



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 08:00 PM UTC

PDB ID : 7XUK / pdb_00007xuk
EMDB ID : EMD-33472
Title : Structure of ATP7B C983S/C985S/D1027A mutant in presence of ATOX1
Authors : Yang, G.; Xu, L.; Guo, J.; Wu, Z.
Deposited on : 2022-05-18
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

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

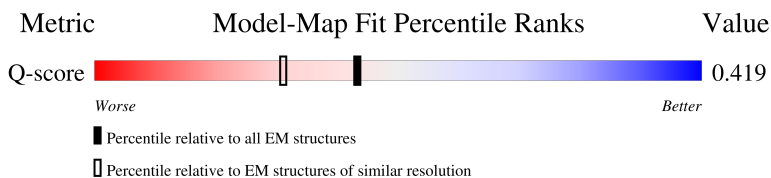
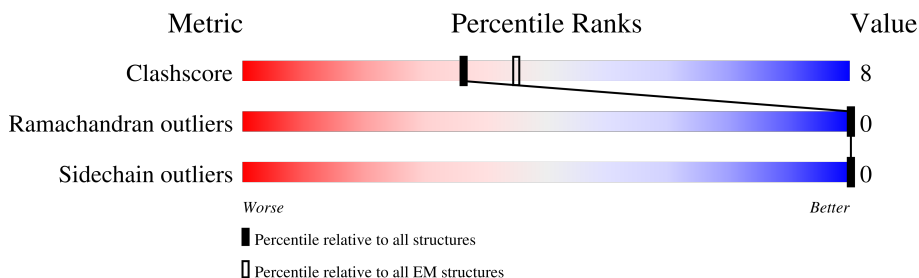
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	1507	9% 43% 11% 46%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6154 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 Copper-transporting ATPase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	816	Total	C	N	O	S	0	0
			6154	3948	1045	1122	39		

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	983	SER	CYS	engineered mutation	UNP P35670
A	985	SER	CYS	engineered mutation	UNP P35670
A	1027	ALA	ASP	engineered mutation	UNP P35670
A	1466	VAL	-	expression tag	UNP P35670
A	1467	ASP	-	expression tag	UNP P35670
A	1468	GLU	-	expression tag	UNP P35670
A	1469	LEU	-	expression tag	UNP P35670
A	1470	THR	-	expression tag	UNP P35670
A	1471	SER	-	expression tag	UNP P35670
A	1472	ARG	-	expression tag	UNP P35670
A	1473	GLY	-	expression tag	UNP P35670
A	1474	ARG	-	expression tag	UNP P35670
A	1475	ASP	-	expression tag	UNP P35670
A	1476	TYR	-	expression tag	UNP P35670
A	1477	LYS	-	expression tag	UNP P35670
A	1478	ASP	-	expression tag	UNP P35670
A	1479	ASP	-	expression tag	UNP P35670
A	1480	ASP	-	expression tag	UNP P35670
A	1481	ASP	-	expression tag	UNP P35670
A	1482	LYS	-	expression tag	UNP P35670
A	1483	TRP	-	expression tag	UNP P35670
A	1484	SER	-	expression tag	UNP P35670
A	1485	HIS	-	expression tag	UNP P35670
A	1486	PRO	-	expression tag	UNP P35670
A	1487	GLN	-	expression tag	UNP P35670
A	1488	PHE	-	expression tag	UNP P35670
A	1489	GLU	-	expression tag	UNP P35670
A	1490	LYS	-	expression tag	UNP P35670

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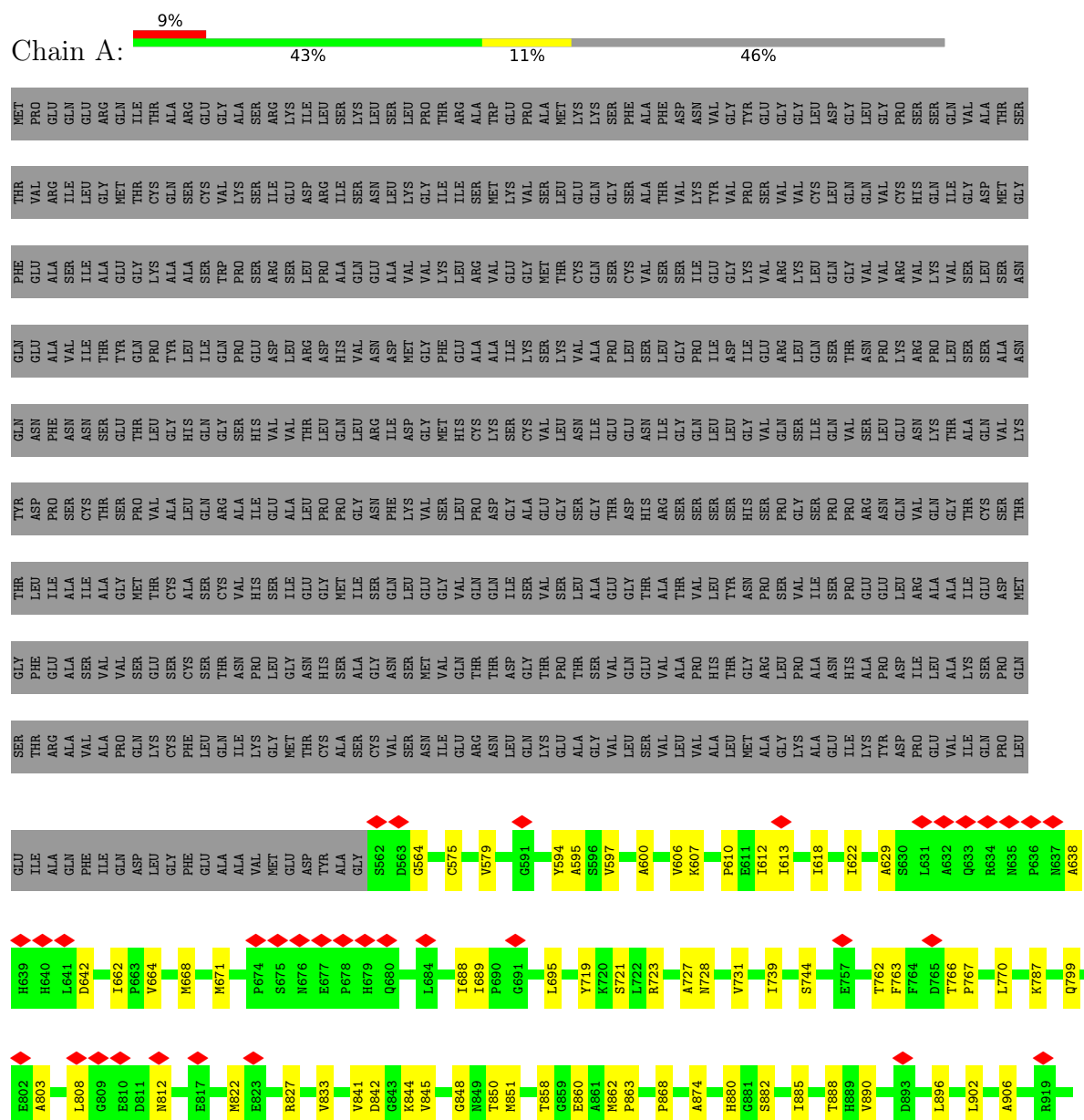
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Chain	Residue	Modelled	Actual	Comment	Reference
A	1491	GLY	-	expression tag	UNP P35670
A	1492	GLY	-	expression tag	UNP P35670
A	1493	GLY	-	expression tag	UNP P35670
A	1494	GLY	-	expression tag	UNP P35670
A	1495	SER	-	expression tag	UNP P35670
A	1496	GLY	-	expression tag	UNP P35670
A	1497	GLY	-	expression tag	UNP P35670
A	1498	SER	-	expression tag	UNP P35670
A	1499	ALA	-	expression tag	UNP P35670
A	1500	TRP	-	expression tag	UNP P35670
A	1501	SER	-	expression tag	UNP P35670
A	1502	HIS	-	expression tag	UNP P35670
A	1503	PRO	-	expression tag	UNP P35670
A	1504	GLN	-	expression tag	UNP P35670
A	1505	PHE	-	expression tag	UNP P35670
A	1506	GLU	-	expression tag	UNP P35670
A	1507	LYS	-	expression tag	UNP P35670

