



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 08:02 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 Full wwPDB EM Validation 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

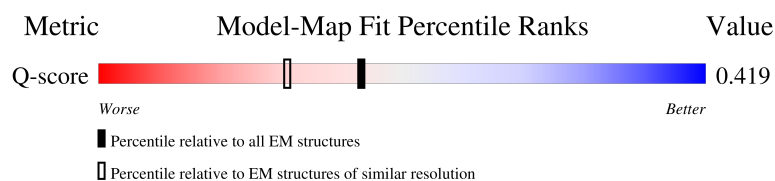
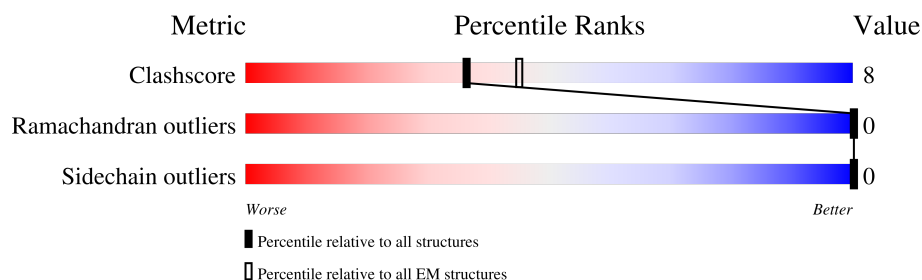
1 Overall quality at a glance

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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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

SER	HIS	VAL	TYR	I1284	D1164	C1104	V1039	S932
PRO	GLN	SER	SER	I1292	V1165	V1106	M1040	G943
GLU	GLU	VAL	GLN	D1296	S1166	S1107	R1041	F947
LYS	LYS	SER	SER	D1296	A1168	M1108	L1044	G948
GLY	GLY	SER	SER	S1310	D1171	E1110	L1045	Q951
GLY	GLY	SER	LEU	I1311	H1172	G1111	G1046	P955
GLY	GLY	LEU	THR	H1312	E1173	I1112	D1047	N956
GLY	GLY	THR	THR	H1312	M1174	L1113	V1048	P957
SER	SER	SER	SER	K1315	K1175	A1114	A1049	N958
GLY	GLY	ASP	ASP	M1324	T1178	H1115	T1050	K959
GLY	GLY	PRO	PRO	L1325	A1179	SER	L1051	H960
ALA	ALA	SER	SER	I1336	I1180	GLU	R1054	I967
TRP	TRP	ARG	ARG	P1337	L1181	ARG	K1055	I968
SER	SER	HIS	HIS	M1344	V1182	PRO		R969
HIS	PRO	ALA	ALA	M1344	A1183	SER		Q973
GLN	ALA	ALA	ALA	M1359	I1184	PRO	A1058	I976
PHE	ALA	ALA	ASP	M1359	D1185	ALA	G1061	L979
GLU	GLU	ASP	ASP	L1371	G1186	SER	T1062	S983
LYS	LYS	ASP	ASP	D1380	V1187	ALA	A1063	S986
	GLY	GLY	GLY	R1383	L1188	HIS	E1064	A990
	LYS	ASP	ASP	R1383	C1189	LEU	A1065	H996
	TRP	TRP	TRP	G1190	G1190	ASN	S1066	L1008
	SER	SER	SER	Q1387	M1191	ALA	GLY	T1009
	LEU	LEU	LEU		I1192	GLY	S1067	G1011
	LEU	LEU	LEU	H1391	A1195	SER	E1068	P1014
	ASN	ASN	ASN	M1392	V1206	PRO	L1071	L1015
	GLY	GLY	GLY	K1393		ALA	A1074	E1016
	ARG	ARG	ARG	P1394	L1209	LYS	E1082	M1017
	ASP	ASP	ASP	L1395	V1216	ASP	L1075	A1018
	GLU	GLU	GLU	T1396		ALA	T1076	H1019
	GLN	GLN	GLN	A1397		VAL	K1077	K1020
	TYR	TYR	TYR	H1403	N1223	PRO	Y1078	I1021
	ILE	VAL	VAL	I1404		GLN	C1079	V1024
	ASP	ASP	ASP	G1405	R1228	THR	K1080	M1025
	GLU	LEU	GLU	MEI	Q1233	F1144	E1081	K1028
	THR	THR	THR	ASP	V1234	S1145	E1082	
	SER	SER	SER	ARG		V1146	L1083	
	ARG	ARG	ARG	TRP	F1240	L1147	G1084	
	GLY	ARG	GLY	TRP		I1148	T1085	
	ASP	ASP	ASP	ASP	K1248	G1149	E1086	
	TYR	TYR	TYR	PRO	K1251	M1150	T1087	
	LYS	LYS	LYS	ARG	V1252	R1151	L1088	
	ASP	ASP	ASP	ALA	Q1253	E1152	G1089	
	ASP	ASP	ASP	THR	E1254	W1153	Y1090	
	ASP	ASP	ASP	THR		L1154	C1091	
	ASP	TRP	TRP	PRO	A1263	R1155	T1092	
	LYS	LYS	LYS	ASP	M1264	R1156	D1093	
TRP	TRP	VAL	VAL	GLN		M1157	F1094	
	SER	SER	SER	SER	D1267	G1158	Q1095	
					Q1277	L1159	A1096	
					G1281	T1160	V1097	
						I1161	P1098	
						S1162	G1099	
						S1163	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 ($\text{\AA}$)	243.36002, 243.36002, 243.36002	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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.

