# wwPDB EM Validation Summary Report (i)

Aug 5, 2026 – 01:16 AM EDT

| | | |
|---|---|---|
| PDB ID | : | 9BKV / pdb_00009bkv |
| EMDB ID | : | EMD-44646 |
| Title | : | DosP R97A bent form |
| Authors | : | Kumar, P.; Kober, D.L. |
| Deposited on | : | 2024-04-29 |
| Resolution | : | 3.43 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

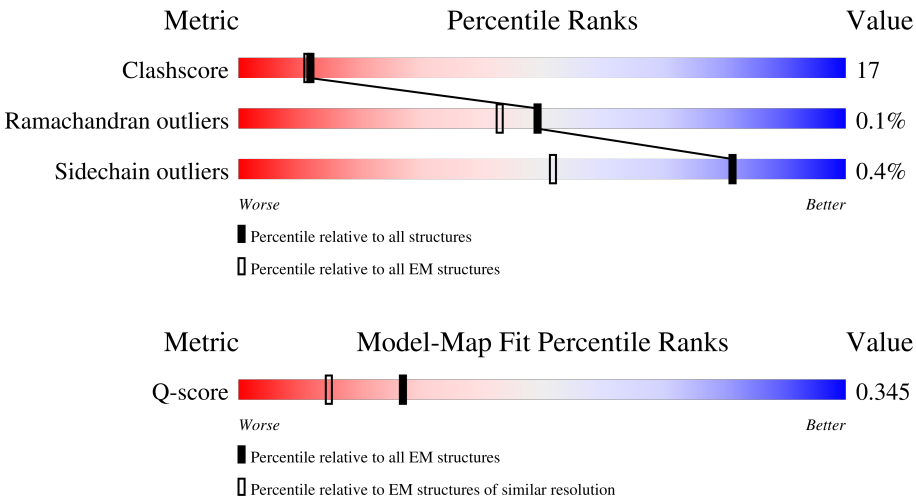
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev133 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Buster-report | : | wwPDB partial adaption of 1.1.7 (2018) |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| EM percentile statistics | : | 202505.v01 (Using data in the EMDB archive up until May 2025) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.50 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.43 Å.

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




| Metric | Whole archive (#Entries) | EM structures (#Entries) | Similar EM resolution (#Entries, resolution range(Å)) |
|---|---|---|---|
| Clashscore | 229148 | 23984 | - |
| Ramachandran outliers | 224038 | 23583 | - |
| Sidechain outliers | 223484 | 23102 | - |
| Q-score | - | 25397 | 13927 ( 2.93 - 3.93 ) |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 807 | 7% 62% 35% · |
| 1 | B | 807 | 6% 62% 34% · |

# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12562 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.

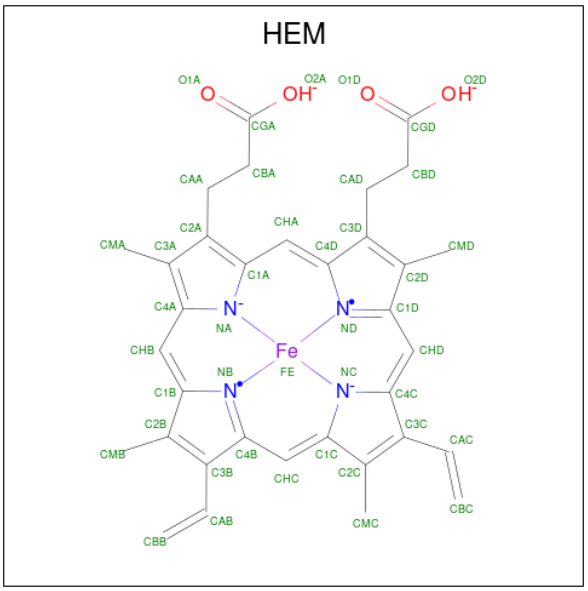
- Molecule 1 is a protein called Oxygen sensor protein DosP.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | A | 788 | 6260 | 3964 | 1093 | 1170 | 33 | 0 | 0 |
| 1 | B | 783 | 6216 | 3936 | 1085 | 1162 | 33 | 0 | 0 |

There are 22 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 1 | MET | - | expression tag | UNP P76129 |
| A | 2 | ARG | - | expression tag | UNP P76129 |
| A | 3 | GLN | - | expression tag | UNP P76129 |
| A | 4 | ASP | - | expression tag | UNP P76129 |
| A | 5 | ALA | - | expression tag | UNP P76129 |
| A | 6 | GLU | - | expression tag | UNP P76129 |
| A | 7 | VAL | - | expression tag | UNP P76129 |
| A | 8 | ILE | - | expression tag | UNP P76129 |
| A | 16 | SER | ASN | conflict | UNP P76129 |
| A | 97 | ALA | ARG | engineered mutation | UNP P76129 |
| A | 195 | THR | ILE | conflict | UNP P76129 |
| B | 1 | MET | - | expression tag | UNP P76129 |
| B | 2 | ARG | - | expression tag | UNP P76129 |
| B | 3 | GLN | - | expression tag | UNP P76129 |
| B | 4 | ASP | - | expression tag | UNP P76129 |
| B | 5 | ALA | - | expression tag | UNP P76129 |
| B | 6 | GLU | - | expression tag | UNP P76129 |
| B | 7 | VAL | - | expression tag | UNP P76129 |
| B | 8 | ILE | - | expression tag | UNP P76129 |
| B | 16 | SER | ASN | conflict | UNP P76129 |
| B | 97 | ALA | ARG | engineered mutation | UNP P76129 |
| B | 195 | THR | ILE | conflict | UNP P76129 |

