



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 12:51 AM UTC

PDB ID : 8Q0G / pdb_00008q0g
EMDB ID : EMD-18053
Title : Release Complex: BAM bound EspP and Compact SurA
Authors : Fenn, K.L.; Ranson, N.A.
Deposited on : 2023-07-28
Resolution : 4.30 Å(reported)
Based on initial models : 8PZ1, 3SLT, 7TTC

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:

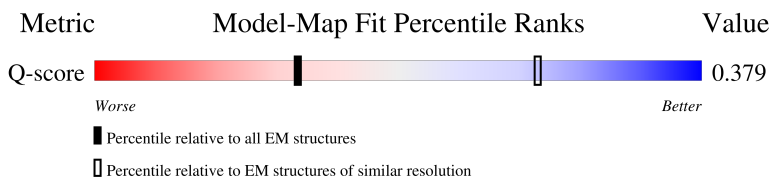
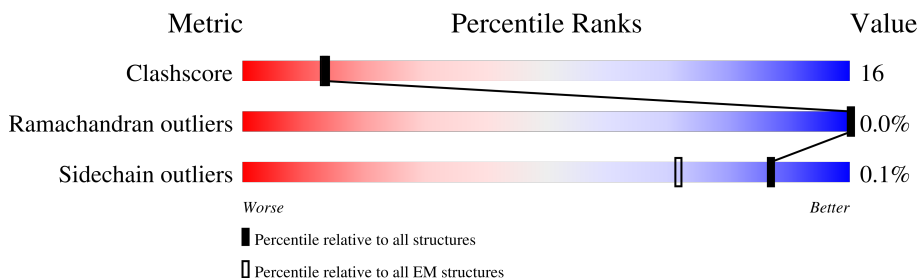
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4585 (3.80 - 4.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	790	
2	B	373	
3	C	320	
4	D	226	

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Mol	Chain	Length	Quality of chain
5	E	104	56%31%13%
6	F	450	52%35%21%44%
7	P	364	71%73%9%18%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15819 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	766	Total	C	N	O	S	0	0
			6041	3812	1023	1190	16		

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	370	Total	C	N	O	S	0	0
			2784	1748	474	556	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	174	Total	C	N	O	S	0	0
			1090	672	196	218	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	32	SER	LYS	conflict	UNP P0A903

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	218	Total	C	N	O	S	0	0
			1761	1109	309	336	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	90	Total	C	N	O	S	0	0
			703	441	123	137	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.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	251	Total	C	N	O	S	0	0
			1920	1189	355	366	10		

There are 43 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-21	GLY	-	expression tag	UNP P0ABZ6
F	-20	SER	-	expression tag	UNP P0ABZ6
F	-19	SER	-	expression tag	UNP P0ABZ6
F	-18	ALA	-	expression tag	UNP P0ABZ6
F	-17	TRP	-	expression tag	UNP P0ABZ6
F	-16	SER	-	expression tag	UNP P0ABZ6
F	-15	HIS	-	expression tag	UNP P0ABZ6
F	-14	PRO	-	expression tag	UNP P0ABZ6
F	-13	GLN	-	expression tag	UNP P0ABZ6
F	-12	PHE	-	expression tag	UNP P0ABZ6
F	-11	GLU	-	expression tag	UNP P0ABZ6
F	-10	LYS	-	expression tag	UNP P0ABZ6
F	-9	GLY	-	expression tag	UNP P0ABZ6
F	-8	GLY	-	expression tag	UNP P0ABZ6
F	-7	GLY	-	expression tag	UNP P0ABZ6
F	-6	SER	-	expression tag	UNP P0ABZ6
F	-5	GLY	-	expression tag	UNP P0ABZ6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-4	GLY	-	expression tag	UNP P0ABZ6
F	-3	GLY	-	expression tag	UNP P0ABZ6
F	-2	SER	-	expression tag	UNP P0ABZ6
F	-1	GLY	-	expression tag	UNP P0ABZ6
F	0	GLY	-	expression tag	UNP P0ABZ6
F	1	SER	-	expression tag	UNP P0ABZ6
F	2	ALA	-	expression tag	UNP P0ABZ6
F	3	TRP	-	expression tag	UNP P0ABZ6
F	4	SER	-	expression tag	UNP P0ABZ6
F	5	HIS	-	expression tag	UNP P0ABZ6
F	6	PRO	-	expression tag	UNP P0ABZ6
F	7	GLN	-	expression tag	UNP P0ABZ6
F	8	PHE	-	expression tag	UNP P0ABZ6
F	9	GLU	-	expression tag	UNP P0ABZ6
F	10	LYS	-	expression tag	UNP P0ABZ6
F	11	SER	-	expression tag	UNP P0ABZ6
F	12	SER	-	expression tag	UNP P0ABZ6
F	13	GLY	-	expression tag	UNP P0ABZ6
F	14	GLU	-	expression tag	UNP P0ABZ6
F	15	ASN	-	expression tag	UNP P0ABZ6
F	16	LEU	-	expression tag	UNP P0ABZ6
F	17	TYR	-	expression tag	UNP P0ABZ6
F	18	PHE	-	expression tag	UNP P0ABZ6
F	19	GLN	-	expression tag	UNP P0ABZ6
F	20	GLY	-	expression tag	UNP P0ABZ6
F	27	CYS	LYS	engineered mutation	UNP P0ABZ6

- Molecule 7 is a protein called Serine protease EspP.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P	299	Total	C	N	O	S	1	0
			1520	900	310	309	1		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	937	GLY	-	expression tag	UNP Q7BSW5
P	938	GLY	-	expression tag	UNP Q7BSW5
P	976	GLY	-	insertion	UNP Q7BSW5
P	977	GLU	-	insertion	UNP Q7BSW5
P	978	ASN	-	insertion	UNP Q7BSW5
P	979	LEU	-	insertion	UNP Q7BSW5

