



wwPDB EM Validation Summary Report ⓘ

Mar 15, 2026 – 12:58 AM UTC

PDB ID : 6V9W / pdb_00006v9w
EMDB ID : EMD-21128
Title : Structure of TRPA1 (ligand-free) with bound calcium, LMNG
Authors : Zhao, J.; Lin King, J.V.; Paulsen, C.E.; Cheng, Y.; Julius, D.
Deposited on : 2019-12-16
Resolution : 3.10 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 ⓘ 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 : 4-5-2 with Phenix2.0
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

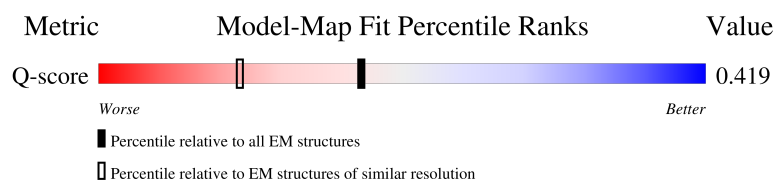
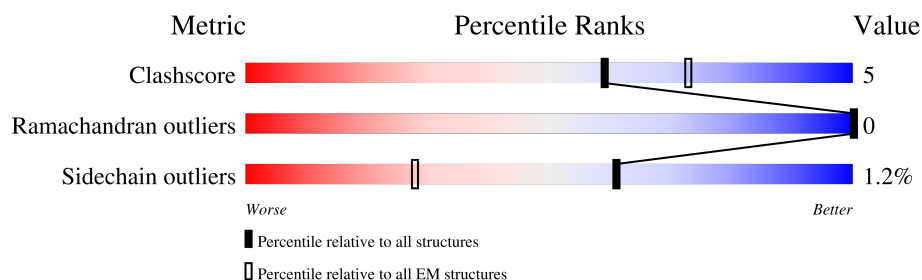
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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 $\leq 5\%$. 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 are 2 unique types of molecules in this entry. The entry contains 18812 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	597	Total	C	N	O	S	0	0
			4702	3088	781	799	34		
1	B	597	Total	C	N	O	S	0	0
			4702	3088	781	799	34		
1	D	597	Total	C	N	O	S	0	0
			4702	3088	781	799	34		
1	C	597	Total	C	N	O	S	0	0
			4702	3088	781	799	34		

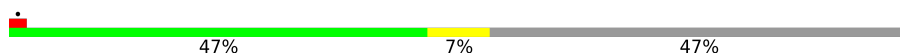
There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

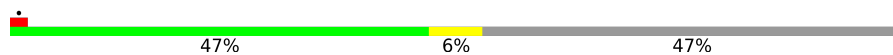
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Ca	0
			1	1	
2	B	1	Total	Ca	0
			1	1	
2	D	1	Total	Ca	0
			1	1	
2	C	1	Total	Ca	0
			1	1	

Chain B:

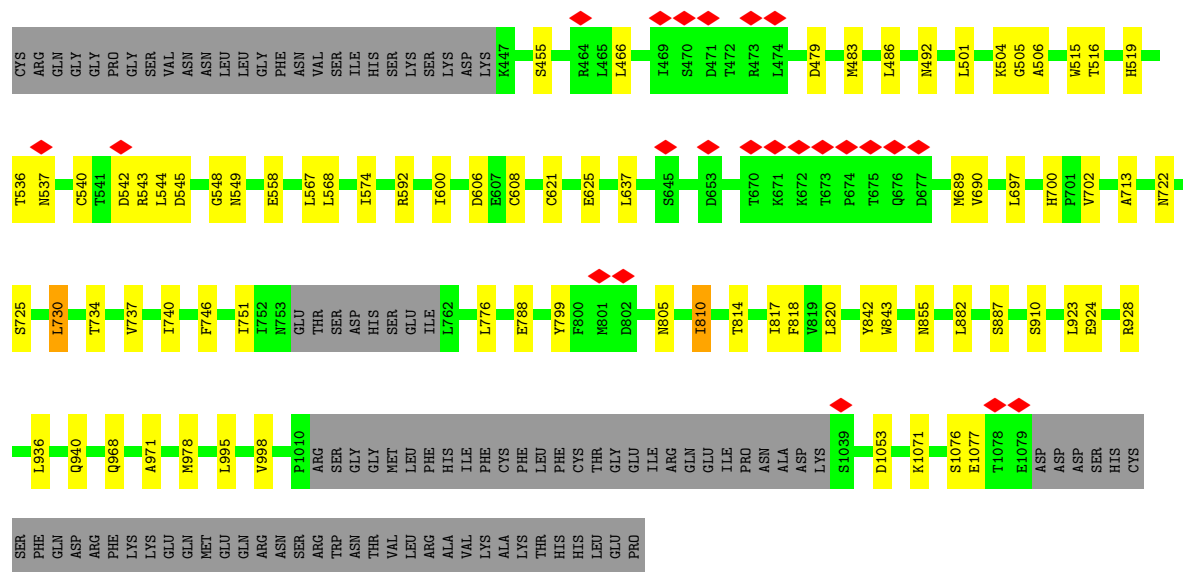


SER	HIS	H700	A883	T516	CYS	LEU	VAL	ILE	THR	LEU	GLN	GLY	ASP	MET
CYS	P701	H702	H519	H519	GLN	SER	ASN	ASN	PRO	LEU	ASN	ALA	MET	LYS
SER	S910	P702	H519	H519	ARG	LEU	THR	THR	HIS	THR	LEU	PRO	THR	THR
PHE	E324	W711	T536	T536	GLY	GLY	THR	THR	GLY	ALA	LYS	LEU	PHE	ARG
ASN	R928	L712	N537	N537	PRO	ALA	ASP	ASP	VAL	VAL	LYS	ARG	LEU	ARG
ASP	A713	L712	N537	N537	GLY	VAL	GLY	GLY	GLN	GLN	GLY	ALA	LEU	MET
ARG	F716	A713	K539	K539	SER	VAL	HIS	CYS	GLN	GLN	GLY	ASN	HIS	LYS
PHE	F716	F716	K539	K539	VAL	ASP	HIS	GLN	ASN	ASN	ALA	PHE	TYR	ARG
LYS	N722	N722	C540	C540	ASN	ILE	GLU	ASN	GLY	GLY	ALA	ASN	ALA	THR
GLY	A971	N722	LYS	LYS	ASN	LYS	THR	MET	ASP	ASP	CYS	MET	ALA	PRO
GLN	R978	S725	D542	D542	LEU	ASN	LEU	MET	LEU	GLU	LYS	ALA	ALA	GLY
MET	V998	S725	R543	R543	LEU	ASN	PHE	PHE	LEU	LEU	GLY	VAL	GLY	VAL
GLN	V998	L730	L544	L544	PHE	GLY	HIS	ASP	ASP	MET	ASN	GLN	GLN	LYS
ARG	P1010	T734	E546	E546	VAL	ASN	ALA	ALA	LEU	MET	TRP	ILE	ILE	PRO
ASN	ARG	T734	D547	D547	SER	PHE	LEU	LEU	CYS	CYS	GLY	ALA	LEU	GLY
SER	SER	V737	G548	G548	ILE	LEU	PHE	PHE	LEU	LEU	CYS	VAL	MET	GLY
ARG	GLY	V737	N549	N549	ILE	LEU	PHE	PHE	LEU	LEU	CYS	VAL	MET	GLY
TRP	GLY	I740	E558	E558	SER	HIS	HIS	ASP	ASP	ASP	PHE	GLN	GLU	VAL
THR	MET	I740	R592	R592	LYS	THR	HIS	GLY	ASN	ASN	PRO	ILE	LYS	VAL
VAL	PHE	F746	L567	L567	SER	VAL	LEU	ALA	ALA	GLN	GLN	ASN	THR	GLY
LEU	HIS	I761	I574	I574	LYS	GLN	LEU	GLU	GLN	ILE	ALA	GLU	ARG	ASP
ALA	ILE	N752	R592	R592	ASP	PRO	ASP	TYR	ASP	ASP	ALA	VAL	SER	VAL
ARG	PHE	N753	GLU	GLU	LYS	TYR	TYR	TYR	PRO	PRO	PHE	VAL	SER	GLY
VAL	CYS	THR	V595	V595	GLY	LEU	ILE	ILE	GLU	GLU	GLY	VAL	LEU	THR
LYS	PHE	THR	V595	V595	LYS	LYS	SER	SER	LYS	LYS	SER	VAL	LEU	ASP
ALA	LEU	SER	T598	T598	ASN	ASN	VAL	VAL	GLY	GLY	LYS	LEU	LEU	GLY
LYS	PHE	ASP	T598	T598	ASN	ASN	VAL	VAL	ARG	ARG	LYS	LEU	LEU	ASP
THR	CYS	THR	I599	I599	LEU	LEU	GLY	GLY	CYS	CYS	GLY	GLU	HIS	PHE
HIS	THR	SER	I600	I600	ARG	ARG	ALA	ALA	ALA	GLY	GLY	GLU	GLY	LYS
HIS	GLY	GLU	I600	I600	PRO	PRO	ALA	ALA	THR	THR	MET	THR	MET	GLY
LEU	GLU	ILE	D606	D606	GLU	GLU	ILE	ILE	ALA	ILE	ILE	ALA	ASP	SER
GLU	ILE	L762	E697	E697	PHE	PHE	ASN	ASN	ILE	ILE	ILE	ILE	ASP	LEU
ARG	ARG	L776	C608	C608	MET	MET	LYS	LYS	HIS	HIS	ILE	ASP	TYR	LYS
GLN	GLU	L776	C621	C621	GLN	GLN	ILE	ILE	PHE	PHE	LEU	VAL	GLY	VAL
ILE	ILE	M801	D802	D802	ILE	GLN	GLY	GLY	ALA	ALA	ARG	ASN	THR	PHE
ASN	ASN	D802	E625	E625	ILE	ILE	GLY	GLY	THR	THR	GLY	GLU	PRO	THR
ALA	ALA	I810	L637	L637	LYS	LYS	ARG	ARG	GLY	GLY	GLY	GLY	LEU	SER
ASP	ASP	I810	L637	L637	LYS	GLU	SER	SER	ALA	ALA	HIS	ASN	CYS	ALA
S1039	S1039	T814	S645	S645	GLN	LEU	PHO	PHO	THR	THR	GLY	GLY	ALA	TYR
D1053	D1053	T814	S645	S645	GLN	VAL	THR	THR	GLU	GLU	TYR	VAL	VAL	ALA
L1067	L1067	I817	D653	D653	ASP	MET	ILE	ILE	ILE	ILE	THR	THR	GLU	GLN
I1068	I1068	F818	D653	D653	ASP	ASP	LEU	LEU	VAL	VAL	ARG	VAL	GLY	ASN
K1071	K1071	V819	D653	D653	ASP	GLY	ILE	ILE	VAL	VAL	GLN	VAL	ASN	ASN
E1077	E1077	L820	K671	K671	ASP	ASP	THR	THR	LYS	LYS	LEU	GLN	ASN	PHE
T1078	T1078	Y840	K672	K672	GLY	ASN	ALA	ALA	MET	MET	HIS	ILE	ILE	ASN
E1079	E1079	F841	K672	K672	GLY	ASP	SER	SER	ILE	ILE	GLY	GLY	GLY	GLN
ASP	ASP	Y842	P674	P674	CYS	THR	ALA	ALA	SER	SER	PHE	THR	VAL	LYS
ASP	ASP	N855	P674	P674	THR	PRO	TTP	TTP	SER	SER	ASN	THR	LYS	LYS
E1079	E1079	L880	Q676	Q676	LEU	LEU	ILE	ILE	GLY	GLY	ASN	ASN	PHE	LEU
ASP	ASP	L881	Q677	Q677	HIS	HIS	VAL	VAL	GLY	GLY	ASN	ASN	LEU	LYS
ASP	ASP	L882	M689	M689	TYR	TYR	ASN	ASN	VAL	VAL	LYS	GLY	SER	GLY
ASP	ASP	L882	V690	V690	ALA	ALA	LEU	LEU	ASP	ASP	ALA	ALA	ARG	ASP
			L697	L697	W515									

Chain D:

[illegible]





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	130595	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	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	33.166	Depositor
Minimum map value	-14.046	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5.8	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: CA

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	0.38	0/4810	0.54	0/6527
1	B	0.38	0/4810	0.54	0/6527
1	C	0.38	0/4810	0.54	0/6527
1	D	0.38	0/4810	0.54	0/6527
All	All	0.38	0/19240	0.54	0/26108

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	4702	0	4733	48	0
1	B	4702	0	4733	45	0
1	C	4702	0	4733	47	0
1	D	4702	0	4733	43	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
All	All	18812	0	18932	175	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 5.

The worst 5 of 175 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:D:600:ILE:HD11	1:D:637:LEU:HD13	1.75	0.69
1:C:740:ILE:HD12	1:C:751:ILE:HD11	1.75	0.69
1:B:740:ILE:HD12	1:B:751:ILE:HD11	1.75	0.69
1:C:600:ILE:HD11	1:C:637:LEU:HD13	1.75	0.68
1:D:740:ILE:HD12	1:D:751:ILE:HD11	1.75	0.67

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	591/1119 (53%)	563 (95%)	28 (5%)	0	100	100
1	B	591/1119 (53%)	563 (95%)	28 (5%)	0	100	100
1	C	591/1119 (53%)	563 (95%)	28 (5%)	0	100	100
1	D	591/1119 (53%)	563 (95%)	28 (5%)	0	100	100
All	All	2364/4476 (53%)	2252 (95%)	112 (5%)	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	496/995 (50%)	490 (99%)	6 (1%)	63	78
1	B	496/995 (50%)	490 (99%)	6 (1%)	63	78
1	C	496/995 (50%)	490 (99%)	6 (1%)	63	78
1	D	496/995 (50%)	490 (99%)	6 (1%)	63	78
All	All	1984/3980 (50%)	1960 (99%)	24 (1%)	61	78

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	810	ILE
1	D	978	MET
1	D	910	SER
1	C	690	VAL
1	B	690	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	519	HIS
1	D	700	HIS
1	C	700	HIS
1	D	520	HIS
1	D	580	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

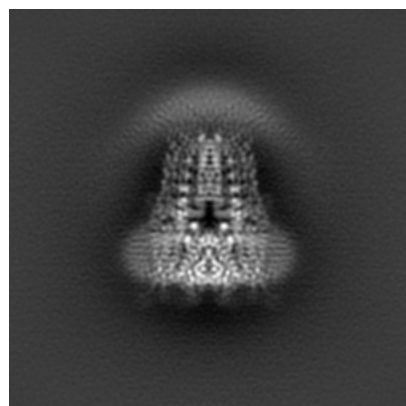
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21128. These allow visual inspection of the internal detail of the map and identification of artifacts.

