



# wwPDB EM Validation Summary Report ⓘ

Sep 21, 2024 – 10:54 am BST

PDB ID : 8PJ5  
EMDB ID : EMD-17700  
Title : Structure of human 48S translation initiation complex after eIF2 release prior  
60S subunit joining (48S-5)  
Authors : Petrychenko, V.; Yi, S.-H.; Liedtke, D.; Peng, B.Z.; Rodnina, M.V.; Fischer,  
N.  
Deposited on : 2023-06-22  
Resolution : 2.90 Å(reported)

This is a wwPDB EM Validation Summary 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.dev112  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : **FAILED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.38.2

## 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 2.90 Å.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

## 2 Entry composition [i](#)

There are 54 unique types of molecules in this entry. The entry contains 113033 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Eukaryotic translation initiation factor 5B.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
|     |       |          | Total | C    | N   | O   | S  |         |       |
| 1   | 0     | 622      | 4928  | 3141 | 851 | 914 | 22 | 0       | 0     |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 2   | 1     | 588      | 3258  | 1986 | 633 | 634 | 5 | 0       | 0     |

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

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
|     |       |          | Total | C   | N   | O   |         |       |
| 3   | 2     | 304      | 1493  | 885 | 304 | 304 | 0       | 0     |

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

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
|     |       |          | Total | C   | N   | O   |         |       |
| 4   | 3     | 213      | 1057  | 631 | 213 | 213 | 0       | 0     |

- Molecule 5 is a protein called Eukaryotic translation initiation factor 3 subunit F.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
|     |       |          | Total | C   | N   | O   |         |       |
| 5   | 4     | 257      | 1272  | 757 | 257 | 258 | 0       | 0     |

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

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
|     |       |          | Total | C   | N   | O   |         |       |
| 6   | 5     | 319      | 1581  | 943 | 319 | 319 | 0       | 0     |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 7   | 6     | 350      | 1917  | 1159 | 376 | 380 | 2 | 0       | 0     |

- Molecule 8 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
|     |       |          | Total | C   | N   | O   | P  |         |       |
| 8   | 7     | 56       | 1300  | 584 | 245 | 410 | 61 | 5       | 0     |

- Molecule 9 is a protein called Eukaryotic translation initiation factor 3 subunit H.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
|     |       |          | Total | C   | N   | O   |         |       |
| 9   | 8     | 317      | 1571  | 936 | 317 | 318 | 0       | 0     |

- Molecule 10 is a protein called 60S ribosomal protein L41.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
|     |       |          | Total | C   | N  | O  | S |         |       |
| 10  | 9     | 24       | 230   | 139 | 62 | 26 | 3 | 0       | 0     |

- Molecule 11 is a RNA chain called 18S rRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
|     |       |          | Total | C     | N    | O     | P    |         |       |
| 11  | A     | 1754     | 37429 | 16718 | 6714 | 12244 | 1753 | 0       | 0     |

- Molecule 12 is a protein called 40S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 12  | B     | 142      | 1166  | 743 | 218 | 199 | 6 | 0       | 0     |

- Molecule 13 is a protein called 40S ribosomal protein S4, X isoform.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 13  | C     | 256      | 2035  | 1302 | 378 | 347 | 8 | 0       | 0     |

- Molecule 14 is a protein called 40S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 14  | D     | 177      | 1477  | 941 | 295 | 239 | 2 | 0       | 0     |

- Molecule 15 is a protein called 40S ribosomal protein S23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 15  | E     | 140      | 1087  | 687 | 215 | 182 | 3 | 0       | 0     |

- Molecule 16 is a protein called 40S ribosomal protein S30.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
|     |       |          | Total | C   | N   | O  | S |         |       |
| 16  | F     | 59       | 461   | 285 | 100 | 75 | 1 | 0       | 0     |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| F     | 125     | PRO      | LYS    | conflict | UNP P62861 |
| F     | 126     | GLY      | LYS    | conflict | UNP P62861 |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 17  | G     | 177      | 1430  | 917 | 260 | 252 | 1 | 0       | 0     |

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

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

- Molecule 19 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 19  | I     | 150      | 1208  | 773 | 229 | 205 | 1 | 0       | 0     |

- Molecule 20 is a protein called 40S ribosomal protein S15a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 20  | J     | 129      | 1034  | 659 | 193 | 176 | 6 | 0       | 0     |

- Molecule 21 is a protein called 40S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 21  | K     | 81       | 617   | 380 | 114 | 118 | 5 | 0       | 0     |

- Molecule 22 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
|     |       |          | Total | C    | N   | O   | S  |         |       |
| 22  | L     | 220      | 1707  | 1104 | 292 | 301 | 10 | 0       | 0     |

- Molecule 23 is a protein called 40S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 23  | M     | 131      | 1064  | 668 | 198 | 194 | 4 | 0       | 0     |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 24  | N     | 207      | 1633  | 1040 | 288 | 297 | 8 | 0       | 0     |

- Molecule 25 is a protein called 40S ribosomal protein S3a.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
|     |       |          | Total | C    | N   | O   | S  |         |       |
| 25  | O     | 211      | 1715  | 1088 | 307 | 306 | 14 | 0       | 0     |

- Molecule 26 is a protein called 40S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 26  | P     | 133      | 997   | 610 | 196 | 185 | 6 | 0       | 0     |

- Molecule 27 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 27  | Q     | 99       | 792   | 492 | 165 | 130 | 5 | 0       | 0     |

- Molecule 28 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 28  | R     | 198      | 1627  | 1021 | 322 | 279 | 5 | 0       | 0     |

- Molecule 29 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 29  | S     | 230      | 1862  | 1164 | 371 | 320 | 7 | 0       | 0     |

- Molecule 30 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 30  | T     | 125      | 1015  | 642 | 199 | 169 | 5 | 0       | 0     |

- Molecule 31 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 31  | V     | 189      | 1495  | 934 | 284 | 270 | 7 | 0       | 0     |

- Molecule 32 is a protein called 40S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 32  | Y     | 141      | 1124  | 715 | 212 | 194 | 3 | 0       | 0     |

- Molecule 33 is a protein called 40S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 33  | Z     | 227      | 1765  | 1125 | 317 | 315 | 8 | 0       | 0     |

- Molecule 34 is a protein called 40S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 34  | a     | 99       | 834   | 544 | 149 | 135 | 6 | 0       | 0     |

- Molecule 35 is a protein called 40S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 35  | b     | 131      | 1072  | 682 | 201 | 182 | 7 | 0       | 0     |

- Molecule 36 is a protein called Receptor of activated protein C kinase 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
|     |       |          | Total | C    | N   | O   | S  |         |       |
| 36  | c     | 313      | 2436  | 1535 | 424 | 465 | 12 | 0       | 0     |

- Molecule 37 is a protein called 40S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 37  | d     | 142      | 1105  | 692 | 213 | 197 | 3 | 0       | 0     |

- Molecule 38 is a protein called 40S ribosomal protein S25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 38  | e     | 82       | 658   | 426 | 121 | 110 | 1 | 0       | 0     |

- Molecule 39 is a protein called 40S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 39  | f     | 149      | 1227  | 770 | 249 | 207 | 1 | 0       | 0     |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 40  | h     | 103      | 817   | 511 | 155 | 147 | 4 | 0       | 0     |

- Molecule 41 is a protein called 40S ribosomal protein S29.



| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 41  | i     | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 419   | 262 | 85 | 67 | 5 |         |       |

- Molecule 42 is a protein called Ubiquitin.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 42  | k     | 71       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 581   | 367 | 109 | 98 | 7 |         |       |

- Molecule 43 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | m     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 950   | 596 | 168 | 177 | 9 |         |       |

- Molecule 44 is a protein called 40S ribosomal protein S28.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 44  | n     | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 506   | 308 | 102 | 94 | 2 |         |       |

- Molecule 45 is a protein called Eukaryotic translation initiation factor 3 subunit G.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 45  | o     | 77       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 616   | 389 | 111 | 116 |         |       |

- Molecule 46 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | q     | 117      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 951   | 590 | 183 | 174 | 4 |         |       |

- Molecule 47 is a protein called Eukaryotic translation initiation factor 3 subunit A.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 47  | u     | 706      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 5383  | 3379 | 982 | 999 | 23 |         |       |

- Molecule 48 is a protein called Eukaryotic translation initiation factor 3 subunit E.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 48  | v     | 384      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2635  | 1657 | 477 | 489 | 12 |         |       |

- Molecule 49 is a RNA chain called Initiator Met-tRNA-i.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 49  | w     | 75       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1604  | 717 | 298 | 515 | 74 |         |       |

- Molecule 50 is a protein called Eukaryotic translation initiation factor 3 subunit D.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 50  | x     | 421      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2831  | 1746 | 521 | 555 | 9 |         |       |

- Molecule 51 is a protein called Eukaryotic translation initiation factor 3 subunit C.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 51  | y     | 531      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4305  | 2711 | 764 | 797 | 33 |         |       |

