



## wwPDB EM Validation Summary Report ⓘ

Mar 22, 2025 – 05:17 PM EDT

PDB ID : 6V9X  
EMDB ID : EMD-21129  
Title : Structure of TRPA1 modified by iodoacetamide, PMAL-C8  
Authors : Zhao, J.; Lin King, J.V.; Paulsen, C.E.; Cheng, Y.; Julius, D.  
Deposited on : 2019-12-16  
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev117  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
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) : 2.41.4

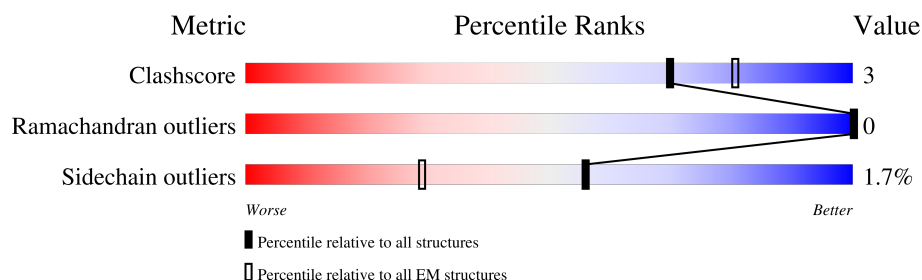
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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  $\leq 5\%$ . 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	1119	
1	B	1119	
1	C	1119	
1	D	1119	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 18084 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 Transient receptor potential cation channel subfamily A member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	571	Total	C	N	O	S	0	0
			4521	2964	750	775	32		
1	B	571	Total	C	N	O	S	0	0
			4521	2964	750	775	32		
1	D	571	Total	C	N	O	S	0	0
			4521	2964	750	775	32		
1	C	571	Total	C	N	O	S	0	0
			4521	2964	750	775	32		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	966	ASP	GLU	engineered mutation	UNP O75762
B	966	ASP	GLU	engineered mutation	UNP O75762
D	966	ASP	GLU	engineered mutation	UNP O75762
C	966	ASP	GLU	engineered mutation	UNP O75762



49%

LYS  
ALA  
LYS  
THR  
HIS  
HIS  
LEU  
GLU  
PRO

- 49%

THR	LEU	GLY	ASP	MET
PRO	GLN	ALA	MET	LYS
LEU	ILE	ASN	ASP	LEU
HIS	LEU	PRO	THR	SER
LEU	LEU	ASN	PHE	LEU
ALA	LYS	ARG	PHE	ARG
VAL	GLY	ASN	LEU	LYS
GLN	GLY	ASN	HIS	MET
ASN	ALA	PHE	TYR	ARG
ASP	PRO	MET	ALA	PRO
LEU	CYS	MET	ALA	GLY
GLU	LYS	ALA	GLU	GLU
MET	SER	PRO	GLY	LYS
ILE	ASN	LEU	GLN	LYS
MET	TRP	ILE	GLU	PRO
CYS	GLY	ALA	LEU	GLN
LEU	CYS	VAL	MET	GLY
ASP	PHE	GLN	GLU	VAL
ASN	PRO	GLY	LYS	VAL
ALA	ILE	GLY	ILE	TYR
ALA	HIS	ASN	THR	GLU
GLN	GLN	ASN	ASP	ASP
ILE	ALA	GLU	ASP	VAL
ASP	ALA	VAL	SER	PRO
PRO	PHE	MET	SER	ASP
VAL	SER	LYS	LEU	GLU
GLU	GLY	VAL	GLU	THR
LYS	SER	LEU	VAL	GLU
GLY	LYS	LEU	LEU	ASP
ARG	GLU	GLU	HIS	PHE
CYS	CYS	HIS	GLU	LYS
THR	MET	ARG	MET	GLU
ALA	GLU	THR	ASP	SER
ILE	ILE	ILE	ASP	LEU
HIS	ILE	ASP	TYR	LYS
PHE	LEU	VAL	GLY	VAL
ALA	ARG	ASN	ASN	VAL
ALA	PHE	LEU	THR	PHE
THR	GLY	GLU	PRO	GLU
GLN	GLU	GLY	LEU	GLY
GLY	GLU	GLU	HIS	SER
ALA	HIS	ASN	CYS	ALA
THR	GLY	GLY	ALA	TYR
ILE	SER	THR	GLU	GLY
VAL	ARG	ALA	LYS	GLN
LYS	GLN	VAL	ASN	ASN
LEU	HIS	ILE	GLN	PHE
MET	LEU	ILE	ILE	ASN
ILE	ILE	ALA	GLU	LYS
SER	ASN	CYS	SER	GLN
SER	PHE	THR	VAL	LYS
TYR	MET	THR	LYS	LYS
SER	ASN	ASN	PHE	LEU
GLY	ASN	ASN	LEU	ARG
SER	GLY	SER	LEU	LYS
VAL	LYS	GLU	ARG	CYS



LEU	ARG	ALA	VAL	LYS	ALA	LYS	THR	HIS	HIS	LEU	GLU	PRO	SER	GLY	GLY	MET	LEU	PHE	HIS	ILE	PHE	CYS	PHE	LEU	PHE	CYS	THR	GLY	GLY	ILE	ARG	GLN	GLU	ILE	PRO	ASN	ALA	ASP	LYS	31039	11042	11078	GLU	ASP	ASP	ASP	SER	SER	HIS	CYS	SER	PHE	GLN	ASP	ARG	PHE	LYS	LYS	GLU	GLN	GLU	MET	GLN	ARG	ASN	THR	VAL
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	190112	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	49.653	Depositor
Minimum map value	-31.670	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	311.1936, 311.1936, 311.1936	wwPDB
Map dimensions	256, 256, 256	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](#)

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

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	0.28	0/4611	0.52	0/6247
1	B	0.28	0/4611	0.52	0/6247
1	C	0.28	0/4611	0.52	0/6247
1	D	0.28	0/4611	0.52	0/6247
All	All	0.28	0/18444	0.52	0/24988

There are no bond length outliers.

There are no bond angle outliers.

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	4521	0	4581	33	0
1	B	4521	0	4581	33	0
1	C	4521	0	4581	33	0
1	D	4521	0	4581	34	0
All	All	18084	0	18324	125	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 3.

