wwPDB EM Validation Summary Report

Sep 18, 2024 – 04:25 pm BST

PDB ID	:	8QP5
EMDB ID	:	EMD-18543
Title	:	Release Complex: BAM bound EspP (SurA released)
Authors	:	Fenn, K.L.; Ranson, N.A.
Deposited on	:	2023-09-29
Resolution	:	4.40 Å(reported)
Based on initial model	:	8PZ1

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:

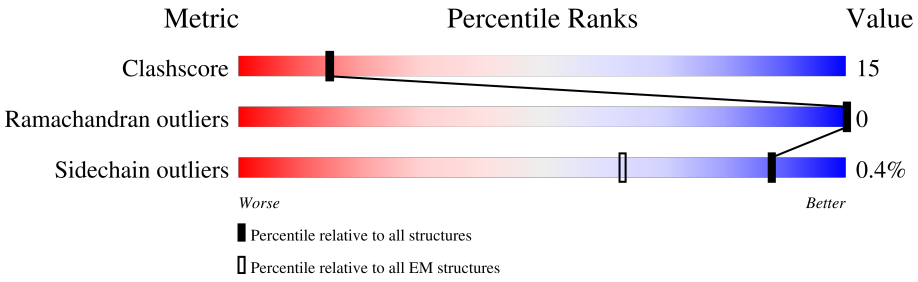
EMDB validation analysis	:	0.0.1.dev112
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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 <=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	790	13% 52% 26% 22%
2	B	373	82% 62% 34% ·
3	C	320	32% 39% 14% 47%
4	D	226	8% 62% 33% ·
5	E	104	11% 52% 33% · 14%
6	P	814	29% 33% · 63%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12554 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 Outer membrane protein assembly factor BamA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	614	Total	C	N	O	S	0	0
			4886	3090	820	962	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	425	CYS	SER	engineered mutation	UNP P0A940

- Molecule 2 is a protein called Outer membrane protein assembly factor BamB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	357	Total	C	N	O	S	0	0
			2674	1677	460	531	6		

- Molecule 3 is a protein called Outer membrane protein assembly factor BamC.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	171	Total	C	N	O	S	0	0
			1036	634	190	209	3		

- Molecule 4 is a protein called Outer membrane protein assembly factor BamD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	216	Total	C	N	O	S	0	0
			1744	1099	307	331	7		

- Molecule 5 is a protein called Outer membrane protein assembly factor BamE.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	89	Total	C	N	O	S	0	0
			693	436	122	133	2		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	114	GLY	-	expression tag	UNP P0A937
E	115	GLY	-	expression tag	UNP P0A937
E	116	HIS	-	expression tag	UNP P0A937
E	117	HIS	-	expression tag	UNP P0A937
E	118	HIS	-	expression tag	UNP P0A937
E	119	HIS	-	expression tag	UNP P0A937
E	120	HIS	-	expression tag	UNP P0A937
E	121	HIS	-	expression tag	UNP P0A937
E	122	HIS	-	expression tag	UNP P0A937
E	123	HIS	-	expression tag	UNP P0A937

- Molecule 6 is a protein called Chaperone SurA,Serine protease EspP.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	299	Total	C	N	O	S	1	0
			1521	900	310	310	1		

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	487	GLY	-	expression tag	UNP P0ABZ6
P	488	SER	-	expression tag	UNP P0ABZ6
P	489	SER	-	expression tag	UNP P0ABZ6
P	490	ALA	-	expression tag	UNP P0ABZ6
P	491	TRP	-	expression tag	UNP P0ABZ6
P	492	SER	-	expression tag	UNP P0ABZ6
P	493	HIS	-	expression tag	UNP P0ABZ6
P	494	PRO	-	expression tag	UNP P0ABZ6
P	495	GLN	-	expression tag	UNP P0ABZ6
P	496	PHE	-	expression tag	UNP P0ABZ6
P	497	GLU	-	expression tag	UNP P0ABZ6
P	498	LYS	-	expression tag	UNP P0ABZ6
P	499	GLY	-	expression tag	UNP P0ABZ6
P	500	GLY	-	expression tag	UNP P0ABZ6
P	501	GLY	-	expression tag	UNP P0ABZ6
P	502	SER	-	expression tag	UNP P0ABZ6
P	503	GLY	-	expression tag	UNP P0ABZ6
P	504	GLY	-	expression tag	UNP P0ABZ6
P	505	GLY	-	expression tag	UNP P0ABZ6
P	506	SER	-	expression tag	UNP P0ABZ6
P	507	GLY	-	expression tag	UNP P0ABZ6
P	508	GLY	-	expression tag	UNP P0ABZ6
P	509	SER	-	expression tag	UNP P0ABZ6

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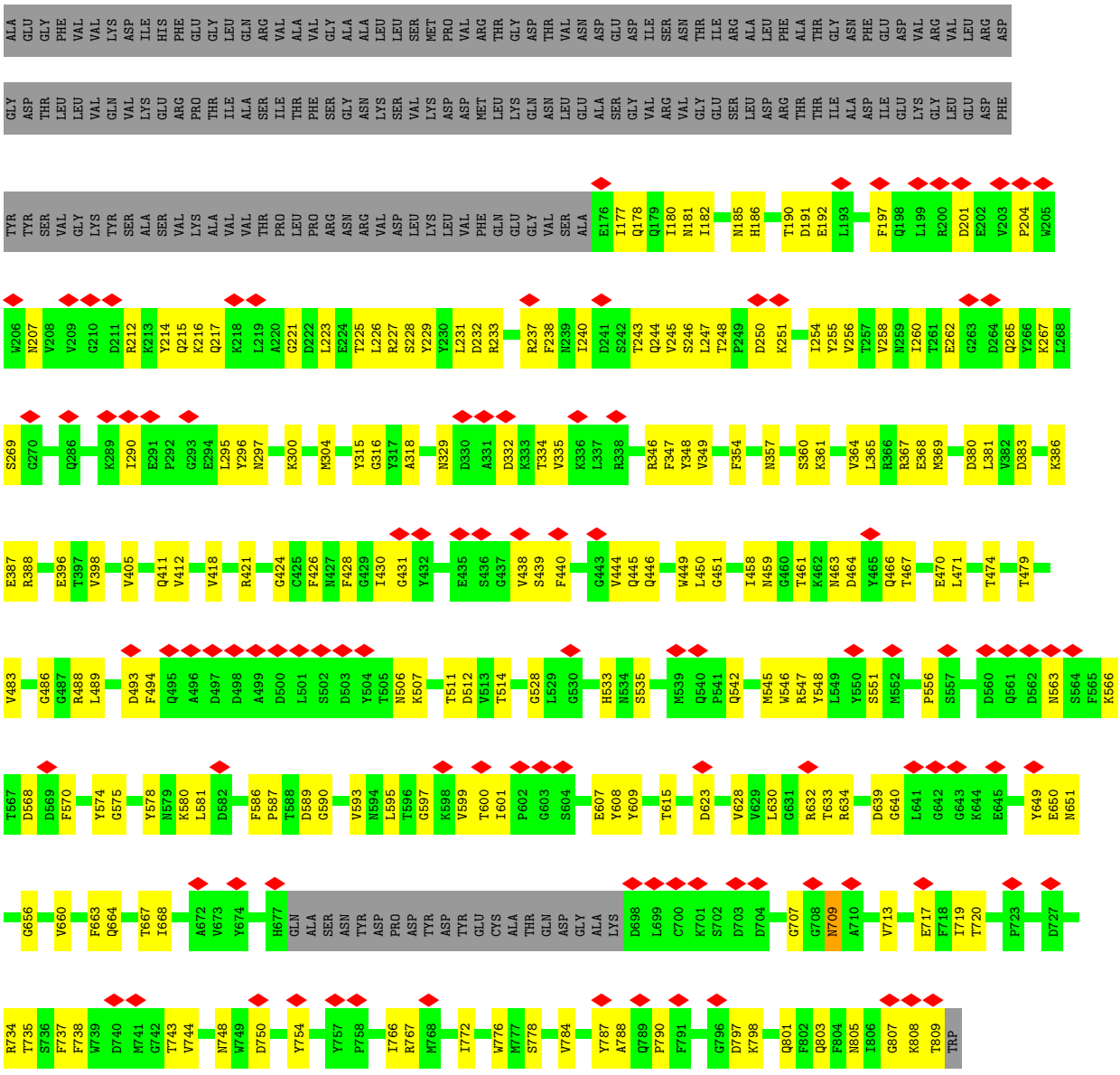
Chain	Residue	Modelled	Actual	Comment	Reference
P	510	ALA	-	expression tag	UNP P0ABZ6
P	511	TRP	-	expression tag	UNP P0ABZ6
P	512	SER	-	expression tag	UNP P0ABZ6
P	513	HIS	-	expression tag	UNP P0ABZ6
P	514	PRO	-	expression tag	UNP P0ABZ6
P	515	GLN	-	expression tag	UNP P0ABZ6
P	516	PHE	-	expression tag	UNP P0ABZ6
P	517	GLU	-	expression tag	UNP P0ABZ6
P	518	LYS	-	expression tag	UNP P0ABZ6
P	519	SER	-	expression tag	UNP P0ABZ6
P	520	SER	-	expression tag	UNP P0ABZ6
P	521	GLY	-	expression tag	UNP P0ABZ6
P	522	GLU	-	expression tag	UNP P0ABZ6
P	523	ASN	-	expression tag	UNP P0ABZ6
P	524	LEU	-	expression tag	UNP P0ABZ6
P	525	TYR	-	expression tag	UNP P0ABZ6
P	526	PHE	-	expression tag	UNP P0ABZ6
P	527	GLN	-	expression tag	UNP P0ABZ6
P	528	GLY	-	expression tag	UNP P0ABZ6
P	535	CYS	LYS	conflict	UNP P0ABZ6
P	937	GLY	-	linker	UNP P0ABZ6
P	938	GLY	-	linker	UNP P0ABZ6
P	976	GLY	-	insertion	UNP Q7BSW5
P	977	GLU	-	insertion	UNP Q7BSW5
P	978	ASN	-	insertion	UNP Q7BSW5
P	979	LEU	-	insertion	UNP Q7BSW5
P	980	TYR	-	insertion	UNP Q7BSW5
P	981	PHE	-	insertion	UNP Q7BSW5
P	982	GLN	-	insertion	UNP Q7BSW5
P	983	GLY	-	insertion	UNP Q7BSW5
P	984	GLY	-	insertion	UNP Q7BSW5
P	1299	CYS	SER	engineered mutation	UNP Q7BSW5