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Copper-transporting ATPase 2



SER	HIS	PRO	GLN	PHE	GLU	GLY	GLY	GLY	GLY	THR	SER	ASP	GLY	LYS	PRO	SER	ALA	TRP	HIS	SER	PRO	ALA	GLN	PHE	GLU	GLY	LYS																											
TYR	VAL	SER	GLN	VAL	SER	LEU	SER	SER	LEU	THR	SER	ASP	GLY	LYS	PRO	SER	ALA	TRP	HIS	SER	PRO	ALA	GLN	PHE	GLU	GLY	LYS																											
I1284	I1292	D1296	S1310	I1311	H1312	K1315	M1324	L1325	I1336	P1337	M1344	M1359	L1371	D1380	R1383	Q1387	H1391	M1392	K1393	P1394	L1395	T1396	A1397	H1403	I1404	G1405	MET	ASP	ASP	TRP	ARG	ASP	SER	TYR	ARG	ASP	LYS	TRP	GLN	VAL	SER													
D1164	V1165	S1166	D1167	A1168	D1171	H1172	E1173	M1174	K1175	T1178	A1179	I1180	L1181	V1182	A1183	I1184	D1185	G1186	V1187	L1188	C1189	G1190	M1191	I1192	A1195	V1206	L1209	V1216	N1223	R1228	Q1233	V1234	F1240	K1248	K1251	V1252	Q1253	E1254	A1263	M1264	D1267	Q1277	G1281											
C1104	K1105	V1106	S1107	M1108	V1109	E1110	G1111	I1112	L1113	A1114	H1115	SER	GLU	ARG	PRO	LEU	SER	ALA	PRO	ALA	SER	HIS	LEU	ASN	GLU	ALA	VAL	PRO	GLN	THR	F1144	S1145	V1146	L1147	I1148	G1149	M1150	R1151	E1152	W1153	L1154	R1155	R1156	M1157	G1158	L1159	T1160	I1161	S1162	S1163				
S932	G943	F947	G948	Q951	P955	N956	P957	N958	K959	H960	I967	I968	R969	Q973	I976	L979	S983	S986	A990	H996	L1008	T1009	K1010	G1011	P1014	L1015	E1016	M1017	A1018	H1019	K1020	I1021	V1024	M1025	K1028	T1031	I1032	G1035	V1036	P1037	R1038													
V1039	M1040	R1041	V1042	L1043	L1044	L1045	G1046	D1047	V1048	A1049	T1050	L1051	R1054	K1055	A1058	G1061	T1062	A1063	E1064	A1065	S1066	S1067	E1068	L1071	A1074	V1075	T1076	K1077	Y1078	C1079	K1080	E1081	E1082	L1083	G1084	T1085	E1086	T1087	L1088	G1089	Y1090	C1091	T1092	D1093	F1094	Q1095	A1096	V1097	P1098	G1099	C1100	G1101	I1102	G1103

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	403645	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 ($e^-/\text{\AA}^2$)	62	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	1300	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.077	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	243.36002, 243.36002, 243.36002	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.014, 1.014, 1.014	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.11	0/6260	0.29	0/8502

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	6154	0	6418	97	0
All	All	6154	0	6418	97	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 8.

The worst 5 of 97 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:575:CYS:SG	1:A:728:ASN:ND2	2.53	0.81
1:A:612:ILE:HG22	1:A:613:ILE:HG23	1.70	0.73
1:A:808:LEU:HB3	1:A:812:ASN:HA	1.71	0.72
1:A:1094:PHE:HA	1:A:1104:CYS:HB3	1.76	0.66
1:A:664:VAL:HG12	1:A:668:MET:HE2	1.79	0.64

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	812/1507 (54%)	778 (96%)	34 (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	676/1258 (54%)	676 (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 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1200	GLN
1	A	1210	GLN
1	A	1256	GLN
1	A	728	ASN
1	A	889	HIS

5.3.3 RNA [i](#)

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.

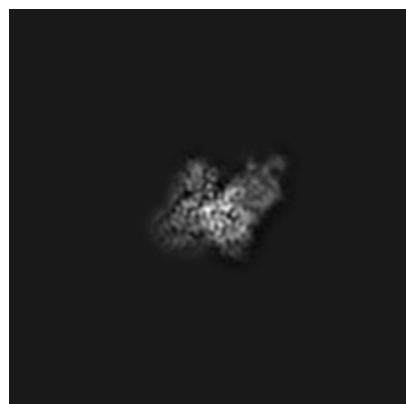
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33472. These allow visual inspection of the internal detail of the map and identification of artifacts.

