



# wwPDB EM Validation Summary Report ⓘ

May 25, 2024 – 08:37 AM EDT

PDB ID : 7NAP  
EMDB ID : EMD-24277  
Title : Human PA28-20S-PA28 proteasome complex  
Authors : Zhao, J.; Makhija, S.; Huang, B.; Cheng, Y.  
Deposited on : 2021-06-22  
Resolution : 3.20 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>.

---

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

EMDB validation analysis : 0.0.1.dev92  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2











Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 5   | S     | 263    | 91% 9%           |
| 6   | F     | 255    | 94% 6%           |
| 6   | T     | 255    | 94% 6%           |
| 7   | G     | 246    | 97% .            |
| 7   | U     | 246    | 97% .            |
| 8   | H     | 277    | 79% . 20%        |
| 8   | V     | 277    | 79% . 20%        |
| 9   | I     | 205    | 99% .            |
| 9   | W     | 205    | 99% .            |
| 10  | J     | 201    | 98% .            |
| 10  | X     | 201    | 98% .            |
| 11  | K     | 263    | 76% 24%          |
| 11  | Y     | 263    | 76% 24%          |
| 12  | L     | 241    | 88% 12%          |
| 12  | Z     | 241    | 88% 12%          |
| 13  | M     | 264    | 81% 19%          |
| 13  | a     | 264    | 81% 19%          |
| 14  | N     | 239    | 85% 15%          |
| 14  | b     | 239    | 85% 15%          |
| 15  | d     | 239    | 91% 9%           |
| 15  | f     | 239    | 88% 12%          |
| 15  | h     | 239    | 90% 10%          |
| 15  | i     | 239    | 90% 9%           |
| 15  | k     | 239    | 91% 9%           |
| 15  | m     | 239    | 88% 12%          |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 15  | o     | 239    |  90% 10% |
| 15  | p     | 239    |  90% 9%  |
| 16  | c     | 249    |  85% 15% |
| 16  | e     | 249    |  85% 15% |
| 16  | g     | 249    |  85% 15% |
| 16  | j     | 249    |  85% 15% |
| 16  | l     | 249    |  85% 15% |
| 16  | n     | 249    |  85% 15% |

## 2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 69762 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 Proteasome subunit alpha type-2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 1   | O     | 229      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1696  | 1101 | 294 | 295 | 6 |         |       |
| 1   | A     | 229      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1696  | 1101 | 294 | 295 | 6 |         |       |

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
|     |       |          | Total | C    | N   | O   | S  |         |       |
| 2   | P     | 249      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1793  | 1146 | 318 | 319 | 10 |         |       |
| 2   | B     | 249      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1793  | 1146 | 318 | 319 | 10 |         |       |

- Molecule 3 is a protein called Proteasome subunit alpha type-7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 3   | Q     | 235      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1703  | 1082 | 314 | 302 | 5 |         |       |
| 3   | C     | 235      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1703  | 1082 | 314 | 302 | 5 |         |       |

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
|     |       |          | Total | C    | N   | O   | S  |         |       |
| 4   | R     | 241      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1751  | 1116 | 301 | 322 | 12 |         |       |
| 4   | D     | 241      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1751  | 1116 | 301 | 322 | 12 |         |       |

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | S     | 239      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1810  | 1144 | 331 | 324 | 11 |         |       |
| 5   | E     | 239      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1810  | 1144 | 331 | 324 | 11 |         |       |

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6   | T     | 240      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1785  | 1145 | 313 | 316 | 11 |         |       |
| 6   | F     | 240      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1785  | 1145 | 313 | 316 | 11 |         |       |

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7   | U     | 239      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1769  | 1133 | 305 | 319 | 12 |         |       |
| 7   | G     | 239      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1769  | 1133 | 305 | 319 | 12 |         |       |

- Molecule 8 is a protein called Proteasome subunit beta type-7.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 8   | V     | 222      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1609  | 1023 | 276 | 299 | 11 |         |       |
| 8   | H     | 222      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1609  | 1023 | 276 | 299 | 11 |         |       |

- Molecule 9 is a protein called Proteasome subunit beta type-3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 9   | W     | 204      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1564  | 1003 | 264 | 278 | 19 |         |       |
| 9   | I     | 204      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1564  | 1003 | 264 | 278 | 19 |         |       |

- Molecule 10 is a protein called Proteasome subunit beta type-2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | X     | 197      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1544  | 998 | 265 | 272 | 9 |         |       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 10  | J     | 197      | 1544  | 998 | 265 | 272 | 9 | 0       | 0     |

- Molecule 11 is a protein called Proteasome subunit beta type-5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 11  | Y     | 200      | 1525  | 968 | 273 | 275 | 9 | 0       | 0     |
| 11  | K     | 200      | 1525  | 968 | 273 | 275 | 9 | 0       | 0     |

- Molecule 12 is a protein called Proteasome subunit beta type-1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
|     |       |          | Total | C    | N   | O   | S  |         |       |
| 12  | Z     | 213      | 1599  | 1022 | 279 | 288 | 10 | 0       | 0     |
| 12  | L     | 213      | 1599  | 1022 | 279 | 288 | 10 | 0       | 0     |

- Molecule 13 is a protein called Proteasome subunit beta type-4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
|     |       |          | Total | C    | N   | O   | S  |         |       |
| 13  | a     | 215      | 1643  | 1043 | 289 | 299 | 12 | 0       | 0     |
| 13  | M     | 215      | 1643  | 1043 | 289 | 299 | 12 | 0       | 0     |

- Molecule 14 is a protein called Proteasome subunit beta type-6.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
|     |       |          | Total | C   | N   | O   | S  |         |       |
| 14  | b     | 202      | 1491  | 939 | 258 | 282 | 12 | 0       | 0     |
| 14  | N     | 202      | 1491  | 939 | 258 | 282 | 12 | 0       | 0     |

- Molecule 15 is a protein called Proteasome activator complex subunit 2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 15  | k     | 217      | 1686  | 1094 | 284 | 304 | 4 | 0       | 0     |
| 15  | m     | 211      | 1648  | 1069 | 279 | 297 | 3 | 0       | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 15  | o     | 216      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1677  | 1087 | 285 | 301 | 4 |         |       |
| 15  | p     | 217      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1695  | 1099 | 287 | 305 | 4 |         |       |
| 15  | d     | 217      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1686  | 1094 | 284 | 304 | 4 |         |       |
| 15  | f     | 211      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1648  | 1069 | 279 | 297 | 3 |         |       |
| 15  | h     | 216      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1677  | 1087 | 285 | 301 | 4 |         |       |
| 15  | i     | 217      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1695  | 1099 | 287 | 305 | 4 |         |       |

- Molecule 16 is a protein called Proteasome activator complex subunit 1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 16  | j     | 212      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1626  | 1049 | 282 | 291 | 4 |         |       |
| 16  | l     | 211      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1641  | 1059 | 282 | 295 | 5 |         |       |
| 16  | n     | 211      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1626  | 1050 | 281 | 289 | 6 |         |       |
| 16  | c     | 212      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1626  | 1049 | 282 | 291 | 4 |         |       |
| 16  | e     | 211      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1641  | 1059 | 282 | 295 | 5 |         |       |
| 16  | g     | 211      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1626  | 1050 | 281 | 289 | 6 |         |       |

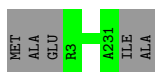


### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

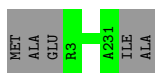
- Molecule 1: Proteasome subunit alpha type-2

Chain O:  98%



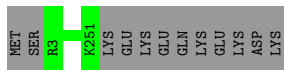
- Molecule 1: Proteasome subunit alpha type-2

Chain A:  98%



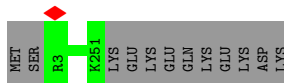
- Molecule 2: Proteasome subunit alpha type-4

Chain P:  95%



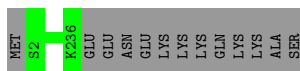
- Molecule 2: Proteasome subunit alpha type-4

Chain B:  95%



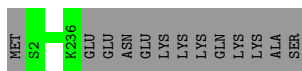
- Molecule 3: Proteasome subunit alpha type-7

