | 644  | OMG  | N9-C8-N7    | -2.61 | 108.56      | 113.40   |
| 1   | 2     | 1842 | 4AC  | C5-C4-N3    | -2.60 | 118.53      | 122.60   |
| 1   | 2     | 166  | A2M  | C4-N9-C8    | 2.59  | 108.45      | 105.74   |
| 1   | 2     | 99   | A2M  | C4-C5-N7    | -2.58 | 107.63      | 110.58   |
| 1   | 2     | 1851 | MA6  | C4-N9-C8    | 2.58  | 108.44      | 105.74   |
| 1   | 2     | 354  | OMU  | O4-C4-C5    | -2.57 | 120.73      | 125.16   |
| 1   | 2     | 590  | A2M  | O4'-C4'-C3' | -2.57 | 100.06      | 105.15   |
| 1   | 2     | 27   | A2M  | C2'-C1'-N9  | -2.56 | 109.54      | 113.75   |
| 1   | 2     | 1288 | OMU  | O4-C4-C5    | -2.55 | 120.77      | 125.16   |
| 1   | 2     | 1232 | PSU  | C5-C6-N1    | -2.54 | 118.61      | 122.14   |
| 1   | 2     | 354  | OMU  | O2-C2-N3    | -2.53 | 116.83      | 121.49   |
| 1   | 2     | 1445 | PSU  | C5-C6-N1    | -2.53 | 118.63      | 122.14   |
| 1   | 2     | 1639 | 7MG  | O6-C6-C5    | -2.53 | 121.42      | 127.62   |
| 1   | 2     | 109  | PSU  | C5-C6-N1    | -2.52 | 118.64      | 122.14   |
| 1   | 2     | 1842 | 4AC  | C4-N3-C2    | 2.52  | 123.44      | 120.11   |
| 1   | 2     | 651  | PSU  | C5-C6-N1    | -2.50 | 118.67      | 122.14   |
| 1   | 2     | 1244 | PSU  | C5-C6-N1    | -2.49 | 118.68      | 122.14   |
| 1   | 2     | 1643 | PSU  | C5-C6-N1    | -2.48 | 118.70      | 122.14   |
| 1   | 2     | 428  | OMU  | O2-C2-N1    | -2.48 | 119.57      | 122.80   |
| 1   | 2     | 512  | A2M  | C4-C5-N7    | -2.46 | 107.77      | 110.58   |
| 1   | 2     | 572  | PSU  | C5-C6-N1    | -2.45 | 118.74      | 122.14   |
| 1   | 2     | 1337 | 4AC  | C5-C4-N3    | -2.44 | 118.78      | 122.60   |
| 1   | 2     | 601  | OMG  | N9-C8-N7    | -2.44 | 108.88      | 113.40   |
| 1   | 2     | 1328 | OMG  | N9-C8-N7    | -2.43 | 108.89      | 113.40   |
| 1   | 2     | 1383 | A2M  | C4-N9-C8    | 2.42  | 108.28      | 105.74   |
| 1   | 2     | 1347 | PSU  | C5-C6-N1    | -2.42 | 118.79      | 122.14   |
| 1   | 2     | 686  | PSU  | C5-C6-N1    | -2.41 | 118.79      | 122.14   |
| 1   | 2     | 1248 | B8N  | C1'-C5-C4   | 2.41  | 121.26      | 117.61   |
| 1   | 2     | 172  | OMU  | O2-C2-N1    | -2.40 | 119.68      | 122.80   |
| 1   | 2     | 1692 | PSU  | C5-C6-N1    | -2.39 | 118.82      | 122.14   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | 2     | 1447 | OMG  | N9-C8-N7    | -2.39 | 108.97      | 113.40   |
| 1   | 2     | 1851 | MA6  | C6-C5-N7    | 2.38  | 137.23      | 133.43   |
| 1   | 2     | 822  | PSU  | C5-C6-N1    | -2.38 | 118.84      | 122.14   |
| 1   | 2     | 1832 | 6MZ  | C4-N9-C8    | 2.36  | 108.21      | 105.74   |
| 1   | 2     | 815  | PSU  | C5-C6-N1    | -2.36 | 118.87      | 122.14   |
| 1   | 2     | 590  | A2M  | C4-N9-C8    | 2.36  | 108.21      | 105.74   |
| 1   | 2     | 159  | A2M  | C4-N9-C8    | 2.35  | 108.21      | 105.74   |
| 1   | 2     | 1288 | OMU  | C1'-N1-C6   | -2.35 | 115.75      | 120.78   |
| 1   | 2     | 1326 | OMU  | C5-C6-N1    | -2.35 | 118.03      | 121.84   |
| 1   | 2     | 1442 | OMU  | O2-C2-N3    | -2.34 | 117.17      | 121.49   |
| 1   | 2     | 1337 | 4AC  | O7-C7-CM7   | -2.34 | 117.89      | 122.05   |
| 1   | 2     | 512  | A2M  | C4-N9-C8    | 2.33  | 108.18      | 105.74   |
| 1   | 2     | 1851 | MA6  | C5-C4-N9    | 2.33  | 108.34      | 105.81   |
| 1   | 2     | 105  | PSU  | C5-C6-N1    | -2.32 | 118.92      | 122.14   |
| 1   | 2     | 668  | A2M  | C3'-C2'-C1' | 2.31  | 107.22      | 102.81   |
| 1   | 2     | 1045 | PSU  | C5-C6-N1    | -2.30 | 118.94      | 122.14   |
| 1   | 2     | 822  | PSU  | O4'-C1'-C2' | 2.30  | 108.33      | 105.15   |
| 1   | 2     | 1850 | MA6  | C4-N9-C8    | 2.30  | 108.15      | 105.74   |
| 1   | 2     | 27   | A2M  | O4'-C1'-N9  | 2.29  | 112.48      | 108.09   |
| 1   | 2     | 1490 | OMG  | N9-C8-N7    | -2.28 | 109.18      | 113.40   |
| 1   | 2     | 1177 | PSU  | C5-C6-N1    | -2.26 | 119.00      | 122.14   |
| 1   | 2     | 1447 | OMG  | O6-C6-C5    | -2.25 | 120.58      | 126.53   |
| 1   | 2     | 512  | A2M  | C2'-C1'-N9  | -2.25 | 110.05      | 113.75   |
| 1   | 2     | 576  | A2M  | C2'-C1'-N9  | -2.25 | 110.05      | 113.75   |
| 1   | 2     | 649  | PSU  | C5-C6-N1    | -2.24 | 119.03      | 122.14   |
| 1   | 2     | 1328 | OMG  | O6-C6-C5    | -2.23 | 120.65      | 126.53   |
| 1   | 2     | 1490 | OMG  | O6-C6-C5    | -2.23 | 120.66      | 126.53   |
| 1   | 2     | 406  | PSU  | C5-C6-N1    | -2.23 | 119.05      | 122.14   |
| 1   | 2     | 428  | OMU  | C5-C6-N1    | -2.21 | 118.24      | 121.84   |
| 1   | 2     | 1238 | PSU  | C5-C6-N1    | -2.21 | 119.07      | 122.14   |
| 1   | 2     | 36   | PSU  | C5-C6-N1    | -2.20 | 119.09      | 122.14   |
| 1   | 2     | 1174 | PSU  | C5-C6-N1    | -2.20 | 119.09      | 122.14   |
| 1   | 2     | 436  | OMG  | O6-C6-C5    | -2.19 | 120.74      | 126.53   |
| 1   | 2     | 1056 | PSU  | C5-C6-N1    | -2.16 | 119.14      | 122.14   |
| 1   | 2     | 683  | OMG  | O6-C6-C5    | -2.16 | 120.84      | 126.53   |
| 1   | 2     | 509  | OMG  | C5-C6-N1    | 2.16  | 118.75      | 113.25   |
| 1   | 2     | 863  | PSU  | C5-C6-N1    | -2.15 | 119.15      | 122.14   |
| 1   | 2     | 644  | OMG  | O6-C6-C5    | -2.14 | 120.87      | 126.53   |
| 1   | 2     | 509  | OMG  | N9-C8-N7    | -2.14 | 109.44      | 113.40   |
| 1   | 2     | 1081 | PSU  | O4'-C1'-C2' | 2.13  | 108.09      | 105.15   |
| 1   | 2     | 1842 | 4AC  | C5-C4-N4    | 2.12  | 126.52      | 122.94   |
| 1   | 2     | 601  | OMG  | O6-C6-C5    | -2.12 | 120.93      | 126.53   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | 2     | 644  | OMG  | C5-C6-N1    | 2.11  | 118.63      | 113.25   |
| 1   | 2     | 509  | OMG  | C2-N1-C6    | -2.10 | 121.30      | 125.11   |
| 1   | 2     | 436  | OMG  | C5-C6-N1    | 2.09  | 118.58      | 113.25   |
| 1   | 2     | 1639 | 7MG  | C2-N1-C6    | -2.09 | 121.32      | 125.11   |
| 1   | 2     | 1447 | OMG  | C5-C6-N1    | 2.09  | 118.57      | 113.25   |
| 1   | 2     | 601  | OMG  | C5-C6-N1    | 2.09  | 118.57      | 113.25   |
| 1   | 2     | 1643 | PSU  | O4'-C1'-C2' | 2.08  | 108.03      | 105.15   |
| 1   | 2     | 681  | PSU  | C5-C6-N1    | -2.08 | 119.26      | 122.14   |
| 1   | 2     | 484  | A2M  | C4-N9-C8    | 2.07  | 107.92      | 105.74   |
| 1   | 2     | 1639 | 7MG  | C6-C5-C4    | -2.07 | 118.76      | 122.40   |
| 1   | 2     | 683  | OMG  | C5-C6-N1    | 2.07  | 118.52      | 113.25   |
| 1   | 2     | 1328 | OMG  | C5-C6-N1    | 2.05  | 118.48      | 113.25   |
| 1   | 2     | 1248 | B8N  | C5-C4-N3    | 2.05  | 119.88      | 116.15   |
| 1   | 2     | 512  | A2M  | C2-N1-C6    | 2.05  | 122.09      | 118.73   |
| 1   | 2     | 1625 | PSU  | C5-C6-N1    | -2.04 | 119.31      | 122.14   |
| 1   | 2     | 1832 | 6MZ  | C2-N1-C6    | 2.03  | 121.98      | 115.24   |
| 1   | 2     | 93   | PSU  | C5-C6-N1    | -2.03 | 119.32      | 122.14   |
| 1   | 2     | 1842 | 4AC  | O2-C2-N1    | 2.03  | 122.87      | 118.90   |
| 1   | 2     | 1445 | PSU  | O4'-C1'-C2' | 2.02  | 107.94      | 105.15   |
| 1   | 2     | 1490 | OMG  | C5-C6-N1    | 2.02  | 118.39      | 113.25   |
| 1   | 2     | 1248 | B8N  | O4'-C1'-C2' | 2.02  | 107.94      | 105.15   |
| 1   | 2     | 590  | A2M  | C1'-N9-C8   | -2.01 | 122.62      | 127.09   |
| 1   | 2     | 296  | PSU  | C5-C6-N1    | -2.01 | 119.35      | 122.14   |
| 1   | 2     | 121  | OMU  | O2-C2-N3    | -2.00 | 117.79      | 121.49   |