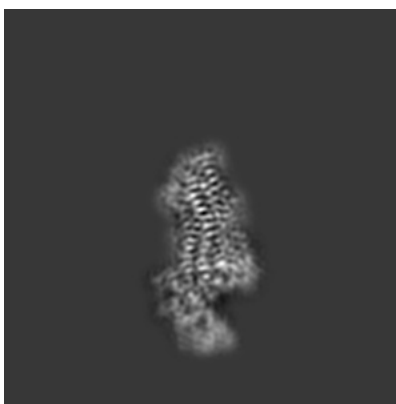
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

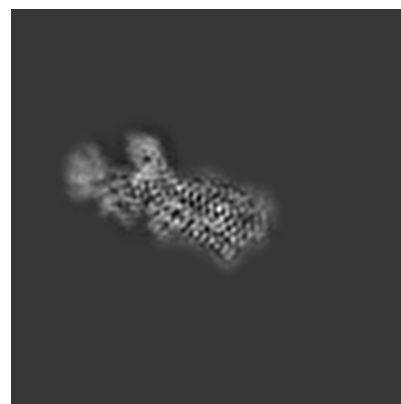
6.1.1 Primary map



X

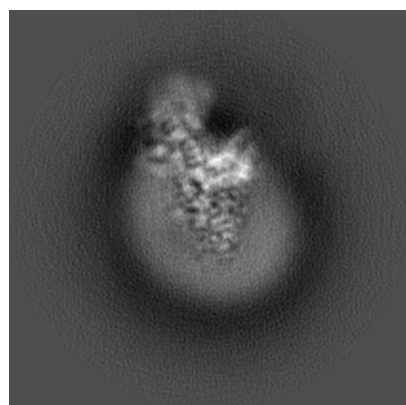


Y

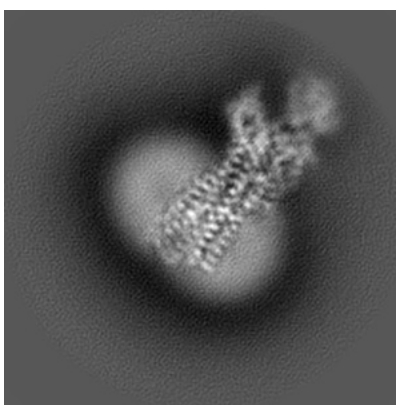


Z

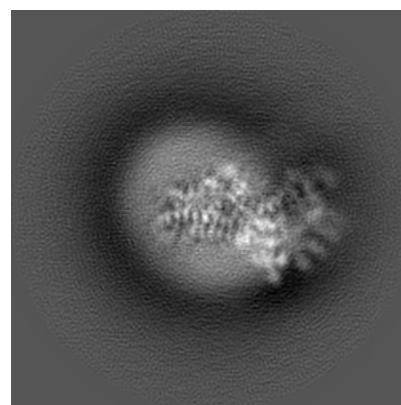
6.1.2 Raw map



X



Y

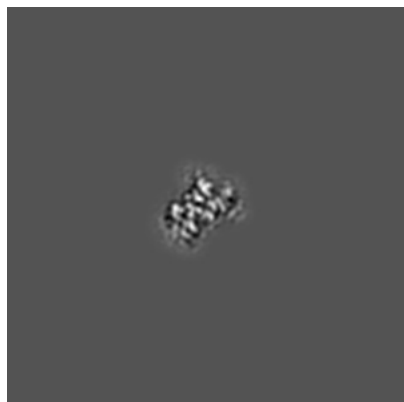


Z

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

6.2 Central slices [i](#)

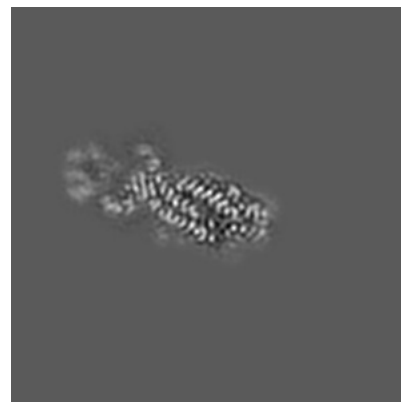
6.2.1 Primary map



X Index: 120

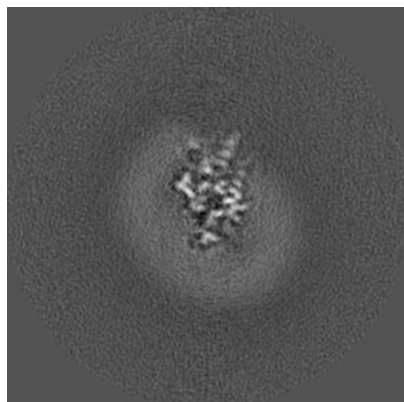


Y Index: 120

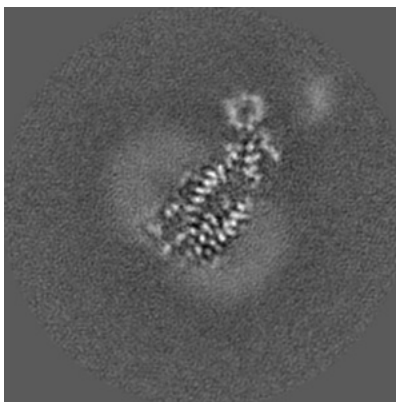


Z Index: 120

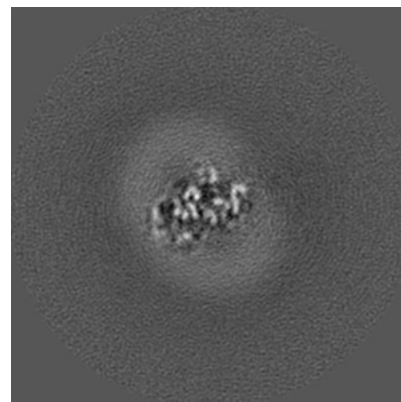
6.2.2 Raw map



X Index: 105



Y Index: 105

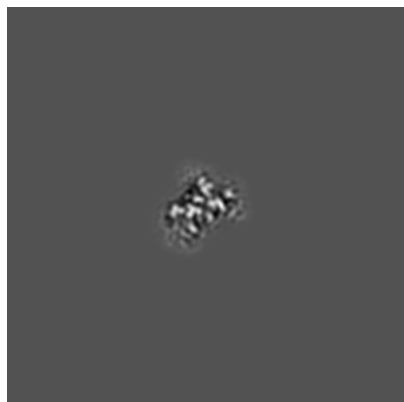


Z Index: 105

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

6.3 Largest variance slices [i](#)

