# Full wwPDB EM Validation Report ⓘ

Apr 26, 2025 – 07:22 am BST

| | | |
|---|---|---|
| PDB ID | : | 8Q15 / pdb_00008q15 |
| EMDB ID | : | EMD-18060 |
| Title | : | CryoEM structure of canonical rice nucleosome core particle |
| Authors | : | Sotelo-Parrilla, P.; Hari Sundar G, V.; Raju, S.; Jha, S.; Gireesh, A.; Gut, F.; Vinothkumar, K.R.; Berger, F.; Shivaprasad, P.V.; Jeyaprakash, A.A. |
| Deposited on | : | 2023-07-30 |
| Resolution | : | 3.60 Å(reported) |

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

We welcome your comments at *validation@mail.wwpdb.org*
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.dev118 |
| MolProbity | : | FAILED |
| 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) | : | 2.43.1 |

# 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 3.60 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 6 unique types of molecules in this entry. The entry contains 10167 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 Histone H2A.2.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 1 | A | 84 | Total<br>639 | C<br>405 | N<br>120 | O<br>114 | 0 | 0 |
| 1 | B | 84 | Total<br>639 | C<br>405 | N<br>120 | O<br>114 | 0 | 0 |

- Molecule 2 is a protein called Histone H2B.4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | C | 88 | Total<br>688 | C<br>443 | N<br>117 | O<br>126 | S<br>2 | 0 | 0 |
| 2 | D | 88 | Total<br>688 | C<br>443 | N<br>117 | O<br>126 | S<br>2 | 0 | 0 |

- Molecule 3 is a protein called Histone H3.2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 3 | E | 73 | Total<br>590 | C<br>373 | N<br>112 | O<br>103 | S<br>2 | 0 | 0 |
| 3 | F | 97 | Total<br>792 | C<br>503 | N<br>151 | O<br>136 | S<br>2 | 0 | 0 |

- Molecule 4 is a protein called Histone H4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 4 | G | 79 | Total<br>630 | C<br>396 | N<br>123 | O<br>110 | S<br>1 | 0 | 0 |
| 4 | H | 78 | Total<br>622 | C<br>392 | N<br>122 | O<br>107 | S<br>1 | 0 | 0 |

- Molecule 5 is a DNA chain called WIDOM 601.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 5 | I | 119 | Total | C | N | O | P | 0 | 0 |
| | | | 2455 | 1160 | 463 | 713 | 119 | | |

- Molecule 6 is a DNA chain called WIDOM 601.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 6 | J | 119 | Total | C | N | O | P | 0 | 0 |
| | | | 2424 | 1150 | 440 | 715 | 119 | | |

MolProbity failed to run properly - this section is therefore empty.

# 3 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 140877 | 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 ($e^-/Å^2$) | 60 | Depositor |
| Minimum defocus (nm) | 500 | Depositor |
| Maximum defocus (nm) | 2600 | Depositor |
| Magnification | Not provided | |
| Image detector | TFS FALCON 4i (4k x 4k) | Depositor |
| Maximum map value | 2.956 | Depositor |
| Minimum map value | -1.795 | Depositor |
| Average map value | 0.005 | Depositor |
| Map value standard deviation | 0.074 | Depositor |
| Recommended contour level | 0.2 | Depositor |
| Map size (Å) | 218.1, 218.1, 218.1 | wwPDB |
| Map dimensions | 300, 300, 300 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.727, 0.727, 0.727 | Depositor |

# 4 Model quality

## 4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

## 4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

## 4.3 Torsion angles

### 4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

### 4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

### 4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

## 4.4 Non-standard residues in protein, DNA, RNA chains

validation-pack failed to run properly - this section is therefore empty.

## 4.5 Carbohydrates

validation-pack failed to run properly - this section is therefore empty.

## 4.6 Ligand geometry

validation-pack failed to run properly - this section is therefore empty.

## 4.7 Other polymers

validation-pack failed to run properly - this section is therefore empty.

## 4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

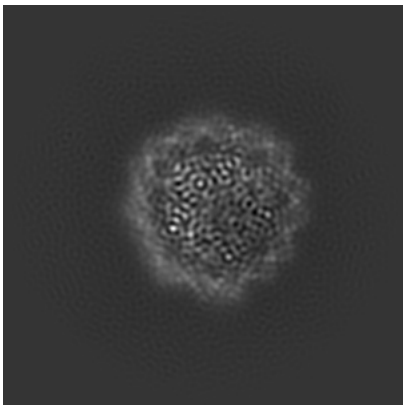
# 5 Map visualisation

This section contains visualisations of the EMDB entry EMD-18060. These allow visual inspection of the internal detail of the map and identification of artifacts.

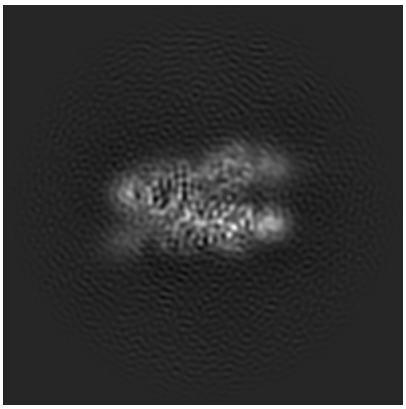
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 5.1 Orthogonal projections