Chain Q:  95%



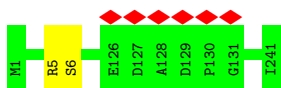
- Molecule 3: Proteasome subunit alpha type-7

Chain C:  95% 5%



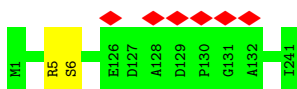
- Molecule 4: Proteasome subunit alpha type-5

Chain R:  99%




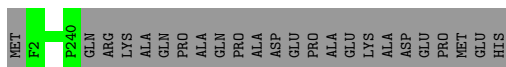
- Molecule 4: Proteasome subunit alpha type-5

Chain D:  99%




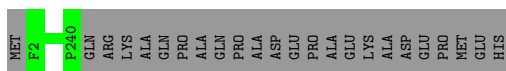
- Molecule 5: Proteasome subunit alpha type-1

Chain S:  91% 9%



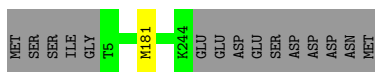
- Molecule 5: Proteasome subunit alpha type-1

Chain E:  91% 9%



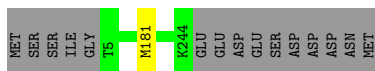
- Molecule 6: Proteasome subunit alpha type-3

Chain T:  94% 6%



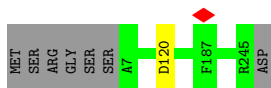
- Molecule 6: Proteasome subunit alpha type-3

Chain F:  94% 6%



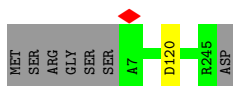
- Molecule 7: Proteasome subunit alpha type-6

Chain U:  97%




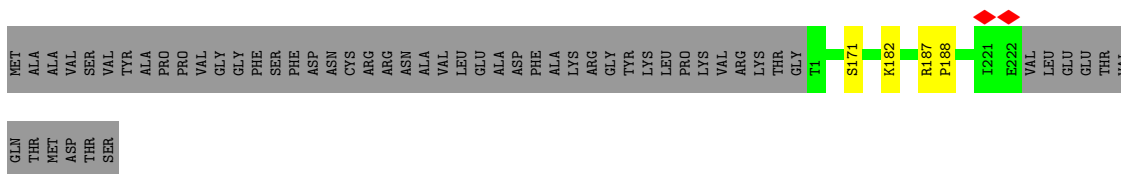
- Molecule 7: Proteasome subunit alpha type-6

Chain G:  97%




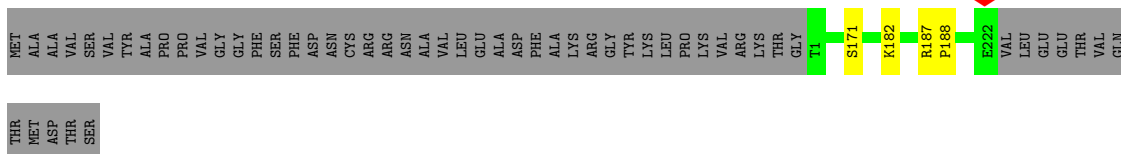
- Molecule 8: Proteasome subunit beta type-7

Chain V:  79% 20%



- Molecule 8: Proteasome subunit beta type-7

Chain H:  79% 20%



- Molecule 9: Proteasome subunit beta type-3

Chain W:  99%



- Molecule 9: Proteasome subunit beta type-3

Chain I:  99%



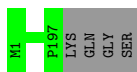
- Molecule 10: Proteasome subunit beta type-2

Chain X:  98%



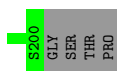
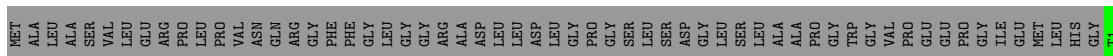
- Molecule 10: Proteasome subunit beta type-2

Chain J:  98%




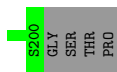
- Molecule 11: Proteasome subunit beta type-5

Chain Y:  76% 24%




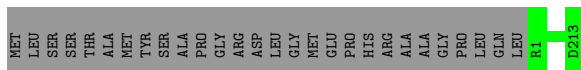
- Molecule 11: Proteasome subunit beta type-5

Chain K:  76% 24%




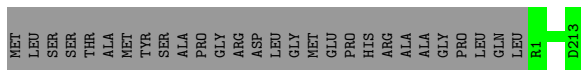
- Molecule 12: Proteasome subunit beta type-1

Chain Z:  88% 12%




- Molecule 12: Proteasome subunit beta type-1

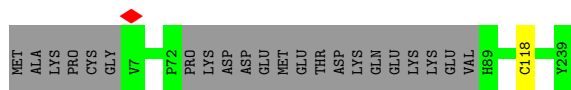
Chain L:  88% 12%



- Molecule 13: Proteasome subunit beta type-4

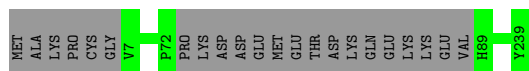
Chain a:  81% 19%





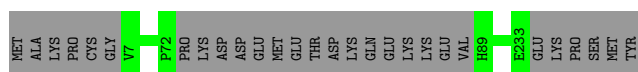
- Molecule 15: Proteasome activator complex subunit 2

Chain d: 91% 9%



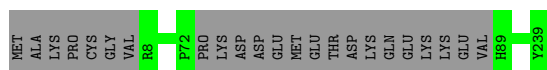
- Molecule 15: Proteasome activator complex subunit 2

Chain f: 88% 12%



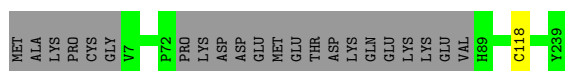
- Molecule 15: Proteasome activator complex subunit 2

Chain h: 90% 10%



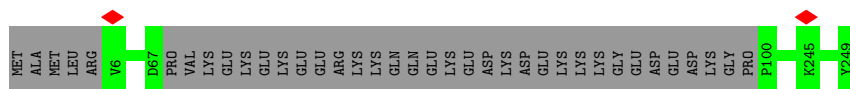
- Molecule 15: Proteasome activator complex subunit 2

Chain i: 90% 9%



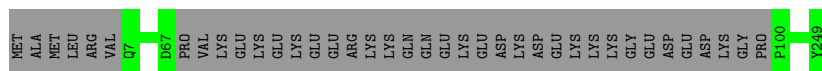
- Molecule 16: Proteasome activator complex subunit 1

Chain j: 85% 15%



- Molecule 16: Proteasome activator complex subunit 1

Chain l: 85% 15%



- Molecule 16: Proteasome activator complex subunit 1

Chain n: 85% 15%



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 22946                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI POLARA 300                          | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 40                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 24.562                                  | Depositor |
| Minimum map value                    | -12.511                                 | Depositor |
| Average map value                    | -0.000                                  | Depositor |
| Map value standard deviation         | 1.000                                   | Depositor |
| Recommended contour level            | 4.0                                     | Depositor |
| Map size (Å)                         | 466.7904, 466.7904, 466.7904            | wwPDB     |
| Map dimensions                       | 384, 384, 384                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.2156, 1.2156, 1.2156                  | Depositor |