- Molecule 52 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 52  | 0     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 52  | A     | 87       | Total | Mg | 0       |
|     |       |          | 87    | 87 |         |
| 52  | P     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 52  | S     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 52  | f     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 53 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



### 3 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 238019                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 45                                      | Depositor |
| Minimum defocus (nm)                 | 200                                     | Depositor |
| Maximum defocus (nm)                 | 2500                                    | Depositor |
| Magnification                        | 59000                                   | Depositor |
| Image detector                       | FEI FALCON III (4k x 4k)                | Depositor |
| Maximum map value                    | 26.872                                  | Depositor |
| Minimum map value                    | -7.142                                  | Depositor |
| Average map value                    | -0.000                                  | Depositor |
| Map value standard deviation         | 1.000                                   | Depositor |
| Recommended contour level            | 3                                       | Depositor |
| Map size (Å)                         | 417.74402, 417.74402, 417.74402         | wwPDB     |
| Map dimensions                       | 432, 432, 432                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.96700007, 0.96700007, 0.96700007      | Depositor |

## 4 Model quality [i](#)

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

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

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### 4.3 Torsion angles [i](#)

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

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#### 4.3.2 Protein sidechains [i](#)

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#### 4.3.3 RNA [i](#)

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

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

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 11  | A2M  | A     | 1678 | 11   | 18,25,26     | 4.37 | 8 (44%)     | 18,36,39    | 3.87 | 4 (22%)     |
| 11  | PSU  | A     | 823  | 11   | 18,21,22     | 1.10 | 1 (5%)      | 22,30,33    | 1.69 | 4 (18%)     |
| 11  | PSU  | A     | 119  | 11   | 18,21,22     | 1.02 | 1 (5%)      | 22,30,33    | 1.56 | 4 (18%)     |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 11  | 5MC  | A     | 1374 | 11    | 18,22,23     | 0.56 | 0        | 26,32,35    | 0.68 | 0        |
| 11  | PSU  | A     | 612  | 11    | 18,21,22     | 1.02 | 1 (5%)   | 22,30,33    | 1.71 | 5 (22%)  |
| 11  | A2M  | A     | 668  | 52,11 | 18,25,26     | 4.24 | 9 (50%)  | 18,36,39    | 3.82 | 5 (27%)  |
| 11  | MA6  | A     | 1851 | 11    | 18,26,27     | 1.35 | 3 (16%)  | 19,38,41    | 3.22 | 2 (10%)  |
| 11  | 5MU  | A     | 814  | 11    | 19,22,23     | 0.42 | 0        | 28,32,35    | 0.82 | 1 (3%)   |
| 11  | A2M  | A     | 27   | 52,11 | 18,25,26     | 4.31 | 9 (50%)  | 18,36,39    | 3.81 | 4 (22%)  |
| 11  | B8N  | A     | 1248 | 11    | 24,29,30     | 3.04 | 7 (29%)  | 29,42,45    | 1.79 | 5 (17%)  |
| 11  | PSU  | A     | 1081 | 11    | 18,21,22     | 1.06 | 1 (5%)   | 22,30,33    | 1.75 | 4 (18%)  |
| 11  | MA6  | A     | 1850 | 11    | 18,26,27     | 1.34 | 3 (16%)  | 19,38,41    | 3.14 | 2 (10%)  |
| 11  | A2M  | A     | 166  | 11    | 18,25,26     | 4.37 | 8 (44%)  | 18,36,39    | 3.83 | 4 (22%)  |
| 11  | UR3  | A     | 1830 | 11    | 19,22,23     | 2.83 | 8 (42%)  | 26,32,35    | 1.57 | 4 (15%)  |
| 11  | PSU  | A     | 1243 | 11    | 18,21,22     | 1.08 | 1 (5%)   | 22,30,33    | 1.77 | 4 (18%)  |
| 11  | OMU  | A     | 121  | 11    | 19,22,23     | 3.01 | 6 (31%)  | 26,31,34    | 1.60 | 5 (19%)  |
| 11  | A2M  | A     | 1031 | 11    | 18,25,26     | 4.37 | 9 (50%)  | 18,36,39    | 3.83 | 4 (22%)  |
| 11  | OMC  | A     | 174  | 52,11 | 19,22,23     | 0.53 | 0        | 26,31,34    | 0.66 | 0        |
| 11  | PSU  | A     | 822  | 11    | 18,21,22     | 1.05 | 1 (5%)   | 22,30,33    | 1.76 | 5 (22%)  |
| 11  | JMH  | A     | 1219 | 52,11 | 18,22,23     | 2.92 | 5 (27%)  | 21,32,35    | 1.71 | 4 (19%)  |
| 11  | OMG  | A     | 509  | 52,11 | 18,26,27     | 1.14 | 2 (11%)  | 19,38,41    | 0.86 | 1 (5%)   |
| 11  | OMG  | A     | 644  | 11    | 18,26,27     | 1.14 | 2 (11%)  | 19,38,41    | 0.84 | 1 (5%)   |
| 11  | OMC  | A     | 517  | 11    | 19,22,23     | 0.55 | 0        | 26,31,34    | 0.77 | 1 (3%)   |
| 11  | A2M  | A     | 159  | 11    | 18,25,26     | 4.29 | 8 (44%)  | 18,36,39    | 3.91 | 4 (22%)  |
| 11  | OMC  | A     | 1703 | 52,11 | 19,22,23     | 0.54 | 0        | 26,31,34    | 0.72 | 1 (3%)   |
| 11  | OMG  | A     | 683  | 11    | 18,26,27     | 1.15 | 2 (11%)  | 19,38,41    | 0.88 | 1 (5%)   |
| 11  | 6MZ  | A     | 1832 | 52,11 | 18,25,26     | 1.77 | 3 (16%)  | 16,36,39    | 2.15 | 4 (25%)  |
| 11  | A2M  | A     | 484  | 11    | 18,25,26     | 4.26 | 9 (50%)  | 18,36,39    | 3.87 | 5 (27%)  |
| 11  | OMU  | A     | 116  | 11    | 19,22,23     | 3.02 | 6 (31%)  | 26,31,34    | 1.58 | 4 (15%)  |

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   |
|-----|------|-------|------|------|---------|-----------|---------|
| 11  | A2M  | A     | 1678 | 11   | -       | 1/5/27/28 | 0/3/3/3 |
| 11  | PSU  | A     | 823  | 11   | -       | 0/7/25/26 | 0/2/2/2 |
| 11  | PSU  | A     | 119  | 11   | -       | 0/7/25/26 | 0/2/2/2 |
| 11  | 5MC  | A     | 1374 | 11   | -       | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 11  | PSU  | A     | 612  | 11    | -       | 0/7/25/26  | 0/2/2/2 |
| 11  | A2M  | A     | 668  | 52,11 | -       | 3/5/27/28  | 0/3/3/3 |
| 11  | MA6  | A     | 1851 | 11    | -       | 3/7/29/30  | 0/3/3/3 |
| 11  | 5MU  | A     | 814  | 11    | -       | 0/7/25/26  | 0/2/2/2 |
| 11  | A2M  | A     | 27   | 52,11 | -       | 2/5/27/28  | 0/3/3/3 |
| 11  | B8N  | A     | 1248 | 11    | -       | 6/16/34/35 | 0/2/2/2 |
| 11  | PSU  | A     | 1081 | 11    | -       | 1/7/25/26  | 0/2/2/2 |
| 11  | MA6  | A     | 1850 | 11    | -       | 0/7/29/30  | 0/3/3/3 |
| 11  | A2M  | A     | 166  | 11    | -       | 0/5/27/28  | 0/3/3/3 |
| 11  | UR3  | A     | 1830 | 11    | -       | 2/7/25/26  | 0/2/2/2 |
| 11  | PSU  | A     | 1243 | 11    | -       | 2/7/25/26  | 0/2/2/2 |
| 11  | OMU  | A     | 121  | 11    | -       | 1/9/27/28  | 0/2/2/2 |
| 11  | A2M  | A     | 1031 | 11    | -       | 1/5/27/28  | 0/3/3/3 |
| 11  | OMC  | A     | 174  | 52,11 | -       | 0/9/27/28  | 0/2/2/2 |
| 11  | PSU  | A     | 822  | 11    | -       | 2/7/25/26  | 0/2/2/2 |
| 11  | JMH  | A     | 1219 | 52,11 | -       | 1/7/25/26  | 0/2/2/2 |
| 11  | OMG  | A     | 509  | 52,11 | -       | 2/5/27/28  | 0/3/3/3 |
| 11  | OMG  | A     | 644  | 11    | -       | 1/5/27/28  | 0/3/3/3 |
| 11  | OMC  | A     | 517  | 11    | -       | 0/9/27/28  | 0/2/2/2 |
| 11  | A2M  | A     | 159  | 11    | -       | 3/5/27/28  | 0/3/3/3 |
| 11  | OMC  | A     | 1703 | 52,11 | -       | 0/9/27/28  | 0/2/2/2 |
| 11  | OMG  | A     | 683  | 11    | -       | 2/5/27/28  | 0/3/3/3 |
| 11  | 6MZ  | A     | 1832 | 52,11 | -       | 2/5/27/28  | 0/3/3/3 |
| 11  | A2M  | A     | 484  | 11    | -       | 1/5/27/28  | 0/3/3/3 |
| 11  | OMU  | A     | 116  | 11    | -       | 1/9/27/28  | 0/2/2/2 |

