



wwPDB EM Validation Summary Report ⓘ

Mar 13, 2024 – 09:45 am GMT

PDB ID : 7ZK9
EMDB ID : EMD-14759
Title : ABCB1 L971C mutant (mABCB1) in the inward facing state
Authors : Parey, K.; Janulienė, D.; Gewering, T.; Zhang, Q.; Moeller, A.
Deposited on : 2022-04-12
Resolution : 4.30 Å (reported)
Based on initial model : 6C0V

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

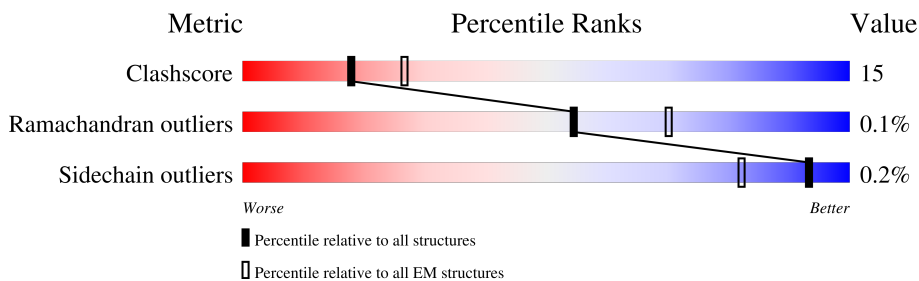
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1260	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8999 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.

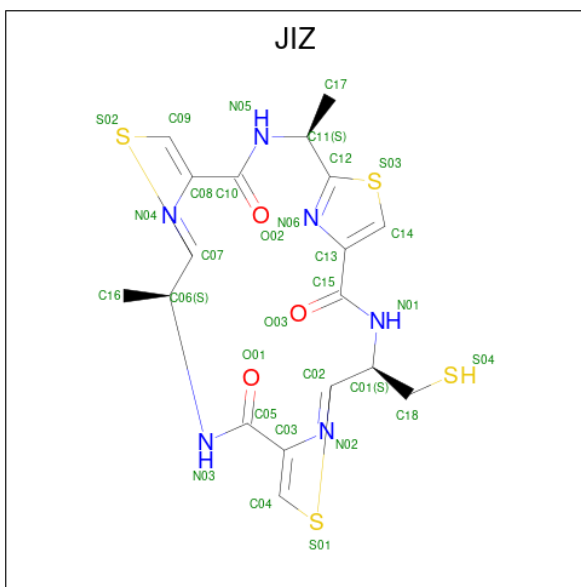
- Molecule 1 is a protein called ATP-dependent translocase ABCB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1157	8968	5763	1527	1648	30	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	GLN	ASN	engineered mutation	UNP P21447
A	87	GLN	ASN	engineered mutation	UNP P21447
A	90	GLN	ASN	engineered mutation	UNP P21447
A	133	ALA	CYS	engineered mutation	UNP P21447
A	427	GLY	CYS	engineered mutation	UNP P21447
A	713	ALA	CYS	engineered mutation	UNP P21447
A	952	ALA	CYS	engineered mutation	UNP P21447
A	971	CYS	LEU	engineered mutation	UNP P21447
A	1070	GLY	CYS	engineered mutation	UNP P21447
A	1121	ARG	CYS	engineered mutation	UNP P21447
A	1223	VAL	CYS	engineered mutation	UNP P21447

- Molecule 2 is (4 {S},11 {S},18 {S})-4,11-dimethyl-18-(sulfanylmethyl)-6,13,20-trithia-3,10,17,22,23,24-hexazatetracyclo[17.2.1.1.1^{5,8}.1^{12,15}]tetracos-1(21),5(24),7,12(23),14,19(22)-hexaene-2,9,16-trione (three-letter code: JIZ) (formula: C₁₈H₁₈N₆O₃S₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
2	A	1	31	18	6	3	4	0

SER	SER	SER	LYS	ASP	SER	GLY	SER	LEU	LEU	ILE	ARG	ARG	ARG	SER	THR	ARG	LYS	SER	ILE	GLY	PRO	HIS	ASP	GLN	ASP	ASP	VAL	P689	F693	W694	R695	K698	S701	W704	F707	V708	I711	F712	A714	I715	I716															
N717	L720	Q721	P722	A723	F724	S725	V726	I727	F728	S729	K730	G738	E742	T743	Q746	N749	L750	F751	L754	I757	I760	I761	S762	F763	I764	I765	F766	F767	L768	Q769	F773	A776	G777	E778	I779	L780	R785	V788	W792	Q795	W799	F800	D801	D802												
P803	K804	N805	T806	T807	L810	N816	A819	Q820	V821	K822	Q834	N835	I836	A837	N838	L839	G840	T841	G842	I843	I844	S846	L847	I848	Y849	G850	L853	T854	L857	L858	A859	I860	I863	I864	A865	I866	A867	G868	V869	V870	E871	M872	K873	M874	L875	S876	G877	Q878	A879	L880	K881					
D882	K883	K884	E885	L886	E887	G888	S889	G890	K891	I892	A893	T894	E895	A896	I897	E898	V904	S905	L906	T907	R908	K911	M915	Q918	S919	L920	Q921	I922	P923	Y924	R925	N926	K929	K930	A931	H932	V933	F934	G935	I936	T937	F938	S939	F940	A943	F955	G956	A957	Y958	L959	V960	T961				
Q962	Q963	L964	M965	L972	V973	G980	A981	M982	A983	V984	G985	Q986	A995	I996	K996	A997	T998	V999	S1000	H1003	I1004	I1005	I1008	E1009	K1010	T1011	P1012	E1013	I1014	D1015	Q1020	G1021	L1022	K1023	P1024	N1025	M1026	L1027	E1028	G1029	M1030	Q1032	F1033	S1034	G1035	V1036	I1037	F1038	R1043	P1044	S1045	I1046				
P1047	V1048	L1049	Q1050	G1051	L1052	S1053	L1054	E1055	V1056	K1057	K1058	G1059	Q1060	T1061	L1062	A1063	L1064	V1065	G1066	S1067	S1068	G1069	S1073	T1074	V1075	V1076	Q1077	L1078	L1079	E1080	R1081	F1082	Y1083	D1084	P1085	M1086	A1087	G1088	S1089	V1090	F1091	L1092	D1093	G1094	K1095	I1097	K1098	Q1099	L1100	M1101	V1102	Q1103	W1104	A1107	Q1108	L1109
Q1114	E1115	P1116	I1117	F1118	D1120	R1121	S1122	I1123	A1124	E1125	M1126	I1127	M1132	S1133	R1134	V1135	Y1138	E1139	E1140	I1141	V1142	R1143	K1146	E1147	A1148	M1149	I1150	H1151	D1152	F1153	I1154	D1155	S1156	L1157	P1158	D1159	K1160	Y1161	M1162	T1163	R1164	V1165	G1166	D1167	K1168	G1169	T1170	Q1171	L1172	S1173	G1174	L1175	Q1176	K1177		
Q1178	R1179	I1180	A1185	R1188	H1191	I1192	L1193	L1194	L1195	D1196	E1197	A1198	T1199	S1200	A1201	L1202	D1203	T1204	E1205	S1206	E1207	K1208	V1209	V1210	Q1211	E1212	A1213	L1214	D1215	K1216	A1217	R1218	E1219	G1220	R1221	T1222	V1223	I1224	V1225	I1226	A1227	H1228	R1229	L1230	S1231	Q1234	M1235	A1236	D1237	L1238	I1239	V1240	V1241	I1242	Q1243	
H1244	G1245	K1246	V1247	K1248	H1249	H1250	G1251	T1252	H1253	Q1254	Q1255	L1256	L1257	A1258	Q1259	K1260																																								