The worst 5 of 125 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:C:682:PRO:HG2	1:C:984:THR:HG22	1.76	0.67
1:C:948:VAL:HA	1:C:951:VAL:HG12	1.77	0.67
1:D:682:PRO:HG2	1:D:984:THR:HG22	1.76	0.67
1:B:682:PRO:HG2	1:B:984:THR:HG22	1.76	0.66
1:A:948:VAL:HA	1:A:951:VAL:HG12	1.77	0.66

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	562/1119 (50%)	539 (96%)	23 (4%)	0	100	100
1	B	562/1119 (50%)	539 (96%)	23 (4%)	0	100	100
1	C	562/1119 (50%)	539 (96%)	23 (4%)	0	100	100
1	D	562/1119 (50%)	539 (96%)	23 (4%)	0	100	100
All	All	2248/4476 (50%)	2156 (96%)	92 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	482/994 (48%)	474 (98%)	8 (2%)	56	74
1	B	482/994 (48%)	474 (98%)	8 (2%)	56	74
1	C	482/994 (48%)	474 (98%)	8 (2%)	56	74
1	D	482/994 (48%)	474 (98%)	8 (2%)	56	74
All	All	1928/3976 (48%)	1896 (98%)	32 (2%)	56	74

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	969	LYS
1	C	984	THR
1	B	969	LYS
1	B	959	LEU
1	C	999	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1061	GLN
1	C	700	HIS
1	D	460	ASN
1	C	855	ASN
1	D	855	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	YCM	B	621	1	7,9,10	1.76	1 (14%)	5,10,12	1.47	1 (20%)
1	YCM	D	621	1	7,9,10	1.77	1 (14%)	5,10,12	1.47	1 (20%)
1	YCM	C	621	1	7,9,10	1.76	1 (14%)	5,10,12	1.48	1 (20%)
1	YCM	A	621	1	7,9,10	1.76	1 (14%)	5,10,12	1.47	1 (20%)

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
1	YCM	B	621	1	-	1/6/8/10	-
1	YCM	D	621	1	-	1/6/8/10	-
1	YCM	C	621	1	-	1/6/8/10	-
1	YCM	A	621	1	-	1/6/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	621	YCM	CE-NZ2	3.95	1.45	1.32
1	B	621	YCM	CE-NZ2	3.95	1.45	1.32
1	D	621	YCM	CE-NZ2	3.94	1.45	1.32
1	A	621	YCM	CE-NZ2	3.94	1.45	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	621	YCM	CB-CA-C	2.71	118.15	110.80
1	A	621	YCM	CB-CA-C	2.70	118.14	110.80
1	D	621	YCM	CB-CA-C	2.69	118.12	110.80
1	B	621	YCM	CB-CA-C	2.69	118.11	110.80

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	621	YCM	C-CA-CB-SG
1	B	621	YCM	C-CA-CB-SG
1	D	621	YCM	C-CA-CB-SG
1	C	621	YCM	C-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides 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.

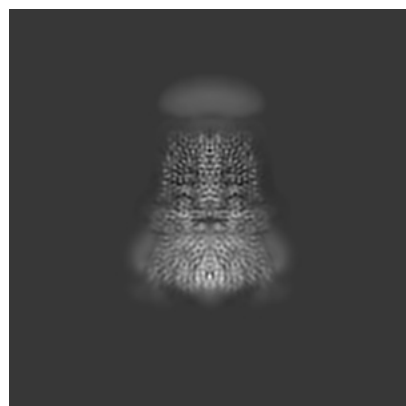
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21129. 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](#)

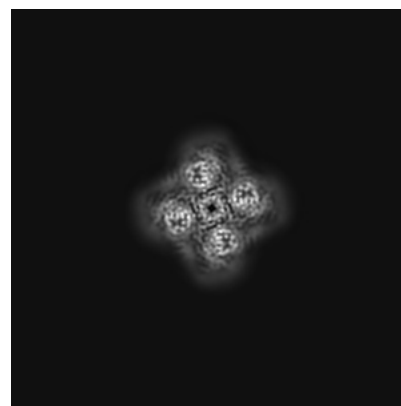
#### 6.1.1 Primary map



X

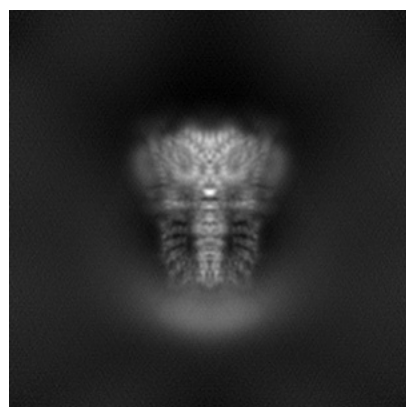


Y

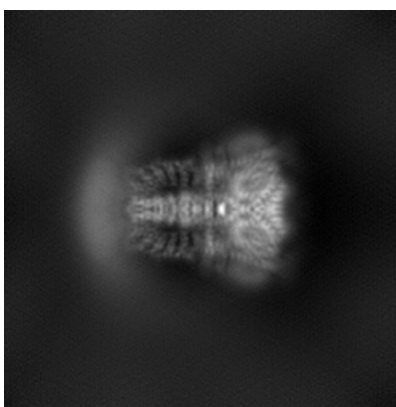


Z

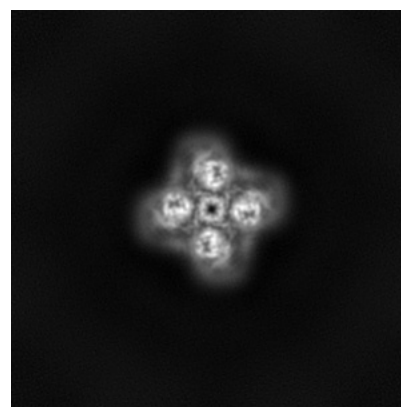
#### 6.1.2 Raw map



X



Y



Z

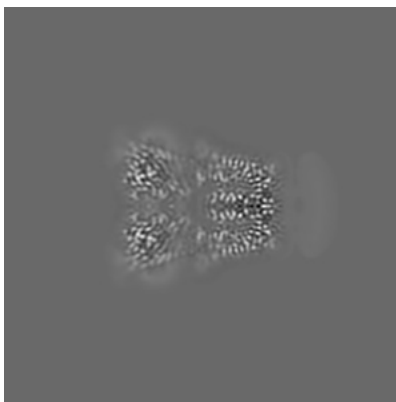
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