The worst 5 of 113 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 11  | A     | 166  | A2M  | C3'-C2' | -12.81 | 1.24        | 1.52     |
| 11  | A     | 1031 | A2M  | C3'-C2' | -12.80 | 1.24        | 1.52     |
| 11  | A     | 1678 | A2M  | C3'-C2' | -12.74 | 1.24        | 1.52     |
| 11  | A     | 27   | A2M  | C3'-C2' | -12.66 | 1.24        | 1.52     |
| 11  | A     | 159  | A2M  | C3'-C2' | -12.49 | 1.25        | 1.52     |

The worst 5 of 92 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 11  | A     | 1851 | MA6  | N1-C6-N6 | -12.57 | 103.83      | 117.06   |
| 11  | A     | 1850 | MA6  | N1-C6-N6 | -12.33 | 104.08      | 117.06   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 11  | A     | 159  | A2M  | C1'-N9-C4 | 10.84 | 145.69      | 126.64   |
| 11  | A     | 1678 | A2M  | C1'-N9-C4 | 10.72 | 145.48      | 126.64   |
| 11  | A     | 484  | A2M  | C1'-N9-C4 | 10.48 | 145.06      | 126.64   |

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | A     | 27  | A2M  | C1'-C2'-O2'-CM' |
| 11  | A     | 116 | OMU  | C1'-C2'-O2'-CM2 |
| 11  | A     | 121 | OMU  | C1'-C2'-O2'-CM2 |
| 11  | A     | 159 | A2M  | C1'-C2'-O2'-CM' |
| 11  | A     | 484 | A2M  | C1'-C2'-O2'-CM' |

There are no ring outliers.

No monomer is involved in short contacts.

## 4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 4.6 Ligand geometry [i](#)

Of 94 ligands modelled in this entry, 93 are monoatomic - leaving 1 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 53  | GTP  | 0     | 1302 | 52   | 26,34,34     | 1.13 | 2 (7%)   | 32,54,54    | 1.51 | 6 (18%)  |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 53  | GTP  | 0     | 1302 | 52   | -       | 5/18/38/38 | 0/3/3/3 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 53  | 0     | 1302 | GTP  | C5-C6 | -4.05 | 1.39        | 1.47     |
| 53  | 0     | 1302 | GTP  | C2-N3 | 2.17  | 1.38        | 1.33     |

The worst 5 of 6 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 53  | 0     | 1302 | GTP  | PB-O3B-PG   | -3.75 | 119.97      | 132.83   |
| 53  | 0     | 1302 | GTP  | C5-C6-N1    | 3.12  | 119.47      | 113.95   |
| 53  | 0     | 1302 | GTP  | C3'-C2'-C1' | 2.98  | 105.46      | 100.98   |
| 53  | 0     | 1302 | GTP  | C8-N7-C5    | 2.98  | 108.66      | 102.99   |
| 53  | 0     | 1302 | GTP  | C2-N1-C6    | -2.81 | 119.92      | 125.10   |

There are no chirality outliers.

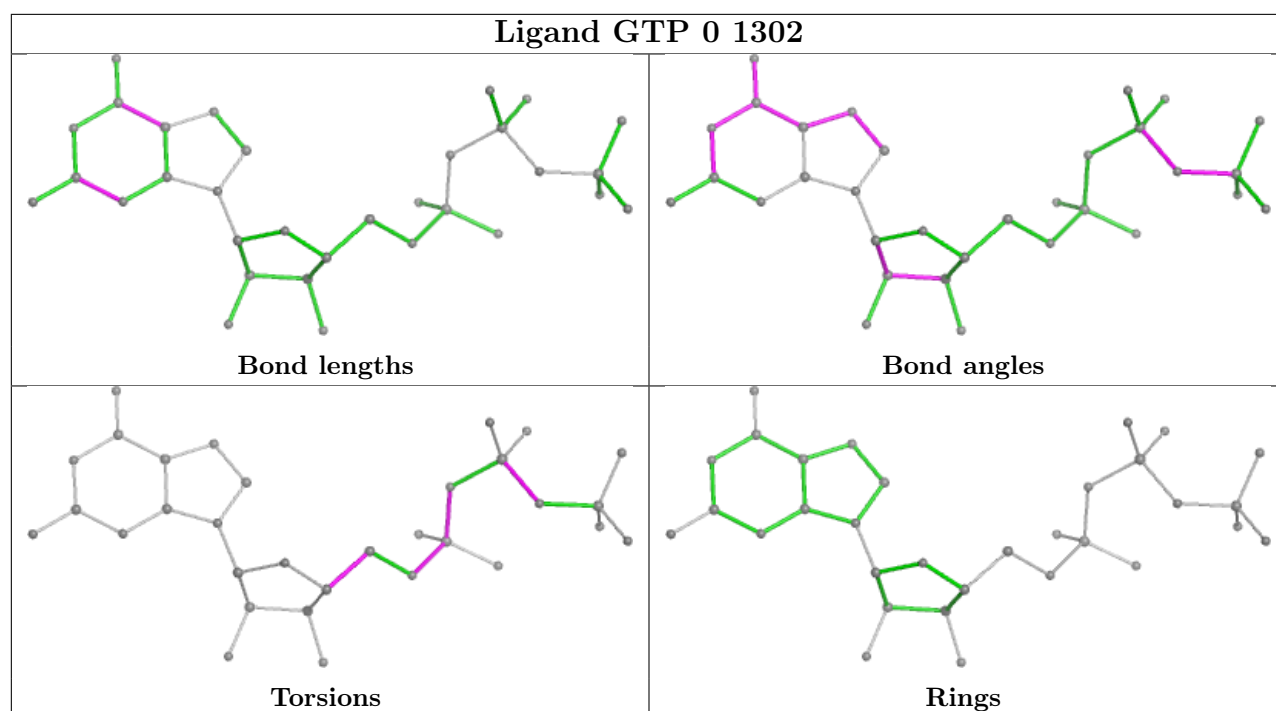
All (5) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 53  | 0     | 1302 | GTP  | PB-O3A-PA-O1A   |
| 53  | 0     | 1302 | GTP  | PG-O3B-PB-O2B   |
| 53  | 0     | 1302 | GTP  | O4'-C4'-C5'-O5' |
| 53  | 0     | 1302 | GTP  | C5'-O5'-PA-O3A  |
| 53  | 0     | 1302 | GTP  | PG-O3B-PB-O1B   |

There are no ring outliers.

No monomer is involved in short contacts.

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



#### 4.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

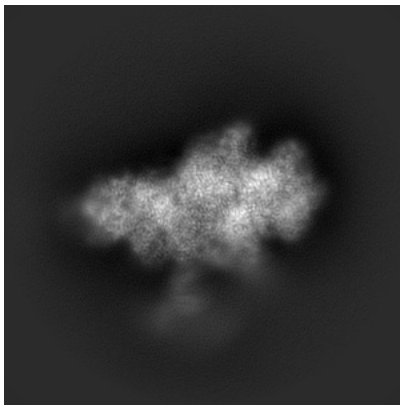
## 5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17700. These allow visual inspection of the internal detail of the map and identification of artifacts.

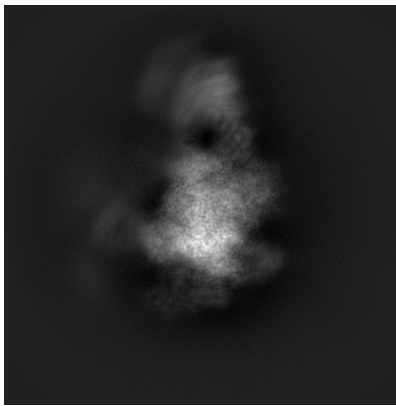
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

