



Full wwPDB EM Validation Report ⓘ

Mar 12, 2025 – 02:22 PM JST

PDB ID : 9JUN
EMDB ID : EMD-61831
Title : Structure of Arabidopsis thaliana ABCB1 in the inward-facing conformation under IAA condition
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.dev117
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.2

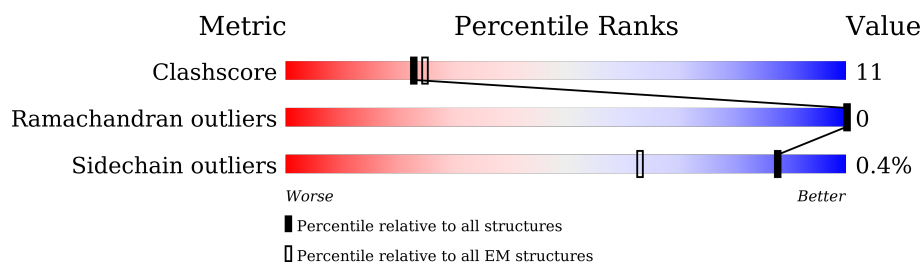
1 Overall quality at a glance

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	<div> <div>37%</div> <div>65%</div> <div>23%</div> <div>12%</div> </div>

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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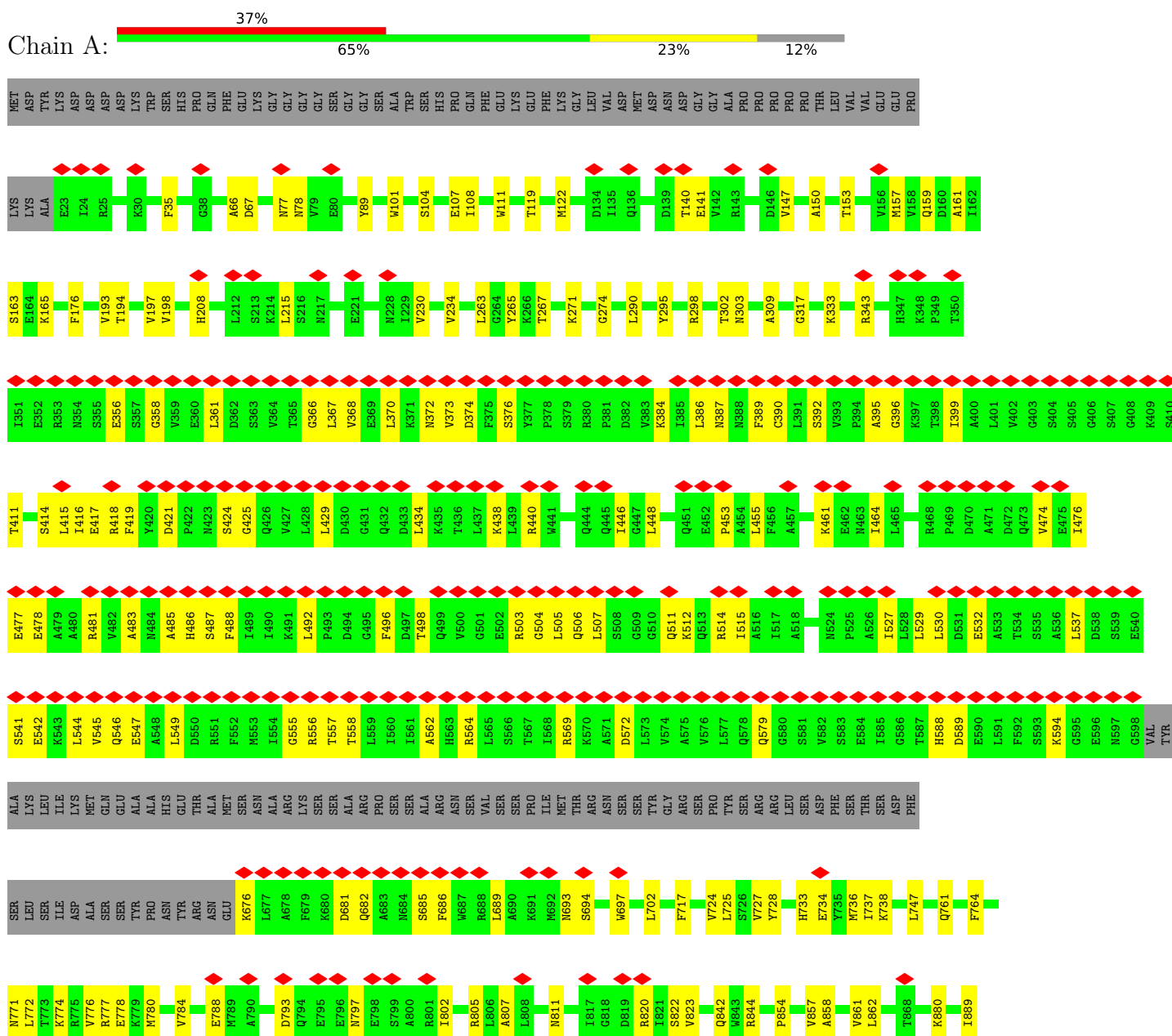
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	HIS	-	expression tag	UNP Q9ZR72
A	-11	PRO	-	expression tag	UNP Q9ZR72
A	-10	GLN	-	expression tag	UNP Q9ZR72
A	-9	PHE	-	expression tag	UNP Q9ZR72
A	-8	GLU	-	expression tag	UNP Q9ZR72
A	-7	LYS	-	expression 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



ARG	G931	R1036	A1097	G1160	R1220
VAL	F966	P1037	I1098	V1161	L1221
LYS		D1038	R1099	Q1162	S1222
GLU	K970	I1039	K1100	L1163	T1223
ASP	L980	Q1040	H1101	S1164	I1224
ALA	T981	I1041	I1102	G1165	R1225
	L982	F1042	A1103	G1166	N1226
	A983	R1043	I1104	G1167	A1227
	F986	D1044	V1105	K1168	H1228
	I987	Q1107	P1106	Q1169	V1229
	K988	L1045	E1108	R1170	I1230
	F991	S1046	P1109	I1171	A1231
	A992	L1047	C1110	A1172	V1232
	K993	R1048	L1111	I1173	I1233
	R994	A1049	T1114	A1174	D1234
	S995	R1050	T1115	R1175	D1235
	E998	A1051	I1116	A1176	G1236
	L999	G1052	Y1117	V1178	K1237
	L1000	K1053	E1118	R1179	V1238
	D1001	T1054	N1119	K1180	A1239
	R1002	L1055	I1120	A1181	E1240
	K1003	A1056	H1124	E1182	Q1241
	T1004	L1057	E1125	I1183	G1242
	E1005	V1058	C1126	M1184	S1243
	I1006	G1059	A1127	L1185	H1244
	E1007	P1060	T1128	L1186	S1245
	P1008	S1061	E1129	D1187	H1246
	D1009	G1062	A1130	E1188	L1247
	D1010	C1063	E1131	A1189	L1248
	P1011	G1064	I1132	T1190	K1249
	D1012	K1065	I1133	S1191	N1250
	T1013	S1066	Q1134	A1192	H1251
	T1014	I1069	A1135	L1193	P1252
	P1015	S1070	A1136	D1194	D1253
	V1016	L1071	T1137	A1195	G1254
	P1017	I1072	L1138	E1196	I1255
	D1018	Q1073	A1139	S1197	Y1256
	R1019	R1074	S1140	E1198	A1257
	L1020	F1075	A1141	R1199	R1258
	R1021	Y1076	H1142	S1200	M1259
	E1023	E1077	K1143	V1201	I1260
	V1024	P1078	F1144	Q1202	Q1261
	E1025	S1079	I1145	E1203	L1262
	L1026	G1081	S1146	A1204	Q1263
	K1027	R1082	A1147	L1205	R1264
	H1028	V1083	L1148	D1206	PHE
	I1029	M1084	P1149	Q1207	THR
	D1030	I1085	E1150	A1208	HIS
	F1031	D1086	G1151	C1209	THR
	S1032	G1087	Y1152	S1210	GLN
	Y1033	K1088	K1153	G1211	VAL
	P1034	D1089	T1154	R1212	ILE
	S1035	I1090	Y1155	T1213	GLY
		R1091	V1156	S1214	MET
		K1092	G1157	I1215	THR
		Y1093	E1158	V1216	SER
		N1094	R1159	V1217	GLY
		L1095		A1218	SER
		K1096		H1219	SER

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	131005	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 ($e^-/\text{\AA}^2$)	50	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	0.128	Depositor
Minimum map value	-0.080	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.025	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	0.26	0/9137	0.48	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	198	0
All	All	8971	0	9116	198	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 11.