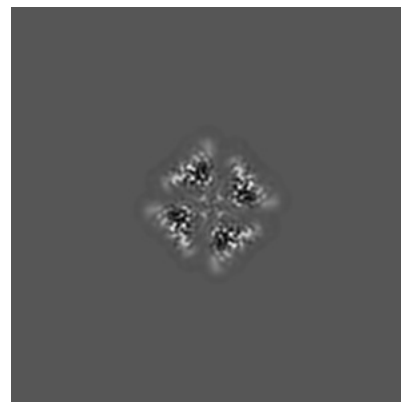
### 6.2.1 Primary map



X Index: 128

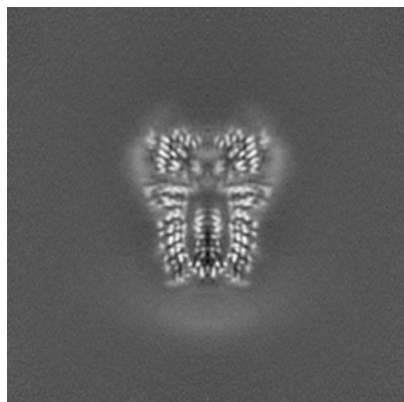


Y Index: 128

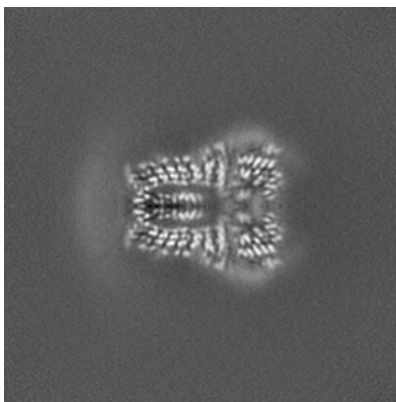


Z Index: 128

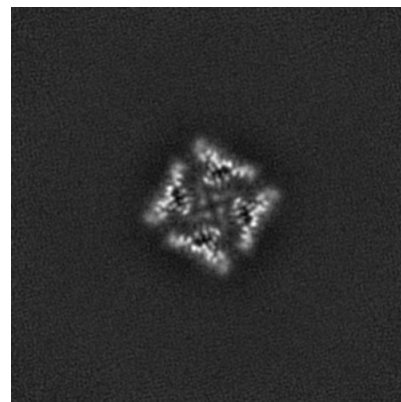
### 6.2.2 Raw map



X Index: 128



Y Index: 128



Z Index: 128

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

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

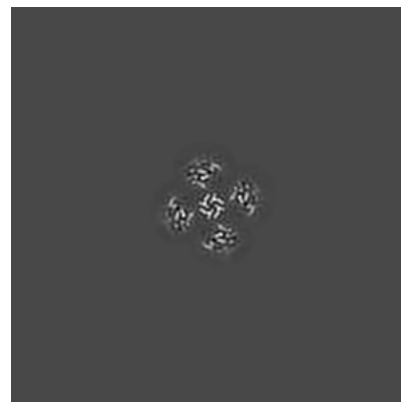
### 6.3.1 Primary map



X Index: 132

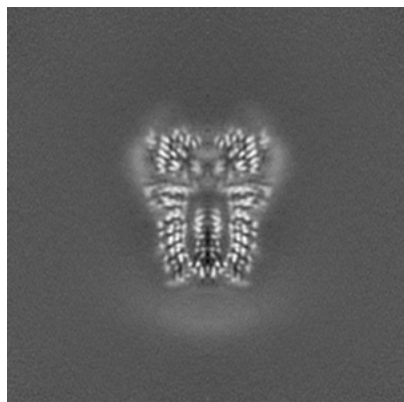


Y Index: 132

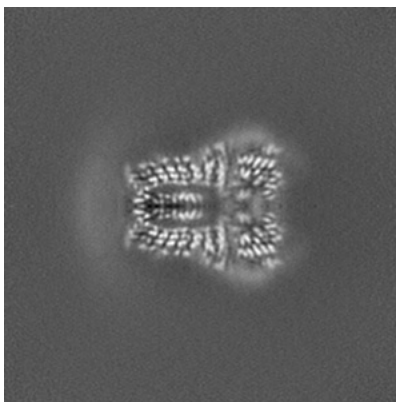


Z Index: 155

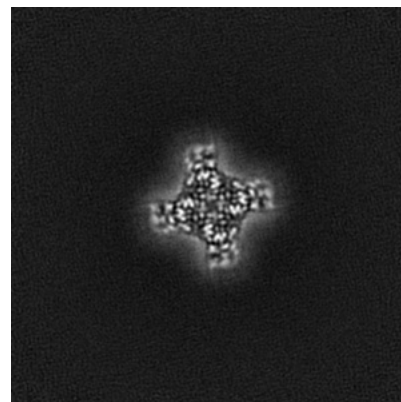
### 6.3.2 Raw map



X Index: 128



Y Index: 128



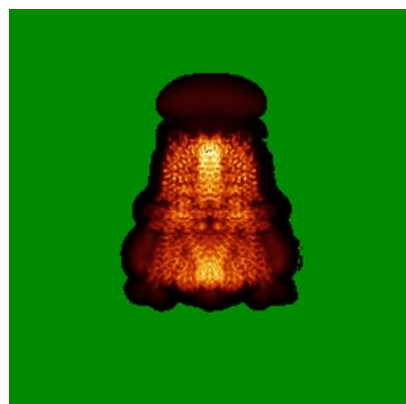
Z Index: 171

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

