



wwPDB EM Validation Summary Report ⓘ

Sep 1, 2025 – 10:09 PM JST

PDB ID : 9JBV / pdb_00009jbv
EMDB ID : EMD-61327
Title : Structure of Engineered Coagulation Factor VIII with Enhanced Secretion and Coagulation Potential
Authors : Kio, H.; Osamu, N.; Tsukasa, O.
Deposited on : 2024-08-27
Resolution : 3.17 Å(reported)

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.dev126
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.45.1

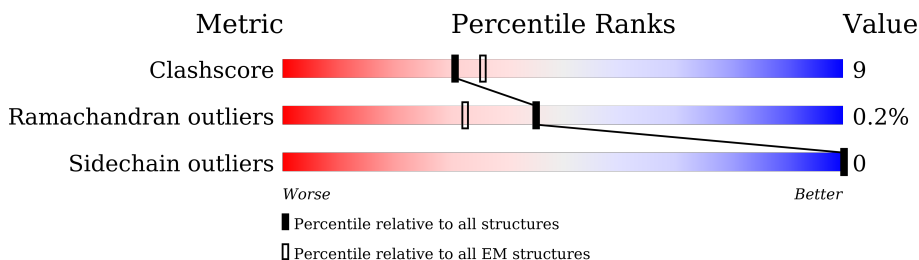
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.17 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	1457	<div> <div>9%</div> <div>69%</div> <div>19%</div> <div>12%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10291 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 Coagulation factor VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1276	Total	C	N	O	S	0	0
			10291	6599	1753	1880	59		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	PRO	ARG	conflict	UNP P00451
A	44	HIS	PRO	conflict	UNP P00451
A	47	THR	ALA	conflict	UNP P00451
A	171	PRO	LEU	conflict	UNP P00451
A	232	ASN	LYS	conflict	UNP P00451
A	236	THR	MET	conflict	UNP P00451
A	247	GLN	TRP	conflict	UNP P00451
A	386	PRO	SER	conflict	UNP P00451
A	429	LEU	GLN	conflict	UNP P00451
A	506	HIS	TYR	conflict	UNP P00451
A	508	GLY	ARG	conflict	UNP P00451
A	520	MET	PHE	conflict	UNP P00451
A	558	LEU	MET	conflict	UNP P00451
A	585	MET	ILE	conflict	UNP P00451
A	622	PRO	LEU	conflict	UNP P00451
A	661	VAL	ILE	conflict	UNP P00451
A	746	PRO	SER	conflict	UNP P00451
A	755	VAL	ALA	conflict	UNP P00451
A	782	PRO	SER	conflict	UNP P00451
A	784	GLU	GLN	conflict	UNP P00451
A	786	LYS	GLU	conflict	UNP P00451
A	793	PHE	ILE	conflict	UNP P00451
A	806	GLY	ASP	conflict	UNP P00451
A	901	LYS	ARG	conflict	UNP P00451
A	984	ARG	HIS	conflict	UNP P00451
A	1118	VAL	ALA	conflict	UNP P00451
A	1132	GLN	HIS	conflict	UNP P00451
A	1144	LYS	ASN	conflict	UNP P00451

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1210	MET	LYS	conflict	UNP P00451
A	1321	LEU	PHE	conflict	UNP P00451
A	1332	GLN	LYS	conflict	UNP P00451
A	1400	LEU	PHE	conflict	UNP P00451
A	1421	ALA	SER	conflict	UNP P00451
A	1439	ALA	VAL	conflict	UNP P00451
A	1441	HIS	GLN	conflict	UNP P00451
A	1446	LEU	MET	conflict	UNP P00451