All (198) 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:1025:GLU:HB2	1:A:1084:MET:HB3	1.57	0.85
1:A:215:LEU:HB3	1:A:267:THR:HG22	1.58	0.83
1:A:1170:ARG:NH2	1:A:1200:SER:OG	2.21	0.73
1:A:820:ARG:HD3	1:A:986:PHE:HB2	1.71	0.73
1:A:298:ARG:NH1	1:A:737:ILE:HG12	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:805:ARG:NH2	1:A:998:GLU:OE2	2.26	0.68
1:A:358:GLY:HA3	1:A:438:LYS:HG2	1.74	0.68
1:A:418:ARG:NH1	1:A:434:LEU:O	2.27	0.67
1:A:1099:ARG:O	1:A:1179:ARG:NH1	2.30	0.65
1:A:119:THR:HG21	1:A:159:GLN:HB2	1.77	0.65
1:A:150:ALA:HA	1:A:153:THR:HG22	1.78	0.64
1:A:776:VAL:O	1:A:780:MET:HG3	1.97	0.64
1:A:823:VAL:HG11	1:A:982:LEU:HD12	1.79	0.63
1:A:295:TYR:HA	1:A:298:ARG:HH21	1.63	0.62
1:A:1029:ILE:HB	1:A:1045:LEU:HB3	1.81	0.61
1:A:481:ARG:HD3	1:A:485:ALA:HA	1.82	0.61
1:A:1124:HIS:HB3	1:A:1127:ALA:HB2	1.82	0.60
1:A:461:LYS:HB3	1:A:496:PHE:HB3	1.82	0.60
1:A:503:ARG:NH1	1:A:506:GLN:OE1	2.35	0.60
1:A:367:LEU:HB3	1:A:395:ALA:HB2	1.83	0.60
1:A:527:ILE:HD12	1:A:556:ARG:HE	1.67	0.60
1:A:1252:PRO:HA	1:A:1256:TYR:HB3	1.83	0.59
1:A:387:ASN:ND2	1:A:579:GLN:O	2.36	0.59
1:A:66:ALA:HB2	1:A:309:ALA:HB2	1.84	0.59
1:A:1050:ARG:NH1	1:A:1051:ALA:O	2.36	0.59
1:A:1104:ILE:HG22	1:A:1106:PRO:HD3	1.83	0.59
1:A:1110:CYS:HB2	1:A:1175:ARG:HH22	1.68	0.58
1:A:727:VAL:HG12	1:A:736:MET:HG3	1.85	0.58
1:A:807:ALA:O	1:A:811:ASN:ND2	2.36	0.58
1:A:820:ARG:CD	1:A:986:PHE:HB2	2.34	0.58
1:A:1025:GLU:OE2	1:A:1048:ARG:NH1	2.31	0.58
1:A:530:LEU:HB3	1:A:558:THR:HA	1.86	0.57
1:A:861:VAL:HG23	1:A:981:THR:HB	1.85	0.57
1:A:761:GLN:NE2	1:A:822:SER:OG	2.37	0.57
1:A:1104:ILE:HD11	1:A:1185:LEU:HD12	1.87	0.57
1:A:527:ILE:HD13	1:A:556:ARG:HH21	1.70	0.56
1:A:1186:LEU:HB2	1:A:1216:VAL:HA	1.86	0.56
1:A:265:TYR:OH	1:A:771:ASN:OD1	2.24	0.55
1:A:1116:ILE:HA	1:A:1119:ASN:HD22	1.69	0.55
1:A:111:TRP:HB3	1:A:163:SER:O	2.06	0.55
1:A:446:ILE:HD13	1:A:527:ILE:HG23	1.89	0.55
1:A:77:ASN:OD1	1:A:78:ASN:N	2.40	0.55
1:A:298:ARG:HH12	1:A:737:ILE:HG12	1.73	0.54
1:A:780:MET:HE3	1:A:999:LEU:HD23	1.88	0.54
1:A:107:GLU:HG3	1:A:108:ILE:N	2.23	0.53
1:A:366:GLY:O	1:A:556:ARG:NH2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1085:ILE:HG21	1:A:1090:ILE:HD11	1.89	0.53
1:A:390:CYS:SG	1:A:392:SER:OG	2.66	0.53
1:A:481:ARG:HA	1:A:485:ALA:HA	1.91	0.53
1:A:147:VAL:HG12	1:A:889:ILE:HD13	1.90	0.53
1:A:455:LEU:HD11	1:A:515:ILE:HG21	1.91	0.53
1:A:1220:ARG:NE	1:A:1222:SER:O	2.41	0.53
1:A:368:VAL:HG12	1:A:429:LEU:HG	1.90	0.53
1:A:1188:GLU:HA	1:A:1218:ALA:HA	1.91	0.53
1:A:453:PRO:HG2	1:A:512:LYS:HG3	1.92	0.52
1:A:564:ARG:HH21	1:A:594:LYS:HB2	1.74	0.52
1:A:793:ASP:OD2	1:A:1076:TYR:OH	2.22	0.52
1:A:1052:GLY:N	1:A:1213:THR:OG1	2.38	0.52
1:A:733:HIS:O	1:A:737:ILE:HG13	2.11	0.51
1:A:1026:LEU:O	1:A:1029:ILE:HG12	2.09	0.51
1:A:1117:TYR:HB2	1:A:1152:TYR:HB3	1.93	0.51
1:A:483:ALA:O	1:A:514:ARG:NH2	2.29	0.51
1:A:356:GLU:HG3	1:A:440:ARG:HH12	1.74	0.51
1:A:1013:THR:HG21	1:A:1094:ASN:HB2	1.91	0.51
1:A:1114:THR:HG23	1:A:1115:THR:HG23	1.93	0.51
1:A:399:ILE:HG23	1:A:557:THR:HG23	1.91	0.51
1:A:805:ARG:NH2	1:A:999:LEU:HB2	2.26	0.50
1:A:464:ILE:HG21	1:A:476:ILE:HG23	1.92	0.50
1:A:1024:VAL:HG12	1:A:1085:ILE:HG13	1.94	0.50
1:A:474:VAL:O	1:A:478:GLU:HG2	2.11	0.50
1:A:504:GLY:N	1:A:506:GLN:OE1	2.44	0.50
1:A:1069:ILE:HD12	1:A:1185:LEU:HB3	1.93	0.50
1:A:374:ASP:HB3	1:A:421:ASP:O	2.11	0.50
1:A:854:PRO:HA	1:A:857:VAL:HG22	1.92	0.50
1:A:995:SER:O	1:A:998:GLU:HG3	2.11	0.50
1:A:1026:LEU:HB2	1:A:1047:LEU:HB3	1.93	0.49
1:A:505:LEU:HD12	1:A:507:LEU:H	1.78	0.49
1:A:290:LEU:HD13	1:A:724:VAL:HG21	1.94	0.49
1:A:295:TYR:HA	1:A:298:ARG:HE	1.76	0.49
1:A:1082:ARG:NH1	1:A:1089:ASP:OD1	2.39	0.49
1:A:1059:GLY:HA2	1:A:1232:VAL:HG13	1.95	0.49
1:A:1090:ILE:HD12	1:A:1098:ILE:HG13	1.94	0.49
1:A:777:ARG:NH2	1:A:811:ASN:OD1	2.46	0.48
1:A:682:GLN:HG2	1:A:686:PHE:HE2	1.78	0.48
1:A:572:ASP:OD1	1:A:572:ASP:N	2.47	0.48
1:A:492:LEU:HD13	1:A:498:THR:HG21	1.95	0.48
1:A:1012:ASP:OD1	1:A:1012:ASP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1062:GLY:H	1:A:1065:LYS:HD3	1.79	0.48
1:A:1027:LYS:HG3	1:A:1082:ARG:HB2	1.95	0.48
1:A:263:LEU:O	1:A:267:THR:HG23	2.14	0.48
1:A:988:LYS:O	1:A:991:GLN:HG3	2.13	0.48
1:A:1254:GLY:O	1:A:1258:ARG:NH1	2.45	0.47
1:A:1073:GLN:HE22	1:A:1102:ILE:HG21	1.78	0.47
1:A:532:GLU:HG3	1:A:562:ALA:H	1.78	0.47
1:A:1028:HIS:O	1:A:1081:GLY:HA2	2.14	0.47
1:A:208:HIS:HE1	1:A:271:LYS:HA	1.80	0.47
1:A:373:VAL:O	1:A:424:SER:OG	2.30	0.47
1:A:370:LEU:HD21	1:A:373:VAL:HG12	1.97	0.47
1:A:416:ILE:HG21	1:A:529:LEU:HD21	1.96	0.47