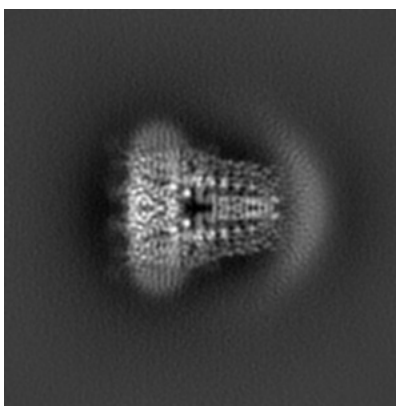
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

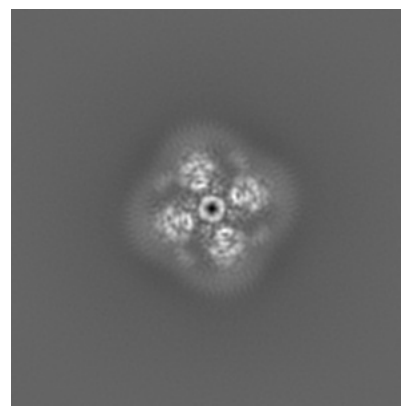
6.1.1 Primary map



X

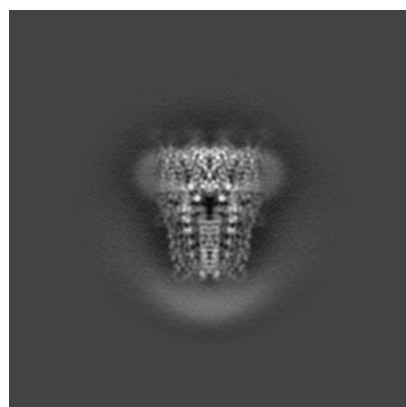


Y

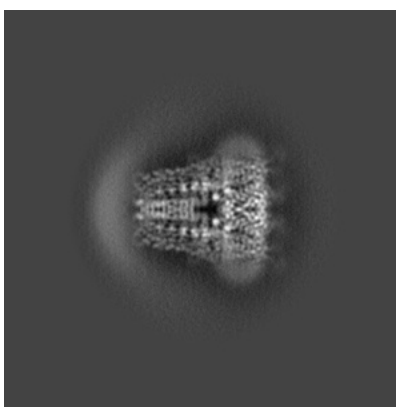


Z

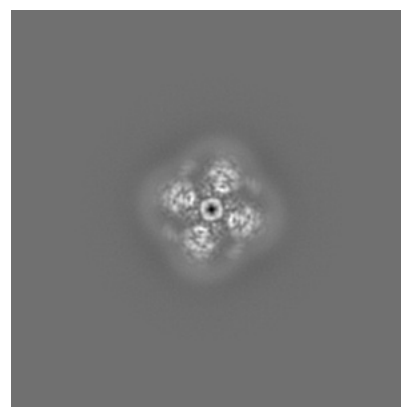
6.1.2 Raw map



X



Y

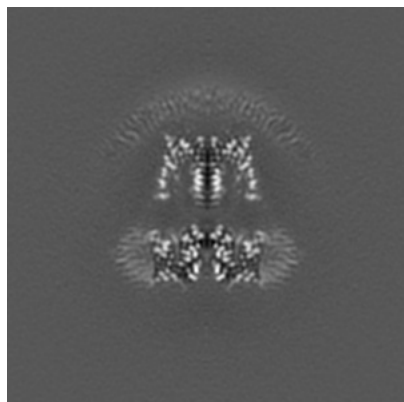


Z

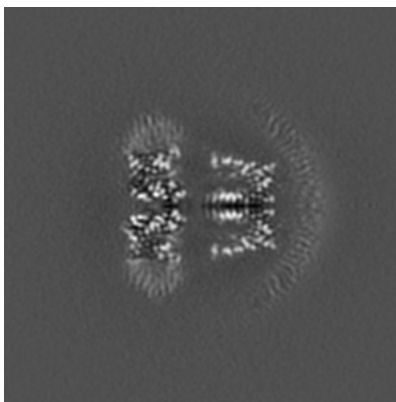
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

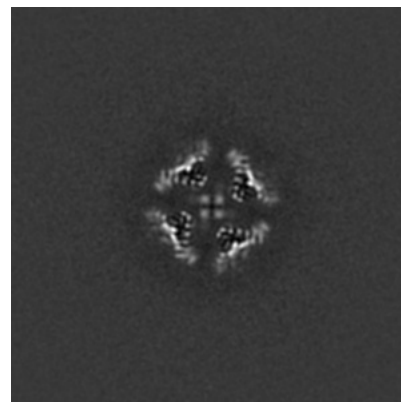
6.2.1 Primary map



X Index: 128

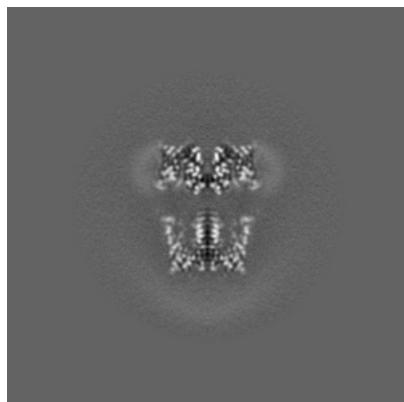


Y Index: 128

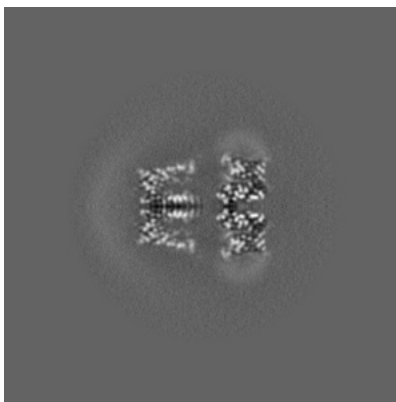


Z Index: 128

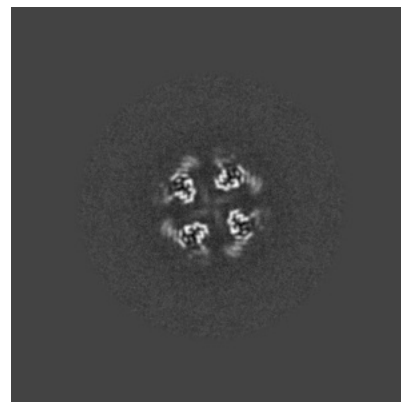
6.2.2 Raw map



X Index: 170



Y Index: 170

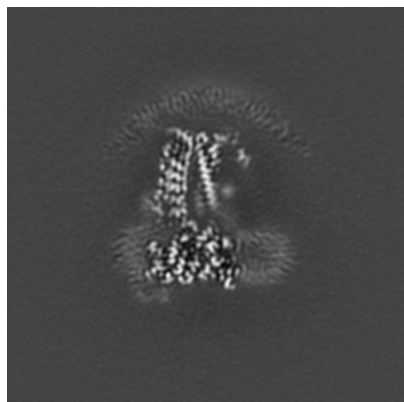


Z Index: 170

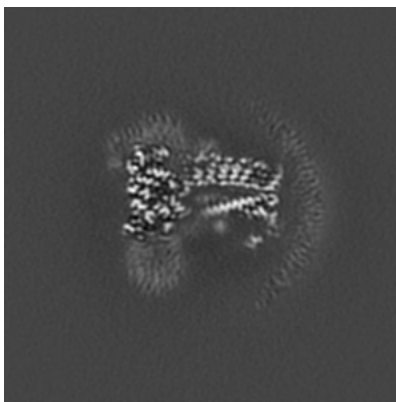
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

