



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 05:56 AM UTC

PDB ID : 9JUI / pdb_00009juj
EMDB ID : EMD-61827
Title : Structure of Arabidopsis thaliana ABCB1 in the inward-facing conformation
Authors : Chen, Q.; Su, N.; Guo, J.
Deposited on : 2024-10-08
Resolution : 3.40 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

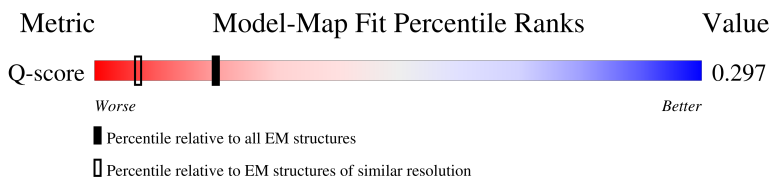
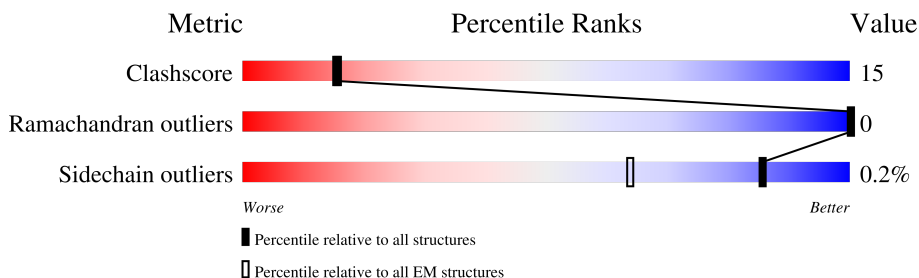
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	1327	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8971 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 ABC transporter B family member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1165	Total	C	N	O	S	0	0
			8971	5736	1543	1651	41		

There are 41 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-40	MET	-	initiating methionine	UNP Q9ZR72
A	-39	ASP	-	expression tag	UNP Q9ZR72
A	-38	TYR	-	expression tag	UNP Q9ZR72
A	-37	LYS	-	expression tag	UNP Q9ZR72
A	-36	ASP	-	expression tag	UNP Q9ZR72
A	-35	ASP	-	expression tag	UNP Q9ZR72
A	-34	ASP	-	expression tag	UNP Q9ZR72
A	-33	ASP	-	expression tag	UNP Q9ZR72
A	-32	LYS	-	expression tag	UNP Q9ZR72
A	-31	TRP	-	expression tag	UNP Q9ZR72
A	-30	SER	-	expression tag	UNP Q9ZR72
A	-29	HIS	-	expression tag	UNP Q9ZR72
A	-28	PRO	-	expression tag	UNP Q9ZR72
A	-27	GLN	-	expression tag	UNP Q9ZR72
A	-26	PHE	-	expression tag	UNP Q9ZR72
A	-25	GLU	-	expression tag	UNP Q9ZR72
A	-24	LYS	-	expression tag	UNP Q9ZR72
A	-23	GLY	-	expression tag	UNP Q9ZR72
A	-22	GLY	-	expression tag	UNP Q9ZR72
A	-21	GLY	-	expression tag	UNP Q9ZR72
A	-20	GLY	-	expression tag	UNP Q9ZR72
A	-19	SER	-	expression tag	UNP Q9ZR72
A	-18	GLY	-	expression tag	UNP Q9ZR72
A	-17	GLY	-	expression tag	UNP Q9ZR72
A	-16	SER	-	expression tag	UNP Q9ZR72
A	-15	ALA	-	expression tag	UNP Q9ZR72
A	-14	TRP	-	expression tag	UNP Q9ZR72
A	-13	SER	-	expression tag	UNP Q9ZR72

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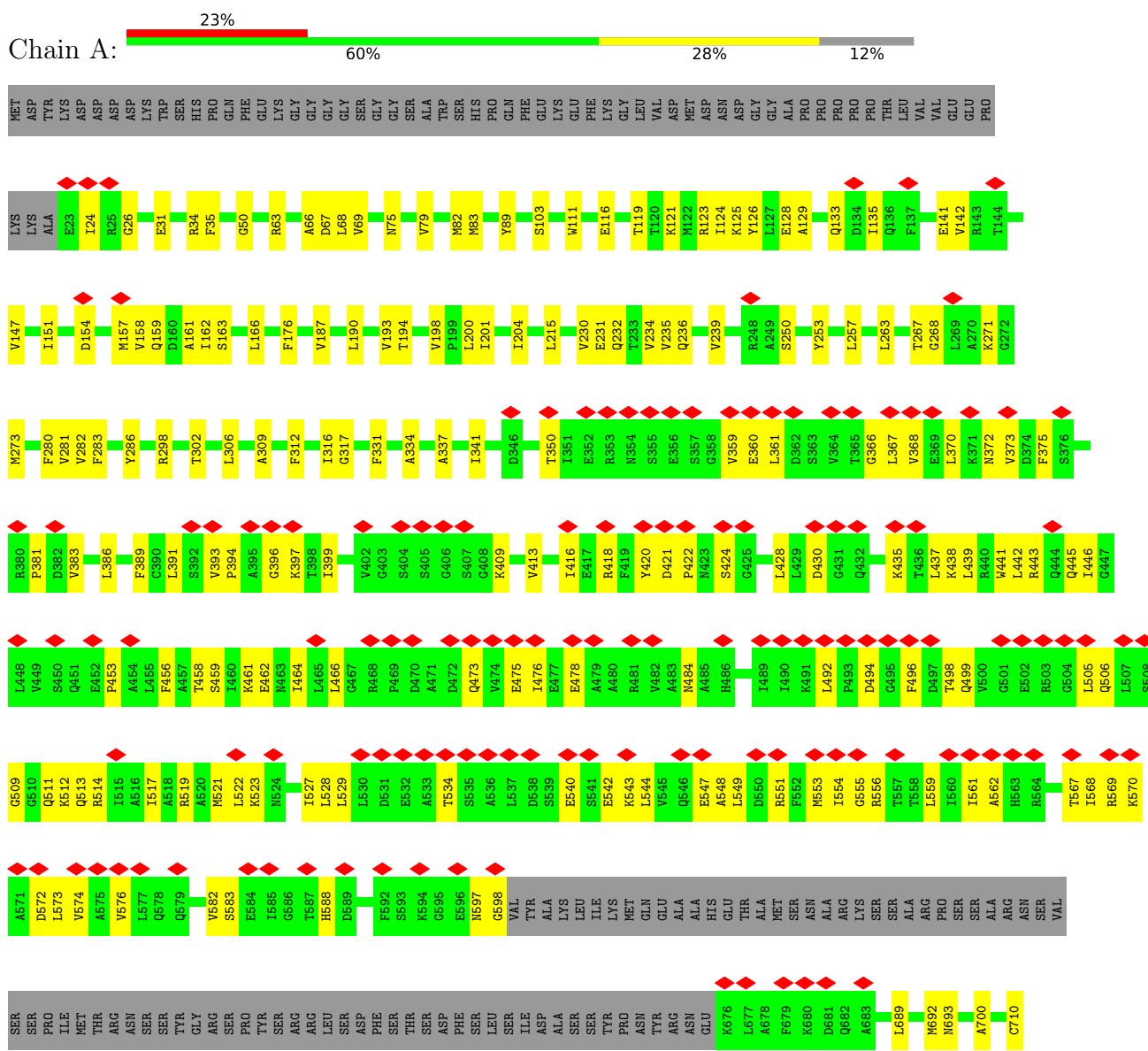
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	HIS	-	expression tag	UNP Q9ZR72
A	-11	PRO	-	expression tag	UNP Q9ZR72
A	-10	GLN	-	expression tag	UNP Q9ZR72
A	-9	PHE	-	expression tag	UNP Q9ZR72
A	-8	GLU	-	expression tag	UNP Q9ZR72
A	-7	LYS	-	expression tag	UNP Q9ZR72
A	-6	GLU	-	expression tag	UNP Q9ZR72
A	-5	PHE	-	expression tag	UNP Q9ZR72
A	-4	LYS	-	expression tag	UNP Q9ZR72
A	-3	GLY	-	expression tag	UNP Q9ZR72
A	-2	LEU	-	expression tag	UNP Q9ZR72
A	-1	VAL	-	expression tag	UNP Q9ZR72
A	0	ASP	-	expression tag	UNP Q9ZR72

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: ABC transporter B family member 1