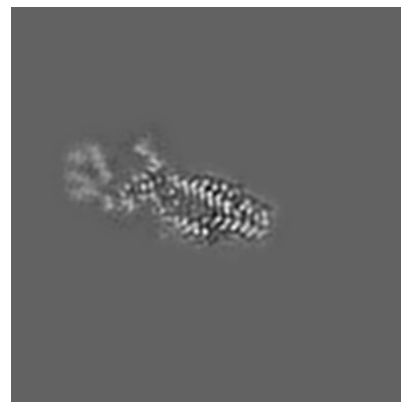
6.3.1 Primary map



X Index: 119

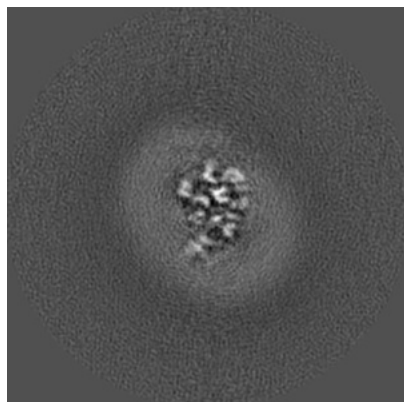


Y Index: 121

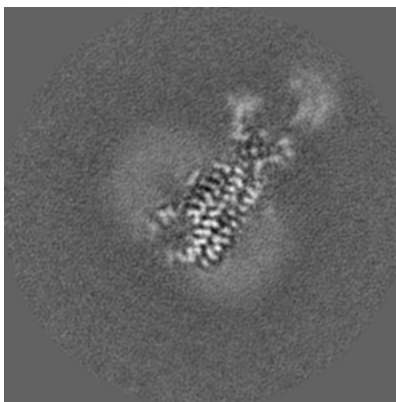


Z Index: 122

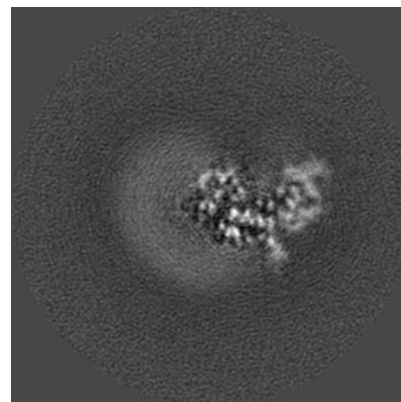
6.3.2 Raw map



X Index: 100



Y Index: 101

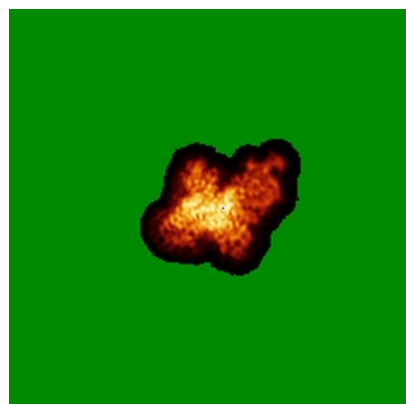


Z Index: 123

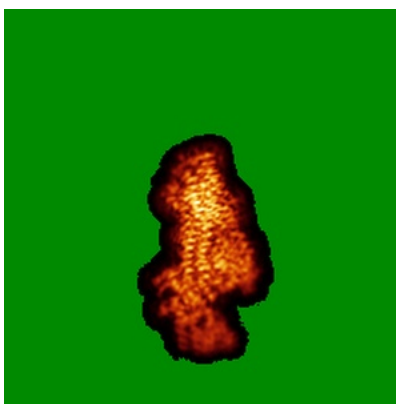
The images above show the largest variance slices of the map in three orthogonal directions.

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

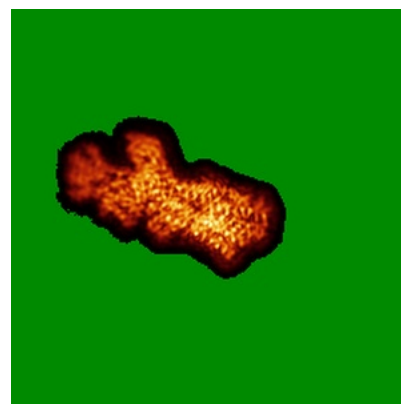
6.4.1 Primary map



X

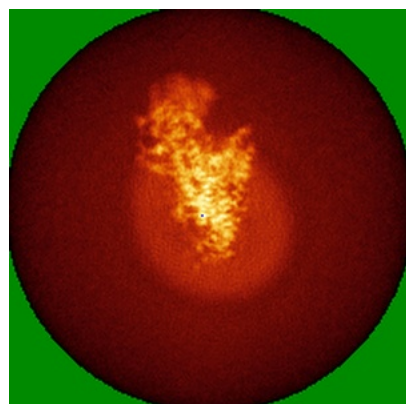


Y

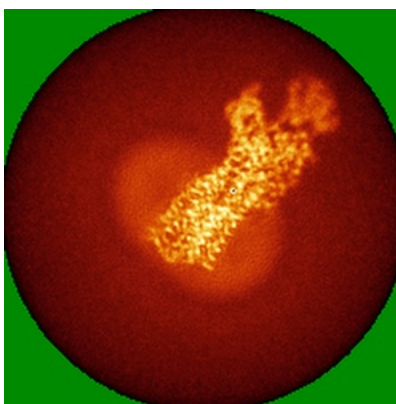


Z

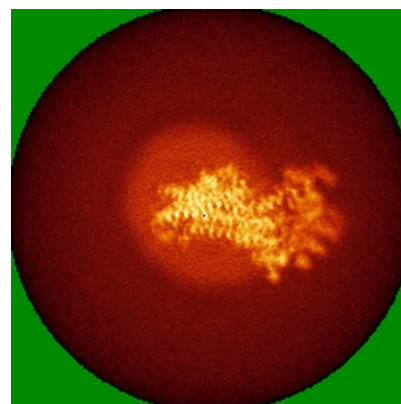
6.4.2 Raw map



X



Y

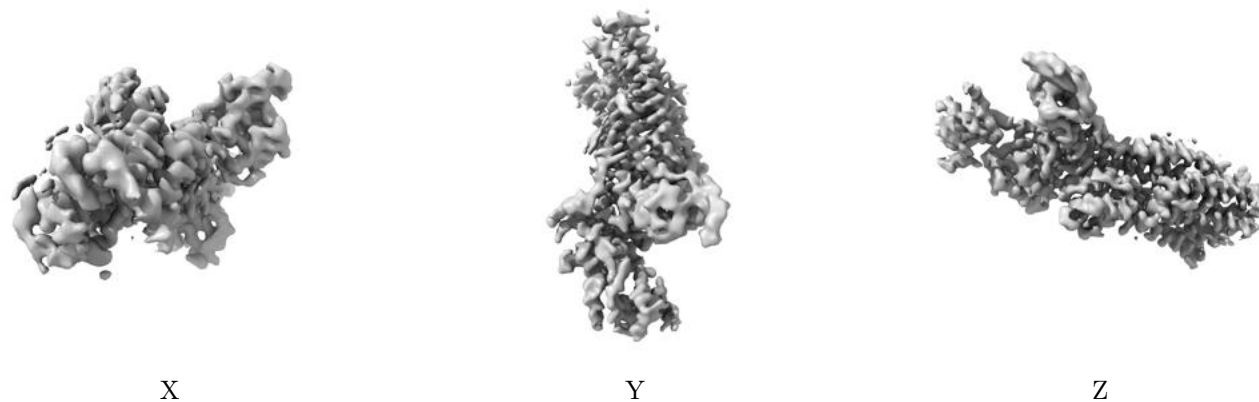


Z

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.