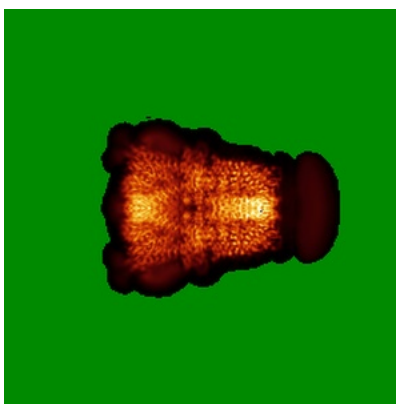


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

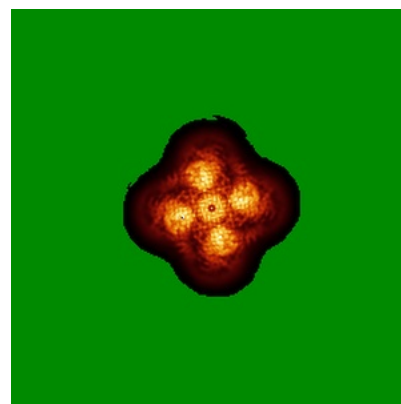
### 6.4.1 Primary map



X

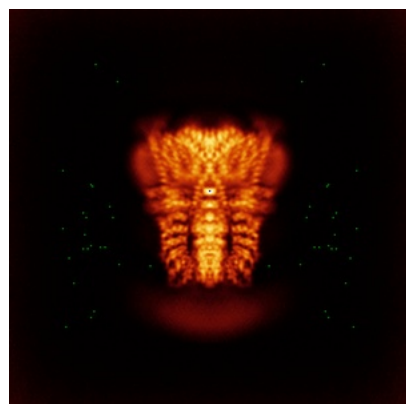


Y

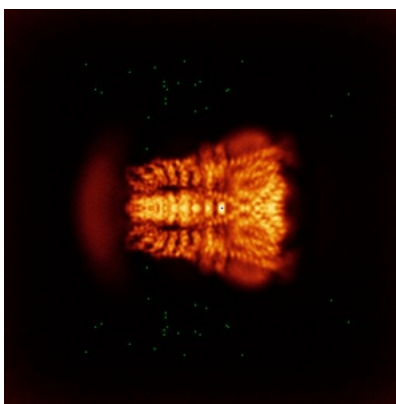


Z

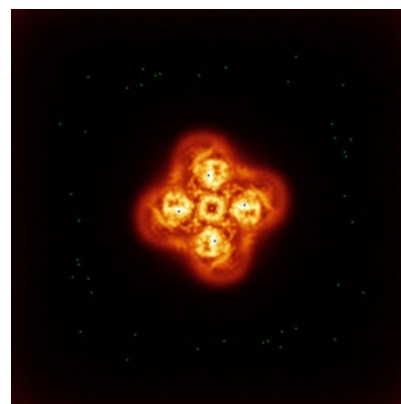
### 6.4.2 Raw map



X



Y

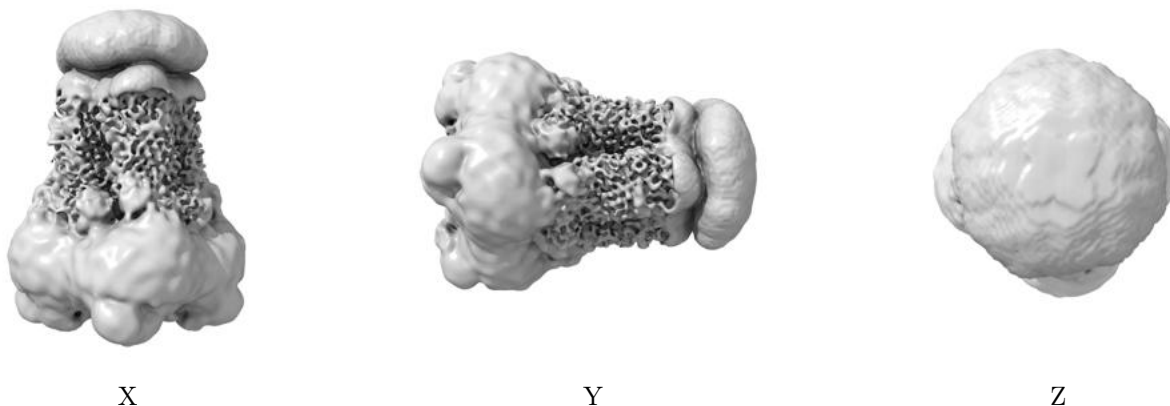


Z

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.

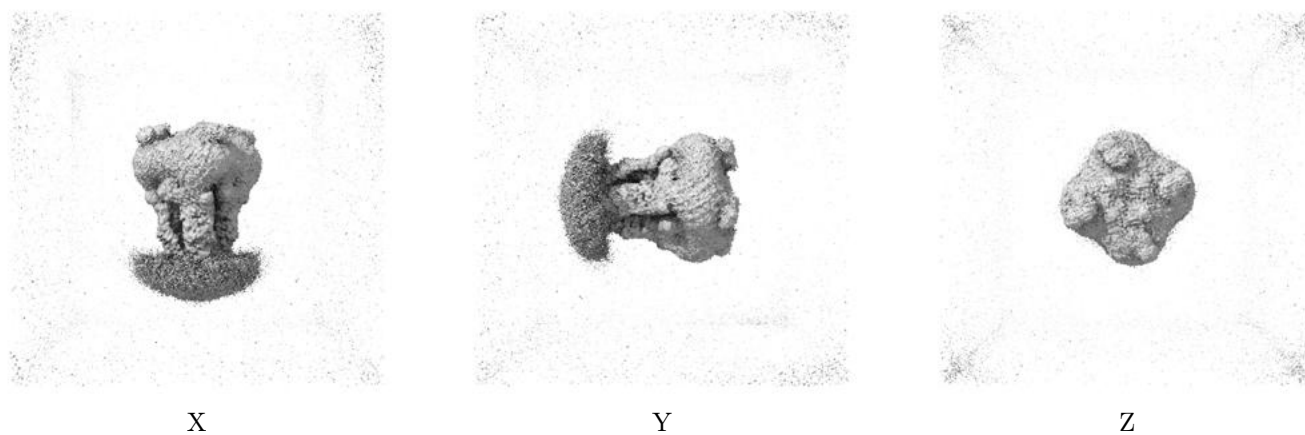
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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



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.

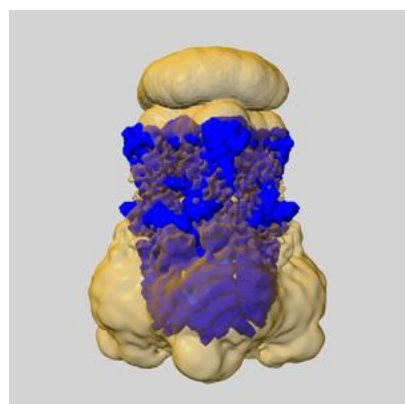
## 6.6 Mask visualisation [i](#)

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

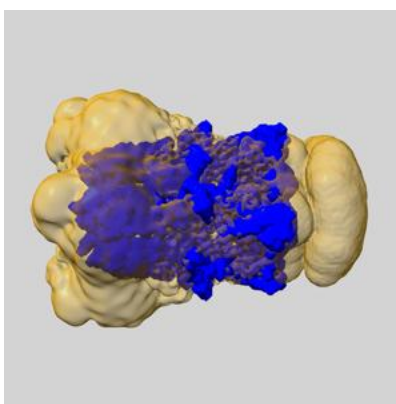
A mask typically either:

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

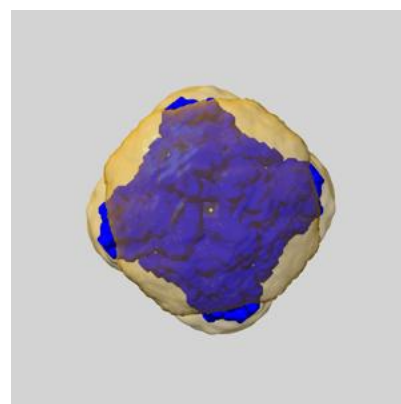
### 6.6.1 emd\_21129\_msk\_1.map [i](#)



X



Y

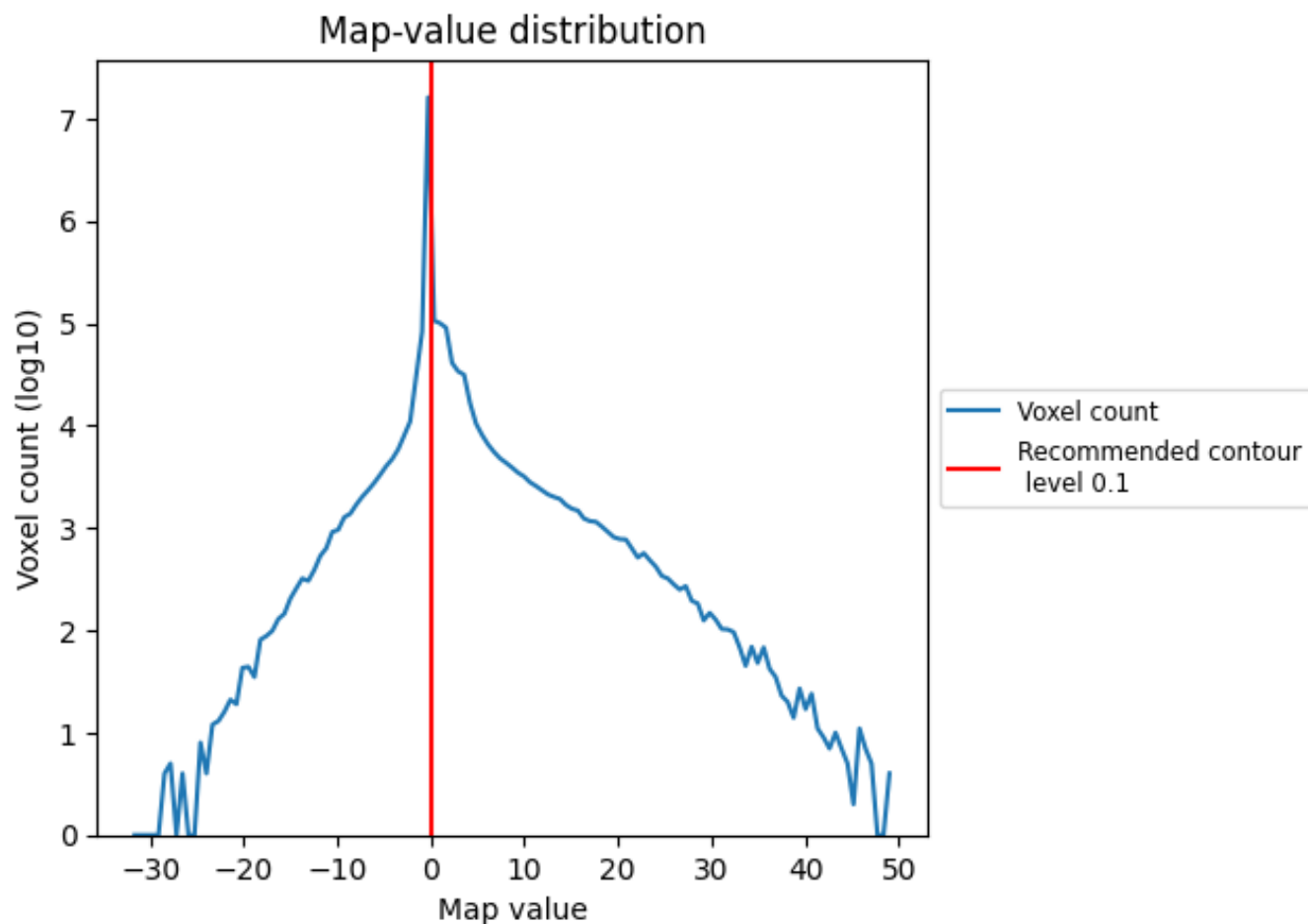


Z

## 7 Map analysis [i](#)

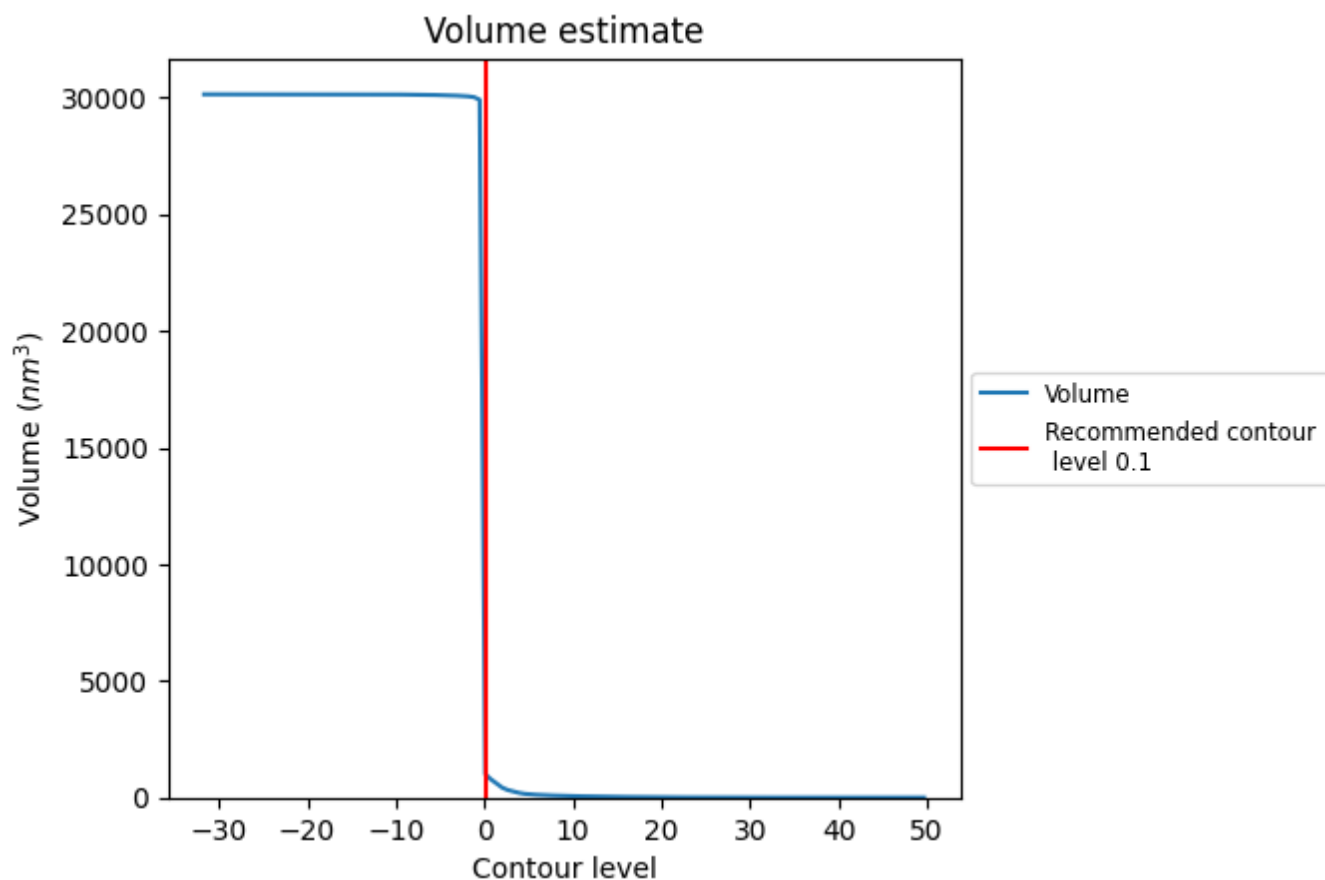
This section contains the results of statistical analysis of the map.