All (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:MET:HE3	1:A:695:LEU:HD22	1.78	0.64
1:A:1037:PRO:HG3	1:A:1071:LEU:HA	1.81	0.63
1:A:1032:ILE:HD11	1:A:1234:VAL:HG11	1.81	0.63
1:A:851:MET:SD	1:A:880:HIS:ND1	2.71	0.63
1:A:833:VAL:O	1:A:882:SER:HA	1.99	0.62
1:A:613:ILE:HD12	1:A:618:ILE:HD11	1.81	0.62
1:A:902:LEU:HD11	1:A:1010:LYS:HE2	1.82	0.62
1:A:594:TYR:HB3	1:A:607:LYS:HG2	1.83	0.60
1:A:1040:MET:HE3	1:A:1195:ALA:HB3	1.83	0.60
1:A:842:ASP:OD1	1:A:874:ALA:N	2.34	0.59
1:A:1010:LYS:NZ	1:A:1292:ILE:O	2.35	0.59
1:A:1228:ARG:NH1	1:A:1397:ALA:O	2.35	0.59
1:A:1102:ILE:HG13	1:A:1148:ILE:HB	1.86	0.57
1:A:1061:GLY:HA2	1:A:1076:THR:HG22	1.87	0.57
1:A:1014:PRO:HA	1:A:1017:MET:HB3	1.86	0.57
1:A:579:VAL:HG23	1:A:597:VAL:HG13	1.86	0.56
1:A:1173:GLU:OE2	1:A:1223:ASN:ND2	2.38	0.55
1:A:1253:GLN:OE1	1:A:1277:GLN:NE2	2.40	0.54
1:A:1097:VAL:HB	1:A:1100:CYS:HB2	1.89	0.54
1:A:1146:VAL:HG22	1:A:1184:ILE:HG12	1.89	0.54
1:A:1024:VAL:HG11	1:A:1209:LEU:HD13	1.90	0.54
1:A:858:THR:OG1	1:A:860:GLU:OE1	2.22	0.54
1:A:1281:GLY:N	1:A:1296:ASP:OD1	2.39	0.54
1:A:766:THR:OG1	1:A:767:PRO:HD3	2.08	0.53
1:A:1038:ARG:HE	1:A:1039:VAL:H	1.56	0.53
1:A:1019:HIS:O	1:A:1315:LYS:NZ	2.42	0.53
1:A:744:SER:HB2	1:A:763:PHE:H	1.74	0.52
1:A:564:GLY:HA3	1:A:610:PRO:HG3	1.93	0.51
1:A:763:PHE:HZ	1:A:973:GLN:HB2	1.75	0.51
1:A:1025:MET:HG2	1:A:1264:MET:HG3	1.92	0.51
1:A:1100:CYS:SG	1:A:1156:ARG:NH2	2.84	0.51
1:A:1042:VAL:HG13	1:A:1192:ILE:HG13	1.92	0.51
1:A:1171:ASP:OD1	1:A:1172:HIS:N	2.42	0.51
1:A:906:ALA:HA	1:A:1011:GLY:H	1.76	0.51
1:A:845:VAL:HA	1:A:885:ILE:HG22	1.93	0.50
1:A:943:GLY:HA3	1:A:967:ILE:HG21	1.93	0.50
1:A:1018:ALA:HA	1:A:1021:ILE:HD12	1.94	0.50
1:A:1182:VAL:HG13	1:A:1189:CYS:HB2	1.92	0.49
1:A:719:TYR:OH	1:A:723:ARG:NH1	2.45	0.49
1:A:851:MET:SD	1:A:851:MET:N	2.86	0.49
1:A:969:ARG:NH2	1:A:973:GLN:OE1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1028:LYS:HA	1:A:1032:ILE:HG22	1.95	0.48
1:A:766:THR:O	1:A:770:LEU:N	2.46	0.48
1:A:983:SER:HB3	1:A:1359:MET:HG2	1.96	0.48
1:A:744:SER:OG	1:A:762:THR:HB	2.14	0.48
1:A:1174:MET:HE3	1:A:1174:MET:HA	1.95	0.48
1:A:1181:LEU:HD21	1:A:1188:LEU:HD11	1.96	0.47
1:A:1251:LYS:O	1:A:1254:GLU:HG3	2.14	0.47
1:A:827:ARG:NE	1:A:888:THR:O	2.48	0.47
1:A:600:ALA:HB1	1:A:996:MET:HE1	1.97	0.47
1:A:1054:ARG:HD2	1:A:1083:LEU:HD22	1.95	0.47
1:A:688:ILE:HG13	1:A:689:ILE:N	2.30	0.47
1:A:1054:ARG:HH22	1:A:1115:HIS:HB2	1.81	0.46
1:A:1162:SER:O	1:A:1166:SER:OG	2.22	0.46
1:A:1079:CYS:HA	1:A:1082:GLU:HG2	1.98	0.45
1:A:1344:MET:HE3	1:A:1344:MET:O	2.16	0.45
1:A:739:ILE:HG22	1:A:976:ILE:HD11	1.99	0.44
1:A:595:ALA:HB2	1:A:606:VAL:HG13	2.00	0.43
1:A:1154:LEU:HD22	1:A:1159:LEU:HD22	2.00	0.43
1:A:638:ALA:O	1:A:642:ASP:HB2	2.18	0.43
1:A:932:SER:OG	1:A:979:LEU:HD23	2.18	0.43
1:A:727:ALA:HB1	1:A:731:VAL:HG21	2.01	0.43
1:A:787:LYS:HB2	1:A:1371:LEU:HD11	2.01	0.42
1:A:1055:LYS:HB2	1:A:1113:LEU:HD21	2.01	0.42
1:A:721:SER:HB2	1:A:728:ASN:OD1	2.19	0.42
1:A:1031:THR:HG23	1:A:1284:ILE:HG21	2.02	0.42
1:A:848:GLY:N	1:A:868:PRO:HG3	2.34	0.42
1:A:1021:ILE:HD13	1:A:1263:ALA:HB2	2.00	0.42
1:A:1078:TYR:O	1:A:1081:GLU:HG3	2.19	0.42
1:A:1092:THR:HG23	1:A:1105:LYS:HB3	2.01	0.42
1:A:1240:PHE:HA	1:A:1403:HIS:HB3	2.02	0.42
1:A:1312:HIS:O	1:A:1312:HIS:ND1	2.51	0.42
1:A:948:GLY:O	1:A:951:GLN:HG3	2.20	0.42
1:A:841:VAL:HG11	1:A:890:VAL:HG22	2.01	0.42
1:A:1310:SER:OG	1:A:1311:ILE:N	2.52	0.42
1:A:862:MET:HA	1:A:863:PRO:HD3	1.91	0.42
1:A:844:LYS:HB3	1:A:844:LYS:HE3	1.81	0.41
1:A:990:ALA:HB1	1:A:1324:ASN:HB3	2.01	0.41
1:A:1184:ILE:HD12	1:A:1189:CYS:SG	2.60	0.41
1:A:799:GLN:HB3	1:A:896:LEU:HD23	2.02	0.41
1:A:983:SER:OG	1:A:986:SER:OG	2.26	0.41
1:A:1008:LEU:HD23	1:A:1008:LEU:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1171:ASP:O	1:A:1175:LYS:HG3	2.21	0.41
1:A:1336:ILE:HB	1:A:1337:PRO:HD3	2.03	0.41
1:A:1181:LEU:HD12	1:A:1190:GLY:O	2.20	0.41
1:A:1206:VAL:HG23	1:A:1216:VAL:HG21	2.03	0.41
1:A:803:ALA:HB2	1:A:822:MET:HE1	2.04	0.40
1:A:850:THR:OG1	1:A:851:MET:N	2.54	0.40
1:A:662:ILE:HD13	1:A:662:ILE:HA	1.97	0.40
1:A:1380:ASP:OD1	1:A:1383:ARG:N	2.49	0.40
1:A:622:ILE:HG21	1:A:629:ALA:HB2	2.04	0.40
1:A:1325:LEU:HD23	1:A:1325:LEU:HA	1.84	0.40

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. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	640	HIS
1	A	707	GLN
1	A	717	GLN
1	A	728	ASN
1	A	889	HIS
1	A	914	GLN
1	A	958	ASN
1	A	1200	GLN
1	A	1210	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](#)

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.

