



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 10:52 AM UTC

PDB ID : 7XUO / pdb_00007xuo
EMDB ID : EMD-33476
Title : Structure of ATP7B C983S/C985S/D1027A mutant with cisplatin in presence of ATOX1
Authors : Yang, G.; Xu, L.; Chang, S.; Guo, J.; Wu, Z.
Deposited on : 2022-05-19
Resolution : 3.60 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

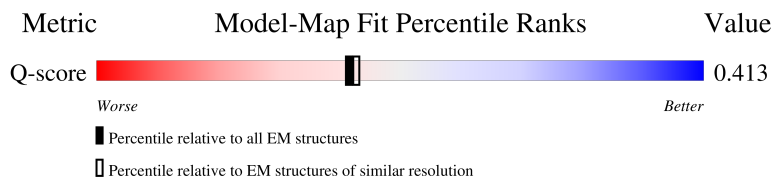
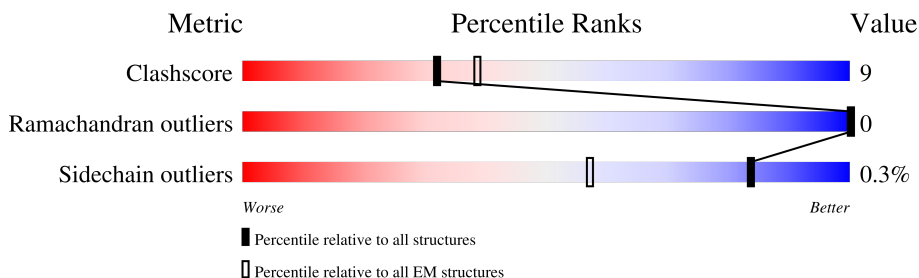
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

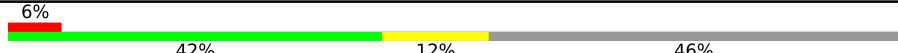
The reported resolution of this entry is 3.60 Å.

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	12797 (3.10 - 4.10)

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	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6155 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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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

- Molecule 2 is PLATINUM (II) ION (CCD ID: PT) (formula: Pt) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Pt	0
			1	1	

ILE	VAL	ASP	GLU	LEU	THR	SER	ARG	GLY	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	GLN	VAL	LYS	TRP	SER	SER	HIS	PRO	GLN	PHE	GLU	GLY	LYS	GLY	GLY	GLY	SER	GLY	GLY	SER	SER	ALA	TRP	SER	HIS	PRO	GLN	PHE	GLU	GLU	LYS											
G1405	MET	ASP	ASP	ASP	TRP	ARG	SER	SER	PRO	ARG	ALA	THR	PRO	TRP	ASP	ASP	GLN	VAL	SER	TYR	VAL	SER	GLN	VAL	SER	LEU	SER	GLY	LYS	PRO	ALA	ALA	ASP	ASP	GLY	ASP	LYS	TRP	SER	LEU	LEU	LEU	ASN	GLY	ARG	ASP	GLU	GLU	GLN	TYR								
R1228	G1235	I1236	N1237	K1238	V1239	F1240	V1243	H1247	K1248	V1249	Q1253	N1257	V1265	Q1277	G1281	V1282	A1295	D1296	L1305	V1308	S1314	N1324	L1325	M1359	S1362	K1374	P1379	Y1384	A1388	M1392	L1395	T1396	A1397	S1398	Q1399	H1403	I1404																					
G1149	N1150	R1151	L1154	R1155	R1156	L1159	T1160	I1161	S1163	D1164	V1165	M1169	T1170	D1171	H1172	M1174	K1175	G1176	Q1177	T1178	A1179	I1180	L1181	V1182	A1183	T1184	V1187	L1188	C1189	G1190	M1191	T1192	A1193	I1194	A1195	V1198	E1201	L1209	D1215	T1216	V1217	L1218	I1219	T1220	G1221	D1222	N1223	R1224										
T1085	E1086	T1087	L1088	G1089	Y1090	C1091	T1092	D1093	F1094	Q1095	A1096	V1097	P1098	G1099	C1100	G1101	C1104	V1109	E1110	G1111	I1112	L1113	A1114	H1115	SER	GLU	ARG	PRO	LEU	SER	ALA	ALA	ALA	SER	HIS	LEU	ASN	GLU	ALA	GLY	SER	LEU	PRO	ALA	ALA	GLU	LYS	ASP	ALA	VAL	PRO	GLN	THR	F1144	S1145	V1146	L1147	I1148
L1008	I1009	K1010	G1011	P1014	L1015	E1016	M1017	A1018	I1021	V1024	T1033	V1036	P1037	R1038	V1039	M1040	R1041	V1042	L1043	L1044	L1045	G1046	D1047	V1048	A1049	T1050	L1053	R1054	L1057	T1062	A1063	E1064	A1065	S1066	S1067	E1068	H1069	P1070	L1071	G1072	V1073	A1074	V1075	T1076	K1077	V1078	E1081	E1082	L1083	G1084								

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	314029	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 ($e^-/\text{\AA}^2$)	54	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.065	Depositor
Minimum map value	-0.041	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.009	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](#)

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

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	0.13	0/6260	0.35	2/8502 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	1081	GLU	CA-C-N	-5.56	111.28	121.52
1	A	1081	GLU	C-N-CA	-5.56	111.28	121.52

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	108	0
2	A	1	0	0	0	0
All	All	6155	0	6418	108	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 108 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:808:LEU:HB3	1:A:812:ASN:HA	1.73	0.70
1:A:1078:TYR:O	1:A:1081:GLU:HG3	1.91	0.70
1:A:1228:ARG:NH1	1:A:1397:ALA:O	2.26	0.69
1:A:1069:HIS:HD2	1:A:1071:LEU:HG	1.58	0.69
1:A:1223:ASN:OD1	1:A:1224:ARG:N	2.27	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	812/1507 (54%)	779 (96%)	33 (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%)	674 (100%)	2 (0%)	86	83