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	443812	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 ($e^-/\text{\AA}^2$)	75	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.571	Depositor
Minimum map value	-0.335	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.13	Depositor
Map size (\AA)	234.36, 234.36, 234.36	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.837, 0.837, 0.837	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.35	0/9132	0.56	0/12342

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	8968	0	9149	271	0
2	A	31	0	0	1	0
All	All	8999	0	9149	271	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.

The worst 5 of 271 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:388:LEU:HA	1:A:448:SER:O	1.75	0.85
1:A:319:SER:O	1:A:320:LYS:HB3	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:854:THR:HG22	1:A:973:VAL:HG21	1.67	0.76
1:A:422:VAL:H	1:A:596:GLY:HA3	1.49	0.76
1:A:1027:LEU:HD22	1:A:1092:LEU:HD21	1.67	0.76

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	1153/1260 (92%)	1091 (95%)	61 (5%)	1 (0%)	51 85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1012	PRO

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	947/1040 (91%)	945 (100%)	2 (0%)	93 96

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

Mol	Chain	Res	Type
1	A	210	LEU
1	A	1084	ASP

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

Mol	Chain	Res	Type
1	A	60	HIS
1	A	1025	ASN
1	A	1032	GLN
1	A	1101	ASN
1	A	1253	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	JIZ	A	1301	-	25,34,34	4.85	15 (60%)	24,49,49	1.56	4 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	JIZ	A	1301	-	-	2/14/38/38	0/3/4/4

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	JIZ	C09-S02	-8.67	1.56	1.70
2	A	1301	JIZ	C14-S03	-8.66	1.57	1.70
2	A	1301	JIZ	C03-N02	8.58	1.64	1.37
2	A	1301	JIZ	C04-S01	-8.00	1.58	1.70
2	A	1301	JIZ	C08-N04	7.84	1.61	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	JIZ	C03-C04-S01	-4.18	106.66	111.79
2	A	1301	JIZ	C08-C09-S02	-3.57	107.41	111.79
2	A	1301	JIZ	C13-C14-S03	-3.35	107.68	111.79
2	A	1301	JIZ	C01-C18-S04	-2.76	111.09	114.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301	JIZ	C02-C01-C18-S04
2	A	1301	JIZ	N01-C01-C18-S04

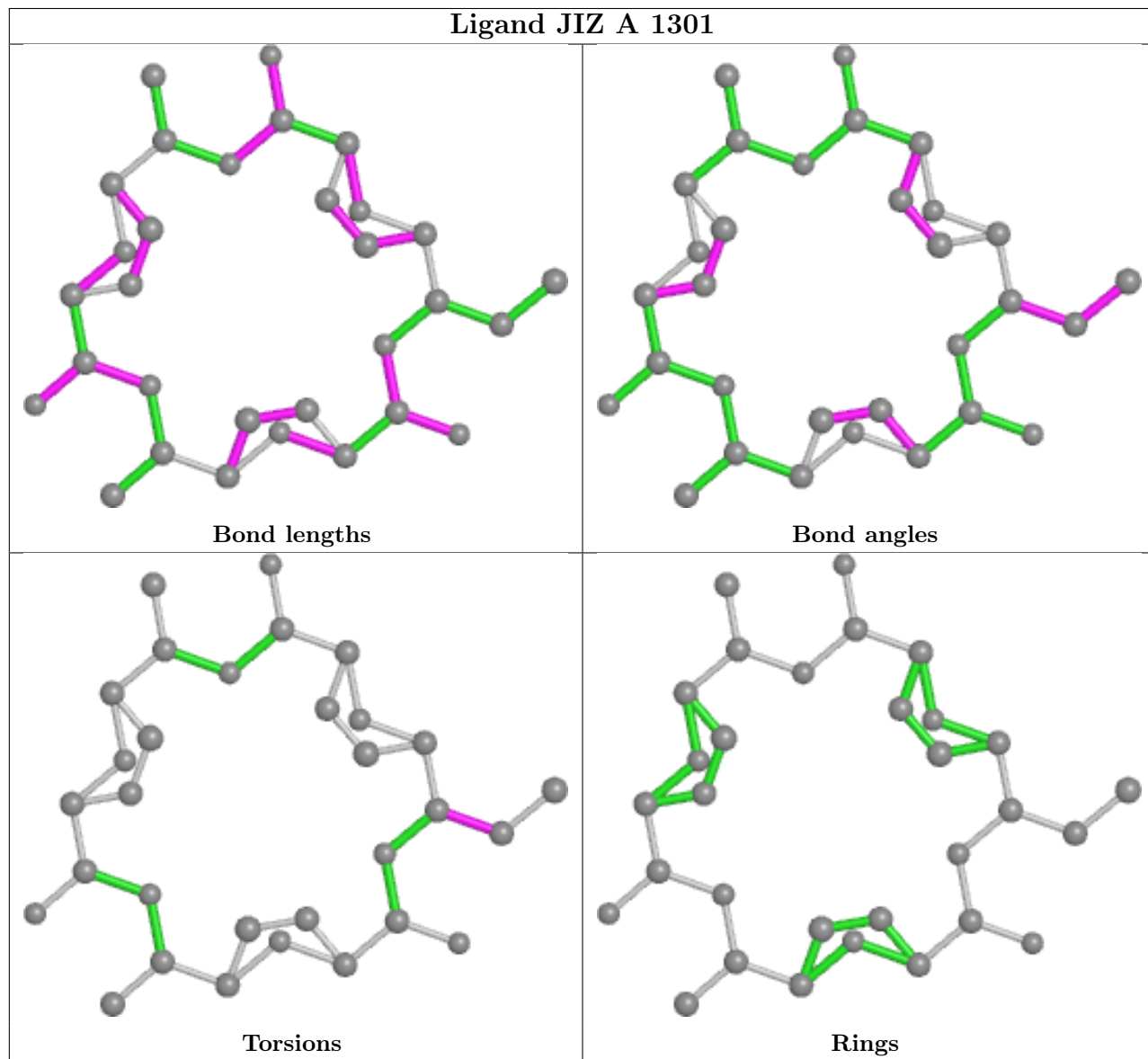
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1301	JIZ	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

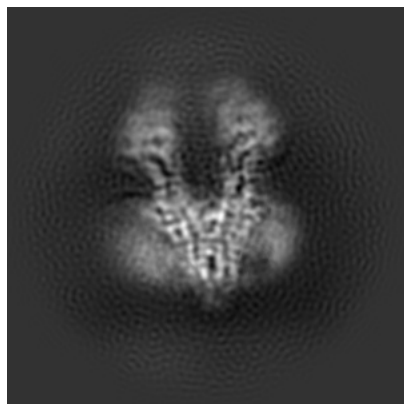
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14759. These allow visual inspection of the internal detail of the map and identification of artifacts.

