



wwPDB EM Validation Summary Report ⓘ

Mar 30, 2026 – 04:44 PM UTC

PDB ID : 7ZGX / pdb_00007zgx
EMDB ID : EMD-14714
Title : S-layer Deinoxanthin Binding Complex, C1 symmetry
Authors : Farci, D.; Piano, D.
Deposited on : 2022-04-04
Resolution : 2.88 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

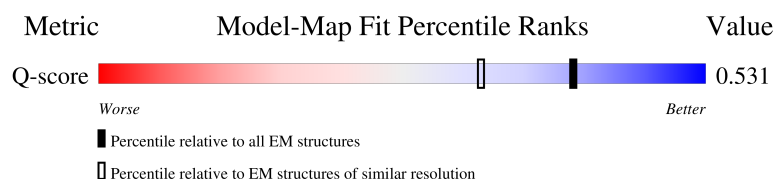
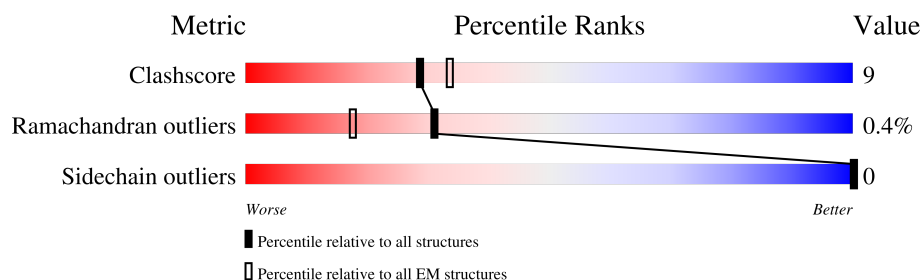
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.88 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	12111 (2.38 - 3.38)

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	1167	6% 64% 17% 19%
1	B	1167	7% 64% 17% 19%
1	C	1167	6% 62% 19% 19%

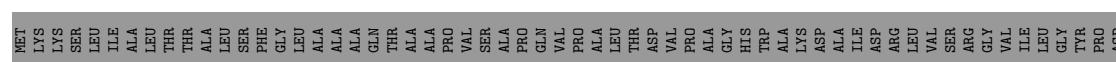
2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 21351 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 S-layer protein SlpA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	949	Total	C	N	O	S	0	0
			7117	4415	1265	1431	6		
1	B	949	Total	C	N	O	S	0	0
			7117	4415	1265	1431	6		
1	C	949	Total	C	N	O	S	0	0
			7117	4415	1265	1431	6		



GLY	THR	ASP	LEU	PHE	ARG	ALA	GLY	THR	ASN	ALA	GLN	ASN	LEU	THR	LYS	THR	ARG	ASP	TYR	GLU	ALA	ALA	SER	ASP	LEU	PHE	ARG	ALA	GLN	ILE	ILE	ALA	ALA	ARG	LEU	GLN	ASP	VAL	ALA	GLN	ARG	ALA	MET	ALA	ARG	GLY	GLY	GLU	THR	GLN	GLY	PRO	ALA	ALA	GLY	THR	GLU	ASP	MET	GLN	ASP	ASP	ILE	THR	GLN	MET	GLN	ASP	ASP	ASP	LEU	GLN	ASN	THR	ALA	ALA	ILE	ARG	VAL	GLN	GLU	ASP	ALA	ALA	TYR	ASP	ALA	LEU	ARG	ALA	ALA	LEU	GLY	VAL	ASP	ASP	ARG	ASN			
SER	ASP	LEU	GLU	GLU	ALA	ALA	ASN	ALA	ASN	VAL	ASN	VAL	SER	LEU	LYS	THR	ASP	ASP	PHE	ALA	ALA	ASN	GLN	LEU	GLU	ILE	ALA	ARG	ILE	ASP	ASP	ASP	GLN	ASP	VAL	VAL	ALA	ARG	ALA	LEU	ARG	ALA	LEU	GLY	VAL	ASP	ASP	ARG	ASN	GLY	GLU	THR	GLN	GLY	PRO	ALA	ALA	GLY	THR	GLU	ASP	MET	GLN	ASP	ASP	ILE	THR	GLN	MET	GLN	ASP	ASP	ASP	LEU	GLN	ASN	THR	ALA	ALA	ILE	ARG	VAL	GLN	GLU	ASP	ALA	ALA	TYR	ASP	ALA	LEU	ARG	ALA	ALA	LEU	GLY	VAL	ASP	ASP	ARG	ASN
ALA	SER	SER	ILE	ALA	ALA	LEU	ASN	ASP	VAL	LEU	LEU	ASN	ASP	THR	THR	THR	THR	THR	PHE	PHE	VAL	GLN	ASP	ARG	VAL	VAL	SER	ALA	VAL	SER	VAL	VAL	GLY	GLY	GLU	GLU	GLN	ASP	ARG	ALA	VAL	SER	ALA	GLY	GLY	GLU	THR	GLN	GLY	PRO	ALA	ALA	GLY	THR	GLU	ASP	MET	GLN	ASP	ASP	ILE	THR	GLN	MET	GLN	ASP	ASP	ASP	LEU	GLN	ASN	THR	ALA	ALA	ILE	ARG	VAL	GLN	GLU	ASP	ALA	ALA	TYR	ASP	ALA	LEU	ARG	ALA	ALA	LEU	GLY	VAL	ASP	ASP	ARG	ASN					
L260	T261	L262	R268	D274	V275	R276	R277	L278	N290	A291	F292	D300	R306	D307	N313	L325	S333	Y334	T335	F338	T339	D340	G341	S342	D353	Y354	K355	V356	P357	T358	G359	K360	V361	I362	K366	G367	R368	G372	F373	N374	T384	D385	I386	F392																																																									
D393	I421	L427	V428	T429	D434	V437	N442	G443	G448	E449	A450	T451	G454	D468	P469	V477	N493	P494	V497	Y506	V511	F512	D513	N514	R519	G520	D521	V525	P533	V534	I535	R549	V562	I571	T572	L577	T578	I581																																																															
H582	Y583	A584	Q585	R588	T597	T598	S599	T600	V604	T605	T606	G608	L611	H612	K614	A615	E623	T626	S627	R628	V629	R630	R631	N632	T633	A634	N635	A636	A637	V638	F644	R647	R651	K652	D653	M654	L655	A656	F657	P662	A663	A664	K665	F666	G667	N668	D669																																																						
T670	F671	G672	V673	S674	L675	Y676	D677	L678	R681	I693	Y696	S702	R703	L709	A710	Y711	F721	L724	D725	R726	Q727	D731	A732	N733	N734	D735	V736	A742	D743	N750	T751	K752	I753	G754	A762	A763	A764	N765	Y774	S778	T779	G780	D784	M789																																																									
G793	A799	I802	F803	L812	D813	S814	N815	R816	P817	Q818	I819	Y820	R821	D822	T826	I829	K833	V834	R835	D842	G846	L847	D857	V858	N859	V860	V863	R864	S865	T866	T867	D868	R869	L872	A878	S879	V885	G886	N887	N888	A889	Y890	R891	T892																																																									
G893	L894	R895	C896	A897	D898	N899	N900	D907	G910	V911	L915	D922	Q923	S924	R925	T926	A927	T928	C929	F930	T931	G941	D942	N943	A944	N945	K949	D950	R954	Y961	V962	P963	T964	T965	A966	T967	A968	T969	D972	V977	D981	Y984	D985	R986	G989	V990																																																							
A991	T1002	N1003	T1004	D1007	T1023	D1024	N1028	V1029	N1036	G1037	Q1038	V1039	Y1042	A1049	N1056	L1066	I1076	G1077	V1078	A1085	Q1086	N1087	R1088	Q1089	Y1090	S1103	N1107	N1108	R1109	R1110	L1113	N1114	G1115	V1118	G1130	T1131	Y1132	S1135	Q1136	K1137	D1138	L1139																																																											
E1143	Y1144	G1145	S1146	G1147	I1148	Q1157	Y1163	F1167																																																																																													