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	860	GLU
1	A	965	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	707	GLN
1	A	724	HIS
1	A	1069	HIS
1	A	1177	GLN
1	A	1256	GLN

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](#)

Of 1 ligands modelled in this entry, 1 is 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

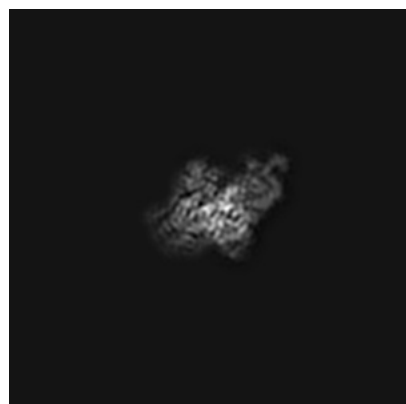
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33476. These allow visual inspection of the internal detail of the map and identification of artifacts.

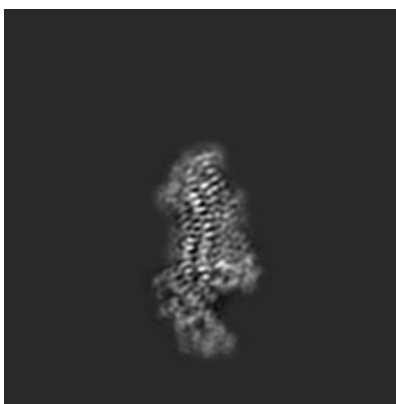
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

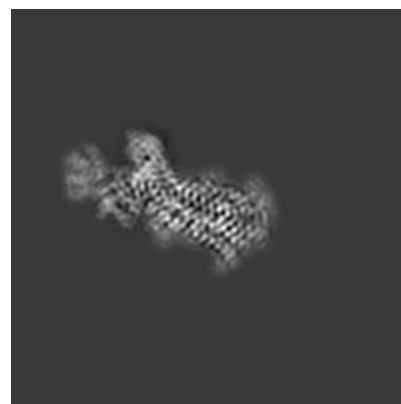
6.1.1 Primary map



X

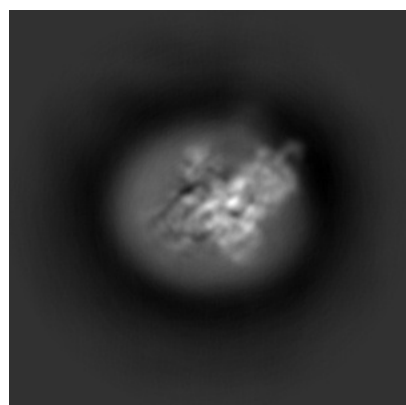


Y

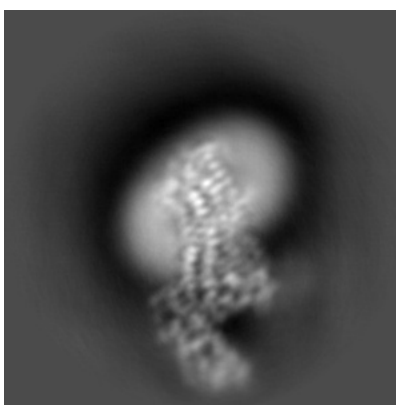


Z

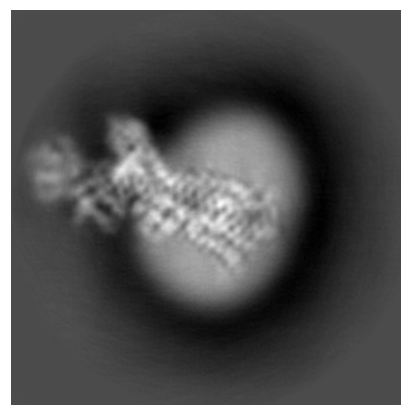
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