GLU ASP ASP ALA	T1223	V1156	K1092	H1028	R906	L713					
	I1224	G1157	Y1093	I1029	R801		F717				
	R1225	E1158	N1094	D1030	Y908			A723			
	N1226	R1159	L1095	F1031	T909				V727		
	A1227	G1160	K1096	S1032	A910					Y728	
	H1228	V1161	A1097	I1039	L912						Y729
	V1229	Q1162	I1098	S1035	P915						
I1230	L1163	R1099	P1037	L916	Y735						
A1231	S1164	K1100	D1038	N811		Y736					
V1232	G1165	H1101	I1039	L945			M736				
I1233	Q1166	A1102	Q1040	A948				I737			
D1234	G1167	A1103	I1041	S949					K738		
D1235	K1168	I1104	F1042	R1043						L746	
D1236	Q1169	E1108	D1044	T962							L747
G1236	R1170	P1109	L1045	V965	L750						
K1237	I1171	L1111	S1046	T979		S751					
A1239	R1175	F1112	L1047	L982			A754				
Q1241	V1178	G1113	R1048	A983				L755			
G1242	R1179	T1114	A1049	K993					M758		
S1243	S1243	T1115	I1116	R994						T759	
H1244	E1182	Y1117	R1050	S995							L760
S1245	I1183	E1118	A1051	E998	Q761						
H1246	M1184	N1119	G1052	L999		H762					
L1247	L1185	I1120	K1053	L1000			W765				
L1248	L1186	A1121	T1054	K1003				D766			
K1249	D1187	Y1122	L1055	T1004					I767		
N1250	E1188	G1123	A1056	E1005						V768	
H1251	A1189	H1124	L1057	I1006							G769
P1252	T1190	E1125	V1058	E1007	E770						
D1253	S1191	C1126	S1061	P1008		N771					
G1254	A1192	A1127	G1062	D1009			L772				
I1255	L1193	T1128	C1063	D1010				T773			
Y1256	D1194	E1129	G1064	P1011					K774		
A1257	A1195	A1130	K1065	D1012						R775	
D1258	E1196	E1131	S1066	L894							V776
M1259	S1197	I1132	I1069	Q883	K779						
I1260	E1198	I1133	S1066	A888		M780					
Q1261	R1199	Q1134	I1069	R893			L781				
D1262	Q1202	L1138	I1072	V1016				V784			
Q1263	E1203	A1139	Q1073	P1017					E788		
R1264	A1204	S1140	R1074	D1018						M789	
PHE		A1141	F1075	R1019							F792
THR	Q1207	H1142	Y1076	L1020	E795						
HIS	A1208	K1143	E1077	R1021		E796					
THR	C1209	F1144	P1078	G1022			N797				
GLN	S1210	I1145	S1079	I904				E798			
VAL	G1211	S1146	S1080	V1024							
ILE	R1212	A1147	G1081	L1026							
GLY	T1213	L1148	R1082	K1027							
MET	S1214	P1149	V1083								
THR	I1215	G1150	M1084								
SER	GLY	G1151	I1085								
SER	SER	Y1152	I1085								
SER	SER	K1153	D1086								
ARG	VAL	T1154	G1087								
VAL	VAL	Y1155	K1088								
LYS		S1222	D1089								
			I1090								
			R1091								

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	96978	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1400	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.107	Depositor
Minimum map value	-0.060	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	223.2, 223.2, 223.2	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	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	0.33	0/9137	0.53	0/12366

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	8971	0	9116	264	0
All	All	8971	0	9116	264	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 15.

