



## Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 09:22 PM UTC

PDB ID : 7NG8 / pdb\_00007ng8  
EMDB ID : EMD-12309  
Title : Trimeric efflux pump Klebsiella TolC in complex with KlebC  
Authors : Webby, M.N.; Housden, N.G.; Kleanthous, C.  
Deposited on : 2021-02-08  
Resolution : 3.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

EMDB validation analysis : 0.0.1.dev132  
MolProbity : **FAILED**  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

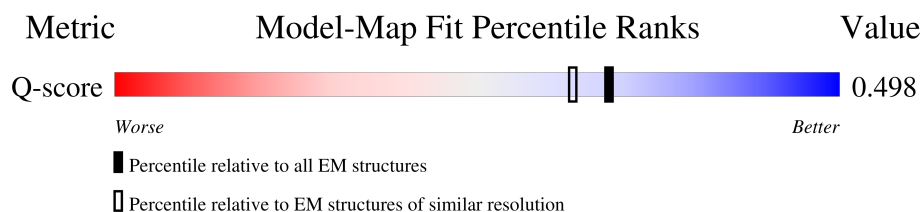
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 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  | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|---------|-----------------------------|----------------------------------------------------------|
| Q-score | 25397                       | 15020 ( 2.70 - 3.70 )                                    |

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

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20173 atoms, of which 9979 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 Outer membrane channel protein.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 1   | A     | 422      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 6468  | 2011 | 3209 | 577 | 668 | 3 |         |       |
| 1   | B     | 422      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 6468  | 2011 | 3209 | 577 | 668 | 3 |         |       |
| 1   | C     | 422      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 6468  | 2011 | 3209 | 577 | 668 | 3 |         |       |

There are 24 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference      |
|-------|---------|----------|--------|----------------|----------------|
| A     | 465     | LEU      | -      | expression tag | UNP A0A1C3Q001 |
| A     | 466     | GLU      | -      | expression tag | UNP A0A1C3Q001 |
| A     | 467     | HIS      | -      | expression tag | UNP A0A1C3Q001 |
| A     | 468     | HIS      | -      | expression tag | UNP A0A1C3Q001 |
| A     | 469     | HIS      | -      | expression tag | UNP A0A1C3Q001 |
| A     | 470     | HIS      | -      | expression tag | UNP A0A1C3Q001 |
| A     | 471     | HIS      | -      | expression tag | UNP A0A1C3Q001 |
| A     | 472     | HIS      | -      | expression tag | UNP A0A1C3Q001 |
| B     | 465     | LEU      | -      | expression tag | UNP A0A1C3Q001 |
| B     | 466     | GLU      | -      | expression tag | UNP A0A1C3Q001 |
| B     | 467     | HIS      | -      | expression tag | UNP A0A1C3Q001 |
| B     | 468     | HIS      | -      | expression tag | UNP A0A1C3Q001 |
| B     | 469     | HIS      | -      | expression tag | UNP A0A1C3Q001 |
| B     | 470     | HIS      | -      | expression tag | UNP A0A1C3Q001 |
| B     | 471     | HIS      | -      | expression tag | UNP A0A1C3Q001 |
| B     | 472     | HIS      | -      | expression tag | UNP A0A1C3Q001 |
| C     | 465     | LEU      | -      | expression tag | UNP A0A1C3Q001 |
| C     | 466     | GLU      | -      | expression tag | UNP A0A1C3Q001 |
| C     | 467     | HIS      | -      | expression tag | UNP A0A1C3Q001 |
| C     | 468     | HIS      | -      | expression tag | UNP A0A1C3Q001 |
| C     | 469     | HIS      | -      | expression tag | UNP A0A1C3Q001 |
| C     | 470     | HIS      | -      | expression tag | UNP A0A1C3Q001 |
| C     | 471     | HIS      | -      | expression tag | UNP A0A1C3Q001 |
| C     | 472     | HIS      | -      | expression tag | UNP A0A1C3Q001 |

- Molecule 2 is a protein called Klebicin C activity.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 2   | D     | 75       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 769   | 249 | 352 | 82 | 84 | 2 |         |       |

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

### 3 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 435603                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 30                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 QUANTUM (4k x 4k)              | Depositor |
| Maximum map value                    | 0.667                                   | Depositor |
| Minimum map value                    | -0.268                                  | Depositor |
| Average map value                    | 0.002                                   | Depositor |
| Map value standard deviation         | 0.020                                   | Depositor |
| Recommended contour level            | 0.145                                   | Depositor |
| Map size (Å)                         | 246.6, 246.6, 246.6                     | wwPDB     |
| Map dimensions                       | 300, 300, 300                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.822, 0.822, 0.822                     | Depositor |

## 4 Model quality [i](#)

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

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

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

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

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

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

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

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

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

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

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

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

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

### 4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such residues in this entry.

## 4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

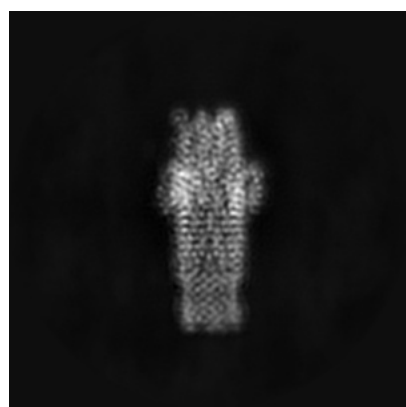
## 5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12309. These allow visual inspection of the internal detail of the map and identification of artifacts.