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	252122	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 ($e^-/\text{\AA}^2$)	1.3	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	1.505	Depositor
Minimum map value	-0.702	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.46	Depositor
Map size (Å)	431.90402, 431.90402, 431.90402	wwPDB
Map dimensions	528, 528, 528	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.818, 0.818, 0.818	Depositor

5 Model quality

5.1 Standard geometry

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	0.26	0/7258	0.48	1/9865 (0.0%)
1	B	0.26	0/7258	0.47	2/9865 (0.0%)
1	C	0.26	0/7258	0.48	3/9865 (0.0%)
All	All	0.26	0/21774	0.48	6/29595 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	632	ASN	CB-CA-C	-6.26	109.34	116.54
1	B	597	THR	CB-CA-C	-5.43	110.29	116.54
1	C	597	THR	CB-CA-C	-5.35	110.39	116.54
1	A	597	THR	CB-CA-C	-5.33	110.41	116.54
1	C	990	VAL	N-CA-C	-5.25	106.77	113.22

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	696	TYR	Peptide

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	7117	0	6745	137	0
1	B	7117	0	6745	130	0
1	C	7117	0	6745	140	0
All	All	21351	0	20235	391	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 9.

The worst 5 of 391 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:819:ILE:HG12	1:A:829:ILE:HG12	1.52	0.91
1:A:519:ARG:HH12	1:A:693:ILE:HG22	1.43	0.84
1:B:549:ARG:HB2	1:B:562:VAL:HG23	1.67	0.77
1:A:733:ASN:OD1	1:A:734:ASN:N	2.18	0.76
1:C:878:ALA:HB1	1:C:894:LEU:HD12	1.68	0.76

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	947/1167 (81%)	826 (87%)	118 (12%)	3 (0%)	36	62
1	B	947/1167 (81%)	838 (88%)	104 (11%)	5 (0%)	24	51
1	C	947/1167 (81%)	844 (89%)	99 (10%)	4 (0%)	30	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2841/3501 (81%)	2508 (88%)	321 (11%)	12 (0%)	31	56

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	598	THR
1	B	986	ARG
1	B	818	GLN
1	C	818	GLN
1	C	1087	ASN

5.3.2 Protein sidechains ⓘ

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	726/891 (82%)	726 (100%)	0	100	100
1	B	726/891 (82%)	726 (100%)	0	100	100
1	C	726/891 (82%)	726 (100%)	0	100	100
All	All	2178/2673 (82%)	2178 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	900	ASN
1	C	840	GLN
1	B	920	ASN
1	C	240	ASN
1	C	1108	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

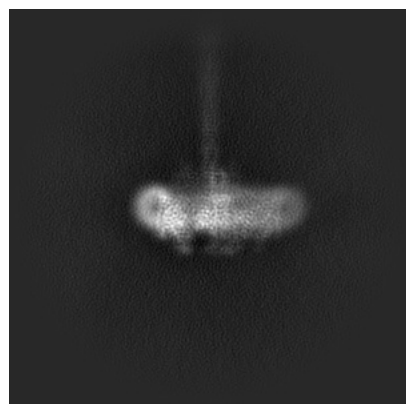
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14714. These allow visual inspection of the internal detail of the map and identification of artifacts.

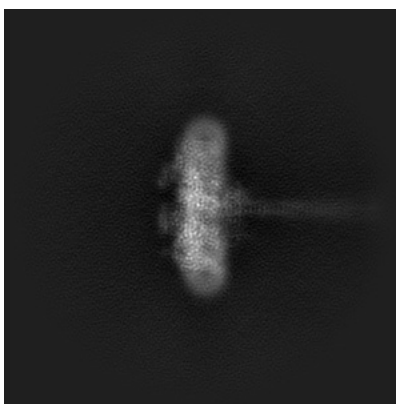
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