All (264) 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:239:VAL:HG11	1:A:1110:CYS:SG	2.25	0.77
1:A:204:ILE:HG13	1:A:281:VAL:HG21	1.67	0.76
1:A:151:ILE:HG22	1:A:882:THR:HG23	1.69	0.74
1:A:820:ARG:O	1:A:824:ILE:HG12	1.87	0.74
1:A:257:LEU:HB3	1:A:774:LYS:HD3	1.67	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:GLU:OE1	1:A:159:GLN:NE2	2.22	0.73
1:A:1104:ILE:HG22	1:A:1185:LEU:HB2	1.71	0.73
1:A:157:MET:SD	1:A:341:ILE:HD12	2.29	0.72
1:A:458:THR:HG22	1:A:459:SER:H	1.55	0.71
1:A:75:ASN:HB2	1:A:82:MET:HB3	1.72	0.70
1:A:441:TRP:O	1:A:445:GLN:NE2	2.25	0.70
1:A:373:VAL:HG11	1:A:389:PHE:HB3	1.74	0.69
1:A:842:GLN:NE2	1:A:843:TRP:O	2.26	0.68
1:A:123:ARG:NH2	1:A:151:ILE:O	2.27	0.68
1:A:234:VAL:HG12	1:A:792:PHE:HE2	1.58	0.68
1:A:372:ASN:HD22	1:A:424:SER:HB2	1.60	0.66
1:A:464:ILE:HG22	1:A:522:LEU:HD12	1.78	0.66
1:A:124:ILE:HD12	1:A:909:THR:HG22	1.78	0.65
1:A:540:GLU:HB2	1:A:543:LYS:HE3	1.78	0.65
1:A:1141:ALA:HA	1:A:1170:ARG:HD2	1.78	0.65
1:A:576:VAL:HB	1:A:583:SER:HB2	1.79	0.65
1:A:1036:ARG:HE	1:A:1039:ILE:HD13	1.61	0.65
1:A:1050:ARG:HB3	1:A:1053:LYS:HB3	1.78	0.64
1:A:1167:GLN:HG2	1:A:1170:ARG:HH21	1.61	0.63
1:A:528:LEU:HD21	1:A:549:LEU:HD12	1.80	0.63
1:A:492:LEU:HD11	1:A:505:LEU:HD21	1.80	0.63
1:A:788:GLU:OE2	1:A:1005:GLU:N	2.32	0.63
1:A:273:MET:HA	1:A:759:THR:HG22	1.80	0.62
1:A:1190:THR:HG1	1:A:1219:HIS:HE2	1.48	0.62
1:A:1115:THR:HB	1:A:1153:LYS:HB2	1.82	0.62
1:A:439:LEU:H	1:A:442:LEU:HD13	1.63	0.62
1:A:824:ILE:HD12	1:A:979:THR:HG23	1.82	0.61
1:A:1114:THR:N	1:A:1118:GLU:OE2	2.32	0.61
1:A:413:VAL:HG22	1:A:529:LEU:HD12	1.81	0.61
1:A:24:ILE:HG22	1:A:26:GLY:H	1.67	0.60
1:A:1078:PRO:HG2	1:A:1091:ARG:HH21	1.66	0.60
1:A:812:ASN:OD1	1:A:813:VAL:N	2.36	0.59
1:A:1212:ARG:HG3	1:A:1213:THR:H	1.68	0.59
1:A:775:ARG:O	1:A:779:LYS:HG2	2.03	0.59
1:A:555:GLY:O	1:A:556:ARG:HD3	2.03	0.58
1:A:809:ASP:OD1	1:A:810:ALA:N	2.37	0.58
1:A:1141:ALA:HB1	1:A:1170:ARG:HH11	1.69	0.58
1:A:119:THR:O	1:A:123:ARG:HG3	2.04	0.57
1:A:823:VAL:HG11	1:A:982:LEU:HD12	1.85	0.57
1:A:461:LYS:NZ	1:A:496:PHE:O	2.36	0.57
1:A:807:ALA:O	1:A:811:ASN:ND2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:LEU:HD13	1:A:391:LEU:HB2	1.88	0.56
1:A:473:GLN:HA	1:A:476:ILE:HD12	1.87	0.56
1:A:568:ILE:HG22	1:A:588:HIS:NE2	2.20	0.56
1:A:298:ARG:HG3	1:A:736:MET:HE1	1.87	0.56
1:A:437:LEU:HB3	1:A:442:LEU:HD11	1.87	0.56
1:A:1021:ARG:CZ	1:A:1023:GLU:HB3	2.36	0.56
1:A:1220:ARG:NH2	1:A:1223:THR:O	2.38	0.55
1:A:35:PHE:HD2	1:A:121:LYS:HG3	1.71	0.55
1:A:511:GLN:HA	1:A:514:ARG:HE	1.72	0.55
1:A:394:PRO:HG2	1:A:397:LYS:HB2	1.89	0.55
1:A:1094:ASN:OD1	1:A:1095:LEU:N	2.39	0.55
1:A:1198:GLU:OE2	1:A:1202:GLN:NE2	2.39	0.55
1:A:83:MET:SD	1:A:949:SER:OG	2.57	0.55
1:A:492:LEU:HD23	1:A:494:ASP:H	1.72	0.55
1:A:567:THR:HA	1:A:570:LYS:HD3	1.88	0.55
1:A:1115:THR:N	1:A:1118:GLU:OE2	2.33	0.55
1:A:458:THR:HG22	1:A:459:SER:N	2.21	0.55
1:A:126:TYR:HD1	1:A:341:ILE:HG23	1.71	0.54
1:A:700:ALA:HB2	1:A:768:VAL:HG21	1.88	0.54
1:A:838:GLY:HA2	1:A:965:VAL:HG22	1.89	0.54
1:A:780:MET:HG2	1:A:1000:LEU:HD11	1.89	0.54
1:A:717:PHE:HD1	1:A:747:LEU:HD11	1.72	0.54
1:A:446:ILE:HG23	1:A:529:LEU:HD23	1.90	0.54
1:A:798:GLU:HB2	1:A:801:ARG:HG2	1.89	0.54
1:A:1220:ARG:HH21	1:A:1224:ILE:HA	1.73	0.54
1:A:466:LEU:HD21	1:A:519:ARG:HH11	1.73	0.53
1:A:727:VAL:HG12	1:A:736:MET:HG3	1.89	0.53
1:A:693:ASN:HB2	1:A:772:LEU:HD13	1.90	0.53
1:A:1102:ILE:HG13	1:A:1183:ILE:HB	1.89	0.53
1:A:232:GLN:O	1:A:236:GLN:HG2	2.09	0.53
1:A:1167:GLN:O	1:A:1170:ARG:HG2	2.08	0.53
1:A:1186:LEU:N	1:A:1215:ILE:O	2.38	0.53
1:A:268:GLY:HA2	1:A:766:ASP:OD2	2.09	0.53
1:A:1021:ARG:CZ	1:A:1086:ASP:HA	2.39	0.53
1:A:574:VAL:HB	1:A:588:HIS:HD2	1.73	0.53
1:A:126:TYR:CD1	1:A:341:ILE:HG23	2.43	0.52
1:A:360:GLU:HA	1:A:441:TRP:CE3	2.45	0.52
1:A:761:GLN:HG3	1:A:762:HIS:N	2.25	0.52
1:A:819:ASP:OD2	1:A:820:ARG:NH1	2.42	0.52
1:A:453:PRO:HG2	1:A:512:LYS:HE2	1.91	0.52
1:A:797:ASN:HB3	1:A:802:ILE:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:905:VAL:O	1:A:909:THR:HG23	2.09	0.52
1:A:854:PRO:HA	1:A:857:VAL:HG22	1.91	0.52
1:A:1220:ARG:HB3	1:A:1224:ILE:HD12	1.91	0.52
1:A:413:VAL:O	1:A:416:ILE:HG22	2.09	0.52
1:A:994:ARG:HD2	1:A:995:SER:N	2.25	0.52
1:A:521:MET:SD	1:A:549:LEU:HD21	2.49	0.51
1:A:215:LEU:HB3	1:A:267:THR:HG22	1.92	0.51
1:A:776:VAL:O	1:A:780:MET:HG3	2.11	0.51
1:A:194:THR:O	1:A:198:VAL:HG23	2.10	0.51
1:A:31:GLU:O	1:A:34:ARG:HG2	2.10	0.51
1:A:157:MET:HE2	1:A:337:ALA:HB1	1.91	0.51
1:A:1021:ARG:H	1:A:1021:ARG:HD3	1.76	0.51
1:A:190:LEU:HA	1:A:193:VAL:HG22	1.93	0.51
1:A:754:ALA:O	1:A:758:ASN:HB2	2.11	0.51
1:A:713:LEU:HD23	1:A:750:LEU:HD22	1.91	0.51
1:A:1057:LEU:HA	1:A:1230:ILE:HG23	1.93	0.50
1:A:1139:ALA:HA	1:A:1204:ALA:HB1	1.93	0.50
1:A:912:LEU:C	1:A:915:PRO:HD2	2.36	0.50
1:A:713:LEU:HD13	1:A:754:ALA:HA	1.93	0.50
1:A:124:ILE:HD13	1:A:908:TYR:CD2	2.47	0.50
1:A:201:ILE:HD13	1:A:282:VAL:HG22	1.94	0.49
1:A:373:VAL:HG13	1:A:386:LEU:HB3	1.93	0.49
1:A:765:TRP:CG	1:A:822:SER:HG	2.30	0.49
1:A:253:TYR:O	1:A:257:LEU:HG	2.13	0.49
1:A:506:GLN:HG3	1:A:509:GLY:H	1.78	0.49
1:A:844:ARG:HA	1:A:847:LEU:HB2	1.94	0.49
1:A:1038:ASP:OD1	1:A:1039:ILE:HD12	2.12	0.49
1:A:1199:ARG:HG2	1:A:1199:ARG:HH11	1.77	0.49
1:A:770:GLU:O	1:A:774:LYS:HG2	2.12	0.49
1:A:542:GLU:OE2	1:A:542:GLU:N	2.28	0.49
1:A:850:VAL:HA	1:A:853:PHE:HB2	1.95	0.49
1:A:1165:GLY:O	1:A:1169:GLN:HG2	2.13	0.49
1:A:1148:LEU:HD13	1:A:1154:THR:HG23	1.94	0.48
1:A:572:ASP:OD1	1:A:573:LEU:N	2.47	0.48
1:A:66:ALA:HB2	1:A:309:ALA:HB2	1.96	0.48
1:A:250:SER:HA	1:A:781:LEU:HD23	1.96	0.48
1:A:466:LEU:HD21	1:A:519:ARG:NH1	2.27	0.48
1:A:476:ILE:HA	1:A:522:LEU:HD11	1.95	0.48
1:A:125:LYS:O	1:A:128:GLU:HG3	2.14	0.48
1:A:1043:ARG:N	1:A:1236:GLY:O	2.47	0.48
1:A:1117:TYR:CE1	1:A:1132:ILE:HD12	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:758:ASN:HA	1:A:761:GLN:HG2	1.96	0.48
1:A:780:MET:HE3	1:A:806:LEU:HG	1.94	0.48
1:A:1103:ALA:HB2	1:A:1179:ARG:HG2	1.95	0.48
1:A:157:MET:O	1:A:334:ALA:HB1	2.14	0.47
1:A:1027:LYS:HD3	1:A:1028:HIS:HB2	1.95	0.47
1:A:1095:LEU:O	1:A:1099:ARG:HB2	2.14	0.47
1:A:747:LEU:HD12	1:A:750:LEU:HD12	1.95	0.47
1:A:283:PHE:HB2	1:A:751:SER:HB3	1.96	0.47
1:A:801:ARG:HE	1:A:801:ARG:HA	1.79	0.47
1:A:66:ALA:HB1	1:A:306:LEU:HD23	1.97	0.47
1:A:1256:TYR:CE2	1:A:1260:ILE:HD11	2.49	0.47
1:A:727:VAL:O	1:A:736:MET:HG3	2.14	0.47
1:A:907:LEU:O	1:A:911:ASN:ND2	2.47	0.47
1:A:540:GLU:O	1:A:543:LYS:HG3	2.14	0.47
1:A:476:ILE:HG12	1:A:522:LEU:HD11	1.96	0.47
1:A:1016:VAL:HG21	1:A:1098:ILE:HG12	1.97	0.47
1:A:389:PHE:HD1	1:A:582:VAL:HB	1.80	0.46
1:A:689:LEU:HD21	1:A:772:LEU:HD21	1.96	0.46
1:A:781:LEU:HA	1:A:784:VAL:HG12	1.96	0.46
1:A:1074:ARG:HH11	1:A:1091:ARG:HA	1.79	0.46
1:A:422:PRO:HG3	1:A:435:LYS:HE2	1.97	0.46
1:A:547:GLU:O	1:A:551:ARG:NH2	2.32	0.46
1:A:79:VAL:HB	1:A:953:LYS:HG2	1.96	0.46
1:A:129:ALA:O	1:A:133:GLN:HG2	2.14	0.46
1:A:393:VAL:HG12	1:A:399:ILE:HD13	1.97	0.46
1:A:734:GLU:O	1:A:738:LYS:HG2	2.15	0.46
1:A:1175:ARG:HA	1:A:1178:VAL:HG12	1.98	0.46
1:A:1080:SER:O	1:A:1082:ARG:NH1	2.49	0.46
1:A:409:LYS:HE2	1:A:561:ILE:HD11	1.97	0.46
1:A:903:LYS:NZ	1:A:906:ARG:HE	2.13	0.46
1:A:544:LEU:O	1:A:548:ALA:N	2.49	0.46
1:A:798:GLU:O	1:A:802:ILE:HG12	2.16	0.46
1:A:758:ASN:OD1	1:A:761:GLN:NE2	2.49	0.45
1:A:823:VAL:HA	1:A:826:GLN:HG2	1.98	0.45
1:A:157:MET:CE	1:A:337:ALA:HB1	2.46	0.45
1:A:366:GLY:HA2	1:A:430:ASP:HB3	1.98	0.45
1:A:710:CYS:HA	1:A:713:LEU:HD12	1.97	0.45
1:A:34:ARG:HG3	1:A:35:PHE:CD1	2.51	0.45
1:A:1228:HIS:ND1	1:A:1229:VAL:HG13	2.31	0.45
1:A:157:MET:HE2	1:A:337:ALA:C	2.42	0.45
1:A:1120:ILE:HG22	1:A:1178:VAL:HG11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1175:ARG:O	1:A:1178:VAL:HG12	2.17	0.45
1:A:597:ASN:OD1	1:A:598:GLY:N	2.49	0.45
1:A:375:PHE:CE1	1:A:421:ASP:HB2	2.52	0.45
1:A:1109:PRO:O	1:A:1168:LYS:HD2	2.16	0.45
1:A:723:ALA:O	1:A:727:VAL:HG23	2.16	0.45
1:A:773:THR:HB	1:A:814:ARG:HB2	1.98	0.45
1:A:68:LEU:HD22	1:A:945:LEU:HD13	1.98	0.45
1:A:280:PHE:HA	1:A:751:SER:HB2	1.99	0.45
1:A:368:VAL:HA	1:A:428:LEU:O	2.17	0.45
1:A:521:MET:HE2	1:A:521:MET:HA	1.99	0.45
1:A:553:MET:SD	1:A:554:ILE:N	2.90	0.45
1:A:475:GLU:HA	1:A:478:GLU:HB2	1.98	0.44
1:A:755:LEU:O	1:A:759:THR:HG23	2.17	0.44
1:A:418:ARG:HD2	1:A:439:LEU:HD13	1.99	0.44
1:A:574:VAL:HB	1:A:588:HIS:CD2	2.51	0.44
1:A:689:LEU:HD11	1:A:772:LEU:HD11	1.99	0.44
1:A:1131:GLU:O	1:A:1134:GLN:HG3	2.17	0.44
1:A:494:ASP:OD2	1:A:498:THR:HG22	2.18	0.44
1:A:200:LEU:O	1:A:204:ILE:HG12	2.18	0.44
1:A:534:THR:HG22	1:A:562:ALA:HB2	2.00	0.44
1:A:141:GLU:HG2	1:A:142:VAL:H	1.81	0.44
1:A:1254:GLY:O	1:A:1258:ARG:NH1	2.26	0.44
1:A:689:LEU:HD22	1:A:993:MET:HE2	1.99	0.44
1:A:350:THR:HG22	1:A:420:TYR:HE2	1.83	0.43
1:A:1109:PRO:HG2	1:A:1168:LYS:HG2	1.99	0.43
1:A:1145:ILE:HG22	1:A:1152:TYR:HB2	2.00	0.43
1:A:1120:ILE:HB	1:A:1132:ILE:HD13	2.00	0.43
1:A:381:PRO:O	1:A:383:VAL:HG13	2.18	0.43
1:A:948:ALA:HB1	1:A:962:THR:HB	2.01	0.43
1:A:312:PHE:O	1:A:316:ILE:HG12	2.18	0.43
1:A:462:GLU:OE2	1:A:903:LYS:HD2	2.19	0.43
1:A:162:ILE:HA	1:A:166:LEU:HB2	2.00	0.43
1:A:443:ARG:O	1:A:523:LYS:NZ	2.49	0.43
1:A:298:ARG:HD3	1:A:737:ILE:HD11	2.00	0.43
1:A:135:ILE:HD12	1:A:893:ARG:HG2	2.00	0.43
1:A:157:MET:HE2	1:A:337:ALA:O	2.19	0.43
1:A:484:ASN:H	1:A:548:ALA:HB2	1.84	0.43
1:A:1124:HIS:HD2	1:A:1126:CYS:HB2	1.82	0.43
1:A:187:VAL:HG22	1:A:302:THR:HG21	2.01	0.42
1:A:232:GLN:HA	1:A:235:VAL:HG22	2.00	0.42
1:A:372:ASN:OD1	1:A:373:VAL:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1109:PRO:HG2	1:A:1168:LYS:HE3	2.01	0.42
1:A:1150:GLU:CD	1:A:1151:GLY:N	2.77	0.42
1:A:1187:ASP:CG	1:A:1188:GLU:H	2.27	0.42
1:A:1261:GLN:HA	1:A:1264:ARG:HE	1.84	0.42
1:A:994:ARG:O	1:A:998:GLU:HG2	2.20	0.42
1:A:1047:LEU:HD11	1:A:1055:LEU:HD23	2.00	0.42
1:A:1054:THR:OG1	1:A:1209:CYS:HB3	2.20	0.42
1:A:458:THR:CG2	1:A:459:SER:H	2.27	0.42
1:A:1045:LEU:HD21	1:A:1047:LEU:HB2	2.01	0.42
1:A:63:ARG:NH1	1:A:67:ASP:OD1	2.53	0.42
1:A:359:VAL:HG12	1:A:361:LEU:H	1.84	0.42
1:A:366:GLY:N	1:A:556:ARG:HH22	2.17	0.42
1:A:789:MET:HB2	1:A:1075:PHE:O	2.20	0.42
1:A:234:VAL:HG12	1:A:792:PHE:CE2	2.47	0.41
1:A:438:LYS:O	1:A:439:LEU:HB3	2.19	0.41
1:A:1199:ARG:HG2	1:A:1199:ARG:NH1	2.35	0.41
1:A:50:GLY:O	1:A:103:SER:HB3	2.20	0.41
1:A:111:TRP:HB3	1:A:163:SER:O	2.20	0.41
1:A:230:VAL:O	1:A:234:VAL:HG22	2.19	0.41
1:A:372:ASN:ND2	1:A:424:SER:HB2	2.32	0.41
1:A:126:TYR:OH	1:A:147:VAL:HG13	2.20	0.41
1:A:569:ARG:NH1	1:A:588:HIS:CE1	2.89	0.41
1:A:161:ALA:O	1:A:166:LEU:N	2.53	0.41
1:A:367:LEU:H	1:A:430:ASP:HB3	1.84	0.41
1:A:396:GLY:HA2	1:A:554:ILE:HA	2.01	0.41
1:A:689:LEU:HA	1:A:692:MET:HG2	2.02	0.41
1:A:69:VAL:HG12	1:A:729:TYR:HE2	1.85	0.41
1:A:250:SER:HA	1:A:781:LEU:CD2	2.50	0.41
1:A:1194:ASP:OD1	1:A:1195:ALA:N	2.53	0.41
1:A:271:LYS:HE3	1:A:762:HIS:ND1	2.35	0.41
1:A:459:SER:HB2	1:A:499:GLN:OE1	2.21	0.41
1:A:527:ILE:HA	1:A:556:ARG:HG3	2.03	0.41
1:A:746:LEU:O	1:A:750:LEU:HG	2.21	0.41
1:A:123:ARG:CZ	1:A:154:ASP:HB3	2.51	0.41
1:A:166:LEU:HA	1:A:331:PHE:HZ	1.85	0.41
1:A:176:PHE:HA	1:A:317:GLY:HA2	2.02	0.41
1:A:484:ASN:HD21	1:A:517:ILE:HB	1.85	0.41
1:A:852:VAL:O	1:A:856:VAL:HG23	2.21	0.41
1:A:884:LEU:HD13	1:A:911:ASN:ND2	2.35	0.41
1:A:67:ASP:HB3	1:A:89:TYR:CZ	2.56	0.41
1:A:116:GLU:HG3	1:A:916:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1038:ASP:OD1	1:A:1038:ASP:N	2.53	0.41
1:A:1116:ILE:HA	1:A:1119:ASN:ND2	2.36	0.40
1:A:119:THR:OG1	1:A:158:VAL:HG13	2.21	0.40
1:A:453:PRO:HG3	1:A:513:GLN:OE1	2.21	0.40
1:A:456:PHE:HE1	1:A:888:ALA:HA	1.86	0.40
1:A:1134:GLN:O	1:A:1138:LEU:HG	2.21	0.40
1:A:1195:ALA:O	1:A:1199:ARG:HG3	2.22	0.40
1:A:555:GLY:C	1:A:556:ARG:HD3	2.46	0.40
1:A:236:GLN:NE2	1:A:1112:PHE:CE1	2.89	0.40
1:A:409:LYS:HD2	1:A:559:LEU:HD13	2.02	0.40
1:A:231:GLU:O	1:A:235:VAL:HG13	2.22	0.40
1:A:765:TRP:HA	1:A:768:VAL:HG12	2.04	0.40
1:A:1052:GLY:HA3	1:A:1212:ARG:HH21	1.86	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	1161/1327 (88%)	1106 (95%)	55 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	949/1087 (87%)	947 (100%)	2 (0%)	87 85