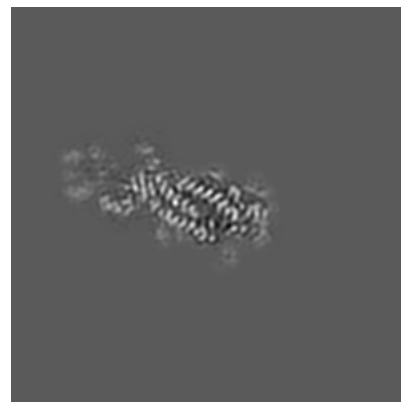
6.2.1 Primary map



X Index: 120

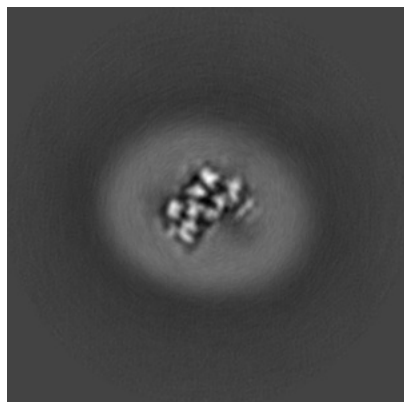


Y Index: 120

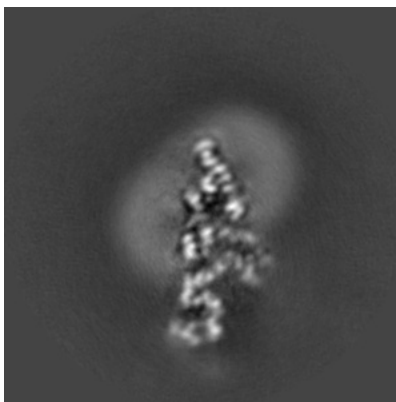


Z Index: 120

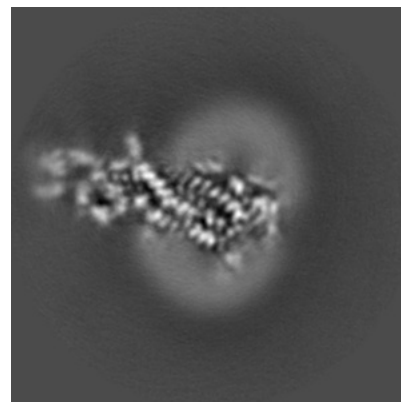
6.2.2 Raw map



X Index: 120



Y Index: 120



Z Index: 120

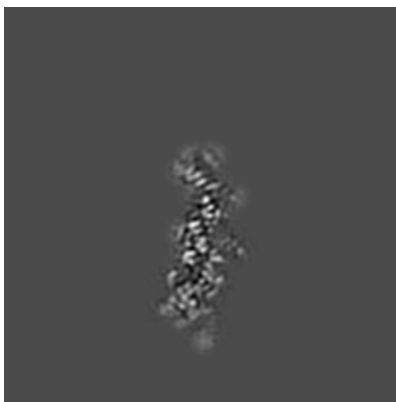
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

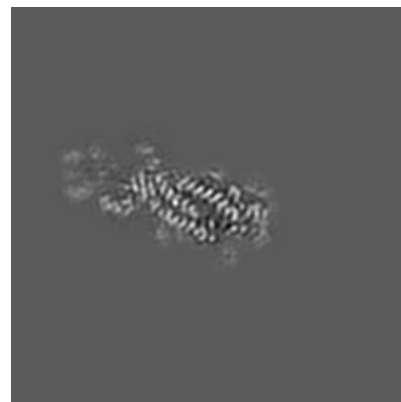
6.3.1 Primary map



X Index: 119

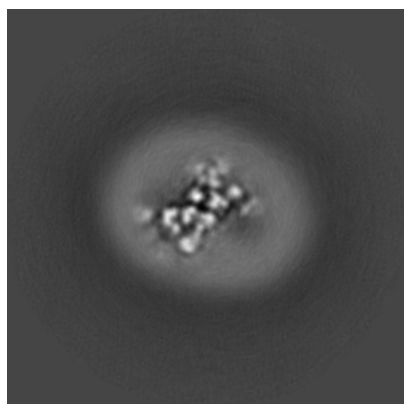


Y Index: 126

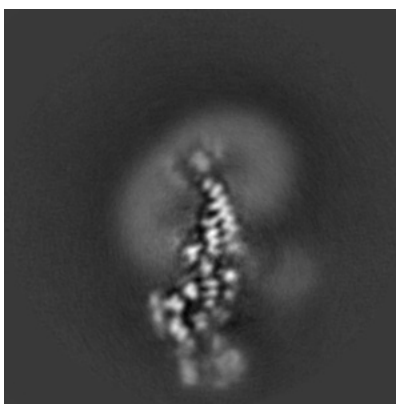


Z Index: 120

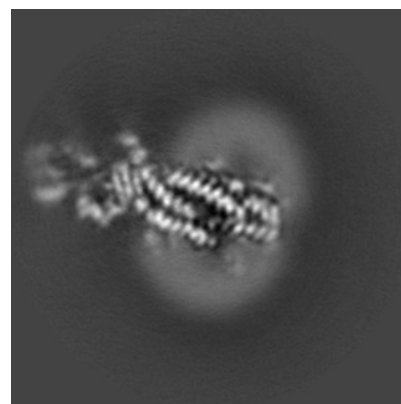
6.3.2 Raw map



X Index: 125



Y Index: 136

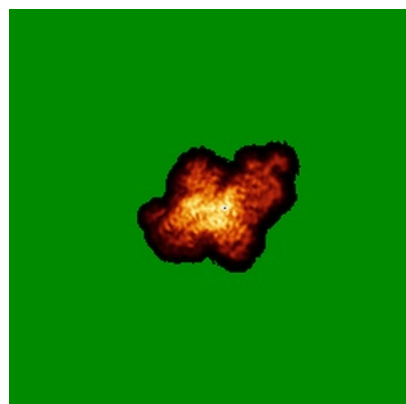


Z Index: 123

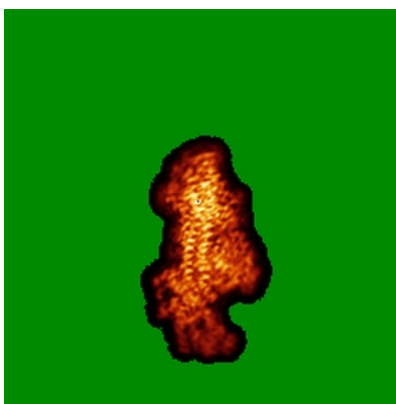
The images above show the largest variance slices of the map in three orthogonal directions.