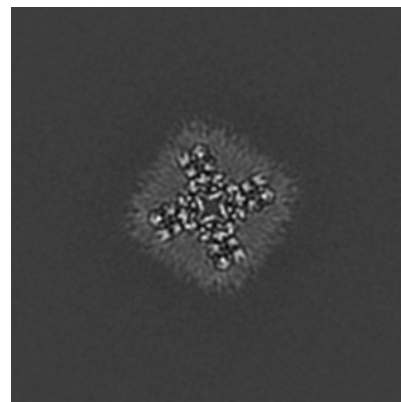
6.3.1 Primary map



X Index: 134

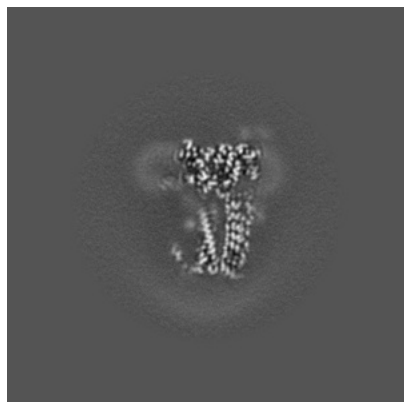


Y Index: 134

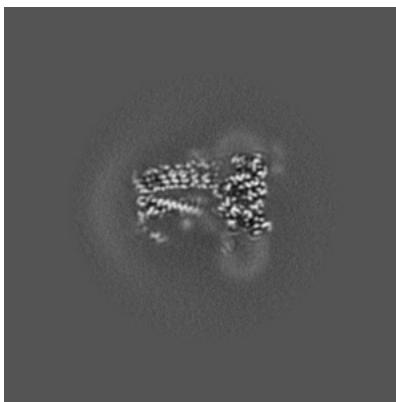


Z Index: 86

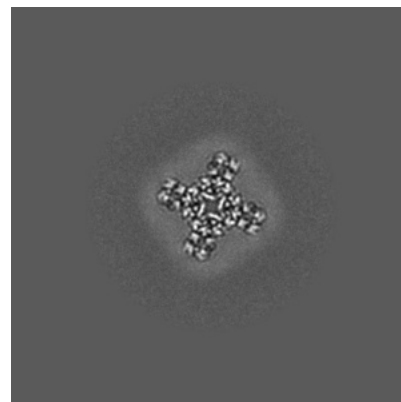
6.3.2 Raw map



X Index: 177



Y Index: 163

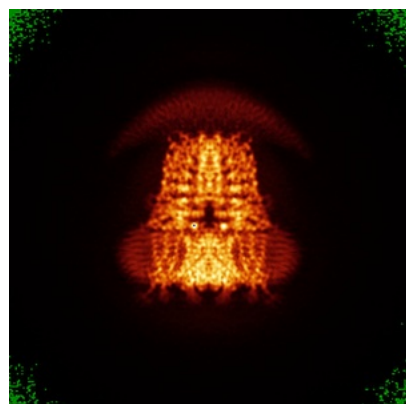


Z Index: 214

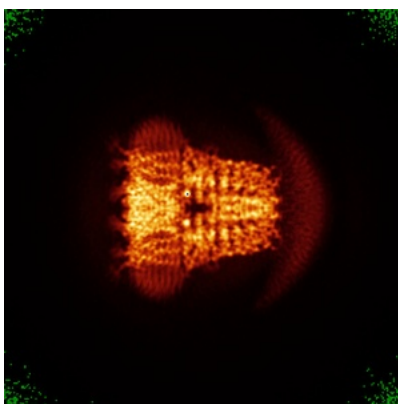
The images above show the largest variance slices of the map in three orthogonal directions.

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

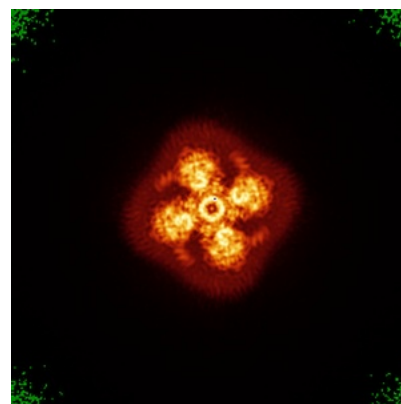
6.4.1 Primary map



X

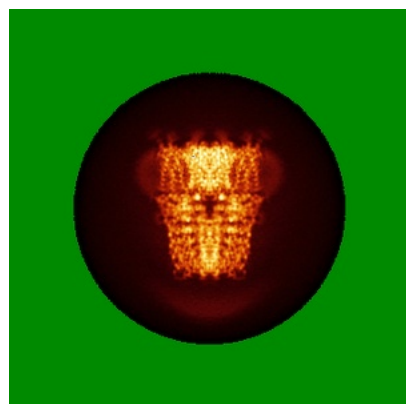


Y

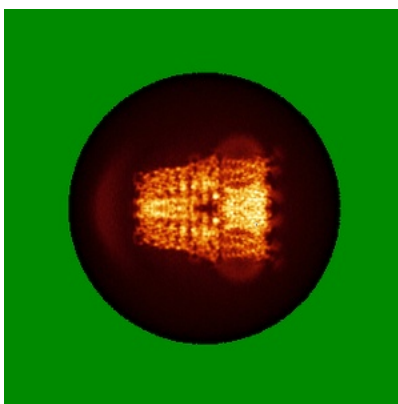


Z

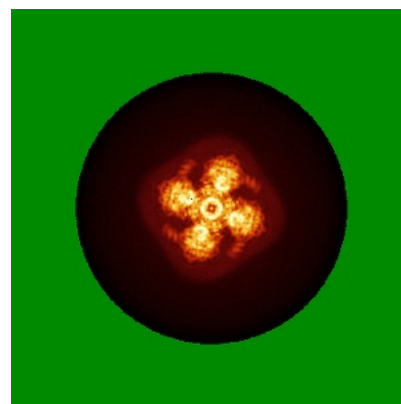
6.4.2 Raw map



X



Y

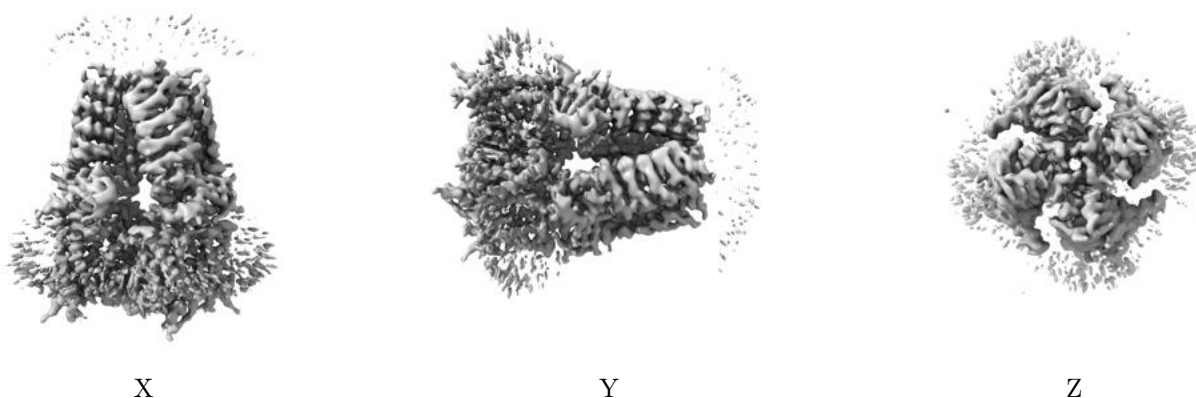


Z

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.