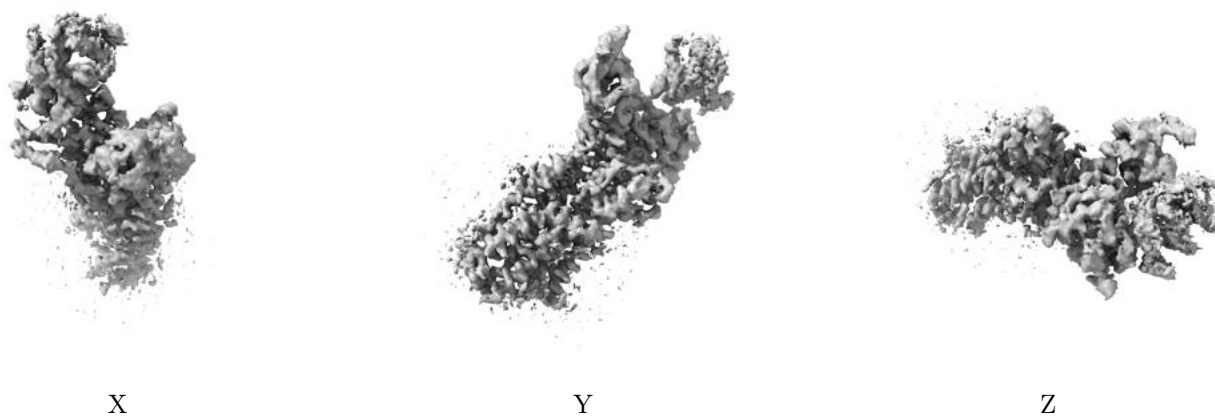
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. 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.

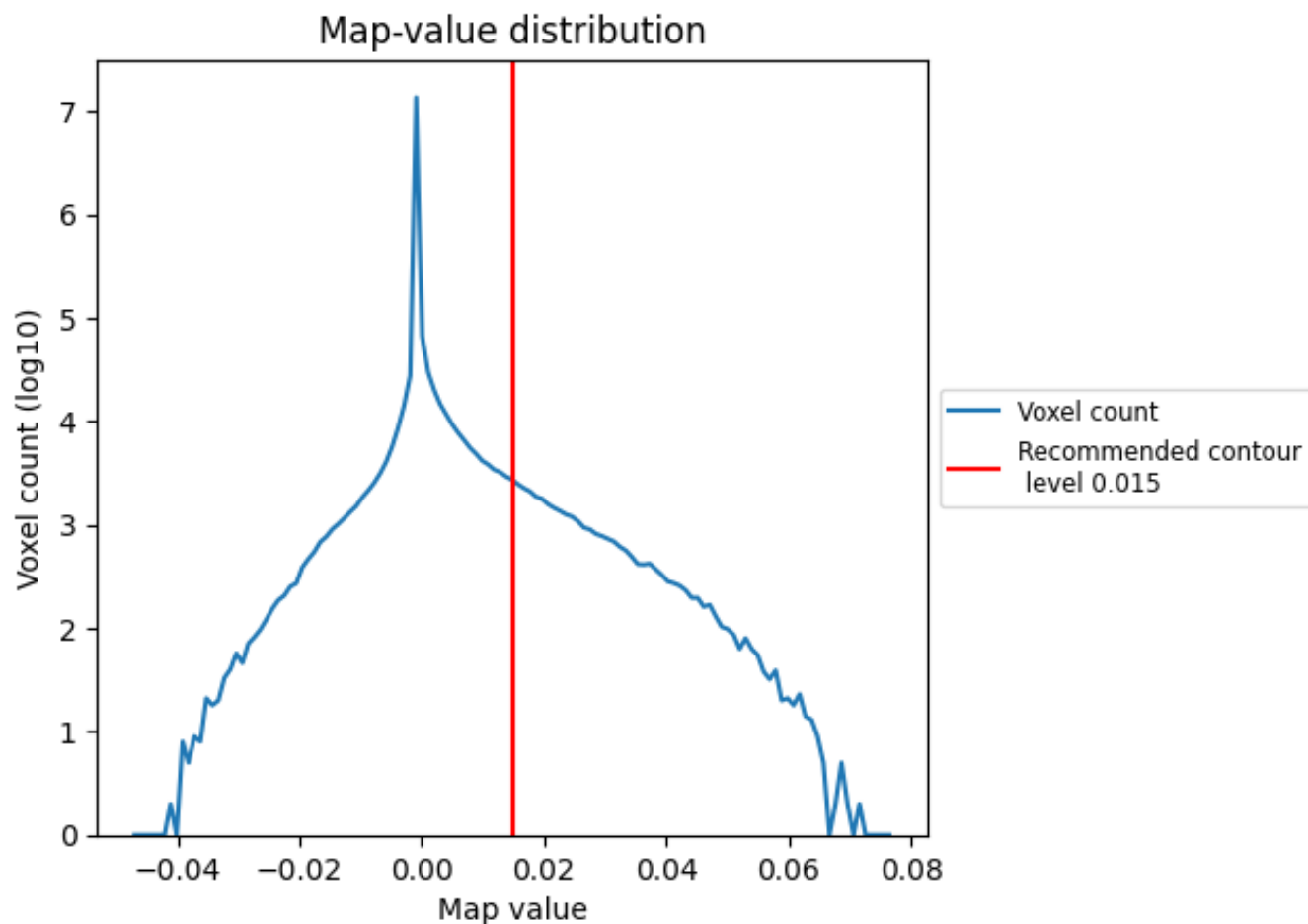
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