## 5 Model quality [i](#)

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

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

| Mol | Chain | Bond lengths |         | Bond angles |               |
|-----|-------|--------------|---------|-------------|---------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5       |
| 1   | A     | 0.34         | 0/1735  | 0.55        | 0/2362        |
| 1   | O     | 0.34         | 0/1735  | 0.55        | 0/2362        |
| 2   | B     | 0.31         | 0/1821  | 0.52        | 0/2477        |
| 2   | P     | 0.31         | 0/1821  | 0.52        | 0/2477        |
| 3   | C     | 0.32         | 0/1729  | 0.57        | 0/2356        |
| 3   | Q     | 0.32         | 0/1729  | 0.57        | 0/2356        |
| 4   | D     | 0.31         | 0/1780  | 0.54        | 0/2417        |
| 4   | R     | 0.31         | 0/1780  | 0.54        | 0/2417        |
| 5   | E     | 0.31         | 0/1845  | 0.58        | 0/2504        |
| 5   | S     | 0.31         | 0/1845  | 0.58        | 0/2504        |
| 6   | F     | 0.35         | 0/1820  | 0.55        | 0/2464        |
| 6   | T     | 0.35         | 0/1820  | 0.54        | 0/2464        |
| 7   | G     | 0.33         | 0/1802  | 0.54        | 1/2449 (0.0%) |
| 7   | U     | 0.33         | 0/1802  | 0.54        | 1/2449 (0.0%) |
| 8   | H     | 0.32         | 0/1636  | 0.58        | 0/2223        |
| 8   | V     | 0.32         | 0/1636  | 0.57        | 0/2223        |
| 9   | I     | 0.33         | 0/1593  | 0.55        | 0/2149        |
| 9   | W     | 0.33         | 0/1593  | 0.55        | 0/2149        |
| 10  | J     | 0.34         | 0/1577  | 0.55        | 0/2138        |
| 10  | X     | 0.34         | 0/1577  | 0.55        | 0/2138        |
| 11  | K     | 0.33         | 0/1556  | 0.56        | 0/2104        |
| 11  | Y     | 0.33         | 0/1556  | 0.56        | 0/2104        |
| 12  | L     | 0.33         | 0/1629  | 0.56        | 0/2201        |
| 12  | Z     | 0.33         | 0/1629  | 0.56        | 0/2201        |
| 13  | M     | 0.33         | 0/1676  | 0.61        | 1/2272 (0.0%) |
| 13  | a     | 0.33         | 0/1676  | 0.61        | 1/2272 (0.0%) |
| 14  | N     | 0.34         | 0/1517  | 0.55        | 0/2056        |
| 14  | b     | 0.34         | 0/1517  | 0.55        | 0/2056        |
| 15  | d     | 0.30         | 0/1720  | 0.51        | 0/2338        |
| 15  | f     | 0.30         | 0/1680  | 0.50        | 0/2281        |
| 15  | h     | 0.30         | 0/1710  | 0.51        | 0/2322        |
| 15  | i     | 0.31         | 0/1729  | 0.52        | 0/2349        |
| 15  | k     | 0.30         | 0/1720  | 0.51        | 0/2338        |
| 15  | m     | 0.30         | 0/1680  | 0.50        | 0/2281        |

| Mol | Chain | Bond lengths |         | Bond angles |                |
|-----|-------|--------------|---------|-------------|----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5        |
| 15  | o     | 0.30         | 0/1710  | 0.51        | 0/2322         |
| 15  | p     | 0.31         | 0/1729  | 0.52        | 0/2349         |
| 16  | c     | 0.30         | 0/1657  | 0.49        | 0/2250         |
| 16  | e     | 0.30         | 0/1672  | 0.51        | 0/2265         |
| 16  | g     | 0.30         | 0/1657  | 0.51        | 0/2247         |
| 16  | j     | 0.30         | 0/1657  | 0.49        | 0/2250         |
| 16  | l     | 0.30         | 0/1672  | 0.52        | 0/2265         |
| 16  | n     | 0.30         | 0/1657  | 0.51        | 0/2247         |
| All | All   | 0.32         | 0/71082 | 0.54        | 4/96448 (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 |
|-----|-------|---------------------|---------------------|
| 4   | D     | 0                   | 1                   |
| 4   | R     | 0                   | 1                   |
| 8   | H     | 0                   | 1                   |
| 8   | V     | 0                   | 1                   |
| All | All   | 0                   | 4                   |

There are no bond length outliers.

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 7   | U     | 120 | ASP  | CB-CG-OD1 | 5.66 | 123.39      | 118.30   |
| 13  | a     | 73  | ASP  | CB-CG-OD1 | 5.63 | 123.36      | 118.30   |
| 13  | M     | 73  | ASP  | CB-CG-OD1 | 5.61 | 123.35      | 118.30   |
| 7   | G     | 120 | ASP  | CB-CG-OD1 | 5.60 | 123.34      | 118.30   |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 4   | D     | 5   | ARG  | Peptide |
| 8   | H     | 187 | ARG  | Peptide |
| 4   | R     | 5   | ARG  | Peptide |
| 8   | V     | 187 | ARG  | Peptide |

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

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 1   | A     | 227/234 (97%) | 225 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 1   | O     | 227/234 (97%) | 225 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 2   | B     | 247/261 (95%) | 244 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 2   | P     | 247/261 (95%) | 244 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 3   | C     | 233/248 (94%) | 228 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 3   | Q     | 233/248 (94%) | 228 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 4   | D     | 239/241 (99%) | 232 (97%)  | 6 (2%)  | 1 (0%)   | 34          | 69  |
| 4   | R     | 239/241 (99%) | 232 (97%)  | 6 (2%)  | 1 (0%)   | 34          | 69  |
| 5   | E     | 237/263 (90%) | 233 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 5   | S     | 237/263 (90%) | 233 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 6   | F     | 238/255 (93%) | 237 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 6   | T     | 238/255 (93%) | 237 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 7   | G     | 237/246 (96%) | 234 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 7   | U     | 237/246 (96%) | 234 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 8   | H     | 220/277 (79%) | 215 (98%)  | 3 (1%)  | 2 (1%)   | 17          | 56  |
| 8   | V     | 220/277 (79%) | 215 (98%)  | 3 (1%)  | 2 (1%)   | 17          | 56  |
| 9   | I     | 202/205 (98%) | 198 (98%)  | 3 (2%)  | 1 (0%)   | 29          | 67  |
| 9   | W     | 202/205 (98%) | 198 (98%)  | 3 (2%)  | 1 (0%)   | 29          | 67  |
| 10  | J     | 195/201 (97%) | 190 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 10  | X     | 195/201 (97%) | 190 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 11  | K     | 198/263 (75%) | 197 (100%) | 1 (0%)  | 0        | 100         | 100 |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 11  | Y     | 198/263 (75%)    | 197 (100%) | 1 (0%)   | 0        | 100         | 100 |
| 12  | L     | 211/241 (88%)    | 208 (99%)  | 3 (1%)   | 0        | 100         | 100 |
| 12  | Z     | 211/241 (88%)    | 208 (99%)  | 3 (1%)   | 0        | 100         | 100 |
| 13  | M     | 213/264 (81%)    | 210 (99%)  | 3 (1%)   | 0        | 100         | 100 |
| 13  | a     | 213/264 (81%)    | 210 (99%)  | 3 (1%)   | 0        | 100         | 100 |
| 14  | N     | 200/239 (84%)    | 198 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 14  | b     | 200/239 (84%)    | 198 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 15  | d     | 213/239 (89%)    | 211 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 15  | f     | 207/239 (87%)    | 205 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 15  | h     | 212/239 (89%)    | 210 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 15  | i     | 213/239 (89%)    | 210 (99%)  | 3 (1%)   | 0        | 100         | 100 |
| 15  | k     | 213/239 (89%)    | 211 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 15  | m     | 207/239 (87%)    | 205 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 15  | o     | 212/239 (89%)    | 210 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 15  | p     | 213/239 (89%)    | 210 (99%)  | 3 (1%)   | 0        | 100         | 100 |
| 16  | c     | 208/249 (84%)    | 207 (100%) | 1 (0%)   | 0        | 100         | 100 |
| 16  | e     | 207/249 (83%)    | 205 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 16  | g     | 207/249 (83%)    | 206 (100%) | 1 (0%)   | 0        | 100         | 100 |
| 16  | j     | 208/249 (84%)    | 207 (100%) | 1 (0%)   | 0        | 100         | 100 |
| 16  | l     | 207/249 (83%)    | 206 (100%) | 1 (0%)   | 0        | 100         | 100 |
| 16  | n     | 207/249 (83%)    | 206 (100%) | 1 (0%)   | 0        | 100         | 100 |
| All | All   | 9128/10282 (89%) | 9007 (99%) | 113 (1%) | 8 (0%)   | 54          | 83  |

5 of 8 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | W     | 31  | ALA  |
| 9   | I     | 31  | ALA  |
| 4   | R     | 6   | SER  |
| 8   | V     | 171 | SER  |
| 4   | D     | 6   | SER  |