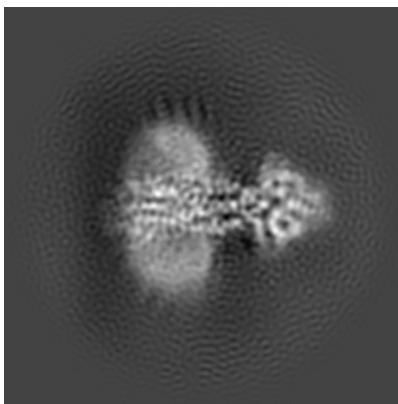
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

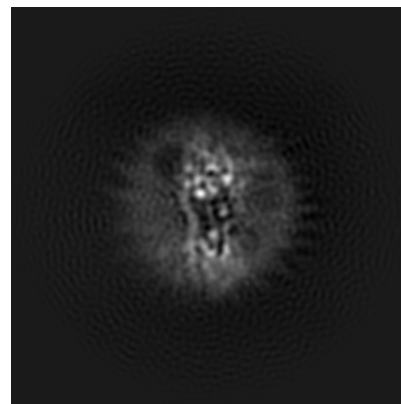
6.1.1 Primary map



X

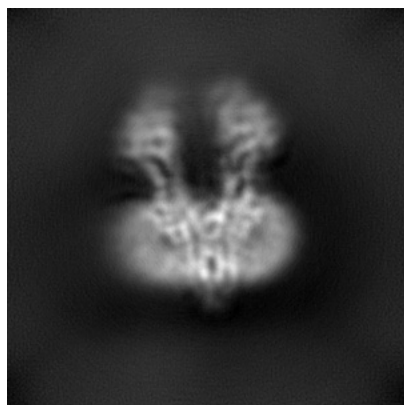


Y

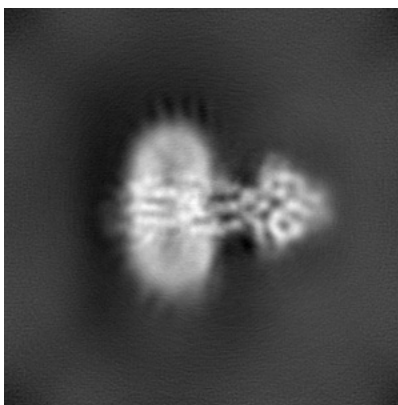


Z

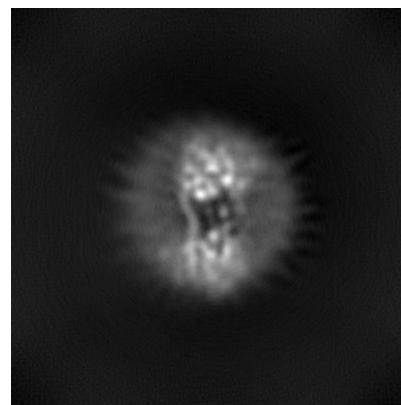
6.1.2 Raw map



X



Y

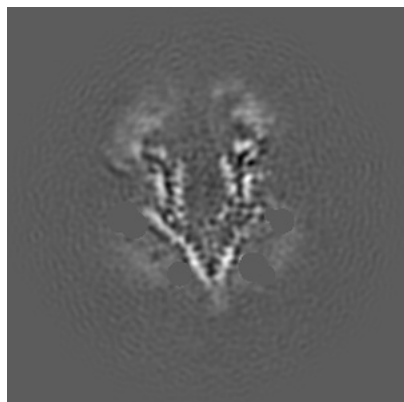


Z

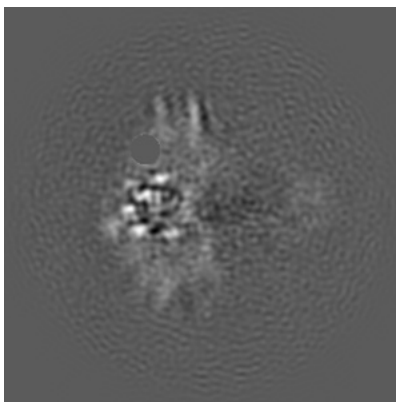
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