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

Mol	Chain	Res	Type
1	A	263	LEU
1	A	286	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	136	GLN
1	A	208	HIS
1	A	236	GLN
1	A	261	GLN
1	A	387	ASN
1	A	445	GLN
1	A	484	ASN
1	A	506	GLN
1	A	863	GLN
1	A	899	ASN
1	A	1124	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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.

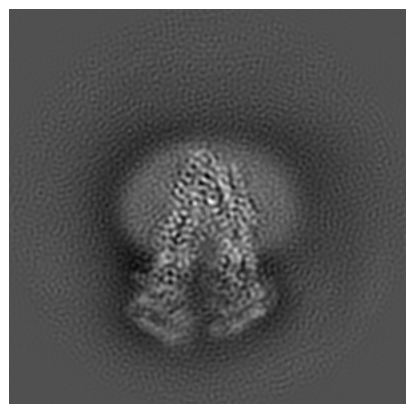
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61827. These allow visual inspection of the internal detail of the map and identification of artifacts.

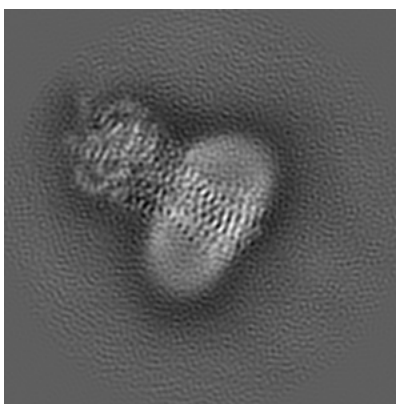
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

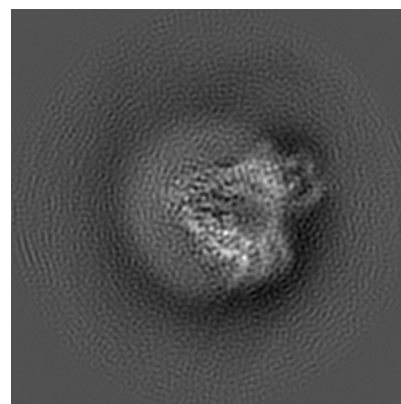
6.1.1 Primary map



X

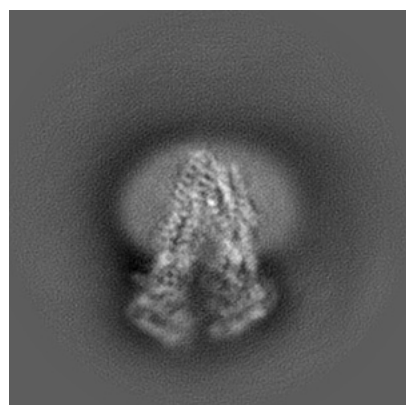


Y

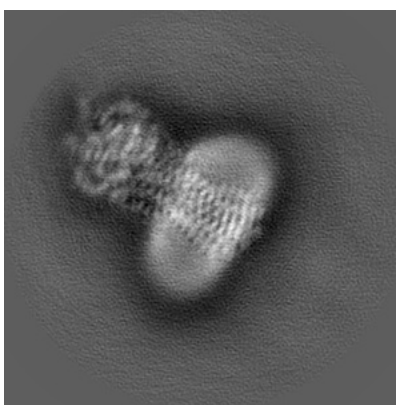


Z

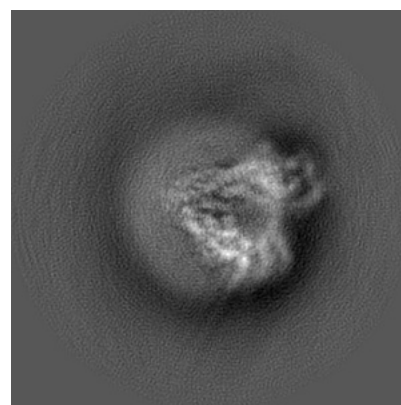
6.1.2 Raw map



X



Y

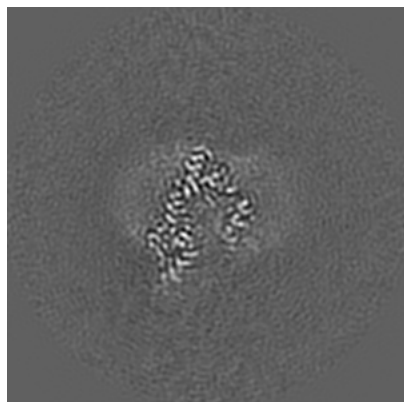


Z

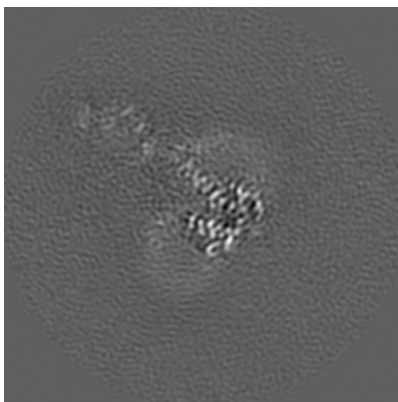
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