3 Residue-property plots (i)

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.

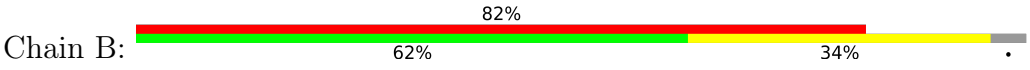
- Molecule 1: Outer membrane protein assembly factor BamA

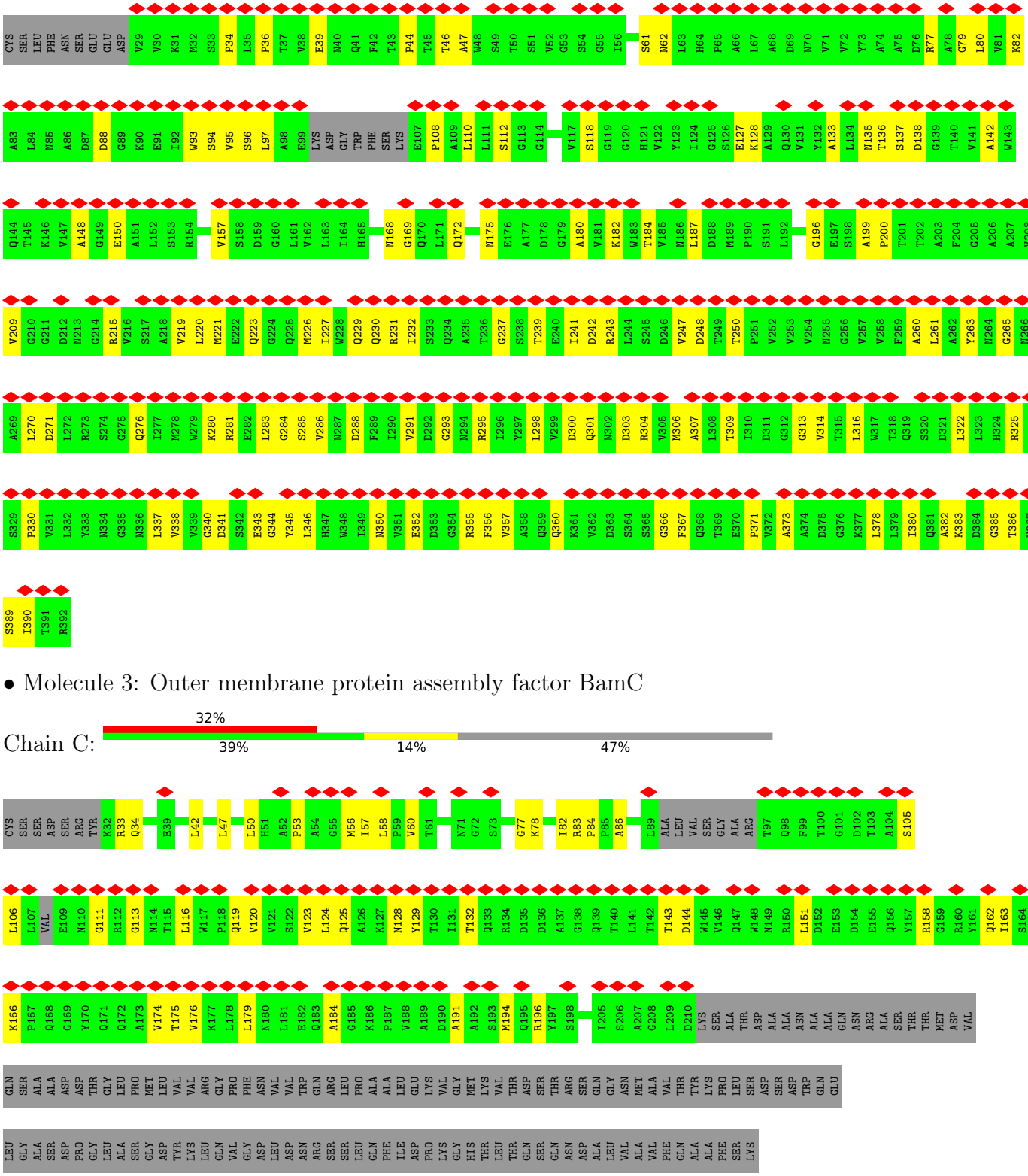
Chain A:



• Molecule 2: Outer membrane protein assembly factor BamB

Chain B:



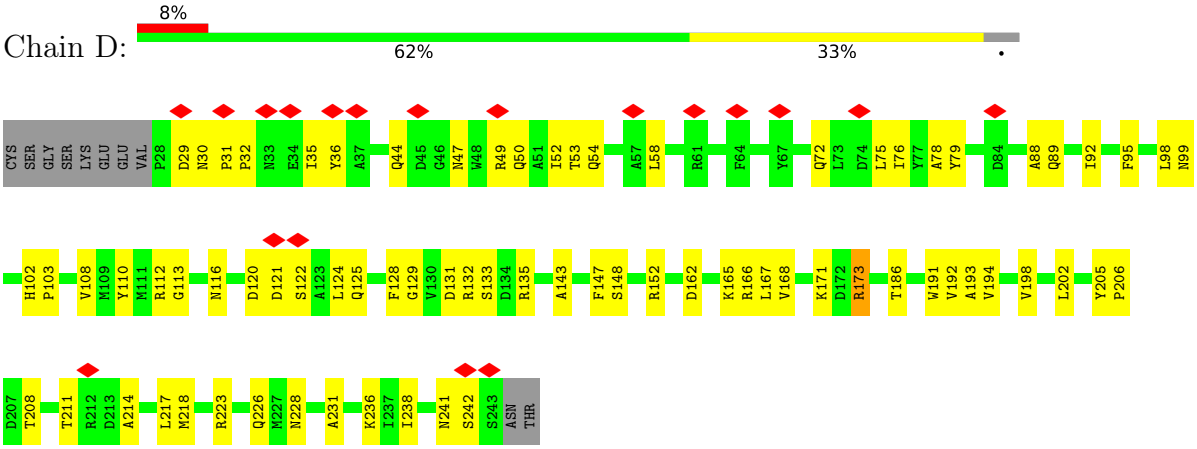


• Molecule 3: Outer membrane protein assembly factor BamC

Chain C:

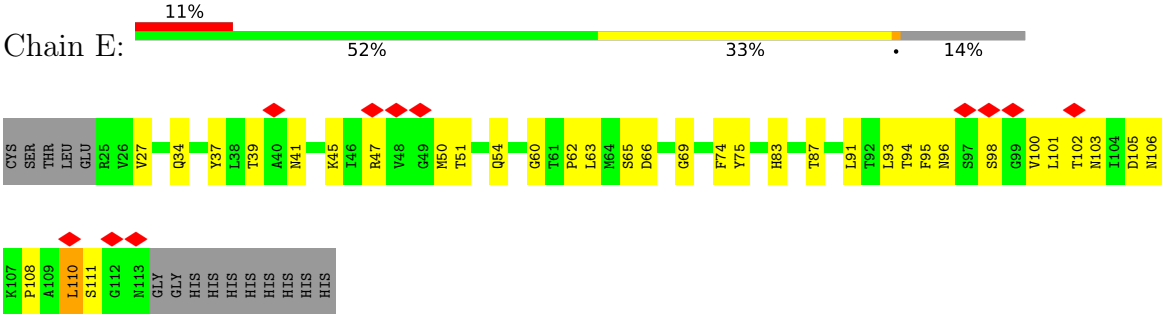
• Molecule 4: Outer membrane protein assembly factor BamD