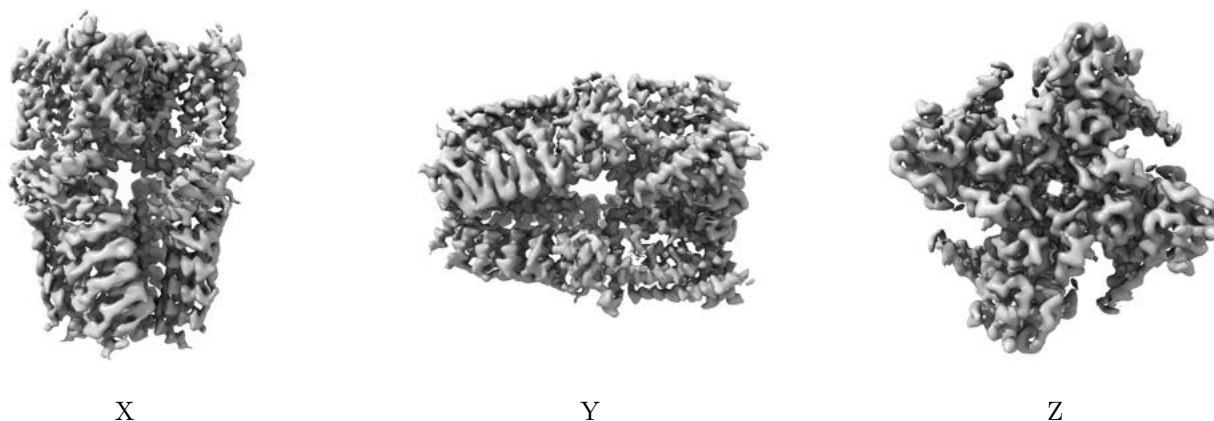
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.8. 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.

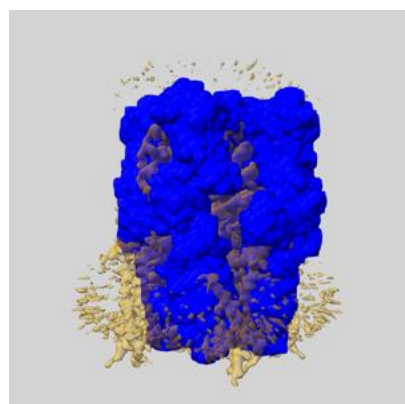
6.6 Mask visualisation [i](#)

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

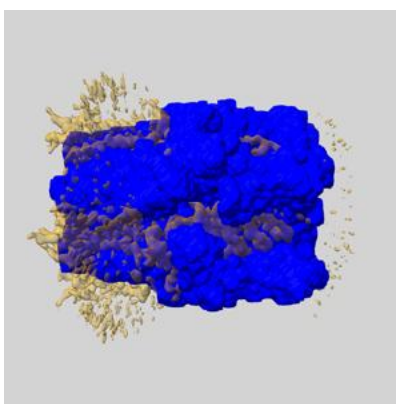
A mask typically either:

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

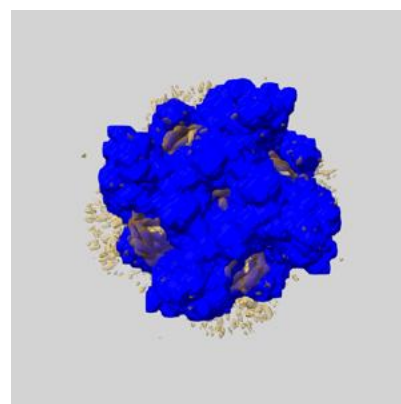
6.6.1 emd_21128_msk_1.map [i](#)