### 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.

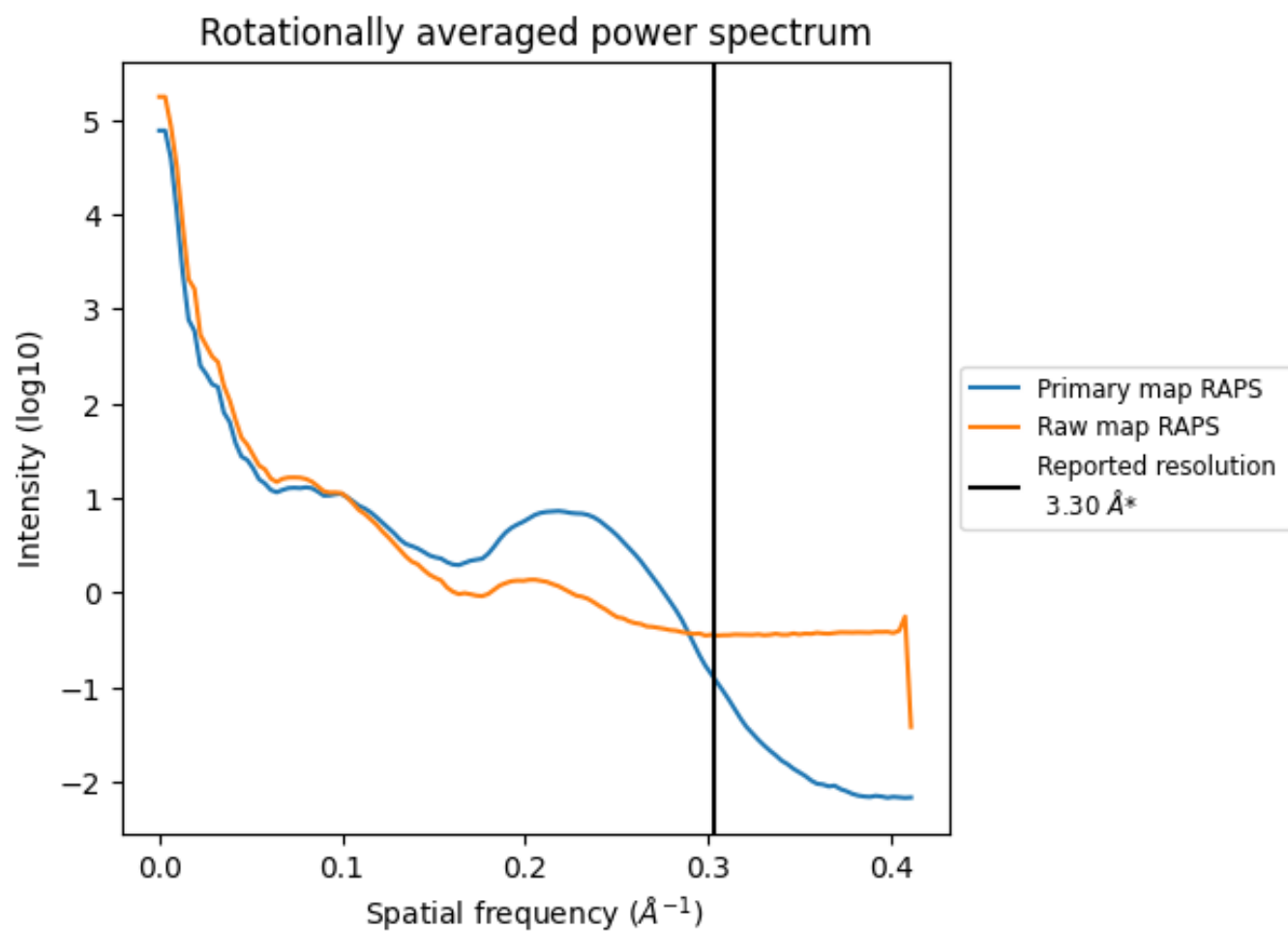
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 995 nm<sup>3</sup>; this corresponds to an approximate mass of 899 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 ⓘ