There are no chirality outliers.

All (46) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 1   | 2     | 512  | A2M  | O4'-C4'-C5'-O5' |
| 1   | 2     | 601  | OMG  | C1'-C2'-O2'-CM2 |
| 1   | 2     | 668  | A2M  | O4'-C4'-C5'-O5' |
| 1   | 2     | 668  | A2M  | C3'-C4'-C5'-O5' |
| 1   | 2     | 1248 | B8N  | O4'-C4'-C5'-O5' |
| 1   | 2     | 1337 | 4AC  | N3-C4-N4-C7     |
| 1   | 2     | 1337 | 4AC  | C5-C4-N4-C7     |
| 1   | 2     | 1850 | MA6  | C5-C6-N6-C10    |
| 1   | 2     | 1851 | MA6  | O4'-C4'-C5'-O5' |
| 1   | 2     | 1851 | MA6  | C5-C6-N6-C10    |
| 1   | 2     | 99   | A2M  | O4'-C4'-C5'-O5' |
| 1   | 2     | 576  | A2M  | C3'-C4'-C5'-O5' |
| 1   | 2     | 1248 | B8N  | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 1   | 2     | 1850 | MA6  | N1-C6-N6-C10    |
| 1   | 2     | 1851 | MA6  | N1-C6-N6-C10    |
| 1   | 2     | 1447 | OMG  | C3'-C4'-C5'-O5' |
| 1   | 2     | 1851 | MA6  | C3'-C4'-C5'-O5' |
| 1   | 2     | 512  | A2M  | C3'-C4'-C5'-O5' |
| 1   | 2     | 576  | A2M  | O4'-C4'-C5'-O5' |
| 1   | 2     | 1045 | PSU  | O4'-C4'-C5'-O5' |
| 1   | 2     | 1850 | MA6  | C5-C6-N6-C9     |
| 1   | 2     | 428  | OMU  | O4'-C4'-C5'-O5' |
| 1   | 2     | 1045 | PSU  | C3'-C4'-C5'-O5' |
| 1   | 2     | 99   | A2M  | C3'-C4'-C5'-O5' |
| 1   | 2     | 1447 | OMG  | O4'-C4'-C5'-O5' |
| 1   | 2     | 1337 | 4AC  | O7-C7-N4-C4     |
| 1   | 2     | 1337 | 4AC  | CM7-C7-N4-C4    |
| 1   | 2     | 1842 | 4AC  | O7-C7-N4-C4     |
| 1   | 2     | 1842 | 4AC  | CM7-C7-N4-C4    |
| 1   | 2     | 428  | OMU  | C3'-C4'-C5'-O5' |
| 1   | 2     | 683  | OMG  | O4'-C4'-C5'-O5' |
| 1   | 2     | 1248 | B8N  | N3-C31-C32-C33  |
| 1   | 2     | 1248 | B8N  | O4'-C1'-C5-C4   |
| 1   | 2     | 1851 | MA6  | C5-C6-N6-C9     |
| 1   | 2     | 1490 | OMG  | C4'-C5'-O5'-P   |
| 1   | 2     | 644  | OMG  | C4'-C5'-O5'-P   |
| 1   | 2     | 1081 | PSU  | C4'-C5'-O5'-P   |
| 1   | 2     | 119  | PSU  | O4'-C4'-C5'-O5' |
| 1   | 2     | 1639 | 7MG  | C2'-C1'-N9-C8   |
| 1   | 2     | 1248 | B8N  | C32-C33-C34-O36 |
| 1   | 2     | 428  | OMU  | C2'-C1'-N1-C6   |
| 1   | 2     | 1248 | B8N  | C32-C33-C34-O35 |
| 1   | 2     | 668  | A2M  | C2'-C1'-N9-C8   |
| 1   | 2     | 590  | A2M  | O4'-C1'-N9-C8   |
| 1   | 2     | 428  | OMU  | O4'-C1'-N1-C6   |
| 1   | 2     | 683  | OMG  | C3'-C4'-C5'-O5' |

There are no ring outliers.