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

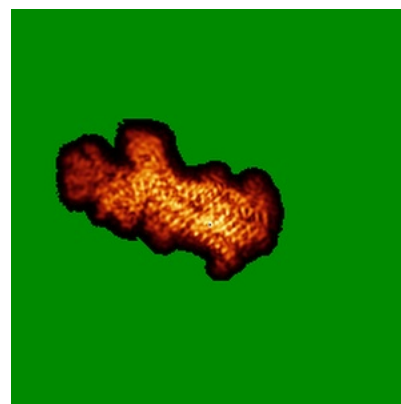
6.4.1 Primary map



X

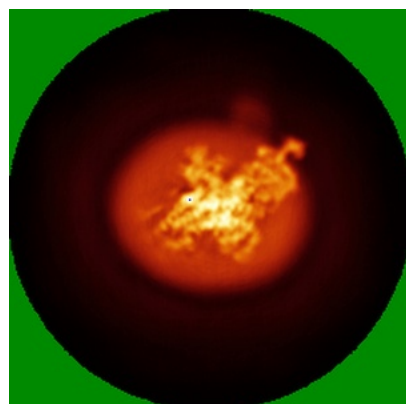


Y



Z

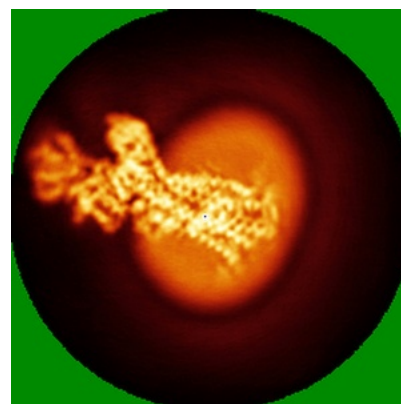
6.4.2 Raw map



X



Y

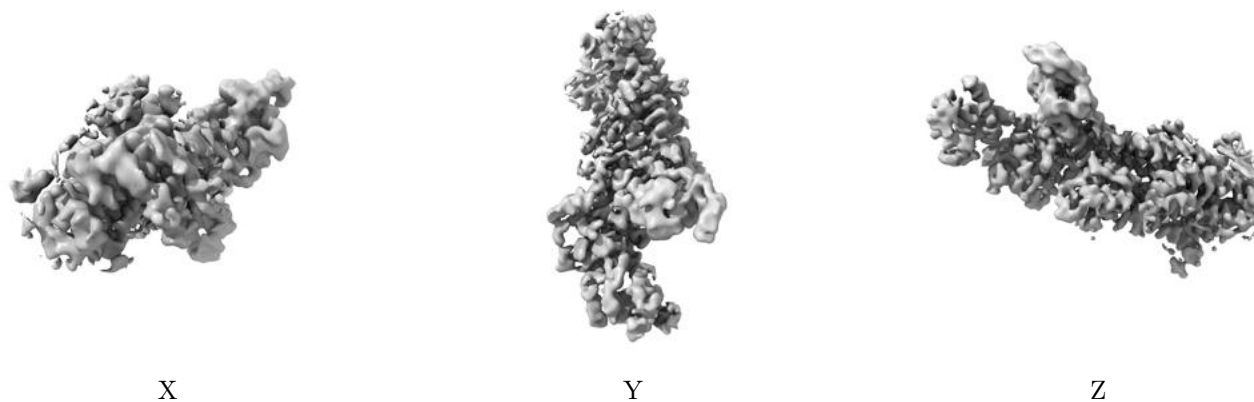


Z

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.

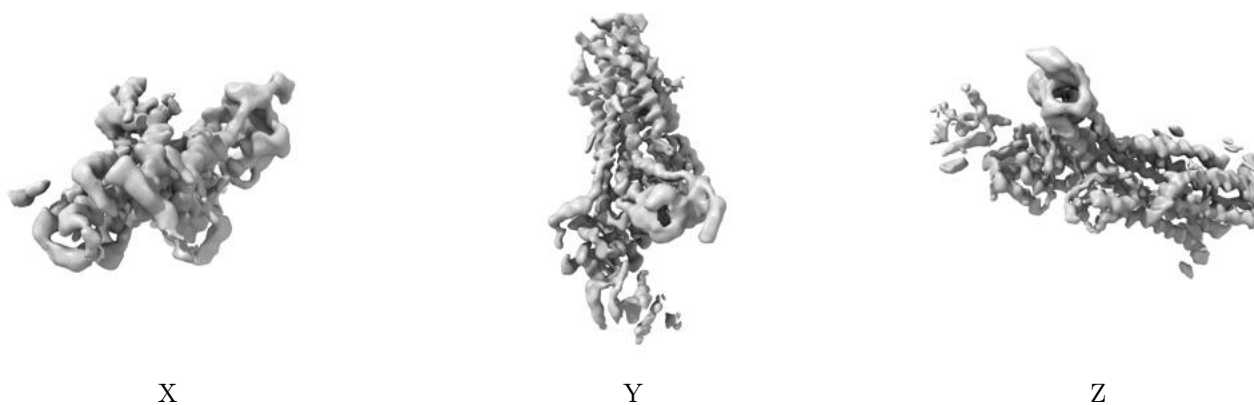
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.009. 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.