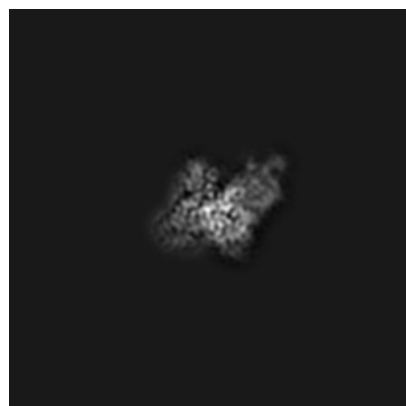
6 Map visualisation [i](#)

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.

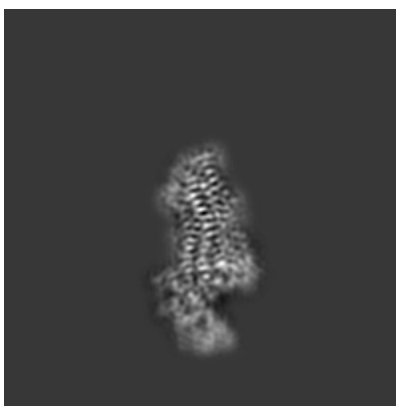
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

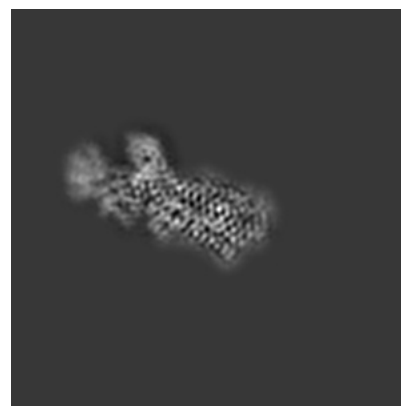
6.1.1 Primary map



X

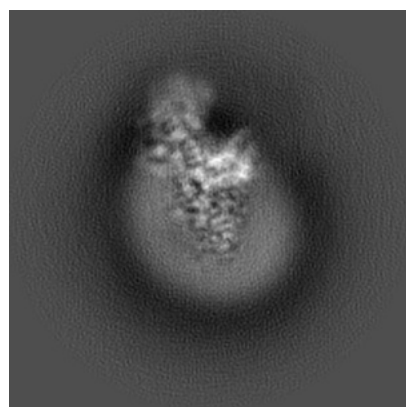


Y

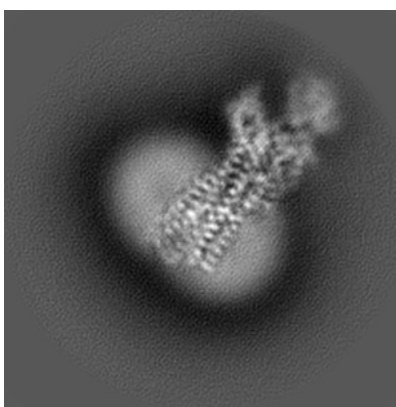


Z

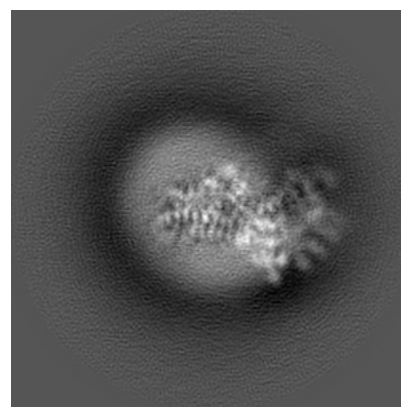
6.1.2 Raw map



X



Y

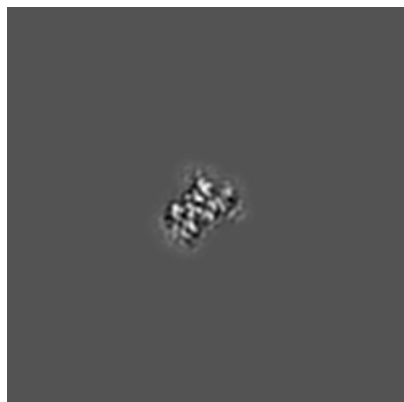


Z

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

6.2 Central slices [i](#)

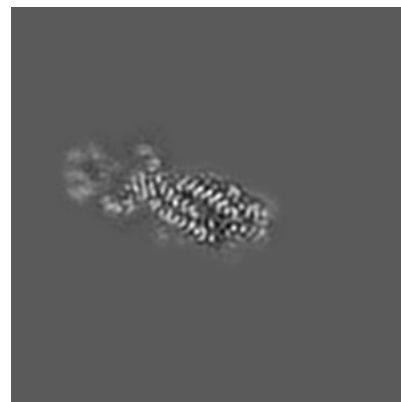
6.2.1 Primary map



X Index: 120

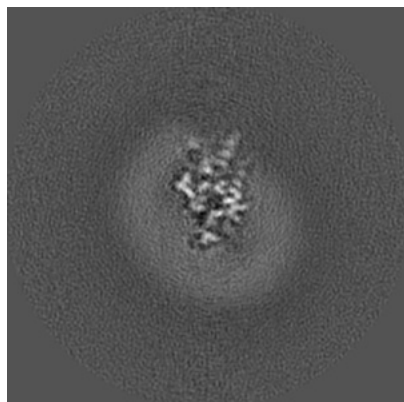


Y Index: 120