10 monomers are involved in 12 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1   | 2     | 1842 | 4AC  | 1       | 0            |
| 1   | 2     | 484  | A2M  | 1       | 0            |
| 1   | 2     | 1232 | PSU  | 1       | 0            |
| 1   | 2     | 1337 | 4AC  | 2       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1   | 2     | 1031 | A2M  | 1       | 0            |
| 1   | 2     | 601  | OMG  | 1       | 0            |
| 1   | 2     | 509  | OMG  | 2       | 0            |
| 1   | 2     | 681  | PSU  | 1       | 0            |
| 1   | 2     | 166  | A2M  | 1       | 0            |
| 1   | 2     | 1383 | A2M  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 166 ligands modelled in this entry, 166 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

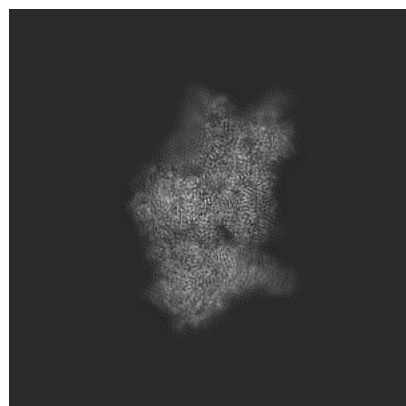
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47929. These allow visual inspection of the internal detail of the map and identification of artifacts.

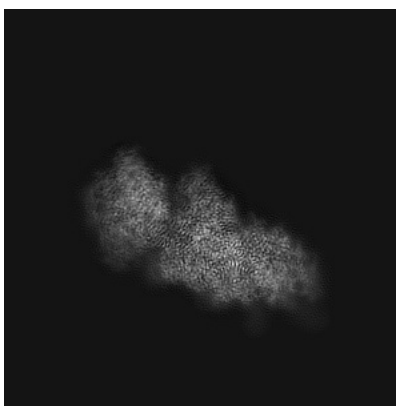
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

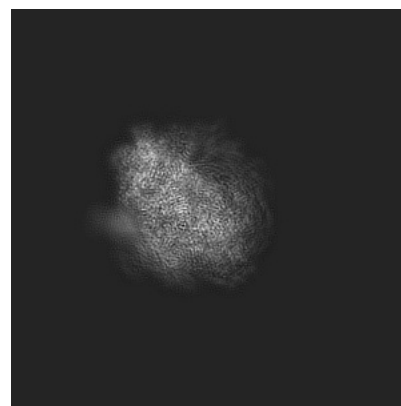
#### 6.1.1 Primary map



X

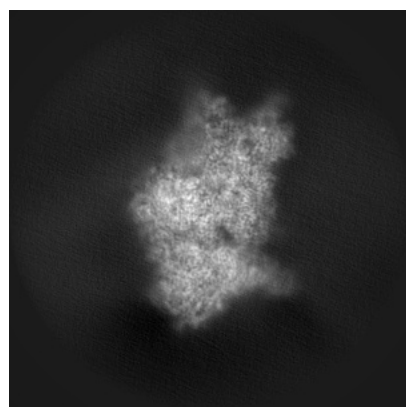


Y

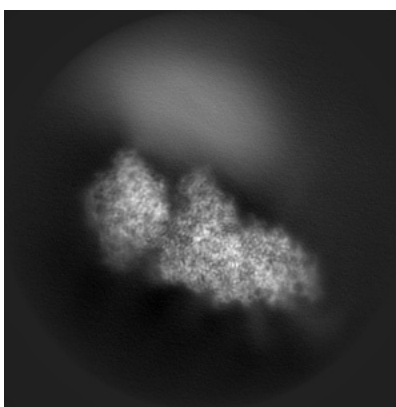


Z

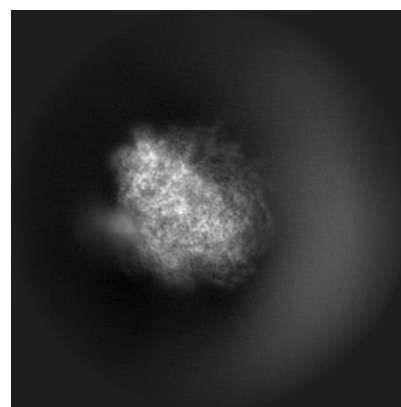
#### 6.1.2 Raw map



X



Y



Z

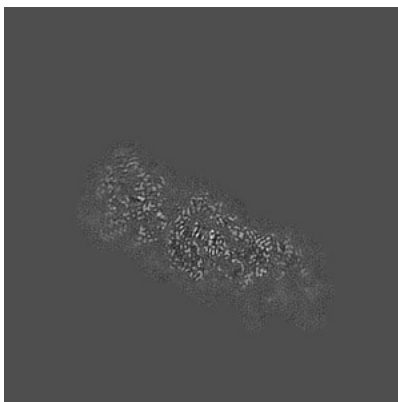
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