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



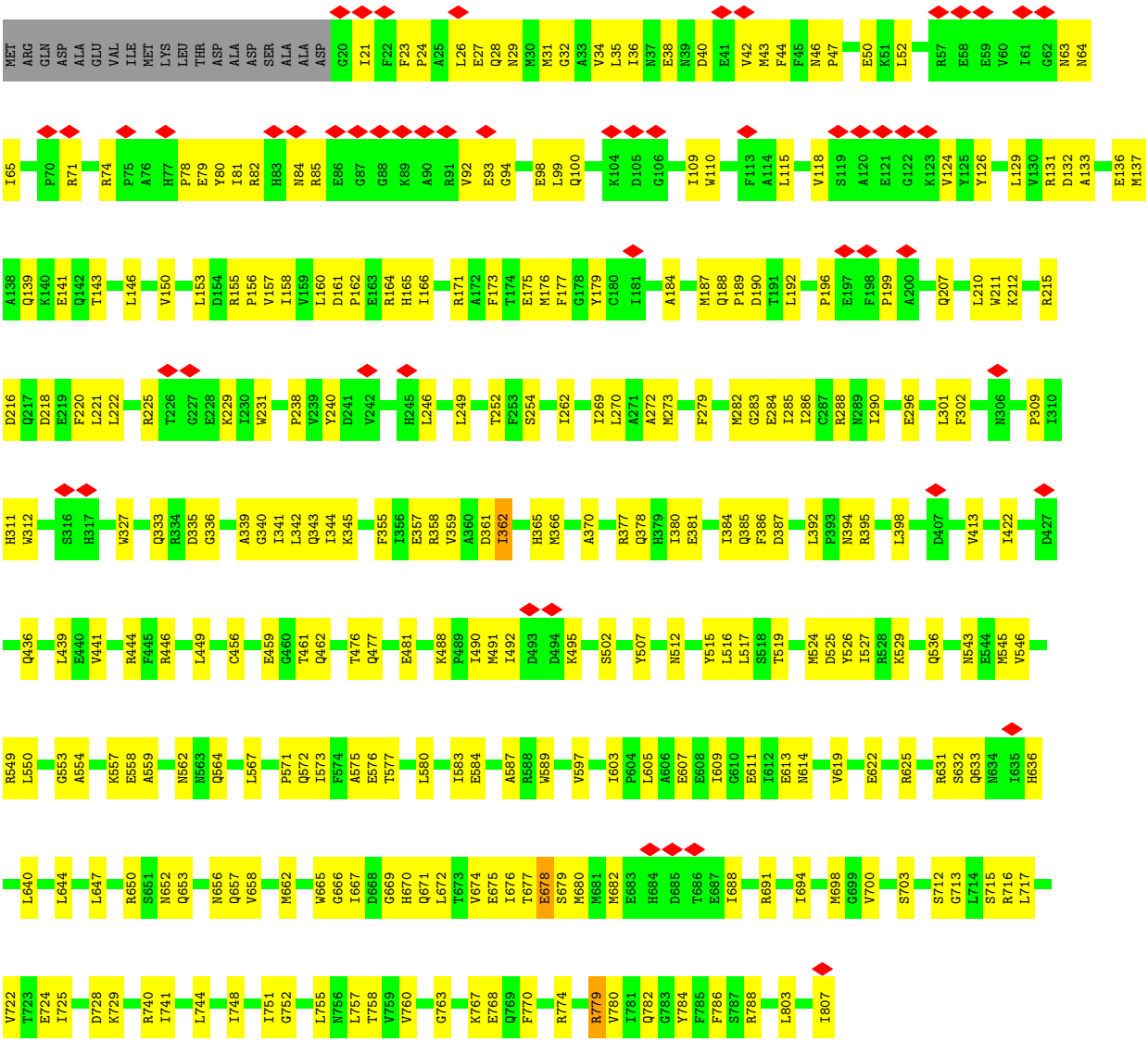

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 2 | A | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 2 | B | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |

# 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: Oxygen sensor protein DosP

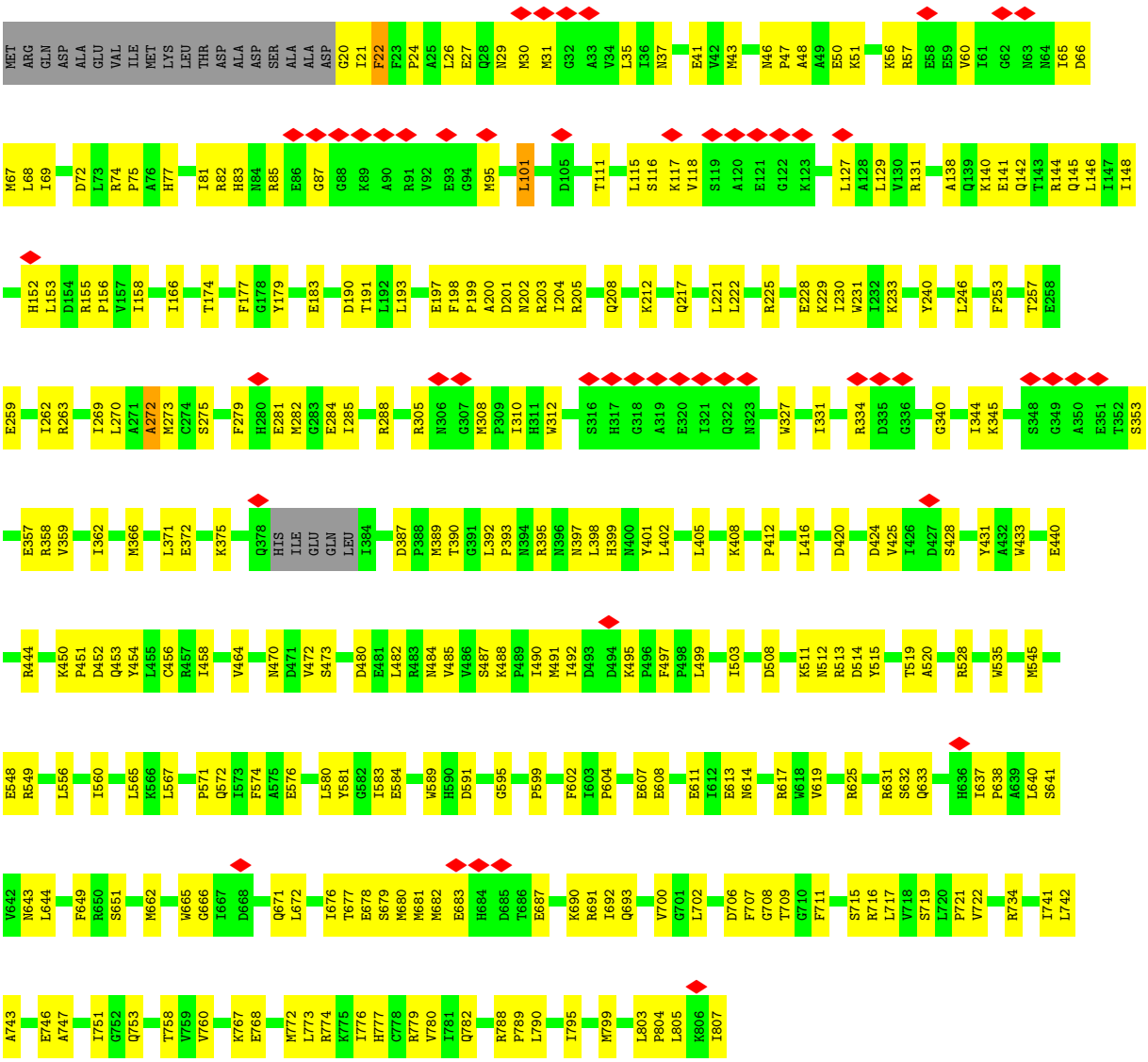
Chain A: 7% 62% 35%




• Molecule 1: Oxygen sensor protein DosP

Chain B:

6%
62%
34%


MET ARG GLN ASP ALA GLU VAL ILE MET LYS LEU THR ASP ALA ASP SER ALA ALA ASP G20 I21 F22 F23 P24 A25 L26 E27 Q28 N29 M30 M31 G32 A33 V34 L35 I36 N37 E41 V42 M43 N46 P47 A48 A49 E50 K51 K56 R57 E58 E59 V60 I61 G62 N63 N64 I65 D66
M67 L68 I69 D72 L73 R74 P75 A76 H77 I81 R82 H83 N84 R85 E86 G87 G88 K89 A90 R91 V92 E93 G94 M95 L101 D105 T111 L115 S116 K117 V118 S119 A120 E121 G122 K123 L127 A128 L129 V130 R131 A138 Q139 K140 E141 Q142 T143 R144 Q145 L146 I147 I148
H152 L153 D154 R155 P156 V157 I158 I166 T174 F177 G178 Y179 E183 D190 T191 L192 L193 E197 F198 P199 A200 D201 N202 R203 I204 R205 Q208 K212 Q217 L221 L222 R225 E228 K229 I230 W231 I232 K233 Y240 L246 F253 T257 E258
E259 I262 R263 I269 L270 A271 A272 M273 C274 S275 F279 H280 E281 M282 G283 E284 I285 R288 R305 N306 G307 M308 P309 I310 H311 W312 S316 H317 G318 A319 E320 I321 Q322 N323 W327 I331 R334 D335 G336 G340 I344 K345 S348 S349 A350 E351 T352 S353
E357 R358 V359 I362 M366 L371 E372 K375 Q378 HIS ILE GLU GLN LEU I384 D387 P388 M389 T390 G391 L392 P393 N394 R395 N396 N397 L398 H399 N400 Y401 L402 L405 K408 P412 L416 D420 D424 V425 I426 D427 S428 Y431 A432 W433 E440
R444 K450 P451 D452 Q453 Y454 L455 C456 R457 I458 V464 N470 D471 V472 S473 D480 E481 L482 R483 N484 V485 V486 S487 K488 P489 I490 M491 I492 D493 D494 K495 P496 F497 P498 L499 I503 D508 K511 N512 R513 D514 Y515 T519 A520 R528 W535 M545
E548 R549 L556 I560 L565 K566 L567 P571 Q572 I573 F574 A575 E576 L580 Y581 G582 I583 E584 W589 H590 D591 G595 P599 F602 I603 P604 E607 E608 E611 I612 E613 N614 R617 W618 V619 R625 R631 S632 Q633 H636 I637 P638 A639 L640 S641
V642 N643 L644 F649 R650 S651 M662 W665 G666 I667 D668 Q671 L672 I676 T677 E678 S679 M680 M681 M682 E683 H684 D685 T686 E687 K690 R691 I692 Q693 V700 G701 L702 D706 F707 G708 T709 G710 F711 S715 R716 L717 V718 S719 L720 P721 V722 R734 I741 L742
A743 E746 A747 I751 G752 Q753 T758 V759 V760 K767 E768 M772 L773 R774 K775 I776 H777 C778 R779 V780 I781 Q782 R788 P789 L790 I795 M799 L803 P804 L805 K806 I807