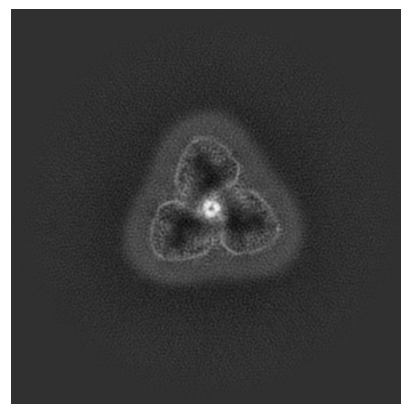
6.1.1 Primary map



X

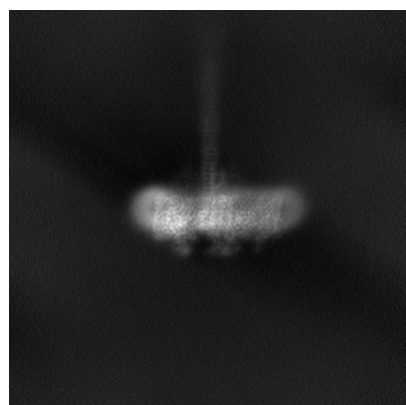


Y

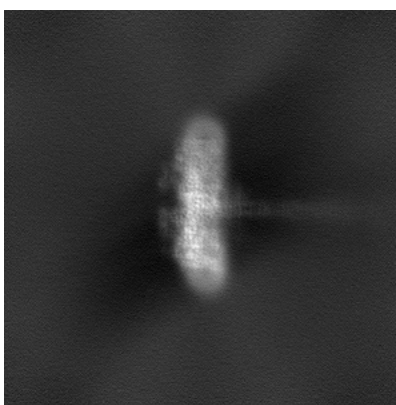


Z

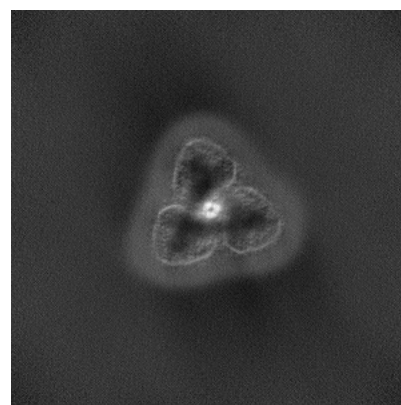
6.1.2 Raw map



X



Y

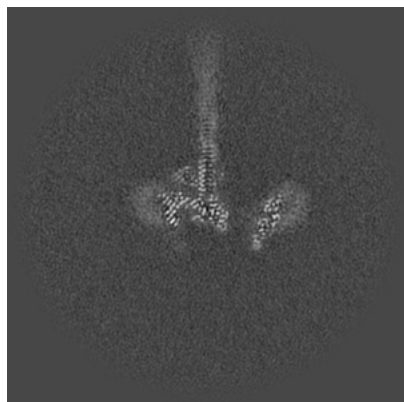


Z

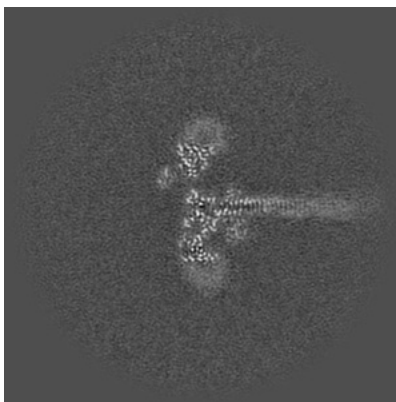
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

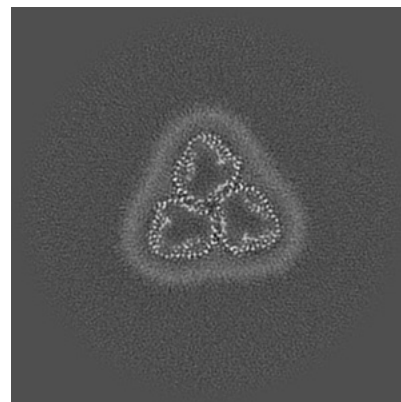
6.2.1 Primary map



X Index: 264

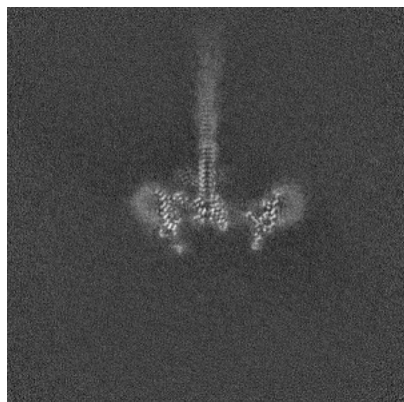


Y Index: 264

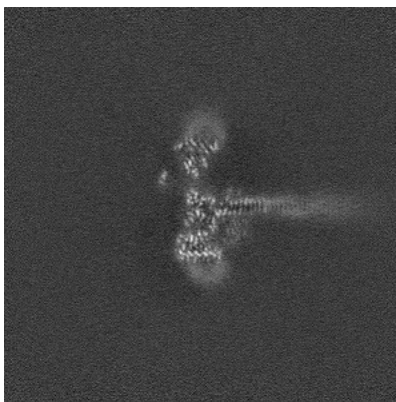


Z Index: 264

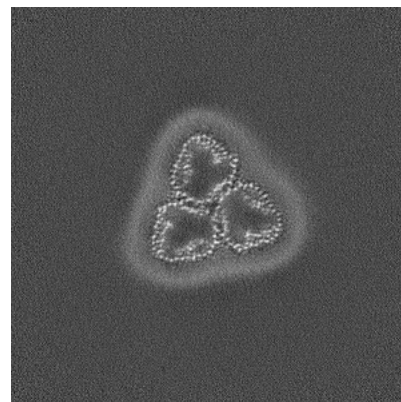
6.2.2 Raw map



X Index: 264



Y Index: 264

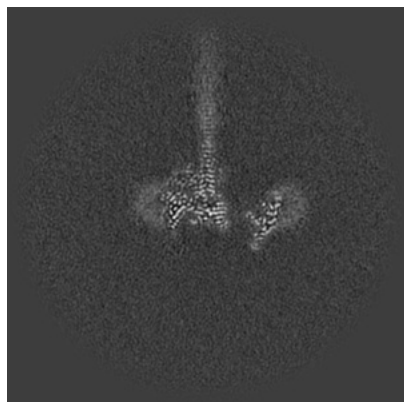


Z Index: 264

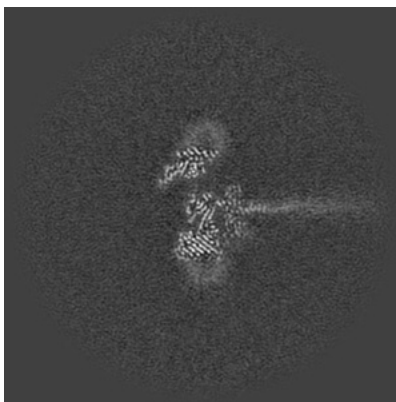
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