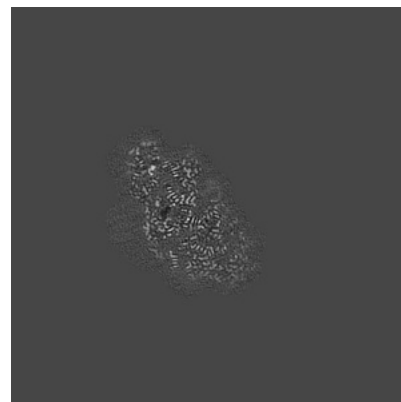
### 6.2.1 Primary map



X Index: 250

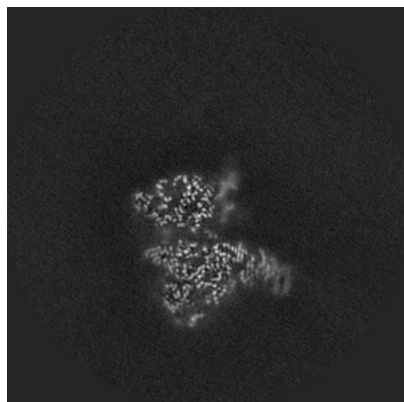


Y Index: 250

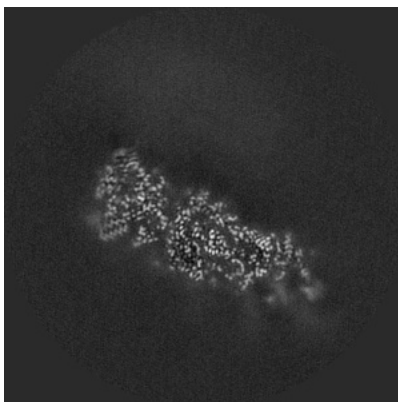


Z Index: 250

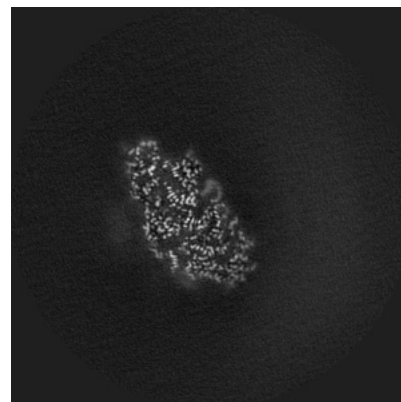
### 6.2.2 Raw map



X Index: 250



Y Index: 250

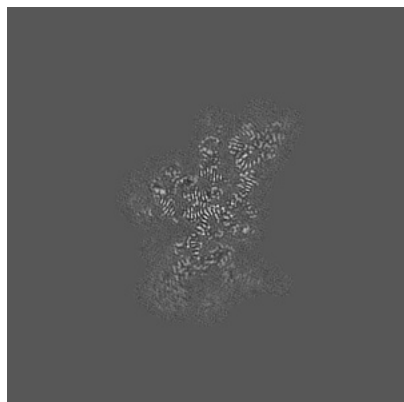


Z Index: 250

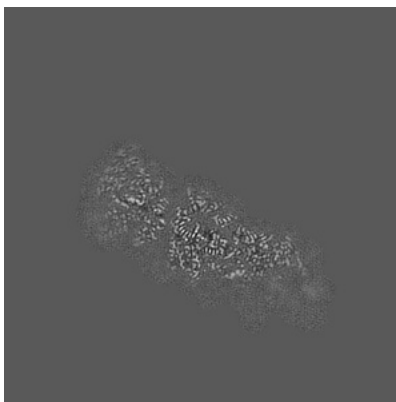
The images above show central slices of the map in three orthogonal directions.

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

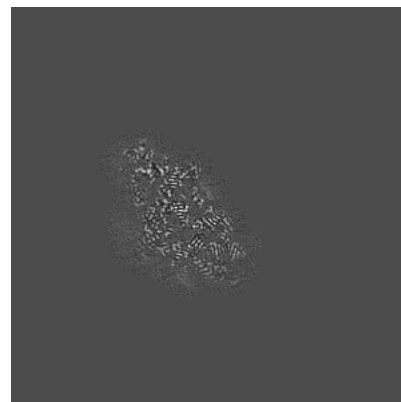
### 6.3.1 Primary map



X Index: 214

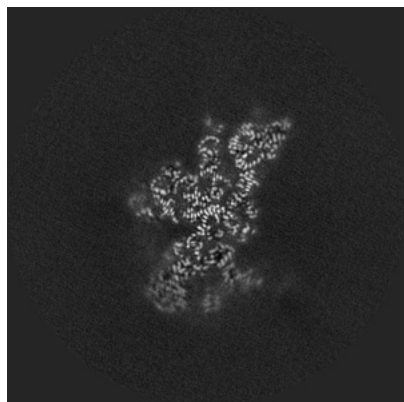


Y Index: 248

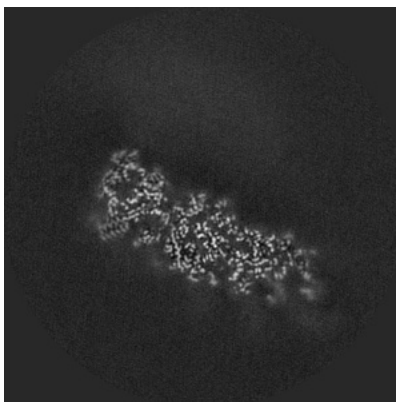


Z Index: 260

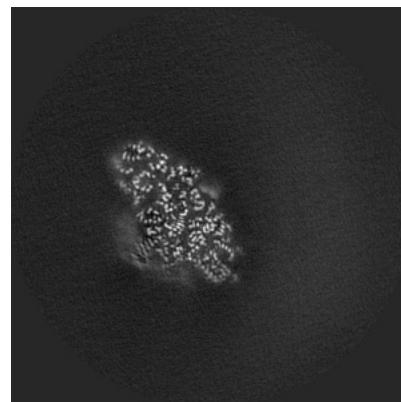
### 6.3.2 Raw map



X Index: 214



Y Index: 253



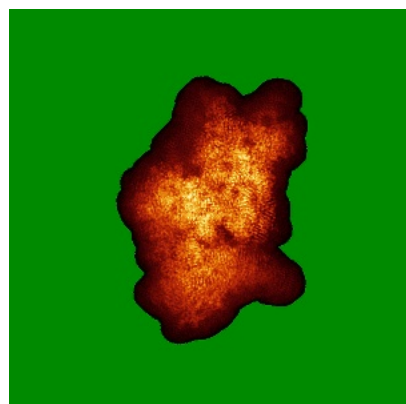
Z Index: 265

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

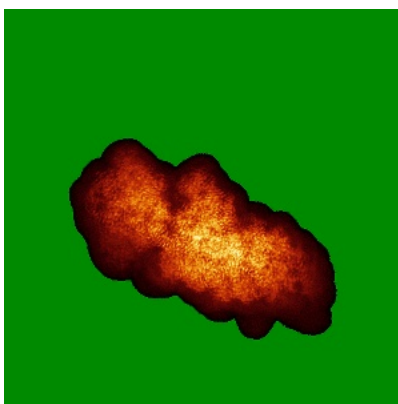


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

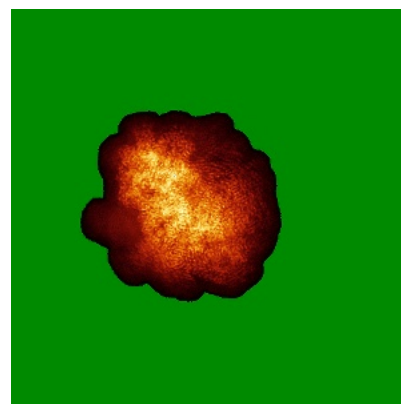
### 6.4.1 Primary map



X

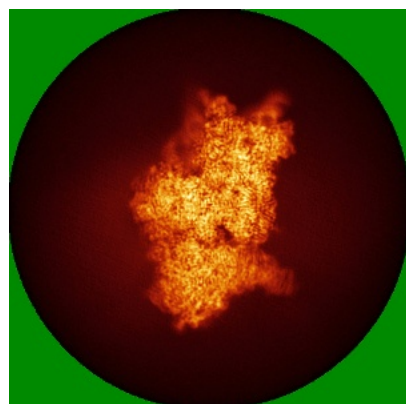


Y

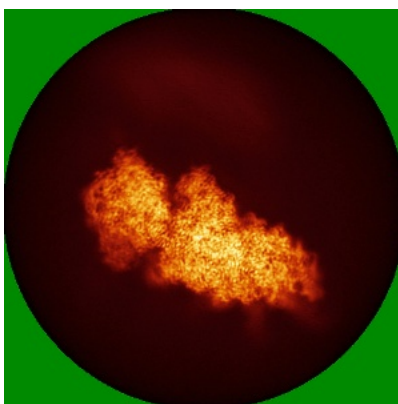


Z

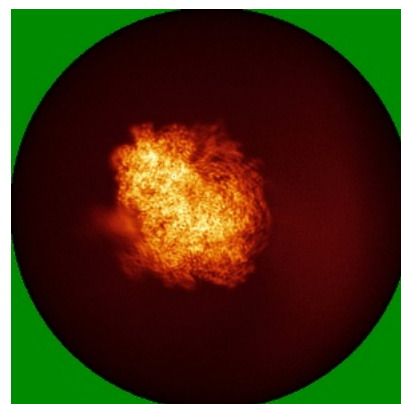
### 6.4.2 Raw map



X



Y



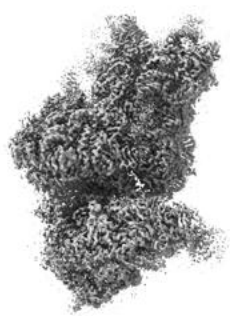
Z

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



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

### 6.5.1 Primary map



X



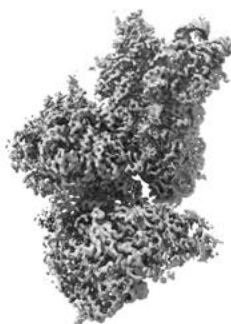
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