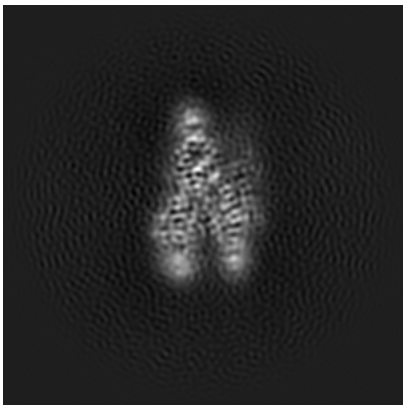
### 5.1.1 Primary map



X

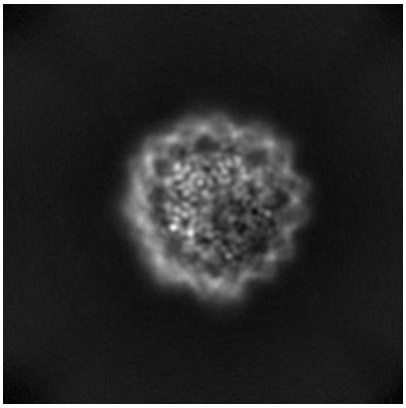


Y

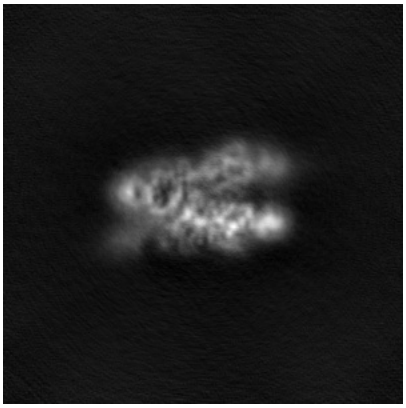


Z

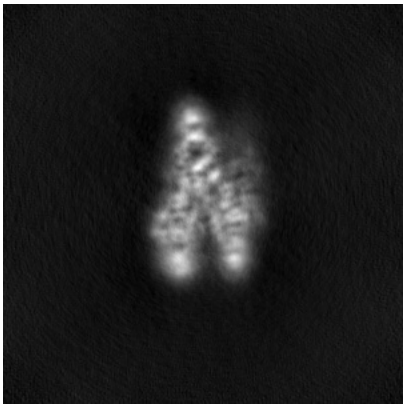
### 5.1.2 Raw map



X



Y

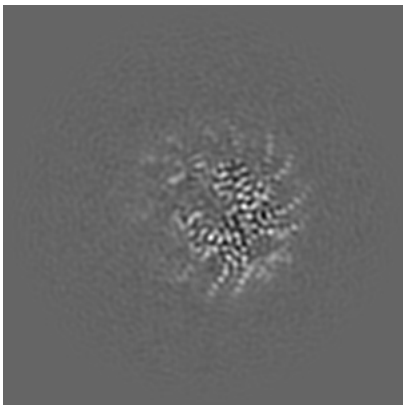


Z

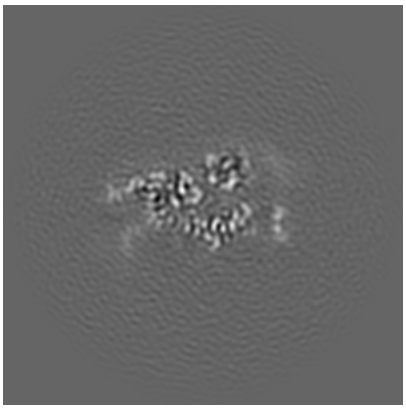
The images above show the map projected in three orthogonal directions.

## 5.2 Central slices (i)

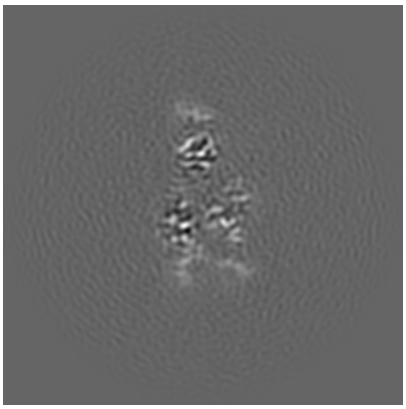
### 5.2.1 Primary map



X Index: 150

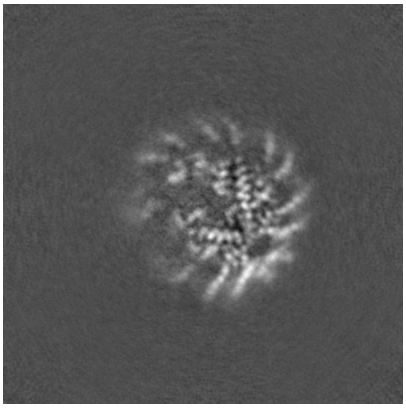


Y Index: 150

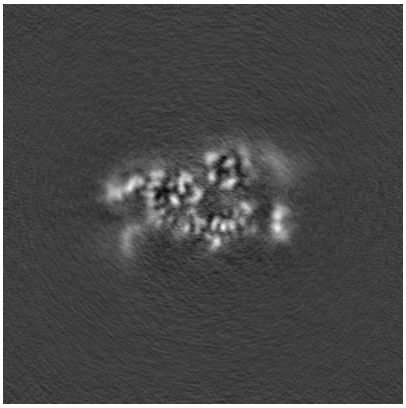


Z Index: 150

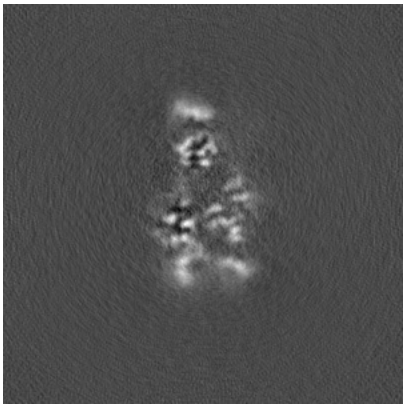
### 5.2.2 Raw map



X Index: 150



Y Index: 150

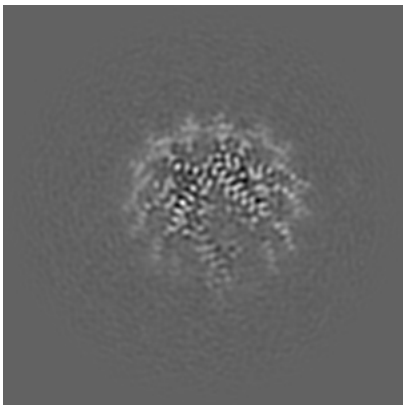


Z Index: 150

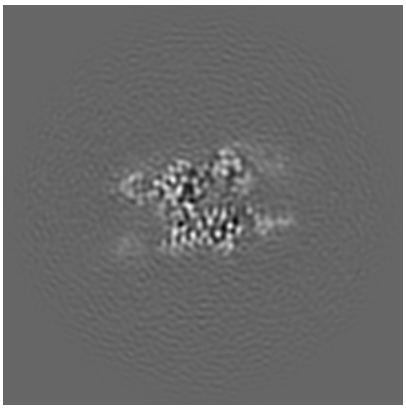
The images above show central slices of the map in three orthogonal directions.