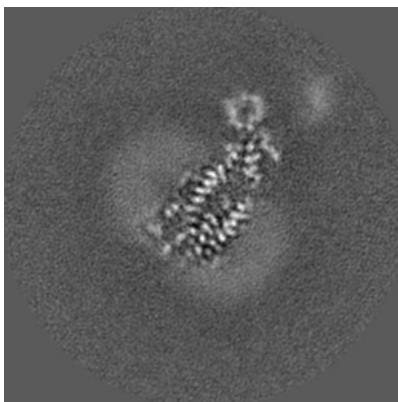


Z Index: 120

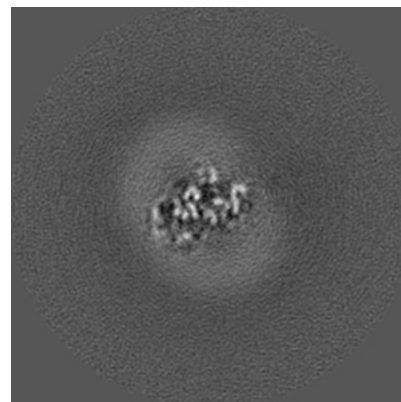
6.2.2 Raw map



X Index: 105



Y Index: 105

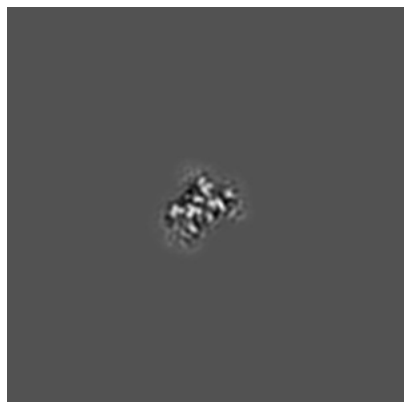


Z Index: 105

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

6.3 Largest variance slices [i](#)

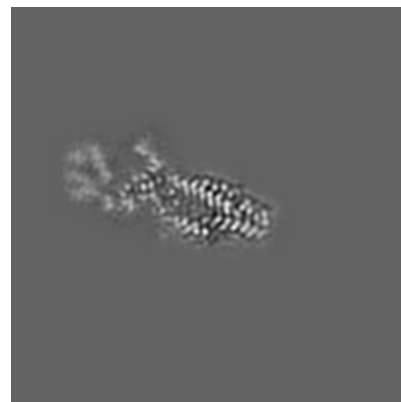
6.3.1 Primary map



X Index: 119

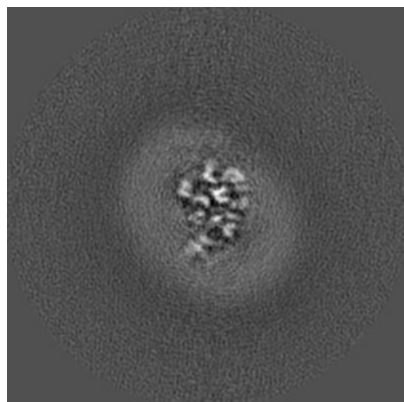


Y Index: 121

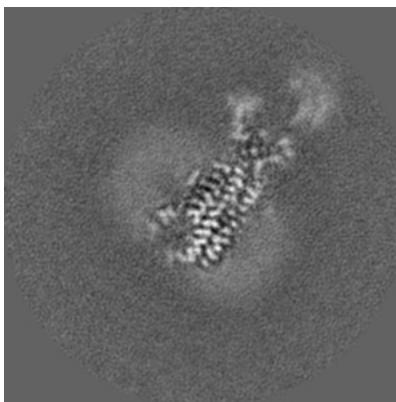


Z Index: 122

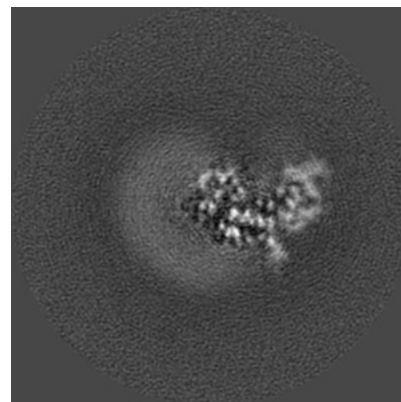
6.3.2 Raw map



X Index: 100



Y Index: 101

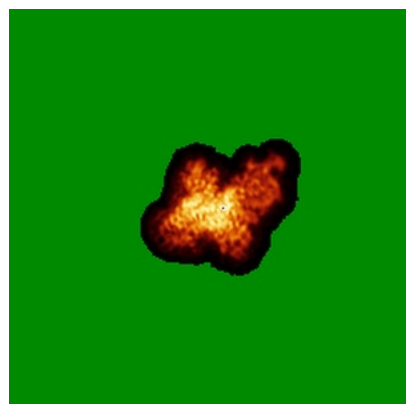


Z Index: 123

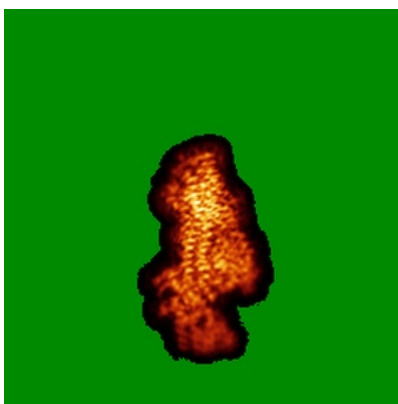
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