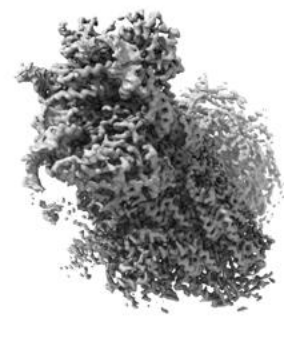
### 6.5.2 Raw map



X



Y



Z

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

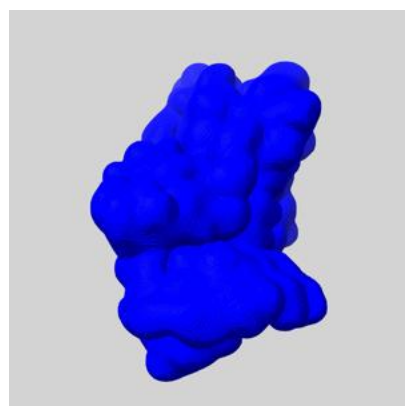
## 6.6 Mask visualisation [i](#)

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

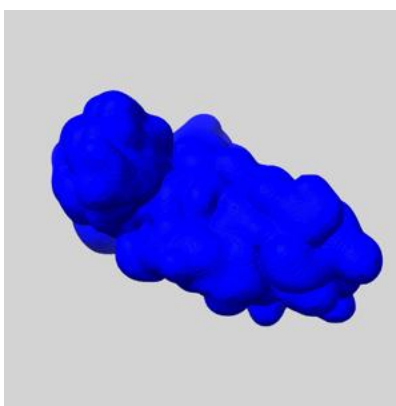
A mask typically either:

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

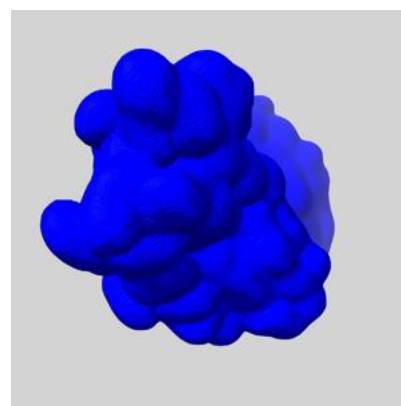
### 6.6.1 emd\_47929\_msk\_1.map [i](#)