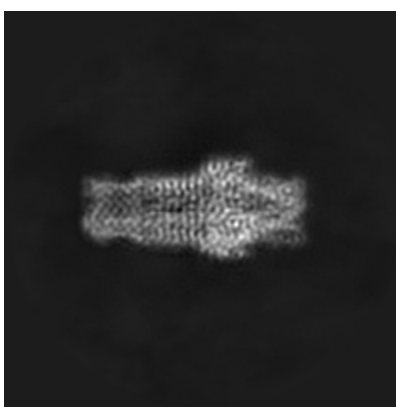
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

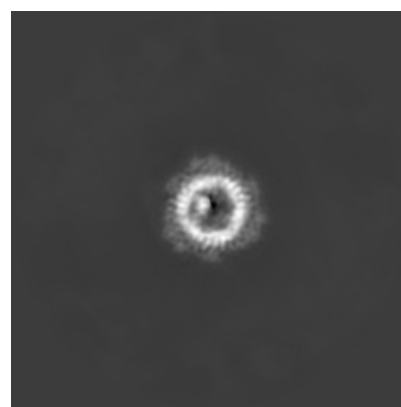
#### 5.1.1 Primary map



X



Y

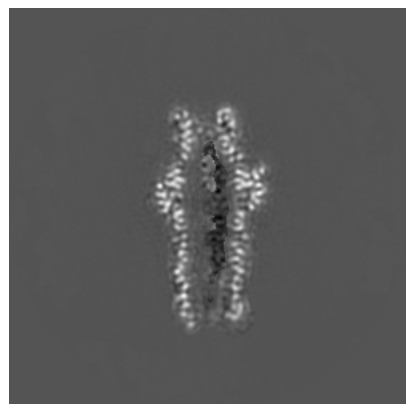


Z

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

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

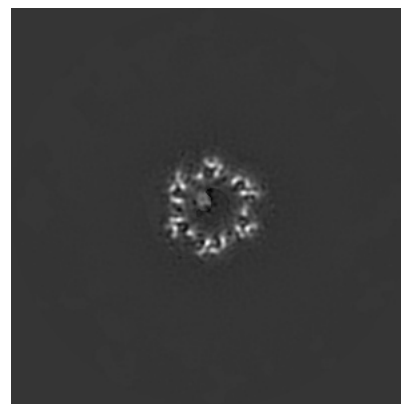
#### 5.2.1 Primary map



X Index: 150



Y Index: 150



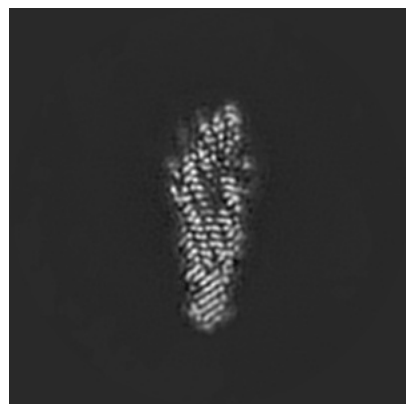
Z Index: 150



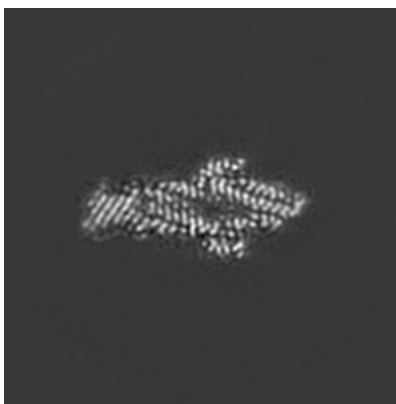
The images above show central slices of the map in three orthogonal directions.