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

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 |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1   | A     | 158/191 (83%) | 158 (100%) | 0        | 100         | 100 |
| 1   | O     | 158/191 (83%) | 158 (100%) | 0        | 100         | 100 |
| 2   | B     | 159/221 (72%) | 159 (100%) | 0        | 100         | 100 |
| 2   | P     | 159/221 (72%) | 159 (100%) | 0        | 100         | 100 |
| 3   | C     | 152/211 (72%) | 152 (100%) | 0        | 100         | 100 |
| 3   | Q     | 152/211 (72%) | 152 (100%) | 0        | 100         | 100 |
| 4   | D     | 173/203 (85%) | 173 (100%) | 0        | 100         | 100 |
| 4   | R     | 173/203 (85%) | 173 (100%) | 0        | 100         | 100 |
| 5   | E     | 181/224 (81%) | 181 (100%) | 0        | 100         | 100 |
| 5   | S     | 181/224 (81%) | 181 (100%) | 0        | 100         | 100 |
| 6   | F     | 167/212 (79%) | 166 (99%)  | 1 (1%)   | 86          | 94  |
| 6   | T     | 167/212 (79%) | 166 (99%)  | 1 (1%)   | 86          | 94  |
| 7   | G     | 175/210 (83%) | 175 (100%) | 0        | 100         | 100 |
| 7   | U     | 175/210 (83%) | 175 (100%) | 0        | 100         | 100 |
| 8   | H     | 165/228 (72%) | 164 (99%)  | 1 (1%)   | 86          | 94  |
| 8   | V     | 165/228 (72%) | 164 (99%)  | 1 (1%)   | 86          | 94  |
| 9   | I     | 164/174 (94%) | 163 (99%)  | 1 (1%)   | 86          | 94  |
| 9   | W     | 164/174 (94%) | 163 (99%)  | 1 (1%)   | 86          | 94  |
| 10  | J     | 156/171 (91%) | 156 (100%) | 0        | 100         | 100 |
| 10  | X     | 156/171 (91%) | 156 (100%) | 0        | 100         | 100 |
| 11  | K     | 146/202 (72%) | 146 (100%) | 0        | 100         | 100 |
| 11  | Y     | 146/202 (72%) | 146 (100%) | 0        | 100         | 100 |
| 12  | L     | 161/199 (81%) | 161 (100%) | 0        | 100         | 100 |
| 12  | Z     | 161/199 (81%) | 161 (100%) | 0        | 100         | 100 |
| 13  | M     | 166/215 (77%) | 166 (100%) | 0        | 100         | 100 |
| 13  | a     | 166/215 (77%) | 166 (100%) | 0        | 100         | 100 |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 14  | N     | 149/181 (82%)   | 149 (100%)  | 0        | 100         | 100 |
| 14  | b     | 149/181 (82%)   | 149 (100%)  | 0        | 100         | 100 |
| 15  | d     | 174/212 (82%)   | 174 (100%)  | 0        | 100         | 100 |
| 15  | f     | 172/212 (81%)   | 172 (100%)  | 0        | 100         | 100 |
| 15  | h     | 173/212 (82%)   | 173 (100%)  | 0        | 100         | 100 |
| 15  | i     | 175/212 (82%)   | 174 (99%)   | 1 (1%)   | 86          | 94  |
| 15  | k     | 174/212 (82%)   | 174 (100%)  | 0        | 100         | 100 |
| 15  | m     | 172/212 (81%)   | 172 (100%)  | 0        | 100         | 100 |
| 15  | o     | 173/212 (82%)   | 173 (100%)  | 0        | 100         | 100 |
| 15  | p     | 175/212 (82%)   | 174 (99%)   | 1 (1%)   | 86          | 94  |
| 16  | c     | 165/224 (74%)   | 165 (100%)  | 0        | 100         | 100 |
| 16  | e     | 170/224 (76%)   | 170 (100%)  | 0        | 100         | 100 |
| 16  | g     | 167/224 (75%)   | 167 (100%)  | 0        | 100         | 100 |
| 16  | j     | 165/224 (74%)   | 165 (100%)  | 0        | 100         | 100 |
| 16  | l     | 170/224 (76%)   | 170 (100%)  | 0        | 100         | 100 |
| 16  | n     | 167/224 (75%)   | 167 (100%)  | 0        | 100         | 100 |
| All | All   | 6936/8724 (80%) | 6928 (100%) | 8 (0%)   | 93          | 98  |

5 of 8 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | i     | 118 | CYS  |
| 9   | I     | 98  | ARG  |
| 6   | F     | 181 | MET  |
| 15  | p     | 118 | CYS  |
| 8   | H     | 182 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 146 | GLN  |
| 10  | J     | 63  | ASN  |
| 16  | g     | 27  | ASN  |
| 9   | I     | 32  | GLN  |
| 12  | L     | 151 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 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.

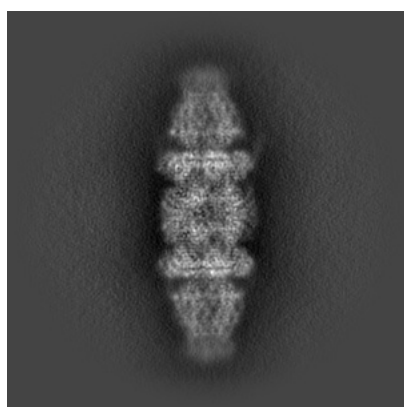
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24277. These allow visual inspection of the internal detail of the map and identification of artifacts.

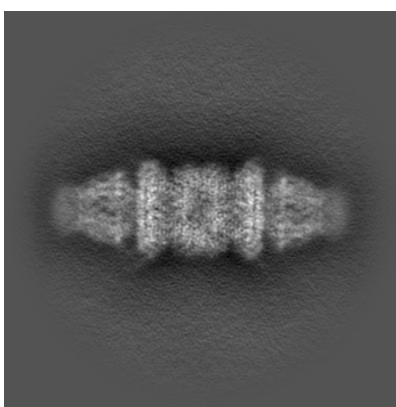
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

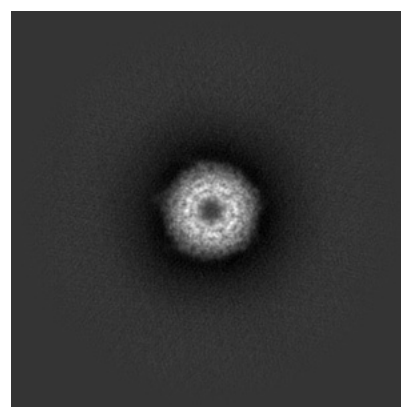
#### 6.1.1 Primary map



X



Y

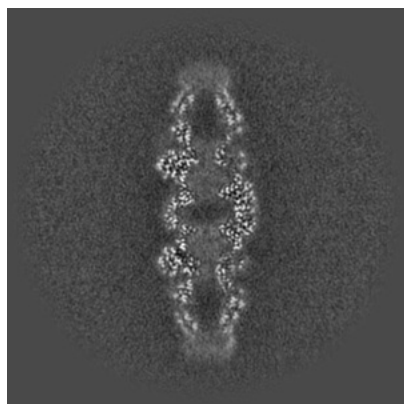


Z

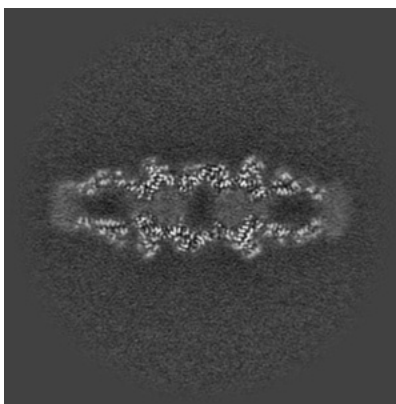
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