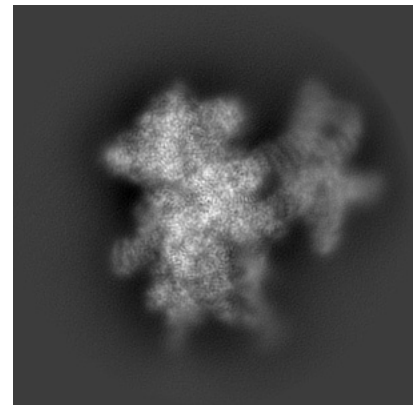
#### 5.1.1 Primary map



X

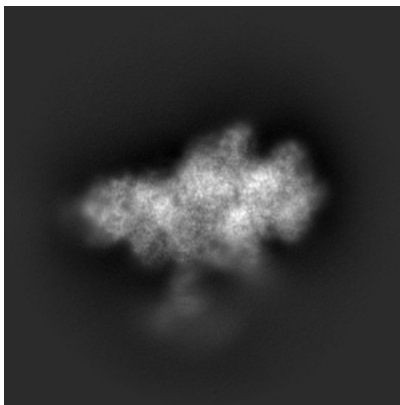


Y

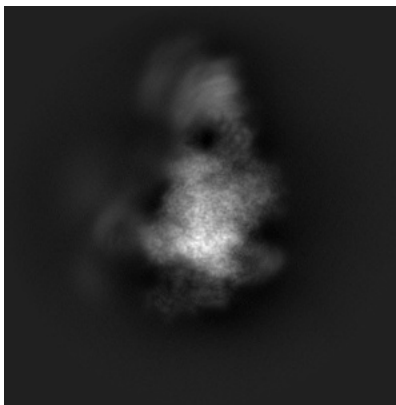


Z

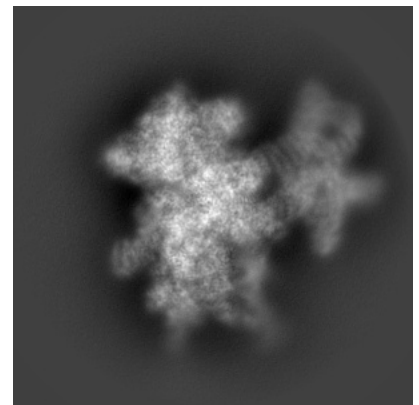
#### 5.1.2 Raw map



X



Y

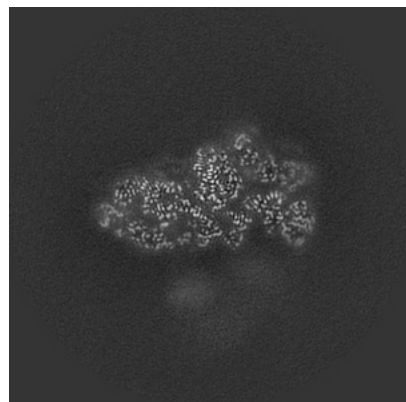


Z

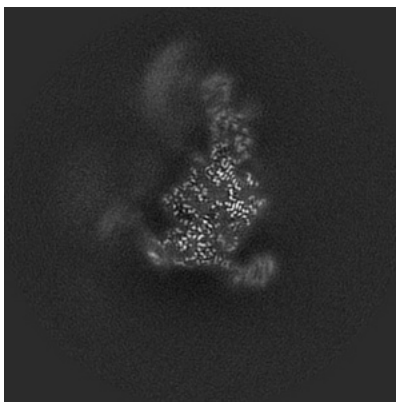
The images above show the map projected in three orthogonal directions.

## 5.2 Central slices [i](#)

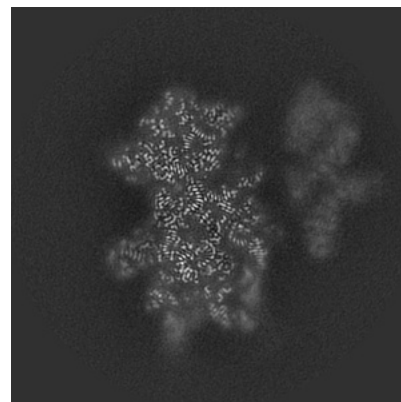
### 5.2.1 Primary map



X Index: 216

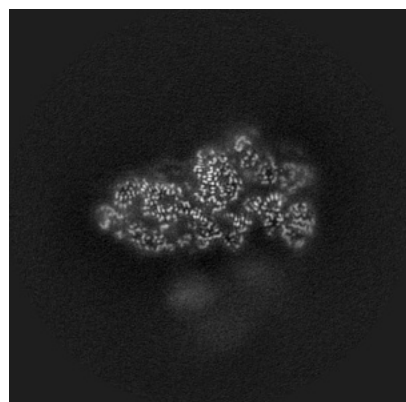


Y Index: 216

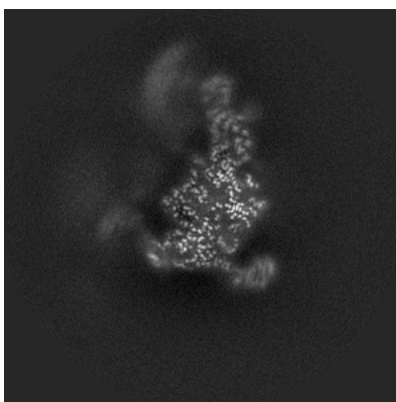


Z Index: 216

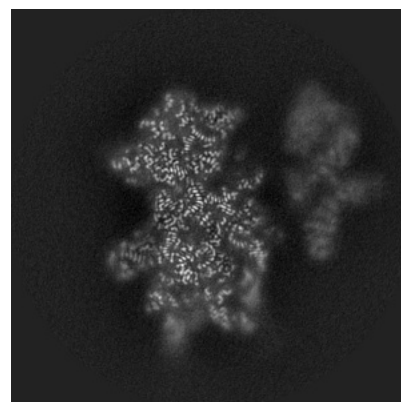
### 5.2.2 Raw map



X Index: 180



Y Index: 180

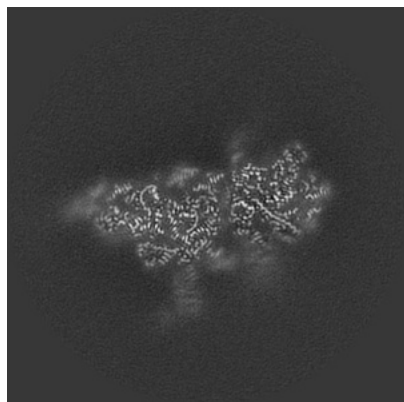


Z Index: 180

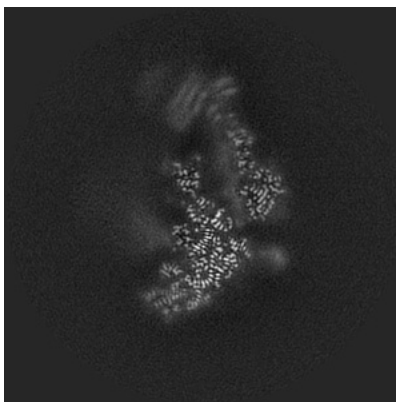
The images above show central slices of the map in three orthogonal directions.

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

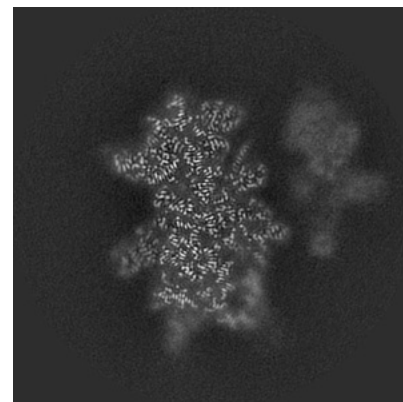
### 5.3.1 Primary map



X Index: 176

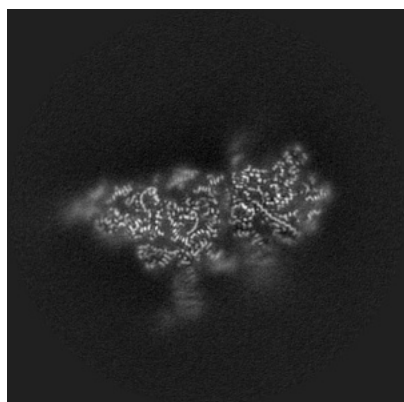


Y Index: 259

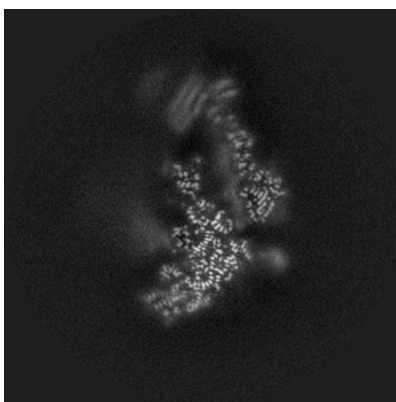


Z Index: 210

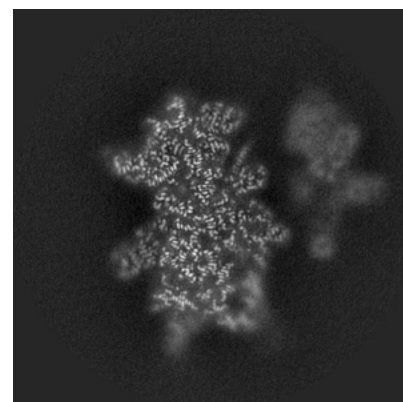
### 5.3.2 Raw map



X Index: 147



Y Index: 216

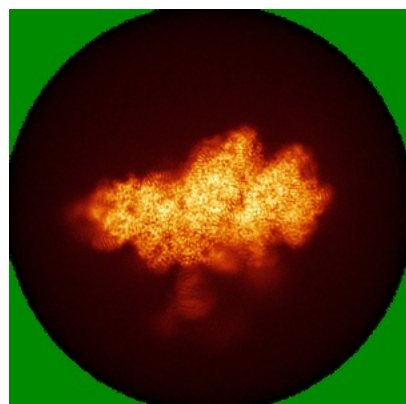


Z Index: 175

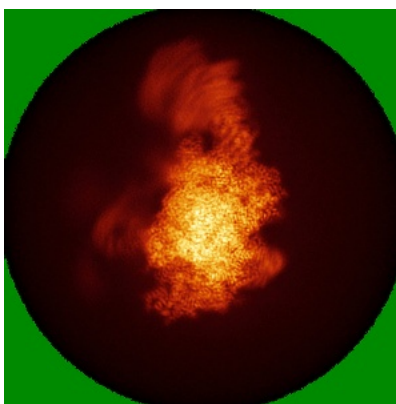
The images above show the largest variance slices of the map in three orthogonal directions.