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 391512 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | TFS KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 50 | Depositor |
| Minimum defocus (nm) | 800 | Depositor |
| Maximum defocus (nm) | 2000 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value | 5.963 | Depositor |
| Minimum map value | -2.397 | Depositor |
| Average map value | -0.001 | Depositor |
| Map value standard deviation | 0.084 | Depositor |
| Recommended contour level | 1 | Depositor |
| Map size (Å) | 426.2, 426.2, 426.2 | wwPDB |
| Map dimensions | 320, 320, 320 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.3318751, 1.3318751, 1.3318751 | Depositor |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM

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 | 0.24 | 0/6388 | 0.45 | 1/8654 (0.0%) |
| 1 | B | 0.24 | 0/6342 | 0.47 | 2/8590 (0.0%) |
| All | All | 0.24 | 0/12730 | 0.46 | 3/17244 (0.0%) |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 272 | ALA | CA-C-N | -5.90 | 110.14 | 121.94 |
| 1 | B | 272 | ALA | C-N-CA | -5.90 | 110.14 | 121.94 |
| 1 | A | 779 | ARG | N-CA-CB | -5.34 | 108.08 | 114.17 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 6260 | 0 | 6239 | 222 | 0 |
| 1 | B | 6216 | 0 | 6195 | 230 | 0 |
| 2 | A | 43 | 0 | 30 | 5 | 0 |
| 2 | B | 43 | 0 | 30 | 4 | 0 |
| All | All | 12562 | 0 | 12494 | 438 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

The worst 5 of 438 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:394:ASN:OD1 | 1:A:395:ARG:N | 2.06 | 0.87 |
| 1:A:269:ILE:HD11 | 1:A:286:ILE:HG12 | 1.57 | 0.84 |
| 1:A:502:SER:HB2 | 1:A:524:MET:HE1 | 1.59 | 0.82 |
| 1:B:141:GLU:HA | 1:B:144:ARG:HD2 | 1.62 | 0.81 |
| 1:A:713:GLY:HA2 | 1:A:716:ARG:HE | 1.49 | 0.79 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 786/807 (97%) | 741 (94%) | 43 (6%) | 2 (0%) | 36 | 66 |
| 1 | B | 779/807 (96%) | 726 (93%) | 53 (7%) | 0 | 100 | 100 |
| All | All | 1565/1614 (97%) | 1467 (94%) | 96 (6%) | 2 (0%) | 49 | 78 |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 188 | GLN |
| 1 | A | 803 | LEU |

### 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 | 683/698 (98%) | 679 (99%) | 4 (1%) | 78 | 80 |
| 1 | B | 678/698 (97%) | 676 (100%) | 2 (0%) | 86 | 84 |
| All | All | 1361/1396 (98%) | 1355 (100%) | 6 (0%) | 81 | 82 |

5 of 6 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 678 | GLU |
| 1 | B | 22 | PHE |
| 1 | B | 101 | LEU |
| 1 | A | 516 | LEU |
| 1 | A | 362 | ILE |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 570 | GLN |
| 1 | B | 753 | GLN |
| 1 | B | 142 | GLN |
| 1 | B | 289 | ASN |
| 1 | B | 397 | 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 oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

2 ligands 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 | $\#\|Z\| > 2$ |
| 2 | HEM | B | 901 | 1 | 50,50,50 | 1.29 | 5 (10%) | 67,82,82 | 0.93 | 0 |
| 2 | HEM | A | 901 | - | 50,50,50 | 1.37 | 10 (20%) | 67,82,82 | 0.84 | 0 |

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 |
|---|---|---|---|---|---|---|---|
| 2 | HEM | B | 901 | 1 | - | 3/14/54/54 | - |
| 2 | HEM | A | 901 | - | - | 0/14/54/54 | - |

The worst 5 of 15 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | A | 901 | HEM | CAB-C3B | 3.15 | 1.55 | 1.47 |
| 2 | A | 901 | HEM | CAC-C3C | 3.04 | 1.55 | 1.47 |
| 2 | B | 901 | HEM | CAC-C3C | 3.01 | 1.55 | 1.47 |
| 2 | B | 901 | HEM | CAB-C3B | 2.91 | 1.55 | 1.47 |
| 2 | A | 901 | HEM | FE-ND | 2.69 | 2.03 | 1.94 |

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | B | 901 | HEM | C2A-CAA-CBA-CGA |
| 2 | B | 901 | HEM | CAA-CBA-CGA-O1A |
| 2 | B | 901 | HEM | CAA-CBA-CGA-O2A |

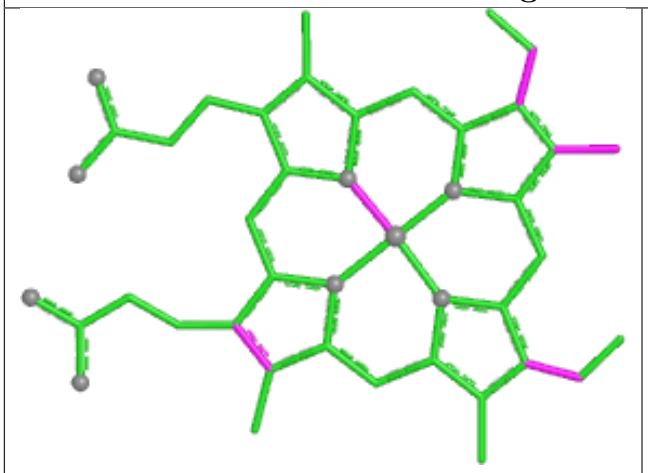
There are no ring outliers.

2 monomers are involved in 9 short contacts:

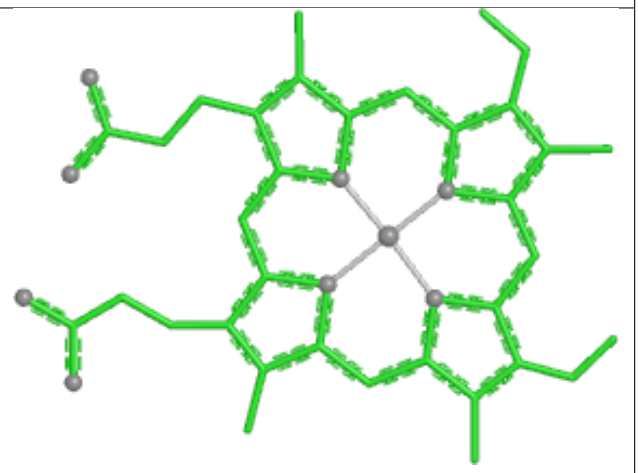
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 2 | B | 901 | HEM | 4 | 0 |
| 2 | A | 901 | HEM | 5 | 0 |

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 then 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.