1:A:35:PHE:CD1	1:A:122:MET:HB2	2.49	0.47
1:A:1217:VAL:HG13	1:A:1218:ALA:H	1.79	0.47
1:A:1217:VAL:HG13	1:A:1218:ALA:N	2.30	0.46
1:A:1221:LEU:HD11	1:A:1263:GLN:HB3	1.97	0.46
1:A:477:GLU:HB3	1:A:481:ARG:HH21	1.80	0.46
1:A:1073:GLN:NE2	1:A:1104:ILE:HD11	2.30	0.46
1:A:372:ASN:HB2	1:A:425:GLY:HA3	1.98	0.46
1:A:681:ASP:OD1	1:A:682:GLN:N	2.48	0.46
1:A:685:SER:HB3	1:A:993:MET:SD	2.56	0.46
1:A:1078:PRO:HB2	1:A:1081:GLY:H	1.82	0.46
1:A:176:PHE:HA	1:A:317:GLY:HA2	1.98	0.45
1:A:483:ALA:HB1	1:A:514:ARG:HE	1.80	0.45
1:A:487:SER:OG	1:A:488:PHE:N	2.46	0.45
1:A:1135:ALA:HA	1:A:1138:LEU:HD12	1.96	0.45
1:A:589:ASP:N	1:A:589:ASP:OD1	2.50	0.45
1:A:1116:ILE:HG13	1:A:1156:VAL:HG11	1.99	0.45
1:A:208:HIS:ND1	1:A:274:GLY:HA3	2.32	0.45
1:A:1006:ILE:HD12	1:A:1074:ARG:HG2	1.97	0.45
1:A:1107:GLN:HG3	1:A:1108:GLU:OE2	2.17	0.45
1:A:157:MET:HG2	1:A:333:LYS:HB3	1.98	0.45
1:A:693:ASN:HD22	1:A:772:LEU:HB2	1.82	0.45
1:A:725:LEU:O	1:A:728:TYR:HB2	2.16	0.45
1:A:537:LEU:HD12	1:A:537:LEU:HA	1.87	0.45
1:A:717:PHE:HD1	1:A:747:LEU:HD11	1.80	0.45
1:A:1074:ARG:HE	1:A:1090:ILE:HG22	1.82	0.45
1:A:1260:ILE:HG22	1:A:1264:ARG:HH21	1.80	0.45
1:A:417:GLU:OE1	1:A:448:LEU:HB2	2.16	0.45
1:A:1187:ASP:OD1	1:A:1188:GLU:N	2.47	0.45
1:A:411:THR:O	1:A:415:LEU:HD23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1010:ASP:H	1:A:1094:ASN:HD22	1.63	0.44
1:A:396:GLY:N	1:A:556:ARG:HH12	2.16	0.44
1:A:1065:LYS:HE3	1:A:1065:LYS:HB2	1.71	0.44
1:A:302:THR:OG1	1:A:303:ASN:N	2.50	0.44
1:A:483:ALA:HB1	1:A:514:ARG:NE	2.32	0.44
1:A:1053:LYS:HE3	1:A:1228:HIS:HB2	2.00	0.44
1:A:545:VAL:O	1:A:549:LEU:HB2	2.18	0.44
1:A:373:VAL:HG11	1:A:386:LEU:HG	1.99	0.44
1:A:1129:GLU:O	1:A:1133:ILE:HG12	2.18	0.44
1:A:418:ARG:O	1:A:418:ARG:HG3	2.18	0.43
1:A:1223:THR:HB	1:A:1225:ARG:HH12	1.83	0.43
1:A:966:PHE:O	1:A:970:MET:HG2	2.18	0.43
1:A:1174:ALA:O	1:A:1178:VAL:HG23	2.19	0.43
1:A:1184:MET:HB2	1:A:1212:ARG:HH22	1.83	0.43
1:A:386:LEU:HD11	1:A:389:PHE:HE2	1.83	0.43
1:A:511:GLN:O	1:A:515:ILE:HG12	2.19	0.43
1:A:1170:ARG:HH22	1:A:1197:SER:HA	1.84	0.43
1:A:477:GLU:HB3	1:A:481:ARG:NH2	2.34	0.43
1:A:702:LEU:HD22	1:A:764:PHE:CE2	2.54	0.42
1:A:1089:ASP:HB3	1:A:1092:LYS:HG2	1.99	0.42
1:A:1116:ILE:O	1:A:1120:ILE:HD12	2.19	0.42
1:A:734:GLU:O	1:A:738:LYS:HG2	2.19	0.42
1:A:1074:ARG:NE	1:A:1090:ILE:HG22	2.33	0.42
1:A:104:SER:HA	1:A:107:GLU:HG2	2.02	0.42
1:A:477:GLU:OE1	1:A:486:HIS:NE2	2.50	0.42
1:A:140:THR:OG1	1:A:141:GLU:OE1	2.36	0.42
1:A:215:LEU:HD23	1:A:215:LEU:HA	1.94	0.42
1:A:101:TRP:CD1	1:A:931:GLY:HA3	2.55	0.42
1:A:361:LEU:HD21	1:A:429:LEU:HD22	2.02	0.42
1:A:374:ASP:O	1:A:415:LEU:HD21	2.19	0.42
1:A:527:ILE:HA	1:A:556:ARG:HG3	2.01	0.42
1:A:980:LEU:HD23	1:A:980:LEU:HA	1.89	0.42
1:A:1041:ILE:HG22	1:A:1042:PHE:H	1.85	0.42
1:A:161:ALA:HA	1:A:165:LYS:HB2	2.01	0.42
1:A:544:LEU:HA	1:A:547:GLU:HG3	2.00	0.42
1:A:555:GLY:C	1:A:556:ARG:HD2	2.40	0.42
1:A:1003:LYS:HD3	1:A:1003:LYS:HA	1.85	0.42
1:A:569:ARG:NH1	1:A:588:HIS:O	2.32	0.42
1:A:1251:HIS:N	1:A:1252:PRO:HD2	2.35	0.42
1:A:689:LEU:HD22	1:A:993:MET:HG3	2.02	0.42
1:A:1023:GLU:HA	1:A:1049:ALA:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:842:GLN:HE21	1:A:844:ARG:H	1.68	0.42
1:A:194:THR:O	1:A:198:VAL:HG23	2.20	0.42
1:A:193:VAL:O	1:A:197:VAL:HG23	2.20	0.41
1:A:376:SER:HB2	1:A:384:LYS:NZ	2.35	0.41
1:A:1101:HIS:O	1:A:1102:ILE:HD13	2.20	0.41
1:A:880:LYS:HB3	1:A:880:LYS:HE2	1.69	0.41
1:A:694:SER:HA	1:A:697:TRP:NE1	2.35	0.41
1:A:1155:TYR:CD2	1:A:1160:GLY:HA2	2.55	0.41
1:A:492:LEU:HD23	1:A:492:LEU:HA	1.86	0.41
1:A:1105:VAL:O	1:A:1105:VAL:HG23	2.20	0.41
1:A:780:MET:O	1:A:784:VAL:HG23	2.20	0.41
1:A:1057:LEU:O	1:A:1217:VAL:HA	2.19	0.41
1:A:1109:PRO:HB2	1:A:1168:LYS:HE2	2.03	0.41
1:A:67:ASP:HB3	1:A:89:TYR:CZ	2.55	0.41
1:A:230:VAL:O	1:A:234:VAL:HG12	2.21	0.41
1:A:541:SER:O	1:A:545:VAL:HG23	2.21	0.41
1:A:1168:LYS:HA	1:A:1171:ILE:HD12	2.03	0.41
1:A:414:SER:HB3	1:A:419:PHE:HD2	1.86	0.41
1:A:542:GLU:O	1:A:546:GLN:OE1	2.38	0.41
1:A:774:LYS:NZ	1:A:778:GLU:OE2	2.41	0.41
1:A:1006:ILE:CD1	1:A:1074:ARG:HG2	2.50	0.41
1:A:1234:ASP:O	1:A:1237:LYS:NZ	2.33	0.41
1:A:788:GLU:HG3	1:A:1006:ILE:HG22	2.02	0.40
1:A:858:ALA:O	1:A:862:LEU:HD23	2.21	0.40
1:A:1201:VAL:O	1:A:1205:LEU:HG	2.21	0.40
1:A:797:ASN:HA	1:A:802:ILE:HD11	2.03	0.40
1:A:1038:ASP:N	1:A:1038:ASP:OD1	2.54	0.40
1:A:396:GLY:H	1:A:556:ARG:HH12	1.70	0.40
1:A:788:GLU:OE1	1:A:1002:ARG:NH1	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	1094 (94%)	67 (6%)	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%)	945 (100%)	4 (0%)	89	93