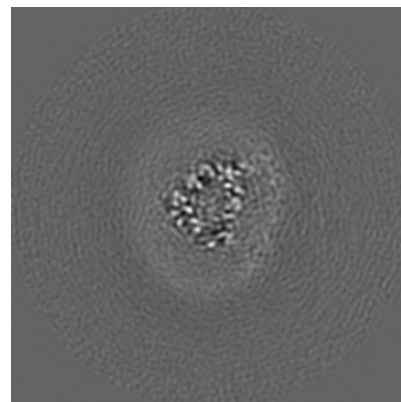
6.2.1 Primary map



X Index: 120

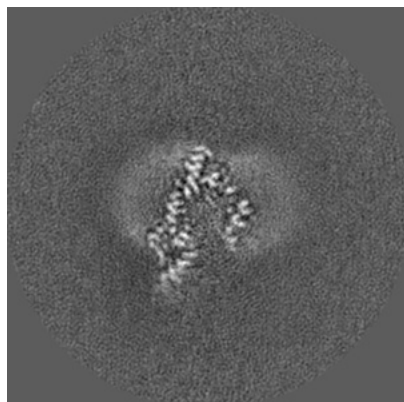


Y Index: 120



Z Index: 120

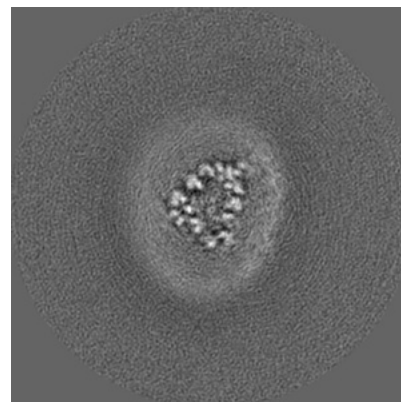
6.2.2 Raw map



X Index: 120



Y Index: 120

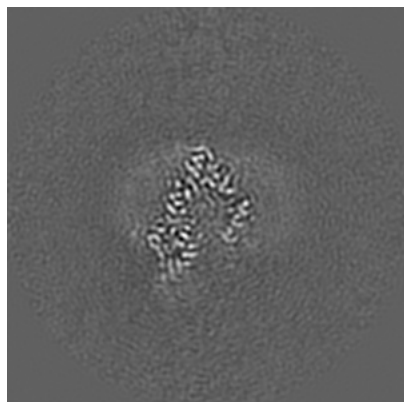


Z Index: 120

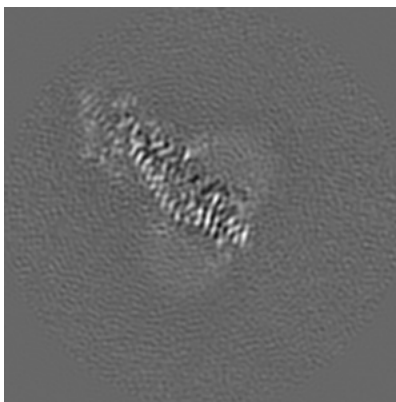
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

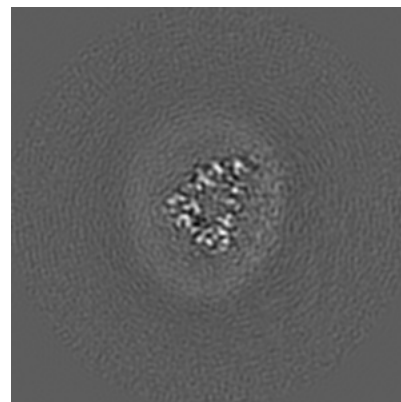
6.3.1 Primary map



X Index: 119

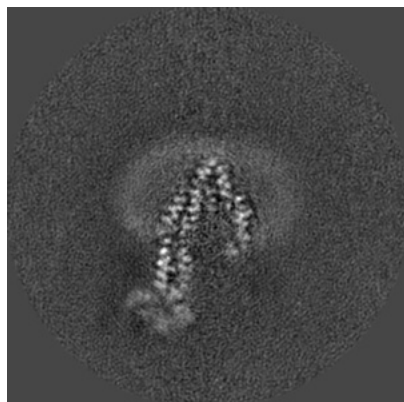


Y Index: 135

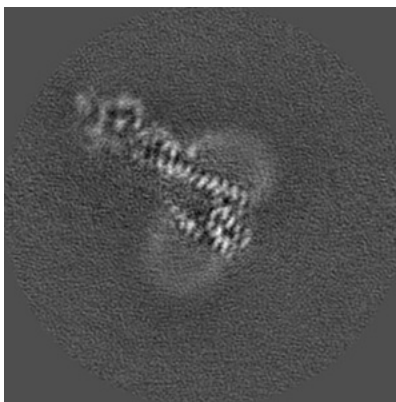


Z Index: 118

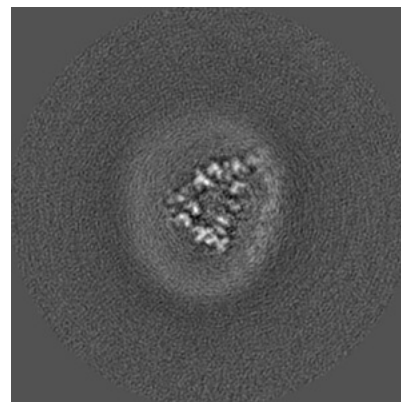
6.3.2 Raw map



X Index: 129



Y Index: 130

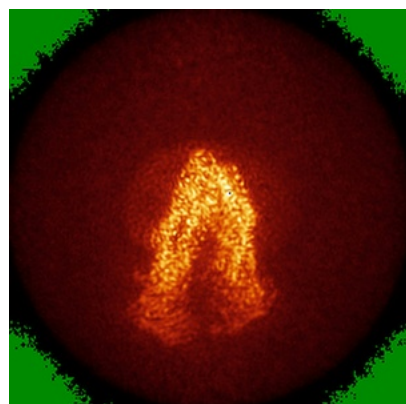


Z Index: 117

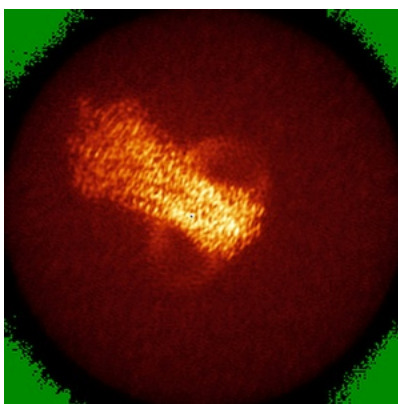
The images above show the largest variance slices of the map in three orthogonal directions.