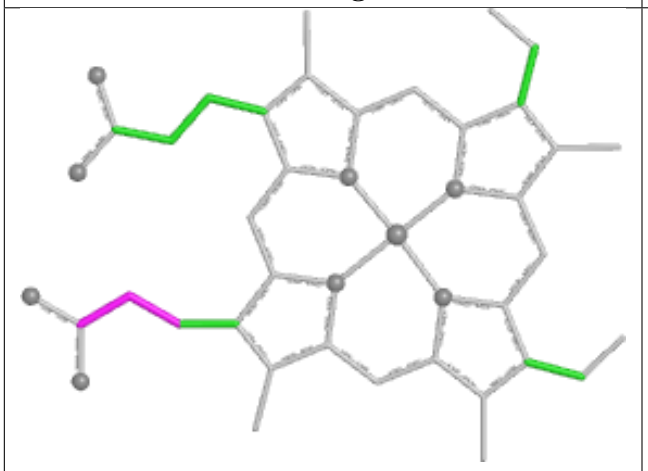
**Ligand HEM B 901**



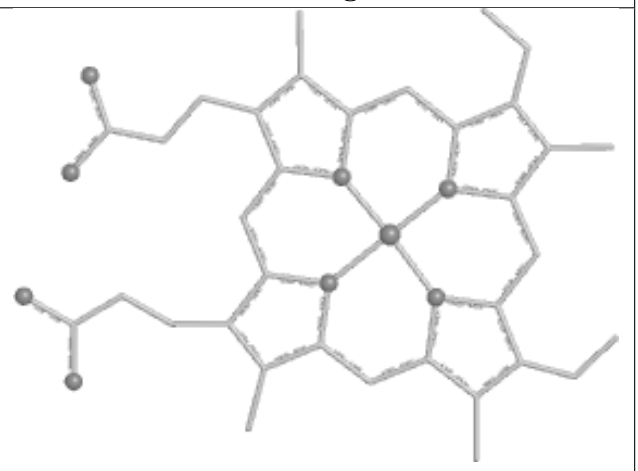
**Bond lengths**



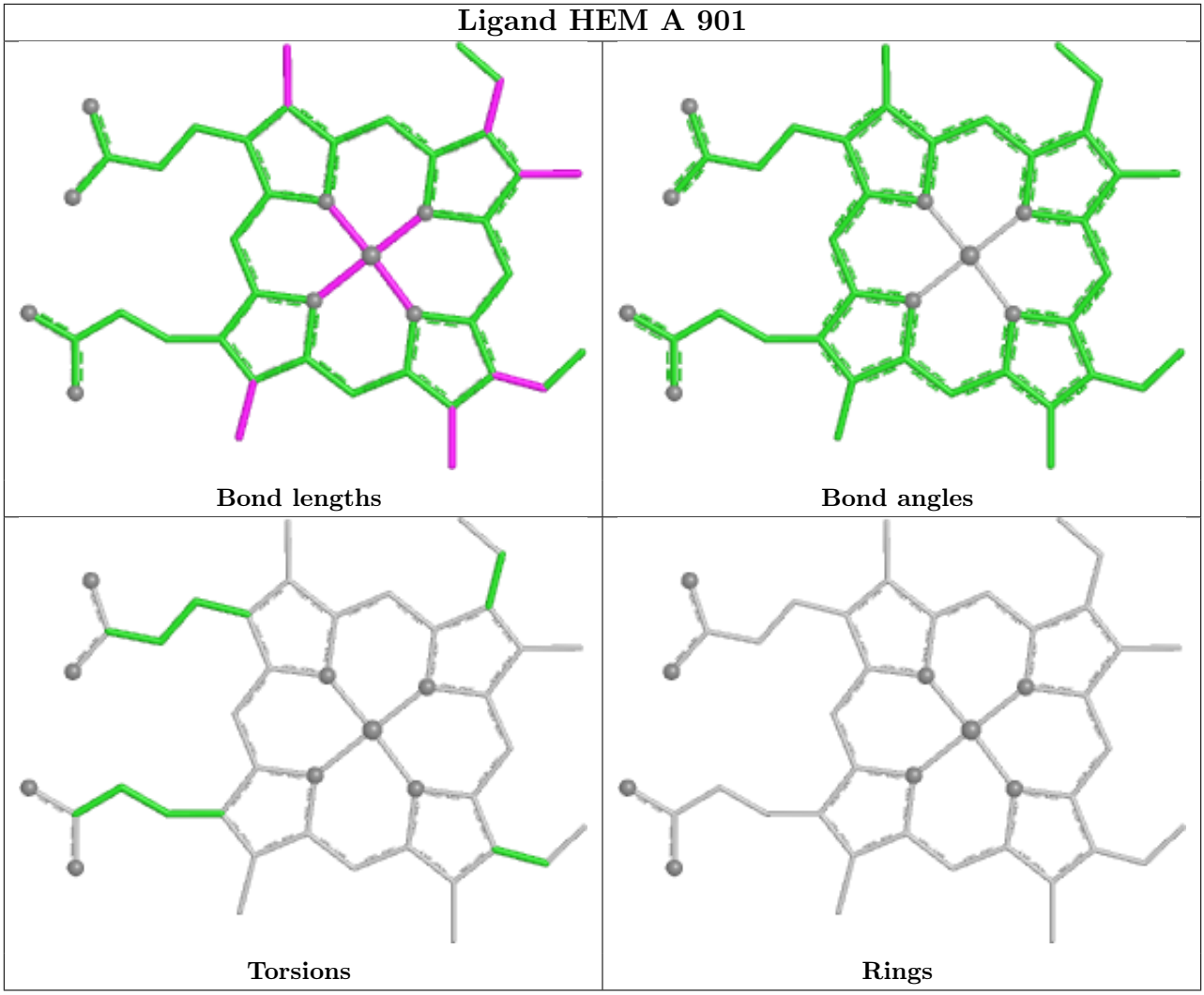
**Bond angles**



**Torsions**



**Rings**




## 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)

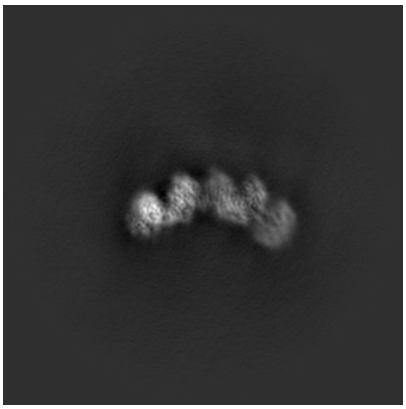
This section contains visualisations of the EMDB entry EMD-44646. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

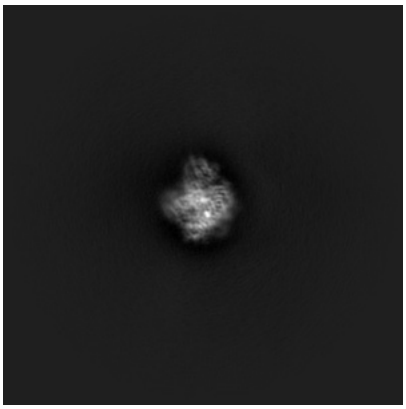
## 6.1 Orthogonal projections (i)