L1446	E1447	V1448	Q1454	Y1457	V1357	D1358	F1359	T1369	T1370	Q1371	G1372	V1373	K1374	S1375	L1376	M1380	E1384	F1385	L1386	I1387	S1388	Q1391	D1392	Q1395	V1396	T1397	L1398	F1399	L1400	Q1401	K1406	V1407	G1410	N1411	Q1412	D1413	S1414	F1415	V1419	D1423	L1427	R1432	I1433	H1434	P1435	Q1436	H1440	H1441	I1442	A1443	L1444	R1445	H1262	M1263	R1275	Y1281	S1282	I1283	R1284	S1285	T1286	L1287	R1288	M1289	E1290	L1291	M1292	G1293	C1294	M1297	S1300	L1303	G1304	M1305	E1306	D1312	A1313	Q1314	I1315	Y1320	L1321	T1322	M1323	M1324	F1325	W1328	S1329	P1330	A1333	R1334	G1339	R1340	R1345	P1346	Q1347	V1348	M1349	M1350	L1355	Q1356	V1049	I1050	M1051	D1052	T1053	M1059	I1065	Y1068	L1069	L1070	S1071	M1072	G1073	N1077	S1080	I1081	H1082	R1091	K1092	E1095	L1100	P1105	G1106	V1107	F1108	W1121	R1122	V1123	E1124	C1125	L1126	I1127	L1131	T1137	L1138	F1139	C1146	L1150	G1151	M1152	A1153	H1156	I1157	R1158	D1159	I1162	G1166	Q1167	Y1168	G1169	Q1170	W1171	L1175	L1178	S1181	G1182	S1183	I1184	T1189	K1190	E1191	P1192	F1193	S1194	K1197	V1198	I1209	M1210	T1211	Q1212	G1213	A1214	R1215	Q1216	K1217	F1218	S1219	S1220	L1221	Y1222	I1223	S1224	Q1225	G1246	T1247	L1248	G1253	N1254	V1255	D1256	S1257	S1258	G1259	I1260	K1261
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	218890	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)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.292	Depositor
Minimum map value	-0.109	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	172.64519, 172.64519, 172.64519	wwPDB
Map dimensions	156, 156, 156	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1067, 1.1067, 1.1067	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	0.13	0/10575	0.29	0/14336

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

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	10291	0	10047	176	0
All	All	10291	0	10047	176	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 9.

The worst 5 of 176 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:673:SER:HB3	1:A:707:TRP:HB3	1.66	0.76
1:A:479:THR:HG22	1:A:533:THR:HG22	1.68	0.76
1:A:1221:LEU:HD13	1:A:1286:THR:HB	1.70	0.74
1:A:107:LEU:HD22	1:A:117:LEU:HB2	1.69	0.73
1:A:906:ARG:HG2	1:A:907:PRO:HD2	1.72	0.71

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	1264/1457 (87%)	1178 (93%)	84 (7%)	2 (0%)	44 73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	423	ASP
1	A	1283	ILE

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	1130/1304 (87%)	1130 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1082	HIS
1	A	1212	GLN
1	A	1434	HIS
1	A	1207	HIS

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Mol	Chain	Res	Type
1	A	1238	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.

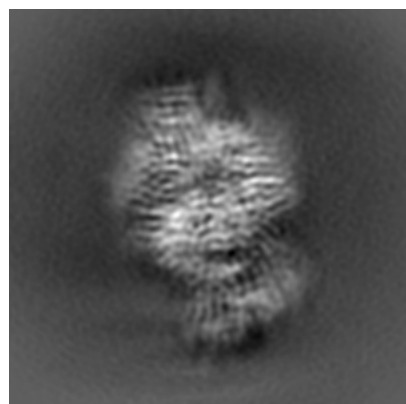
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61327. These allow visual inspection of the internal detail of the map and identification of artifacts.

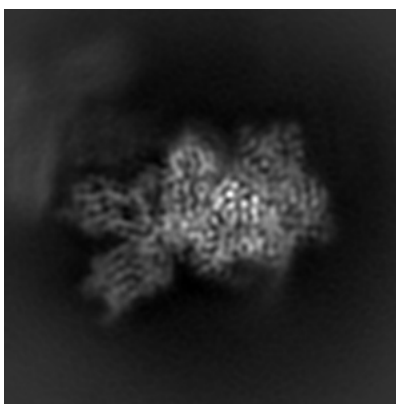
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