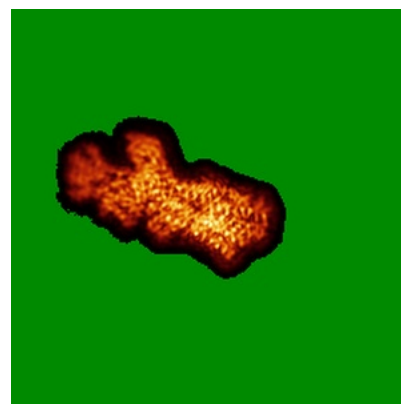
6.4.1 Primary map



X

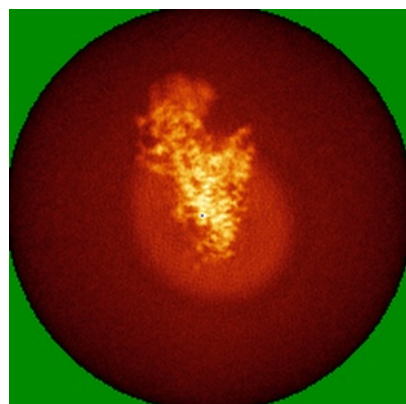


Y

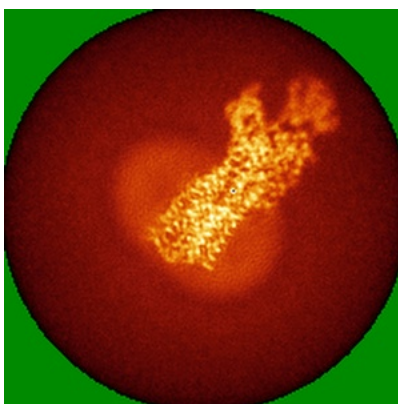


Z

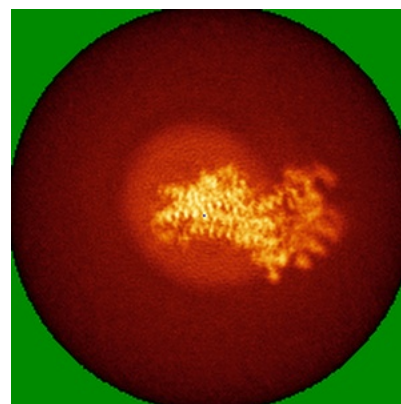
6.4.2 Raw map



X



Y

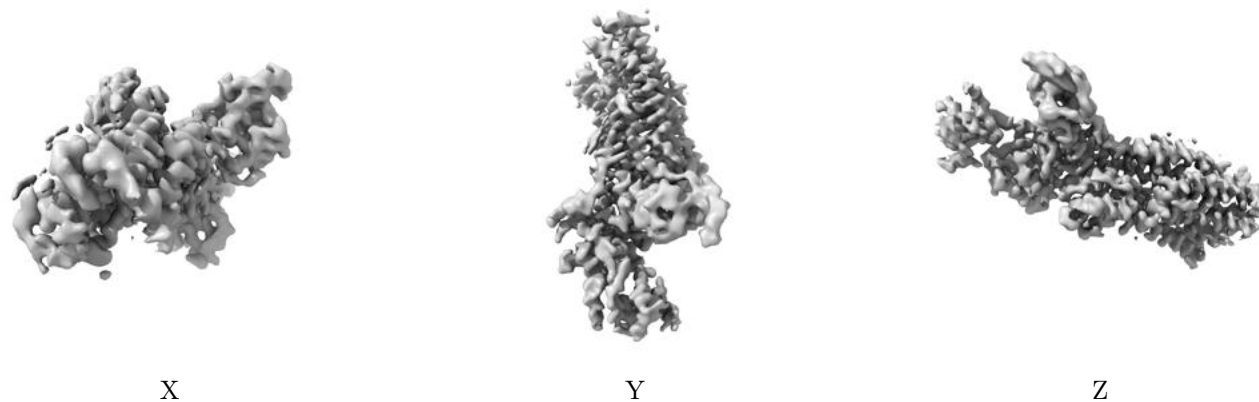


Z

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.

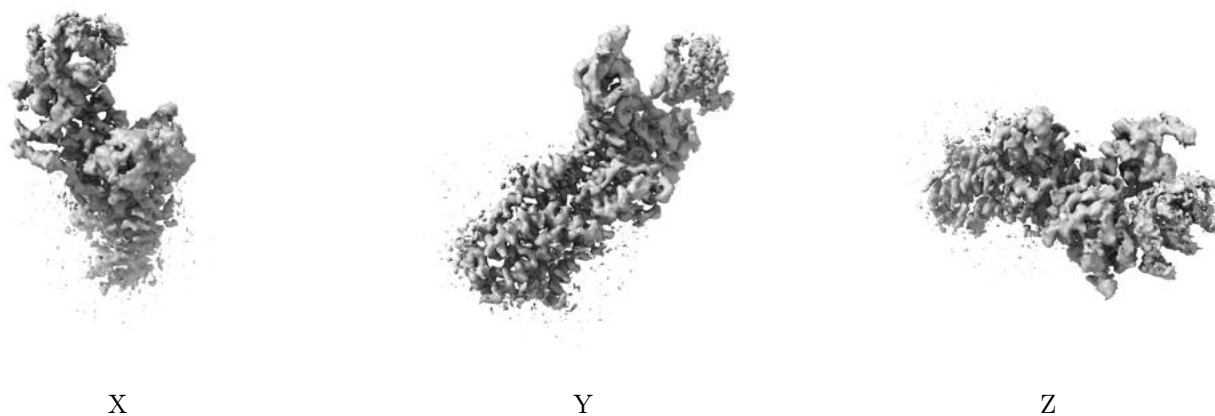
6.5 Orthogonal surface views [i](#)

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.

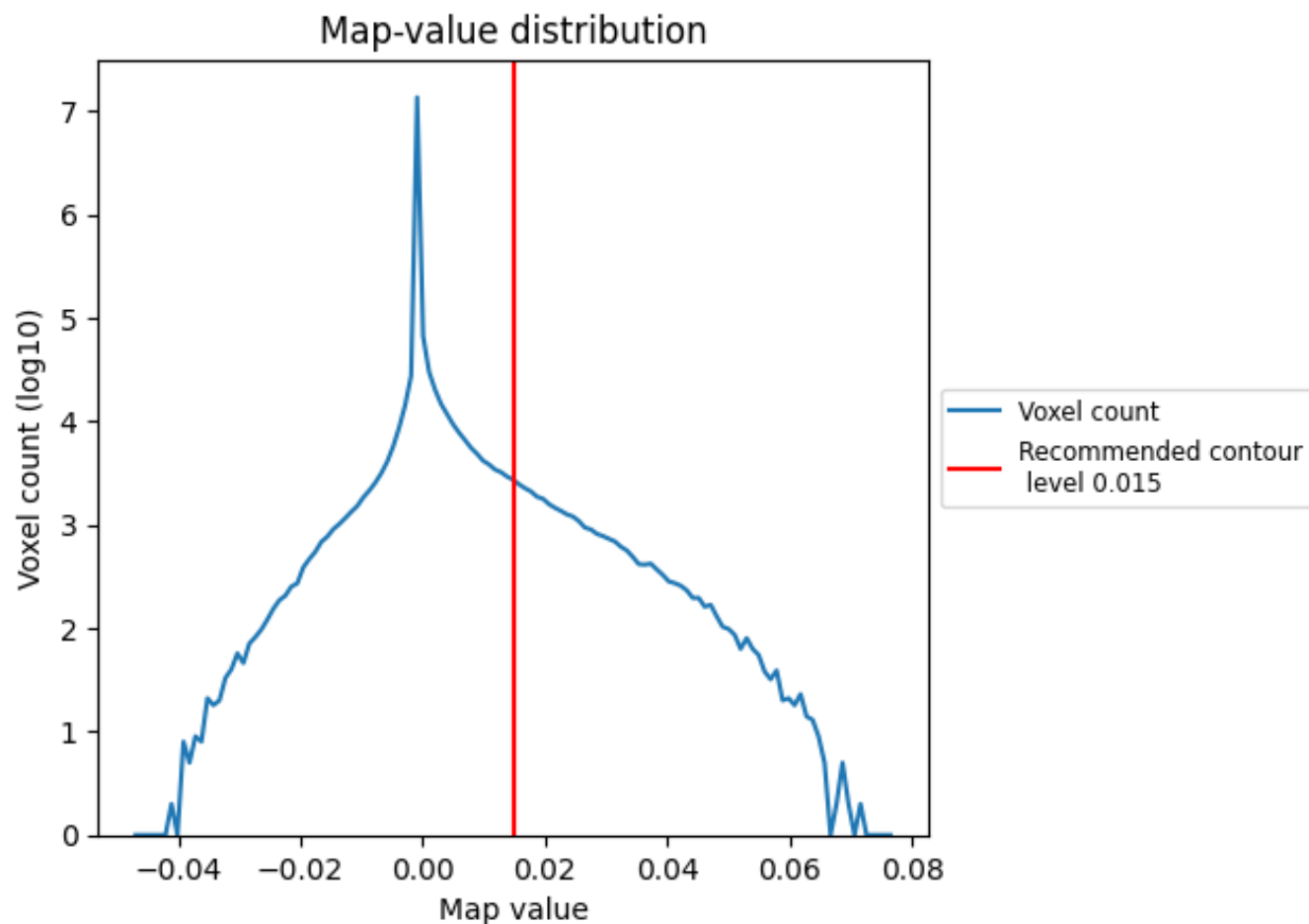
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