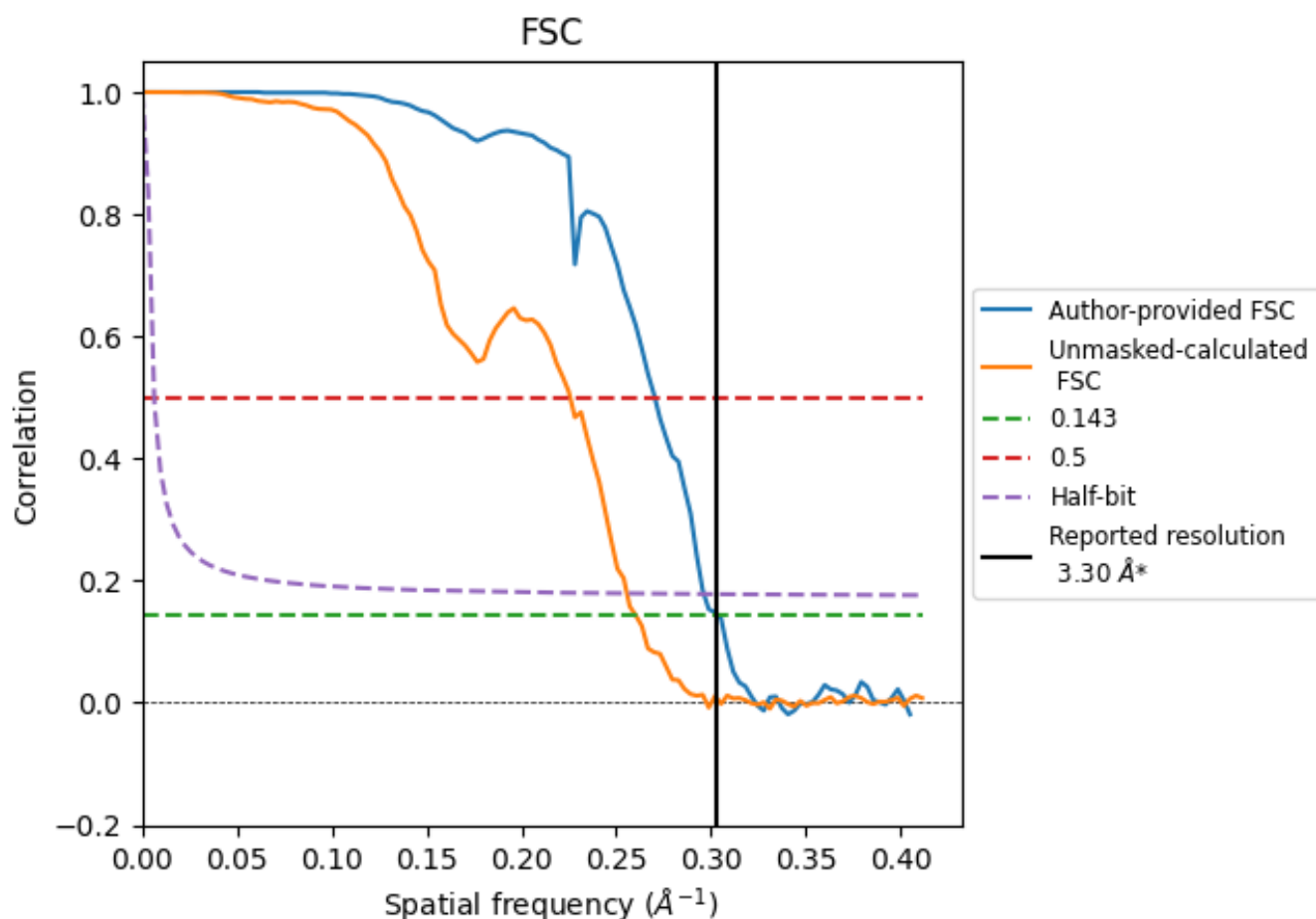


\*Reported resolution corresponds to spatial frequency of  $0.303 \text{ \AA}^{-1}$

## 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  $0.303 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.29	3.70	3.37
Unmasked-calculated*	3.84	4.43	3.91

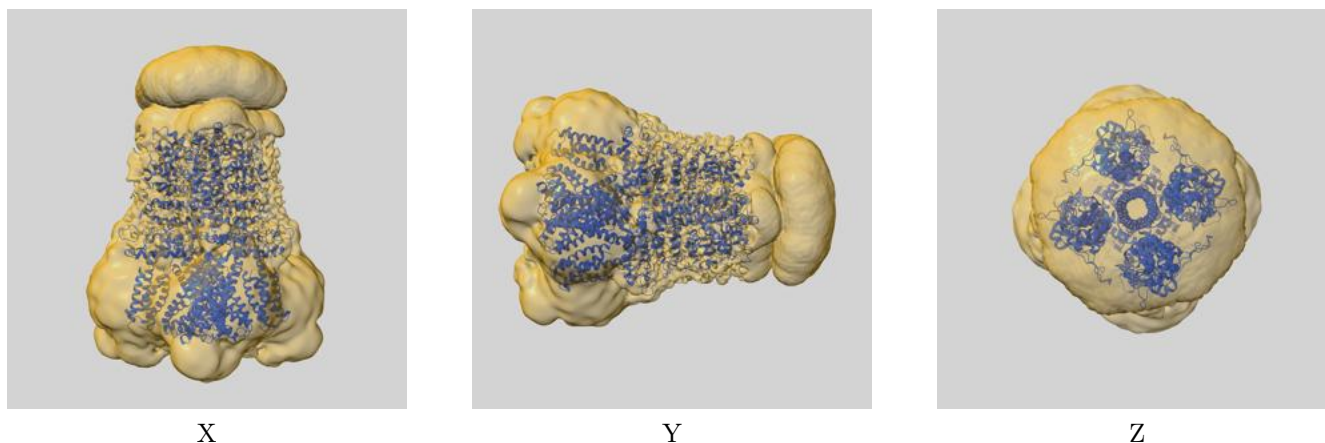
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.84 differs from the reported value 3.3 by more than 10 %



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

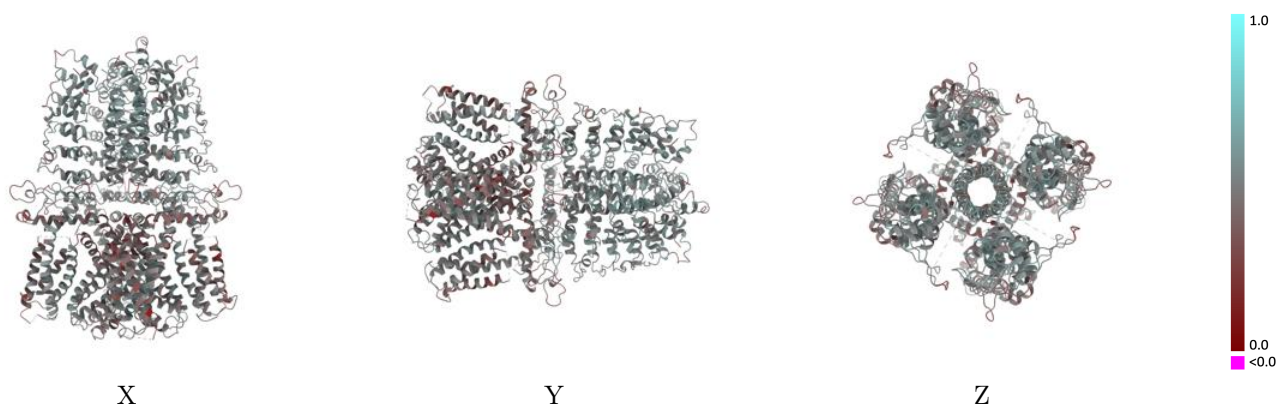
This section contains information regarding the fit between EMDB map EMD-21129 and PDB model 6V9X. Per-residue inclusion information can be found in section [3](#) on page [4](#).