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

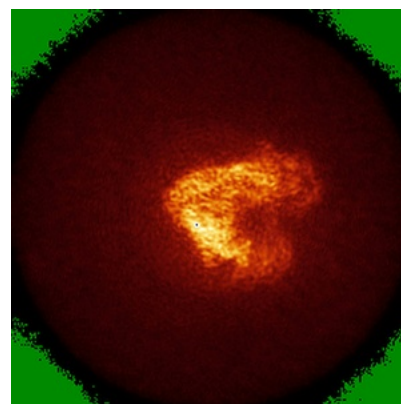
6.4.1 Primary map



X

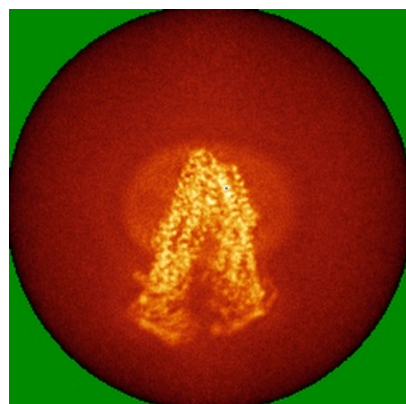


Y

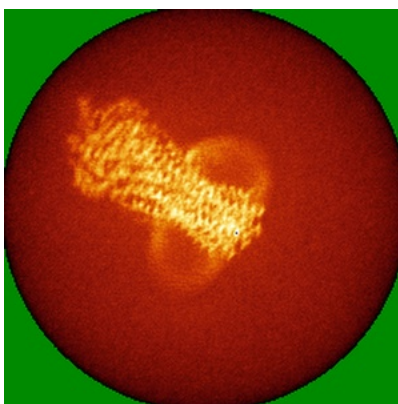


Z

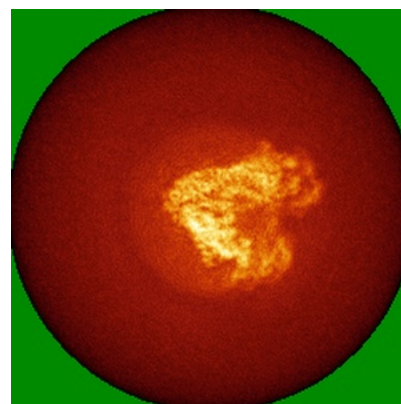
6.4.2 Raw map



X



Y

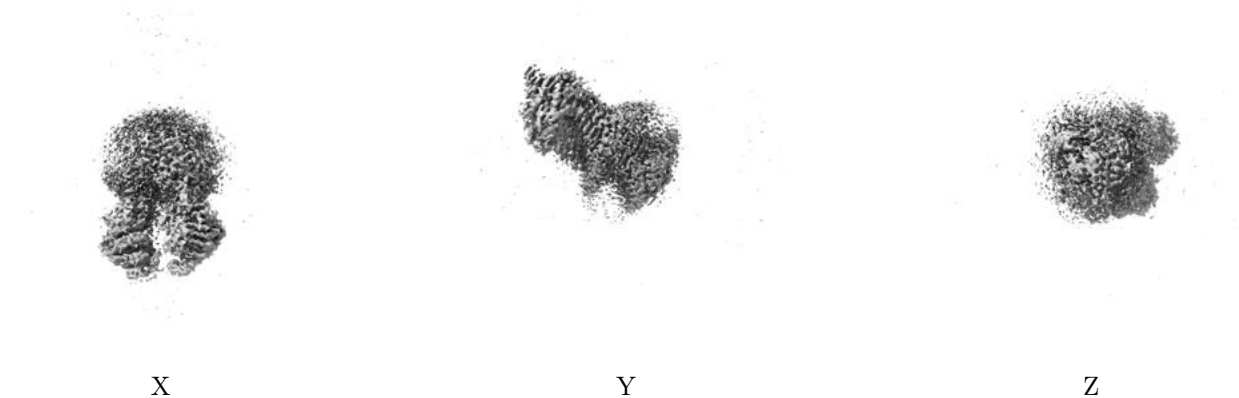


Z

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.

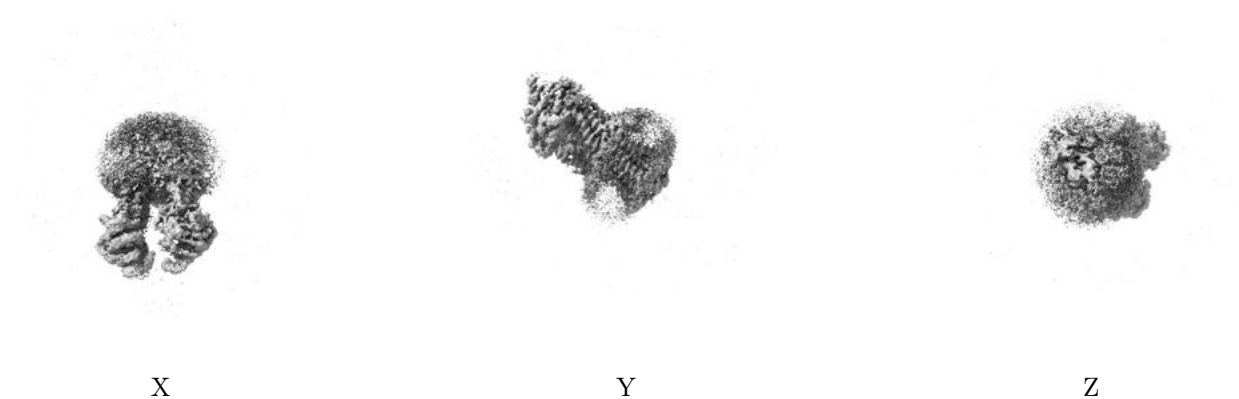
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

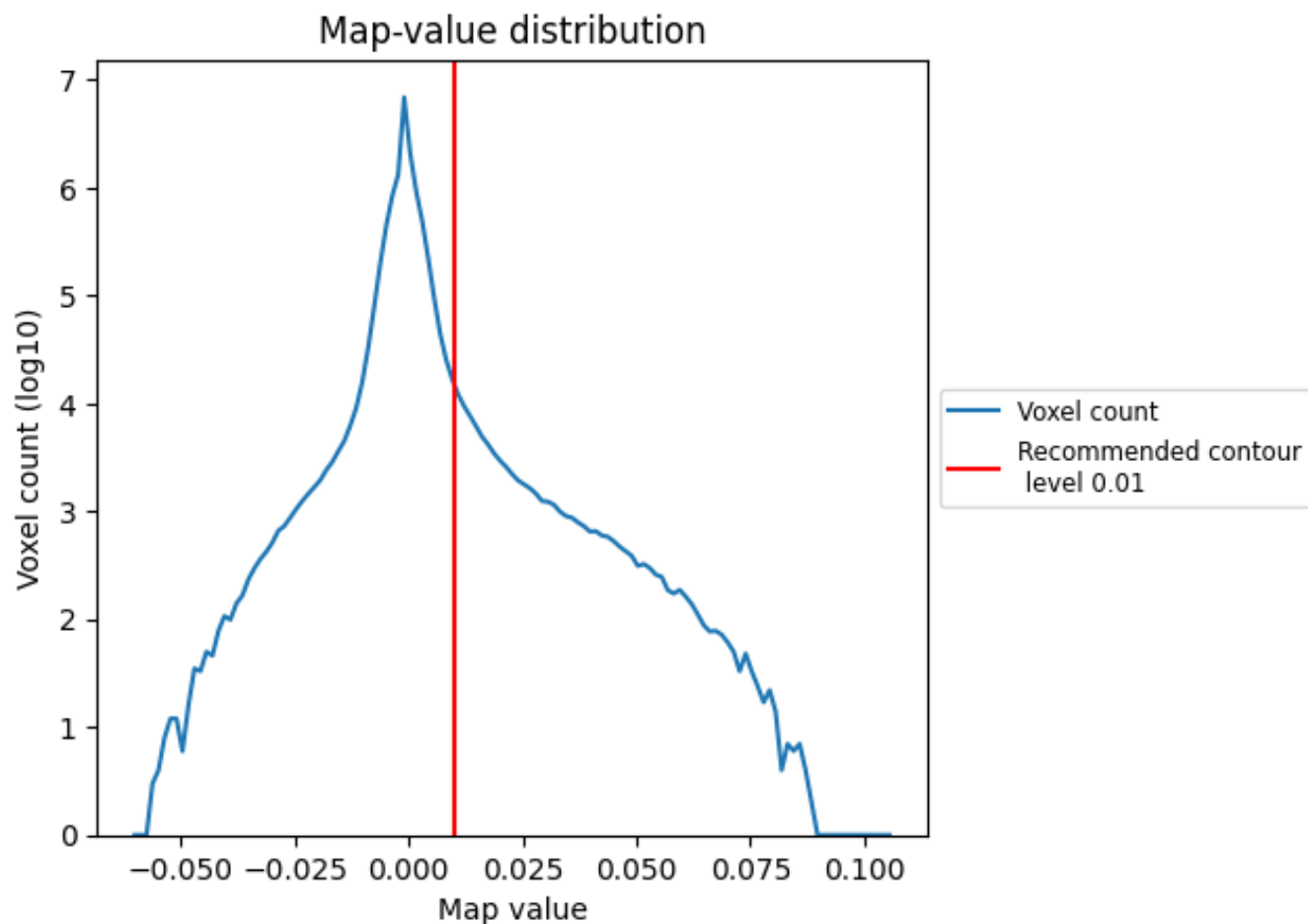
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