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	343	ARG
1	A	676	LYS
1	A	1050	ARG
1	A	1212	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	842	GLN
1	A	1073	GLN
1	A	1169	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.

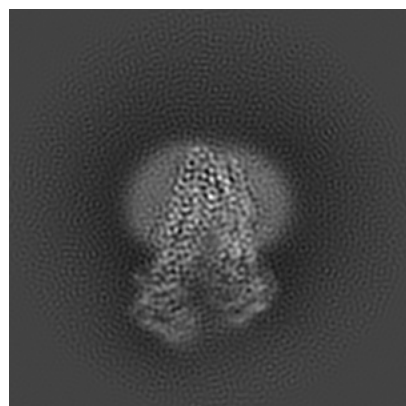
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61831. These allow visual inspection of the internal detail of the map and identification of artifacts.

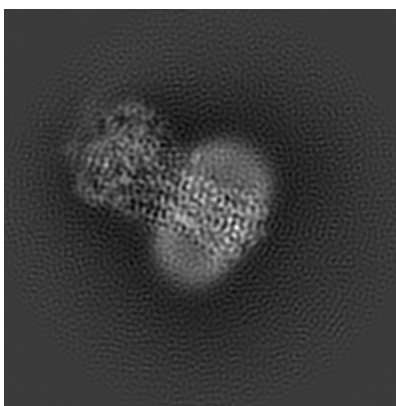
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

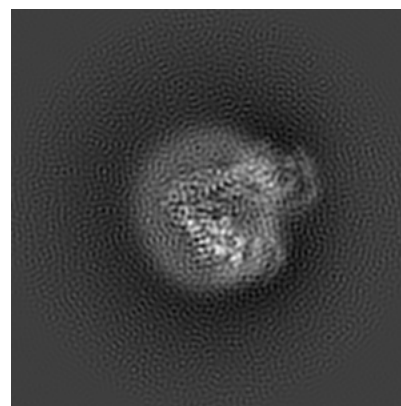
6.1.1 Primary map



X

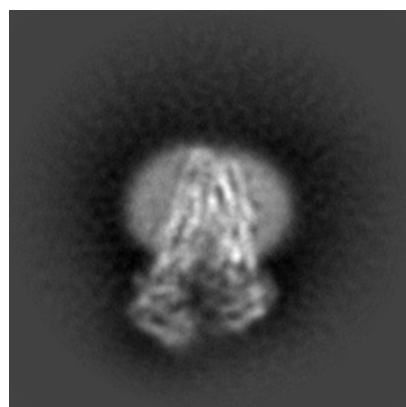


Y

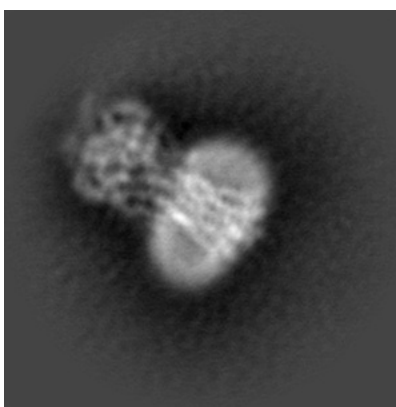


Z

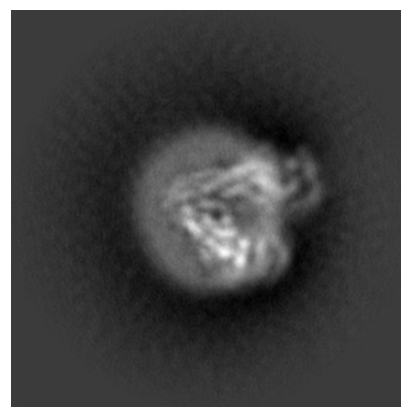
6.1.2 Raw map



X



Y

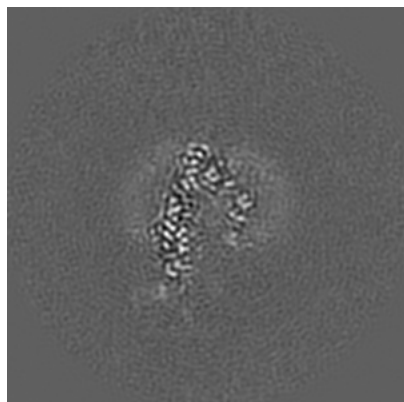


Z

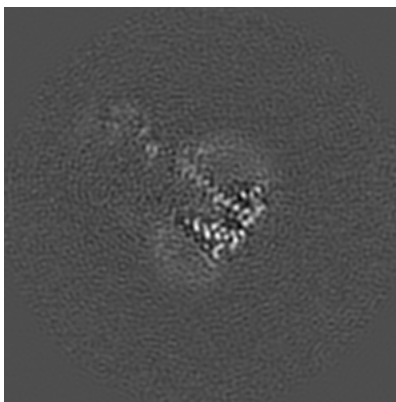
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

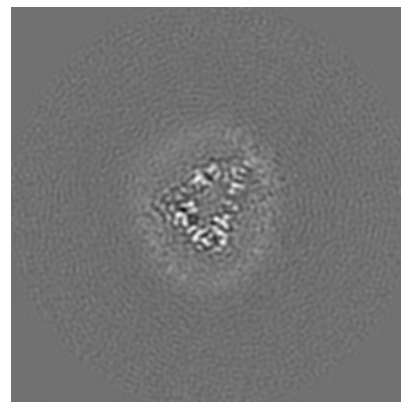
6.2.1 Primary map



X Index: 120

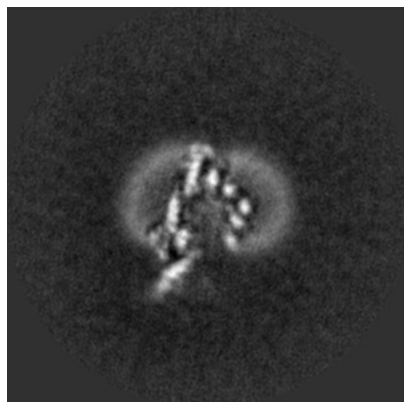


Y Index: 120



Z Index: 120

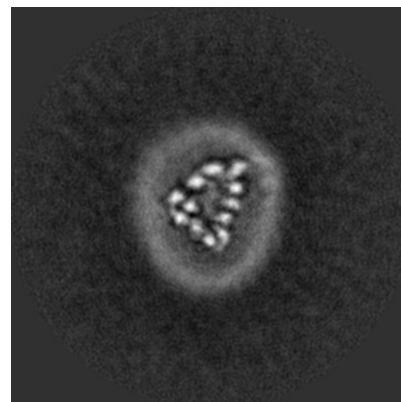
6.2.2 Raw map



X Index: 120



Y Index: 120

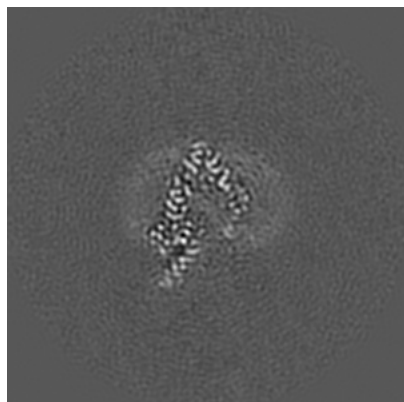


Z Index: 120

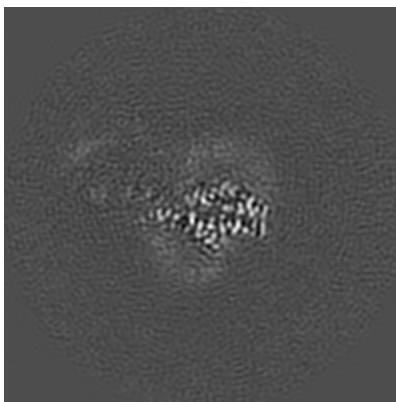
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