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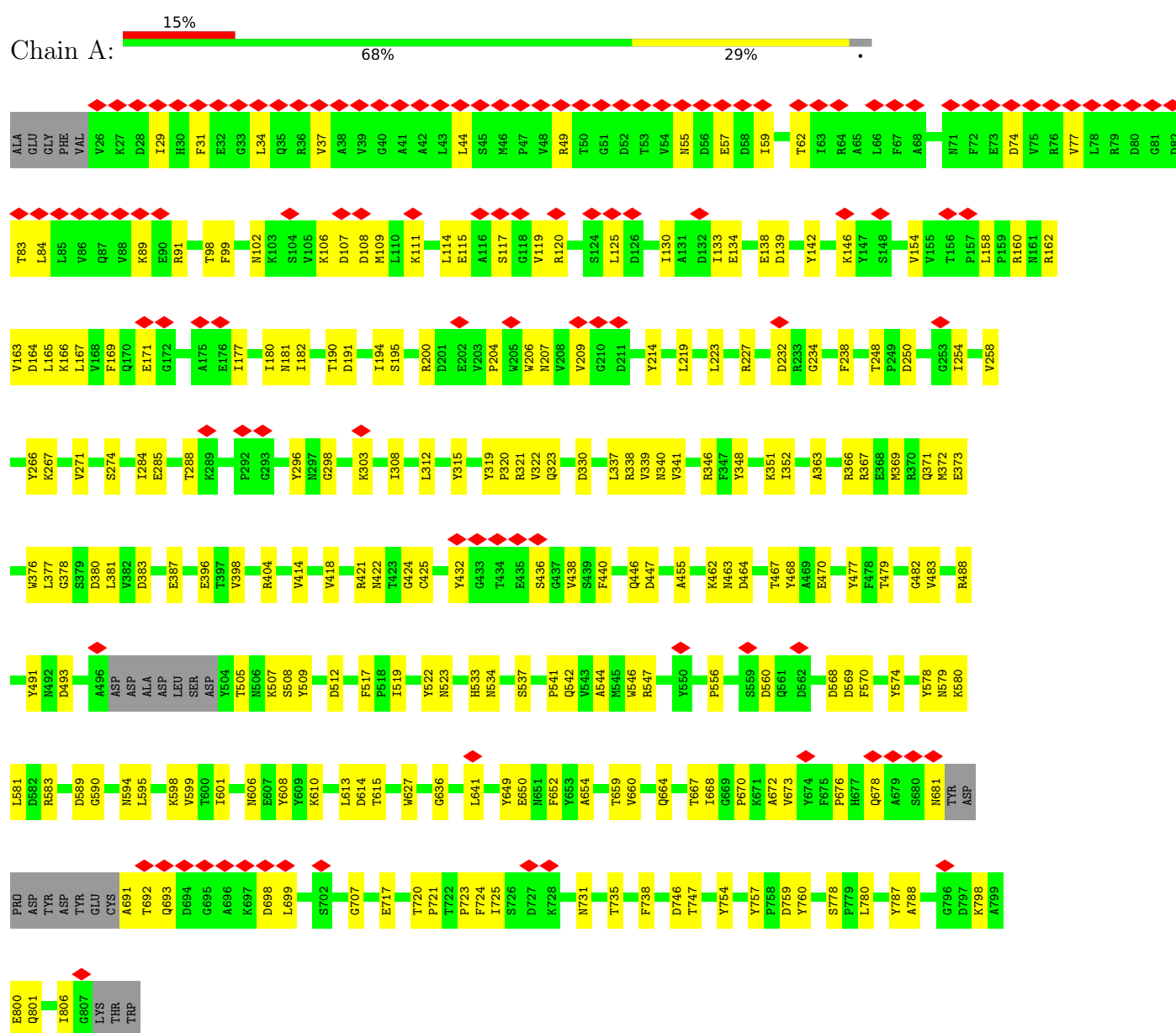
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Chain	Residue	Modelled	Actual	Comment	Reference
P	980	TYR	-	insertion	UNP Q7BSW5
P	981	PHE	-	insertion	UNP Q7BSW5
P	982	GLN	-	insertion	UNP Q7BSW5
P	983	GLY	-	insertion	UNP Q7BSW5
P	984	GLY	-	insertion	UNP Q7BSW5
P	1299	CYS	SER	engineered mutation	UNP Q7BSW5

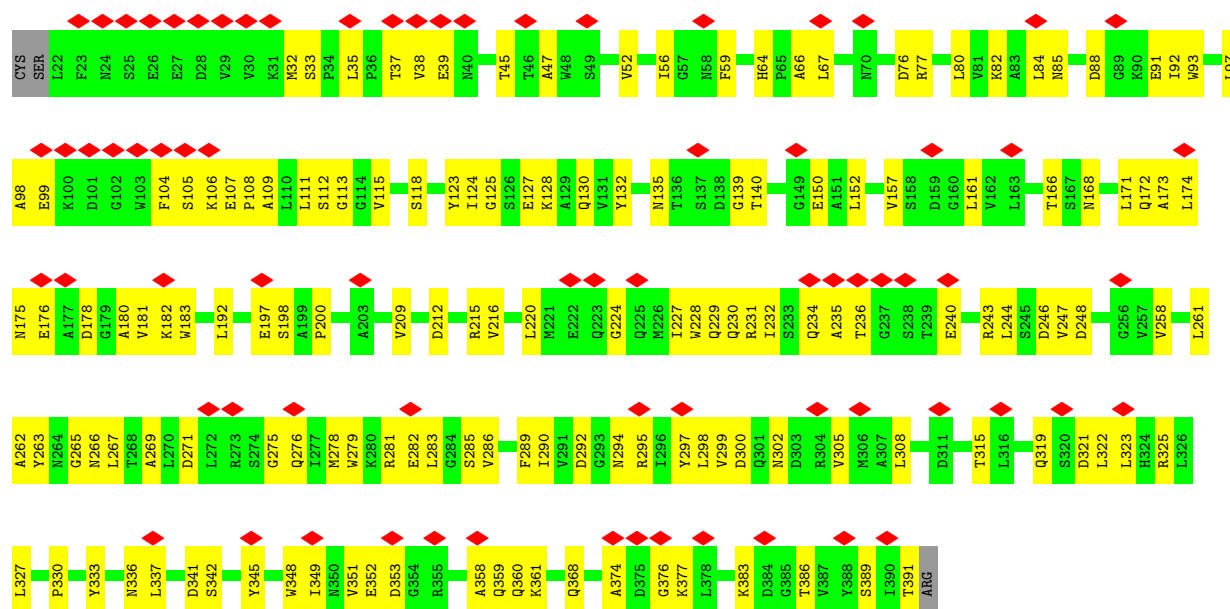
3 Residue-property plots

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



- Molecule 2: Outer membrane protein assembly factor BamB



D1243	Q1182	I1122	D1058	THR	GLY
A1244	F1183	G1123	N1059	VAL	GLY
S1245	A1184	K1124	Y1060	ALA	ASN
G1246	W1185	Y1125	T1061	ASN	ILE
E1247	K1186	Y1126	H1062	L1062	GLU
K1248	D1187	H1127	V1063	A1003	VAL
R1249	Q1188	H1128	Q1064	T1004	SER
I1250	K1189	D1129	V1065	T1005	ALA
K1251	M1190	N1130	G1066	N1006	PRO
G1252	H1191	E1131	V1067	A1007	LYS
E1253	L1192	Y1132	D1068	A1008	ASP
K1254	S1193	T1133	K1069	A1009	ASN
D1255	M1194	A1134	K1070	L1010	GLU
S1256	K1195	T1135	H1071	F1011	ASN
R1257	D1196	F1136	E1072	S1012	VAL
M1258	K1197	A1137	L1073	V1013	LYS
L1259	D1198	G1138	D1074	D1014	ALA
M1260	Y1199	L1139	G1075	Y1015	SER
S1261	N1200	G1140	L1076	K1016	GLN
V1262	P1201	T1141	D1077	A1017	THR
G1263	L1202	R1142	L1078	F1018	ILE
L1264	I1203	D1143	F1079	L1019	GLY
M1265	G1204	Y1144	T1080	N1020	SER
A1266	R1205	S1145	G1081	E1021	ASP
E1267	T1206	T1146	F1082	V1022	VAL
G1268	G1207	H1147	T1083	N1023	THR
	V1208	S1148	V1084	N1024	VAL
D1270	D1209	W1149	T1085	L1025	ILE
M1271	V1210	Y1150	S1089	N1026	THR
V1272	G1211	A1151		K1027	THR
R1273	K1212	G1152	N1028	R1028	ARG
F1274	S1213	A1153	N1029	M1029	THR
G1275	F1214	E1154	A1091	G1030	GLY
L1276	S1215	A1155	S1092	D1031	GLU
E1277	G1216	A1155	A1093	L1032	ASN
F1278	K1217	G1156	D1094	L1033	LEU
E1279	D1218	R1157	V1095	R1033	TYR
K1280	W1219	R1158	F1096	D1034	PHE
S1281	K1220	Y1159	S1097	T1035	GLN
A1282	V1221	H1160	G1098	N1036	GLY
F1283	T1222	V1161	G1099	G1037	ASP
G1284	A1223	T1162	T1100	E1038	ASP
K1285	R1224	E1163	V1103	A1039	LYS
Y1286	A1225	D1164	G1104	G1040	ILE
M1287	G1226	A1165	A1105	A1041	THR
V1288	L1227	W1166	G1106	W1042	SER
D1289	G1228	T1167	L1107	A1043	LEU
A1291	F1231	E1168	Y1108	R1044	THR
V1292	D1232	P1169	A1109	T1045	GLY
M1293	L1233	Q1170	S1110	A1046	TYR
F1294	L1234	A1171	A1111	G1050	ASN
	A1235	L1173	M1112	T1049	
Y1296	N1236	V1174	F1113	S1051	
C1299	G1237	Y1175	D1114	A1052	
F1300	E1238	G1176	S1115	S1053	
G1301	T1239	S1177	G1116	G1054	
	V1240	V1178	A1117	G1055	
H1302	L1241	S1179	D1120	F1056	
	R1242	K1181	L1121	S1057	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	179199	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 ($e^-/\text{\AA}^2$)	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	0.019	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00387	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 [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	0.24	0/6177	0.40	0/8375
2	B	0.18	0/2835	0.41	0/3867
3	C	0.32	0/1102	0.48	0/1512
4	D	0.28	0/1801	0.45	0/2447
5	E	0.34	0/718	0.40	0/979
6	F	0.26	0/1938	0.47	0/2611
7	P	0.13	0/1523	0.34	0/2100
All	All	0.24	0/16094	0.42	0/21891