Chain D:



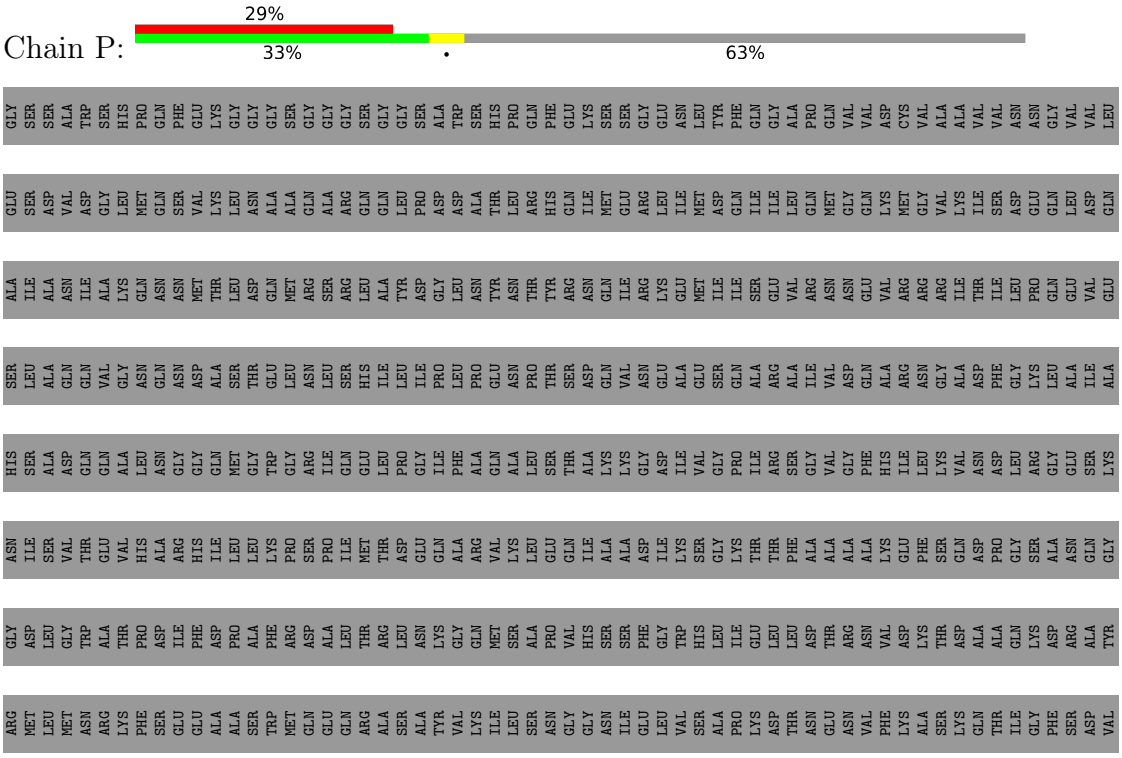
• Molecule 5: Outer membrane protein assembly factor BamE

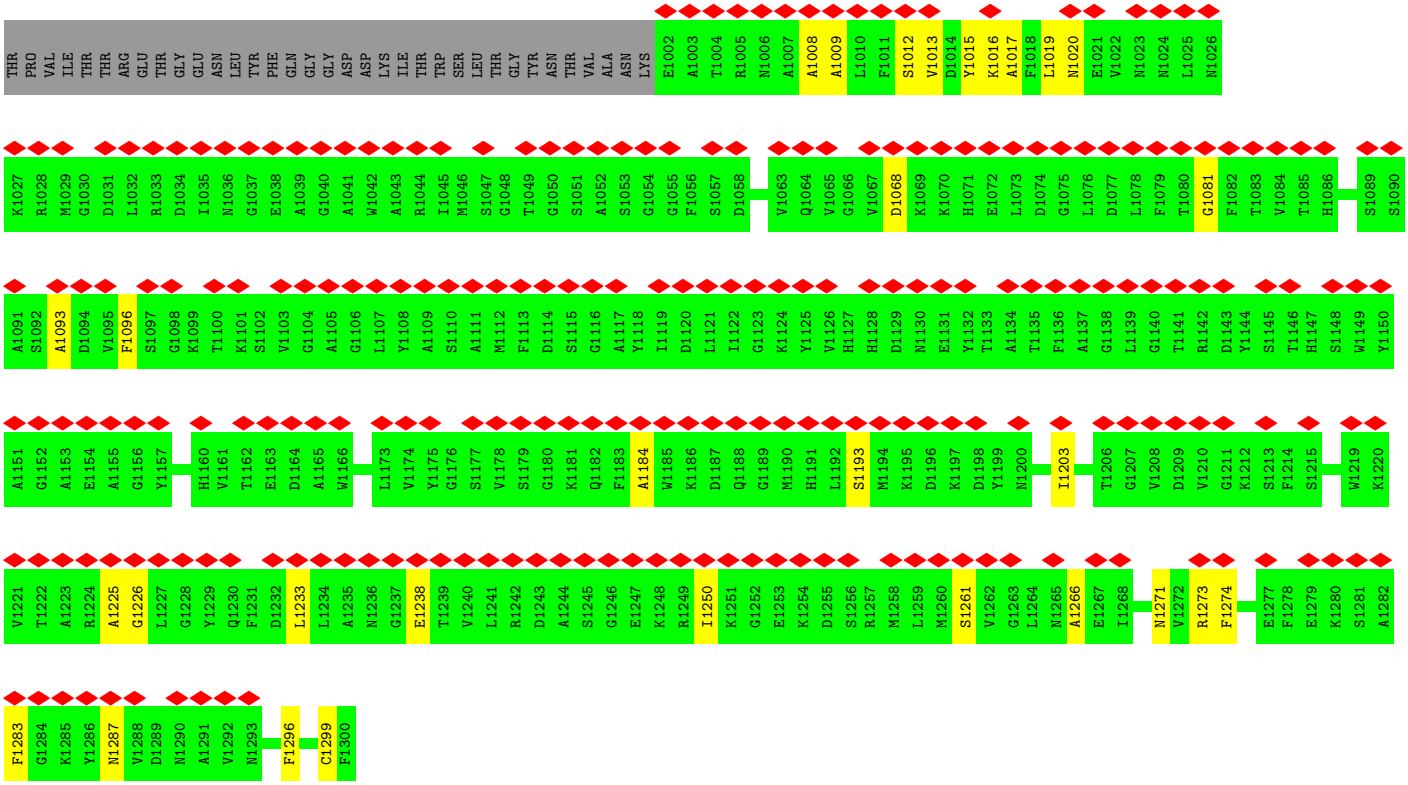
Chain E:



• Molecule 6: Chaperone SurA,Serine protease EspP

Chain P:




THR PRO VAL ILE THR THR ARG GLU THR GLY GLU ASN LEU TYR PHE GLN GLY GLY ASP ASP LYS ILE THR TRP SER LEU THR GLY TYR ASN THR VAL ALA ASN LYS
E1002 A1003 T1004 R1005 N1006 A1007 A1008 A1009 L1010 F1011 S1012 V1013 D1014 Y1015 K1016 A1017 F1018 L1019 N1020 E1021 V1022 N1023 N1024 L1025 N1026
K1027 R1028 M1029 G1030 D1031 L1032 R1033 D1034 I1035 N1036 G1037 E1038 A1039 G1040 A1041 W1042 A1043 R1044 I1045 M1046 S1047 G1048 T1049 G1050 S1051 A1052 S1053 G1054 G1055 F1056 S1057 D1058 V1063 Q1064 V1065 G1066 V1067 D1068 K1069 K1070 H1071 E1072 L1073 D1074 G1075 L1076 D1077 L1078 F1079 T1080 G1081 F1082 T1083 V1084 T1085 H1086 S1089 S1090
A1091 S1092 A1093 D1094 V1095 F1096 S1097 G1098 K1099 T1100 K1101 S1102 V1103 G1104 A1105 G1106 L1107 Y1108 A1109 S1110 A1111 M1112 F1113 D1114 S1115 G1116 A1117 Y1118 I1119 D1120 L1121 I1122 G1123 K1124 Y1125 V1126 H1127 H1128 D1129 N1130 E1131 Y1132 T1133 A1134 T1135 F1136 A1137 G1138 L1139 G1140 T1141 R1142 D1143 Y1144 S1145 T1146 H1147 S1148 W1149 Y1150
A1151 G1152 A1153 E1154 A1155 G1156 Y1157 H1160 V1161 T1162 E1163 D1164 A1165 W1166 L1173 V1174 Y1175 G1176 S1177 V1178 S1179 G1180 K1181 Q1182 F1183 A1184 W1185 K1186 D1187 Q1188 G1189 M1190 H1191 L1192 S1193 M1194 K1195 D1196 K1197 D1198 Y1199 N1200 I1203 T1206 G1207 V1208 D1209 V1210 G1211 K1212 S1213 F1214 S1215 W1219 K1220
V1221 T1222 A1223 R1224 A1225 G1226 L1227 G1228 Y1229 Q1230 F1231 D1232 L1233 L1234 A1235 N1236 G1237 E1238 T1239 V1240 L1241 R1242 D1243 A1244 S1245 G1246 E1247 K1248 R1249 I1250 K1251 G1252 E1253 K1254 D1255 S1256 R1257 M1258 L1259 M1260 S1261 V1262 G1263 L1264 N1265 A1266 E1267 I1268 N1271 V1272 R1273 F1274 E1277 F1278 E1279 K1280 S1281 A1282
F1283 G1284 K1285 Y1286 N1287 V1288 D1289 N1290 A1291 V1292 N1293 F1296 C1299 F1300