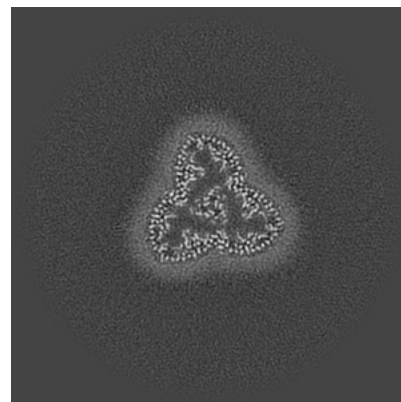
6.3.1 Primary map



X Index: 268

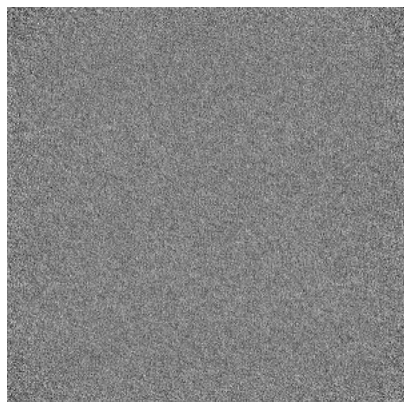


Y Index: 272

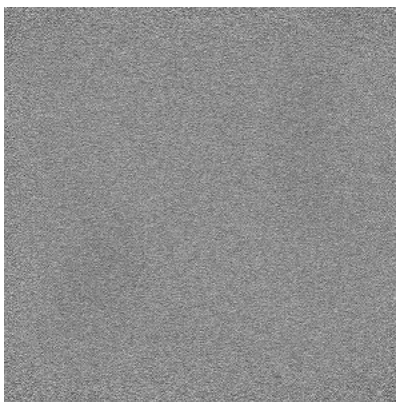


Z Index: 246

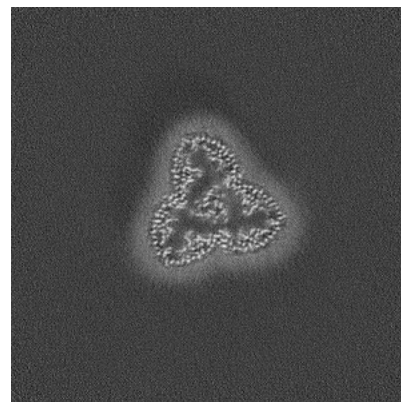
6.3.2 Raw map



X Index: 0



Y Index: 0

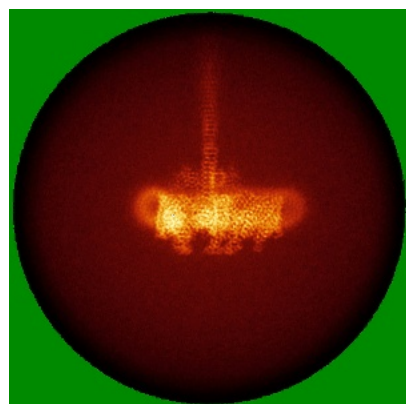


Z Index: 246

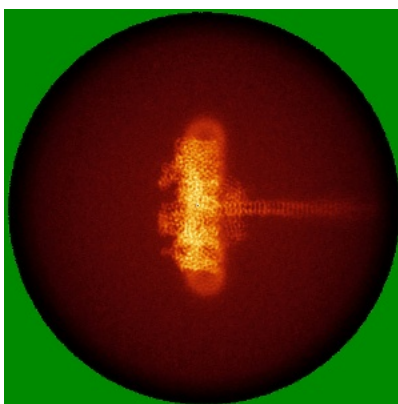
The images above show the largest variance slices of the map in three orthogonal directions.