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	6041	0	5784	172	0
2	B	2784	0	2725	119	0
3	C	1090	0	896	36	0
4	D	1761	0	1699	58	0
5	E	703	0	680	25	0
6	F	1920	0	1923	75	0
7	P	1520	0	800	21	0
All	All	15819	0	14507	482	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 16.

The worst 5 of 482 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:541:PRO:HA	1:A:546:TRP:HE1	1.34	0.89
2:B:299:VAL:HG21	2:B:327:LEU:HD12	1.58	0.86
1:A:422:ASN:ND2	7:P:1299:CYS:SG	2.49	0.85
6:F:183:LEU:HD12	6:F:264:GLY:HA2	1.59	0.84
1:A:440:PHE:HB3	1:A:462:LYS:HB3	1.61	0.82

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	760/790 (96%)	701 (92%)	59 (8%)	0	100	100
2	B	368/373 (99%)	328 (89%)	40 (11%)	0	100	100
3	C	168/320 (52%)	144 (86%)	24 (14%)	0	100	100
4	D	216/226 (96%)	199 (92%)	17 (8%)	0	100	100
5	E	88/104 (85%)	83 (94%)	5 (6%)	0	100	100
6	F	243/450 (54%)	224 (92%)	18 (7%)	1 (0%)	30	66
7	P	298/364 (82%)	279 (94%)	19 (6%)	0	100	100
All	All	2141/2627 (82%)	1958 (92%)	182 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	187	PRO

5.3.2 Protein sidechains ⓘ

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	650/672 (97%)	649 (100%)	1 (0%)	87	85
2	B	301/304 (99%)	301 (100%)	0	100	100
3	C	78/258 (30%)	78 (100%)	0	100	100
4	D	183/190 (96%)	183 (100%)	0	100	100
5	E	78/90 (87%)	78 (100%)	0	100	100
6	F	201/367 (55%)	200 (100%)	1 (0%)	81	81
7	P	15/289 (5%)	15 (100%)	0	100	100
All	All	1506/2170 (69%)	1504 (100%)	2 (0%)	87	88

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

Mol	Chain	Res	Type
1	A	806	ILE
6	F	191	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	359	GLN
4	D	41	GLN
6	F	223	GLN
6	F	186	ASN
2	B	121	HIS

5.3.3 RNA ⓘ

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.

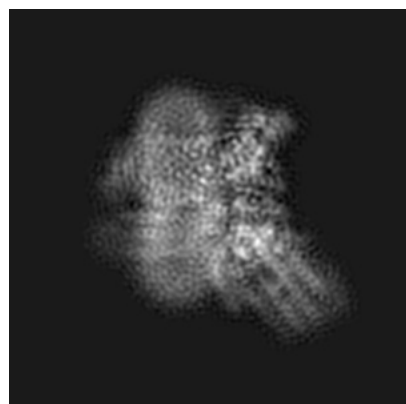
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18053. These allow visual inspection of the internal detail of the map and identification of artifacts.

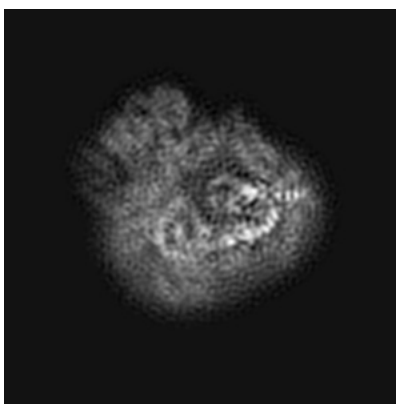
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

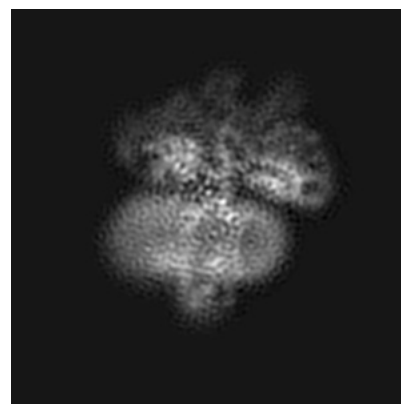
6.1.1 Primary map



X

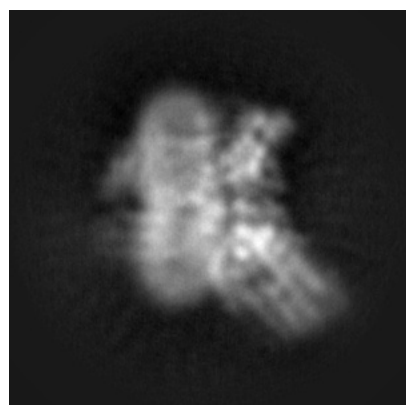


Y

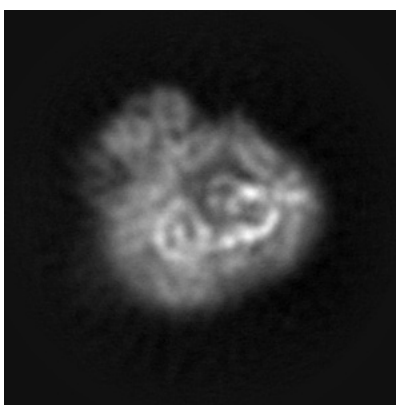


Z

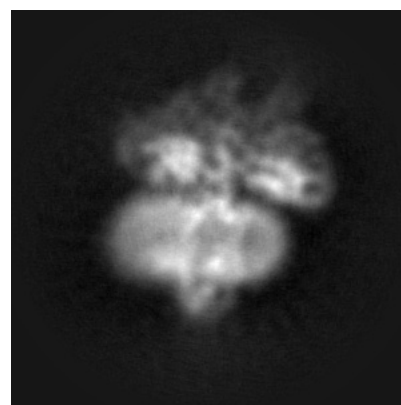
6.1.2 Raw map



X



Y

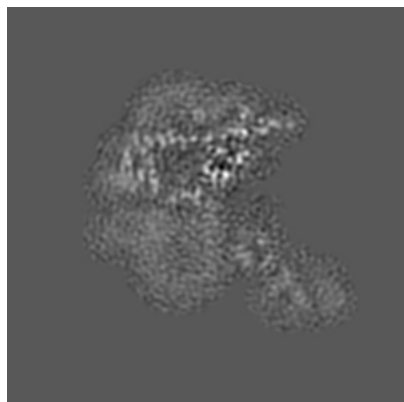


Z

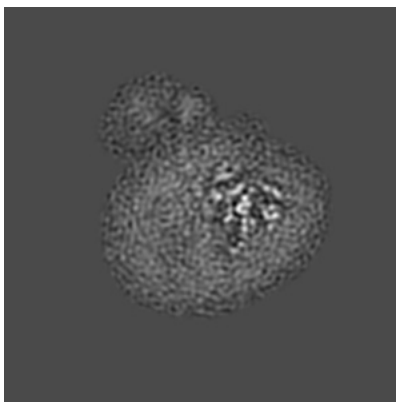
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