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	67655	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 ($e^-/Å^2$)	37.4	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.570	Depositor
Minimum map value	-0.373	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.125	Depositor
Map size (Å)	222.0, 222.0, 222.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.74, 0.74, 0.74	Depositor

5 Model quality

5.1 Standard geometry

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	0.28	0/5009	0.52	0/6795
2	B	0.25	0/2720	0.52	0/3711
3	C	0.33	0/1047	0.52	0/1440
4	D	0.28	0/1784	0.54	1/2423 (0.0%)
5	E	0.27	0/708	0.53	0/965
6	P	0.25	0/1524	0.50	0/2101
All	All	0.28	0/12792	0.52	1/17435 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	167	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4886	0	4615	145	0
2	B	2674	0	2633	83	0
3	C	1036	0	811	34	0
4	D	1744	0	1685	60	0
5	E	693	0	674	31	0
6	P	1521	0	804	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12554	0	11222	351	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 351 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:580:LYS:O	1:A:590:GLY:HA3	1.83	0.78
4:D:192:VAL:H	5:E:34:GLN:HE21	1.31	0.78
2:B:215:ARG:HH21	2:B:229:GLN:HG2	1.48	0.76
1:A:600:THR:HG21	1:A:607:GLU:HA	1.65	0.76
6:P:1238:GLU:HA	6:P:1250:ILE:O	1.87	0.75

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	610/790 (77%)	570 (93%)	40 (7%)	0	100	100
2	B	353/373 (95%)	313 (89%)	40 (11%)	0	100	100
3	C	165/320 (52%)	141 (86%)	24 (14%)	0	100	100
4	D	214/226 (95%)	201 (94%)	13 (6%)	0	100	100
5	E	87/104 (84%)	81 (93%)	6 (7%)	0	100	100
6	P	298/814 (37%)	283 (95%)	15 (5%)	0	100	100
All	All	1727/2627 (66%)	1589 (92%)	138 (8%)	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	524/672 (78%)	522 (100%)	2 (0%)	89 91
2	B	289/304 (95%)	289 (100%)	0	100 100
3	C	67/258 (26%)	66 (98%)	1 (2%)	60 75
4	D	181/190 (95%)	180 (99%)	1 (1%)	84 88
5	E	77/90 (86%)	76 (99%)	1 (1%)	65 77
6	P	16/656 (2%)	16 (100%)	0	100 100
All	All	1154/2170 (53%)	1149 (100%)	5 (0%)	88 91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216	LYS
1	A	709	ASN
3	C	33	ARG
4	D	173	ARG
5	E	110	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	GLN
2	B	230	GLN
4	D	47	ASN
5	E	34	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.

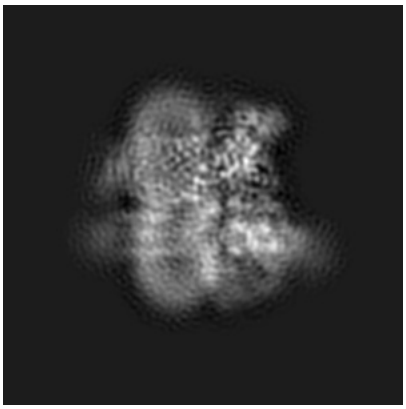
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-18543. These allow visual inspection of the internal detail of the map and identification of artifacts.

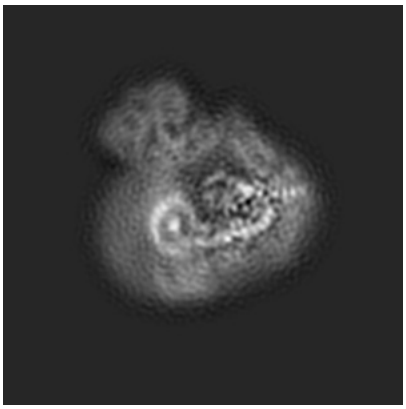
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

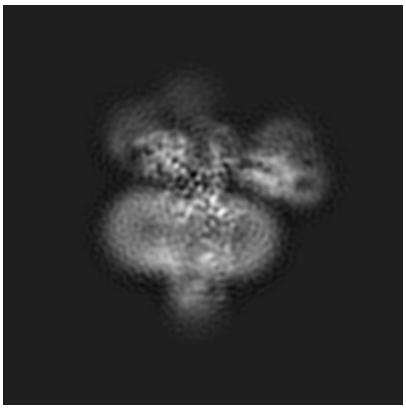
6.1.1 Primary map



X

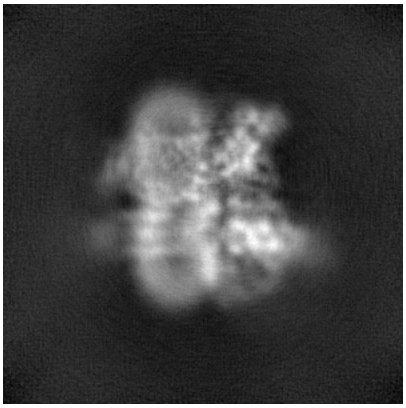


Y



Z

6.1.2 Raw map



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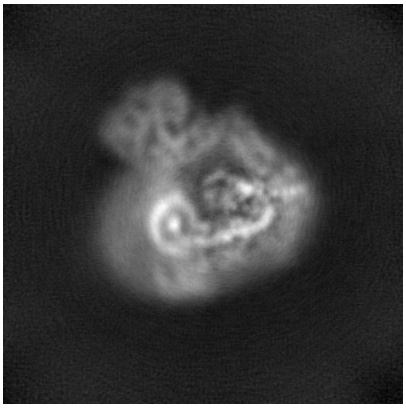
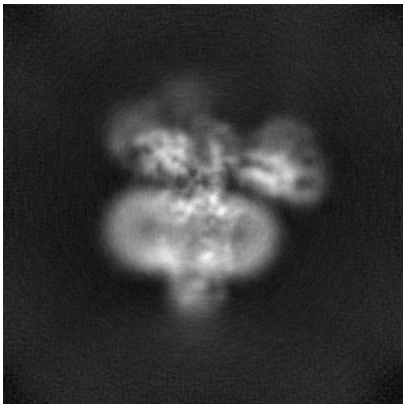


Y

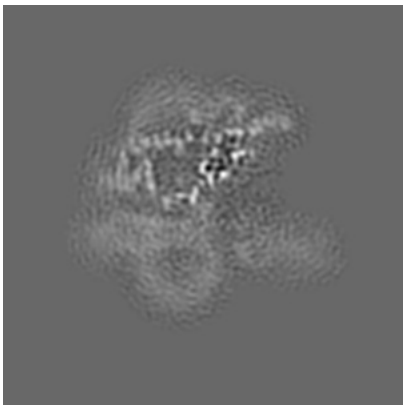


Z

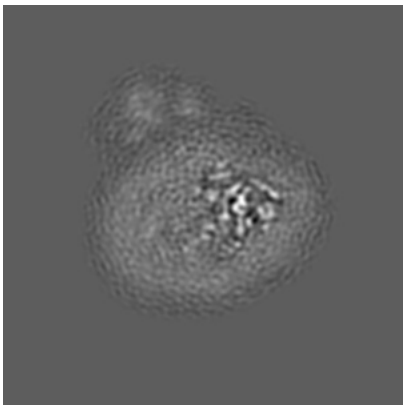
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