X



Y

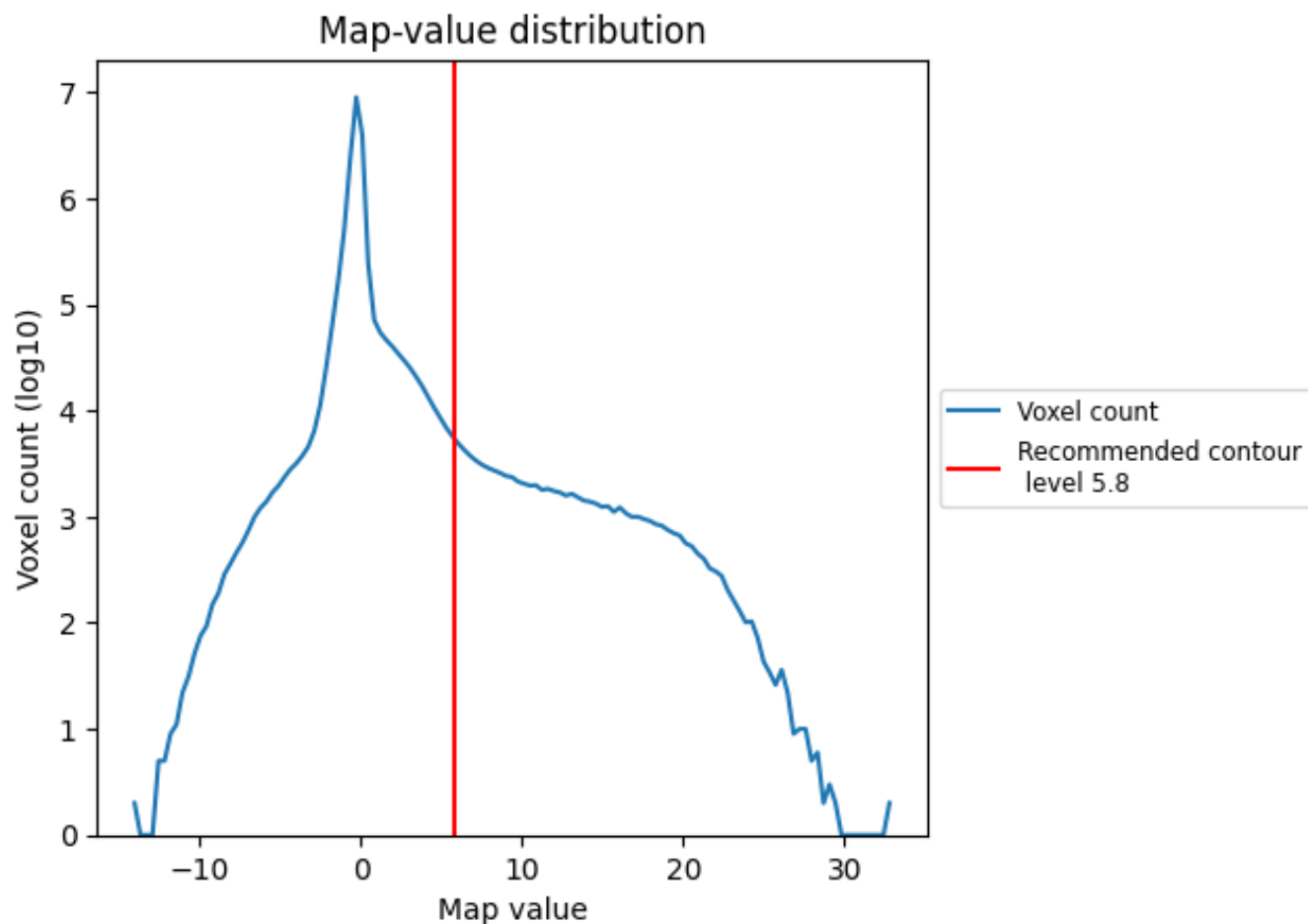


Z

7 Map analysis [i](#)

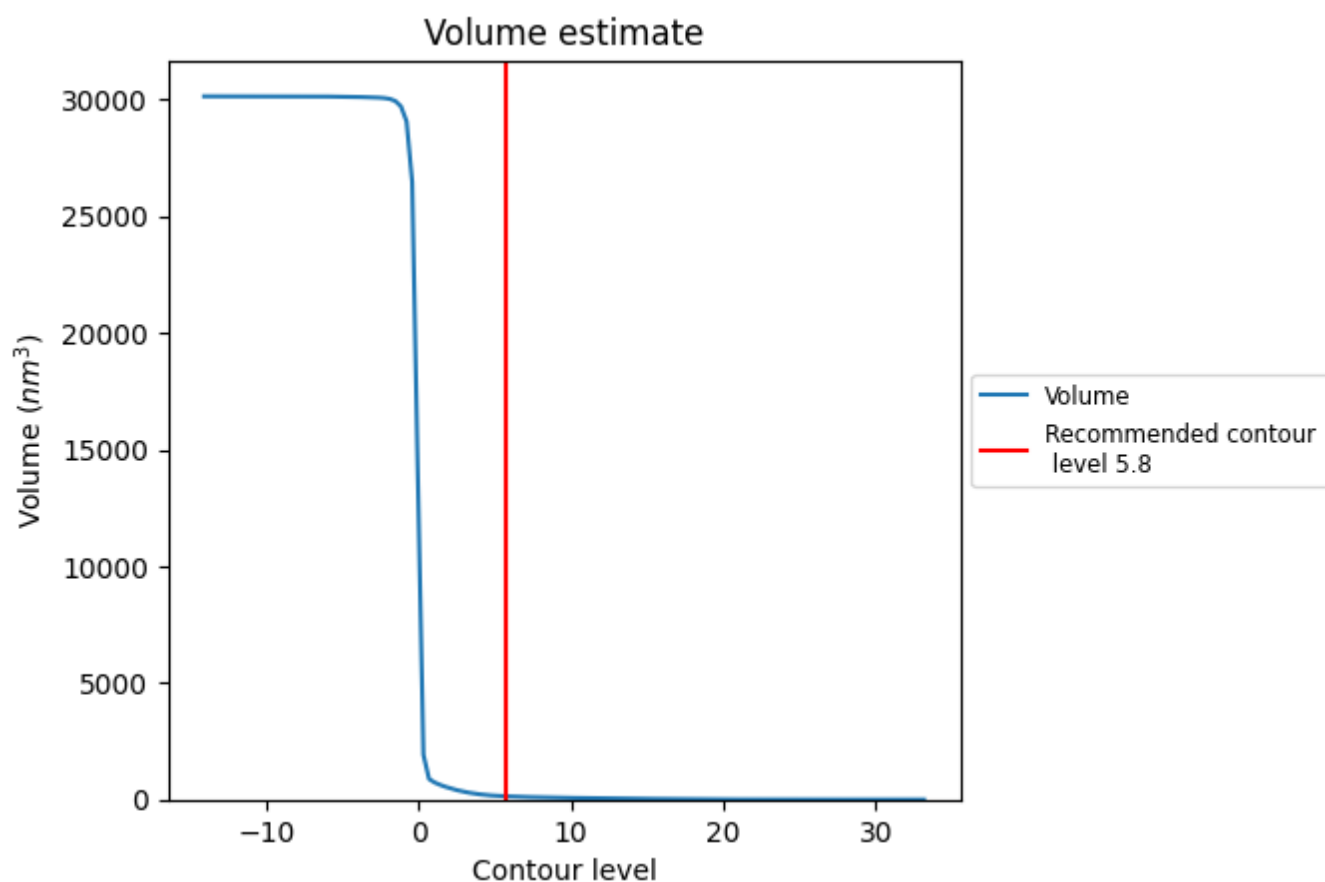
This section contains the results of statistical analysis of the map.

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.

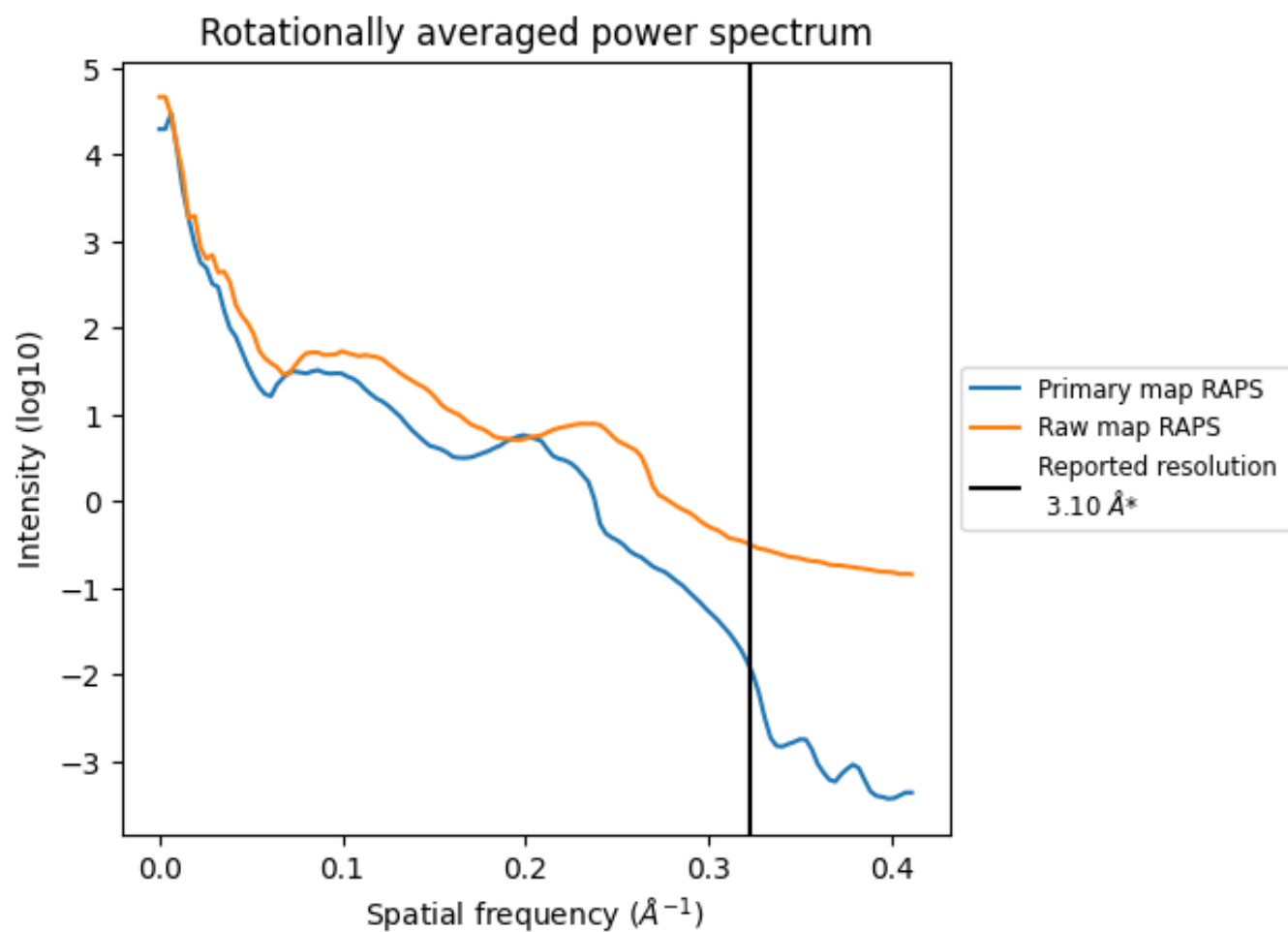
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 139 nm³; this corresponds to an approximate mass of 125 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 ⓘ