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

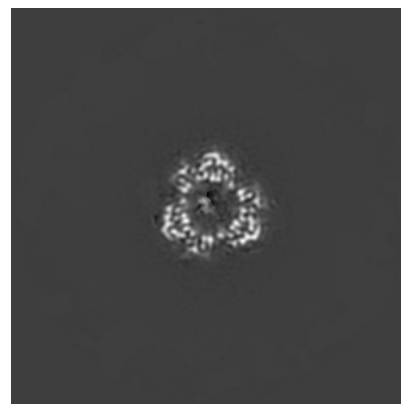
### 5.3.1 Primary map



X Index: 169



Y Index: 132



Z Index: 177

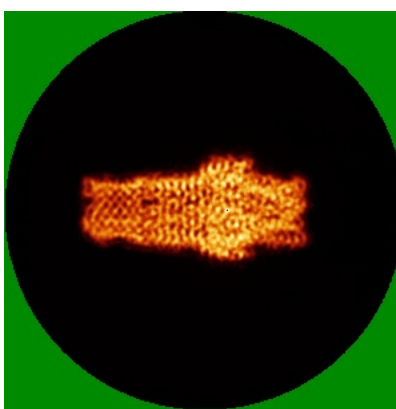
The images above show the largest variance slices of the map in three orthogonal directions.