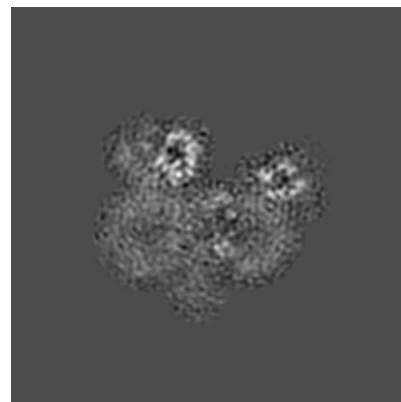
6.2.1 Primary map



X Index: 150

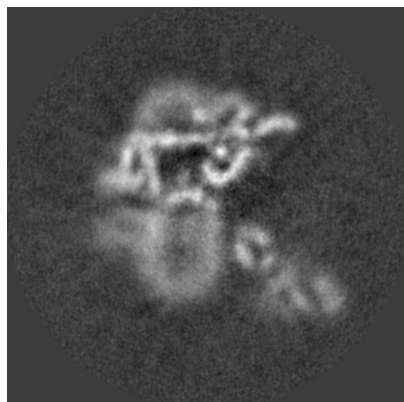


Y Index: 150

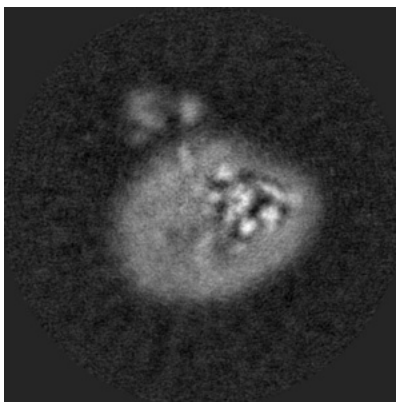


Z Index: 150

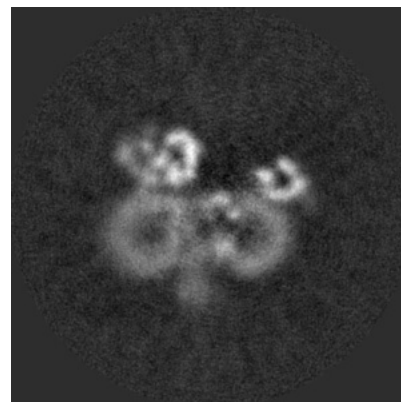
6.2.2 Raw map



X Index: 150



Y Index: 150

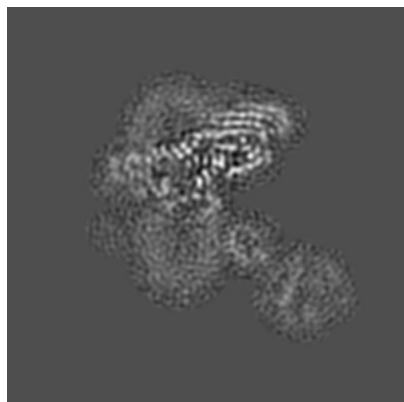


Z Index: 150

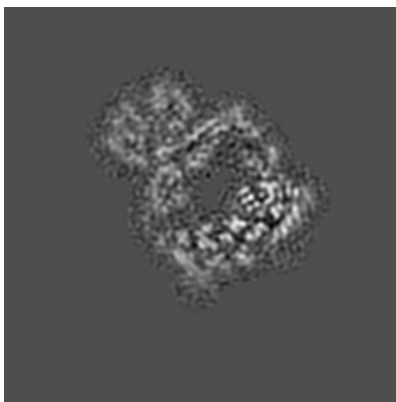
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

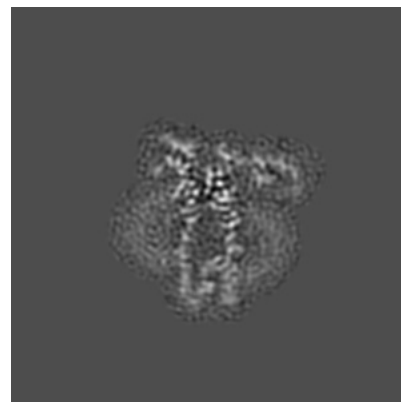
6.3.1 Primary map



X Index: 160

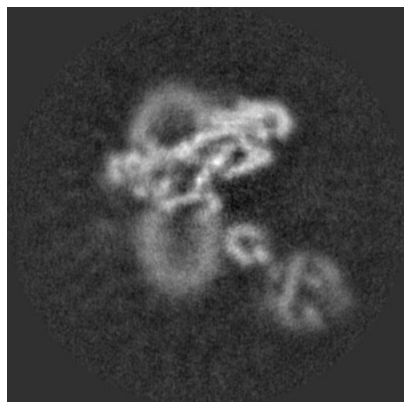


Y Index: 176

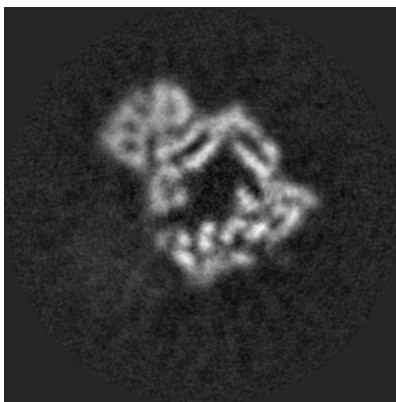


Z Index: 183

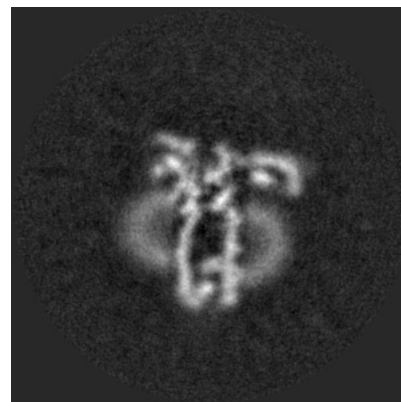
6.3.2 Raw map



X Index: 160



Y Index: 174

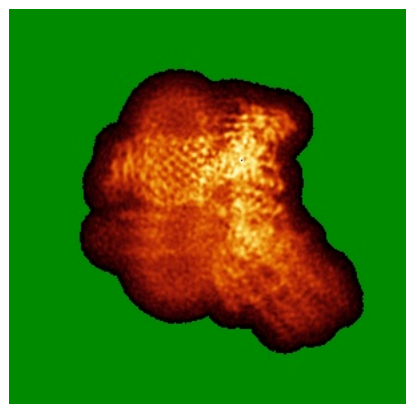


Z Index: 182

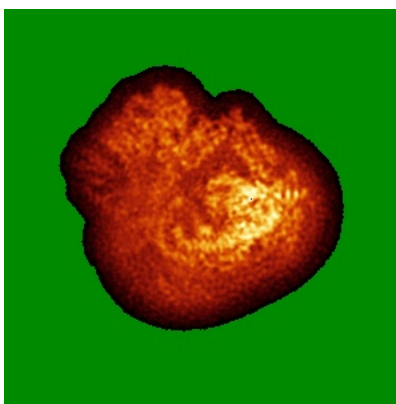
The images above show the largest variance slices of the map in three orthogonal directions.