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

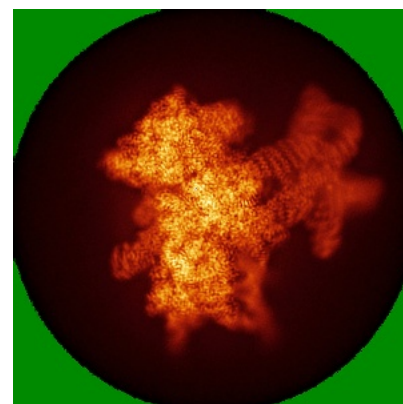
### 5.4.1 Primary map



X

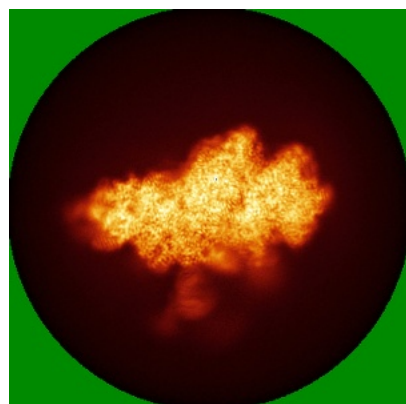


Y

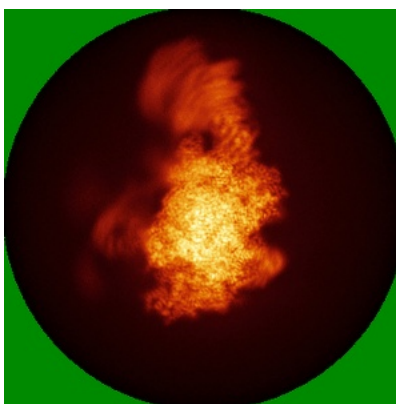


Z

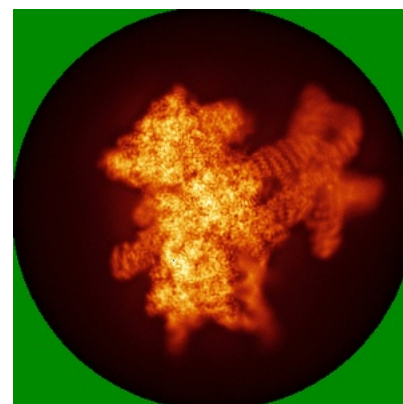
### 5.4.2 Raw map



X



Y

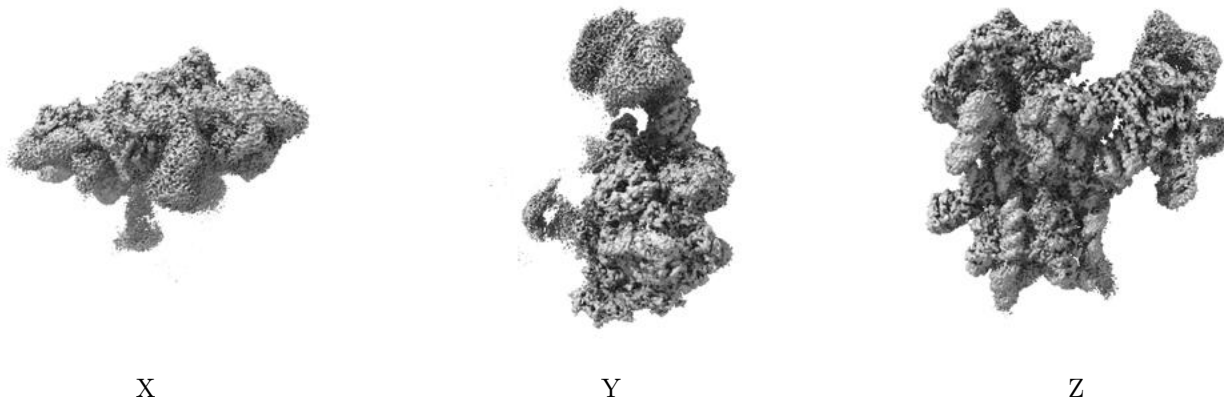


Z

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.

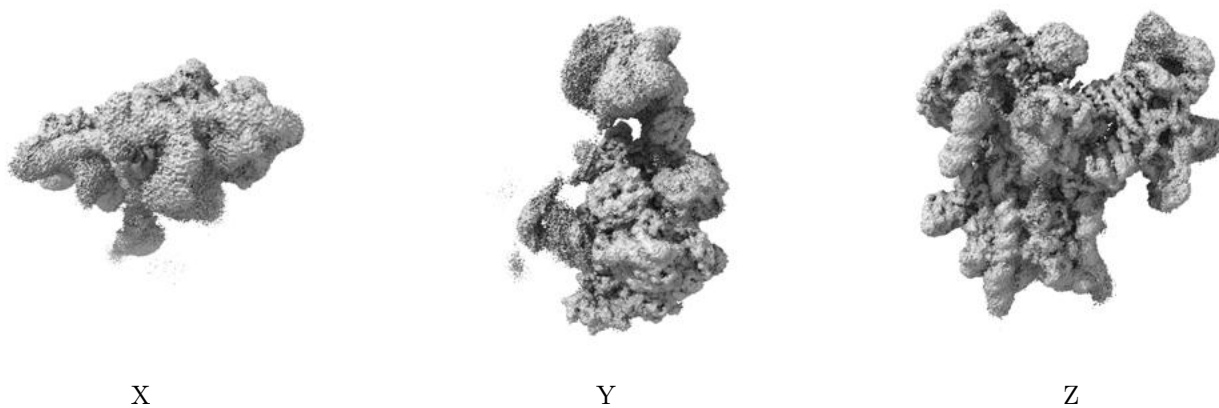
## 5.5 Orthogonal surface views [i](#)

### 5.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 5.5.2 Raw map



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

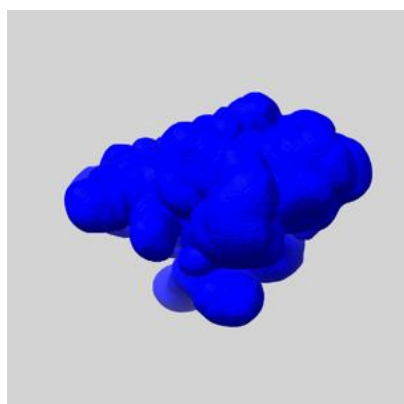
## 5.6 Mask visualisation [i](#)

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

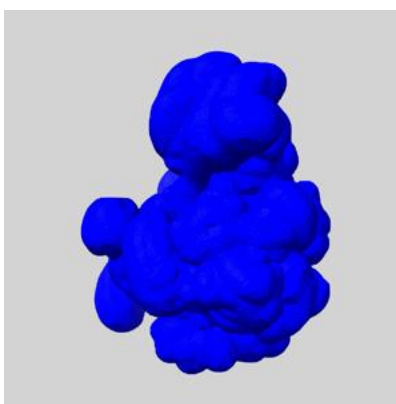
A mask typically either:

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

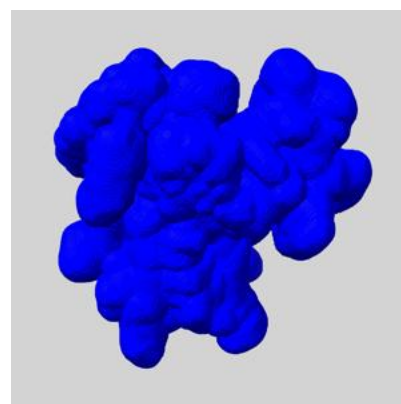
### 5.6.1 emd\_17700\_msk\_1.map [i](#)