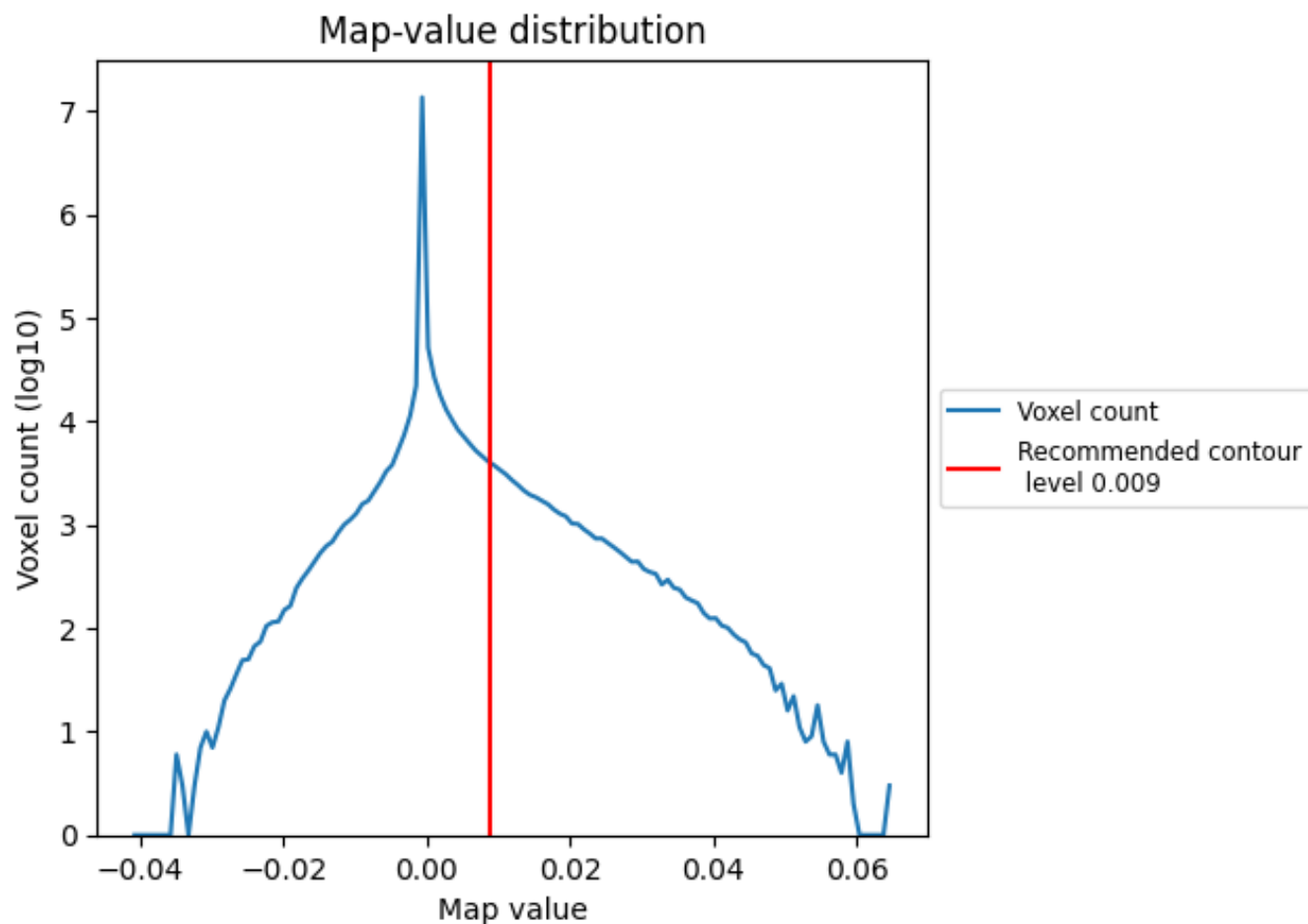
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

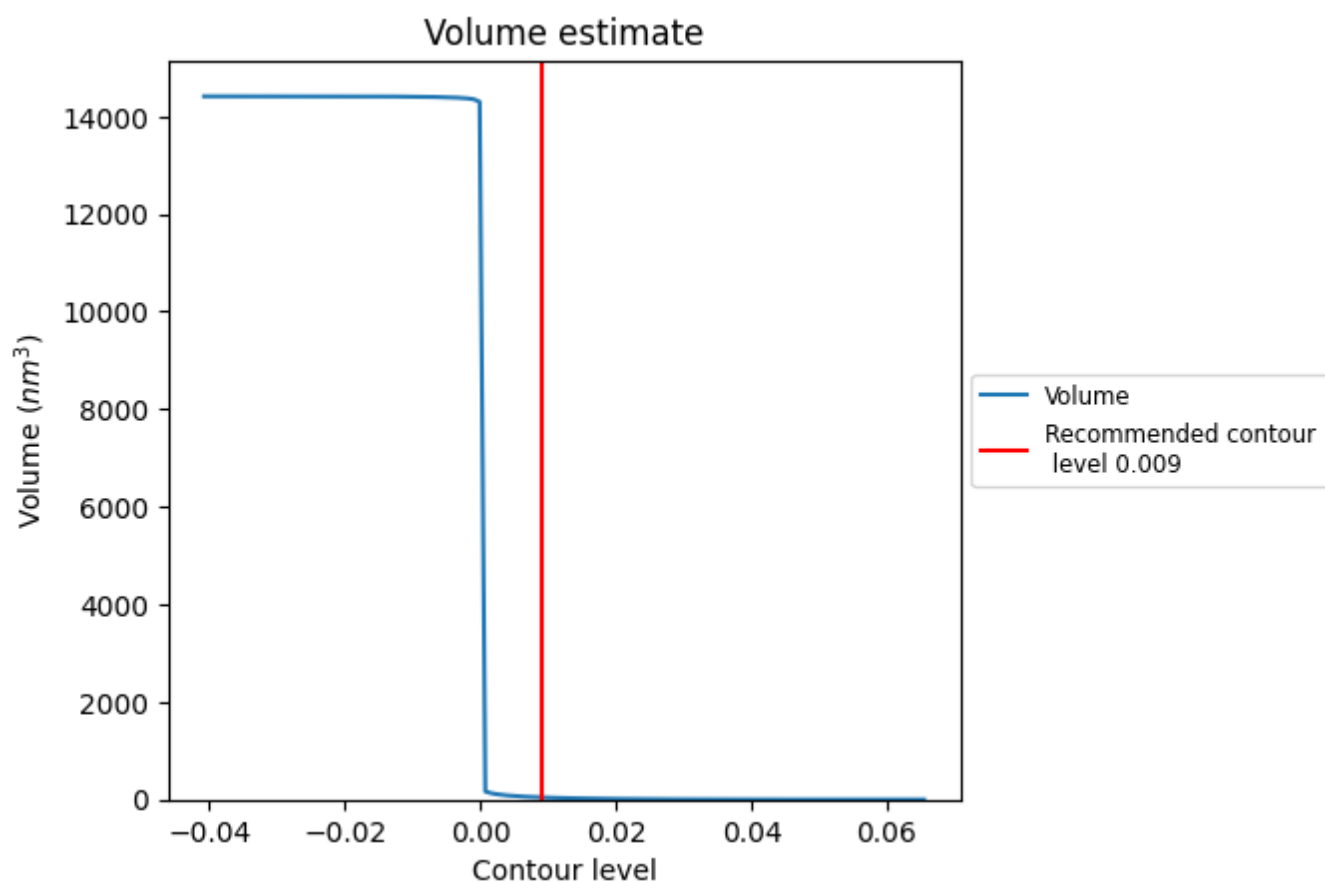
This section contains the results of statistical analysis of the map.