## 5.3 Largest variance slices (i)

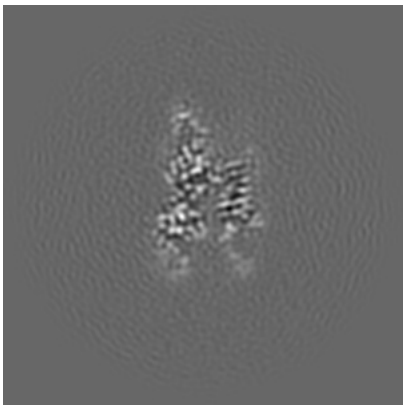
### 5.3.1 Primary map



X Index: 137

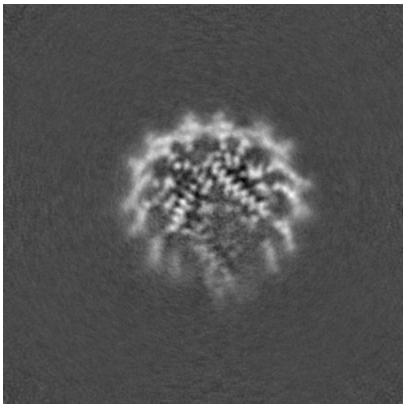


Y Index: 140

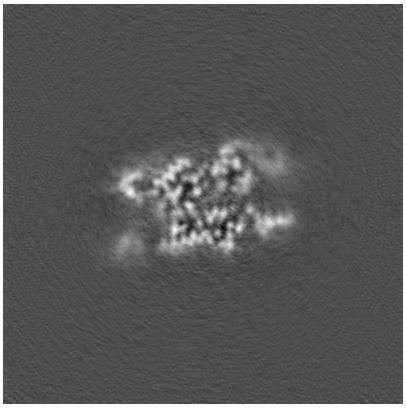


Z Index: 170

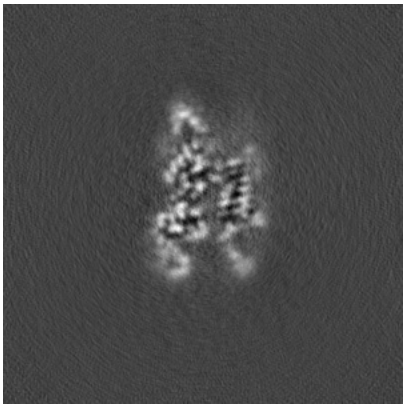
### 5.3.2 Raw map



X Index: 137



Y Index: 140

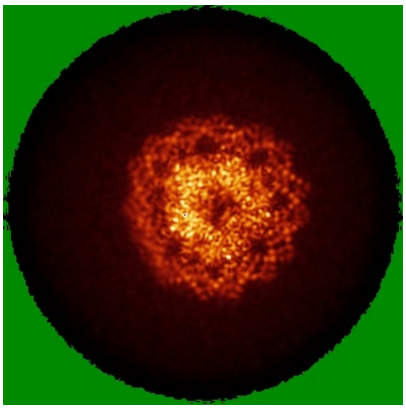


Z Index: 170

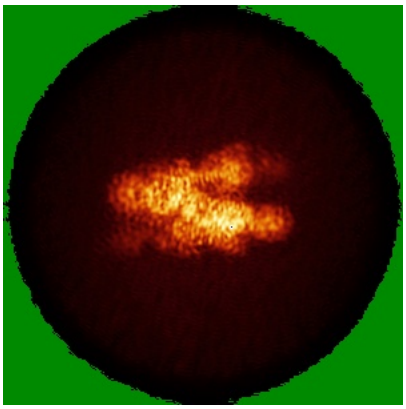
The images above show the largest variance slices of the map in three orthogonal directions.

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

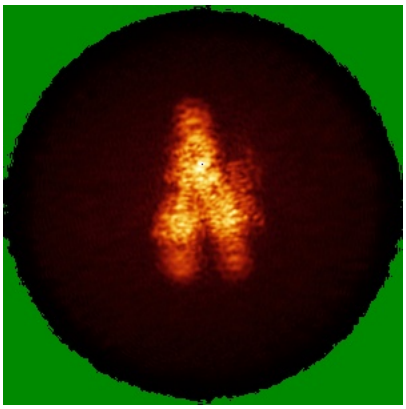
### 5.4.1 Primary map



X

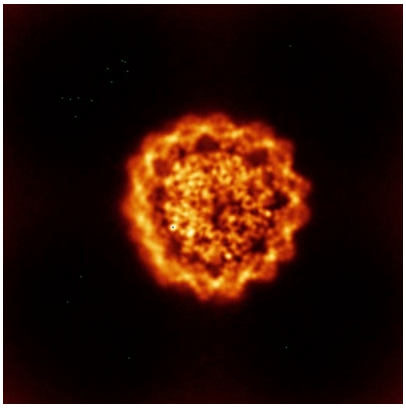


Y

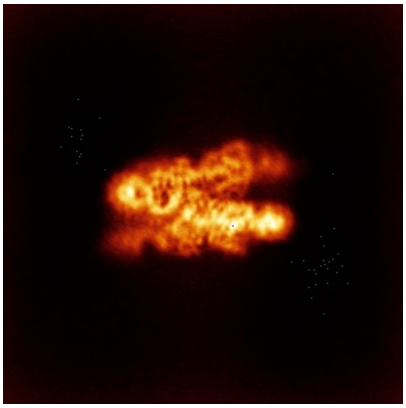


Z

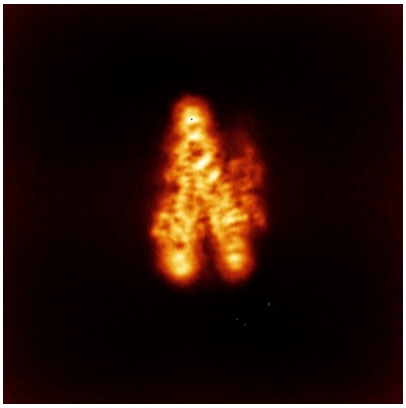
### 5.4.2 Raw map



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.