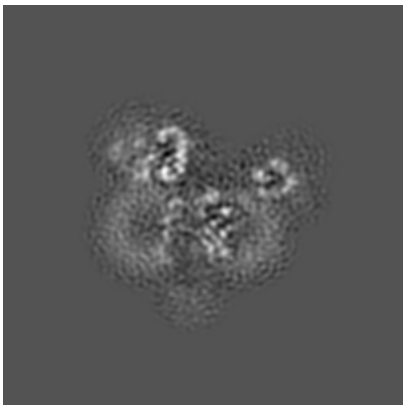
6.2.1 Primary map



X Index: 150

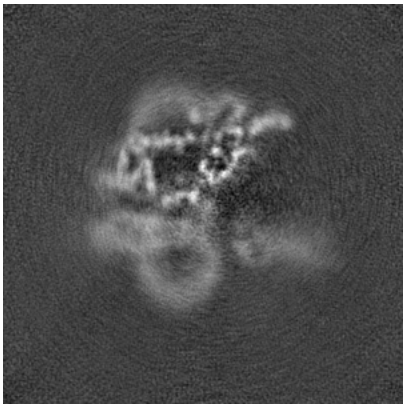


Y Index: 150

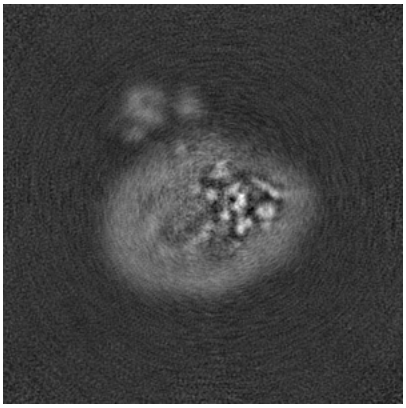


Z Index: 150

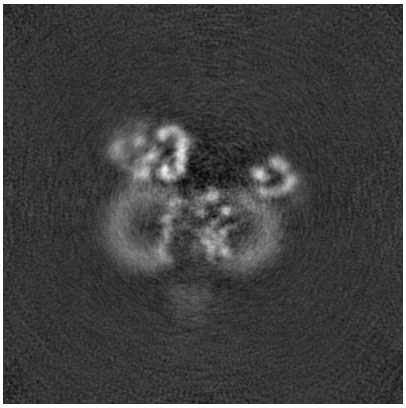
6.2.2 Raw map



X Index: 150



Y Index: 150

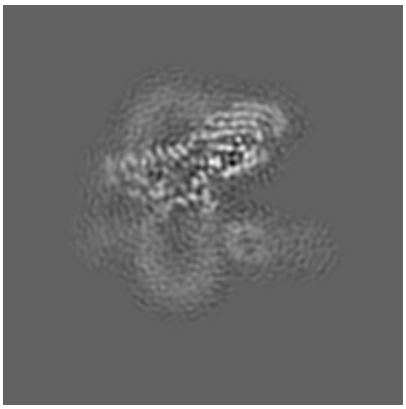


Z Index: 150

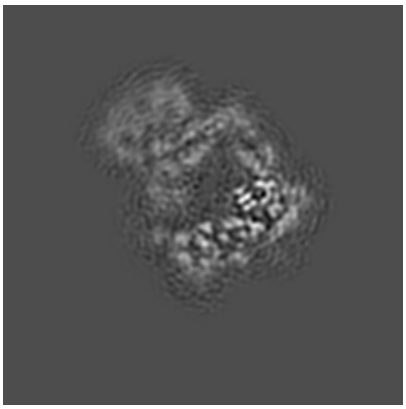
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

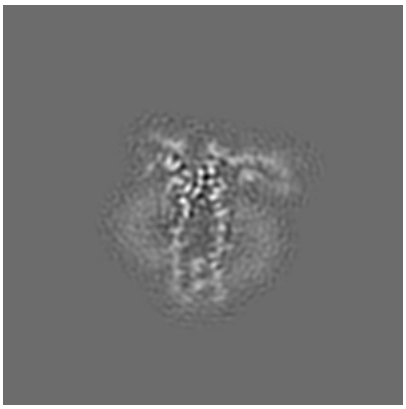
6.3.1 Primary map



X Index: 159

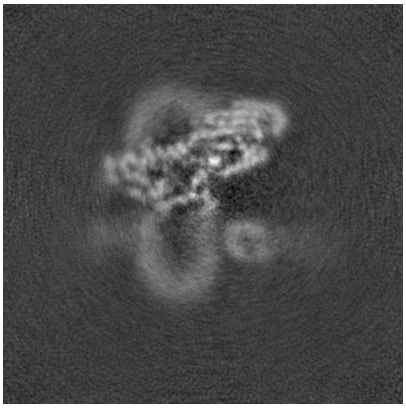


Y Index: 175

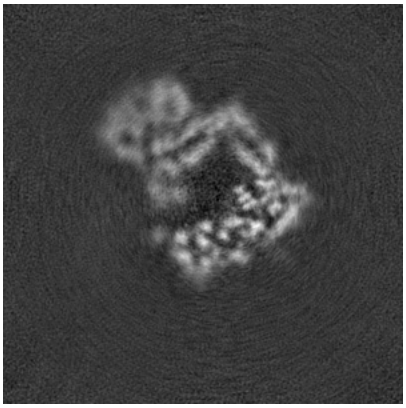


Z Index: 183

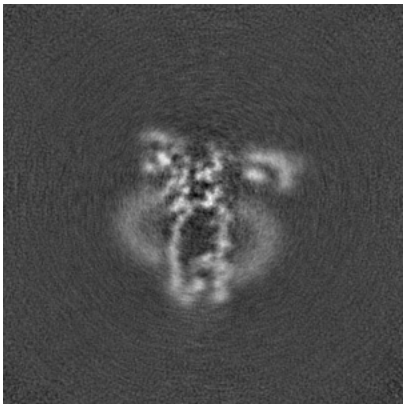
6.3.2 Raw map



X Index: 159



Y Index: 175

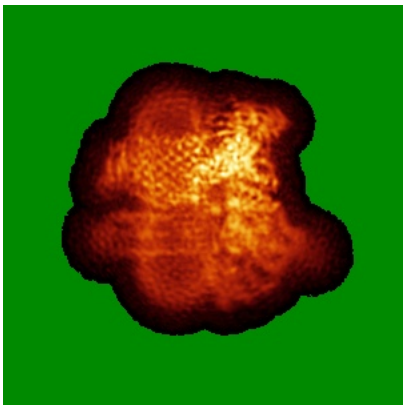


Z Index: 179

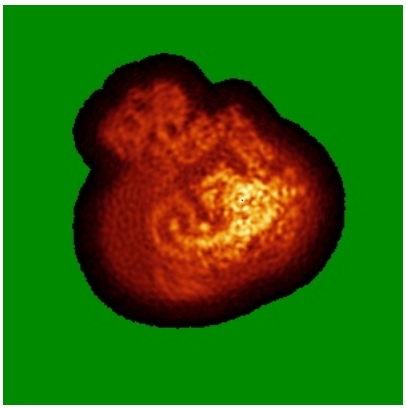
The images above show the largest variance slices of the map in three orthogonal directions.