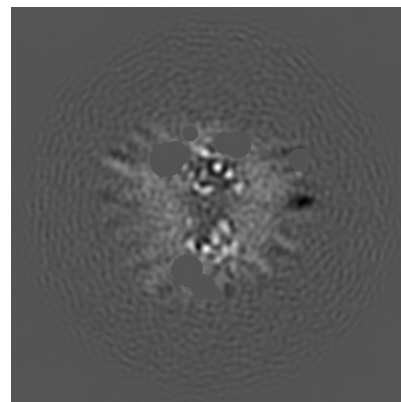
6.2.1 Primary map



X Index: 140

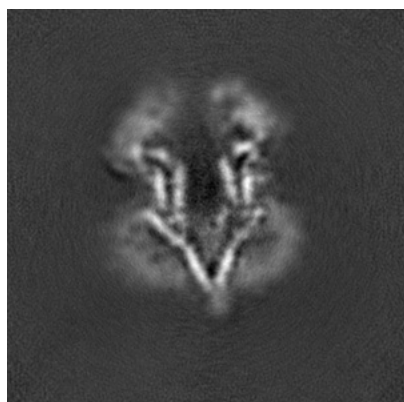


Y Index: 140

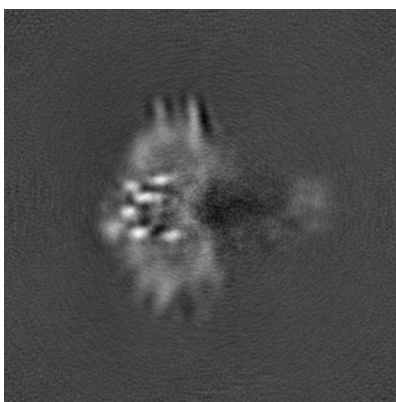


Z Index: 140

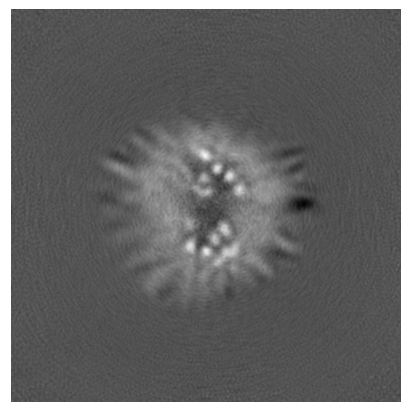
6.2.2 Raw map



X Index: 140



Y Index: 140

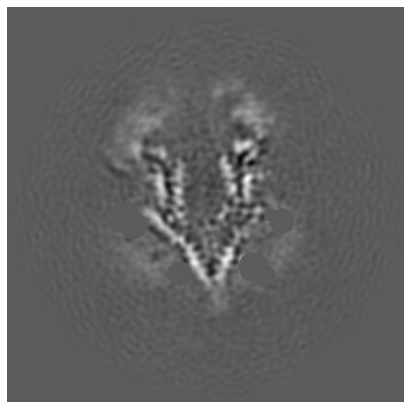


Z Index: 140

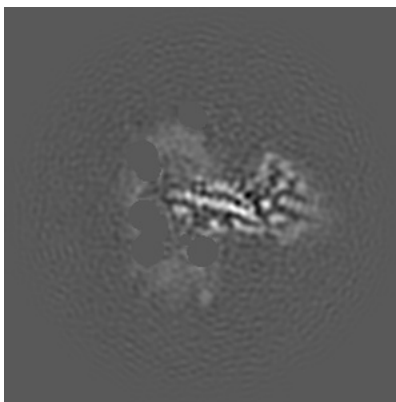
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

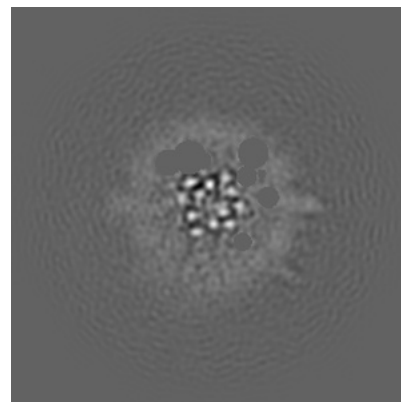
6.3.1 Primary map



X Index: 140

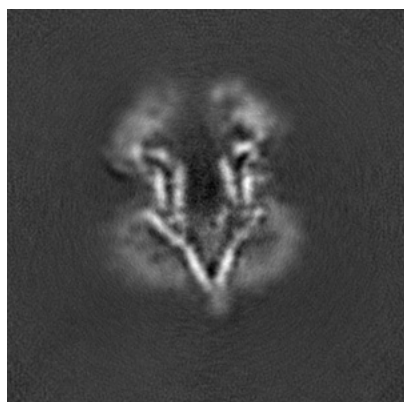


Y Index: 167

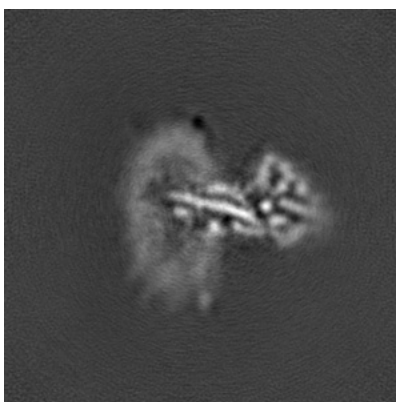


Z Index: 108

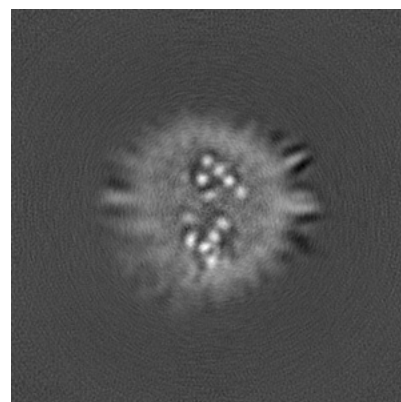
6.3.2 Raw map



X Index: 140



Y Index: 167

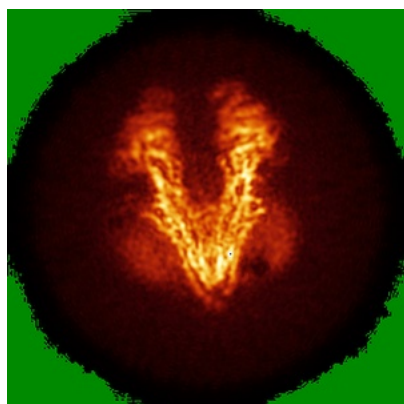


Z Index: 133

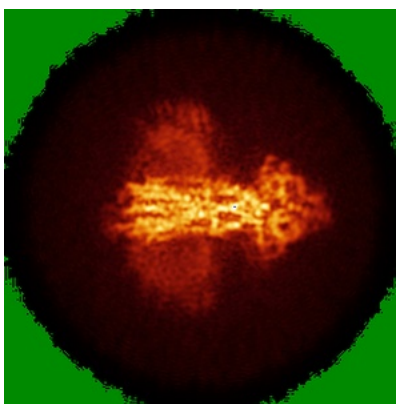
The images above show the largest variance slices of the map in three orthogonal directions.

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

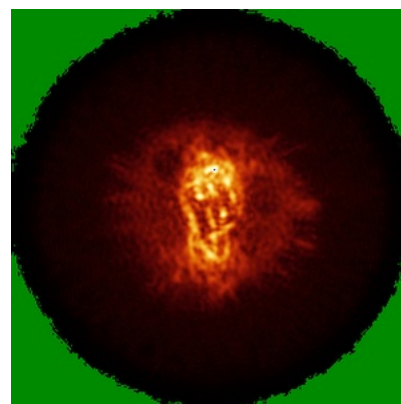
6.4.1 Primary map



X

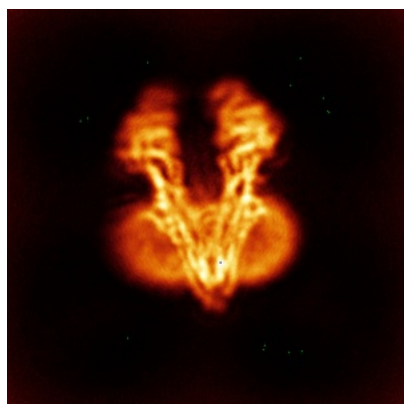


Y

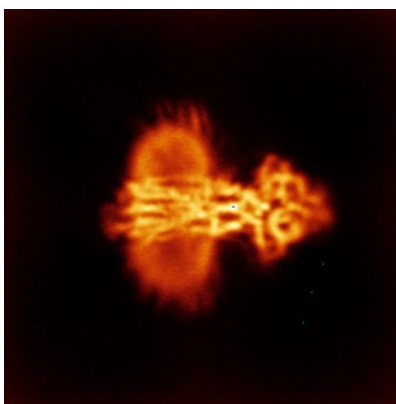


Z

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.