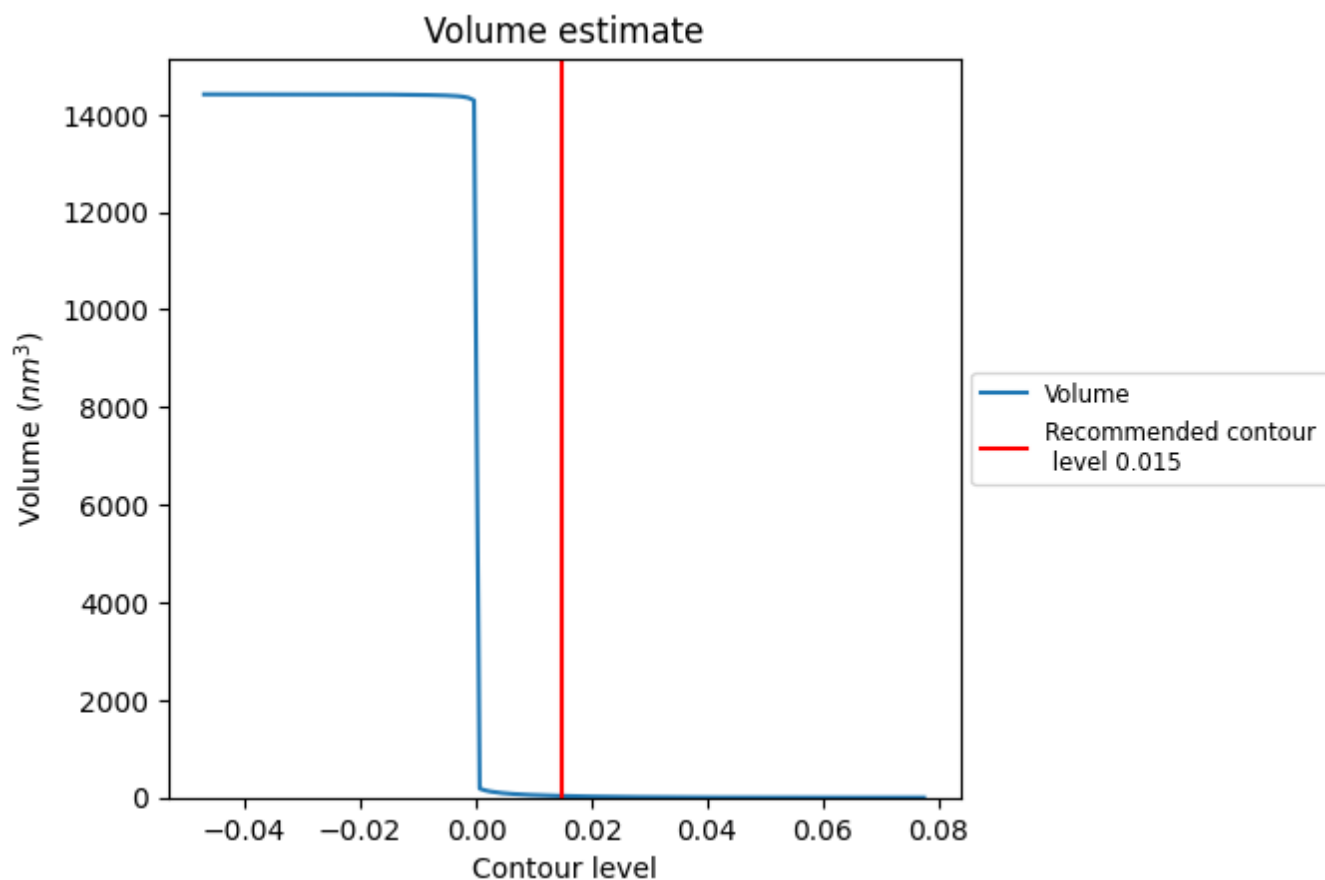
This section contains the results of statistical analysis of the map.

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.

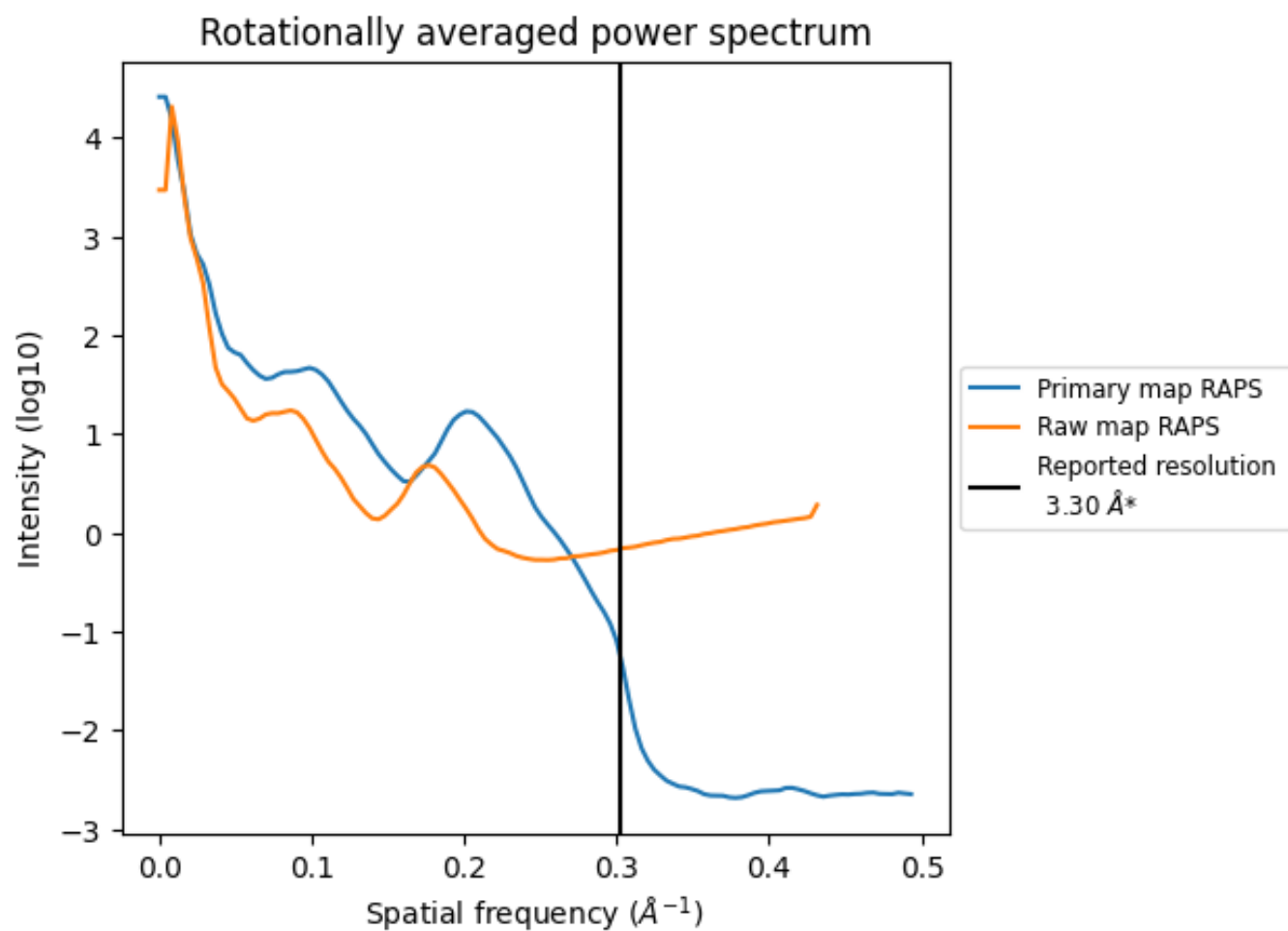
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 33 nm^3 ; this corresponds to an approximate mass of 30 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 ⓘ