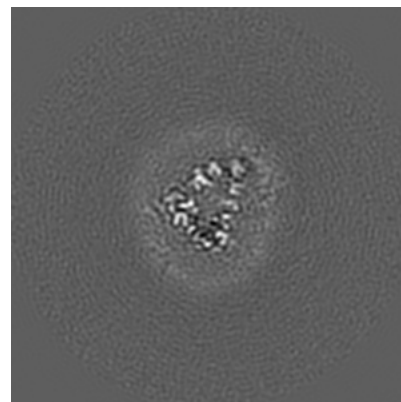
6.3.1 Primary map



X Index: 117

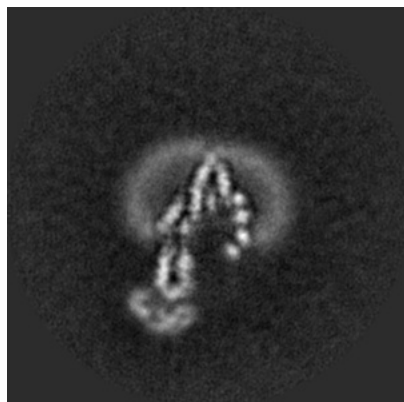


Y Index: 112

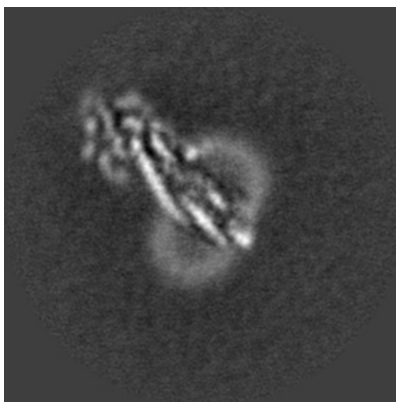


Z Index: 121

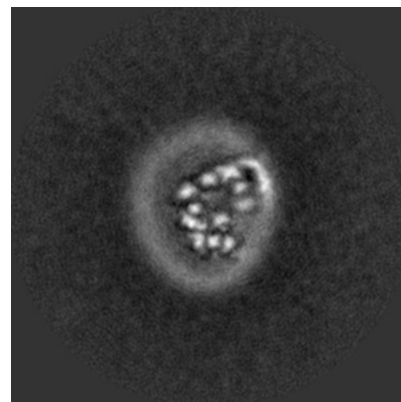
6.3.2 Raw map



X Index: 129



Y Index: 135

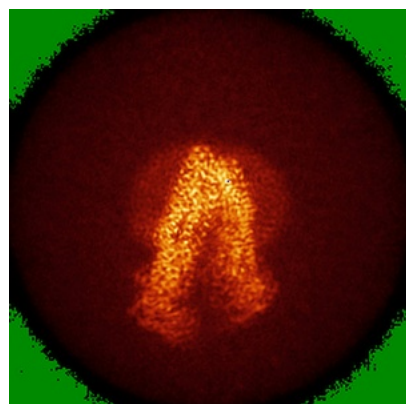


Z Index: 113

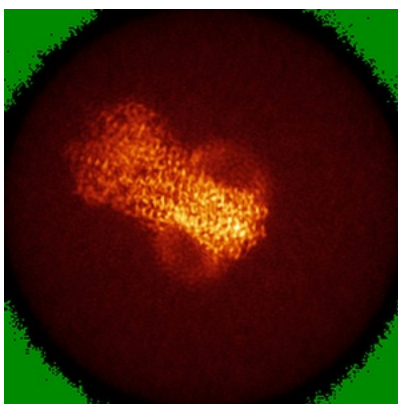
The images above show the largest variance slices of the map in three orthogonal directions.

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

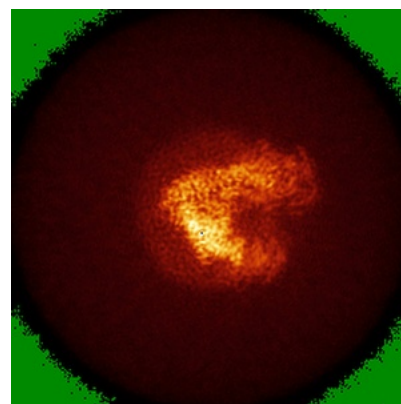
6.4.1 Primary map



X

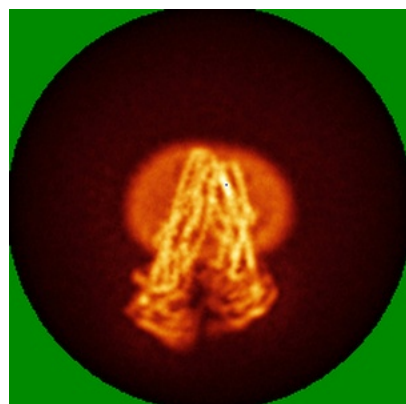


Y

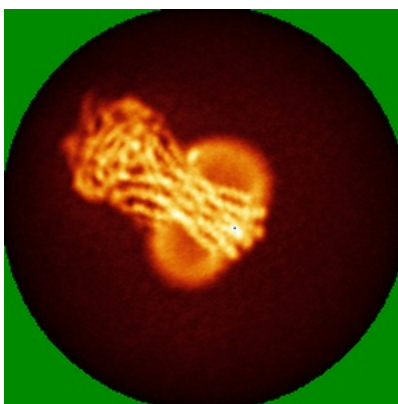


Z

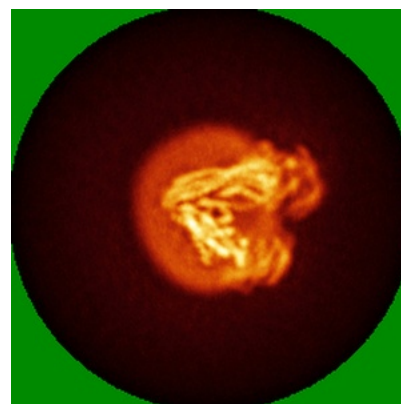
6.4.2 Raw map



X



Y

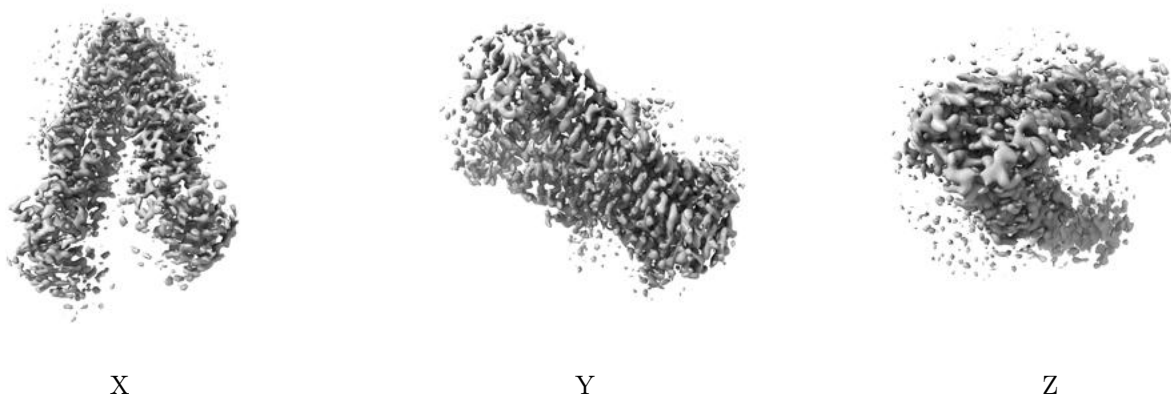


Z

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.

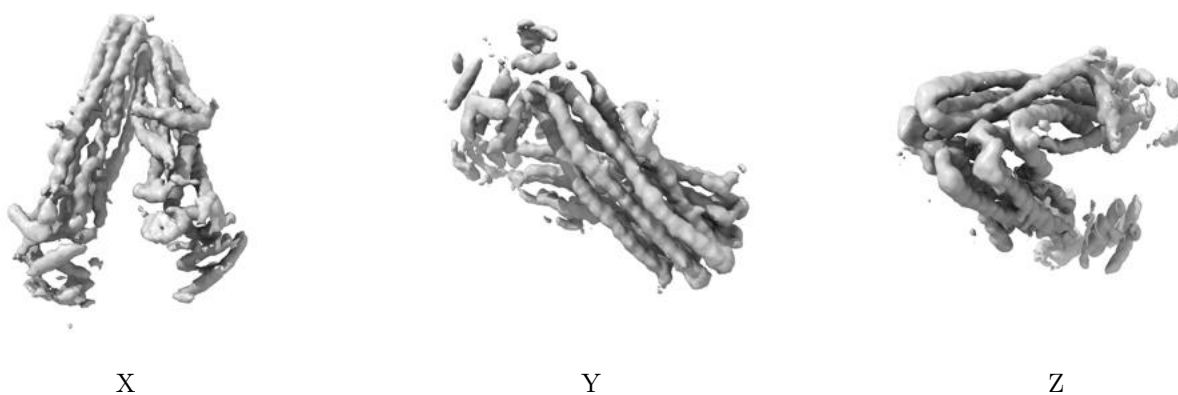
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. 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.