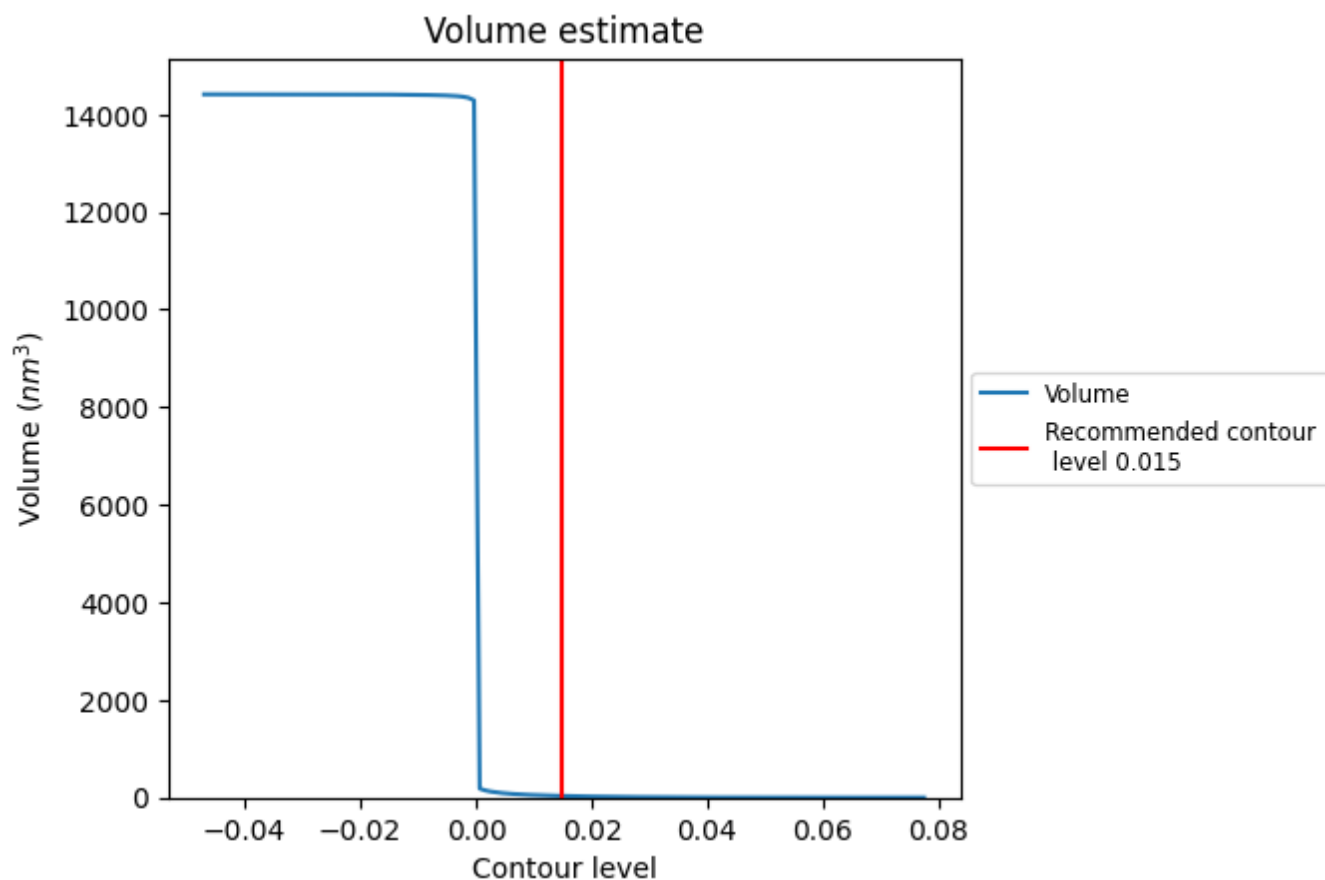
This section contains the results of statistical analysis of the map.

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.

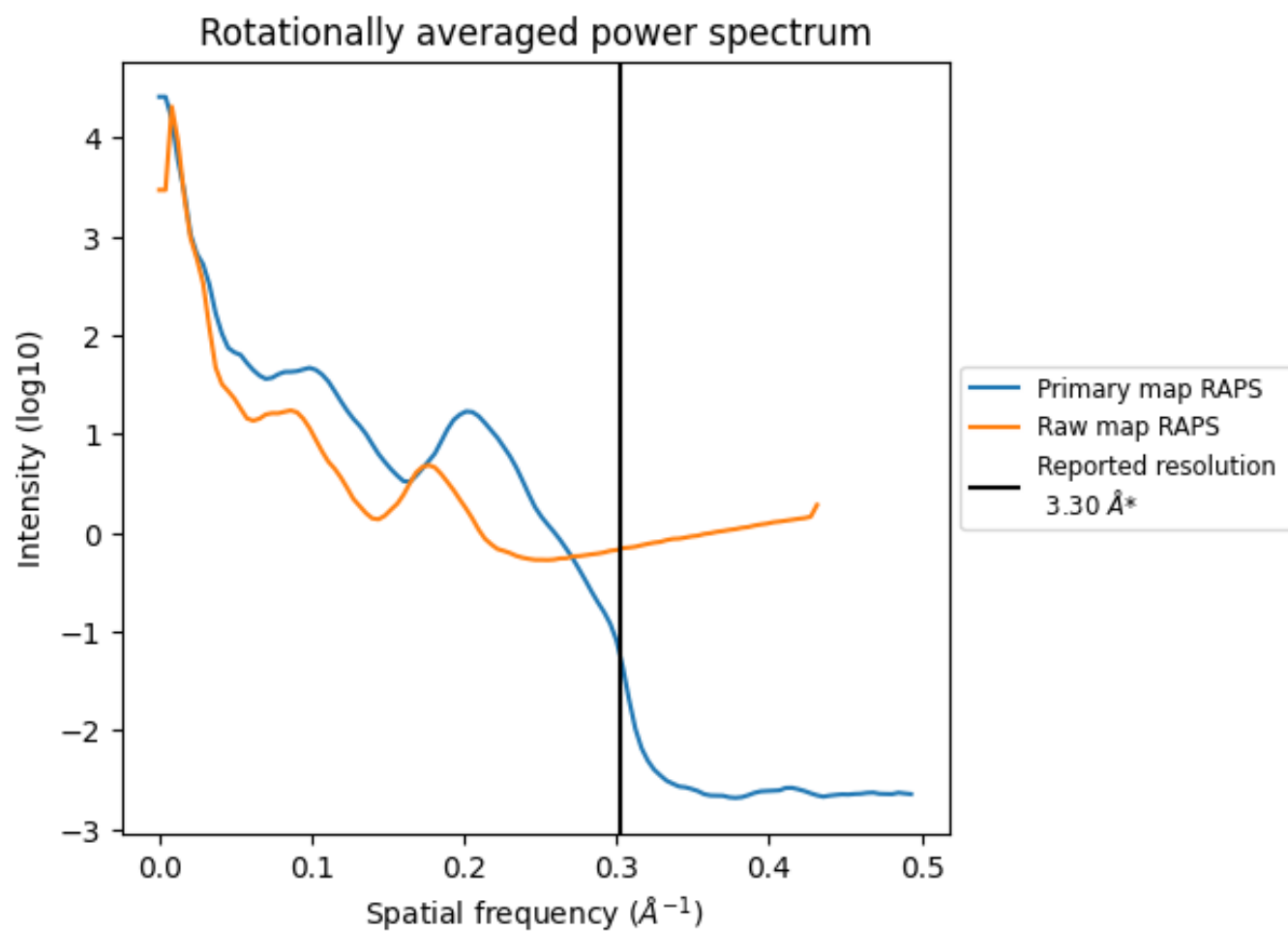
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 33 nm³; 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 ⓘ