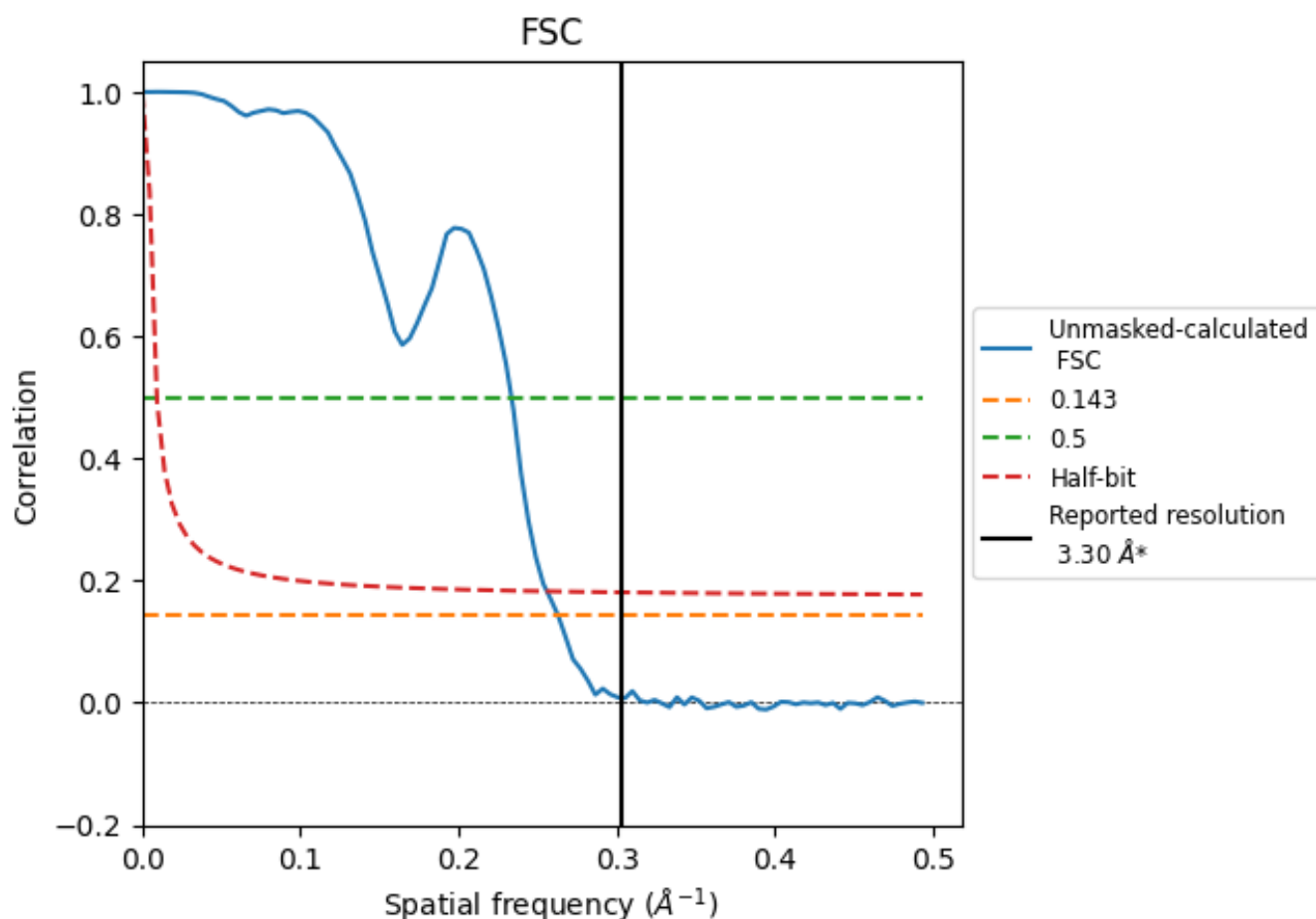


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

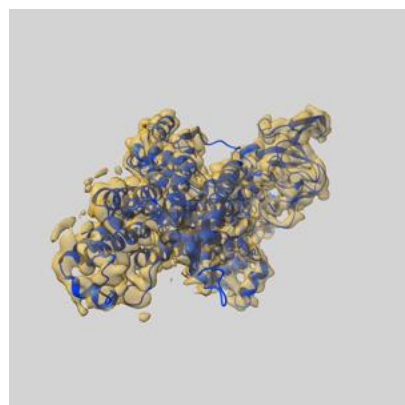
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.80	4.28	3.91

*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 3.80 differs from the reported value 3.3 by more than 10 %

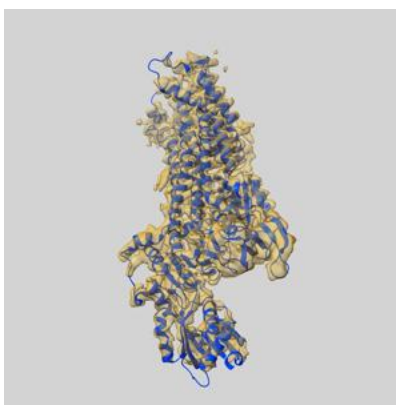
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33472 and PDB model 7XUK. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

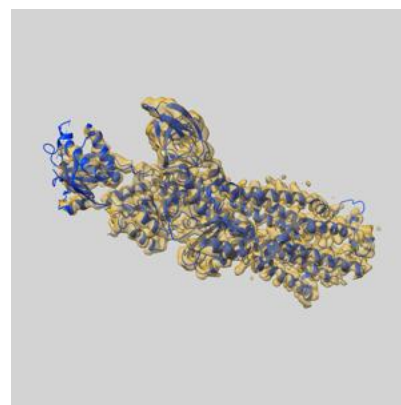
9.1 Map-model overlay [i](#)