X



Y

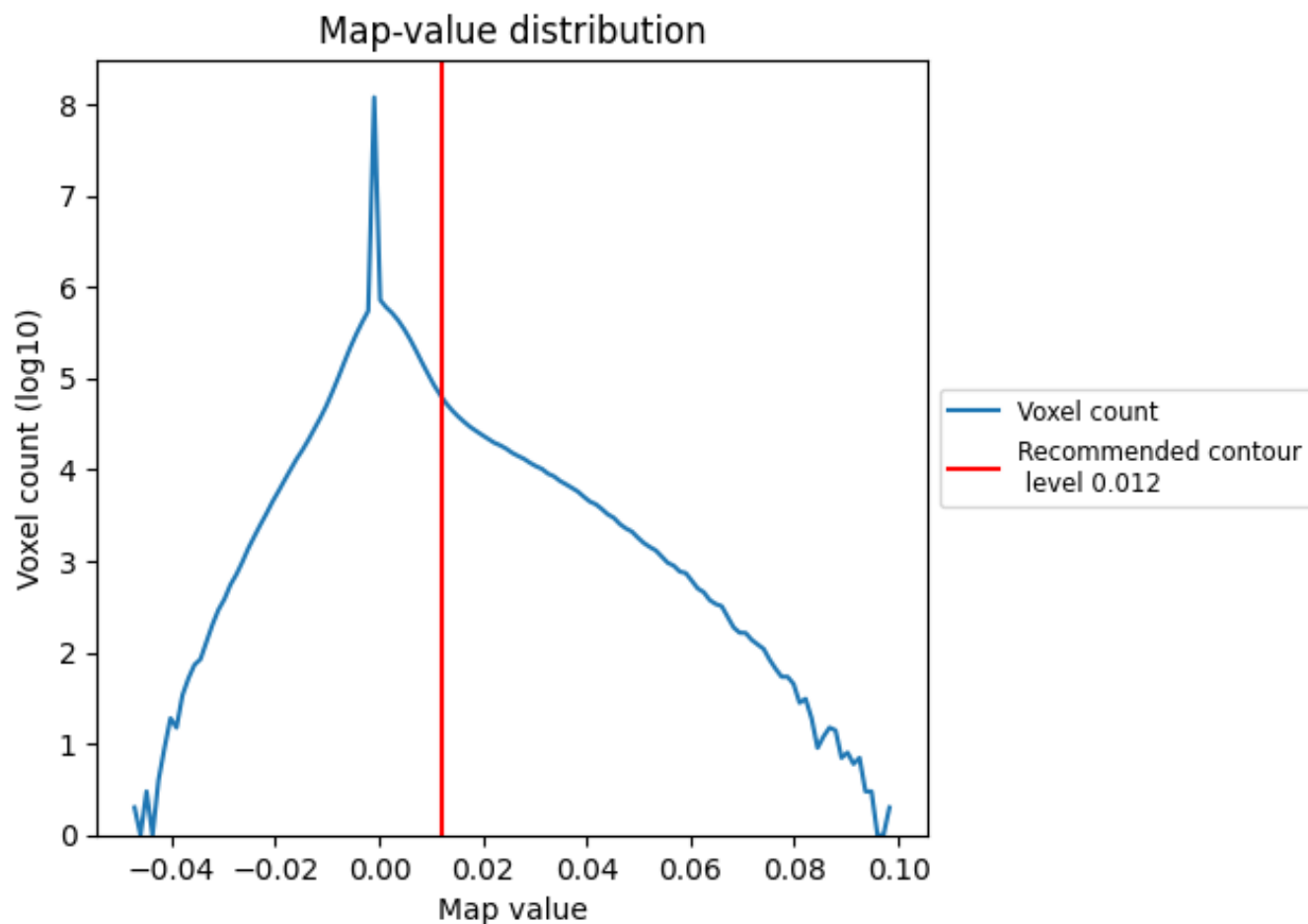


Z

## 7 Map analysis [i](#)

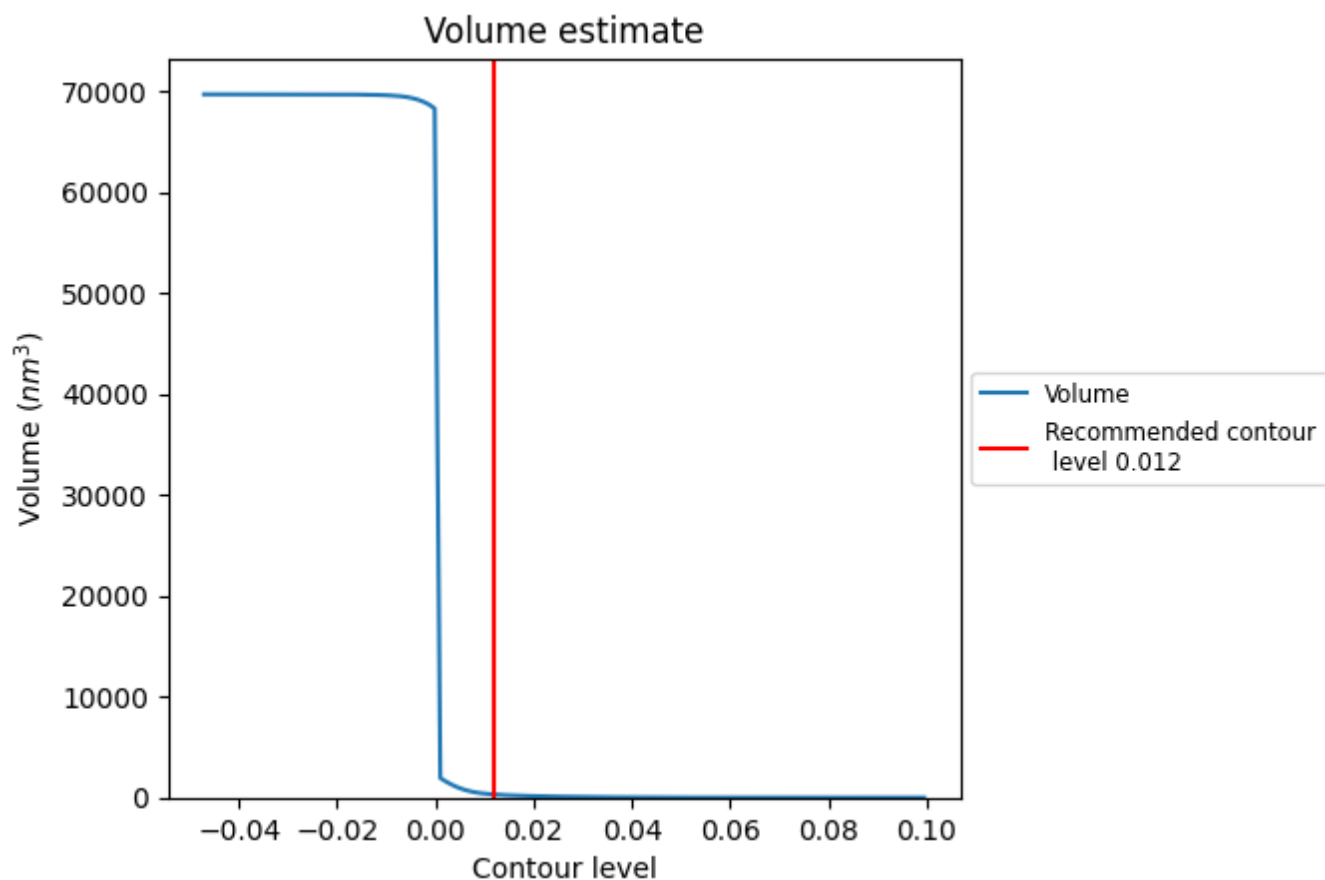
This section contains the results of statistical analysis of the map.

### 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.

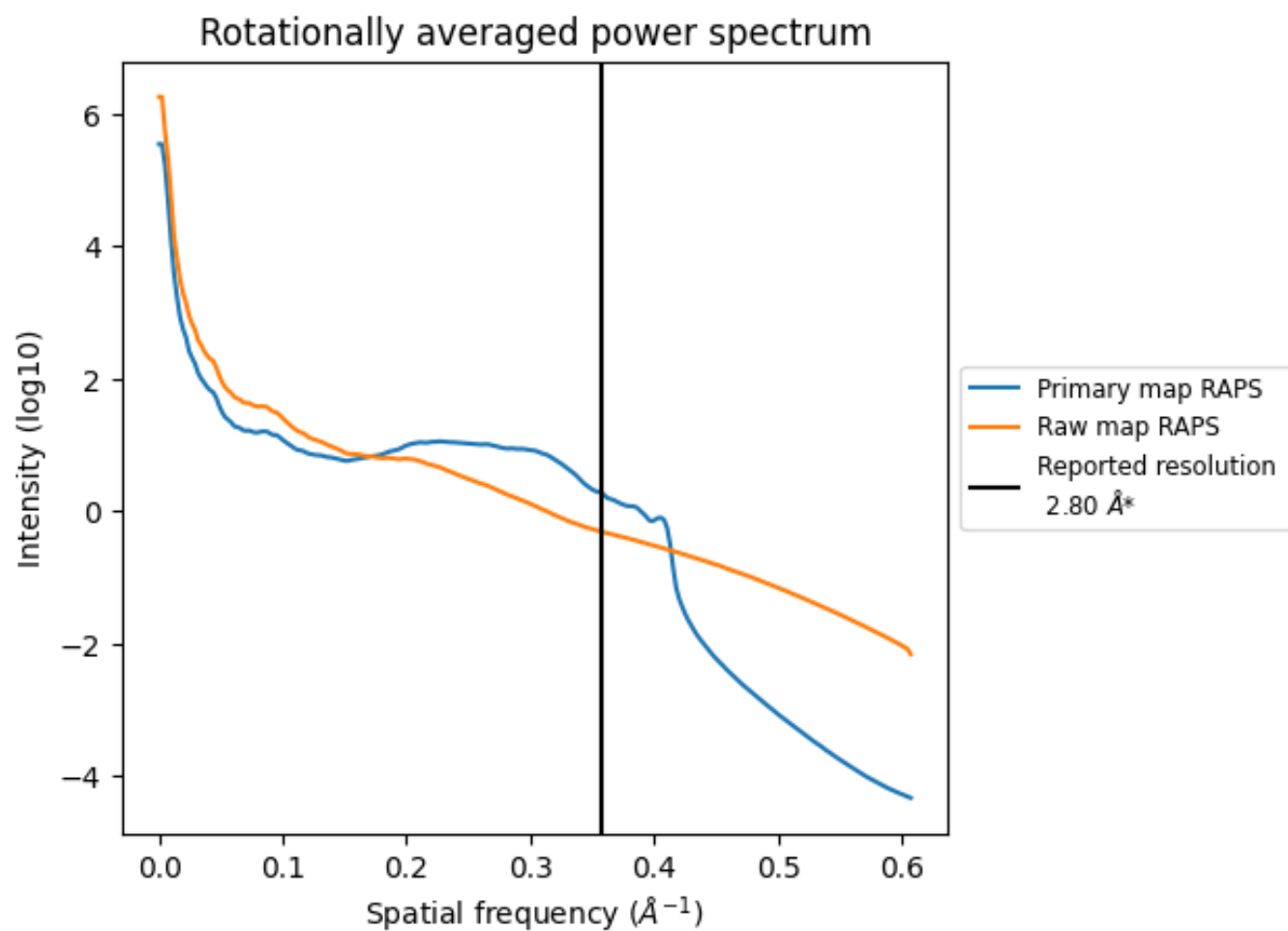
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 304 nm<sup>3</sup>; this corresponds to an approximate mass of 274 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 ⓘ