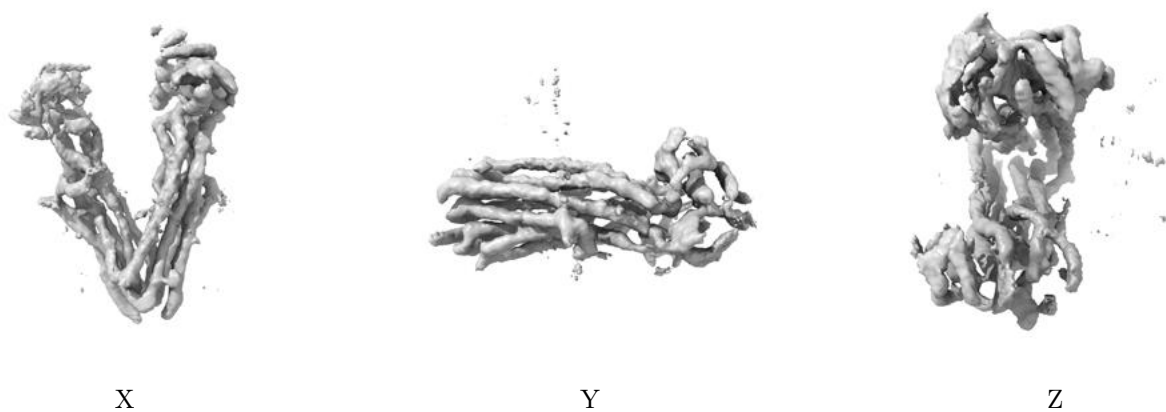
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.13. 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.

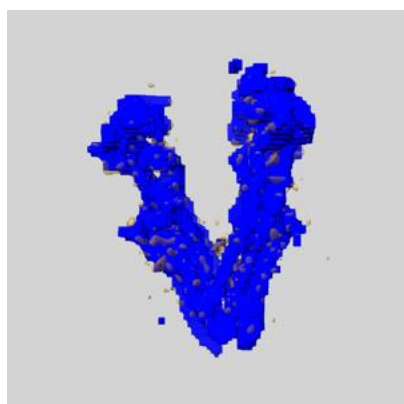
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

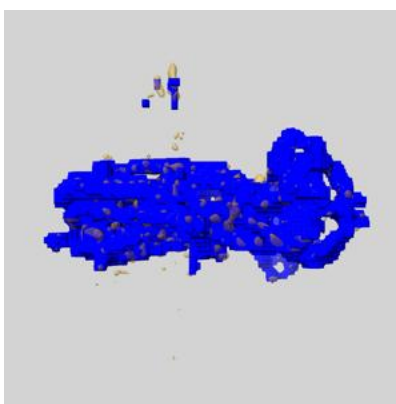
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

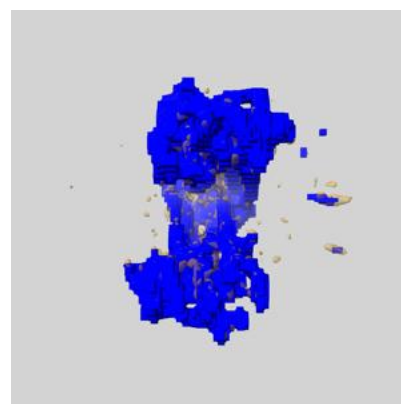
6.6.1 emd_14759_msk_1.map [i](#)