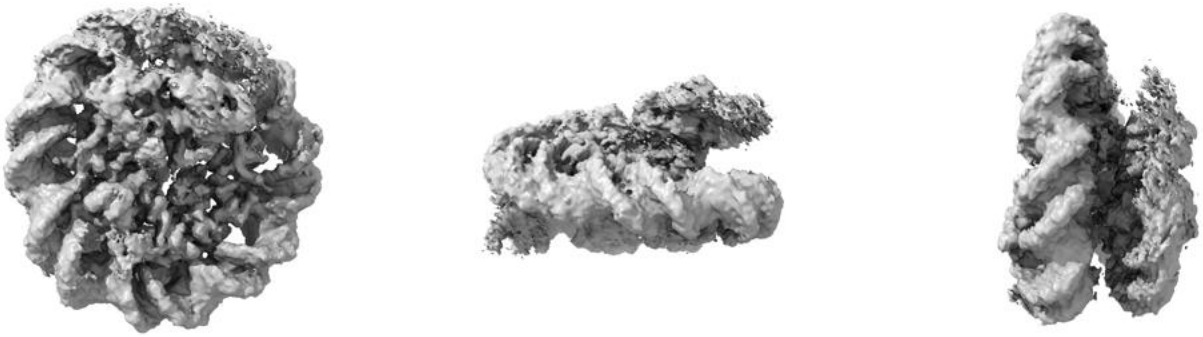
## 5.5 Orthogonal surface views (i)

### 5.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. 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



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.

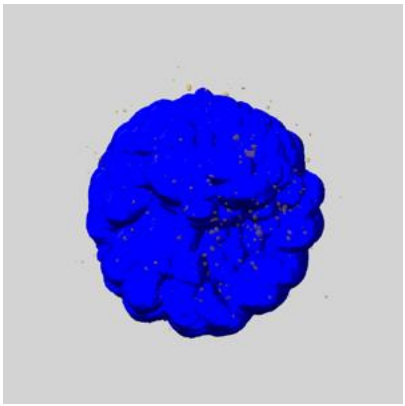
## 5.6 Mask visualisation (i)

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

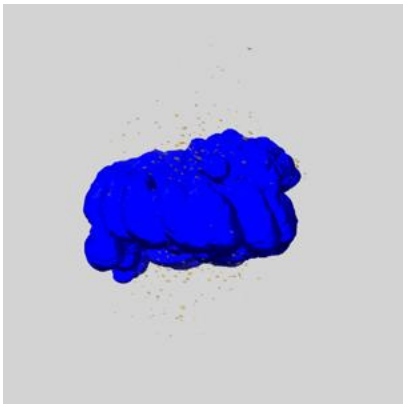
A mask typically either:

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

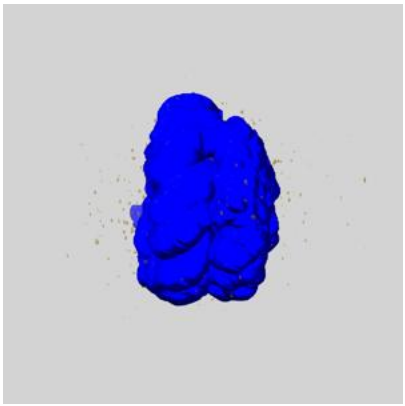
### 5.6.1 emd_18060_msk_1.map (i)