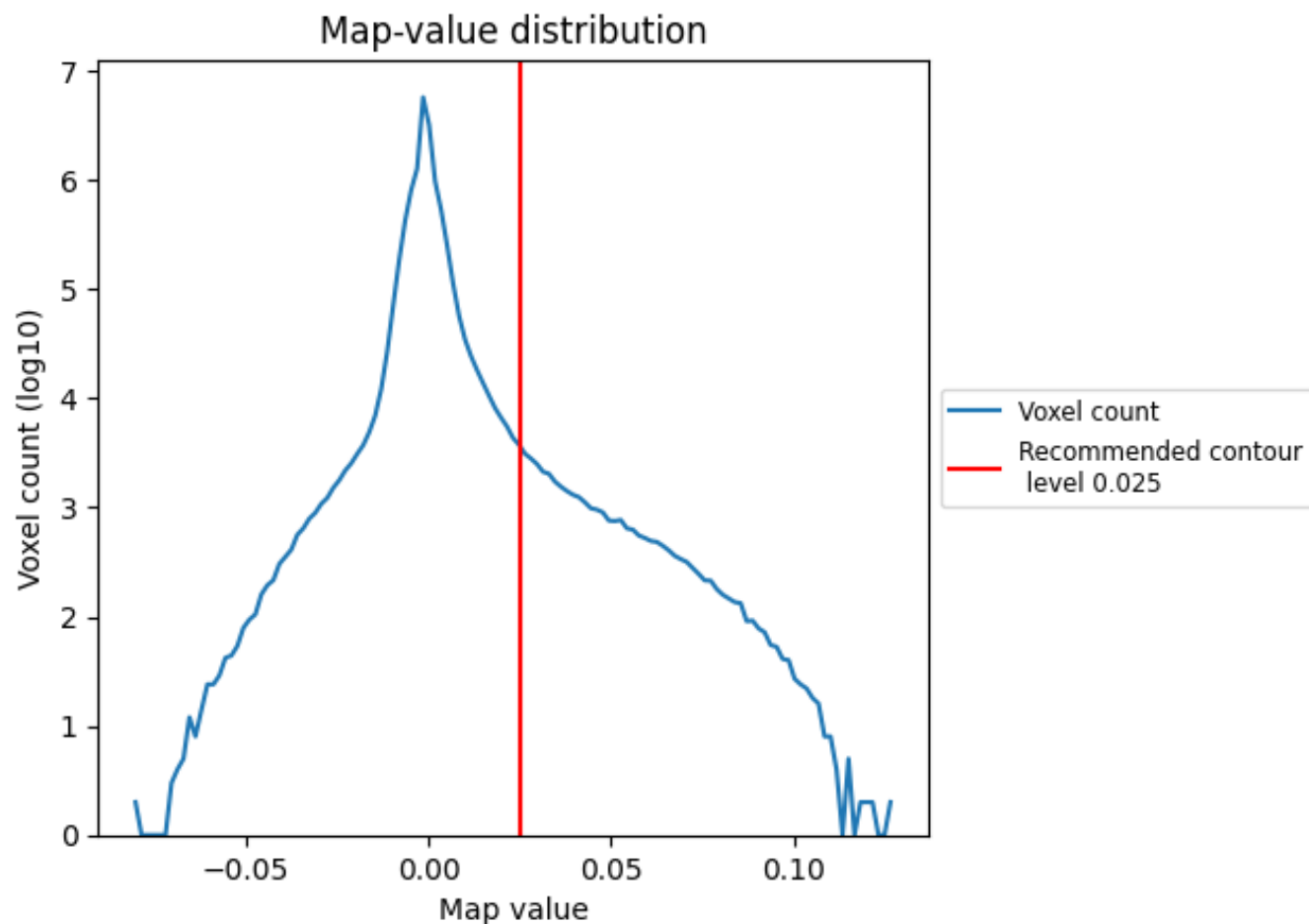
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

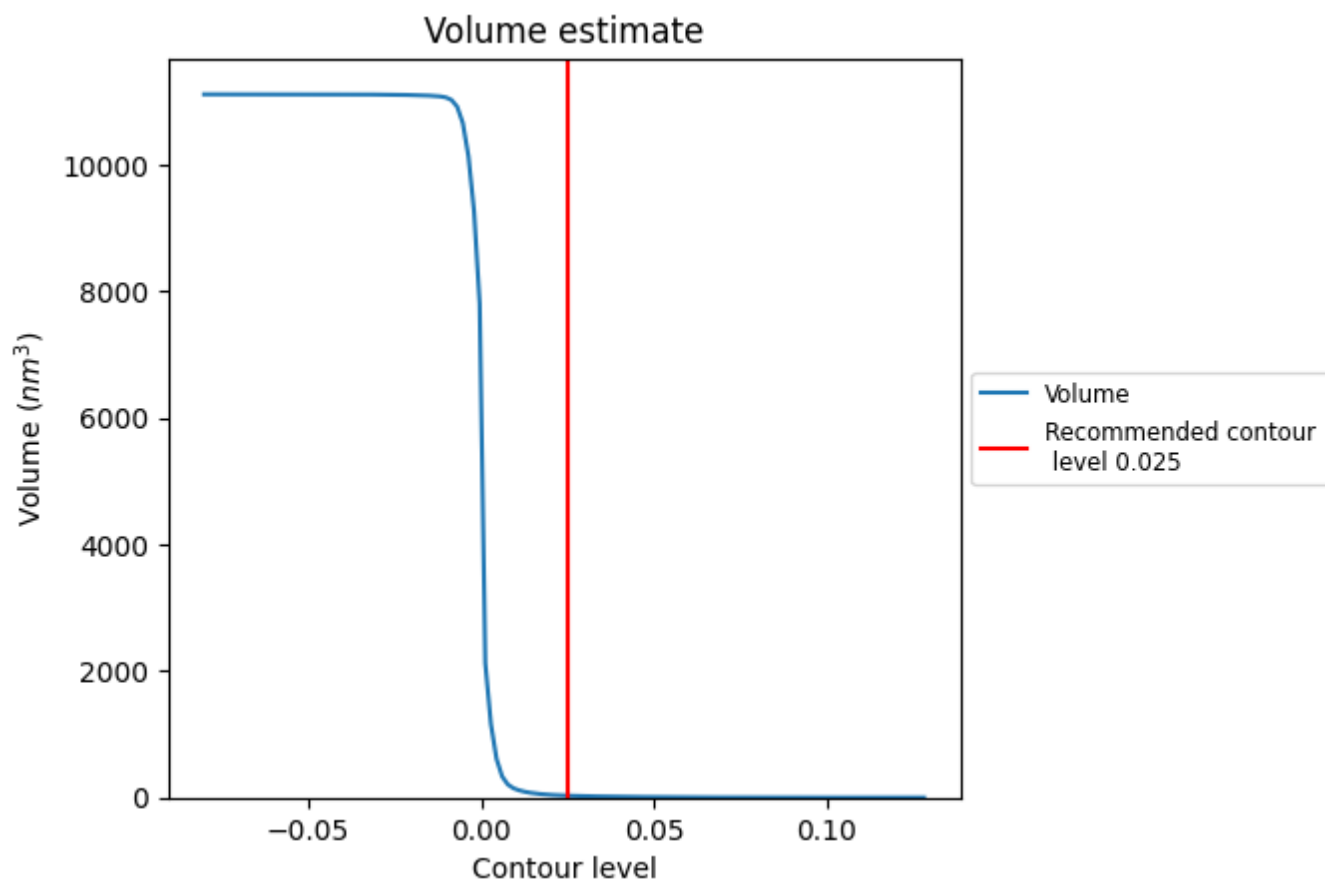
This section contains the results of statistical analysis of the map.

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.