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.

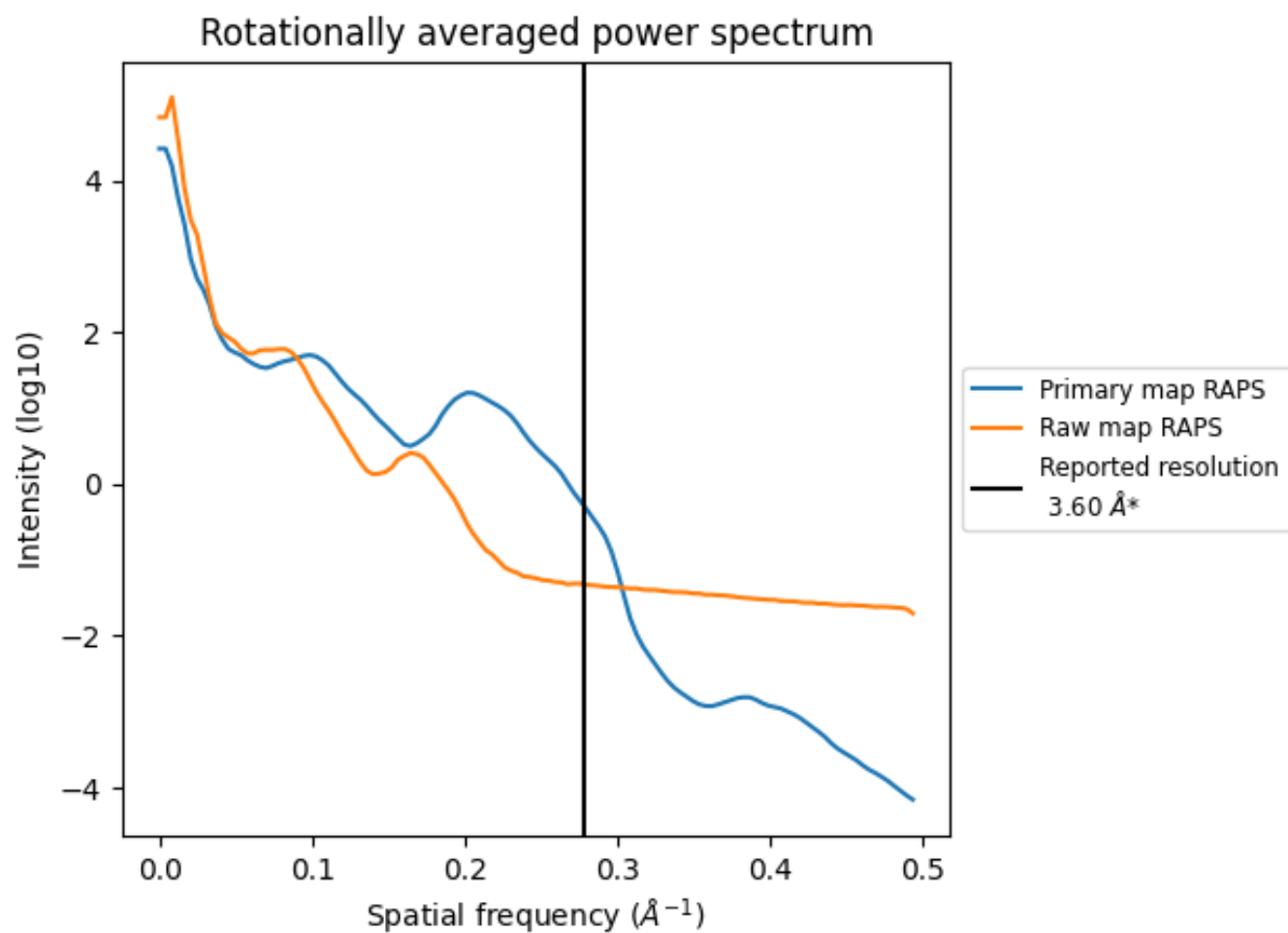
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 45 nm^3 ; this corresponds to an approximate mass of 40 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 ⓘ