X



Y

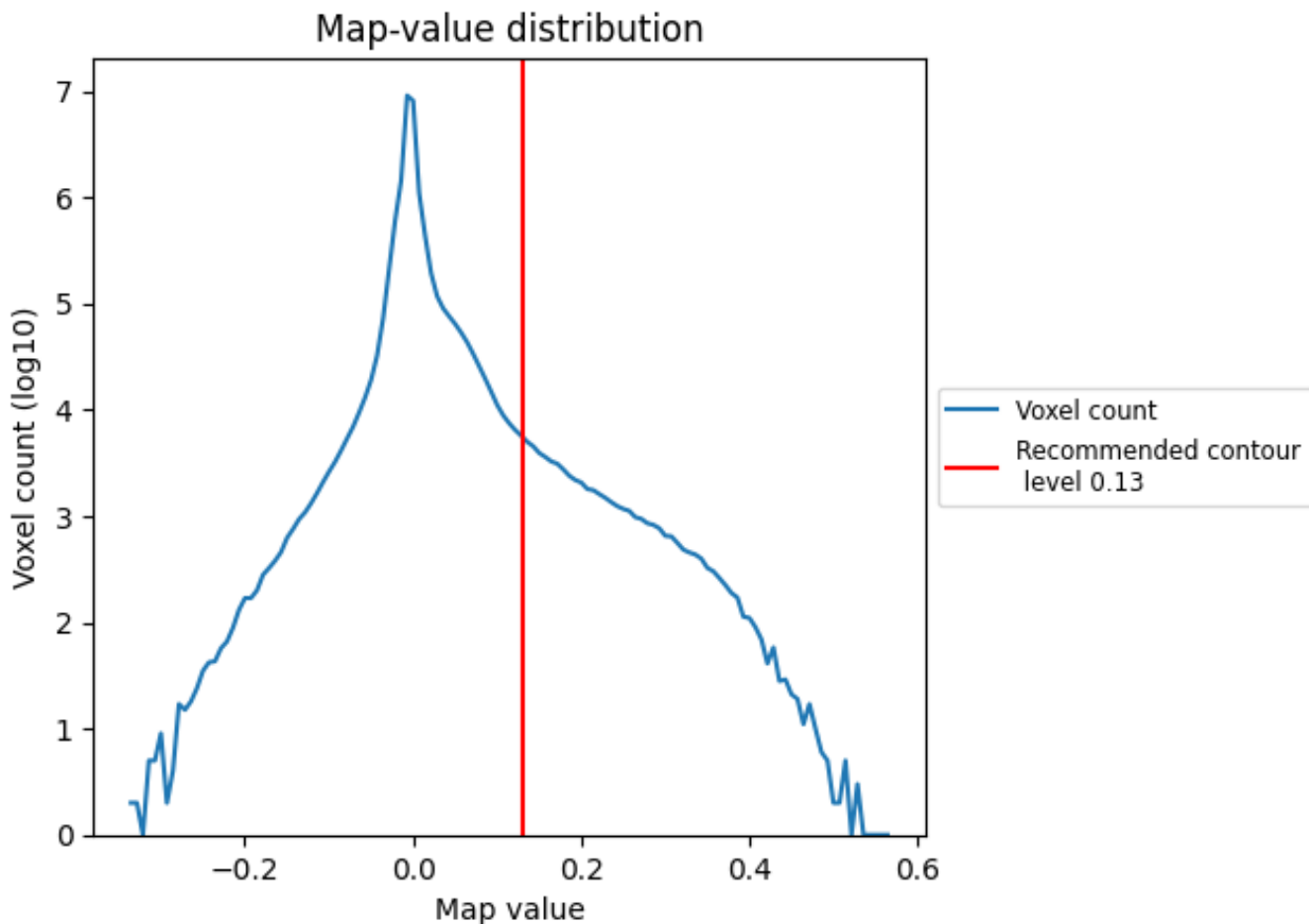


Z

7 Map analysis [i](#)

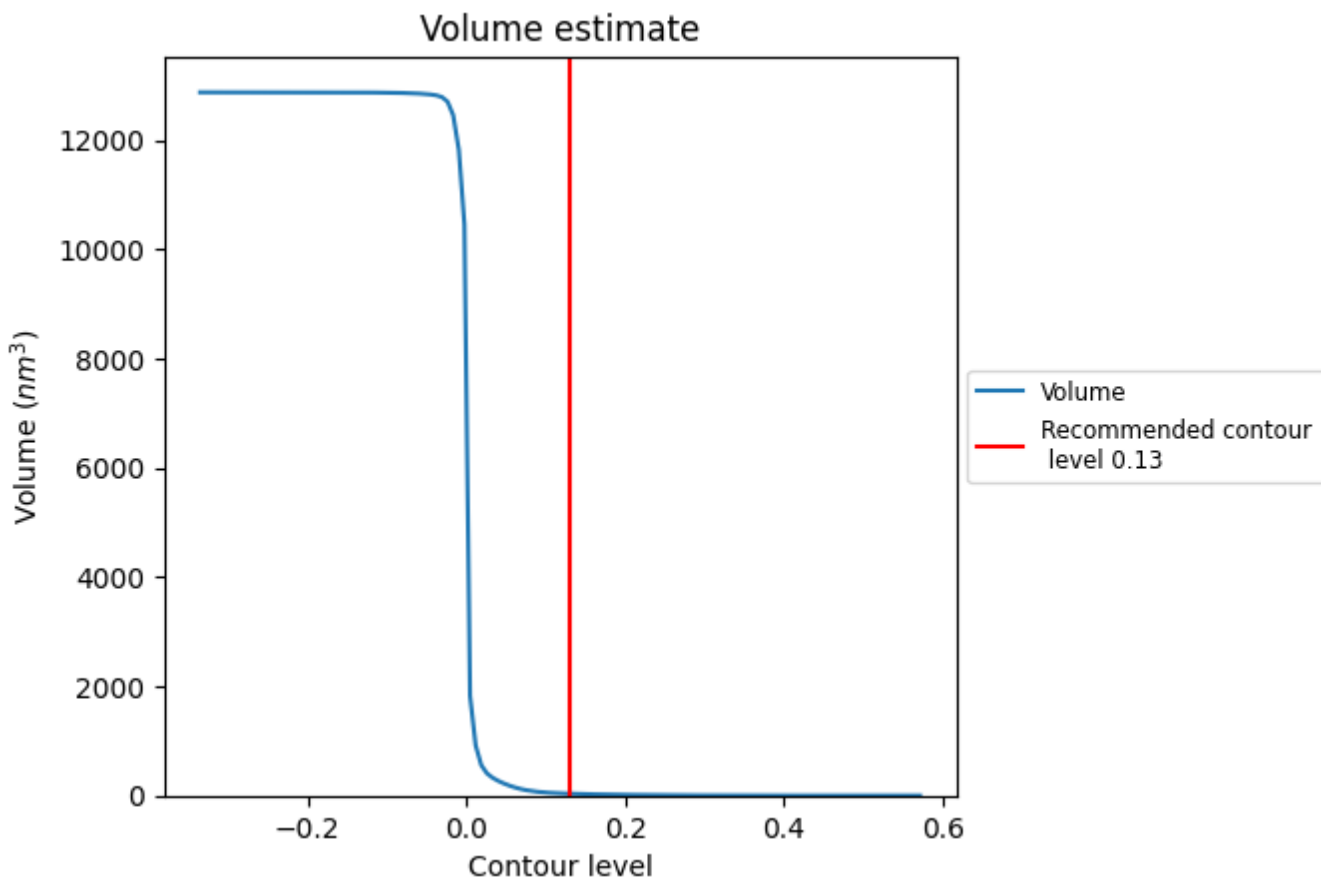
This section contains the results of statistical analysis of the map.

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.

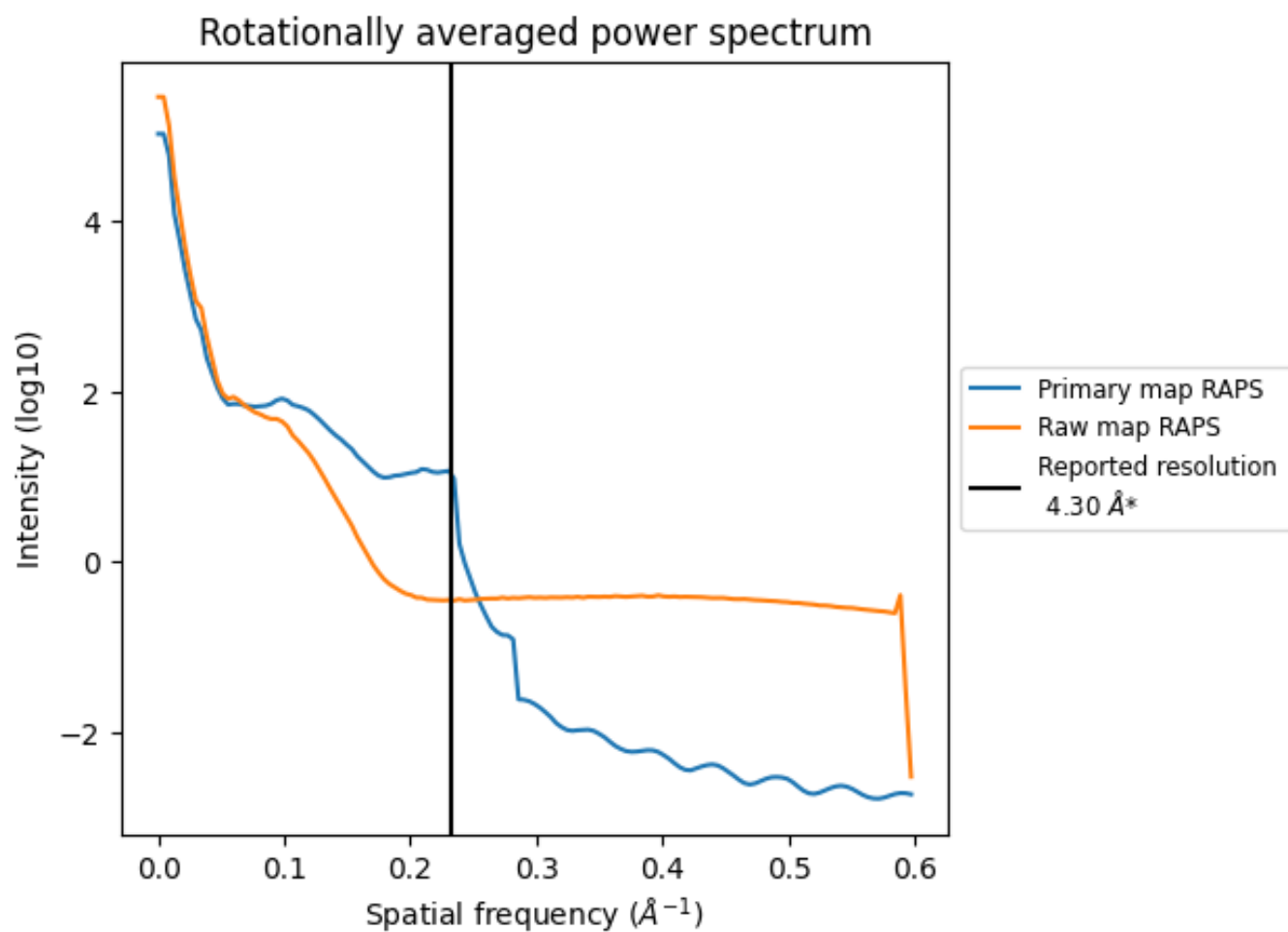
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 35 nm³; this corresponds to an approximate mass of 31 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 [\(i\)](#)