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

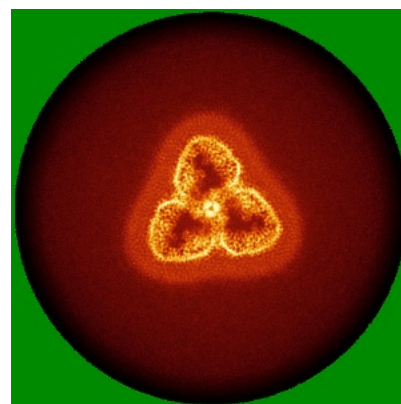
6.4.1 Primary map



X

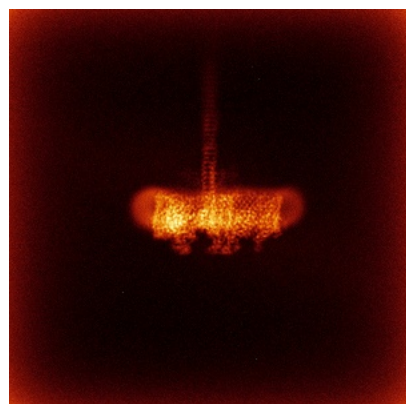


Y

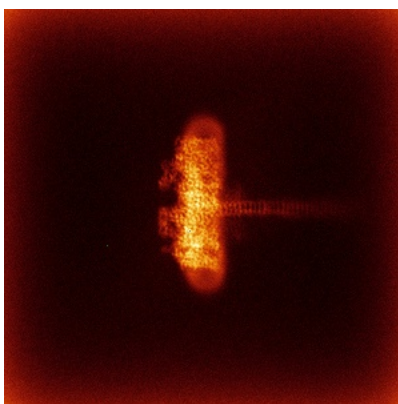


Z

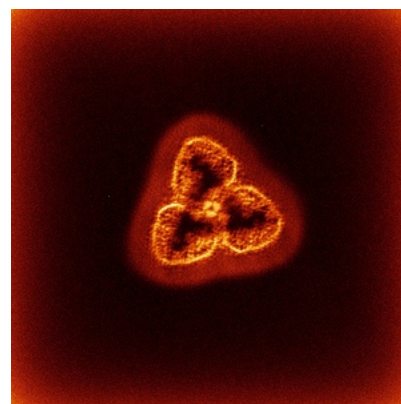
6.4.2 Raw map



X



Y

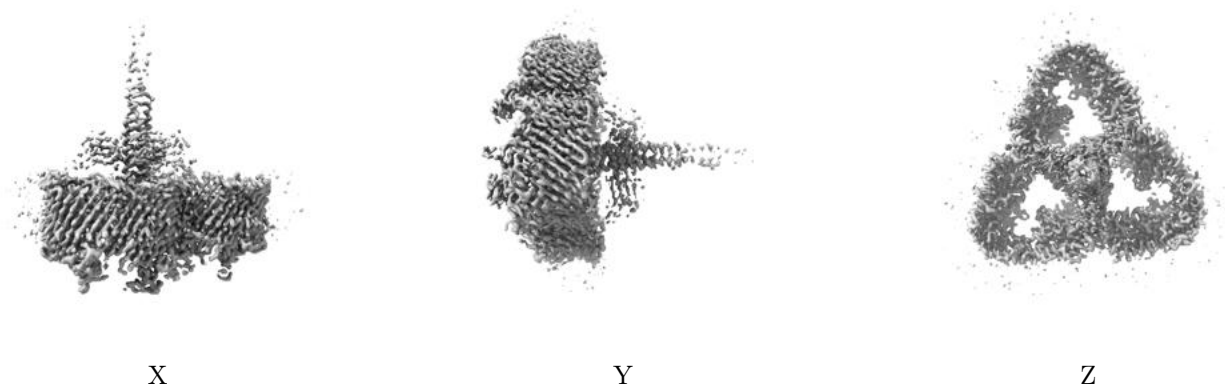


Z

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 0.46. 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.

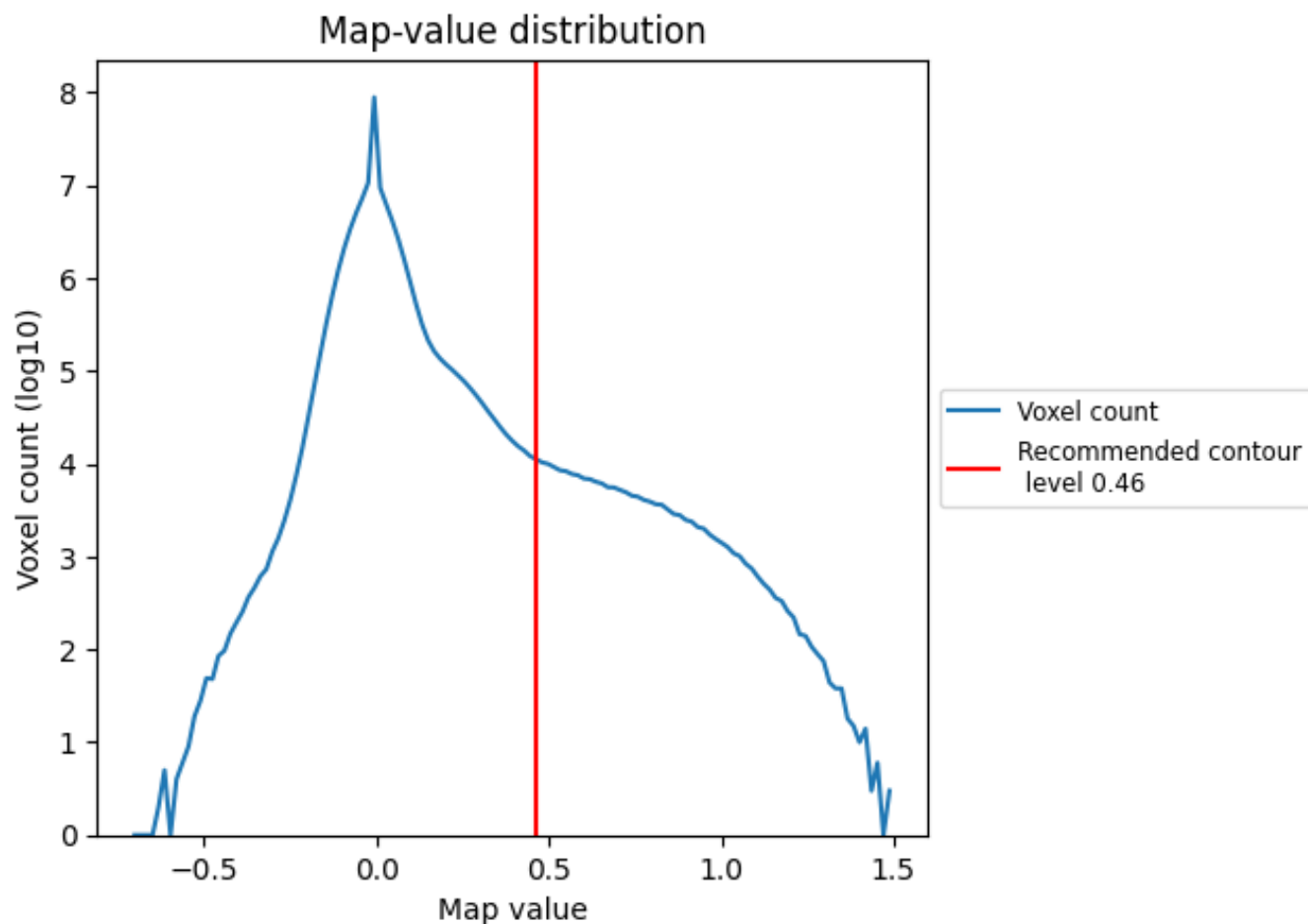
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