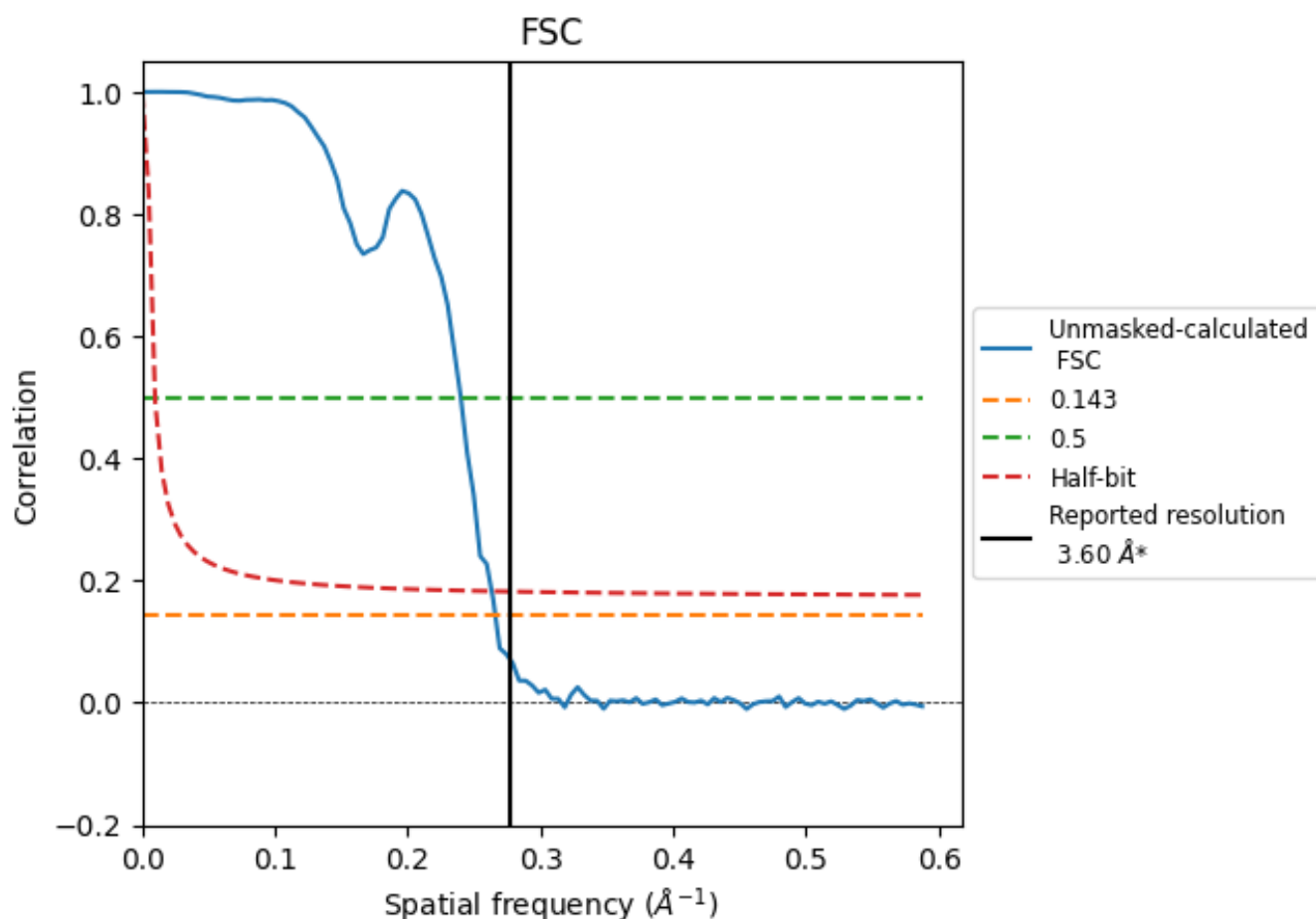


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

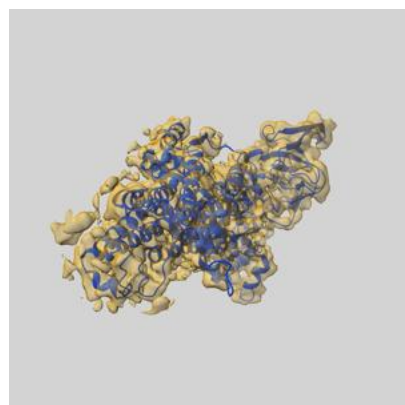
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.76	4.17	3.80

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

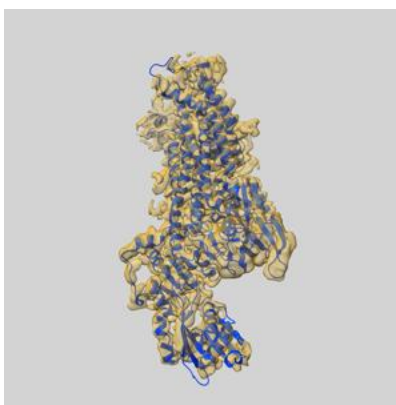
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33476 and PDB model 7XUO. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

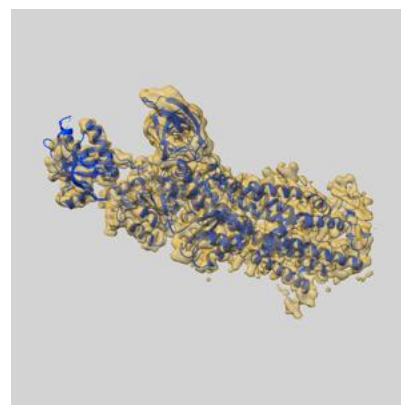
9.1 Map-model overlay [i](#)