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



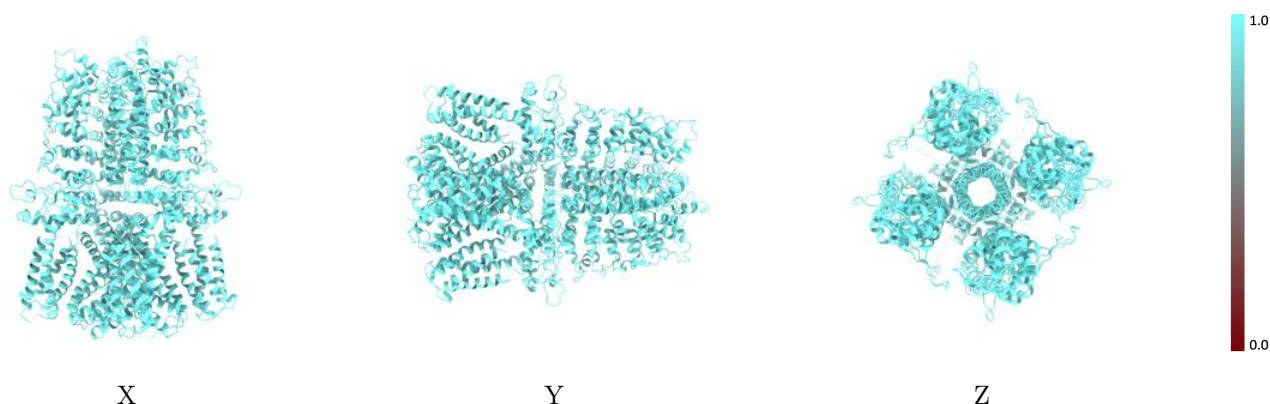
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



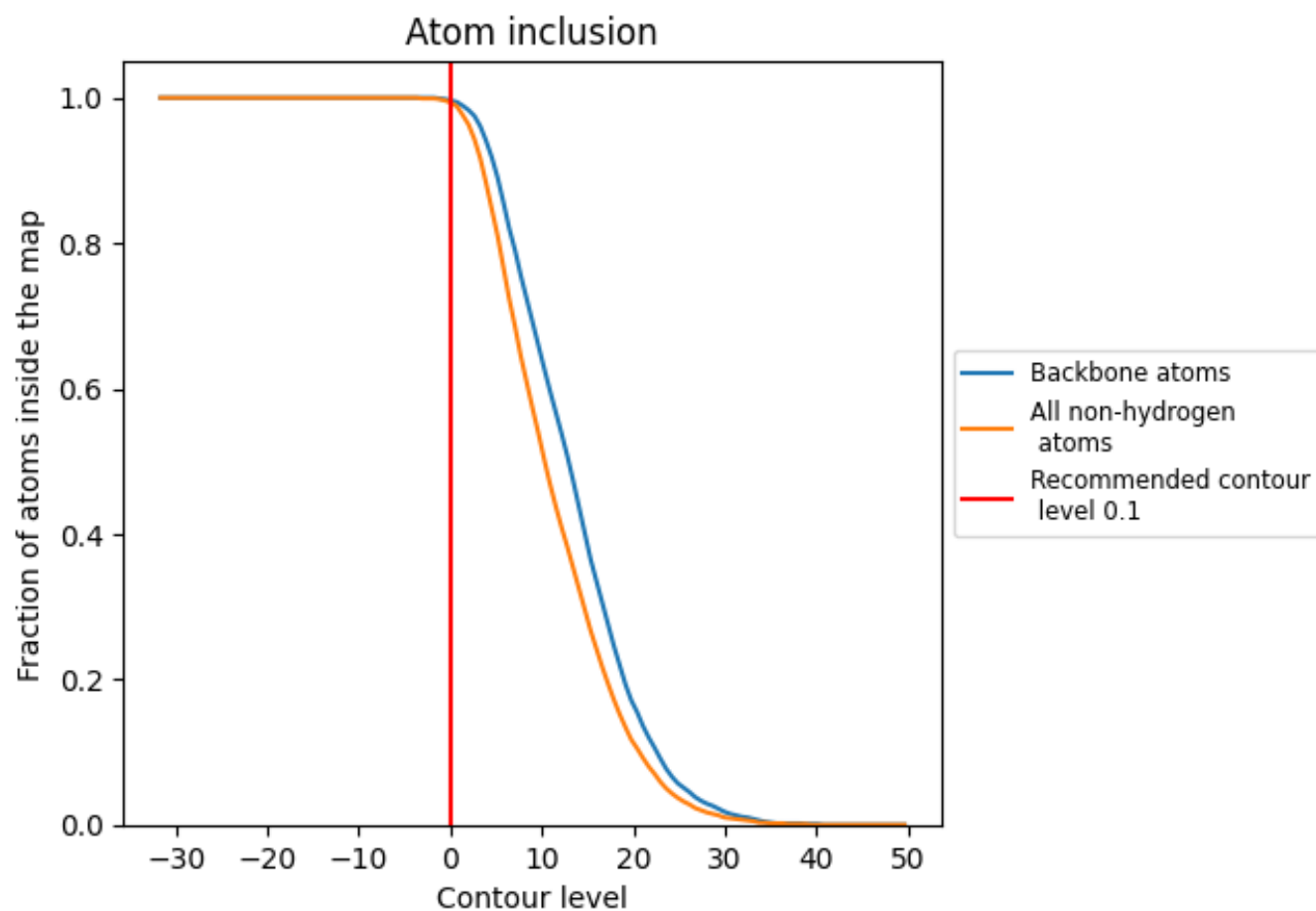
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9930	<div><div></div></div> 0.4750
A	<div><div></div></div> 0.9940	<div><div></div></div> 0.4790
B	<div><div></div></div> 0.9930	<div><div></div></div> 0.4750
C	<div><div></div></div> 0.9930	<div><div></div></div> 0.4730
D	<div><div></div></div> 0.9920	<div><div></div></div> 0.4740