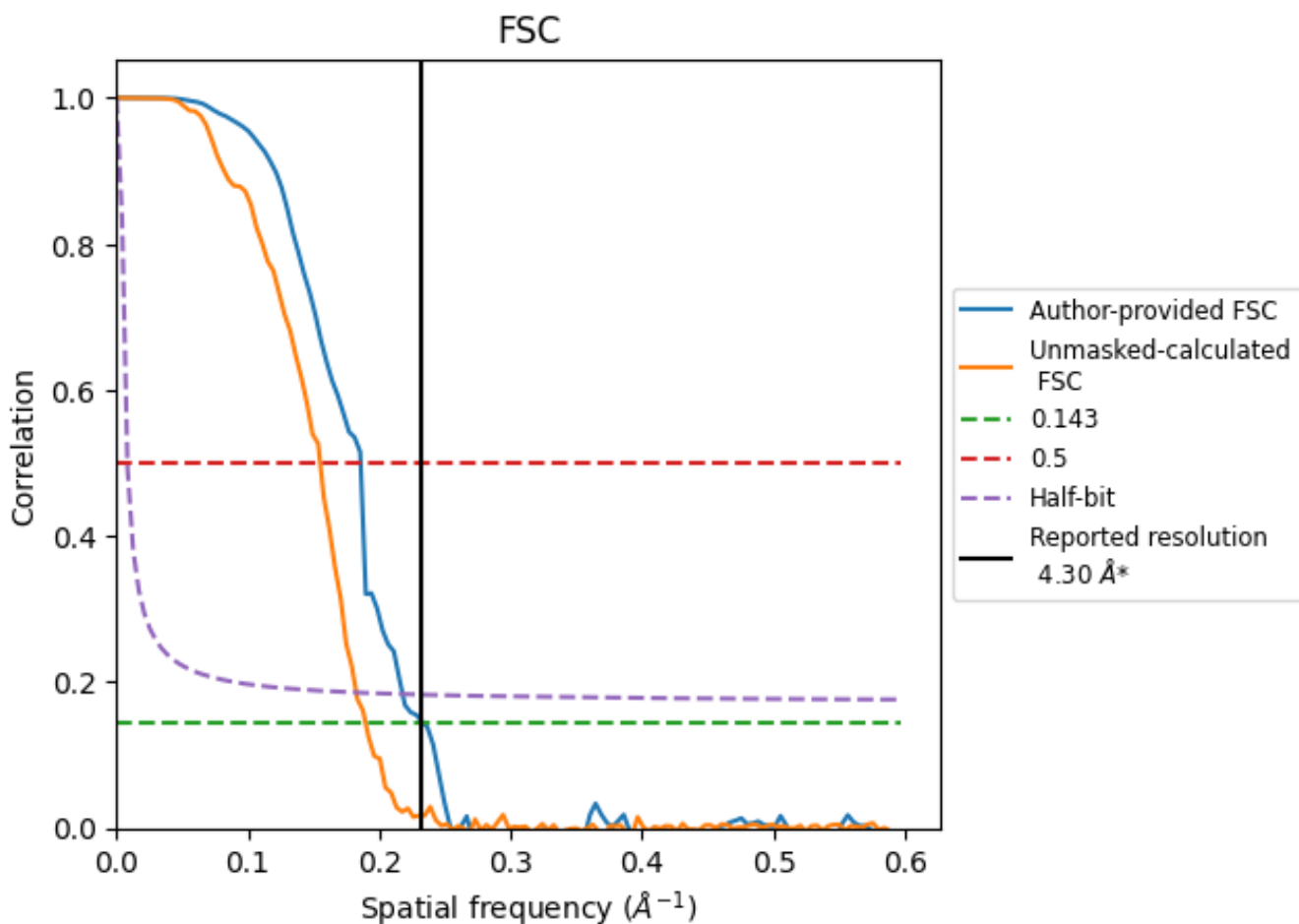


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

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 0.233\AA^{-1}

8.2 Resolution estimates [i](#)

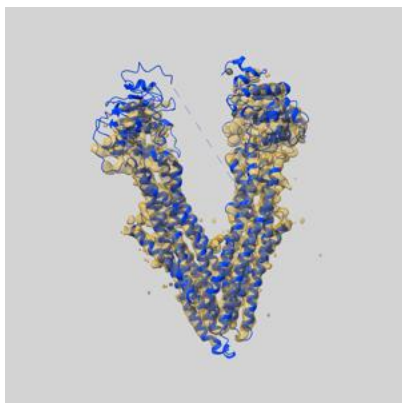
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.27	5.38	4.59
Unmasked-calculated*	5.27	6.45	5.48

*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 5.27 differs from the reported value 4.3 by more than 10 %

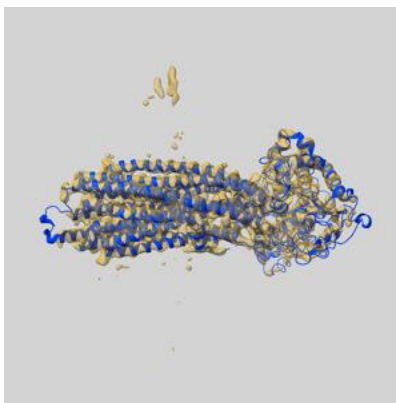
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14759 and PDB model 7ZK9. Per-residue inclusion information can be found in section 3 on page 5.