### 6.1.1 Primary map

X

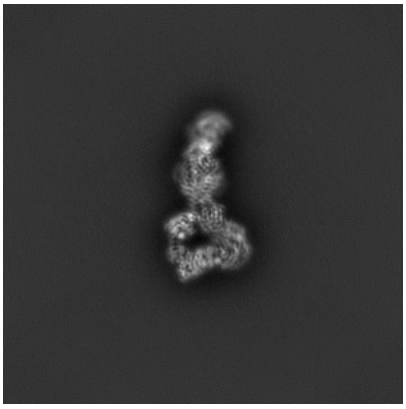


Y

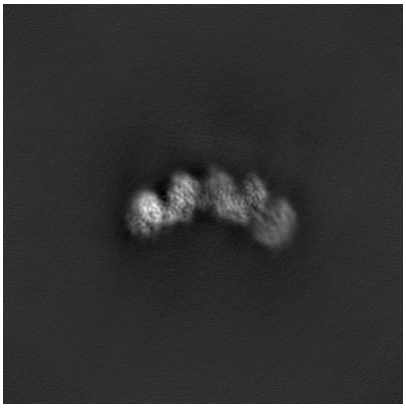


Z

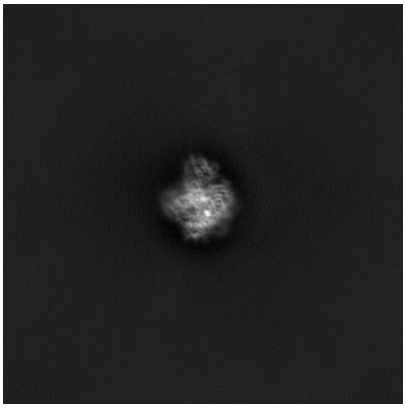
### 6.1.2 Raw map



X



Y

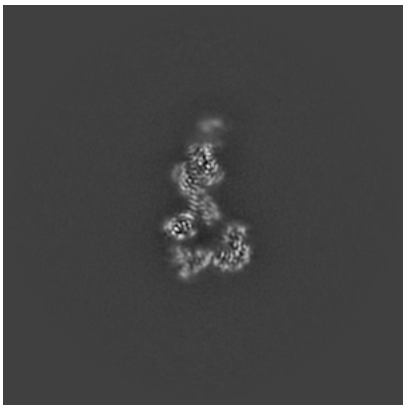


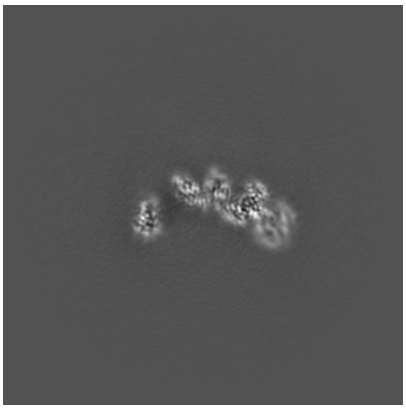
Z

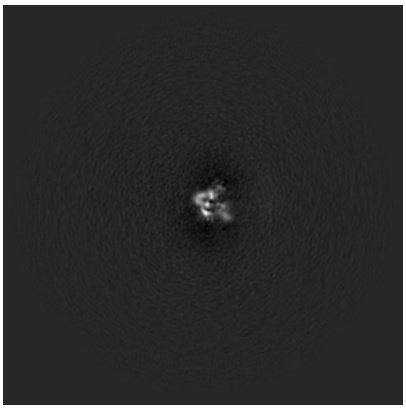
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

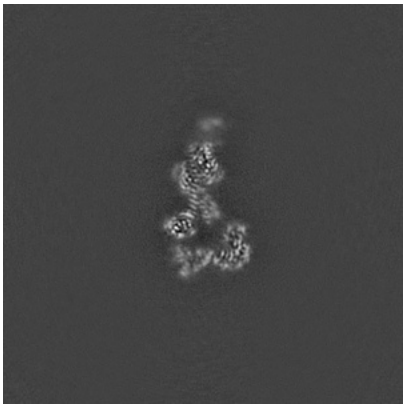
### 6.2.1 Primary map

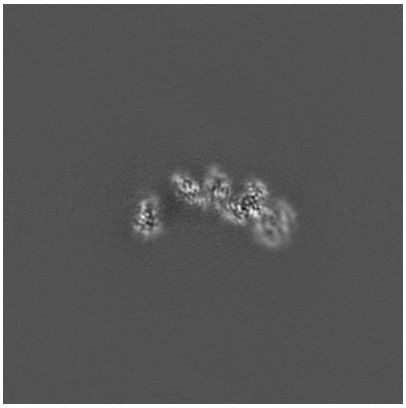

X Index: 160

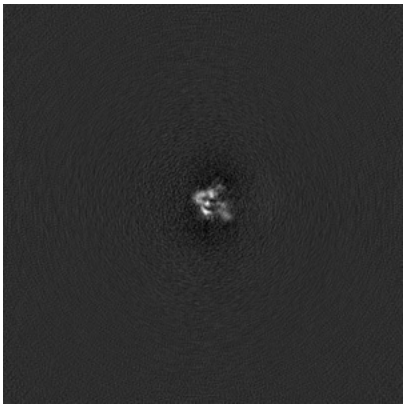

Y Index: 160


Z Index: 160

### 6.2.2 Raw map


X Index: 160


Y Index: 160

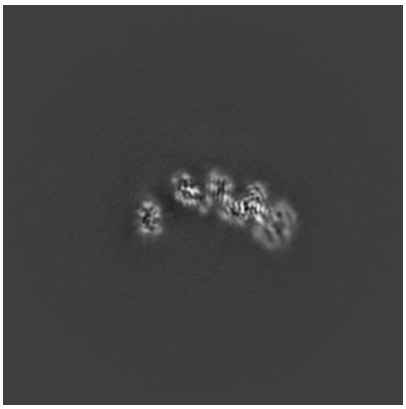

Z Index: 160

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: 157


Y Index: 163

Z Index: 113

### 6.3.2 Raw map

X Index: 157

Y Index: 163

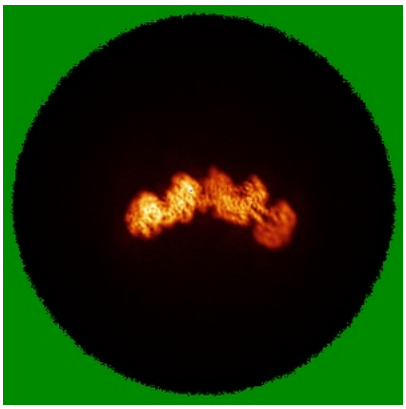
Z Index: 143

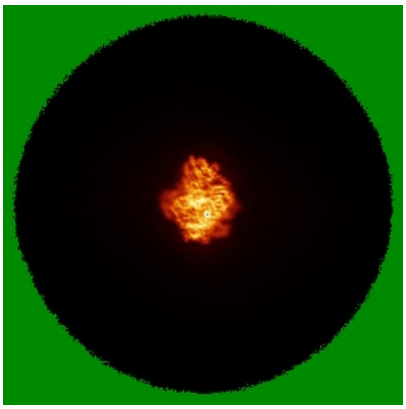
The images above show the largest variance slices of the map in three orthogonal directions.