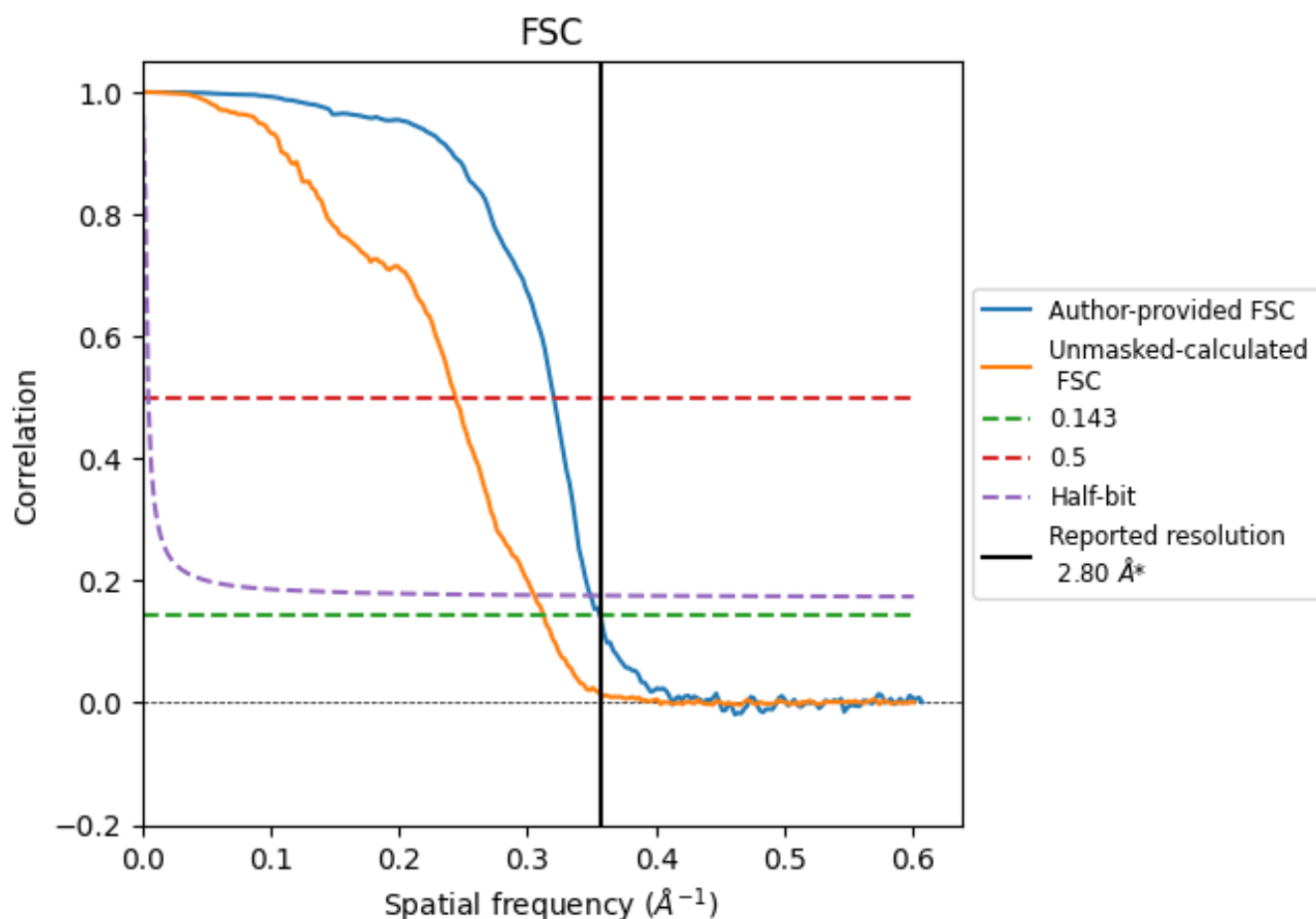


\*Reported resolution corresponds to spatial frequency of  $0.357 \text{ \AA}^{-1}$

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

## 8.2 Resolution estimates [i](#)

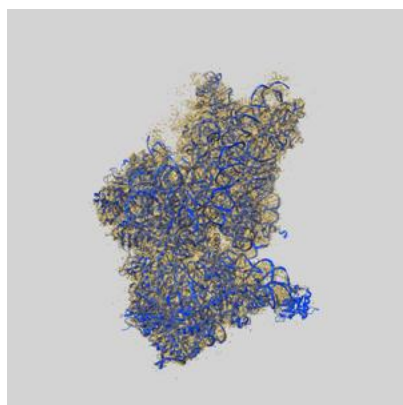
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.80                               | -    | -        |
| Author-provided FSC curve | 2.80                               | 3.12 | 2.86     |
| Unmasked-calculated*      | 3.20                               | 4.10 | 3.28     |

\*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 3.20 differs from the reported value 2.8 by more than 10 %

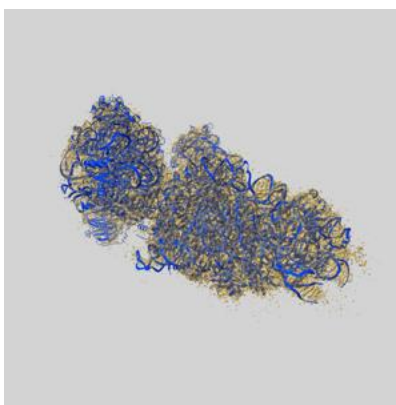
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47929 and PDB model 9ED0. Per-residue inclusion information can be found in section [3](#) on page [11](#).

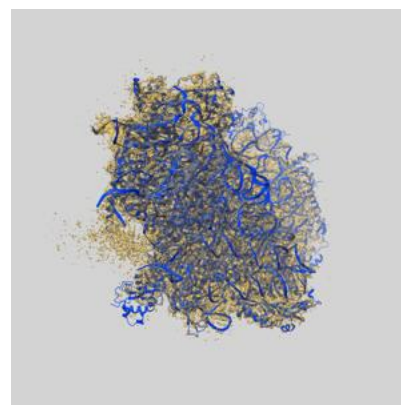
### 9.1 Map-model overlay [i](#)