X



Y



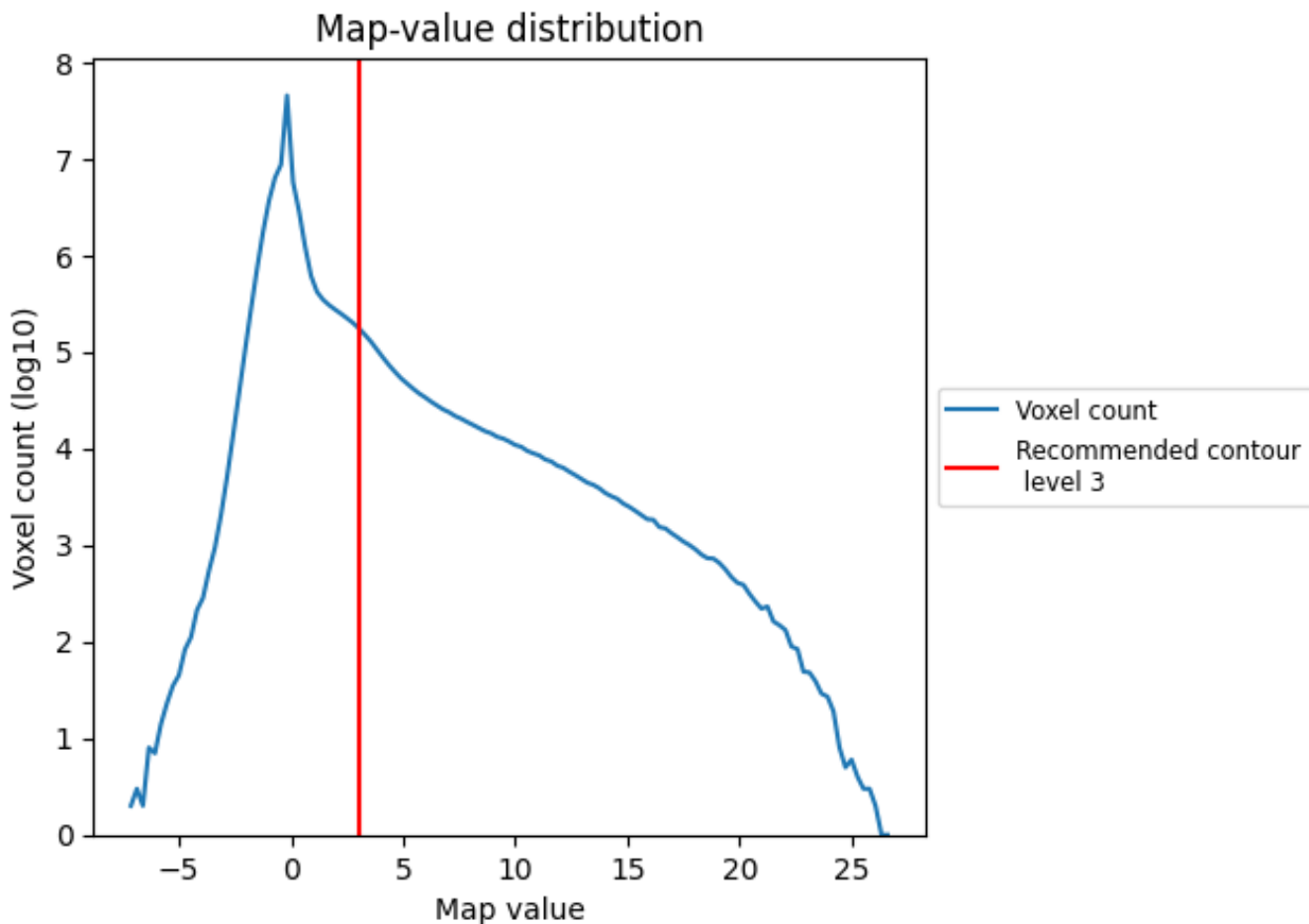
Z



## 6 Map analysis [i](#)

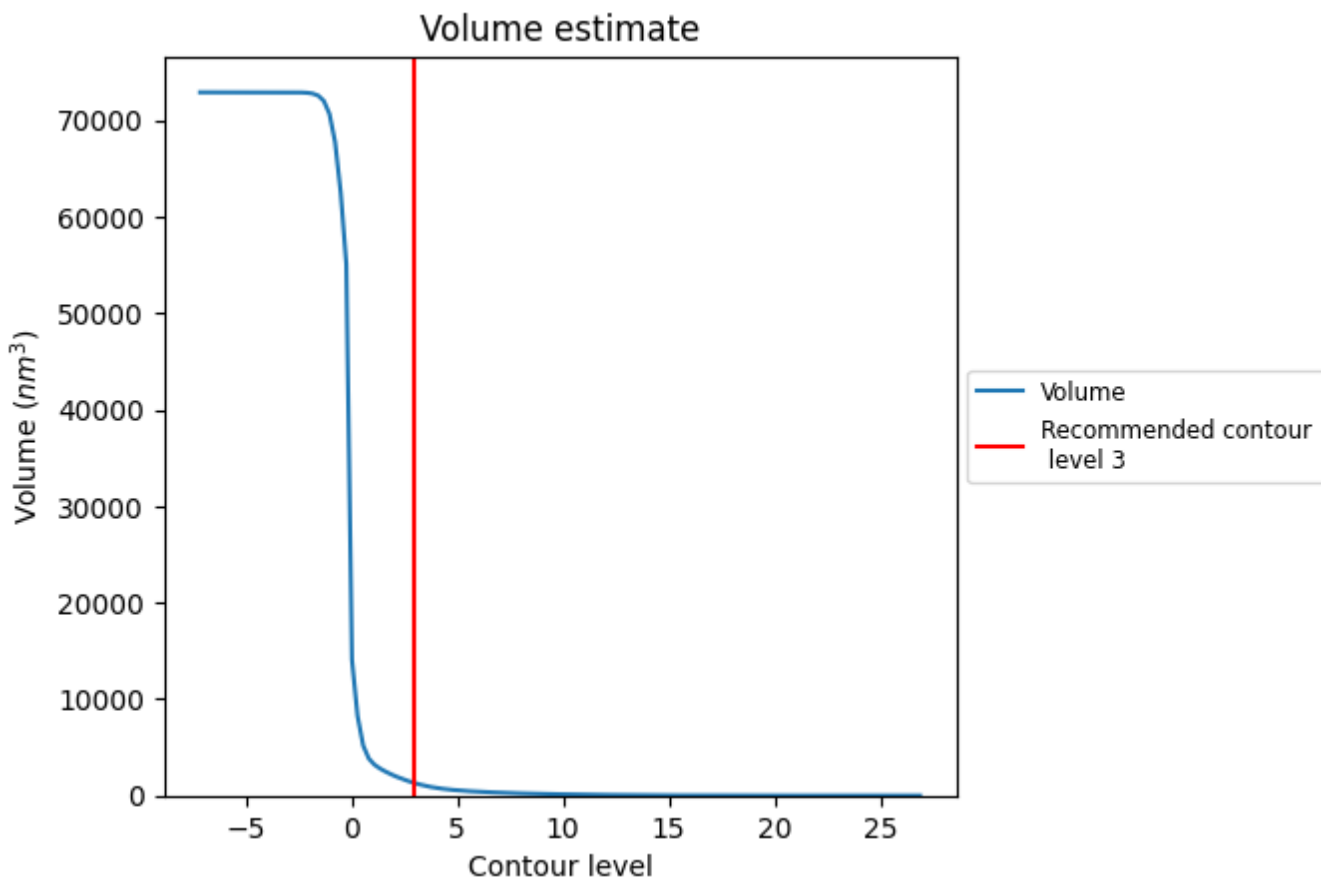
This section contains the results of statistical analysis of the map.

### 6.1 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.

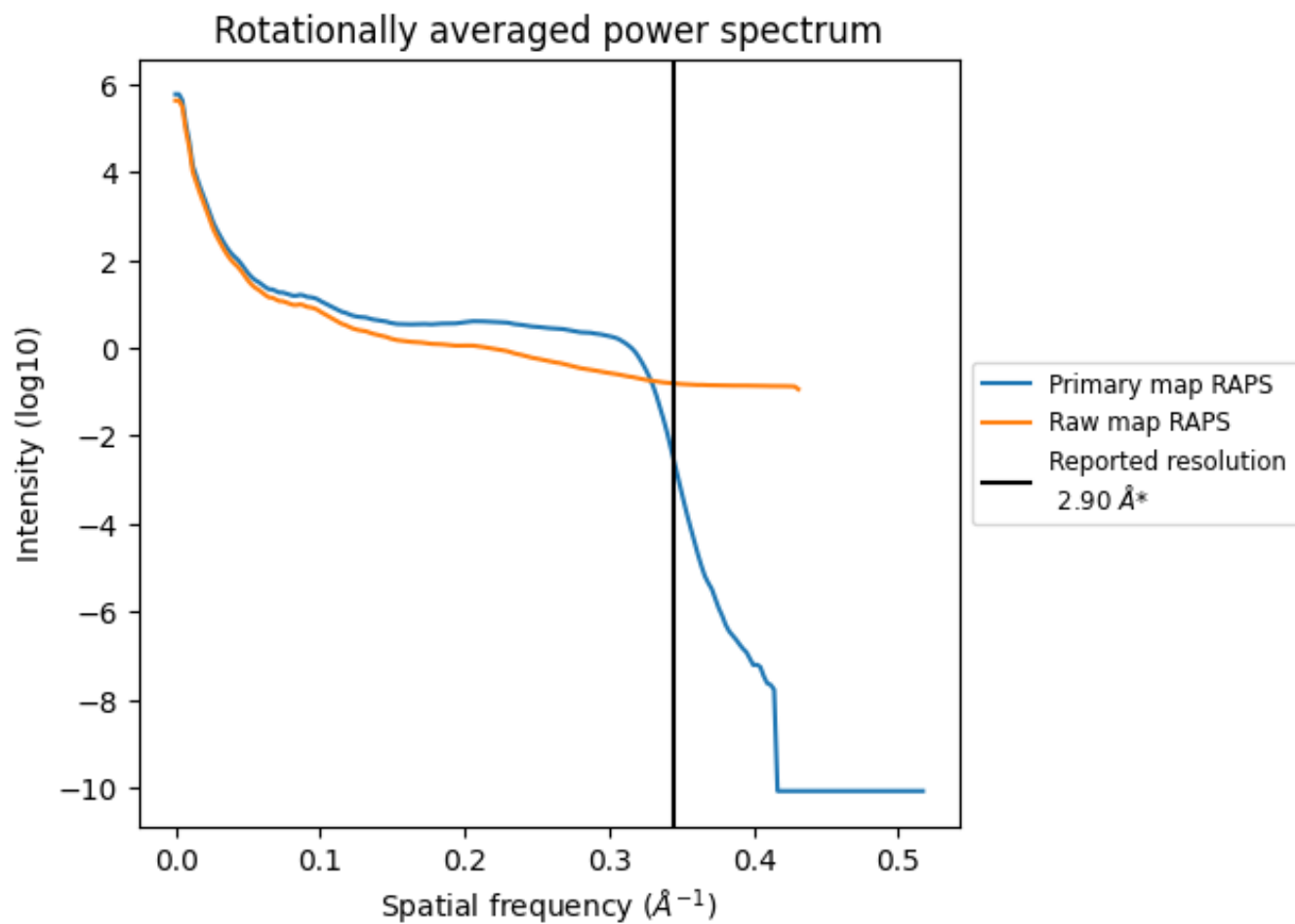
## 6.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1292 nm<sup>3</sup>; this corresponds to an approximate mass of 1167 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.