X



Y

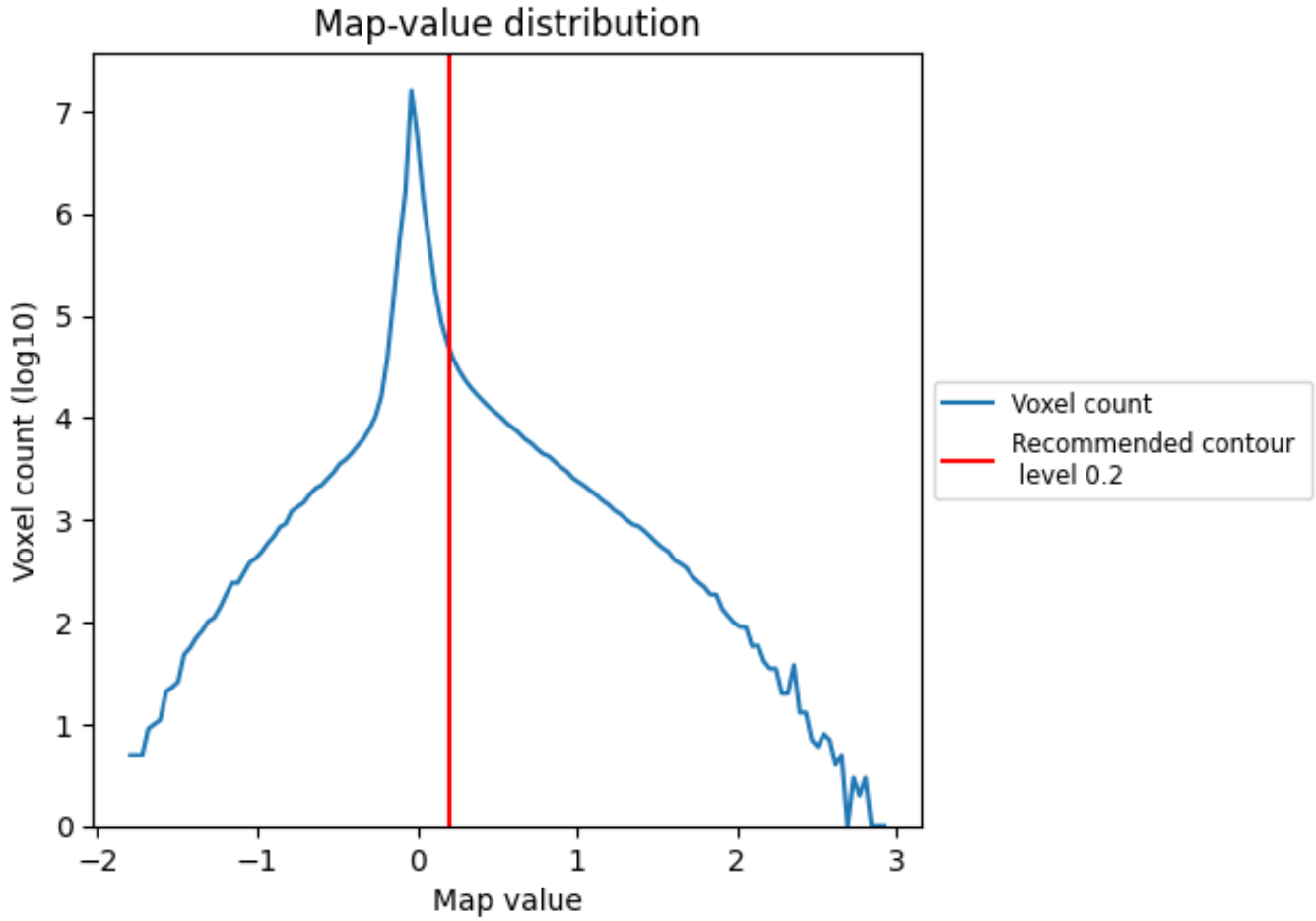


Z

# 6 Map analysis

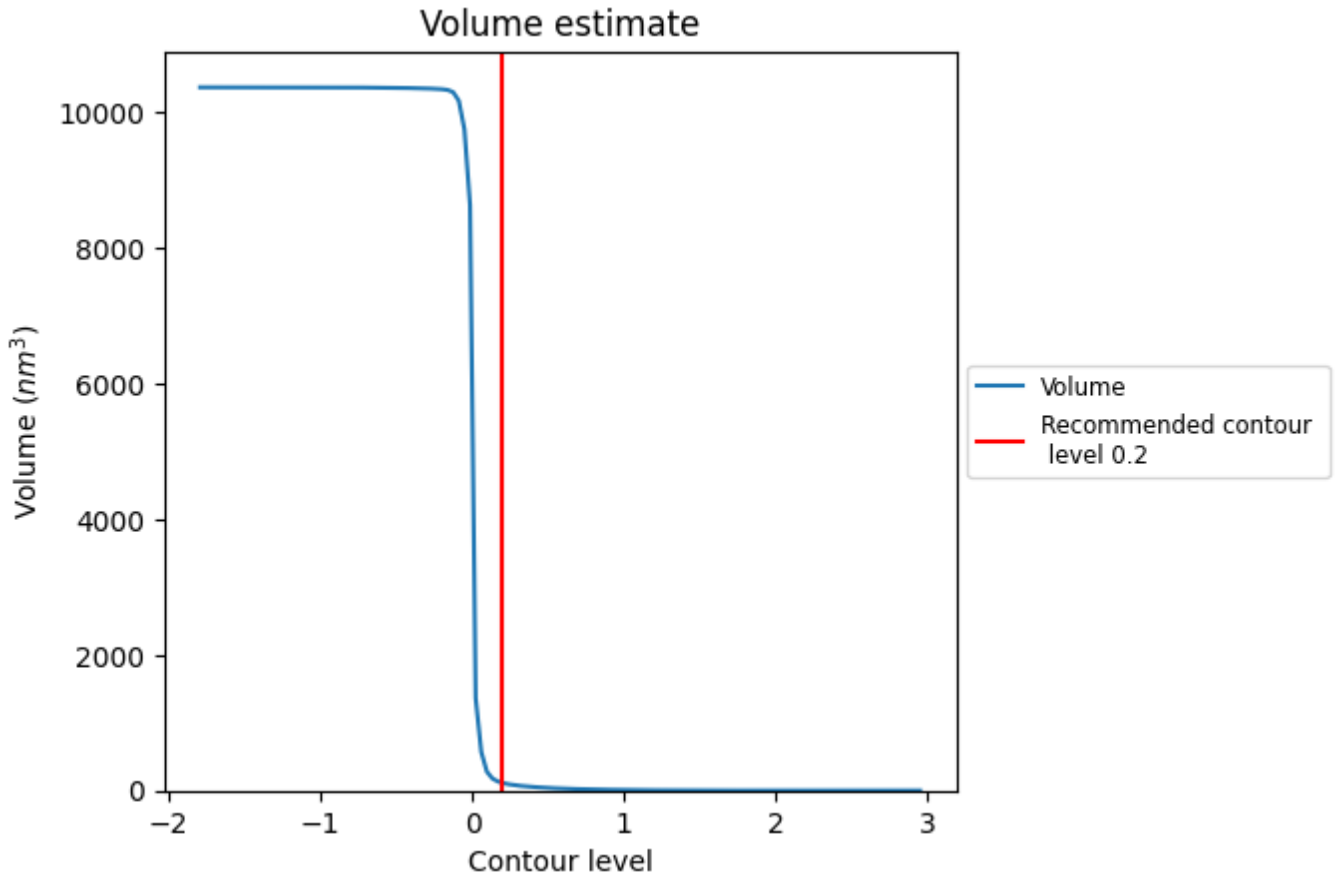
This section contains the results of statistical analysis of the map.