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

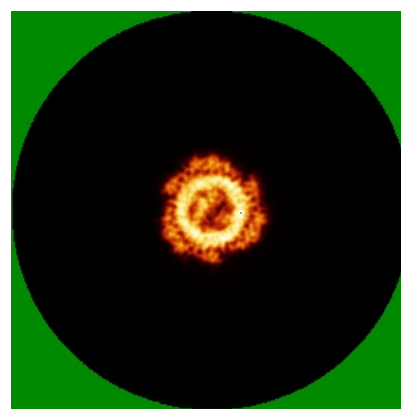
### 5.4.1 Primary map



X



Y

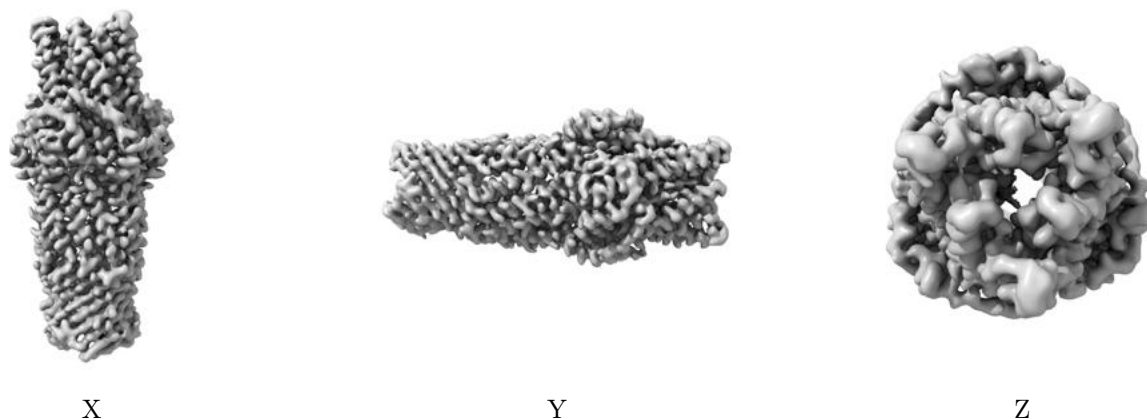


Z

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

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

### 5.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.145. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

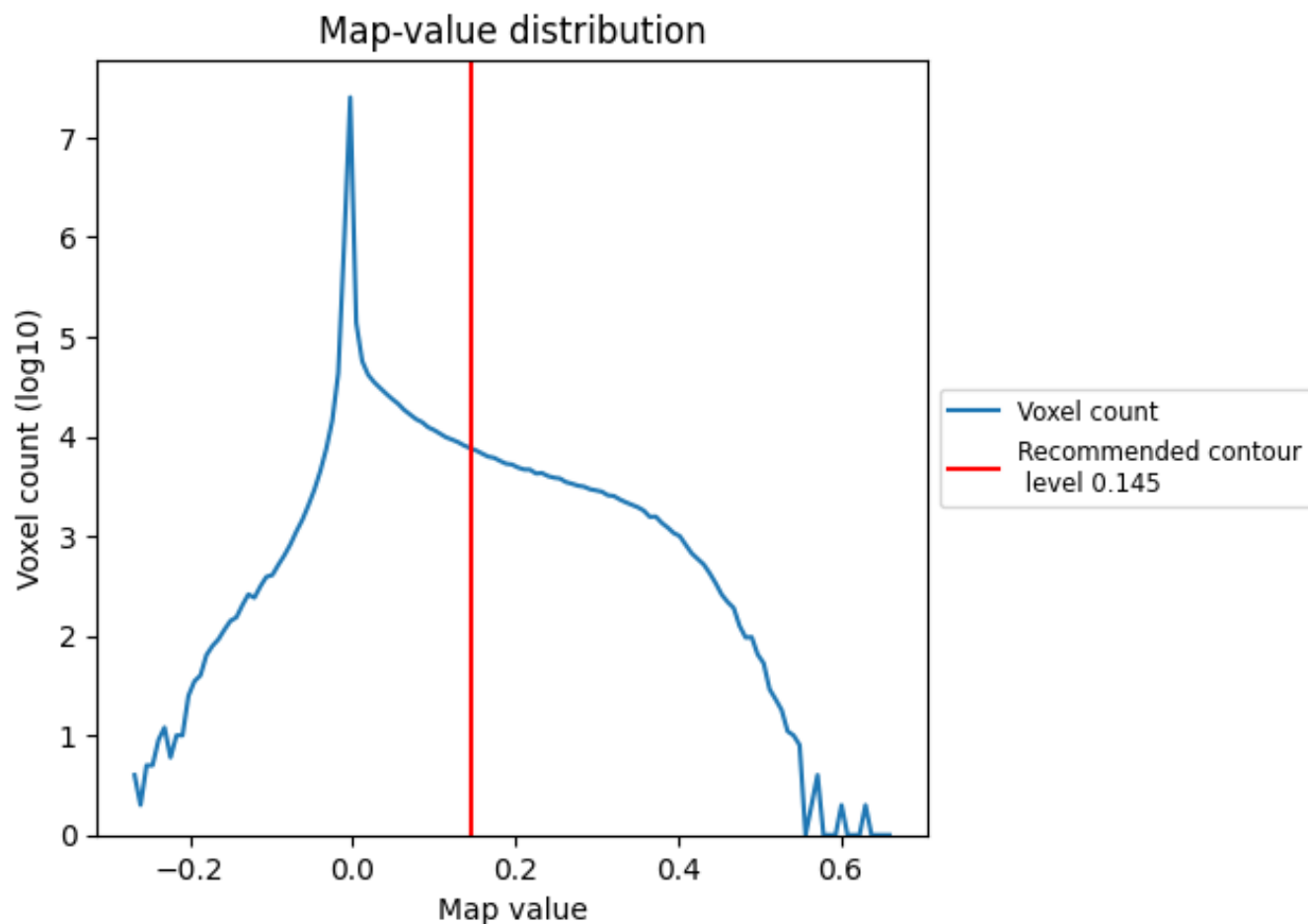
## 5.6 Mask visualisation [i](#)

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

## 6 Map analysis [i](#)

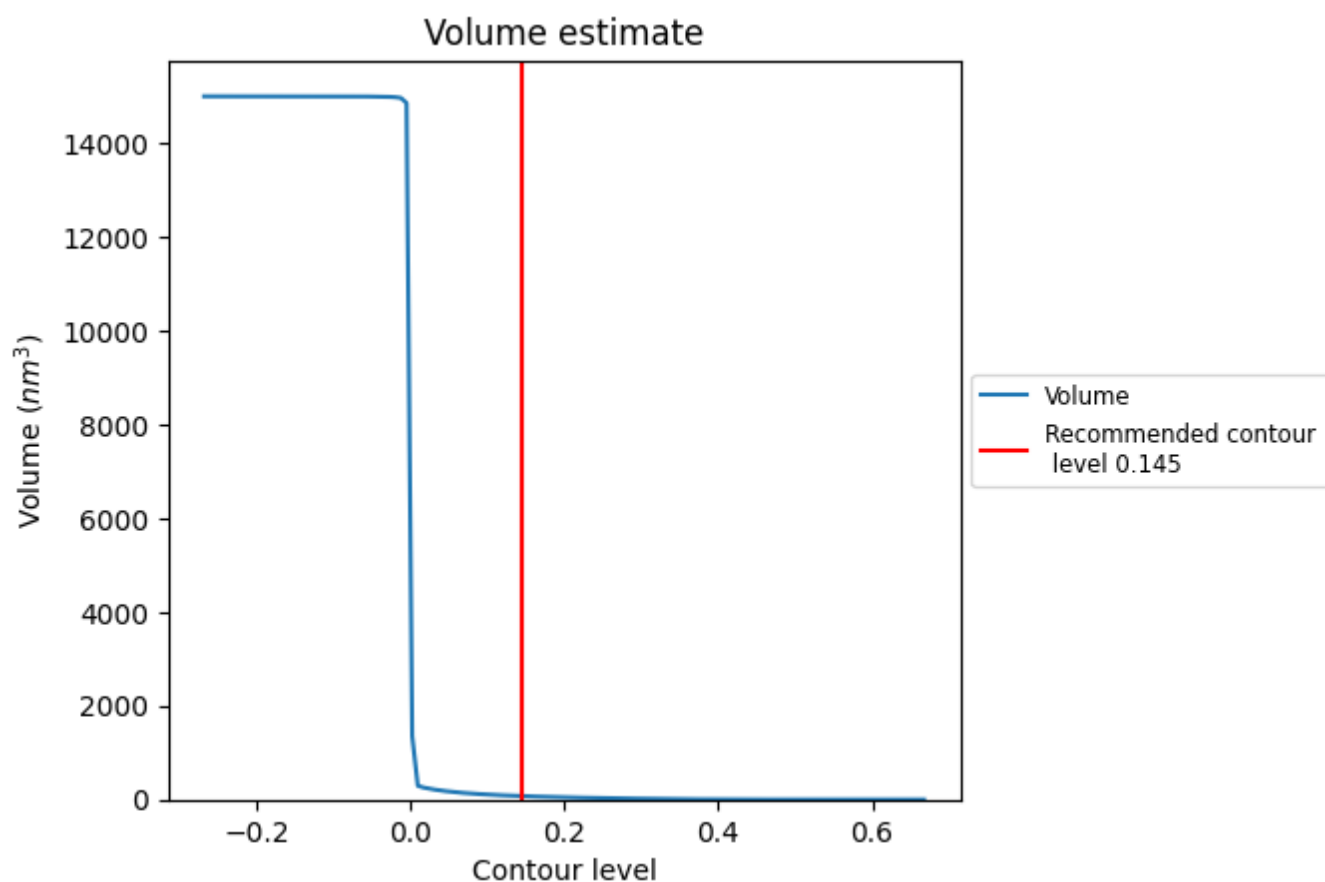
This section contains the results of statistical analysis of the map.