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

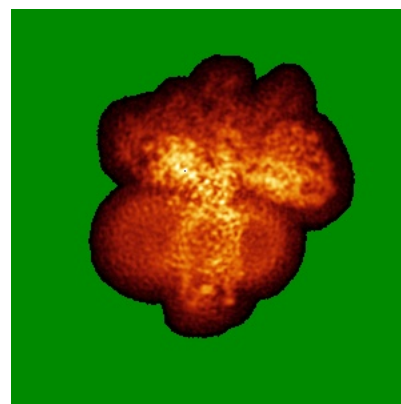
6.4.1 Primary map



X

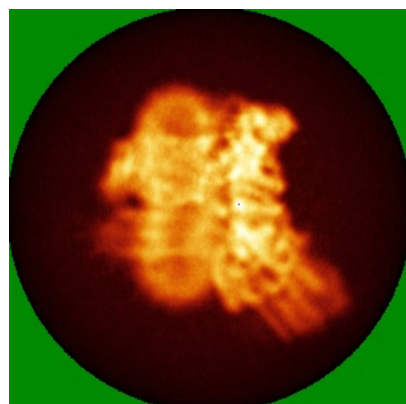


Y

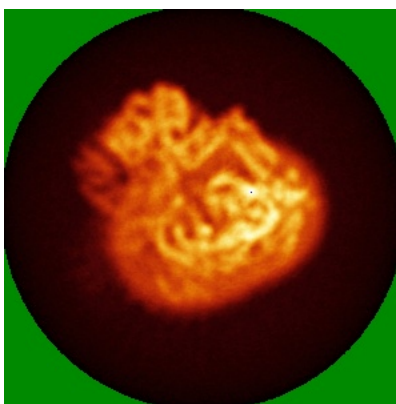


Z

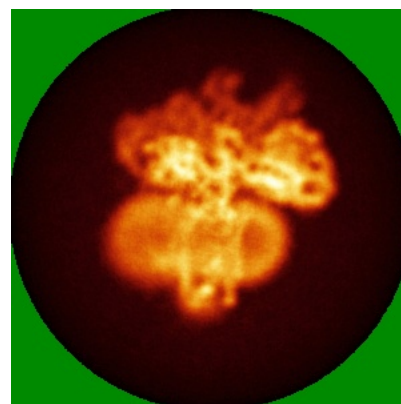
6.4.2 Raw map



X



Y

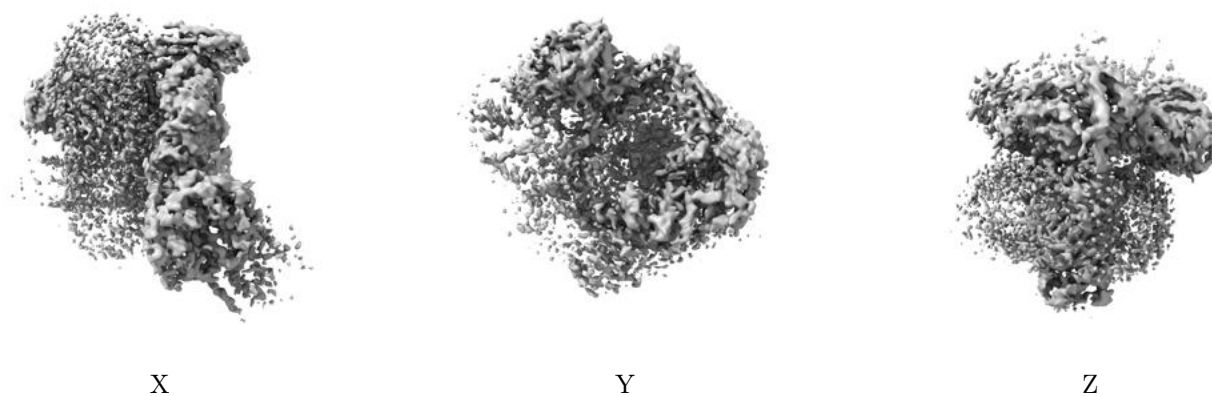


Z

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 0.00387. 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.

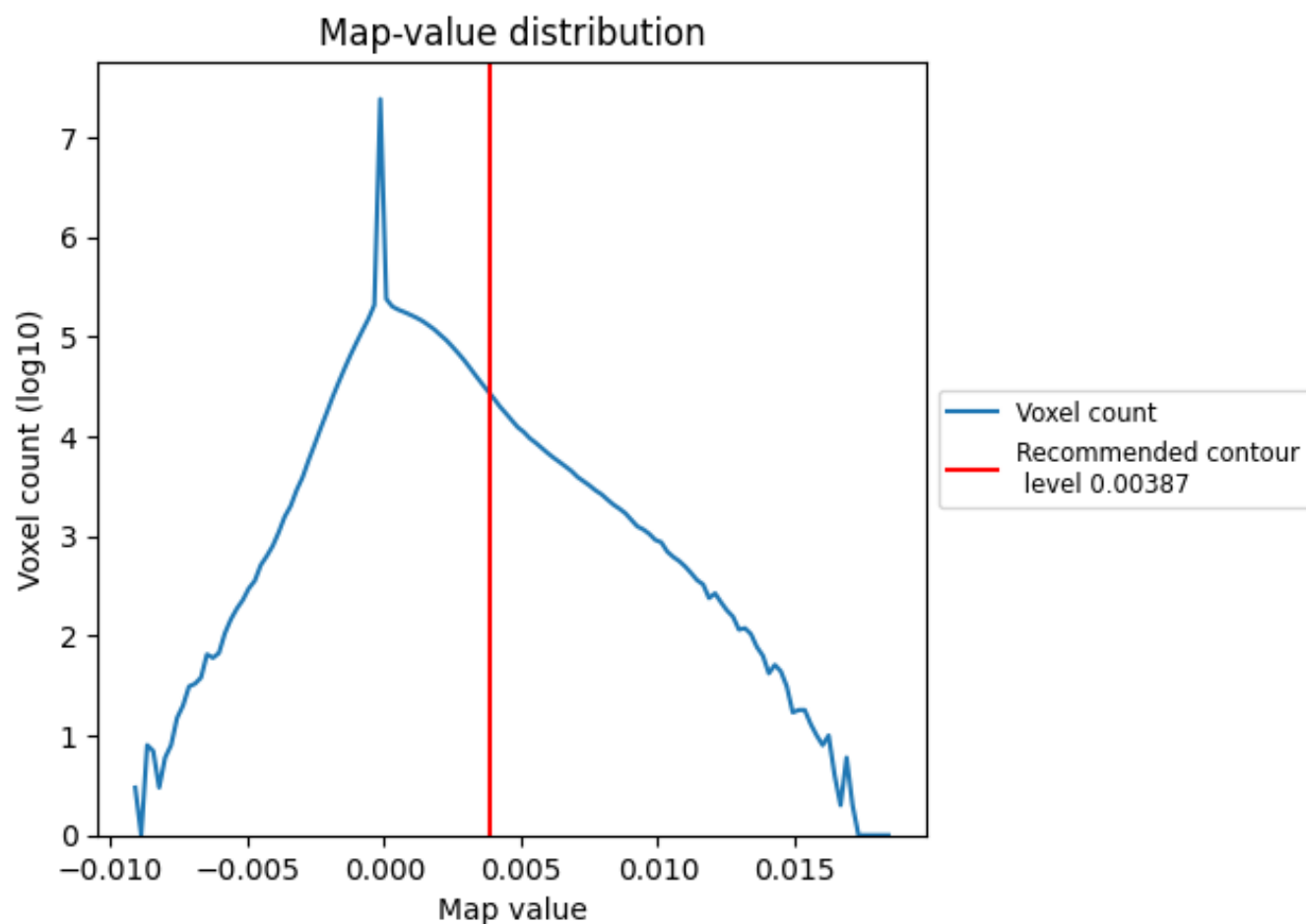
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