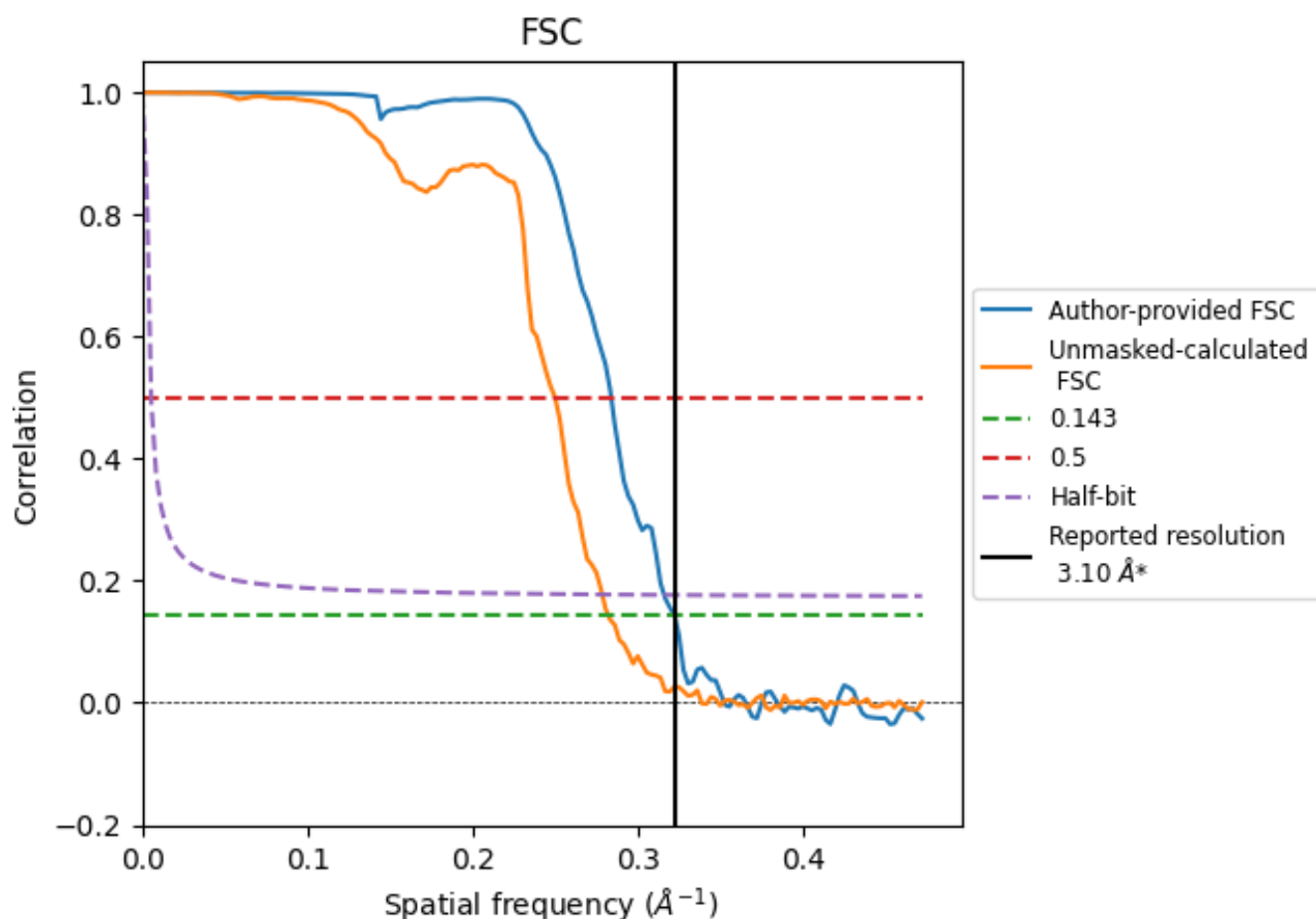


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

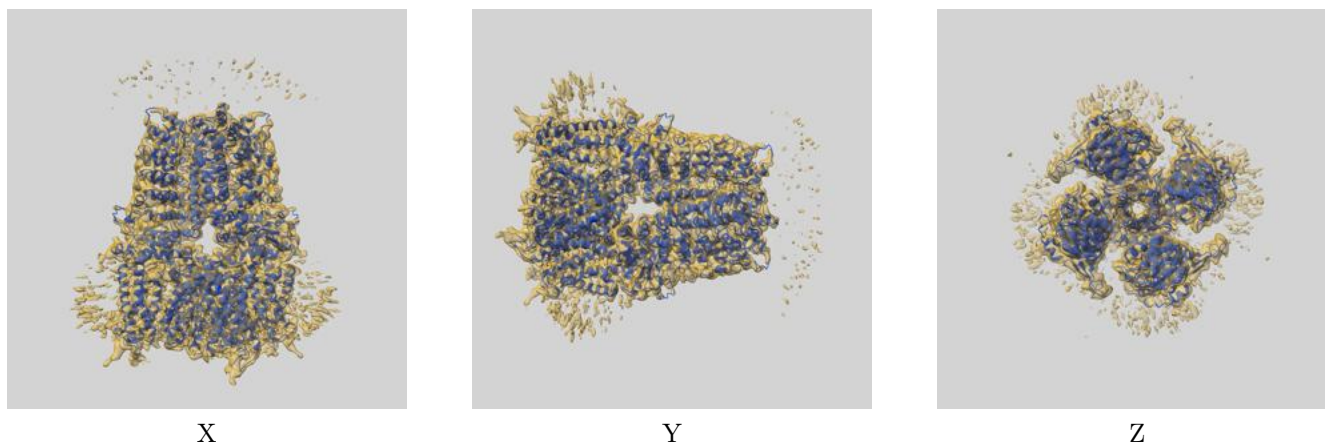
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.11	3.52	3.17
Unmasked-calculated*	3.55	4.00	3.59

*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 3.55 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