X



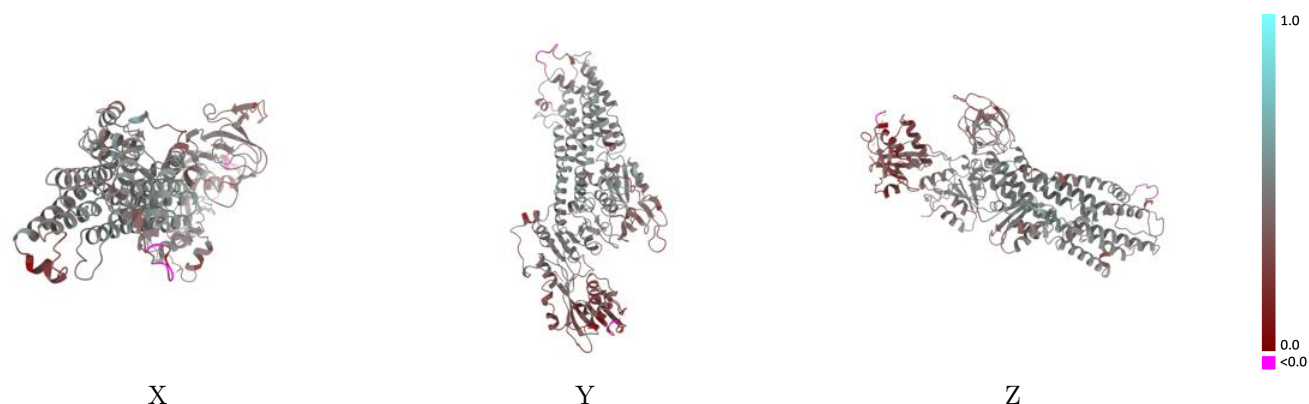
Y



Z

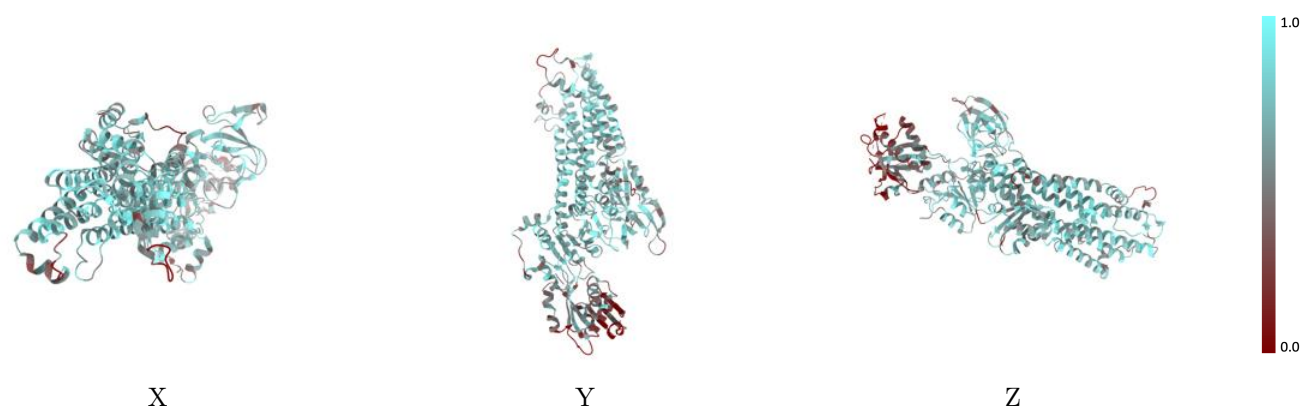
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



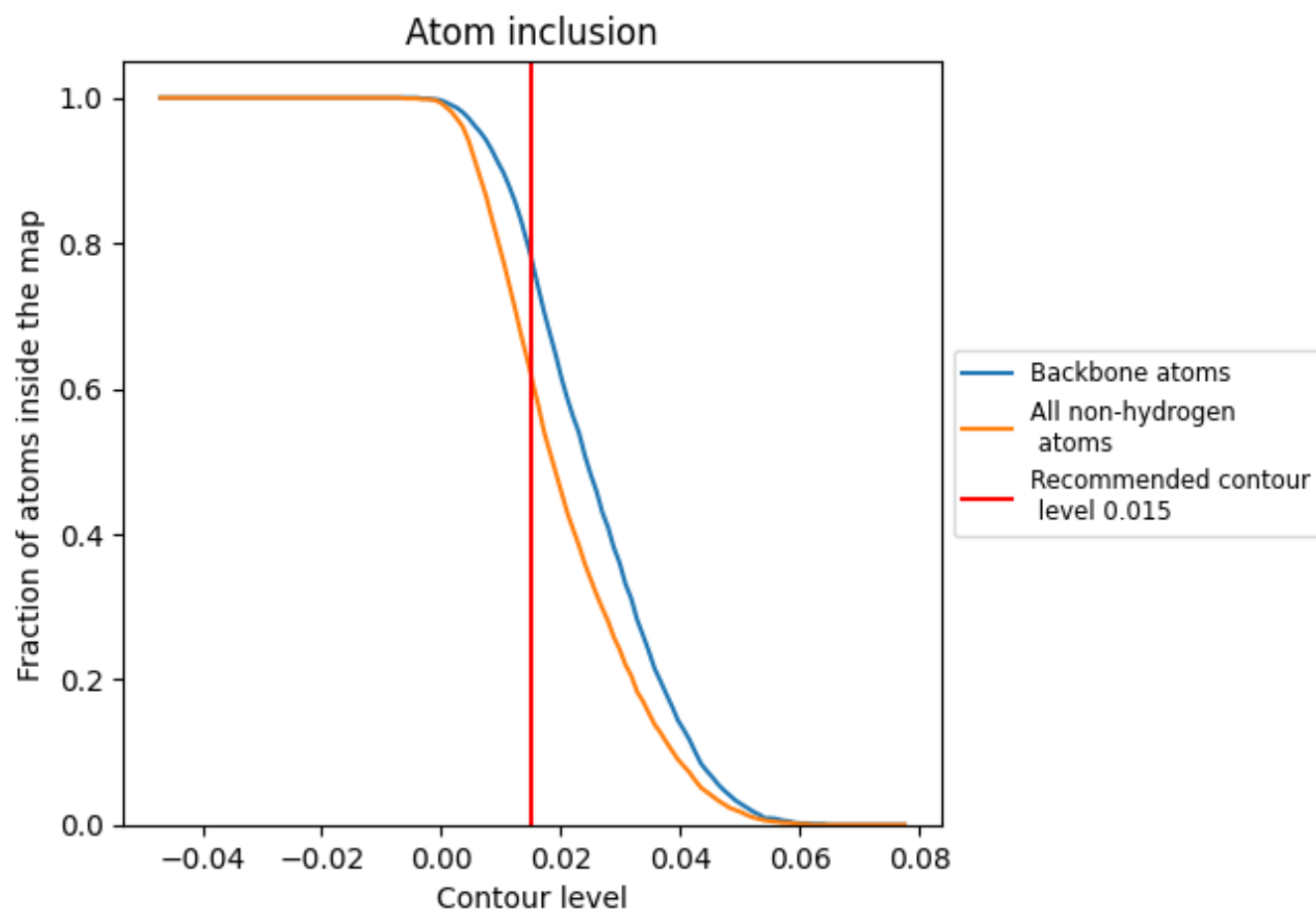
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 62% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6190	0.4190
A	0.6190	0.4190