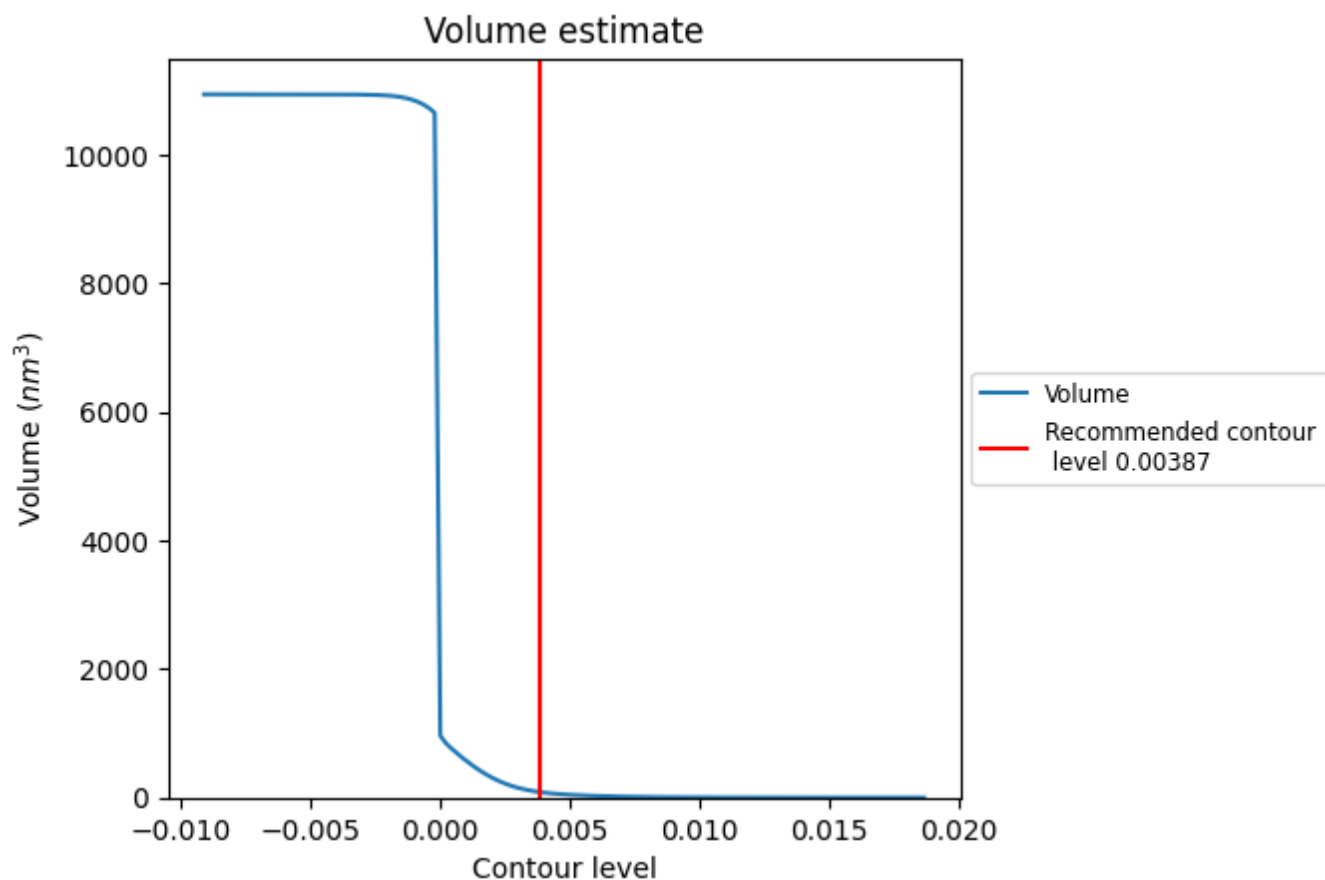
This section contains the results of statistical analysis of the map.

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.

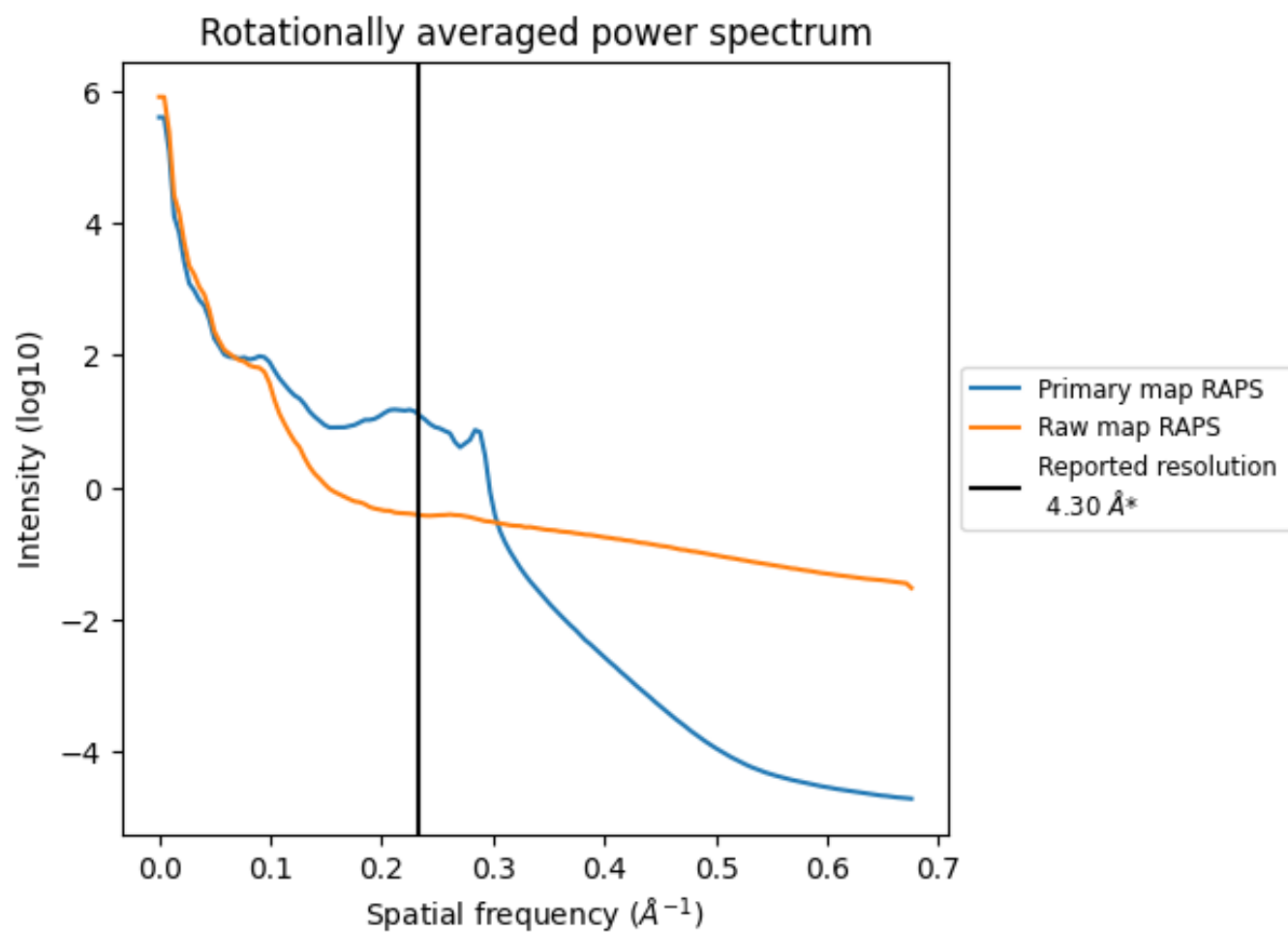
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 84 nm³; this corresponds to an approximate mass of 76 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](#)