## 6.1 Map-value distribution




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.

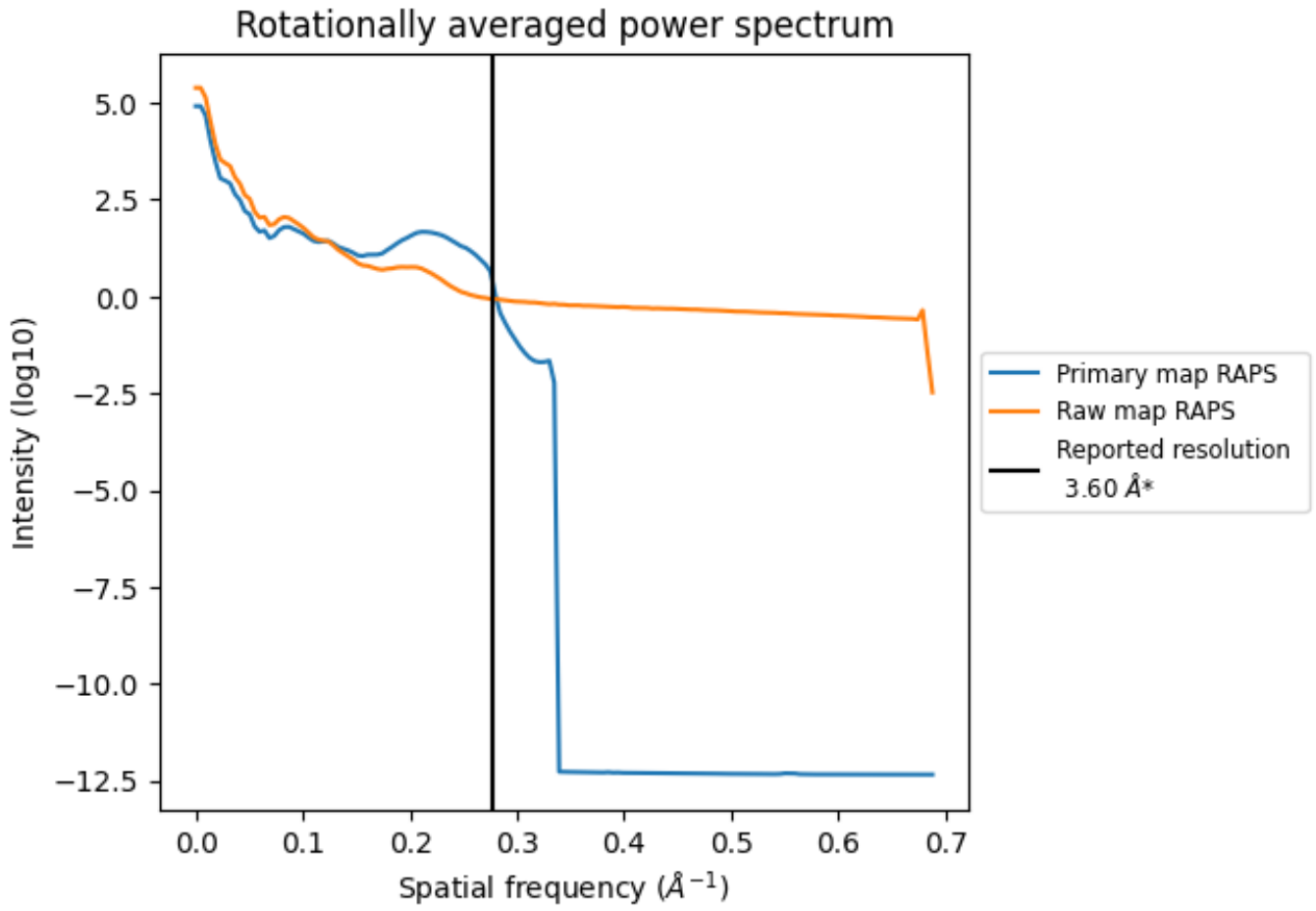
## 6.2 Volume estimate




The volume at the recommended contour level is 114 $nm^3$; this corresponds to an approximate mass of 103 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)