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



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

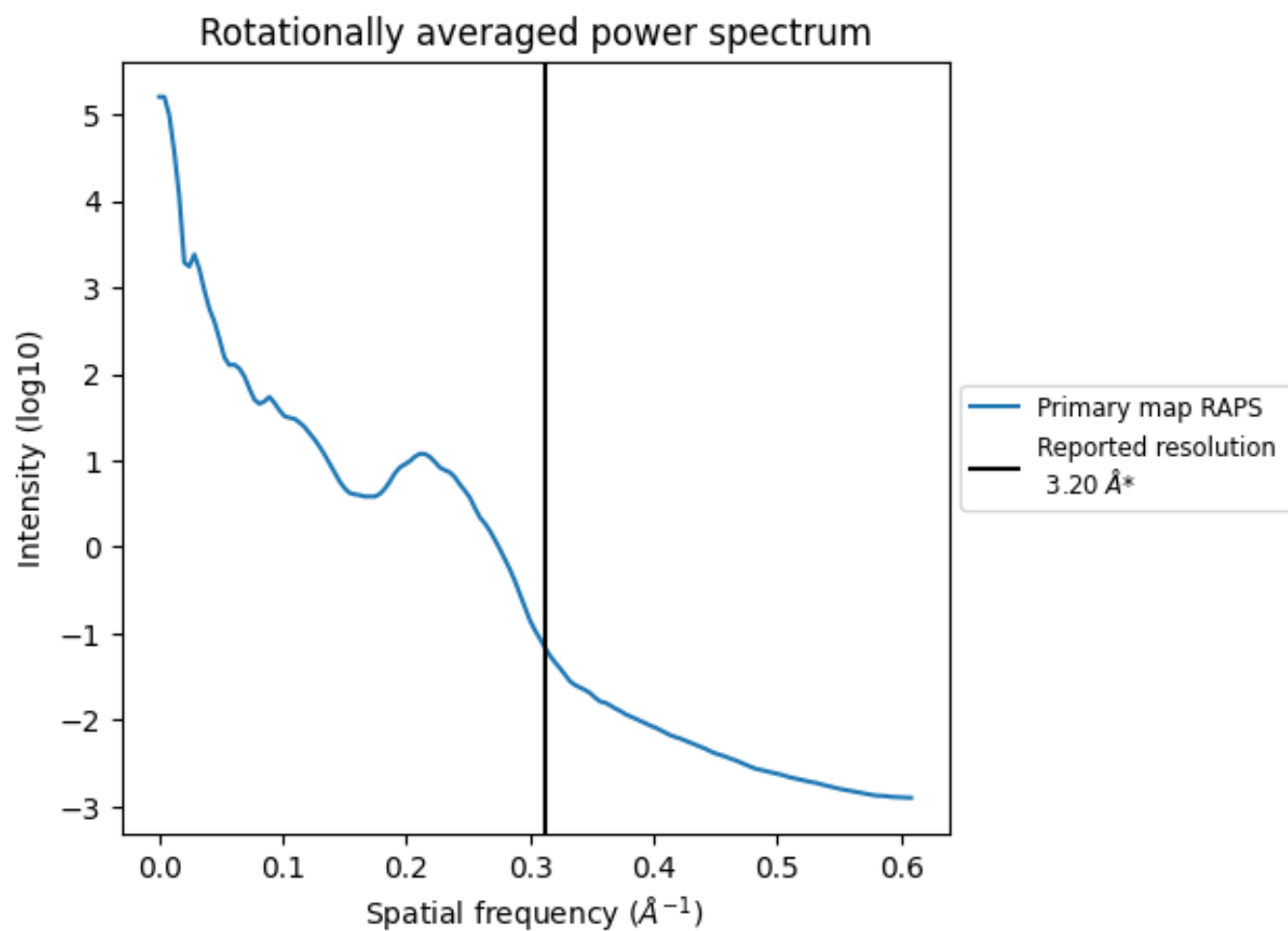
## 6.2 Volume estimate [i](#)