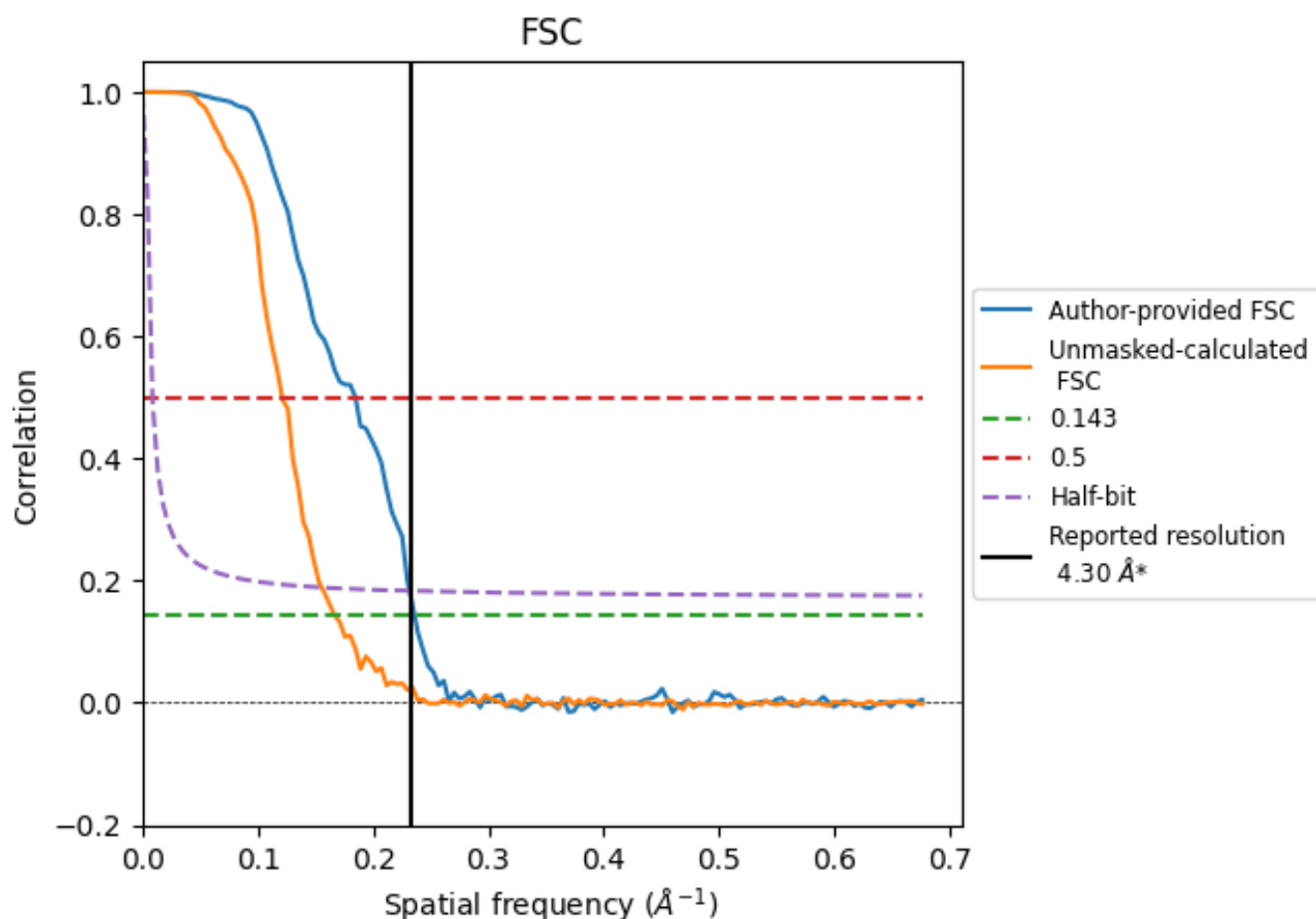


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

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 $0.233 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

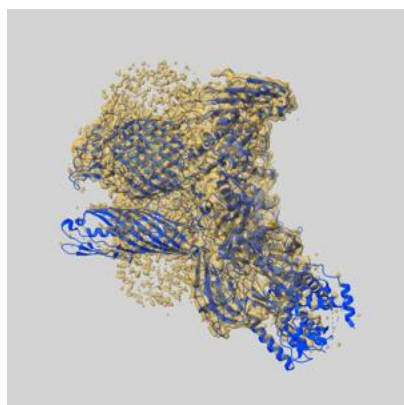
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.24	5.41	4.32
Unmasked-calculated*	6.00	8.25	6.43

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

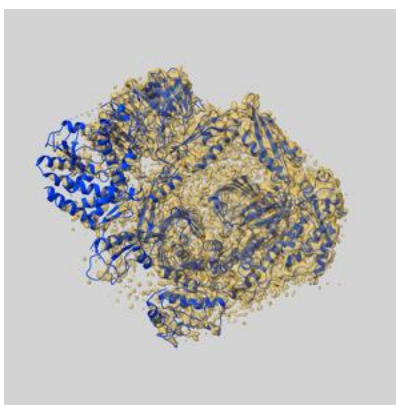
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18053 and PDB model 8Q0G. Per-residue inclusion information can be found in section [3](#) on page [8](#).