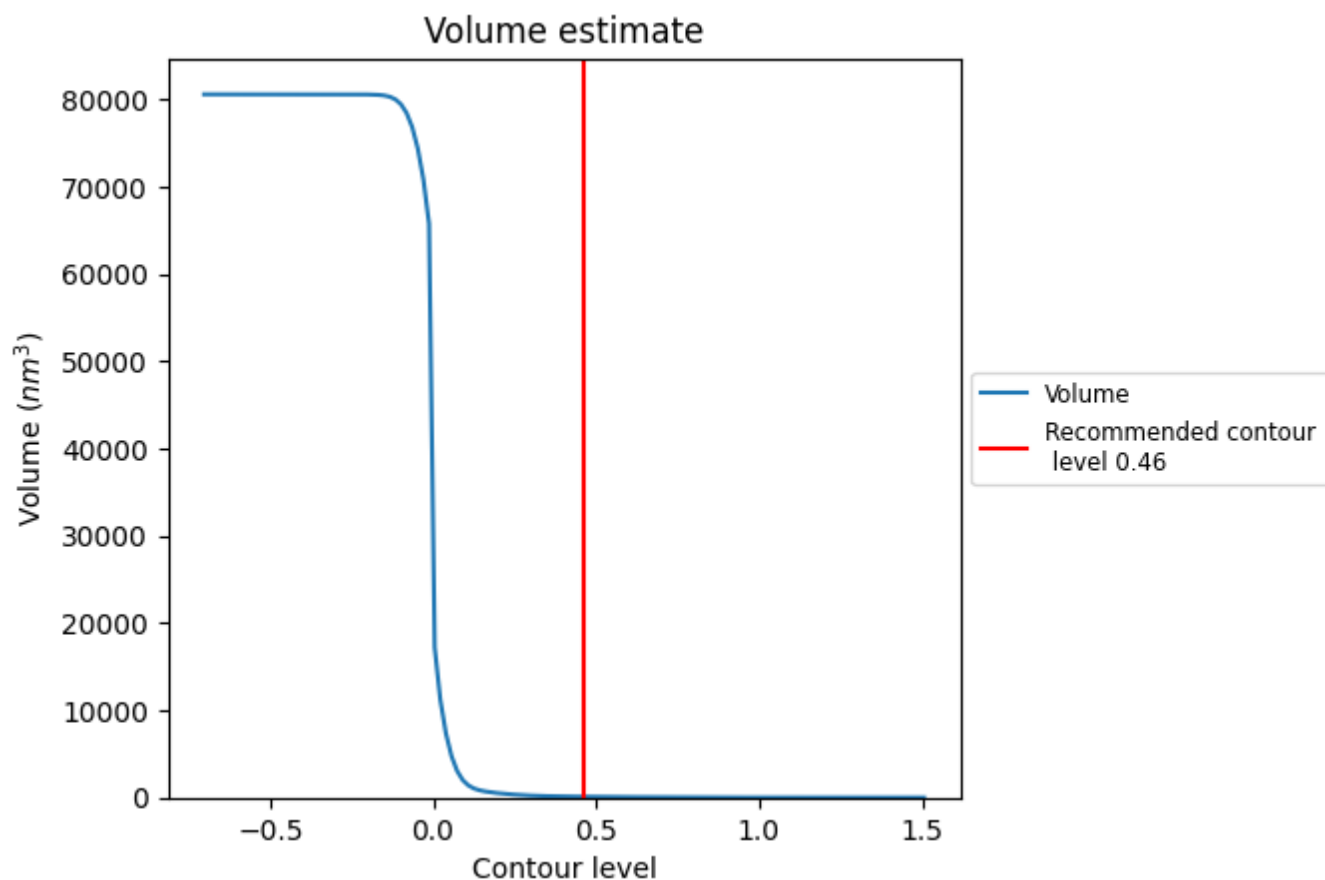
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

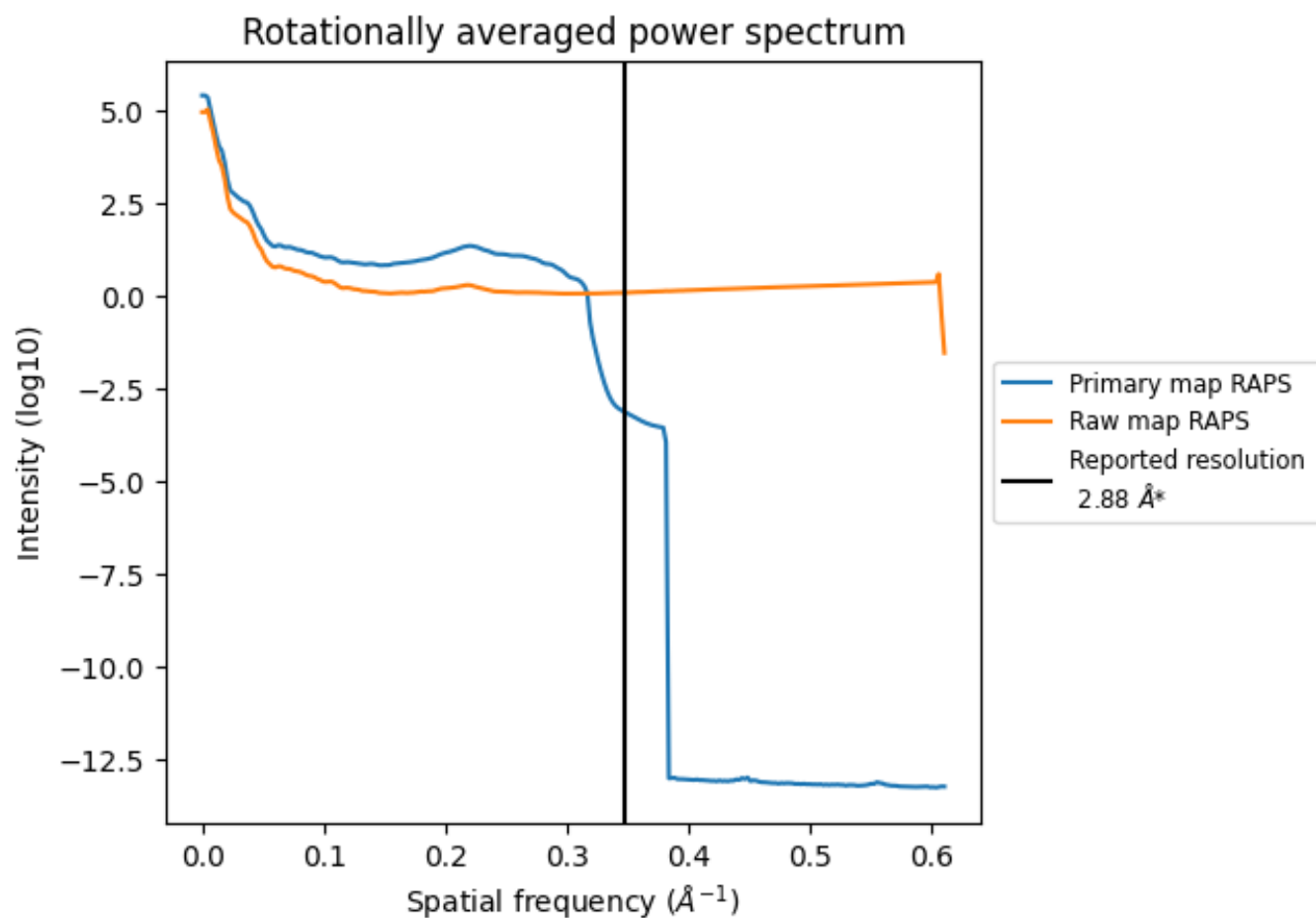
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 97 nm³; this corresponds to an approximate mass of 88 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 ⓘ