The volume at the recommended contour level is 74  $\text{nm}^3$ ; this corresponds to an approximate mass of 67 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 ⓘ

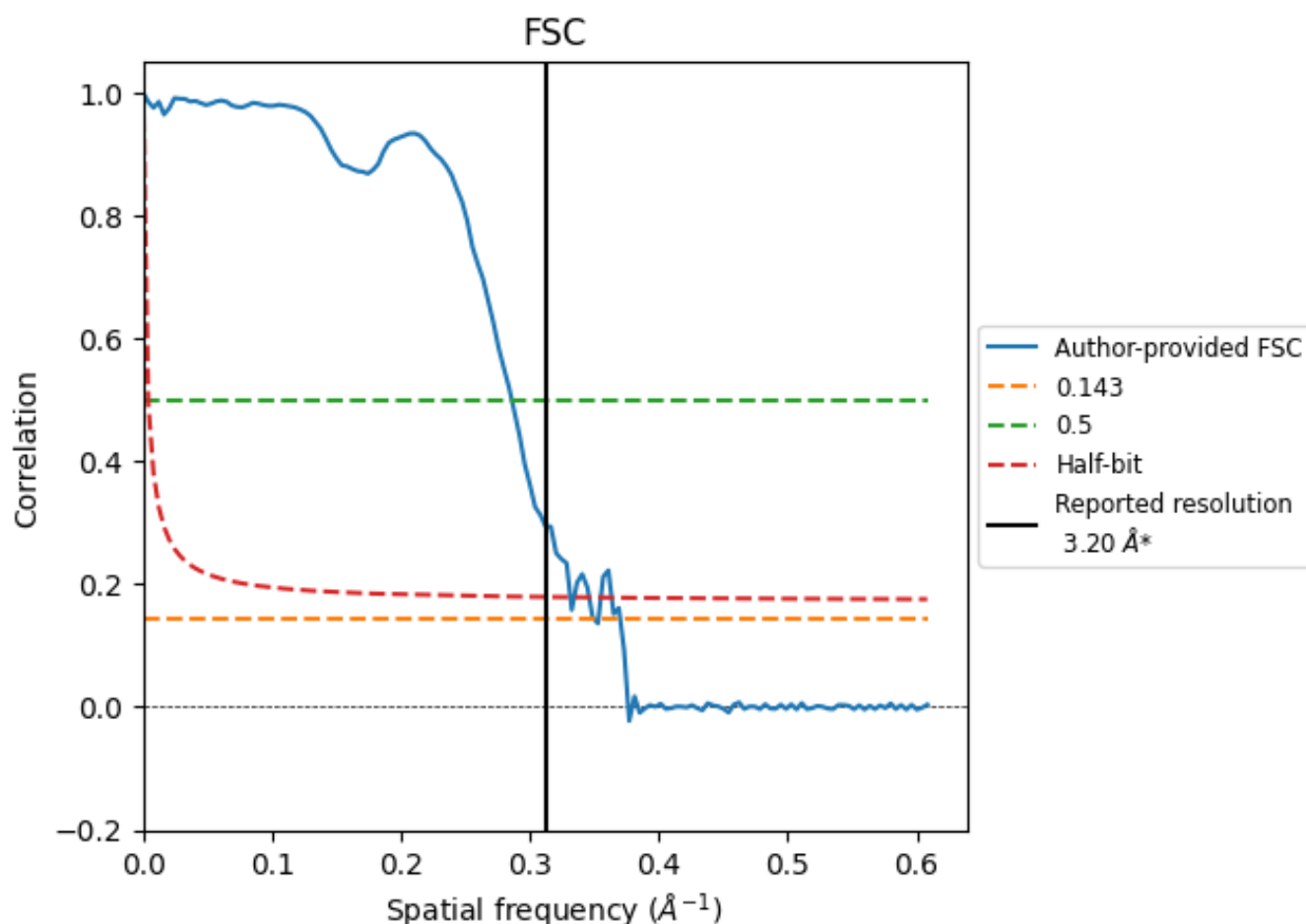


\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 7 Fourier-Shell correlation [i](#)