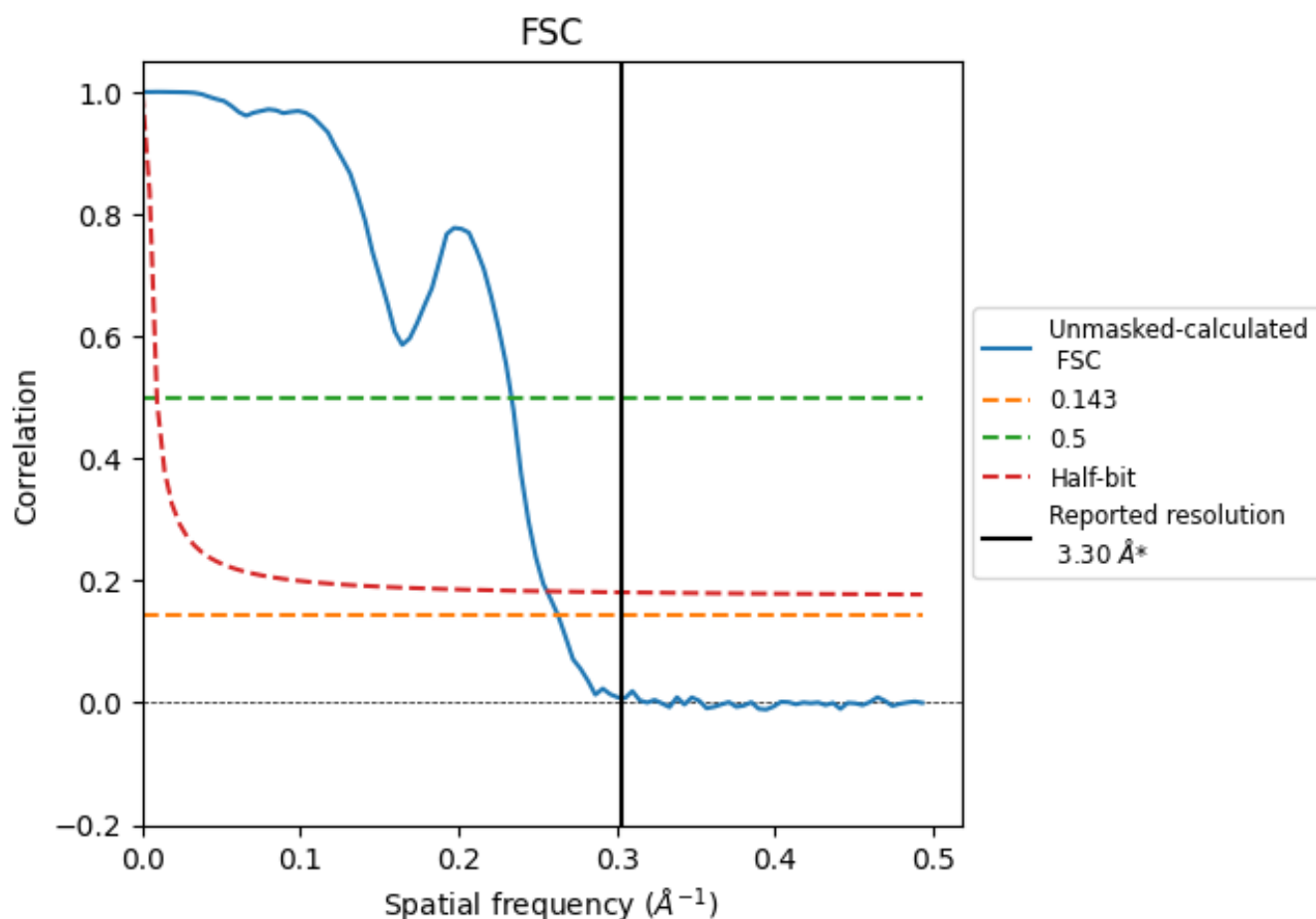


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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

8.2 Resolution estimates [i](#)

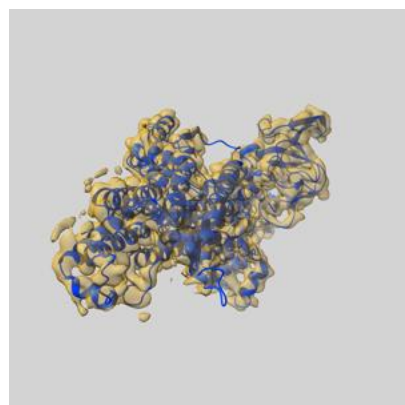
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.80	4.28	3.91

*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 %

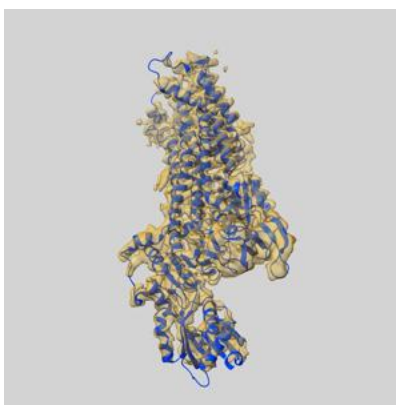
9 Map-model fit [i](#)

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](#).

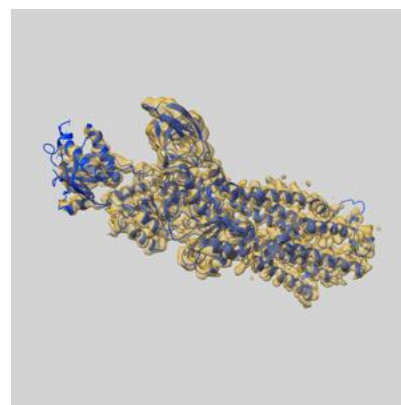
9.1 Map-model overlay [i](#)