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

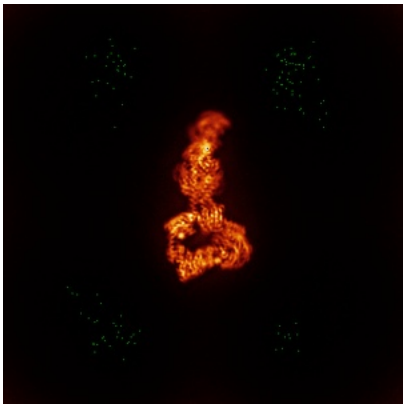
### 6.4.1 Primary map

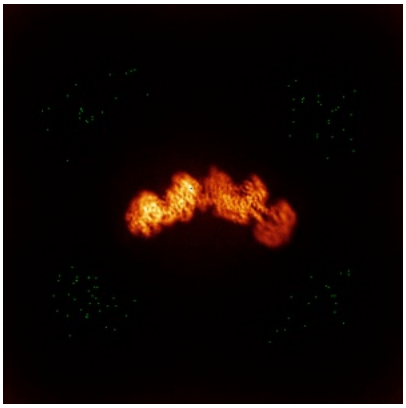
X

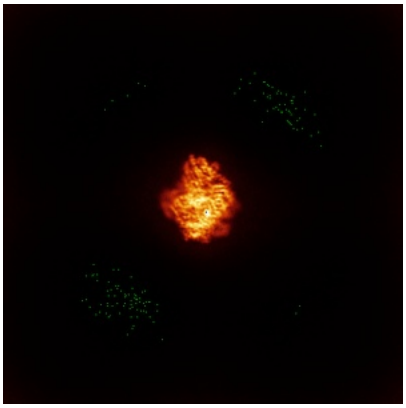

Y


Z

### 6.4.2 Raw map


X


Y


Z

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

## 6.5 Orthogonal surface views (i)

### 6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map

X Y Z

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

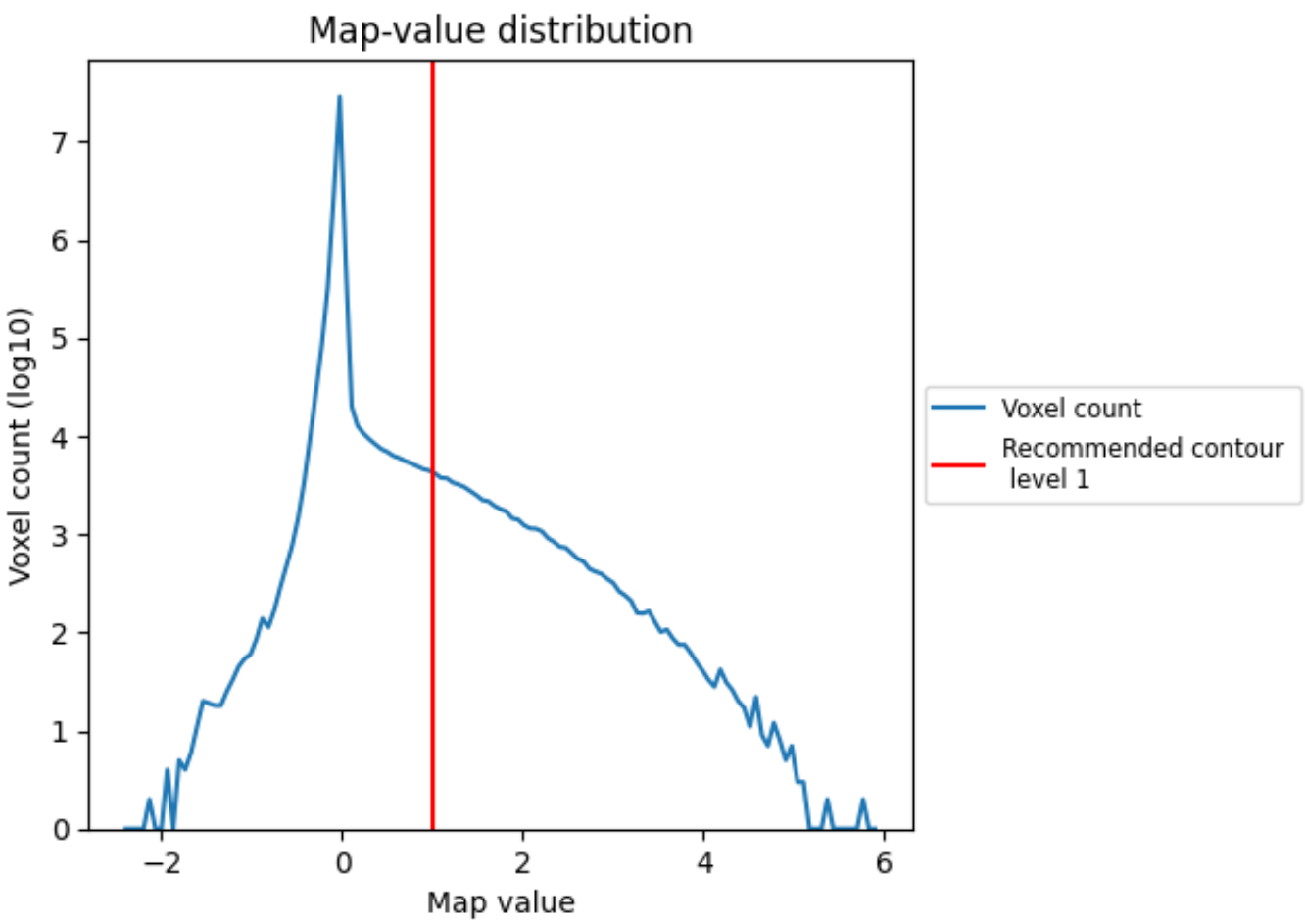
## 6.6 Mask visualisation (i)

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

# 7 Map analysis (i)

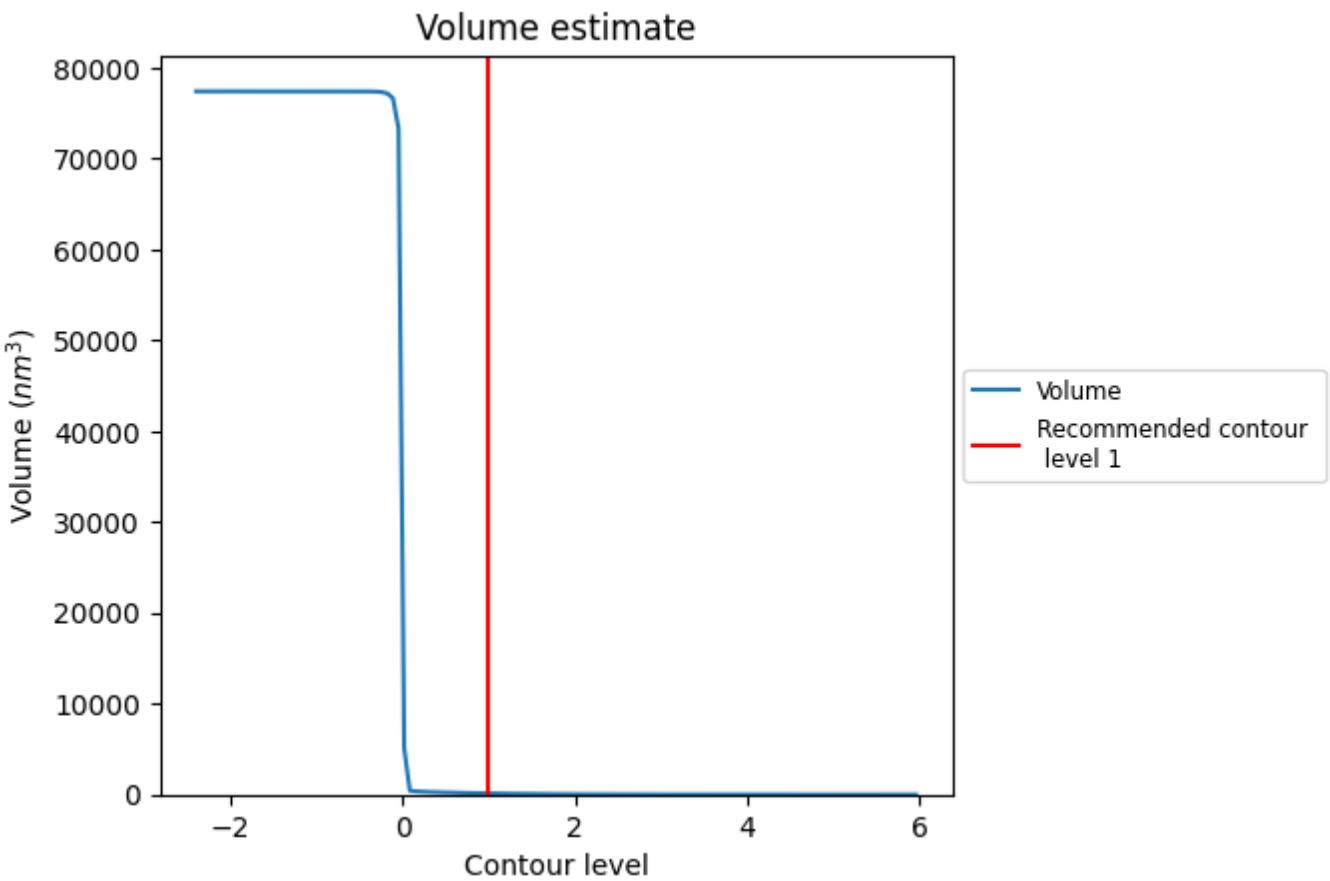
This section contains the results of statistical analysis of the map.