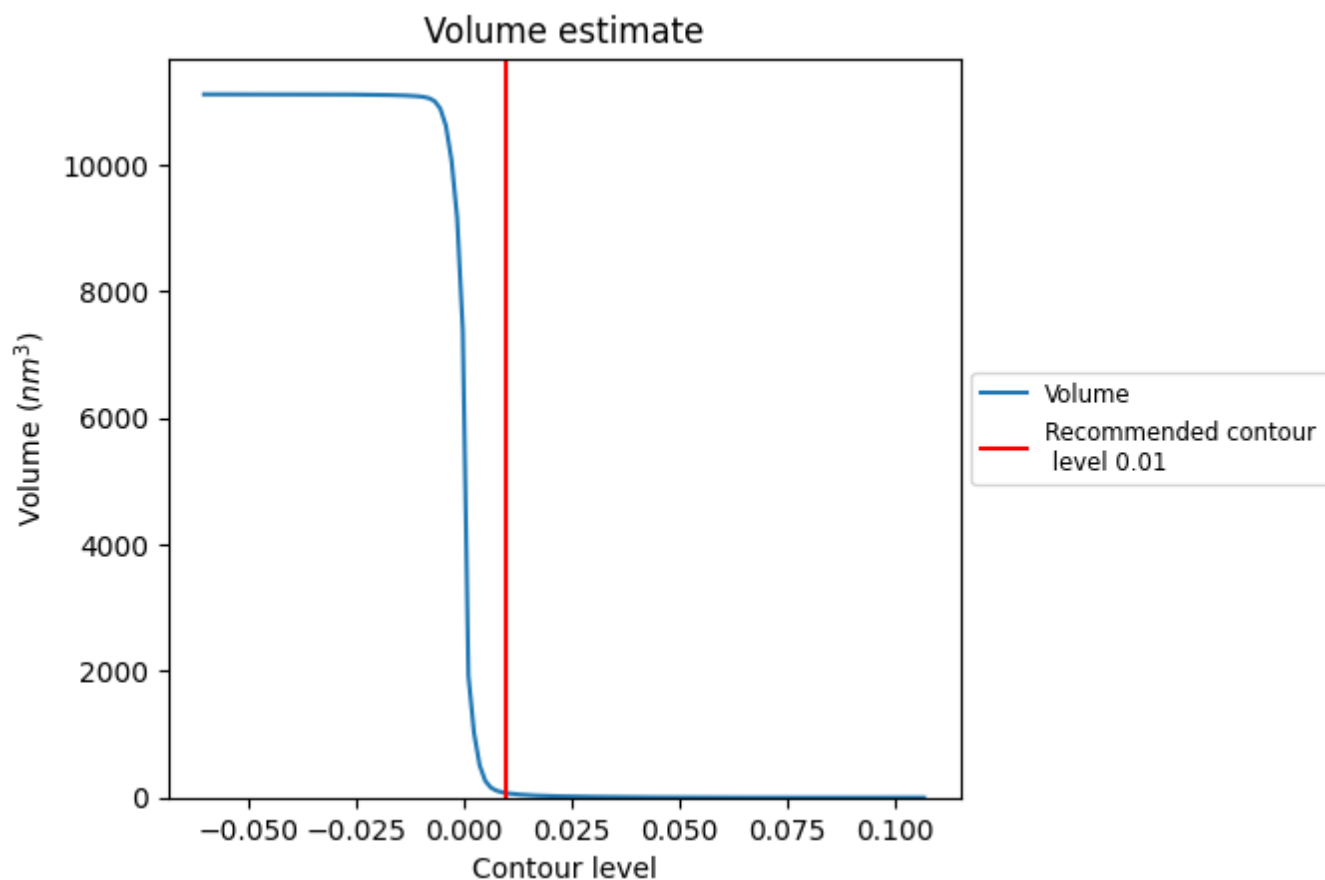
This section contains the results of statistical analysis of the map.

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.

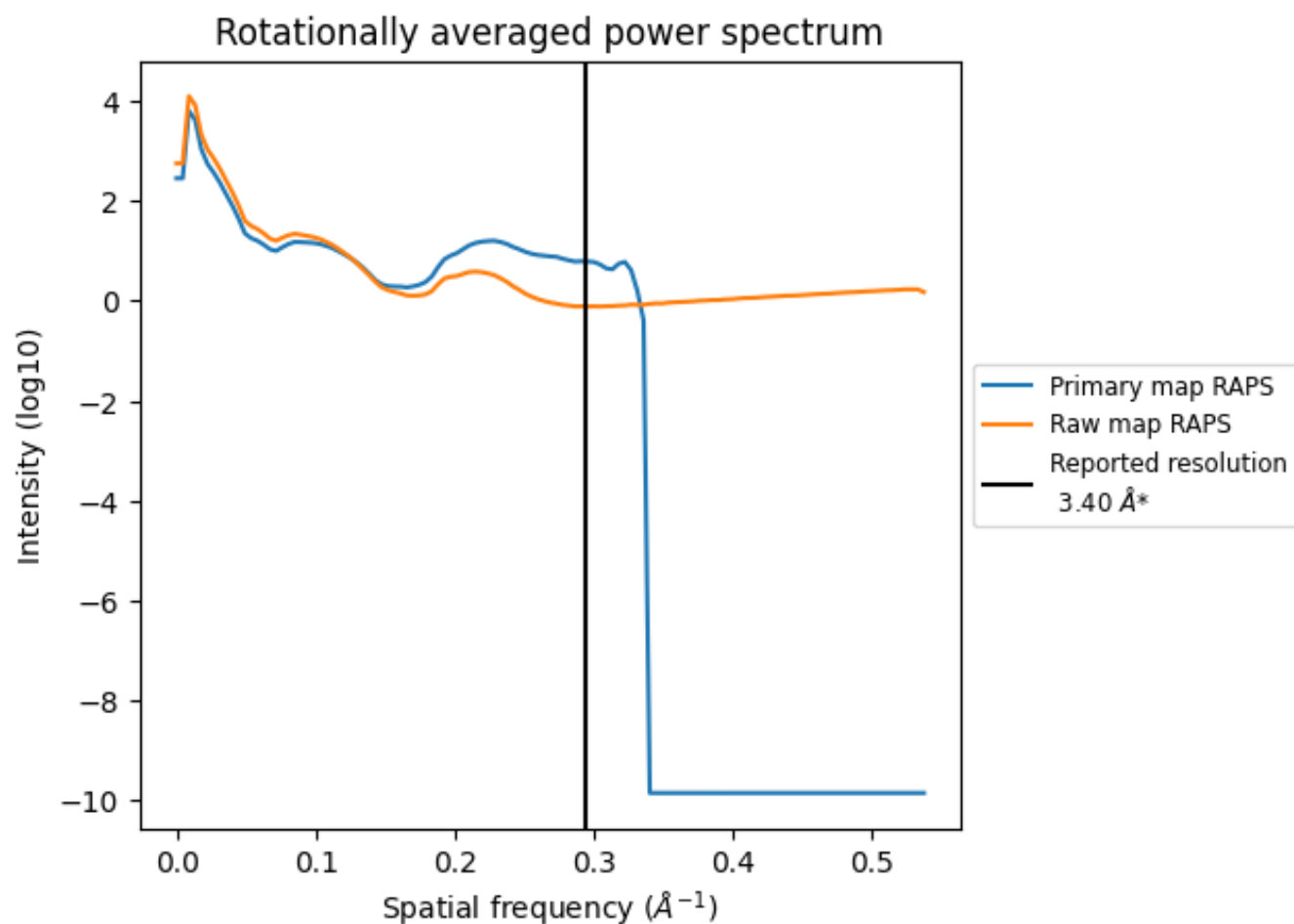
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 71 nm³; this corresponds to an approximate mass of 64 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 ⓘ