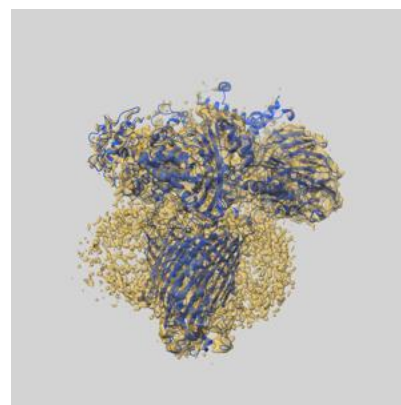
9.1 Map-model overlay [i](#)



X



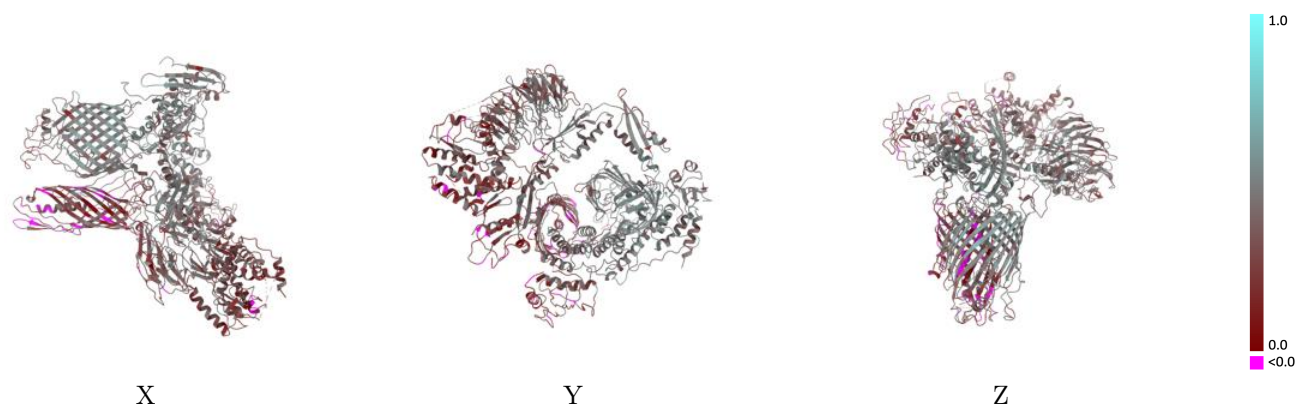
Y



Z

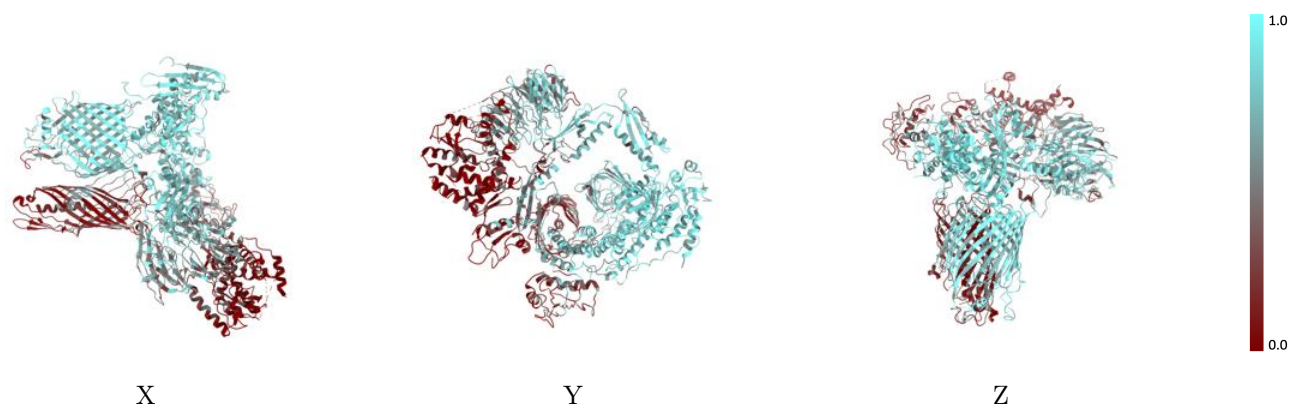
The images above show the 3D surface view of the map at the recommended contour level 0.00387 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



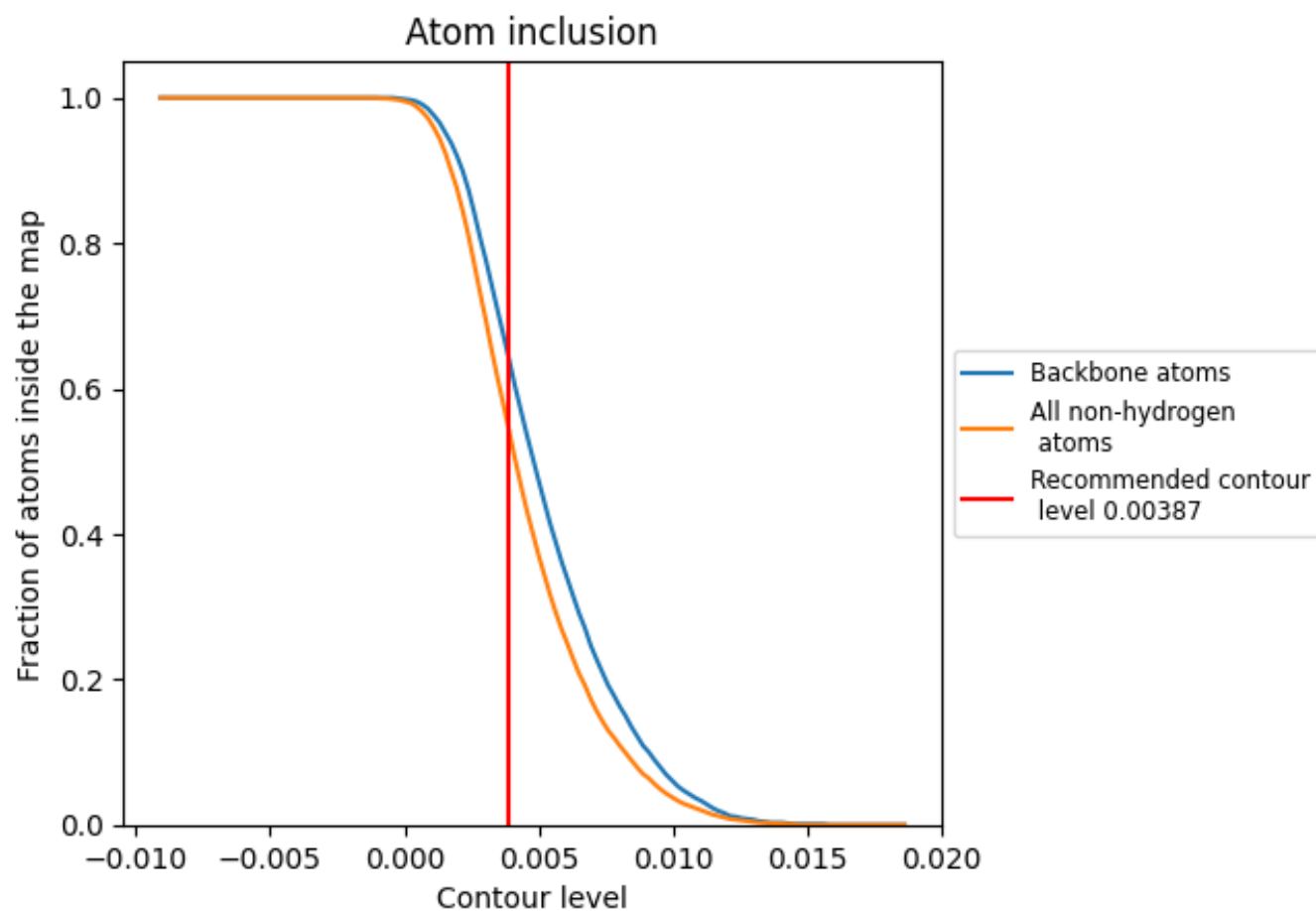
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00387).

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 55% 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 (0.00387) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5480	0.3790
A	0.6760	0.4240
B	0.5810	0.3860
C	0.4260	0.3330
D	0.8050	0.4610
E	0.8000	0.4550
F	0.1260	0.2880
P	0.1970	0.2080

1.0

0.0

<0.0