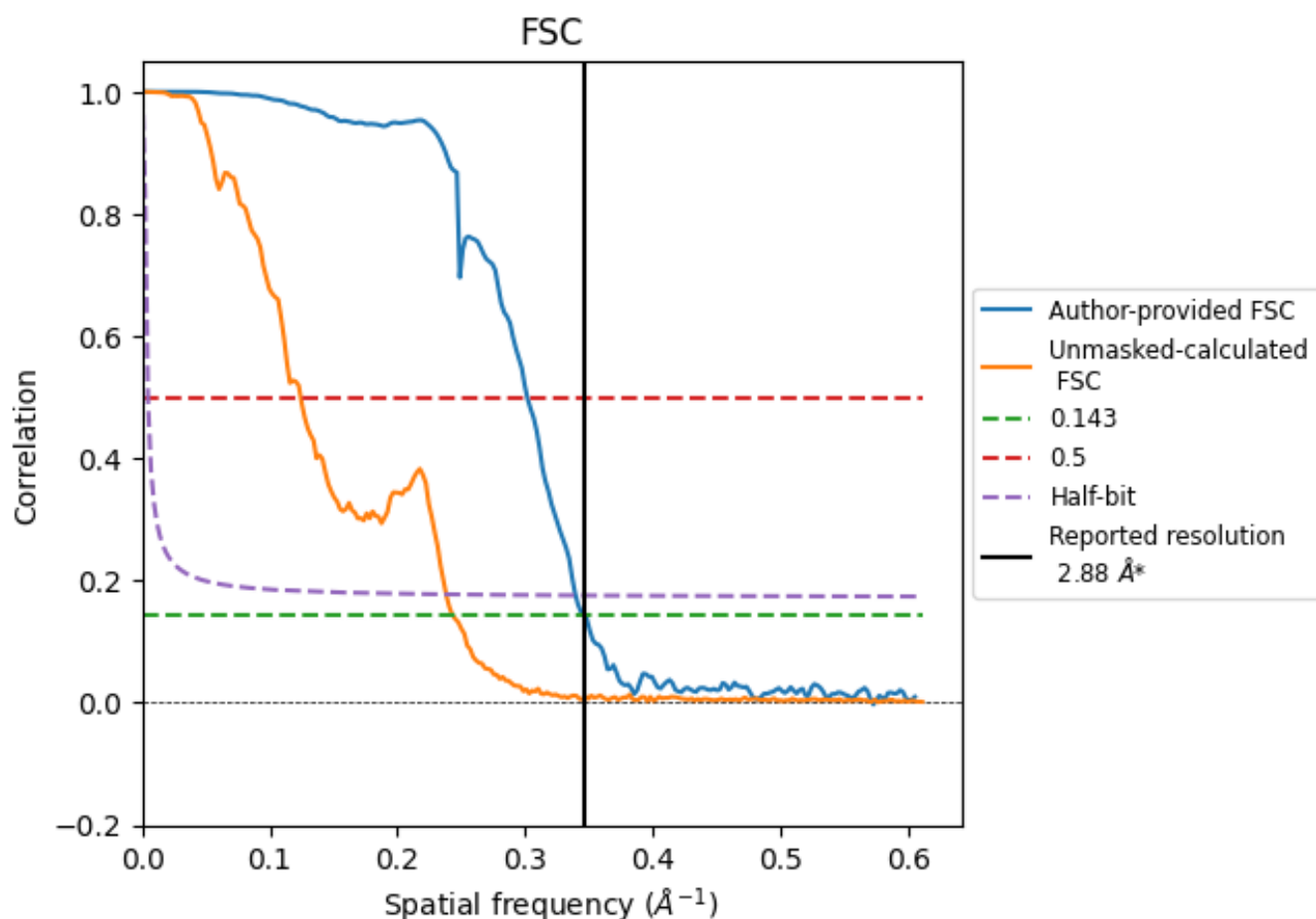


*Reported resolution corresponds to spatial frequency of 0.347 $\text{\AA}^{-1}$

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 $0.347 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

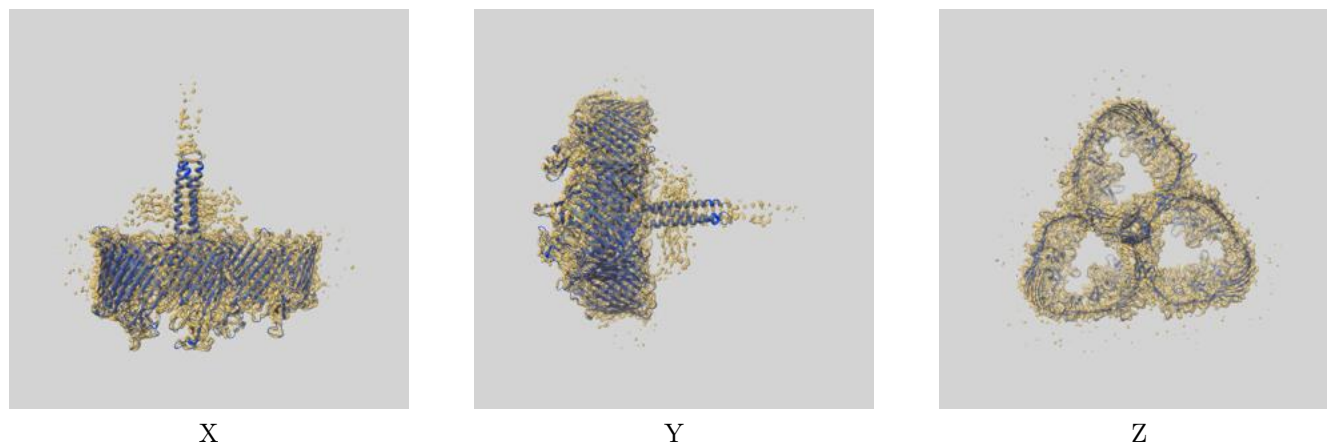
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.88	-	-
Author-provided FSC curve	2.88	3.31	2.94
Unmasked-calculated*	4.11	8.05	4.20