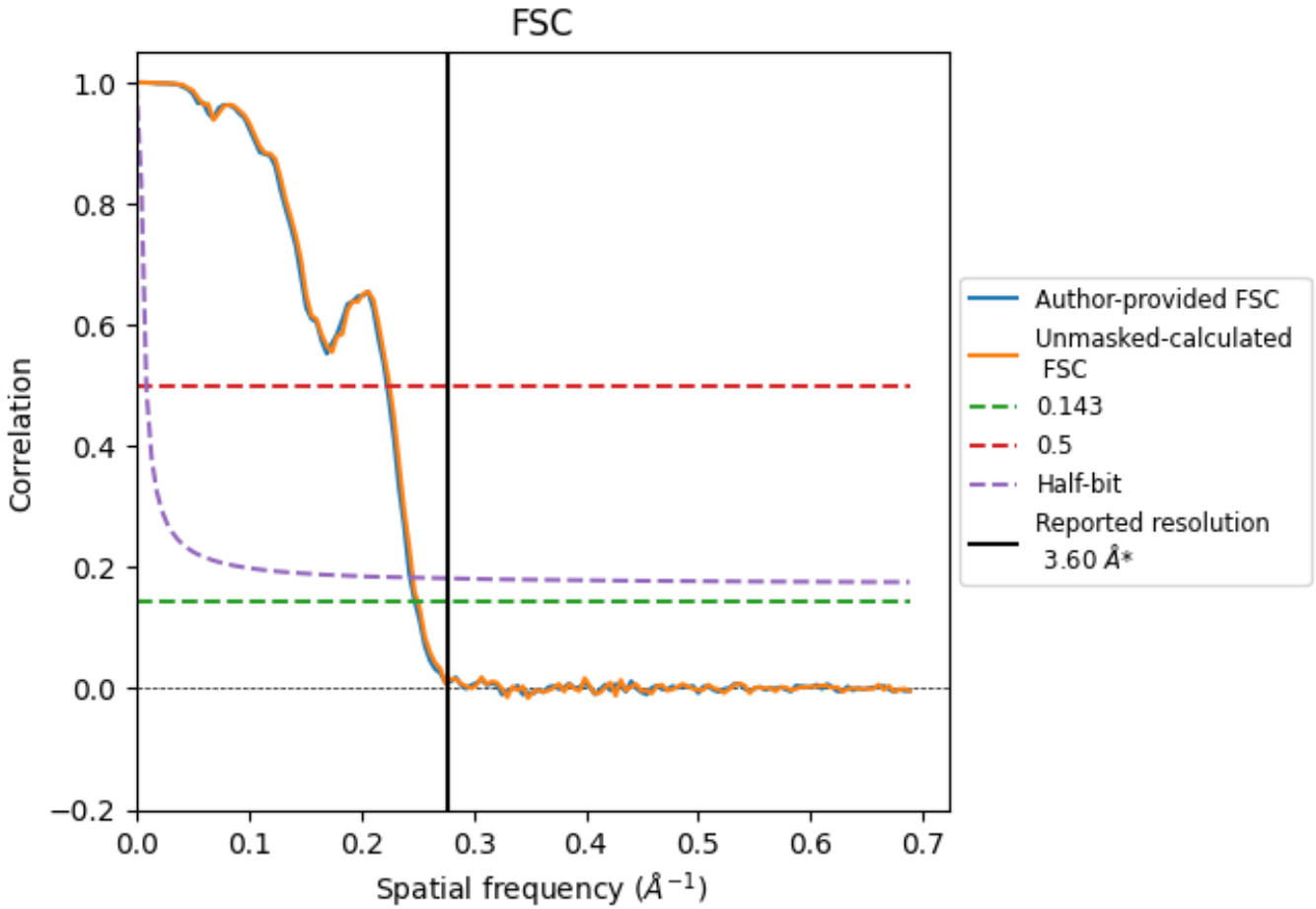



*Reported resolution corresponds to spatial frequency of 0.278 Å$^{-1}$

# 7 Fourier-Shell correlation

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




*Reported resolution corresponds to spatial frequency of 0.278 Å$^{-1}$

## 7.2 Resolution estimates (i)

| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.60 | - | - |
| Author-provided FSC curve | 4.03 | 4.48 | 4.11 |
| Unmasked-calculated* | 3.99 | 4.44 | 4.06 |

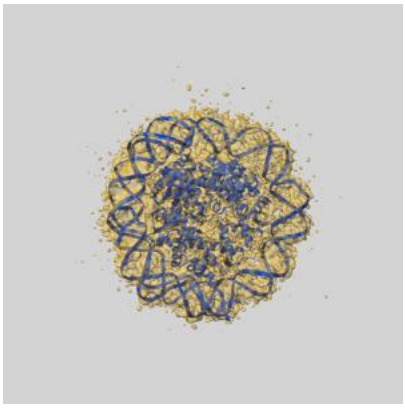
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.03 differs from the reported value 3.6 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.99 differs from the reported value 3.6 by more than 10 %

# 8 Map-model fit

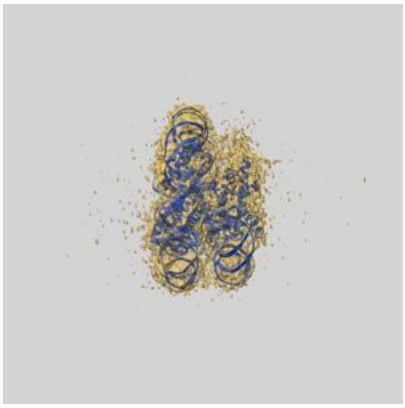
This section contains information regarding the fit between EMDB map EMD-18060 and PDB model 8Q15. Per-residue inclusion information can be found in section ?? on page ??.

## 8.1 Map-model overlay



X

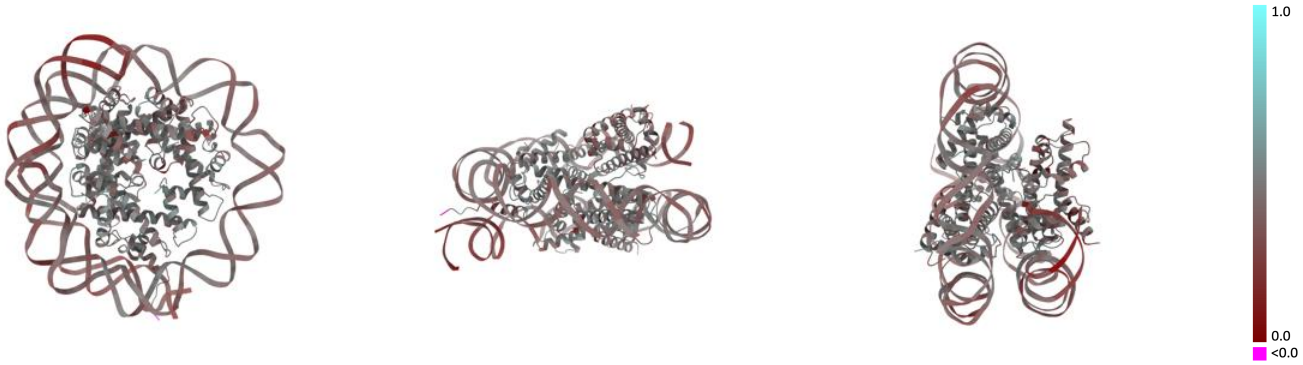
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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.