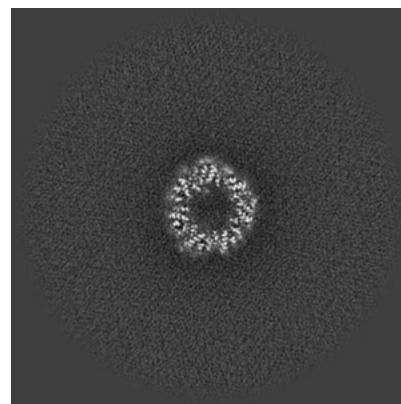
#### 6.2.1 Primary map



X Index: 192



Y Index: 192



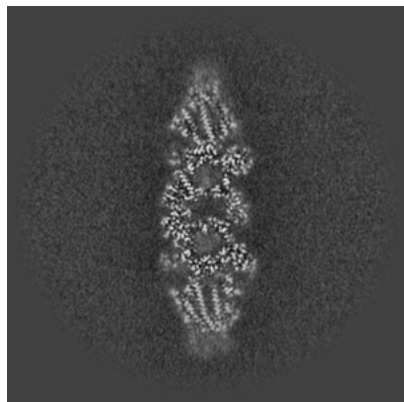
Z Index: 192



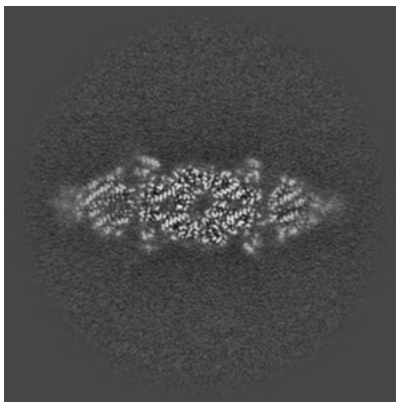
The images above show central slices of the map in three orthogonal directions.

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

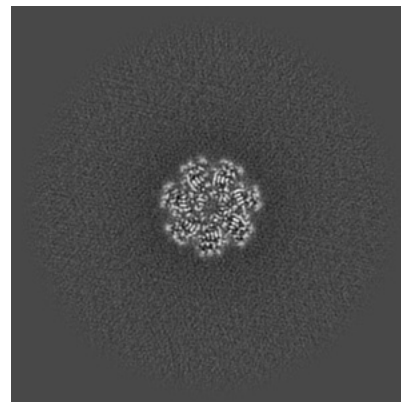
### 6.3.1 Primary map



X Index: 207



Y Index: 211

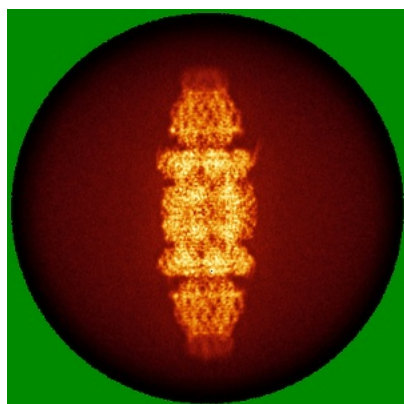


Z Index: 235

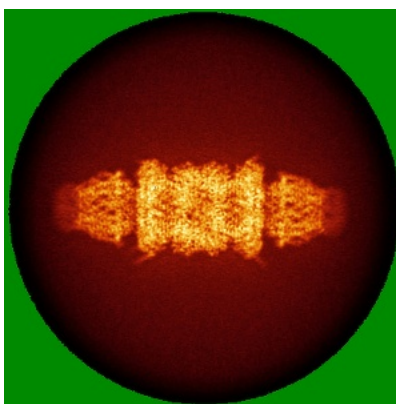
The images above show the largest variance slices of the map in three orthogonal directions.

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

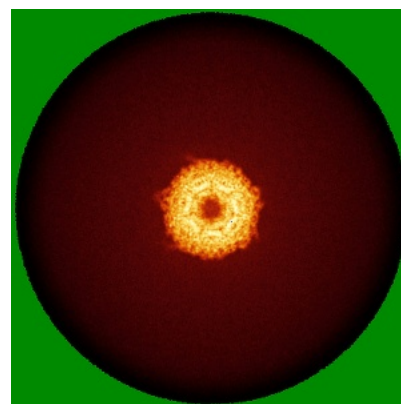
### 6.4.1 Primary map



X



Y

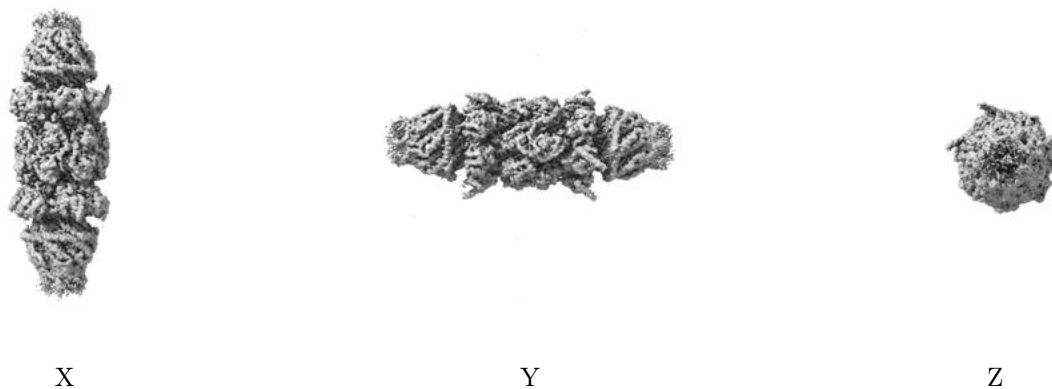


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

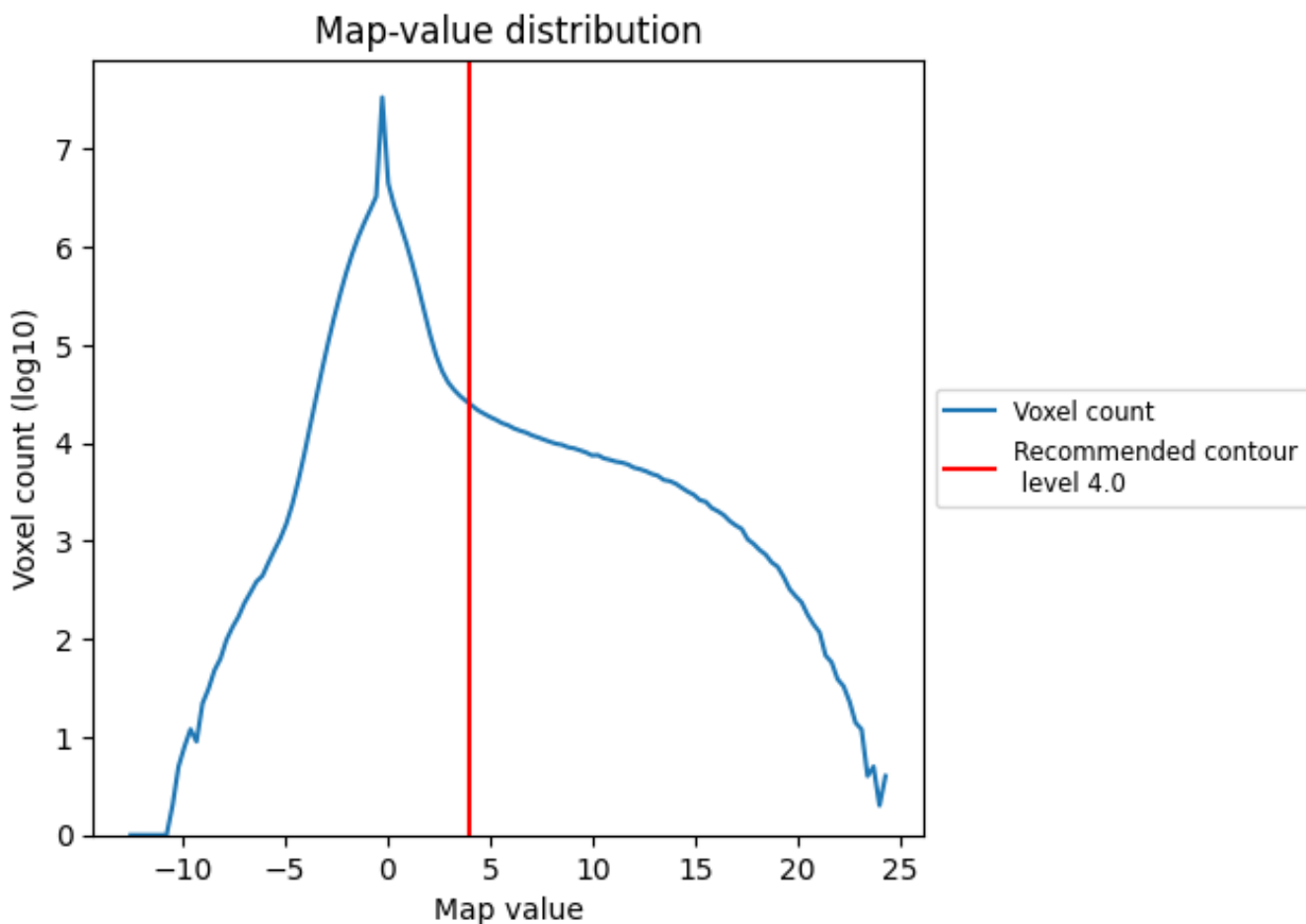
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