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

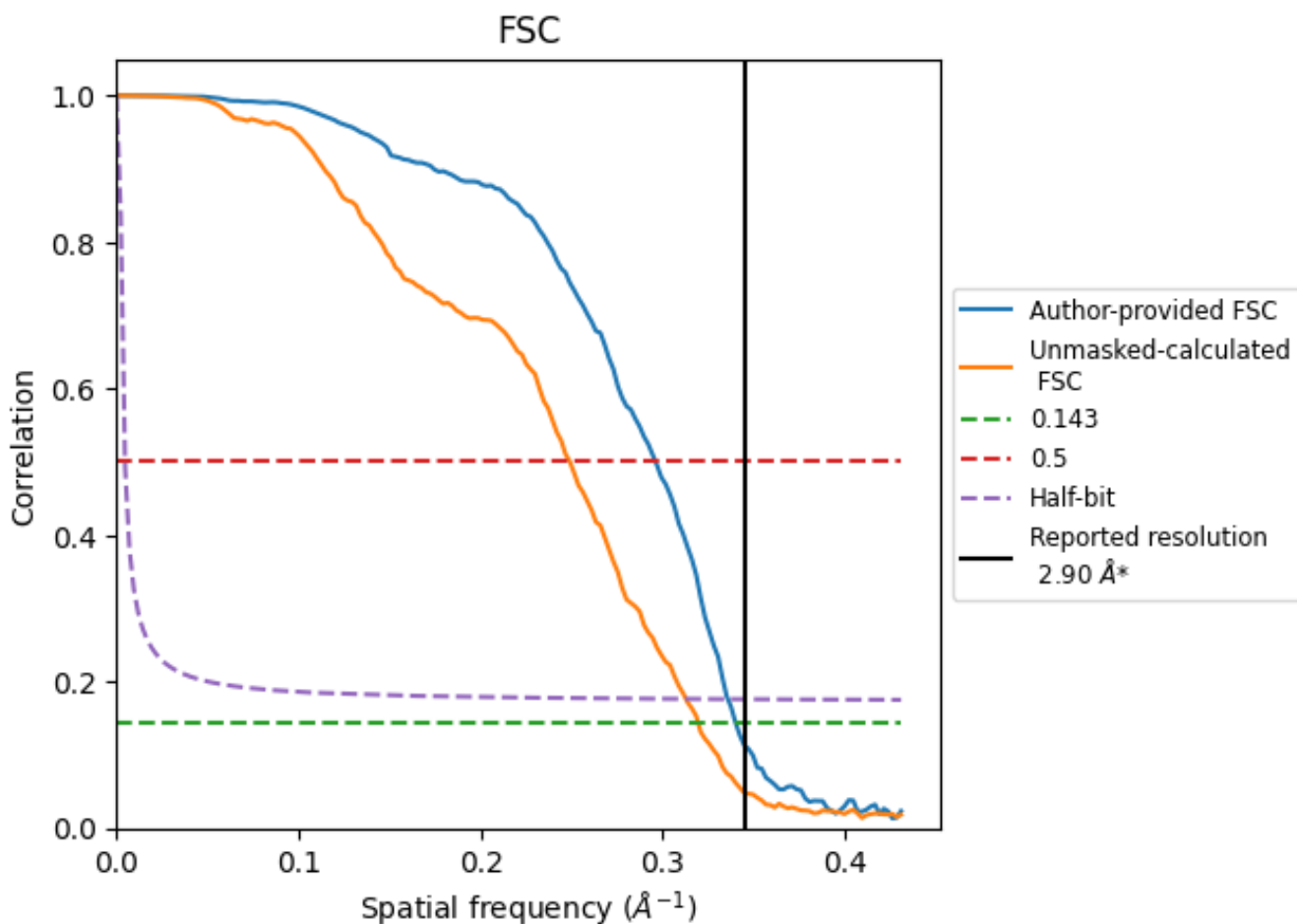


\*Reported resolution corresponds to spatial frequency of 0.345 Å<sup>-1</sup>

## 7 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.

### 7.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.345 Å<sup>-1</sup>

## 7.2 Resolution estimates [i](#)

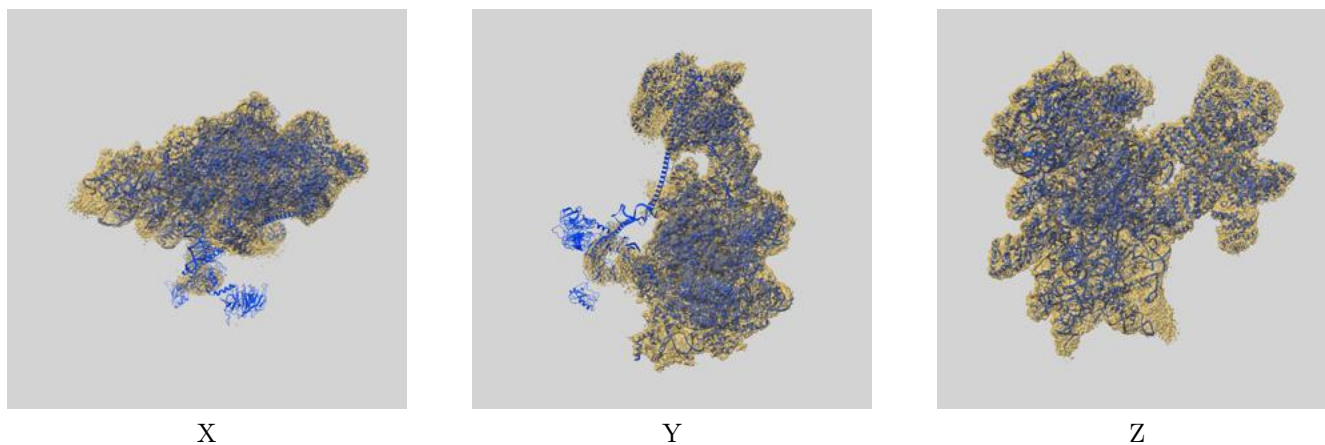
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.90                               | -    | -        |
| Author-provided FSC curve | 2.94                               | 3.38 | 2.98     |
| Unmasked-calculated*      | 3.13                               | 4.01 | 3.20     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

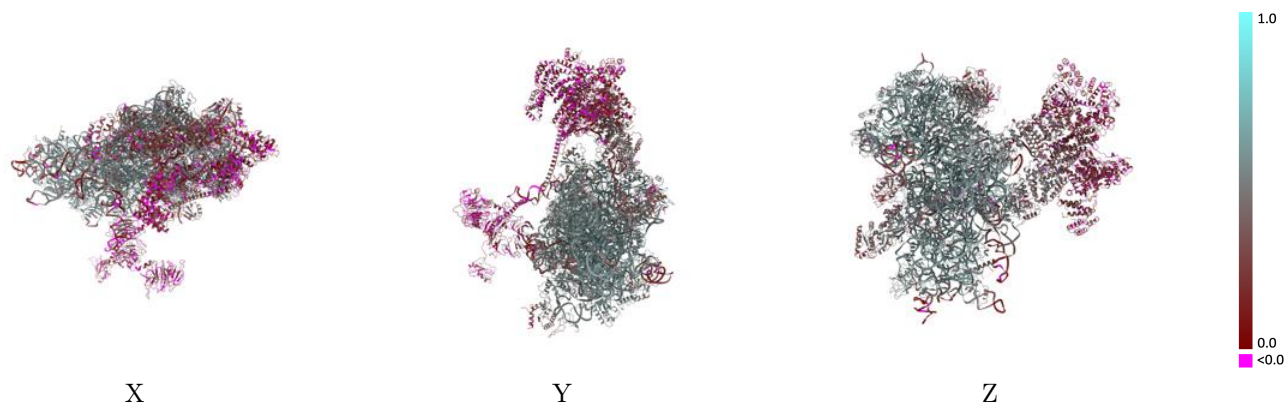
This section contains information regarding the fit between EMDB map EMD-17700 and PDB model 8PJ5. Per-residue inclusion information can be found in section ?? on page ??.