## 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.

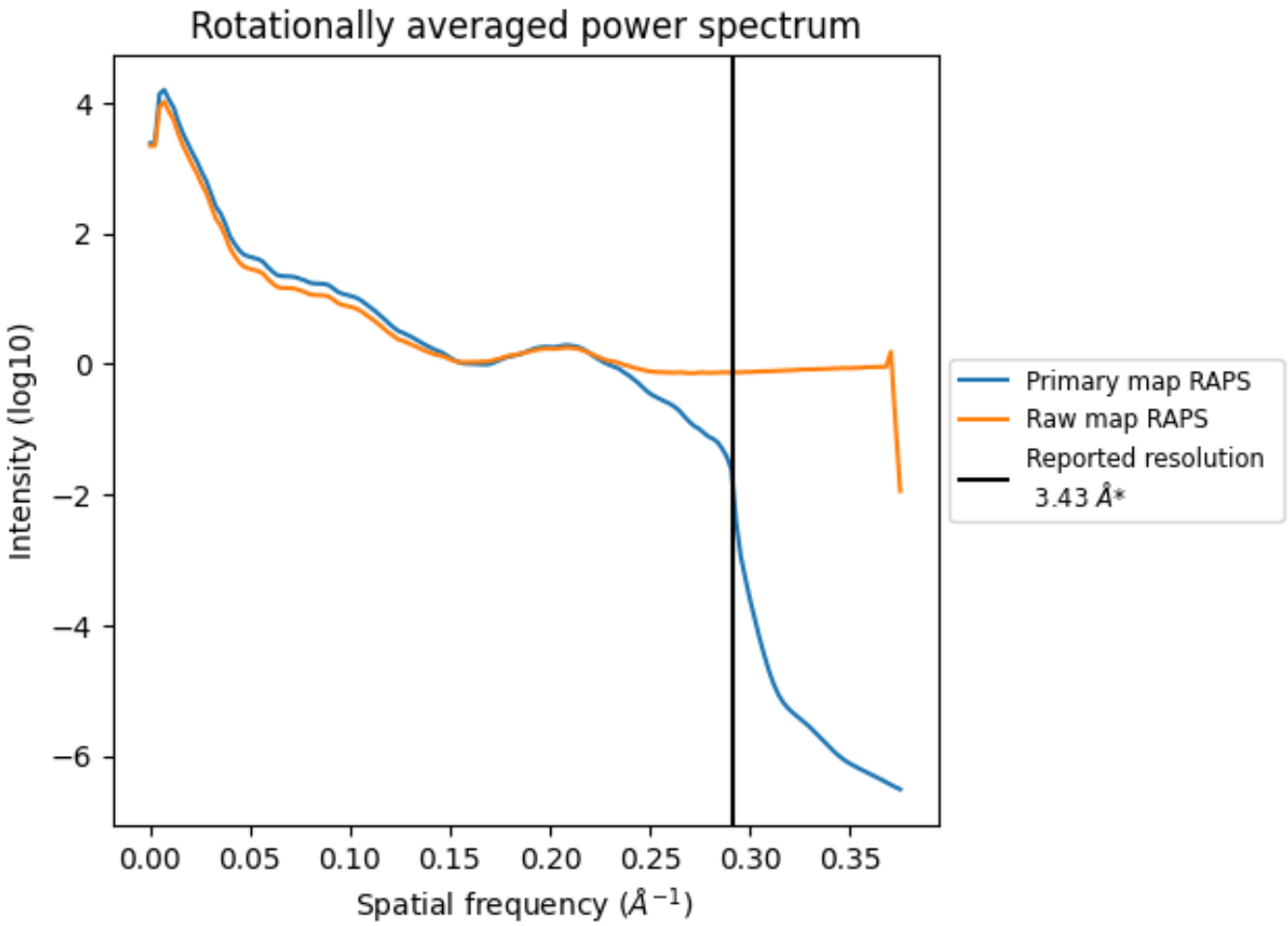
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 129 $nm^3$; this corresponds to an approximate mass of 116 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)

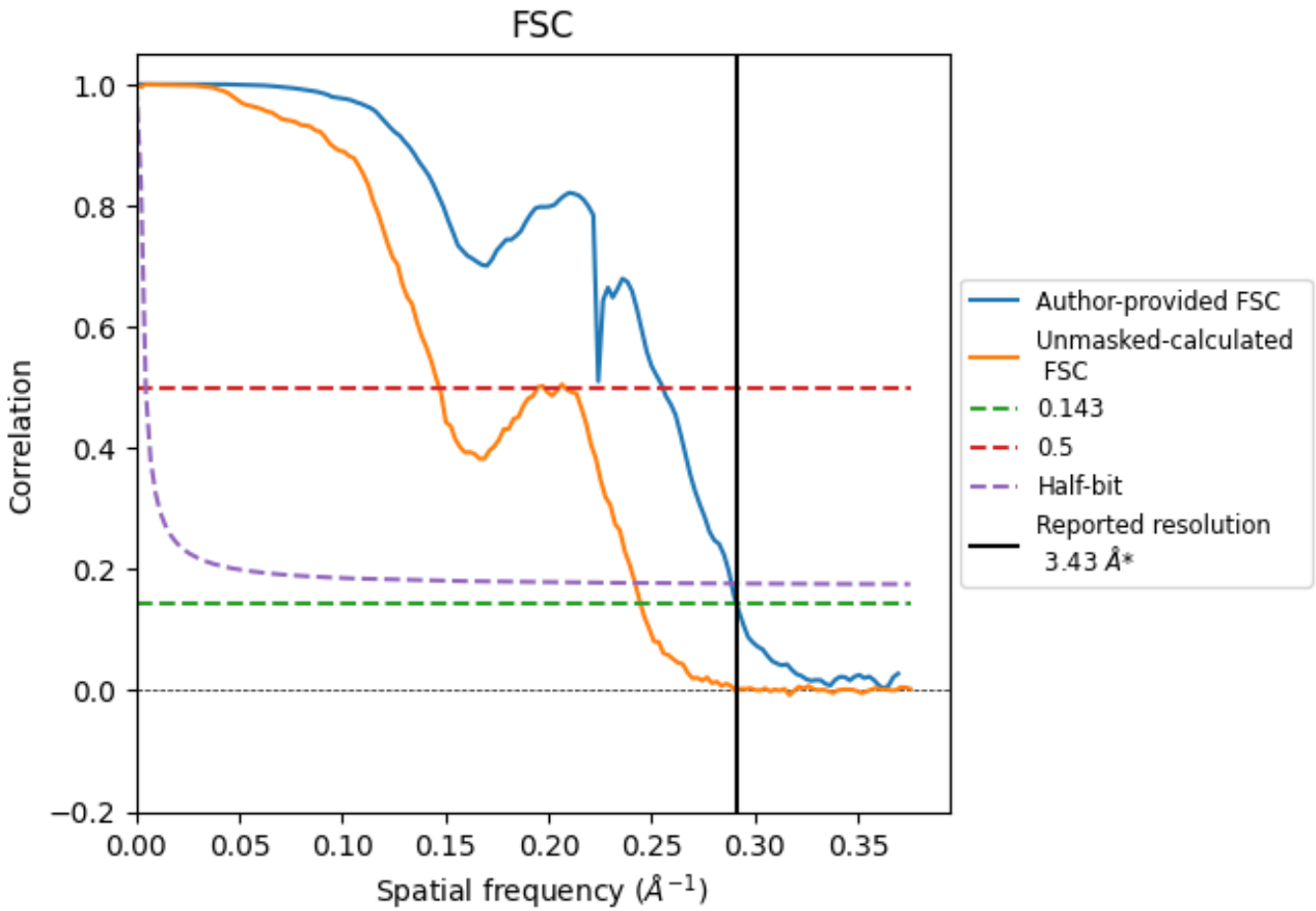



*Reported resolution corresponds to spatial frequency of 0.292 Å$^{-1}$

# 8 Fourier-Shell correlation (i)

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

## 8.1 FSC (i)




*Reported resolution corresponds to spatial frequency of 0.292 Å$^{-1}$

## 8.2 Resolution estimates (i)

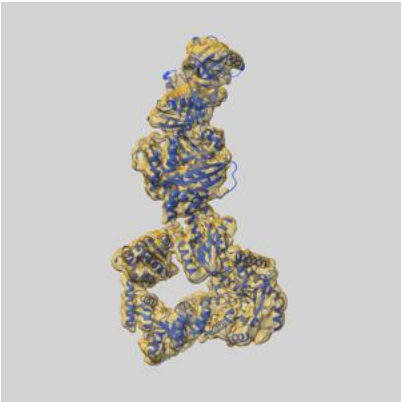
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.43 | - | - |
| Author-provided FSC curve | 3.44 | 3.92 | 3.46 |
| Unmasked-calculated* | 4.09 | 6.81 | 4.13 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.09 differs from the reported value 3.43 by more than 10 %

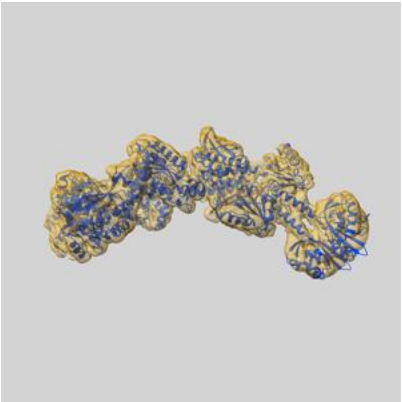
# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-44646 and PDB model 9BKV. Per-residue inclusion information can be found in section 3 on page 5.