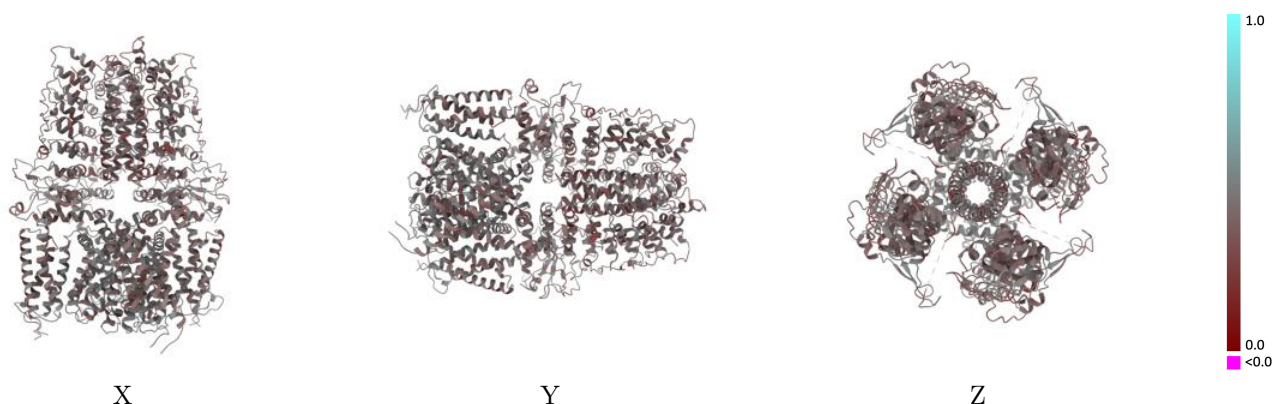
This section contains information regarding the fit between EMDB map EMD-21128 and PDB model 6V9W. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



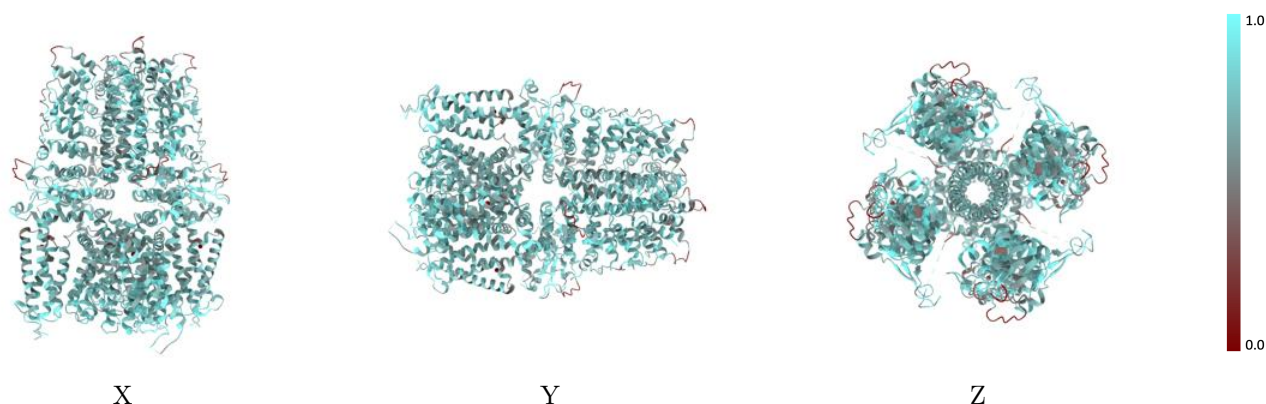
The images above show the 3D surface view of the map at the recommended contour level 5.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



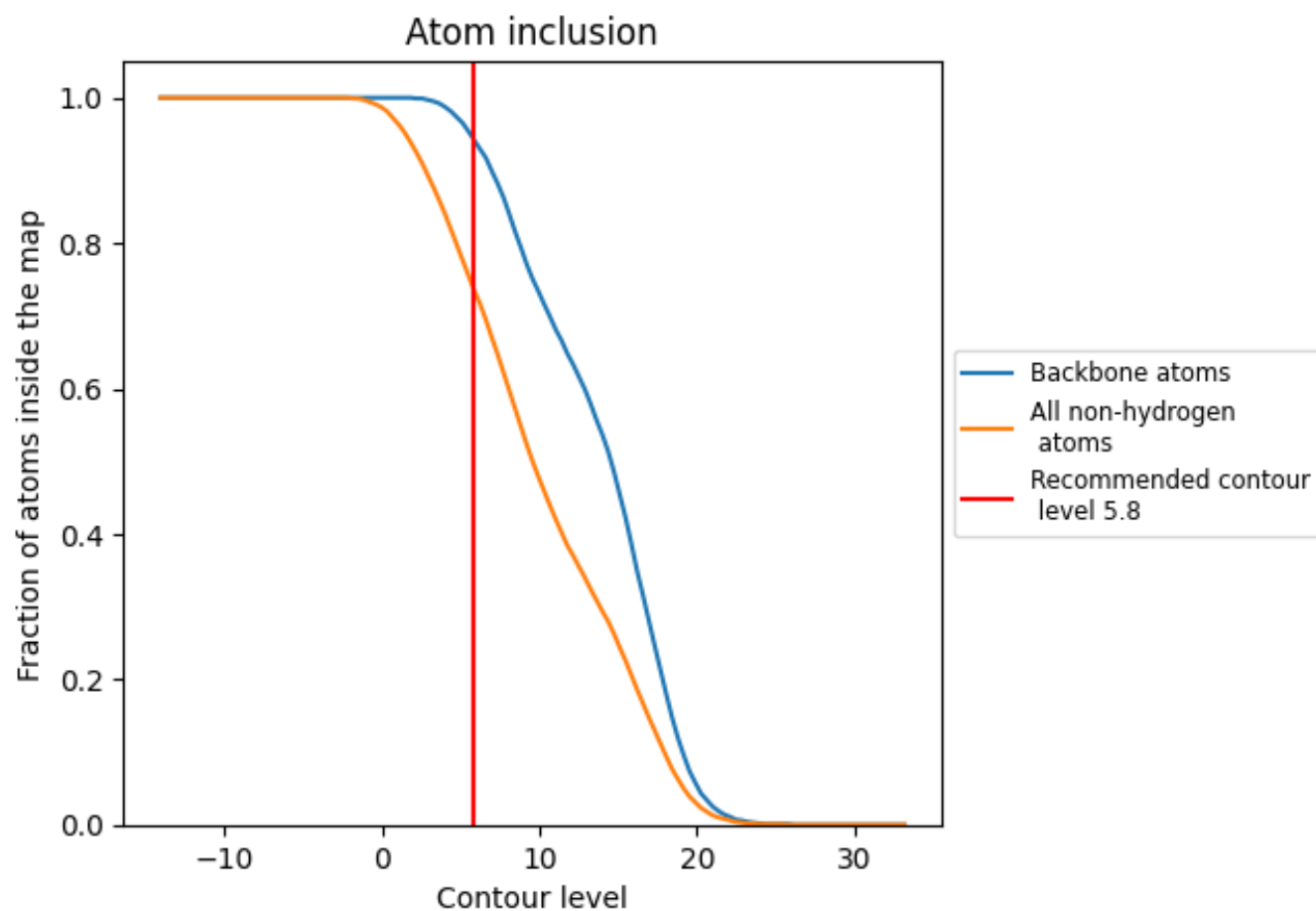
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 74% 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 (5.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7380	0.4190
A	0.7370	0.4210
B	0.7380	0.4190
C	0.7410	0.4200
D	0.7360	0.4180