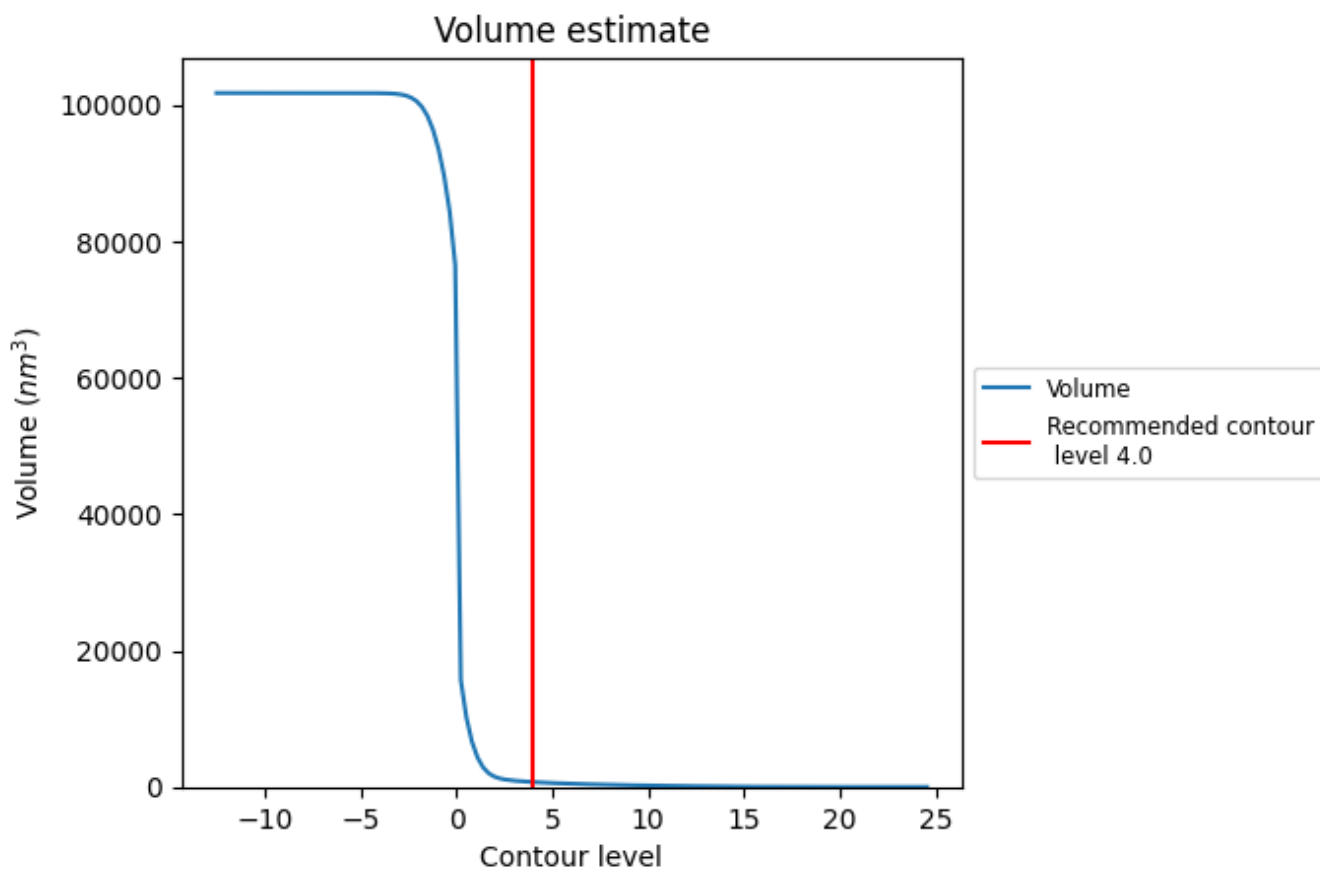
This section contains the results of statistical analysis of the map.

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



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

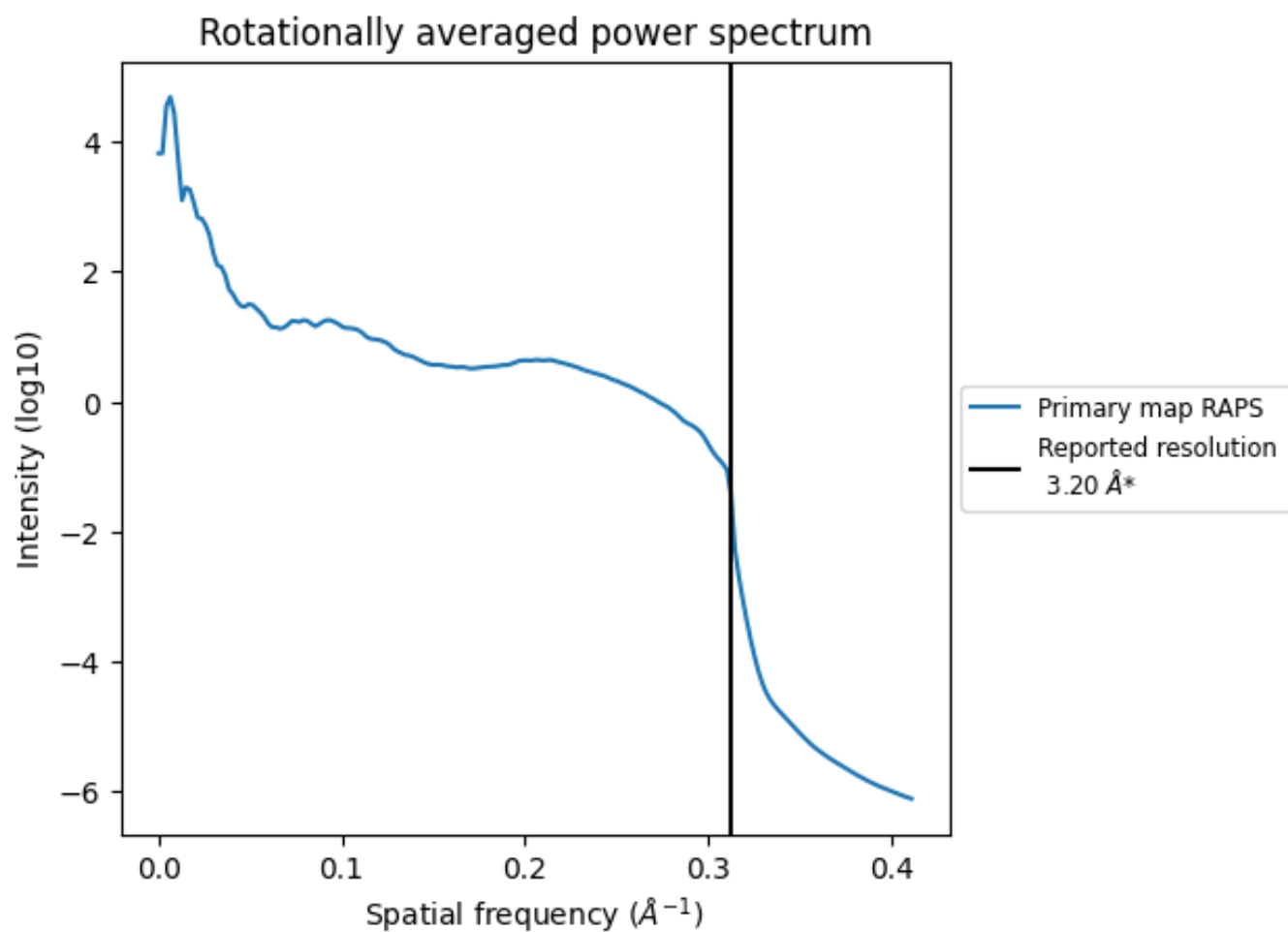
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 718  $\text{nm}^3$ ; this corresponds to an approximate mass of 648 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 i