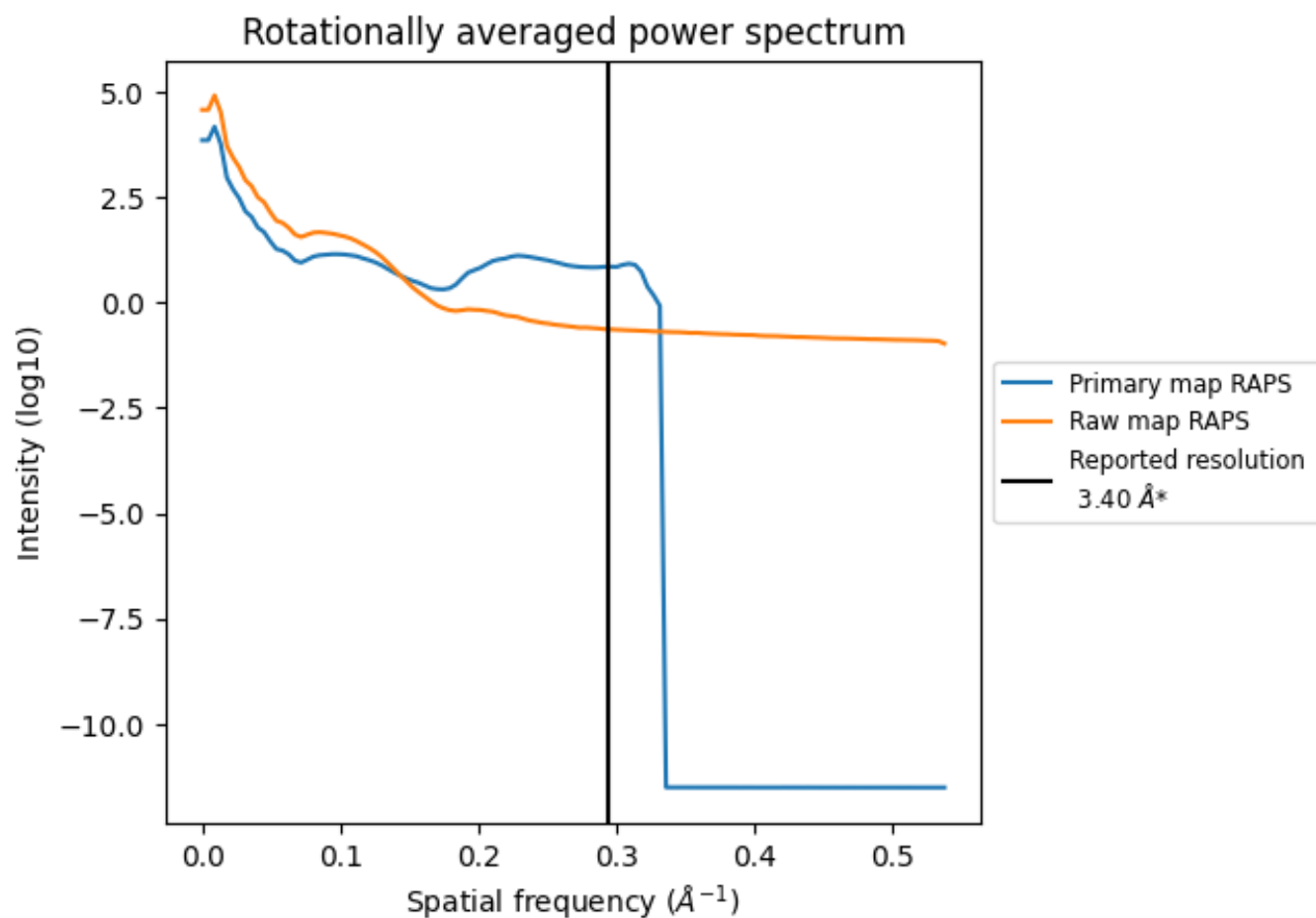
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 30 nm³; this corresponds to an approximate mass of 27 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 ⓘ

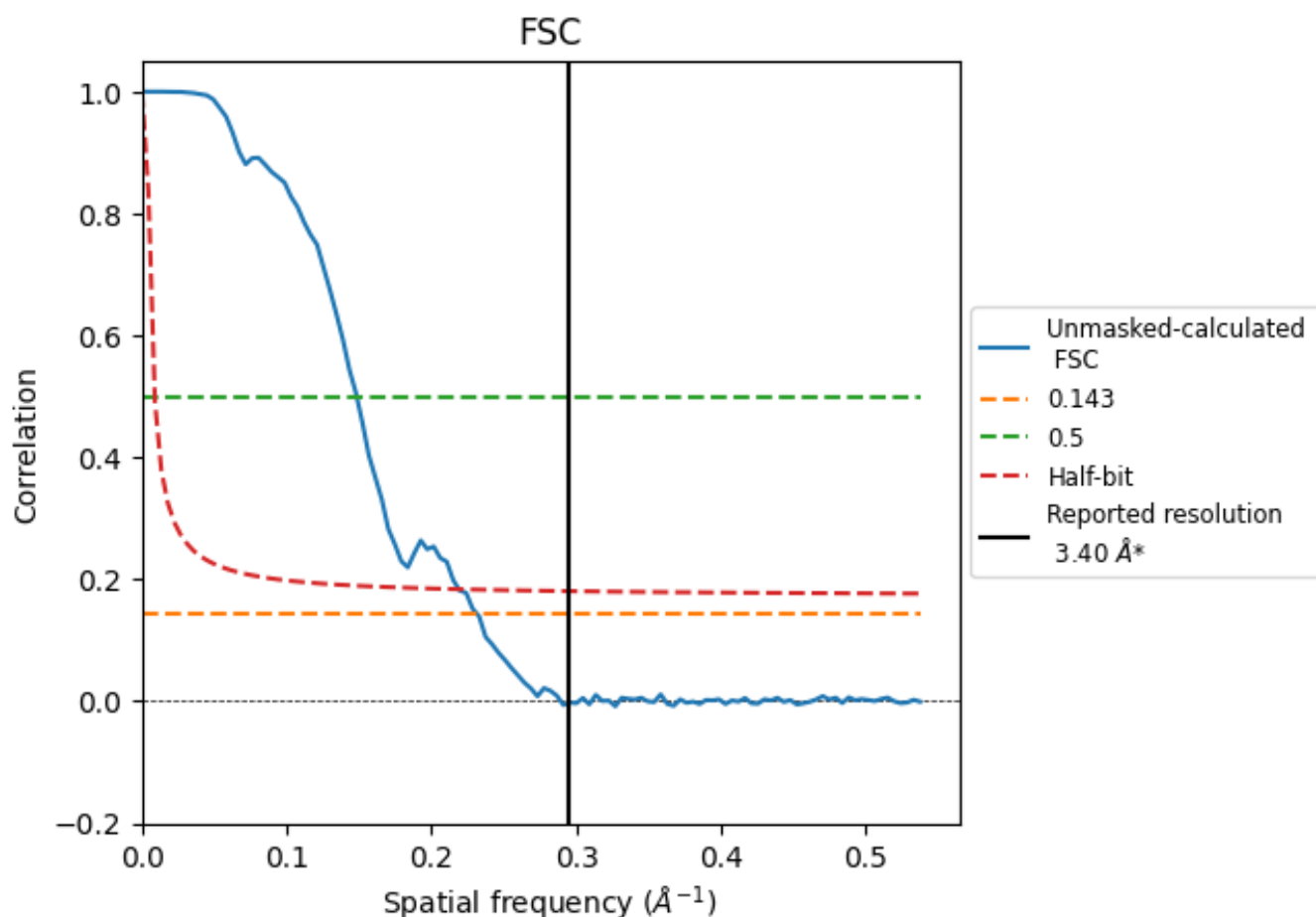


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 \AA^{-1}

8.2 Resolution estimates [i](#)

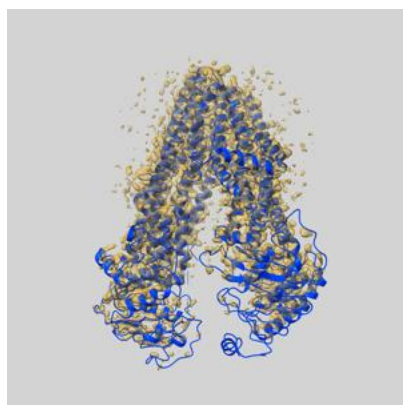
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.32	6.74	4.57

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.32 differs from the reported value 3.4 by more than 10 %