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

### 7.1 FSC [i](#)



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

## 7.2 Resolution estimates [i](#)

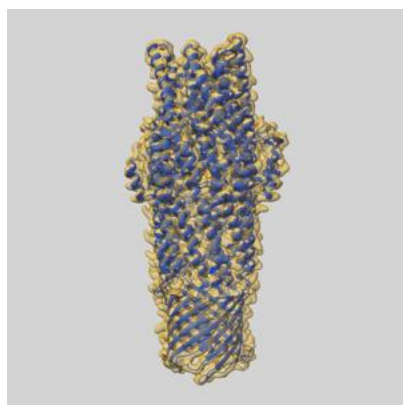
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.20                               | -    | -        |
| Author-provided FSC curve | 2.86                               | 3.50 | 3.02     |
| Unmasked-calculated*      | -                                  | -    | -        |

\*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 2.86 differs from the reported value 3.2 by more than 10 %

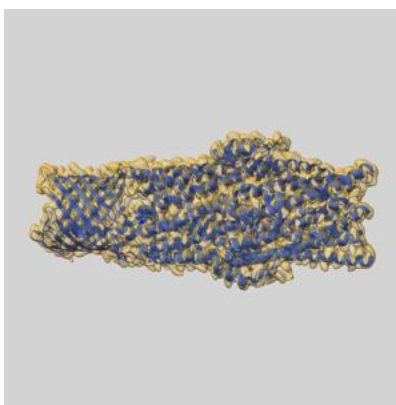
## 8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12309 and PDB model 7NG8. Per-residue inclusion information can be found in section ?? on page ??.

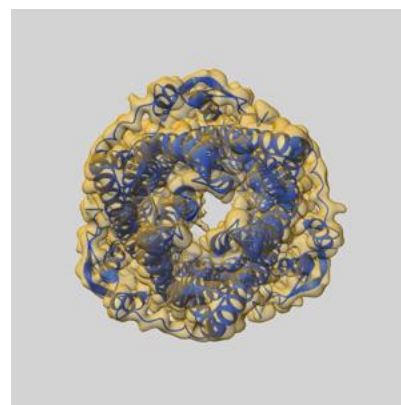
### 8.1 Map-model overlay [i](#)



X



Y

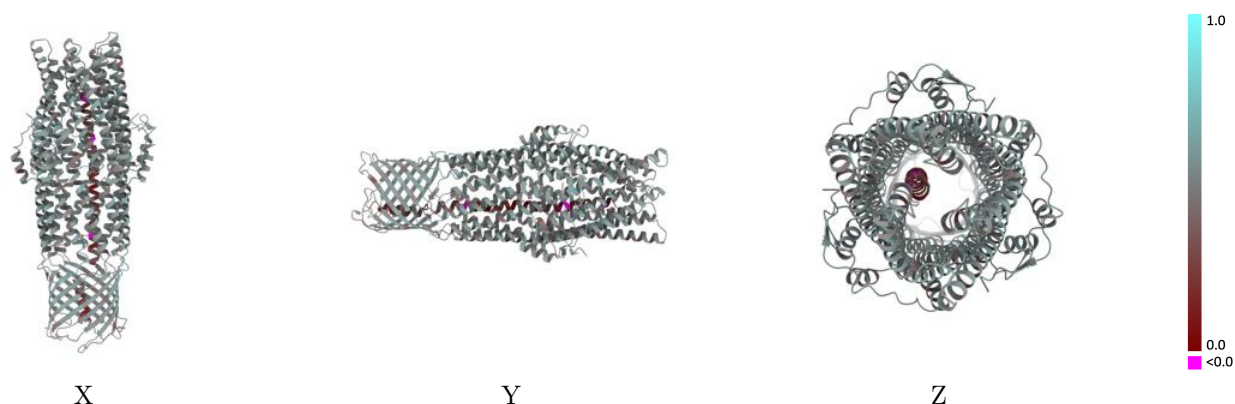


Z

The images above show the 3D surface view of the map at the recommended contour level 0.145 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