X



Y

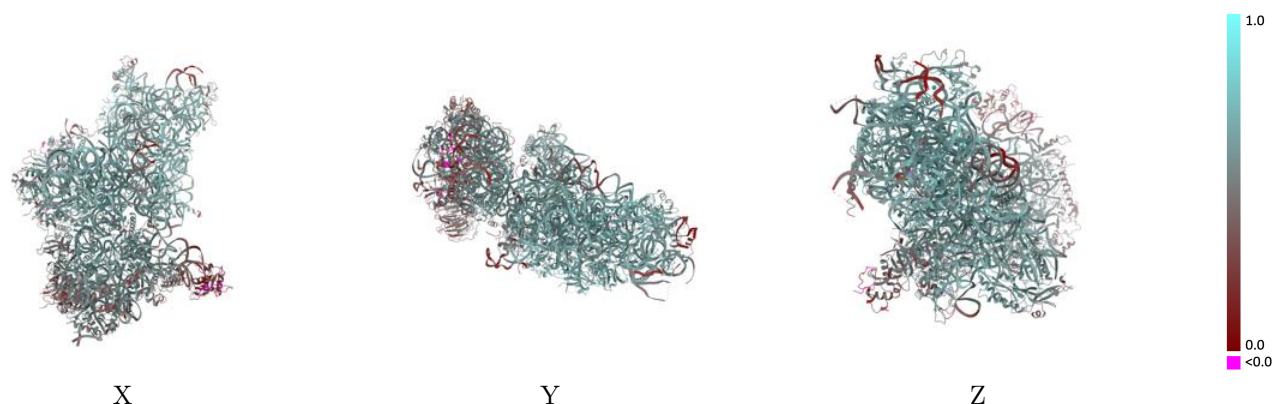


Z

The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

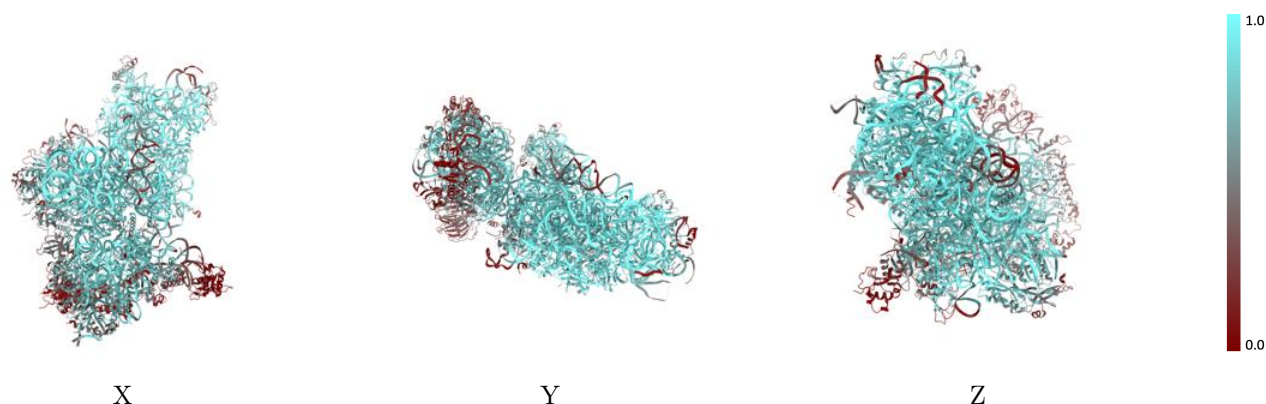


## 9.2 Q-score mapped to coordinate model [i](#)



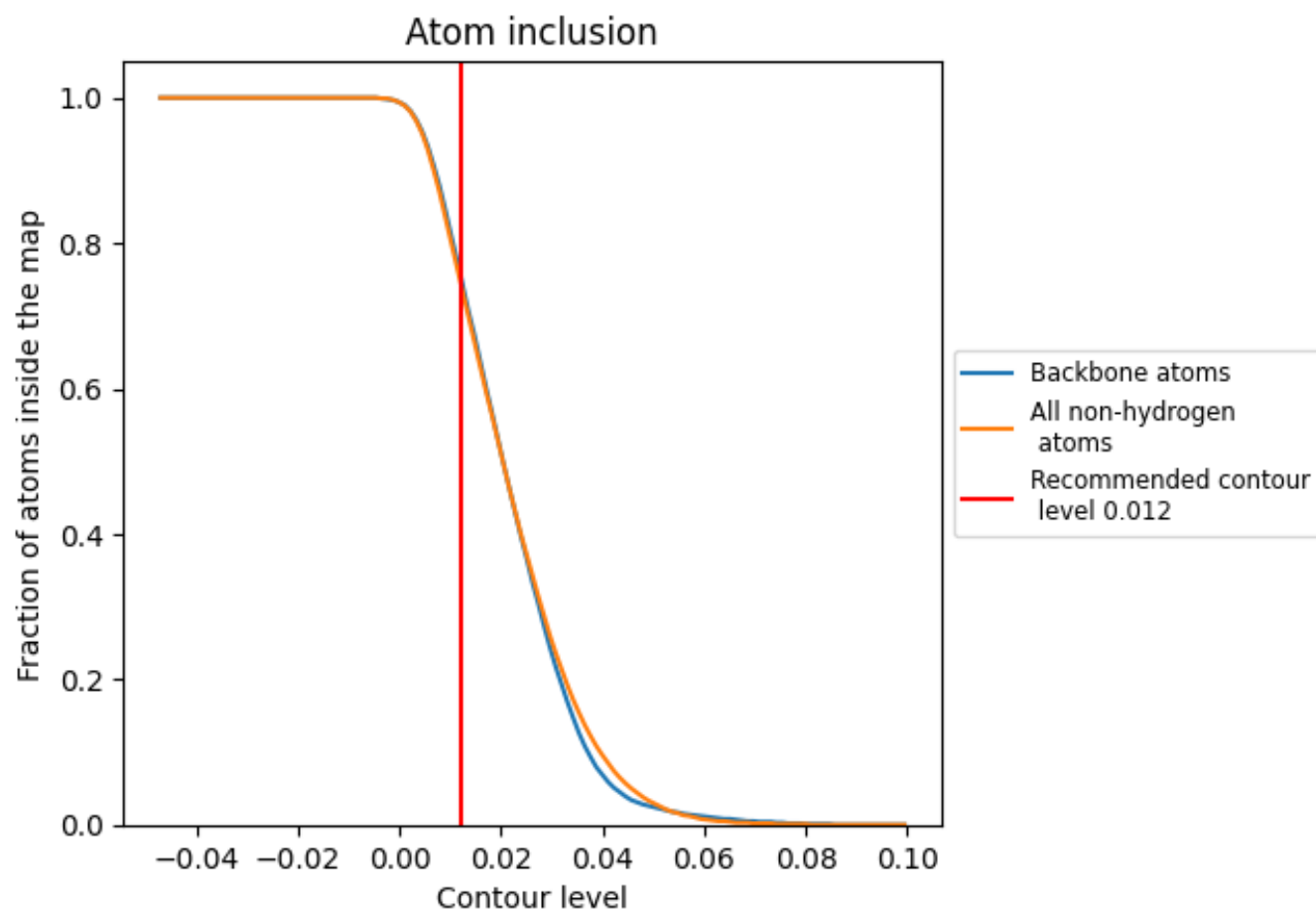
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 75% 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 (0.012) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7460   |  0.5680   |
| 2     |  0.8600   |  0.5950   |
| A     |  0.7230   |  0.5860   |
| B     |  0.6680   |  0.5740   |
| C     |  0.8410   |  0.6360   |
| D     |  0.6570   |  0.5460   |
| E     |  0.9180   |  0.6560   |
| F     |  0.6060   |  0.5270   |
| G     |  0.7500   |  0.5790   |
| H     |  0.2550   |  0.3970   |
| I     |  0.7950   |  0.6030   |
| J     |  0.8870   |  0.6410   |
| K     |  0.5330   |  0.5000   |
| L     |  0.8770   |  0.6390   |
| M     |  0.0190  |  0.2210  |
| N     |  0.7560 |  0.6030 |
| O     |  0.7600 |  0.5990 |
| P     |  0.4110 |  0.4450 |
| Q     |  0.7390 |  0.5770 |
| R     |  0.4100 |  0.4580 |
| S     |  0.3830 |  0.4280 |
| T     |  0.6550 |  0.5410 |
| U     |  0.5270 |  0.5000 |
| V     |  0.7440 |  0.6010 |
| W     |  0.9260 |  0.6570 |
| X     |  0.9150 |  0.6560 |
| Y     |  0.8680 |  0.6400 |
| Z     |  0.1940 |  0.3970 |
| a     |  0.8280 |  0.6190 |
| b     |  0.6160 |  0.5500 |
| c     |  0.5020 |  0.4980 |
| d     |  0.8530 |  0.6280 |
| e     |  0.7260 |  0.5900 |
| f     |  0.0250 |  0.1880 |
| g     |  0.2270 |  0.3680 |



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*Continued from previous page...*

| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| h     |  0.5560 |  0.5080 |
| n     |  0.7900 |  0.6090 |