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.11 differs from the reported value 2.88 by more than 10 %

9 Map-model fit [i](#)

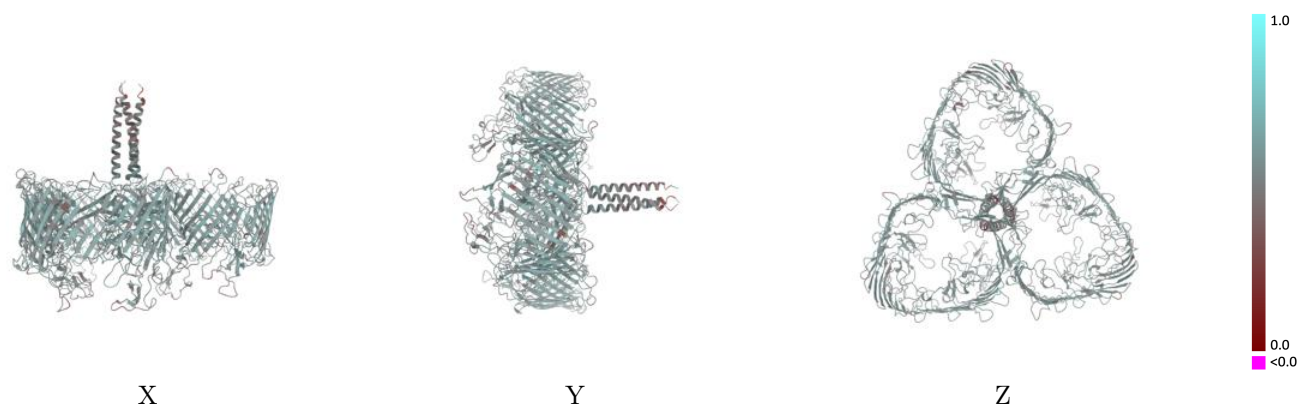
This section contains information regarding the fit between EMDB map EMD-14714 and PDB model 7ZGX. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.46 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](#)



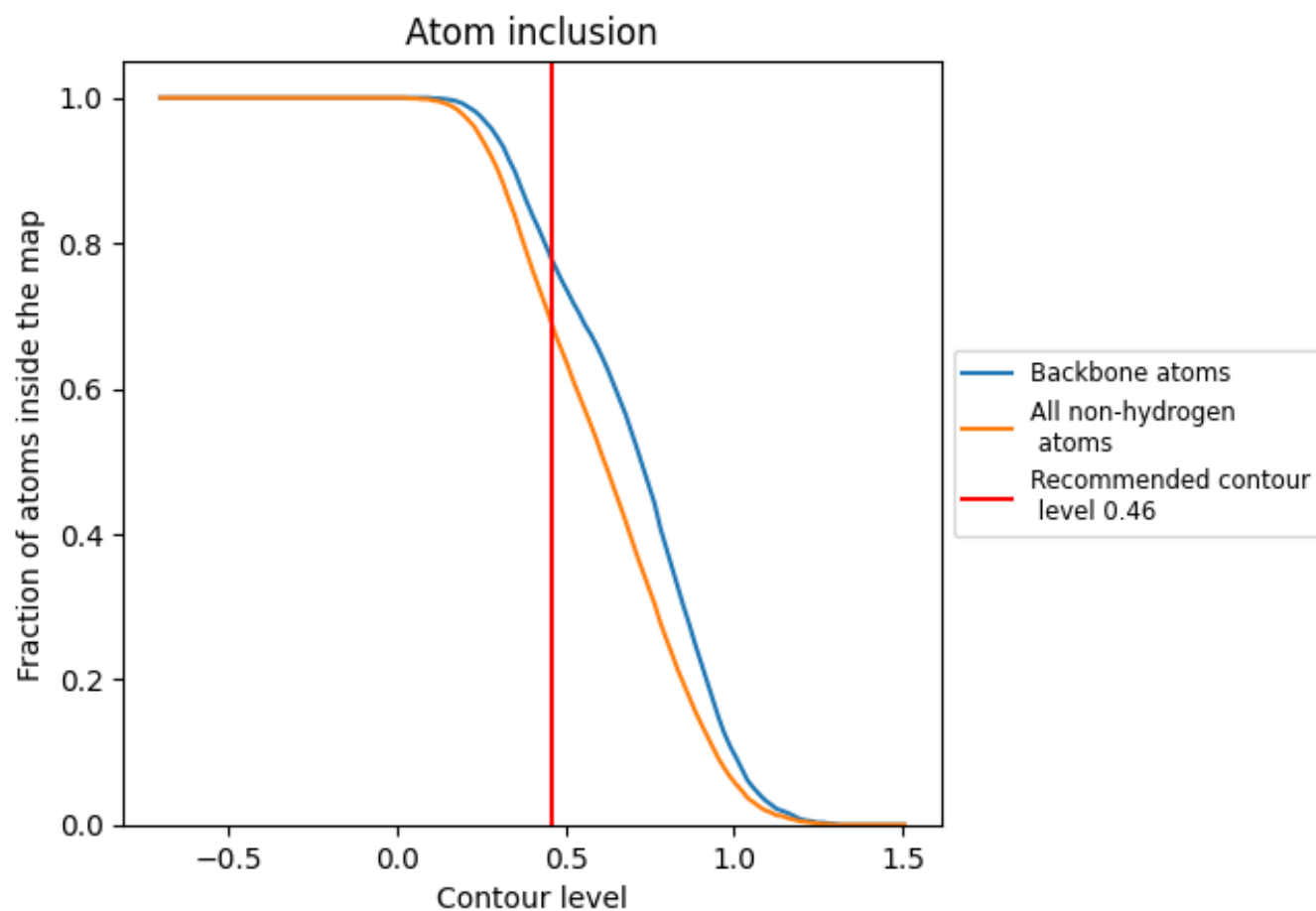
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.46).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 69% 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 (0.46) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6870	0.5310
A	0.6900	0.5300
B	0.6840	0.5310
C	0.6880	0.5320