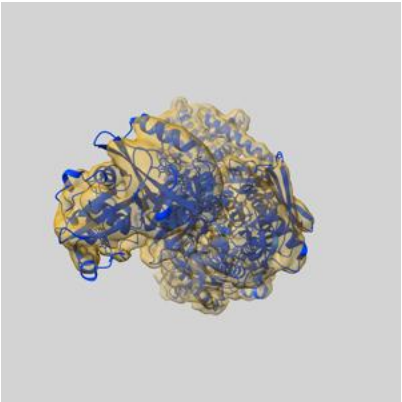
## 9.1 Map-model overlay (i)



X



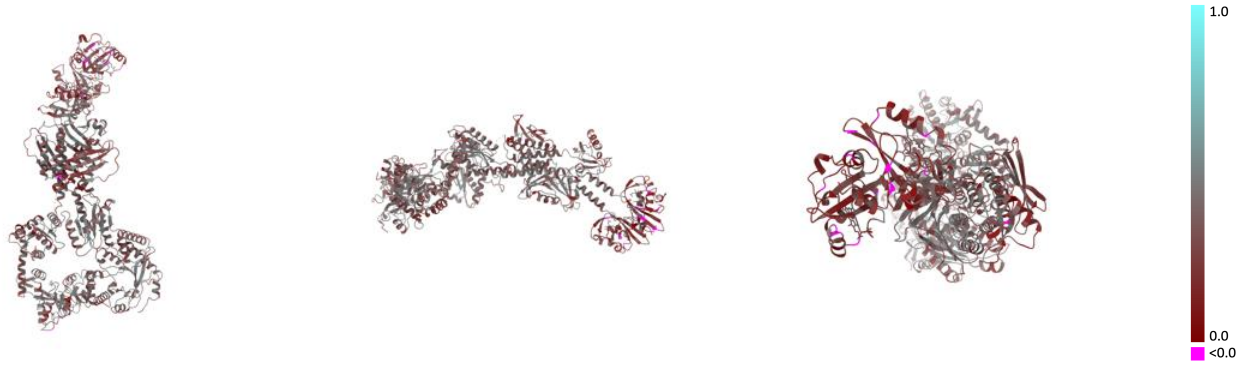
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.0 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.

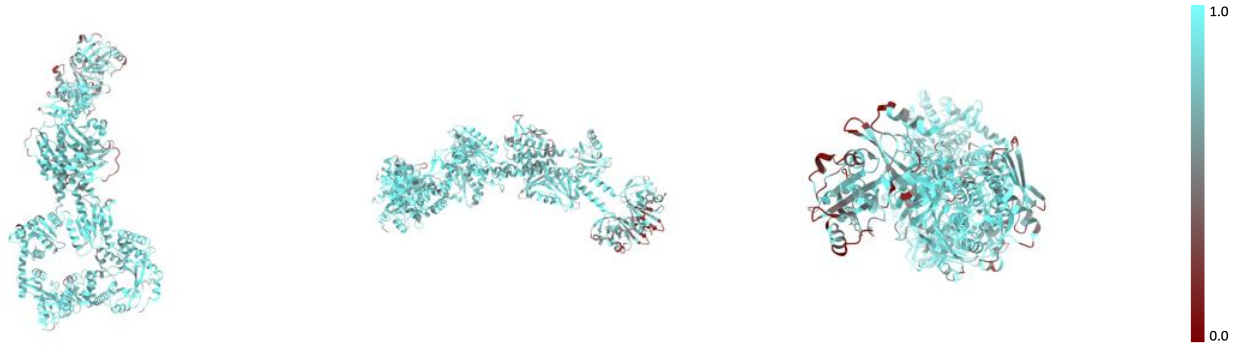
## 9.2 Q-score mapped to coordinate model (i)




X Y Z

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

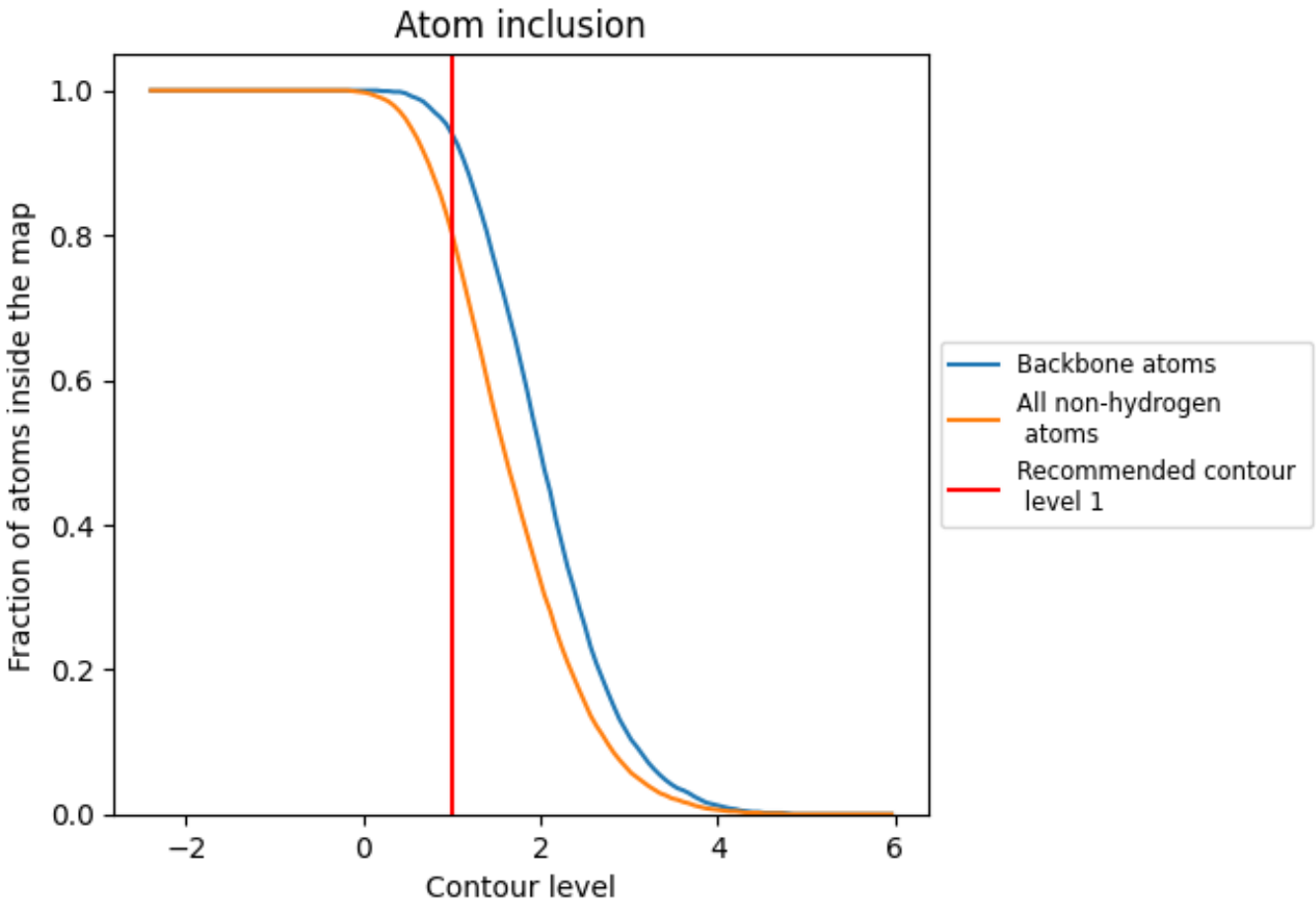
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

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 (1).

## 9.4 Atom inclusion (i)




At the recommended contour level, 94% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (1) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.8030 | 0.3450 |
| A | 0.8060 | 0.3490 |
| B | 0.8000 | 0.3410 |