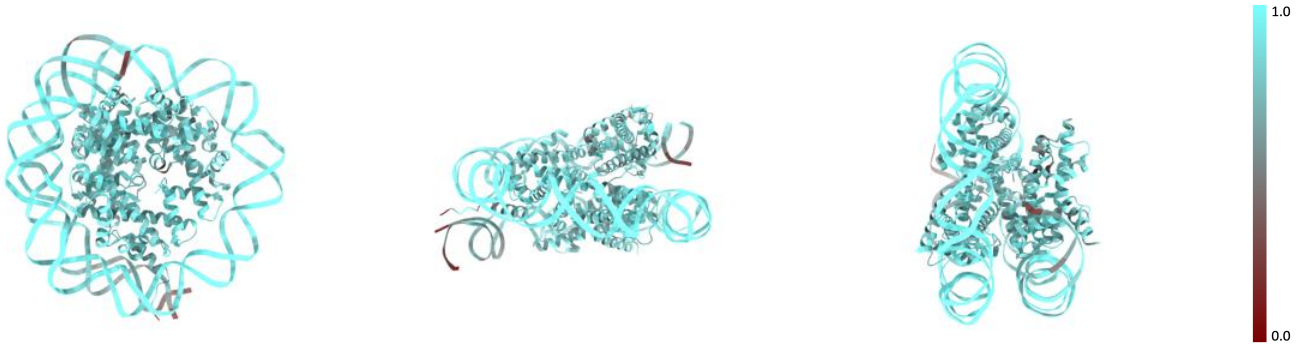
## 8.2 Q-score mapped to coordinate model (i)




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.

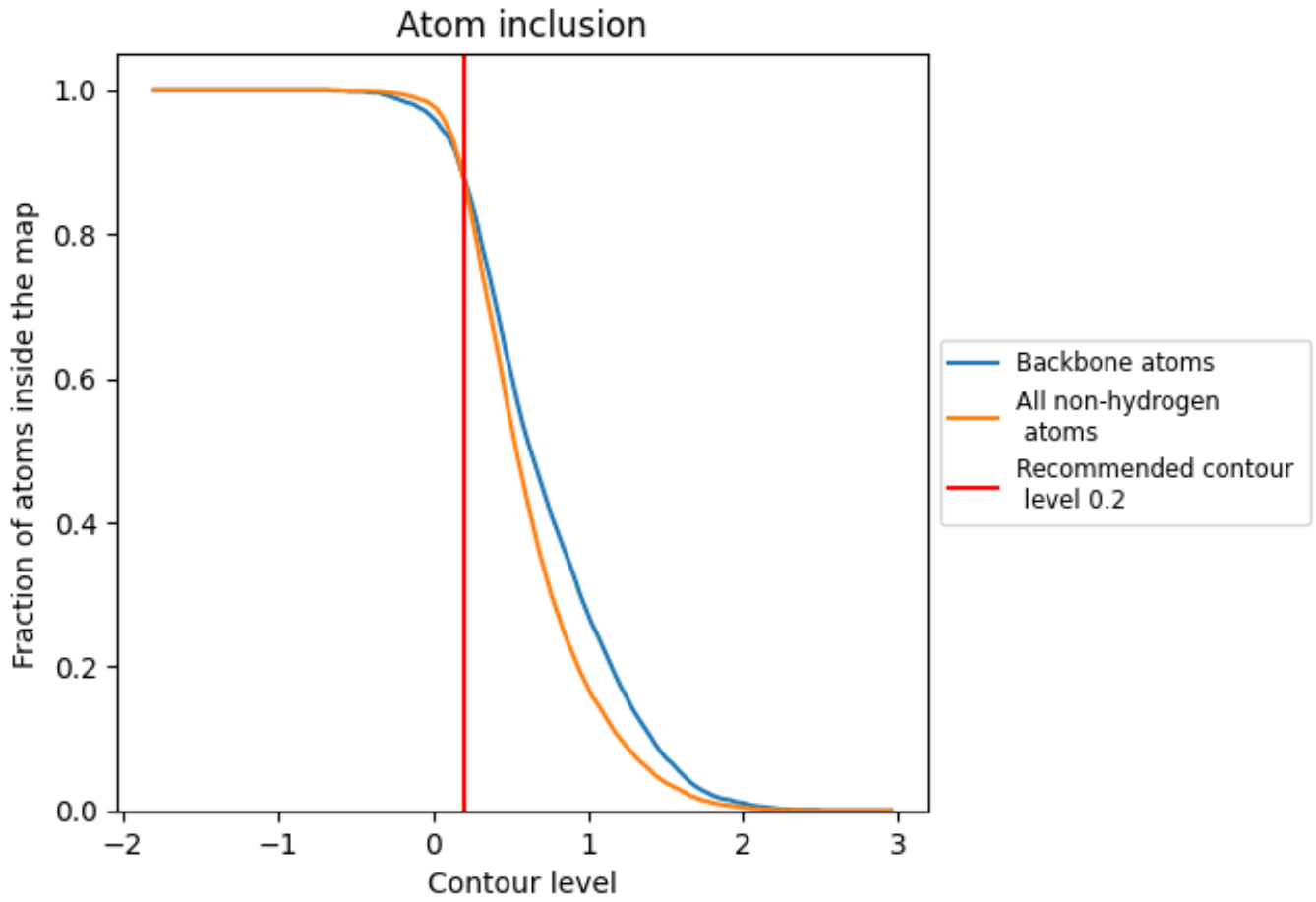
## 8.3 Atom inclusion mapped to coordinate model (i)




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 (0.2).

## 8.4 Atom inclusion (i)




At the recommended contour level, 88% of all backbone atoms, 88% 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 (0.2) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.8780 | 0.4010 |
| A | 0.8240 | 0.4110 |
| B | 0.8690 | 0.4560 |
| C | 0.8310 | 0.4120 |
| D | 0.8700 | 0.4500 |
| E | 0.8790 | 0.4740 |
| F | 0.8580 | 0.4560 |
| G | 0.8860 | 0.4770 |
| H | 0.9030 | 0.4730 |
| I | 0.8960 | 0.3440 |
| J | 0.8890 | 0.3510 |