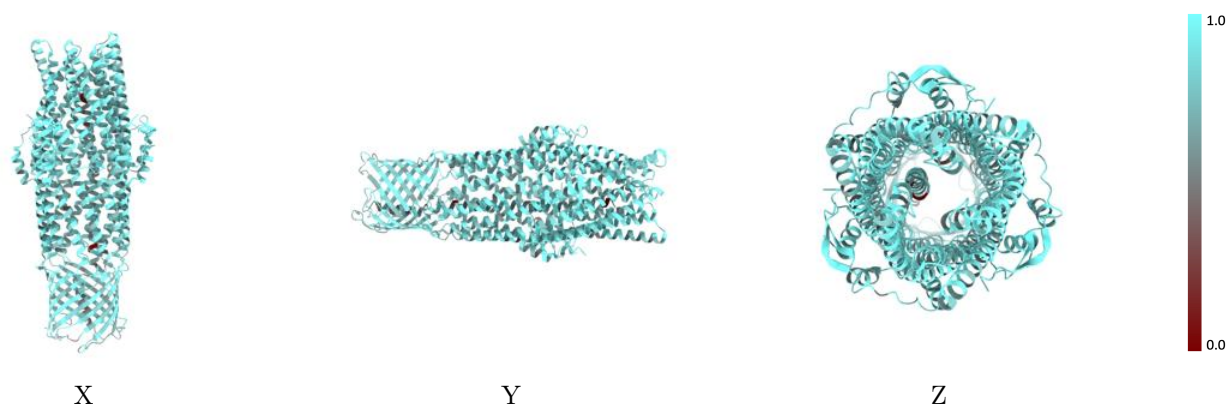


## 8.2 Q-score mapped to coordinate model [i](#)



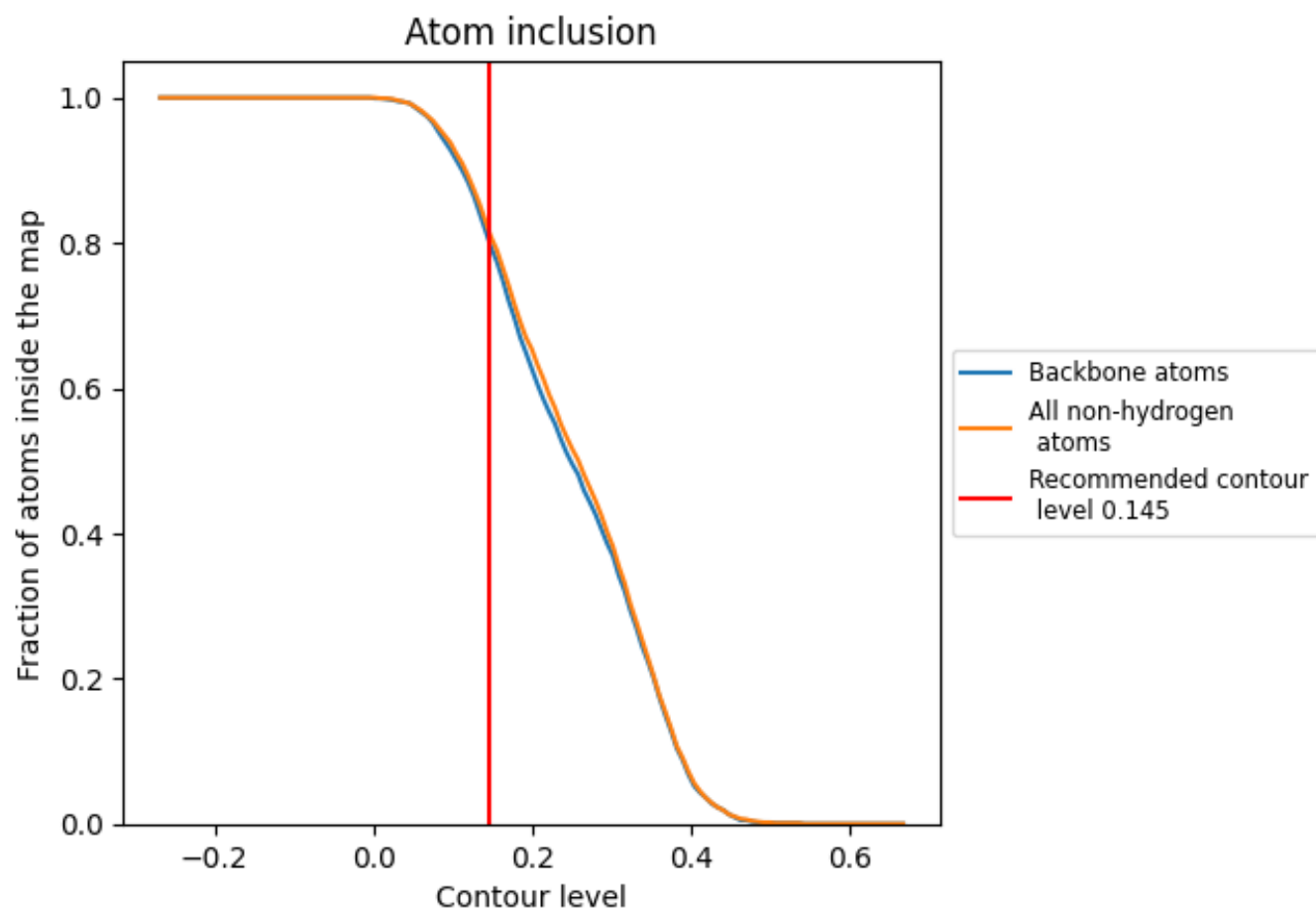
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.145).

## 8.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 82% 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 (0.145) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.8180 | <div></div> 0.4980 |
| A     | <div></div> 0.8370 | <div></div> 0.5100 |
| B     | <div></div> 0.8410 | <div></div> 0.5120 |
| C     | <div></div> 0.8410 | <div></div> 0.5060 |
| D     | <div></div> 0.6980 | <div></div> 0.2410 |