X



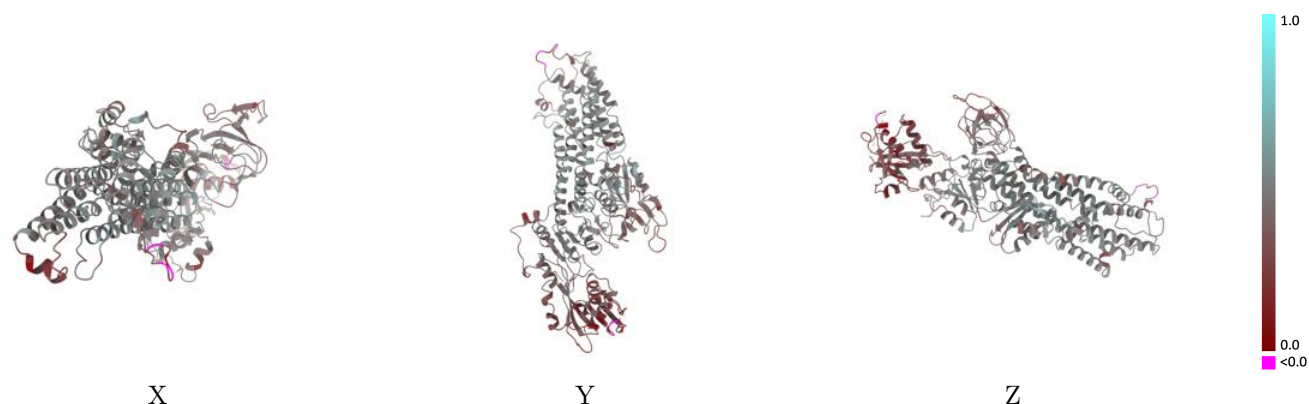
Y



Z

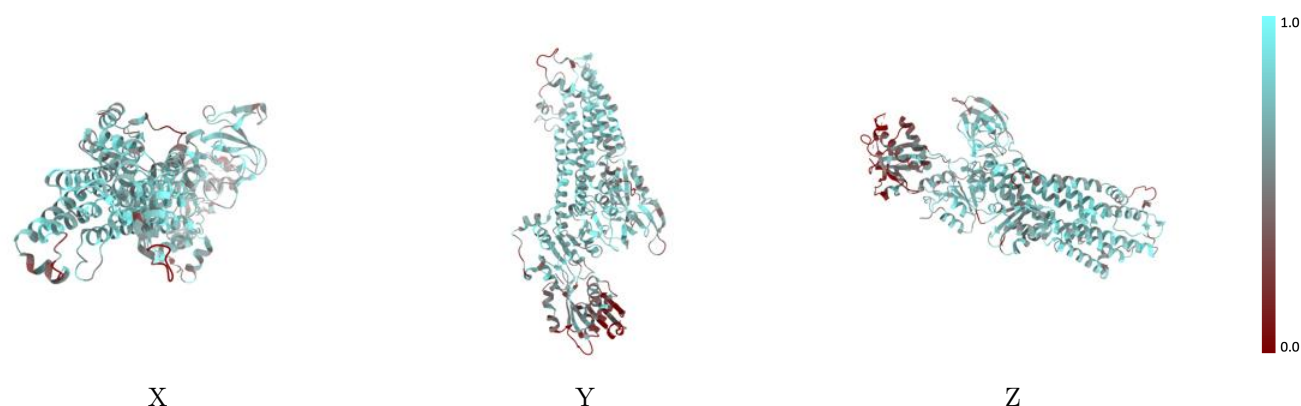
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



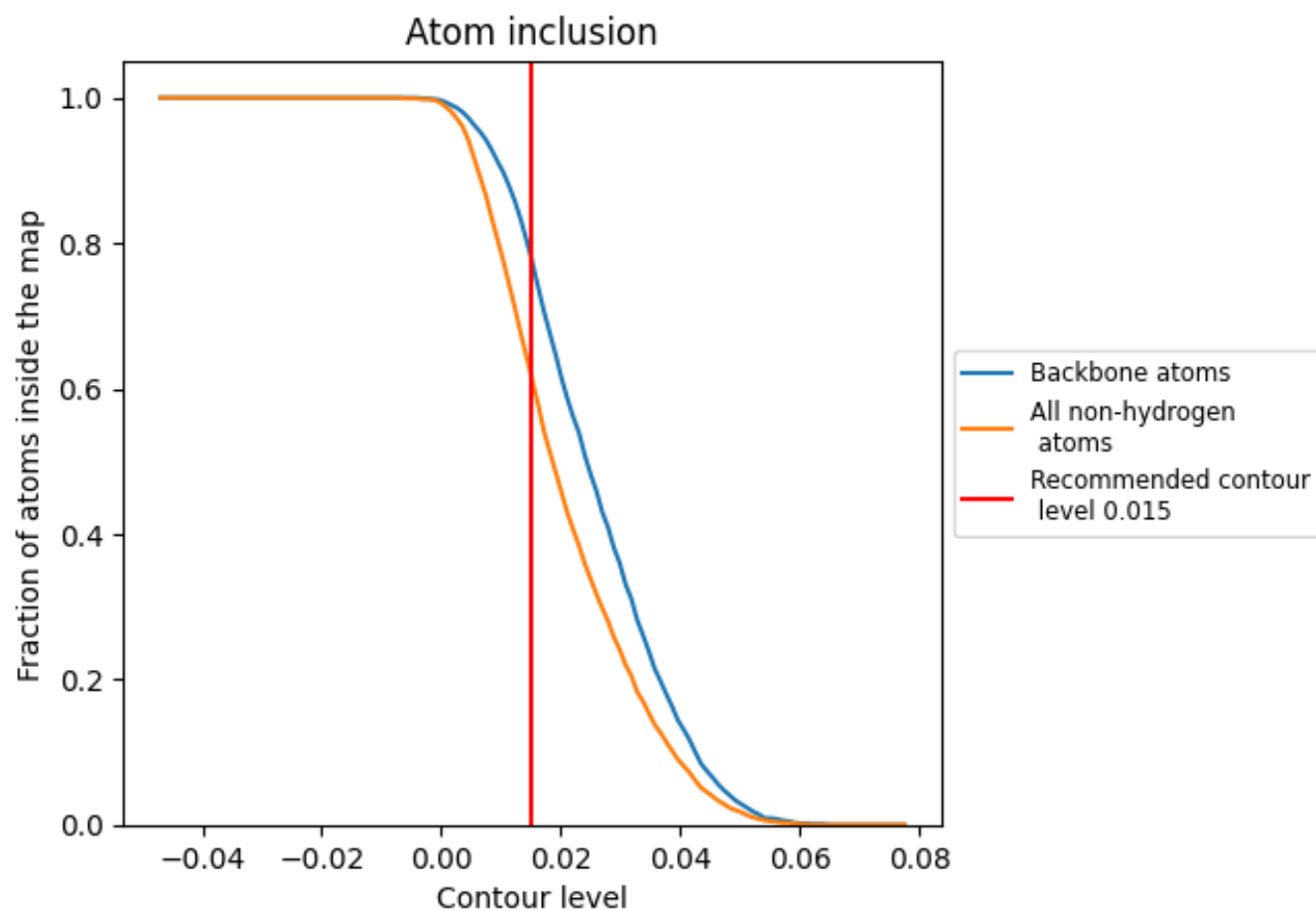
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