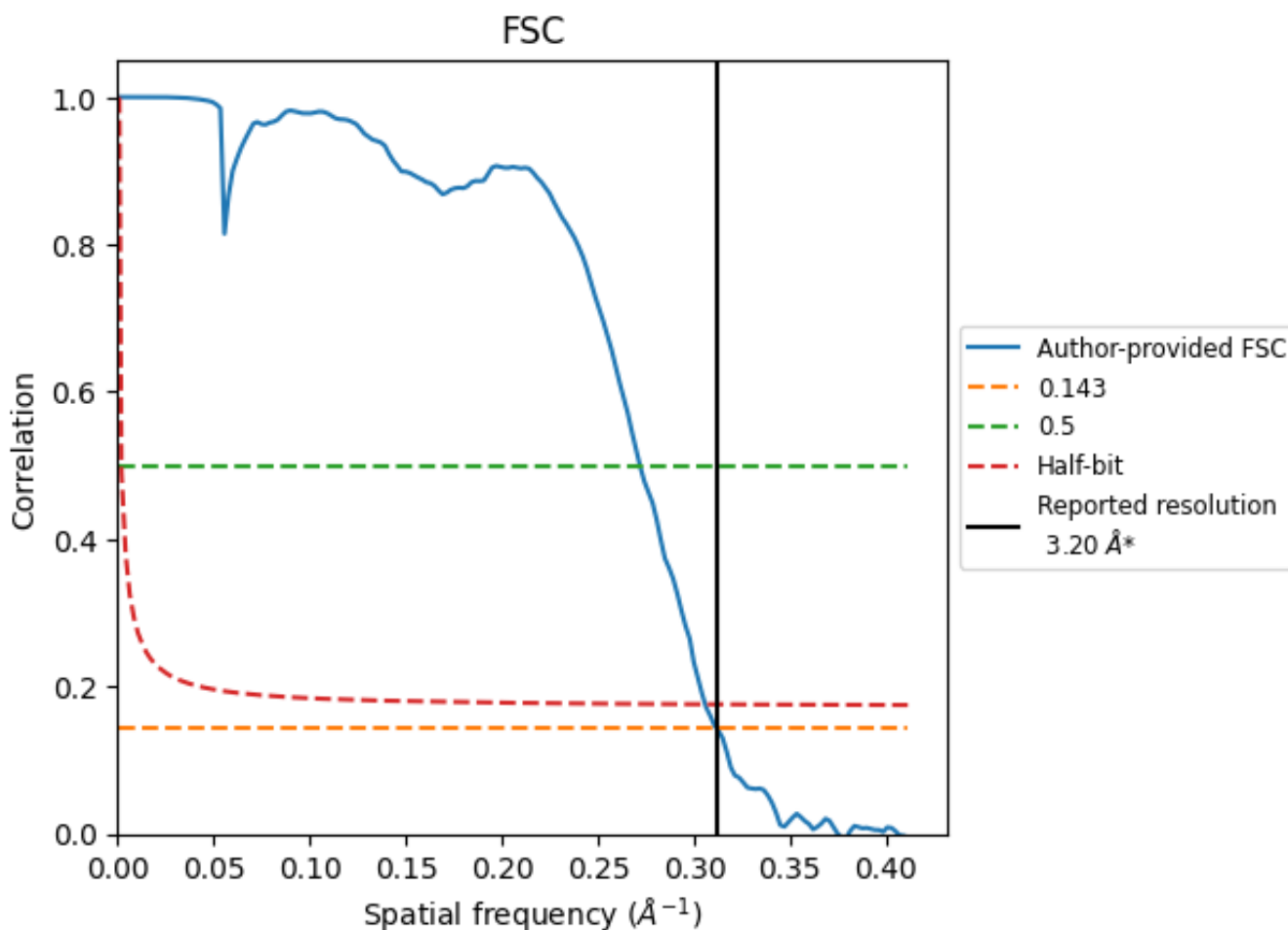


\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [\(i\)](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [\(i\)](#)



\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

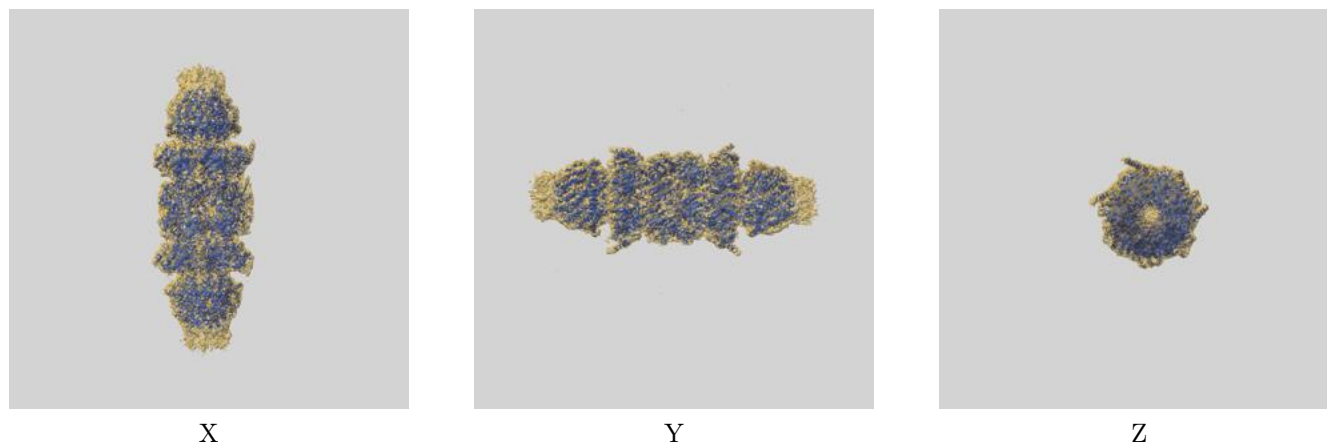
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.20                               | -    | -        |
| Author-provided FSC curve | 3.21                               | 3.68 | 3.27     |
| Unmasked-calculated*      | -                                  | -    | -        |

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

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

This section contains information regarding the fit between EMDB map EMD-24277 and PDB model 7NAP. Per-residue inclusion information can be found in section 3 on page 9.

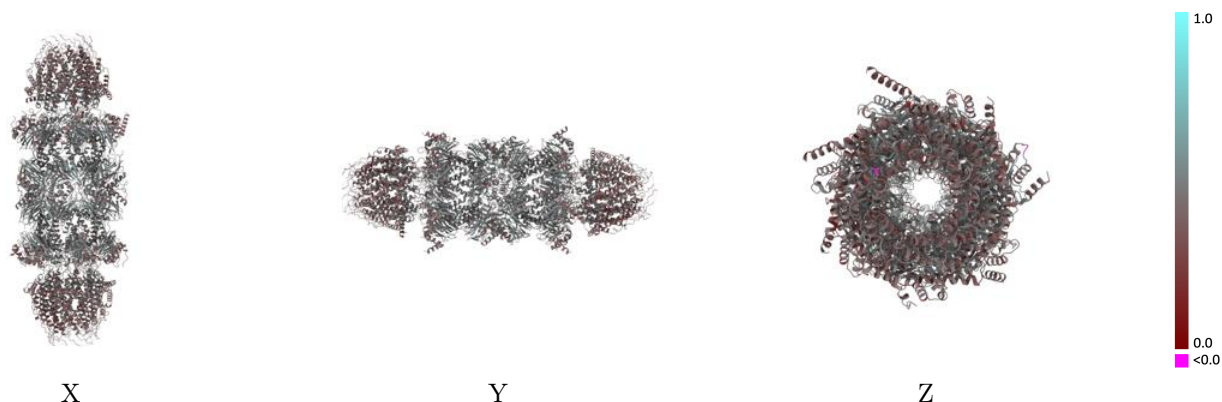
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 4.0 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.