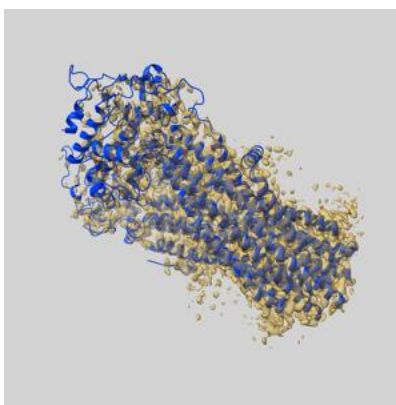
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-61831 and PDB model 9JUN. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

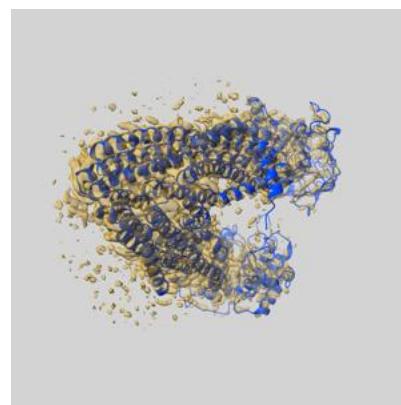
9.1 Map-model overlay [i](#)



X



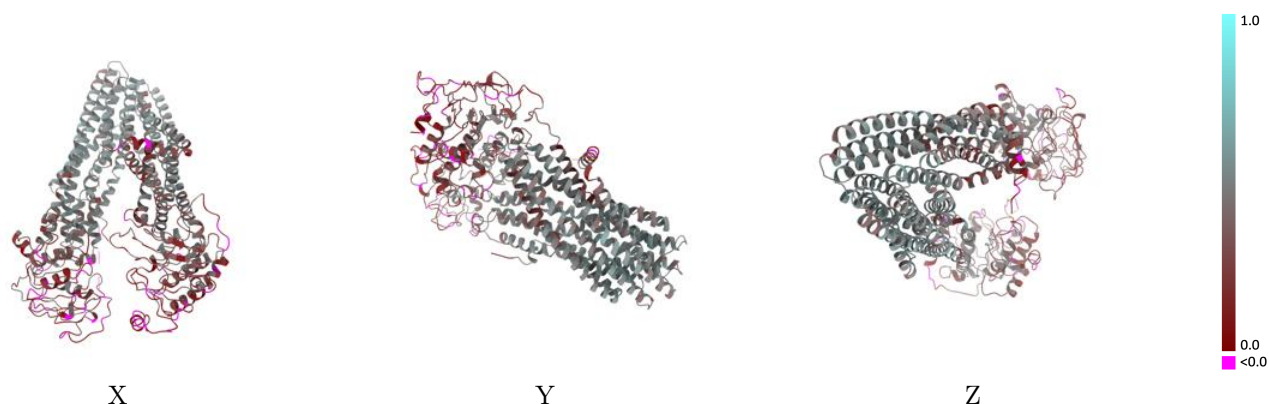
Y



Z

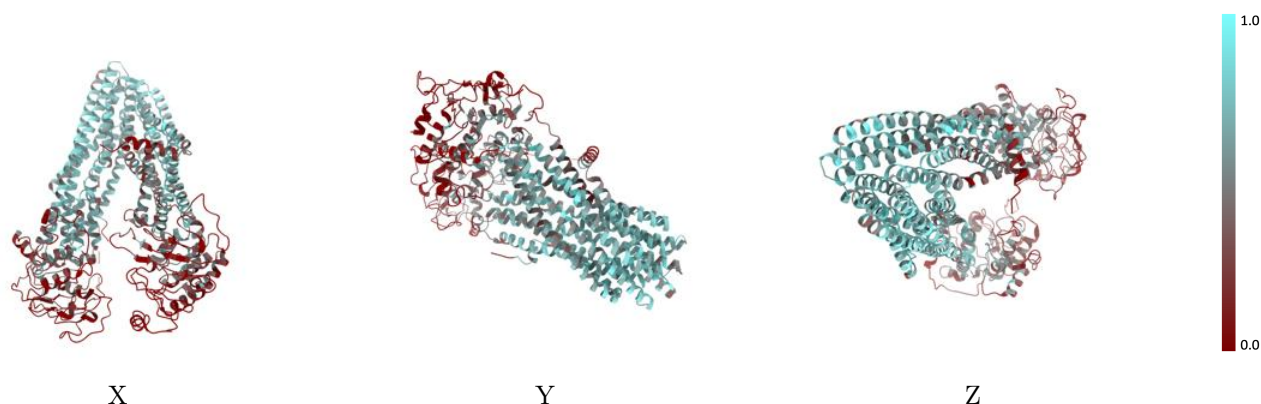
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



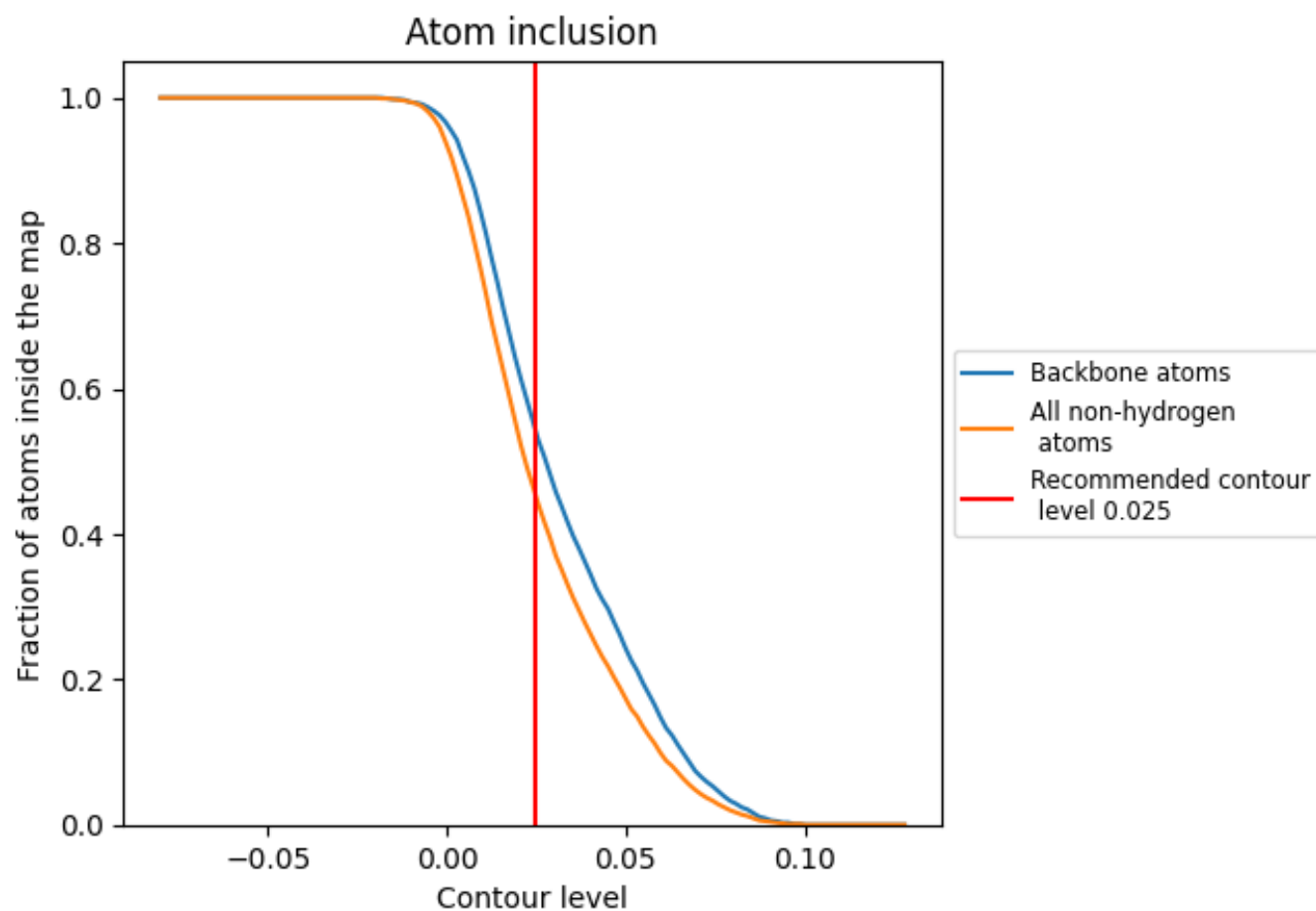
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 45% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4500	<div></div> 0.3620
A	<div></div> 0.4500	<div></div> 0.3620