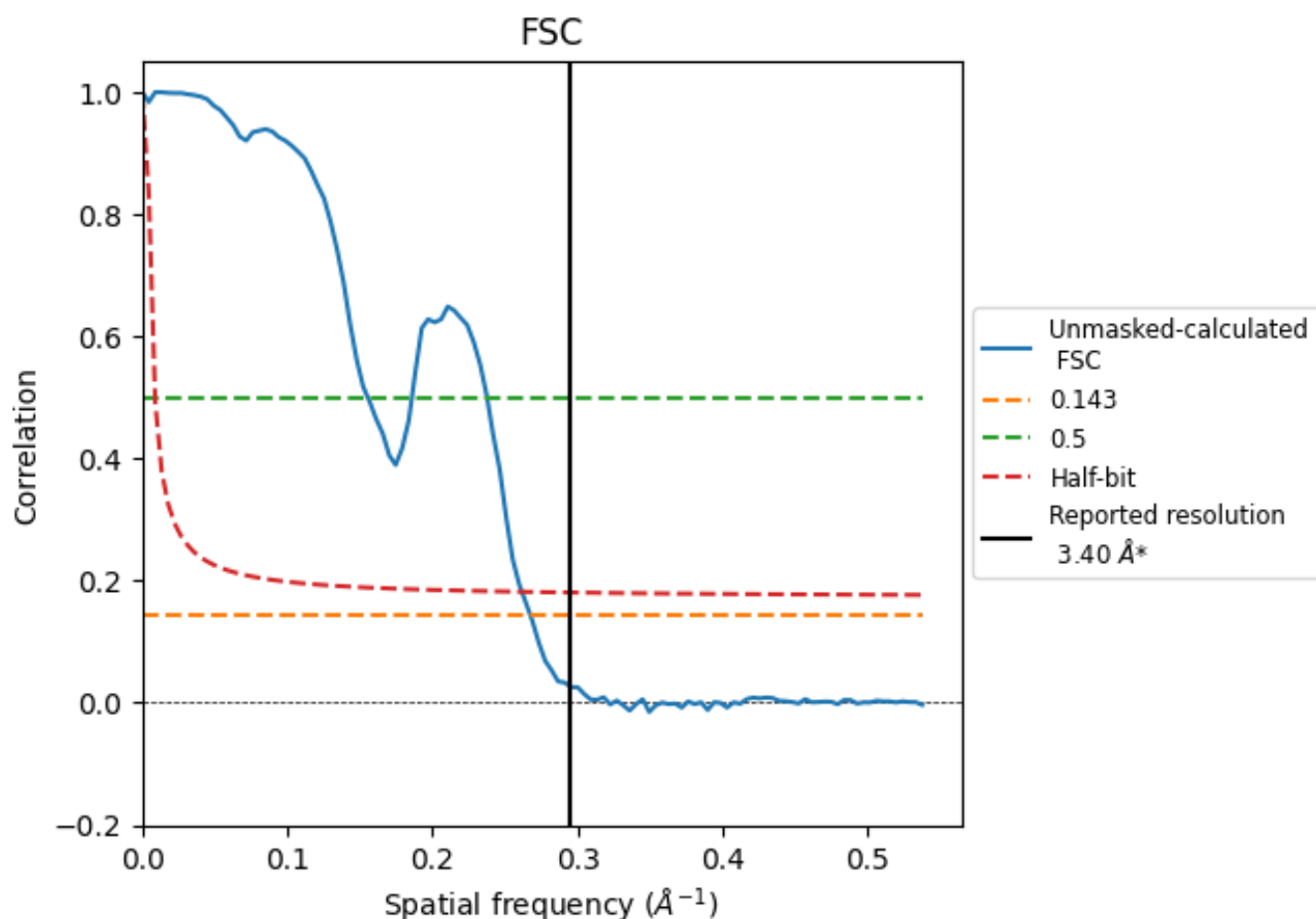


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

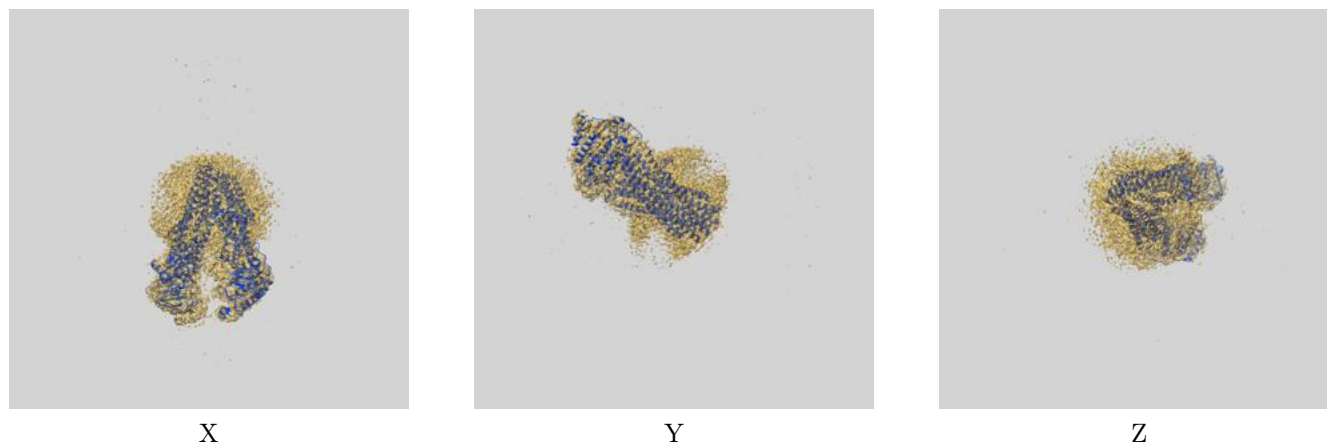
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.74	6.43	3.82

*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 3.74 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

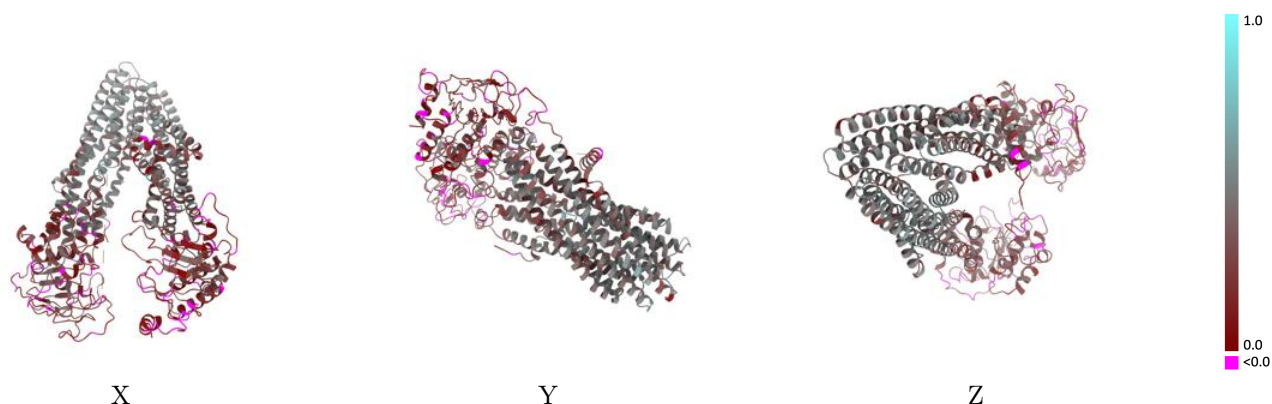
This section contains information regarding the fit between EMDB map EMD-61827 and PDB model 9JUU. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



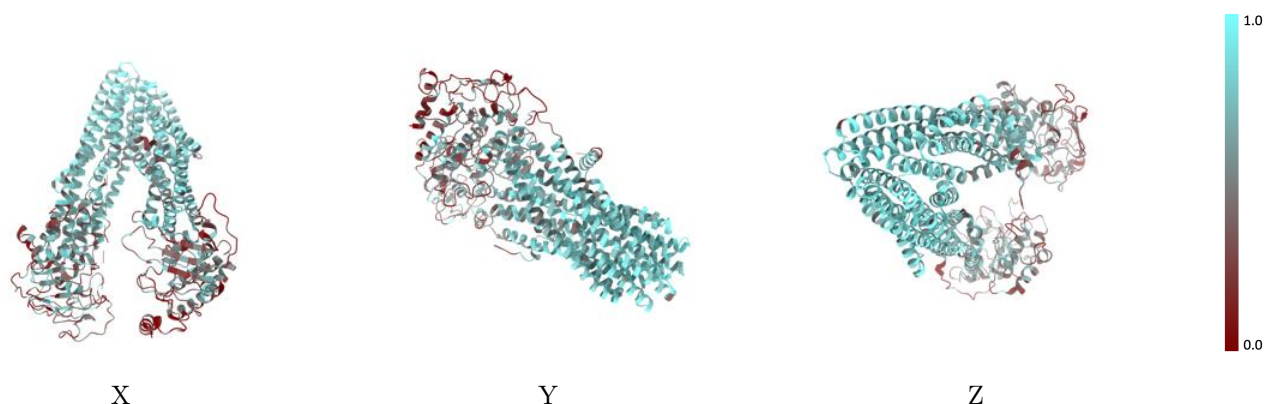
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



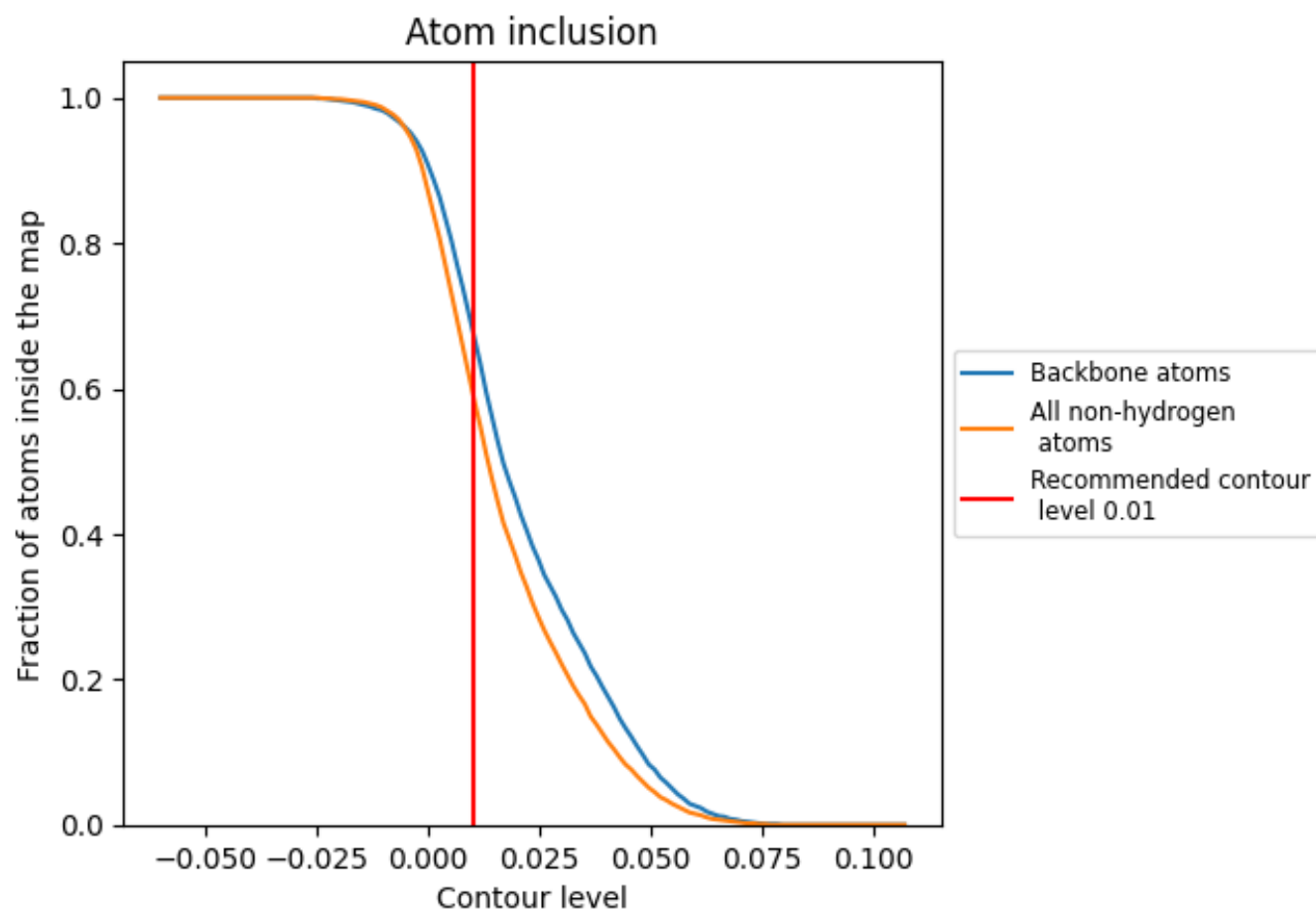
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 59% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5910	0.2970
A	0.5910	0.2970