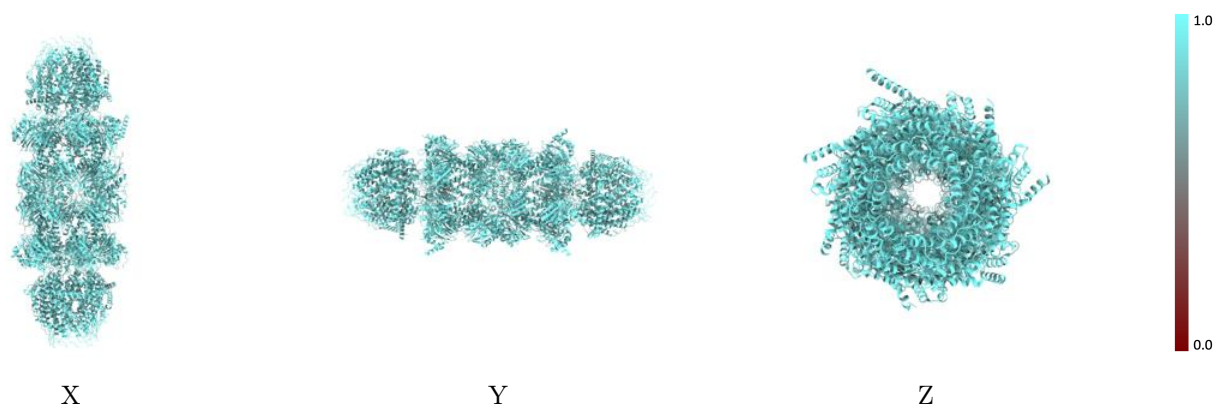


## 9.2 Q-score mapped to coordinate model [\(i\)](#)



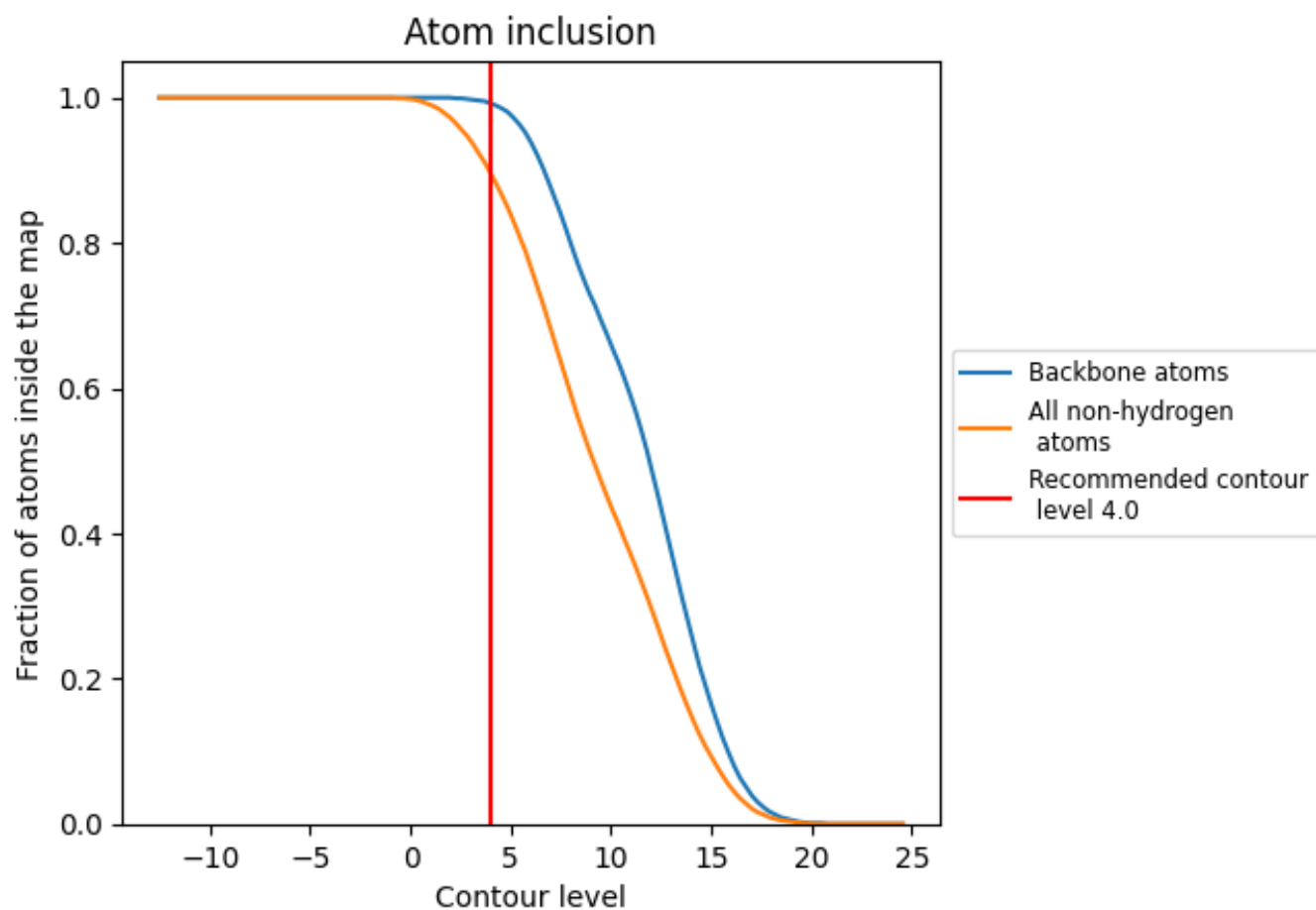
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.0).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 90% 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 (4.0) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.8960   |  0.4450   |
| A     |  0.9070   |  0.4620   |
| B     |  0.9080   |  0.4650   |
| C     |  0.9140   |  0.4560   |
| D     |  0.8840   |  0.4470   |
| E     |  0.9060   |  0.4610   |
| F     |  0.9120   |  0.4600   |
| G     |  0.9060   |  0.4600   |
| H     |  0.9150   |  0.4740   |
| I     |  0.8980   |  0.4750   |
| J     |  0.9020   |  0.4850   |
| K     |  0.9290   |  0.4740   |
| L     |  0.9010   |  0.4740   |
| M     |  0.9140   |  0.4750   |
| N     |  0.9150  |  0.4780  |
| O     |  0.9050 |  0.4590 |
| P     |  0.9110 |  0.4630 |
| Q     |  0.9130 |  0.4560 |
| R     |  0.8920 |  0.4520 |
| S     |  0.9110 |  0.4550 |
| T     |  0.9070 |  0.4610 |
| U     |  0.9110 |  0.4590 |
| V     |  0.9100 |  0.4720 |
| W     |  0.9050 |  0.4750 |
| X     |  0.9050 |  0.4800 |
| Y     |  0.9190 |  0.4680 |
| Z     |  0.9020 |  0.4770 |
| a     |  0.9160 |  0.4800 |
| b     |  0.9090 |  0.4740 |
| c     |  0.8660 |  0.3960 |
| d     |  0.8850 |  0.4090 |
| e     |  0.8830 |  0.4140 |
| f     |  0.8910 |  0.4060 |
| g     |  0.8660 |  0.3960 |
| h     |  0.8710 |  0.3970 |



*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| i     |  0.8670 |  0.3860 |
| j     |  0.8600 |  0.4020 |
| k     |  0.8890 |  0.4160 |
| l     |  0.8790 |  0.4060 |
| m     |  0.8830 |  0.3980 |
| n     |  0.8540 |  0.3920 |
| o     |  0.8600 |  0.3880 |
| p     |  0.8750 |  0.3990 |