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

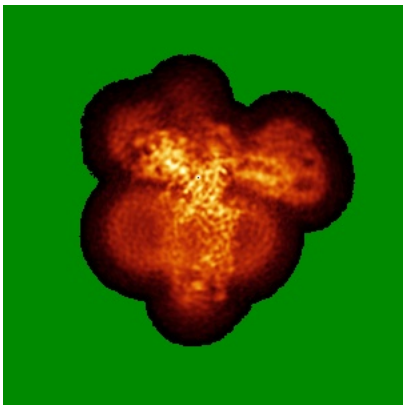
6.4.1 Primary map



X

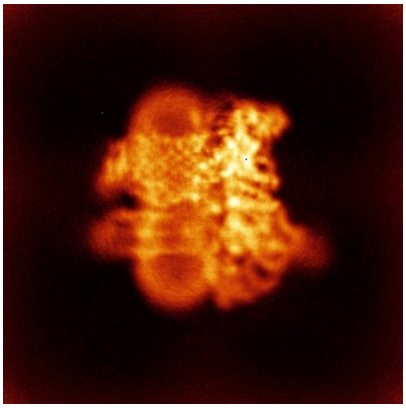


Y

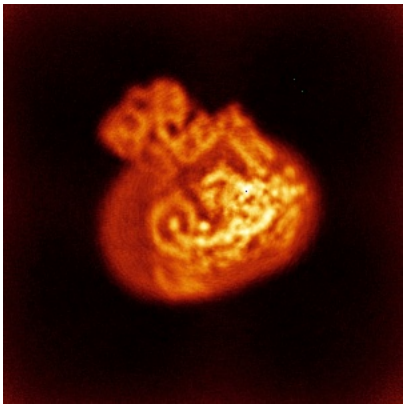


Z

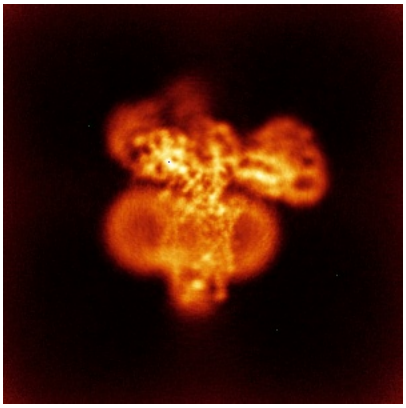
6.4.2 Raw map



X



Y

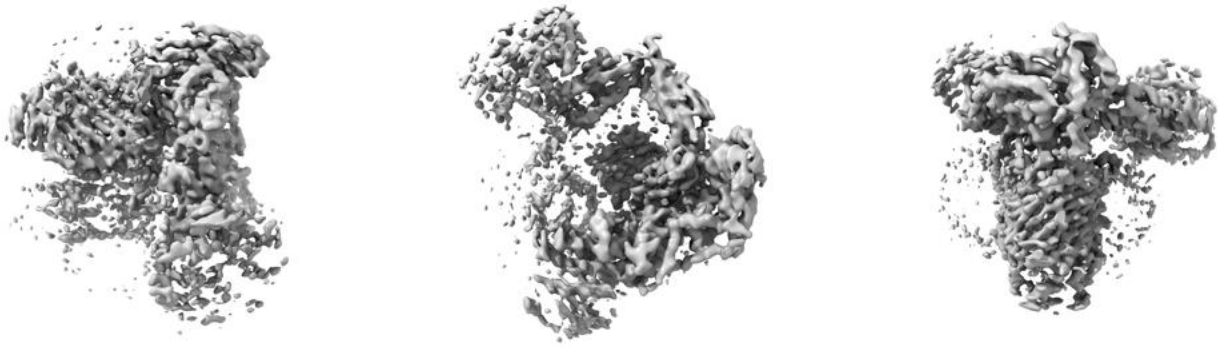


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.125. 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

X Y Z

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.

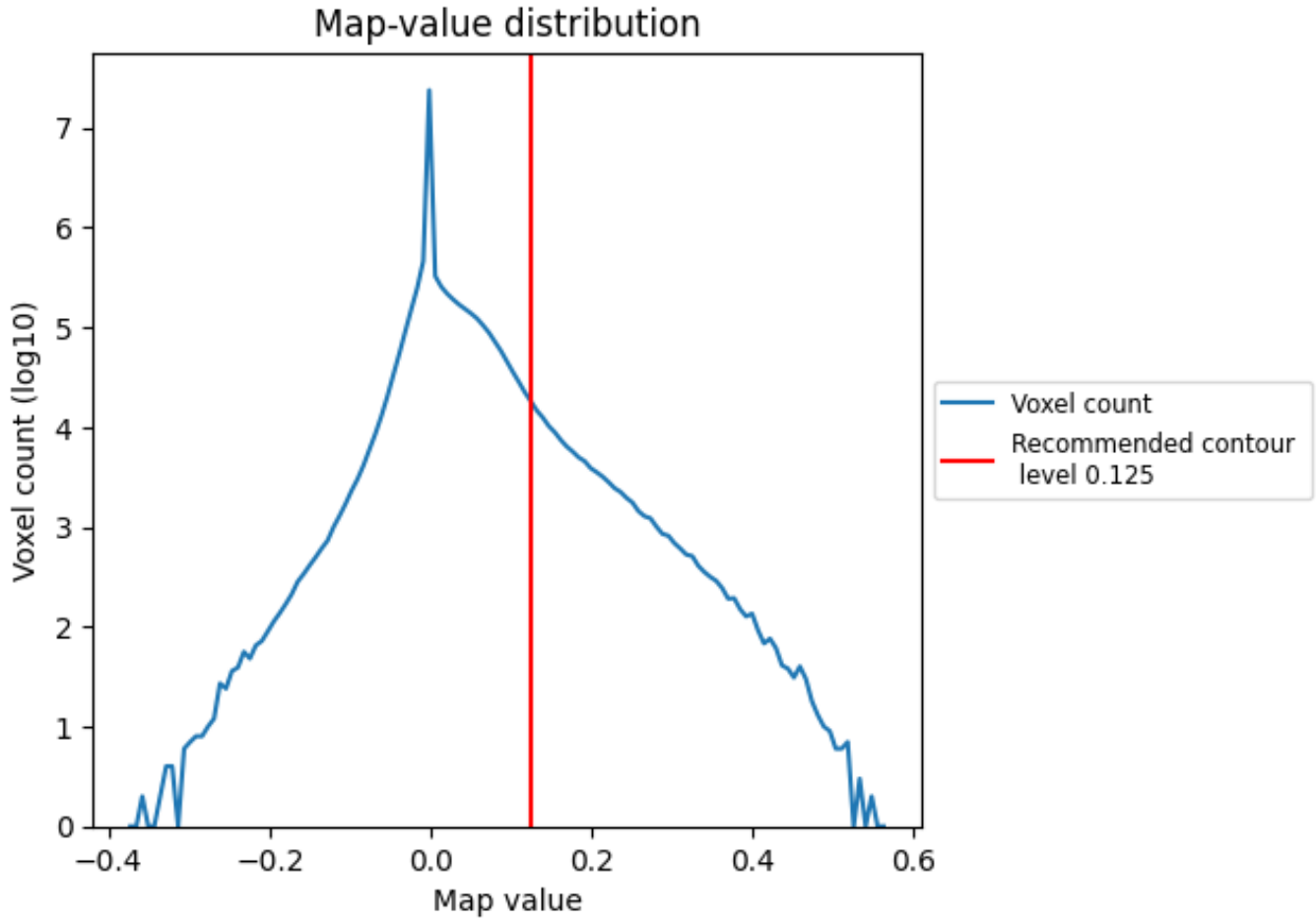
6.6 Mask visualisation (i)

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

7 Map analysis

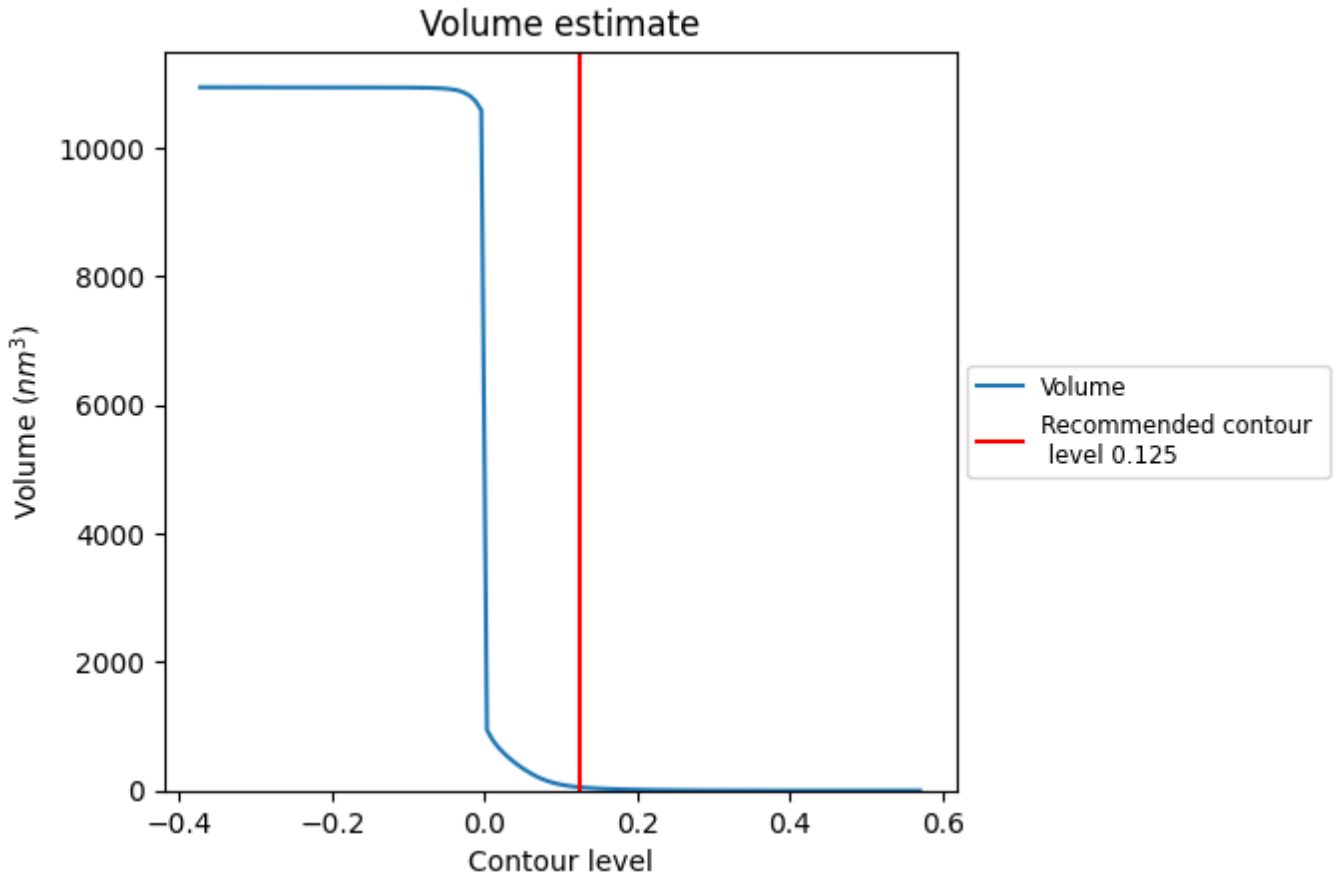
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