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



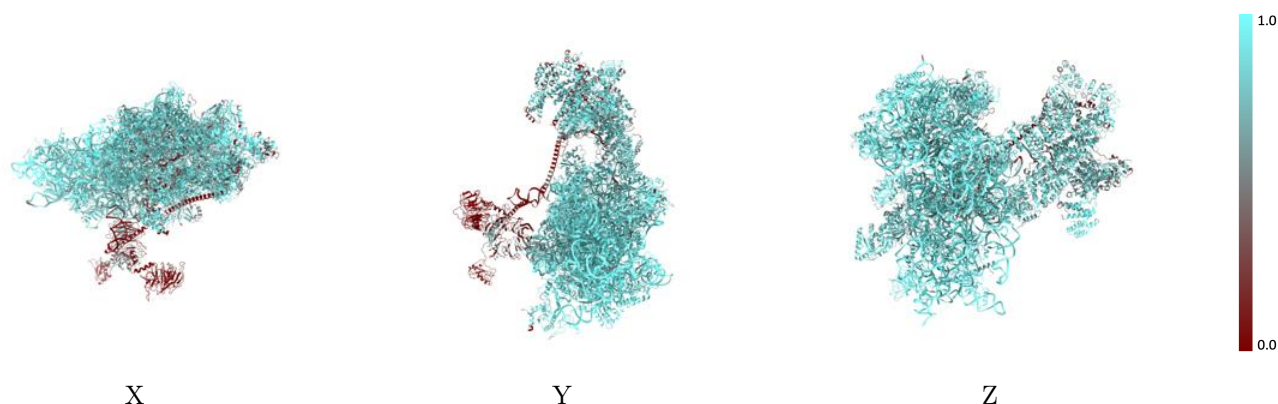
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



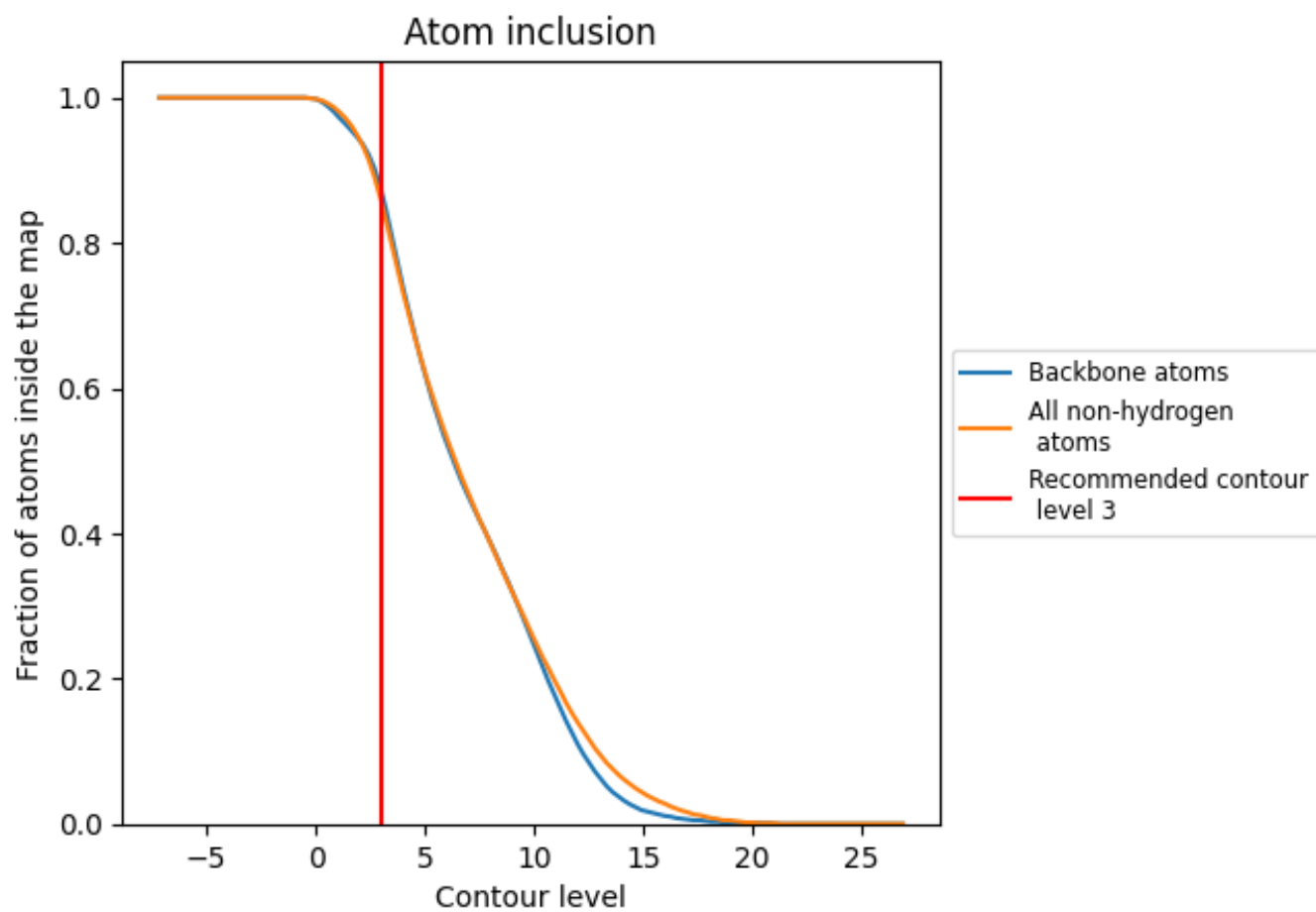
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 8.3 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 (3).

## 8.4 Atom inclusion [i](#)









































































At the recommended contour level, 87% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.



## 8.5 Map-model fit summary



































The table lists the average atom inclusion at the recommended contour level (3) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.8580   |  0.4370   |
| 0     |  0.8160   |  0.3900   |
| 1     |  0.2300   |  0.1250   |
| 2     |  0.0000   |  0.0810   |
| 3     |  0.6210   |  0.1340   |
| 4     |  0.7700   |  0.1600   |
| 5     |  0.7550   |  0.1450   |
| 6     |  0.7550   |  0.1630   |
| 7     |  0.6480   |  0.2570   |
| 8     |  0.6660   |  0.1550   |
| 9     |  0.8660   |  0.5070   |
| A     |  0.9680   |  0.5180   |
| B     |  0.9480   |  0.5560   |
| C     |  0.9540   |  0.5540   |
| D     |  0.9310  |  0.5420  |
| E     |  0.9480 |  0.5580 |
| F     |  0.8610 |  0.5050 |
| G     |  0.8570 |  0.4660 |
| H     |  0.9110 |  0.5190 |
| I     |  0.9260 |  0.5370 |
| J     |  0.9510 |  0.5600 |
| K     |  0.9190 |  0.5250 |
| L     |  0.9100 |  0.5470 |
| M     |  0.8670 |  0.5120 |
| N     |  0.9380 |  0.5440 |
| O     |  0.9280 |  0.5270 |
| P     |  0.9150 |  0.5250 |
| Q     |  0.9300 |  0.5430 |
| R     |  0.9570 |  0.5250 |
| S     |  0.9460 |  0.4950 |
| T     |  0.9430 |  0.5270 |
| V     |  0.9240 |  0.5360 |
| Y     |  0.9670 |  0.5570 |
| Z     |  0.8790 |  0.5170 |
| a     |  0.9360 |  0.5160 |



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| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| b     |  0.9380 |  0.5370 |
| c     |  0.9230 |  0.4990 |
| d     |  0.9560 |  0.5470 |
| e     |  0.8760 |  0.5080 |
| f     |  0.9140 |  0.5130 |
| h     |  0.9110 |  0.4910 |
| i     |  0.9580 |  0.5670 |
| k     |  0.8590 |  0.3870 |
| m     |  0.8110 |  0.3500 |
| n     |  0.8540 |  0.4940 |
| o     |  0.6480 |  0.3030 |
| q     |  0.8250 |  0.5010 |
| u     |  0.6850 |  0.2860 |
| v     |  0.7430 |  0.1900 |
| w     |  0.9360 |  0.3200 |
| x     |  0.7740 |  0.3550 |
| y     |  0.7960 |  0.3640 |