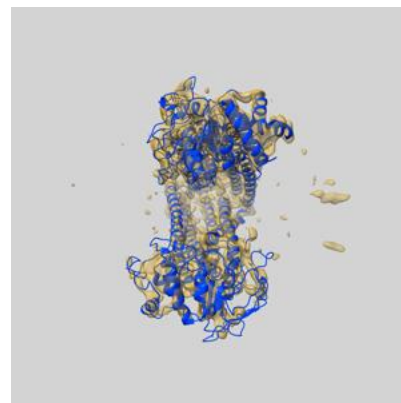
9.1 Map-model overlay [i](#)



X



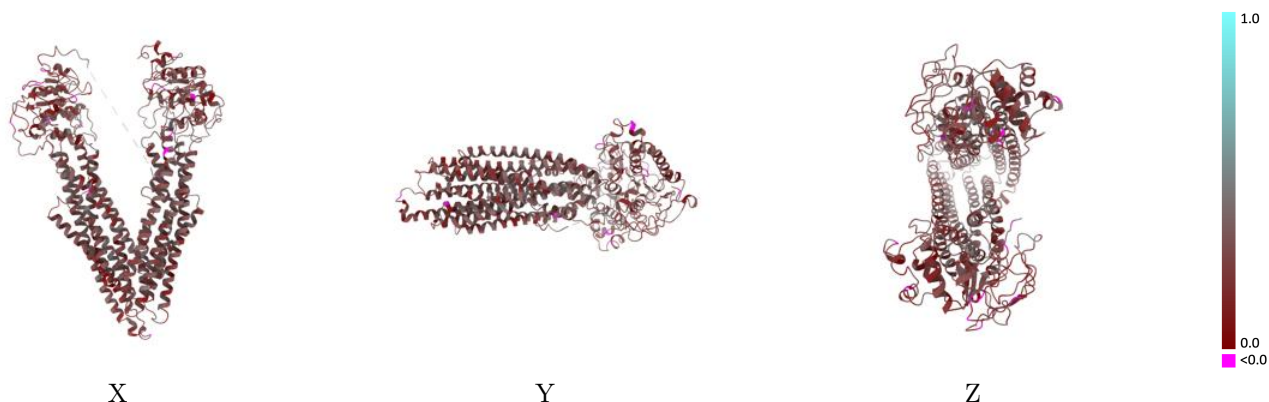
Y



Z

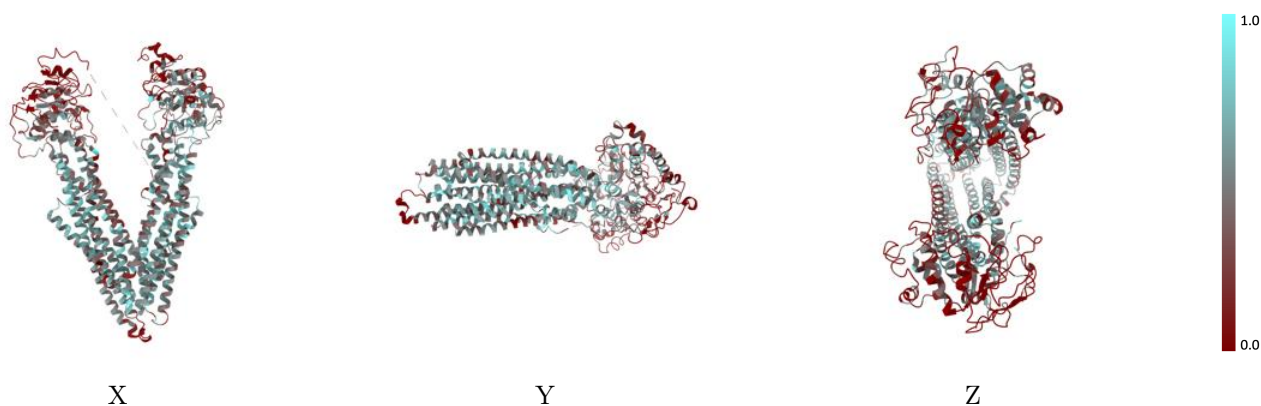
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



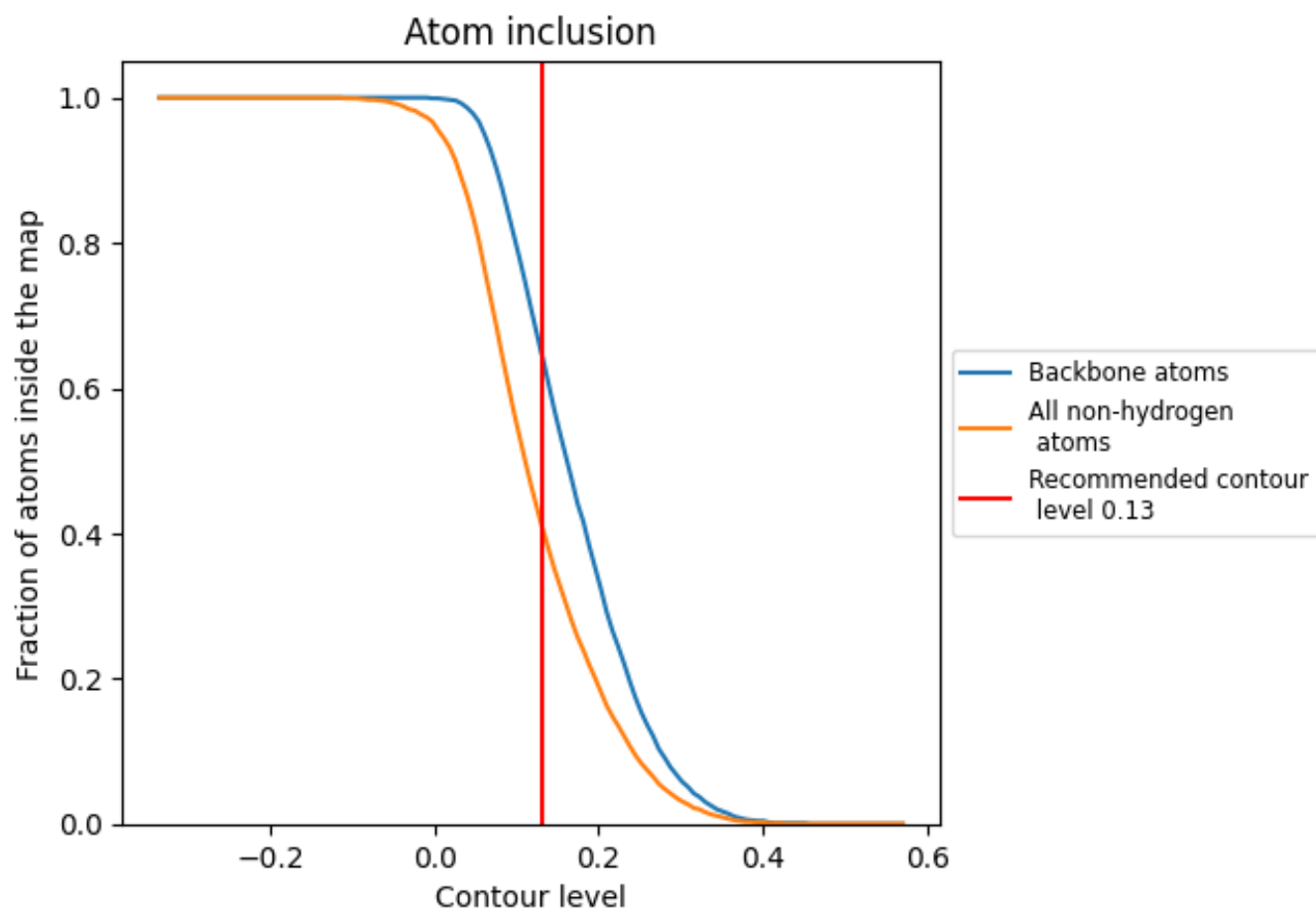
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.13).





9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 41% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4130	 0.2820
A	 0.4120	 0.2820