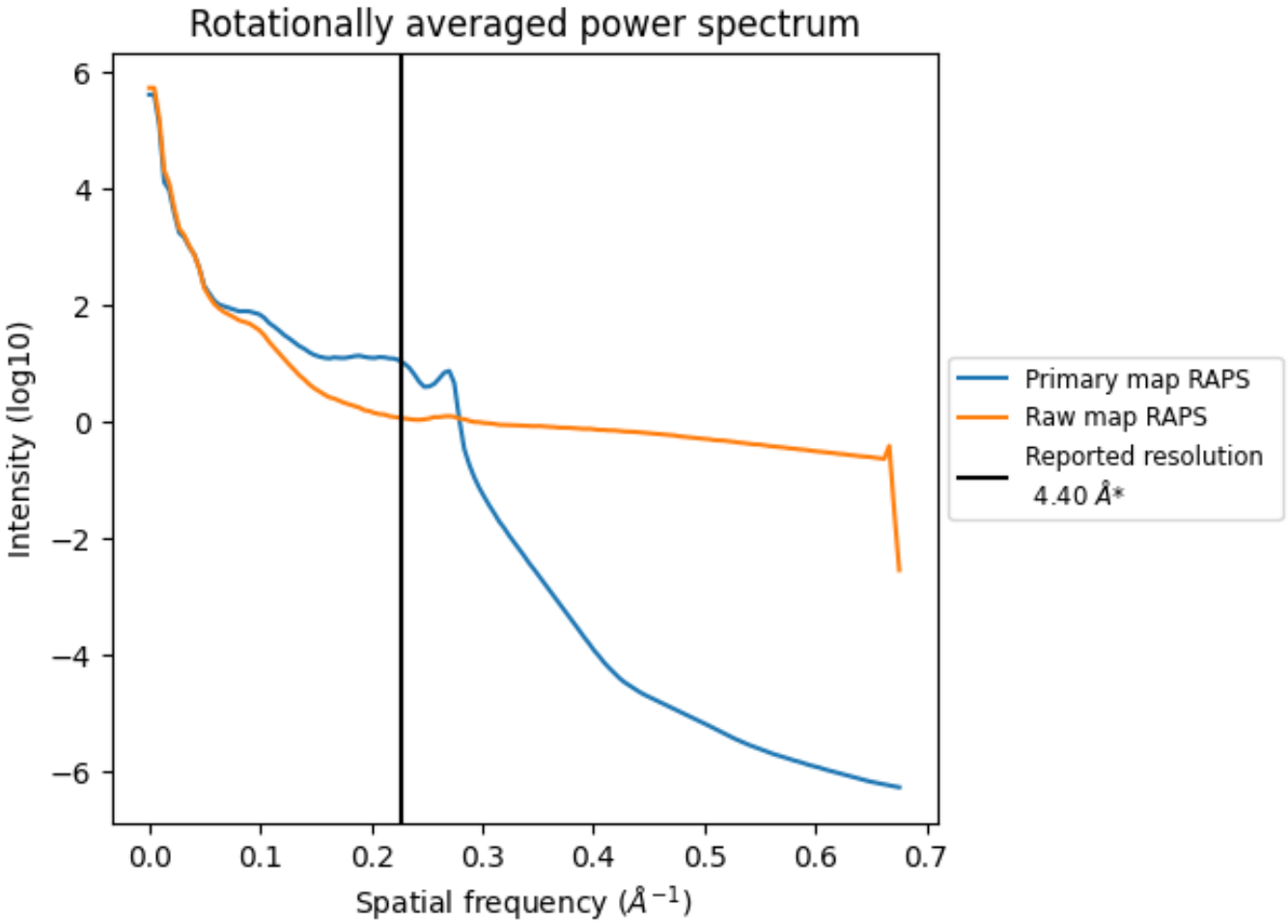
7.2 Volume estimate (i)



The volume at the recommended contour level is 51 nm^3; this corresponds to an approximate mass of 46 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)

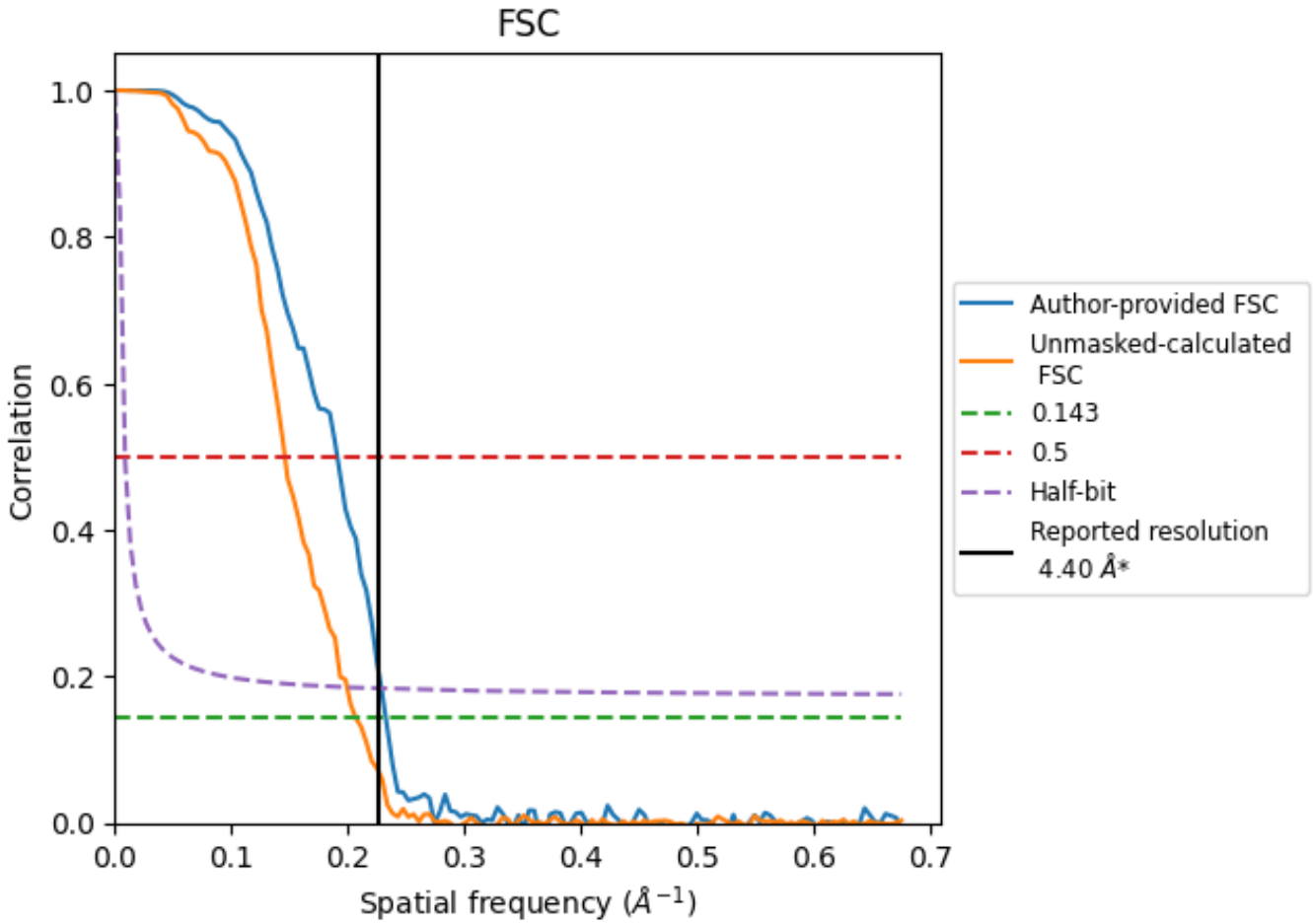


*Reported resolution corresponds to spatial frequency of 0.227 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.227 Å^{-1}

8.2 Resolution estimates (i)

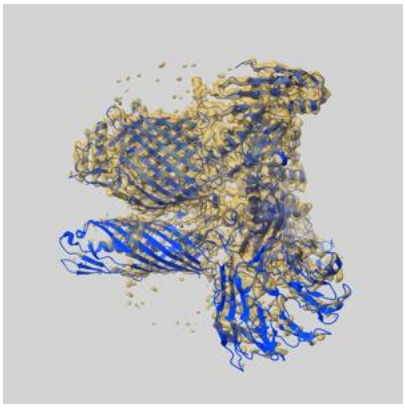
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.29	5.23	4.36
Unmasked-calculated*	4.83	6.84	5.01

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

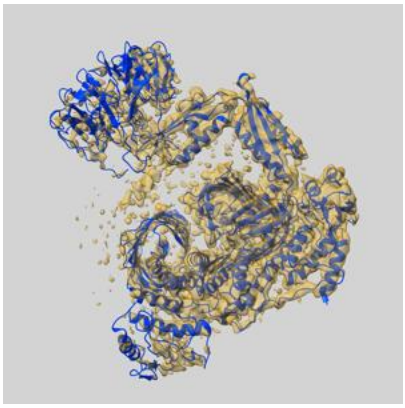
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-18543 and PDB model 8QP5. Per-residue inclusion information can be found in section 3 on page 6.