X



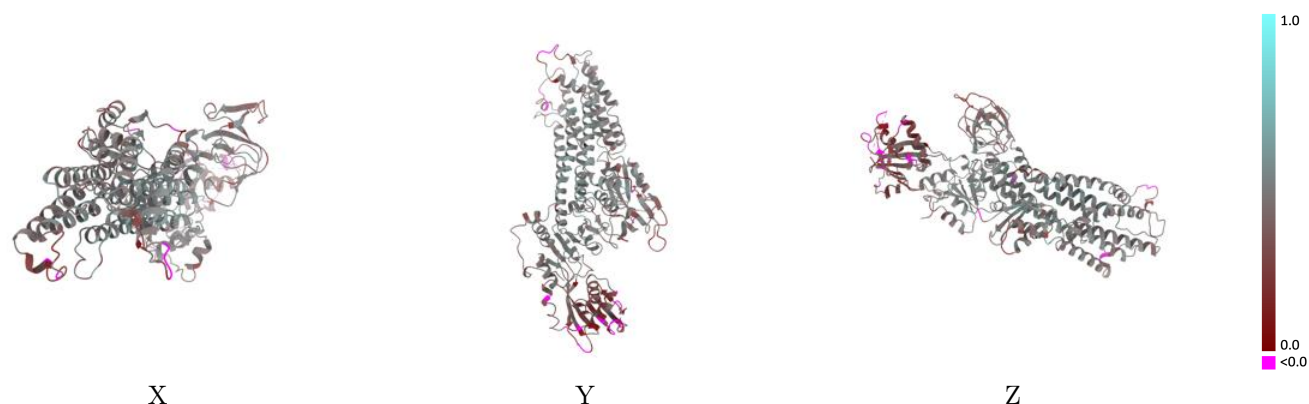
Y



Z

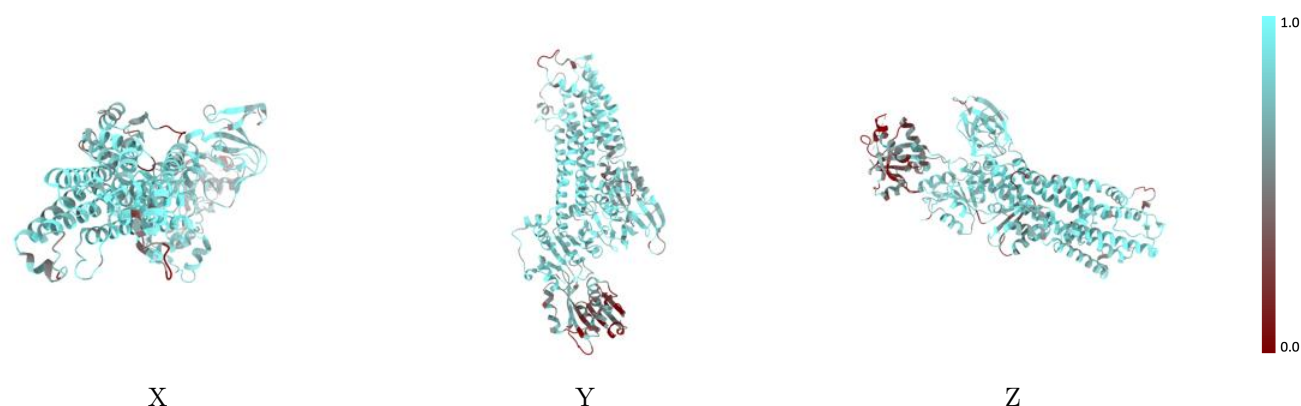
The images above show the 3D surface view of the map at the recommended contour level 0.009 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



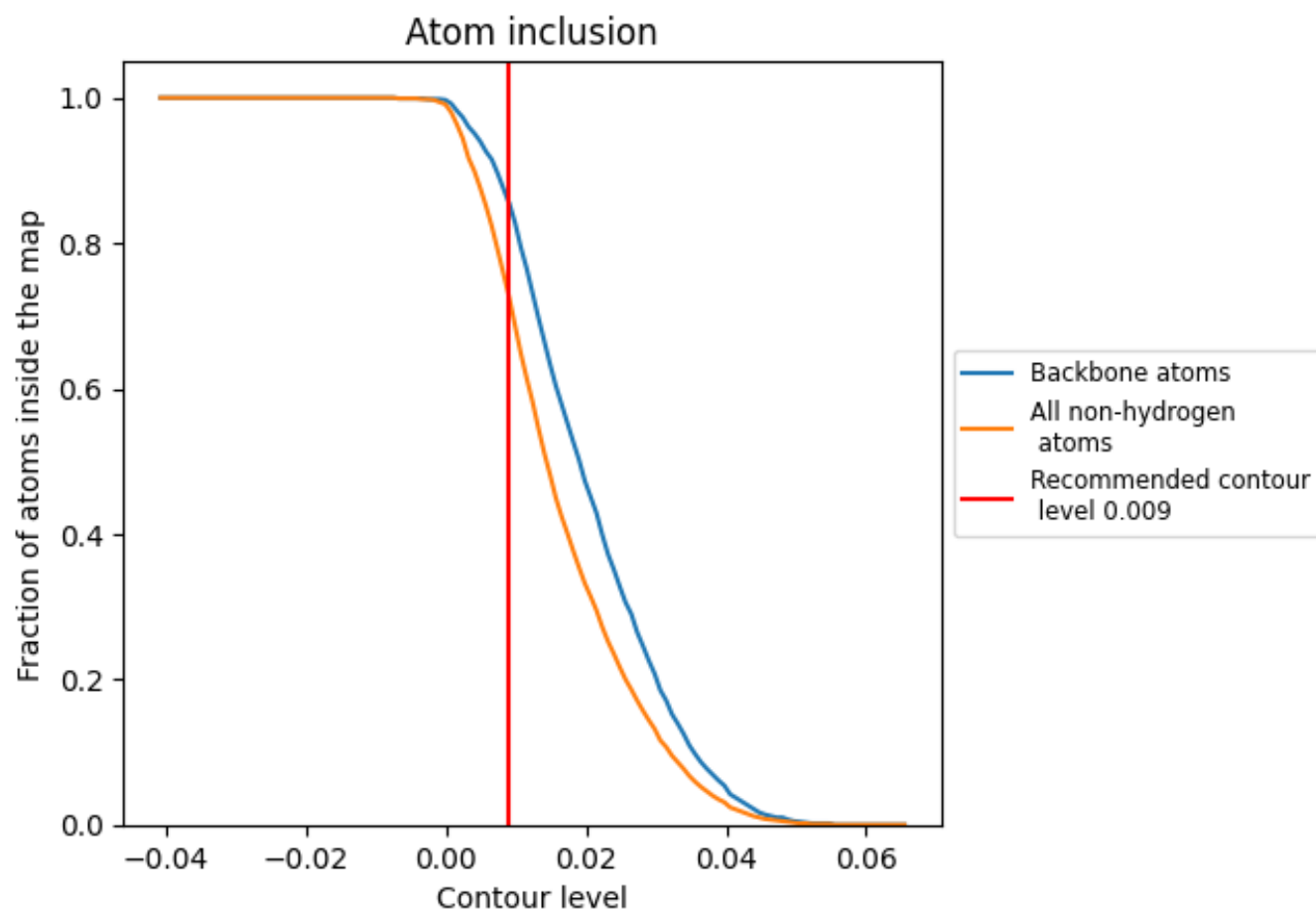
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.009).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 73% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7260	0.4130
A	0.7260	0.4130