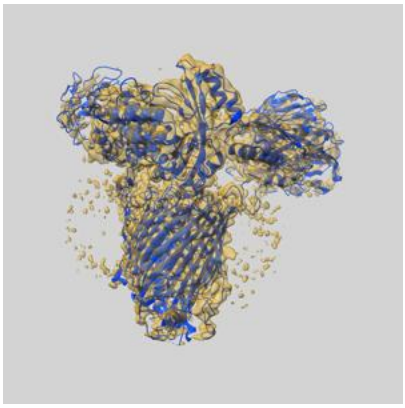
9.1 Map-model overlay



X



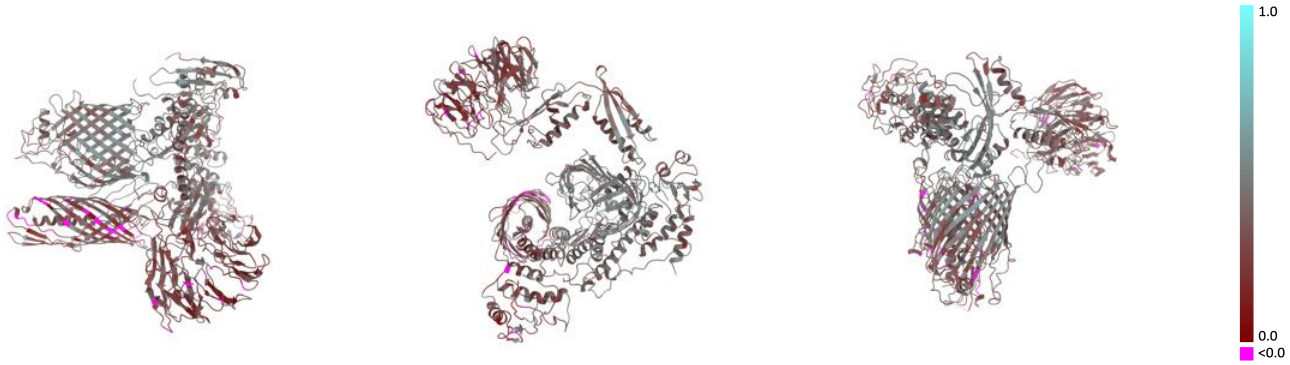
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.125 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.

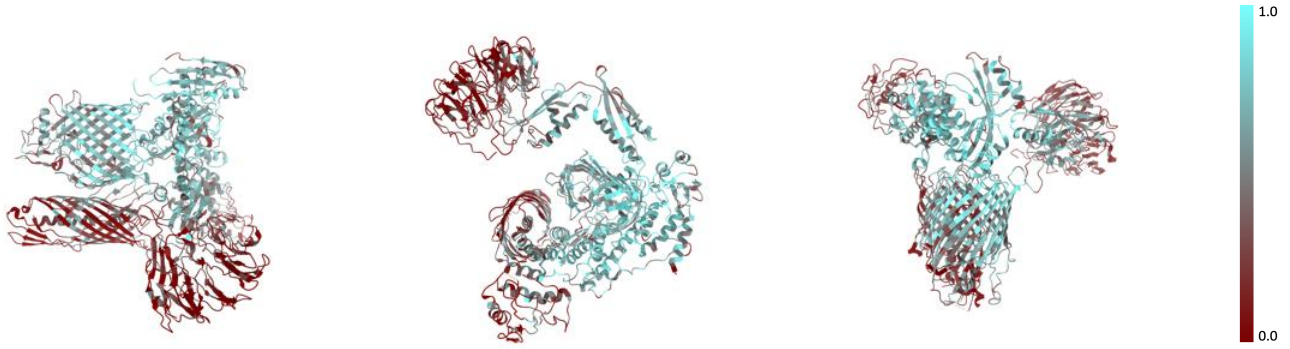
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

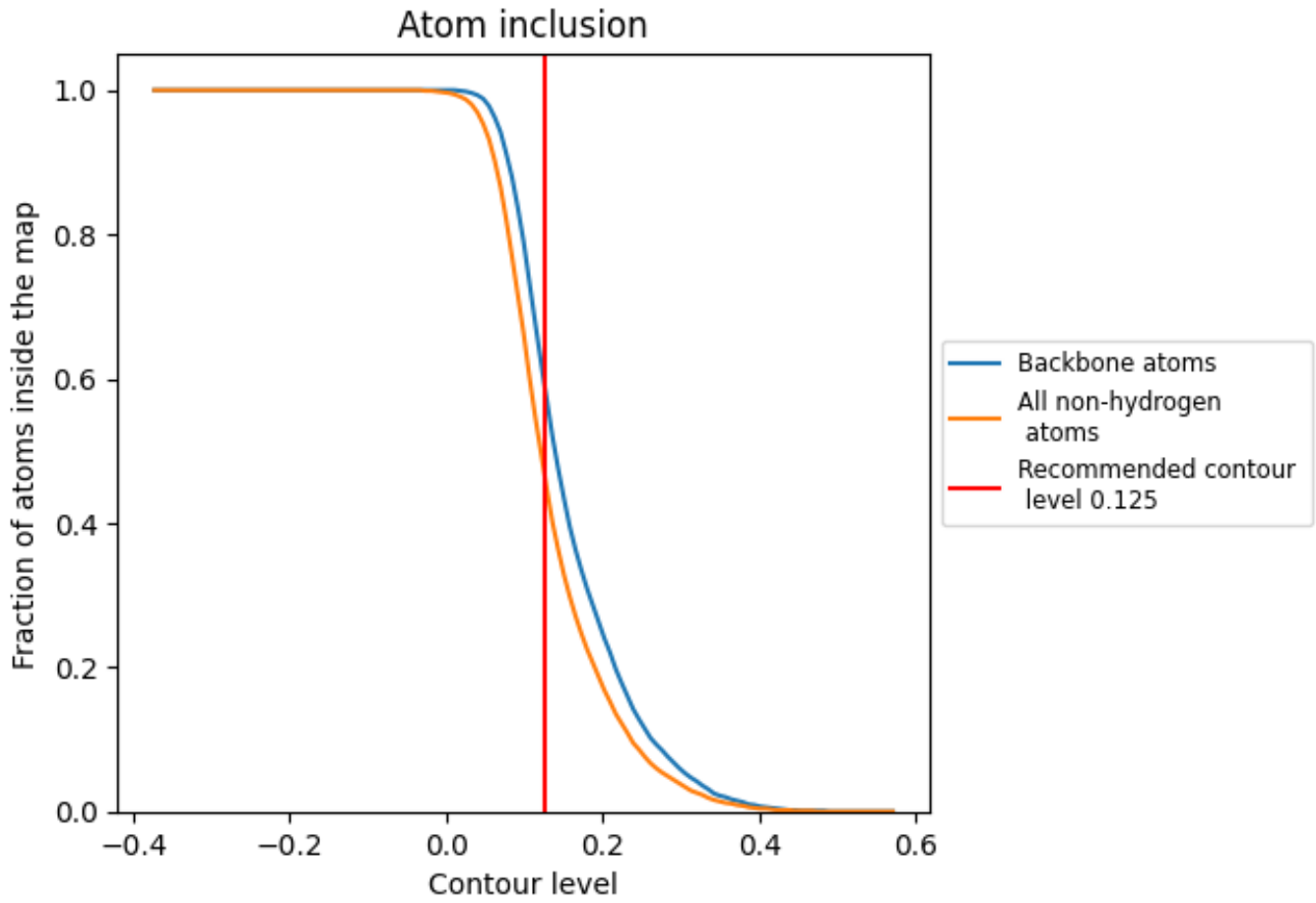
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.125).

9.4 Atom inclusion (i)



At the recommended contour level, 59% of all backbone atoms, 47% 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 (0.125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4680	0.3680
A	0.6110	0.4160
B	0.1850	0.2950
C	0.3820	0.3460
D	0.6820	0.4120
E	0.6600	0.4390
P	0.2420	0.2740