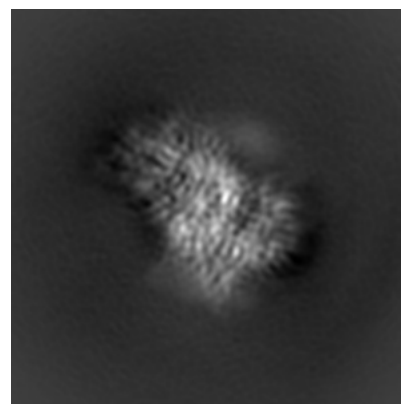
6.1.1 Primary map



X

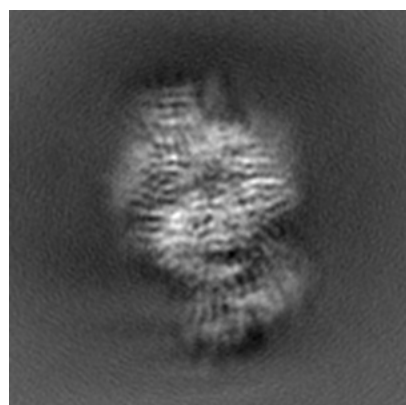


Y

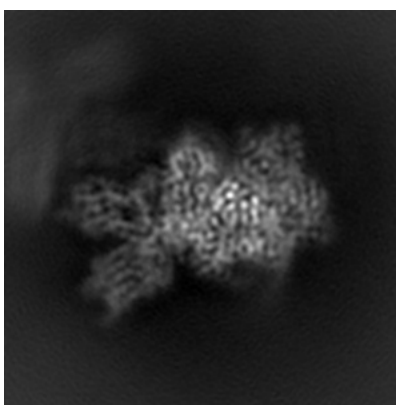


Z

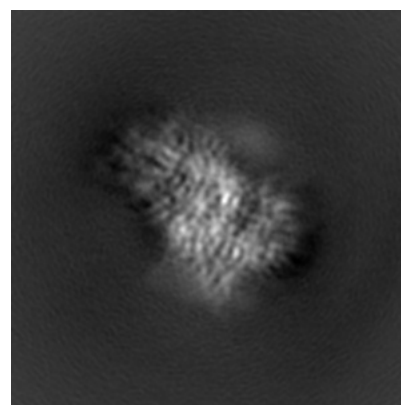
6.1.2 Raw map



X



Y

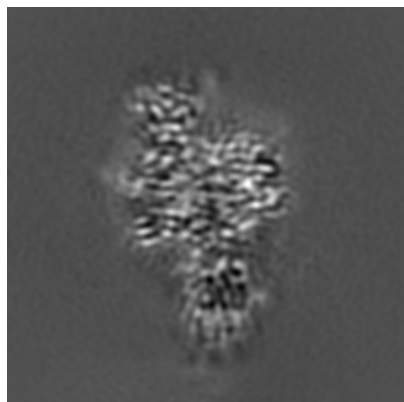


Z

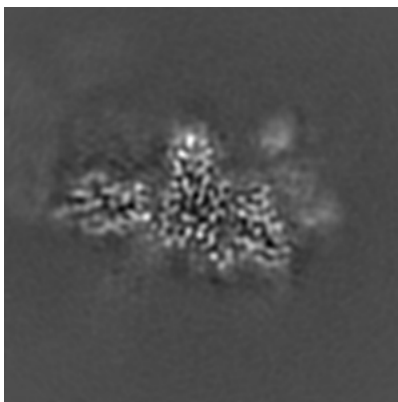
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

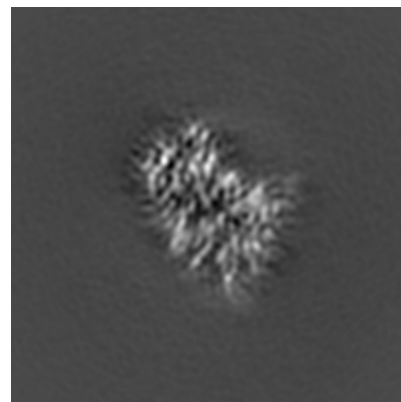
6.2.1 Primary map



X Index: 78

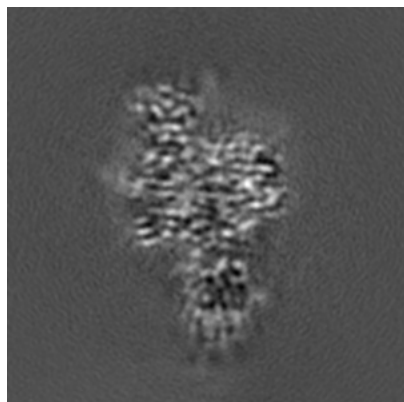


Y Index: 78

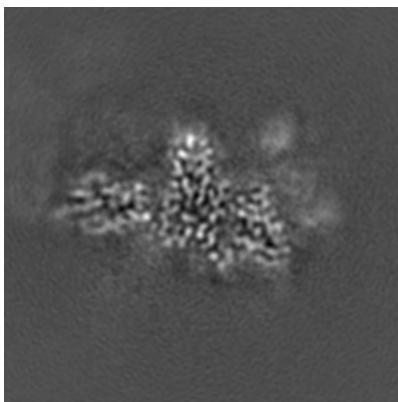


Z Index: 78

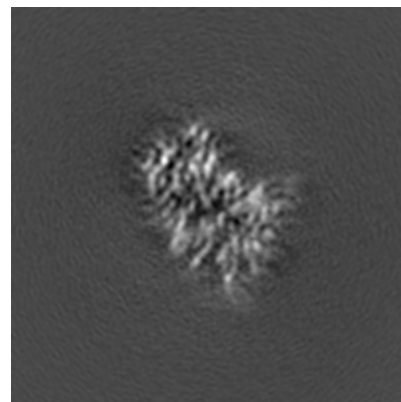
6.2.2 Raw map



X Index: 78



Y Index: 78

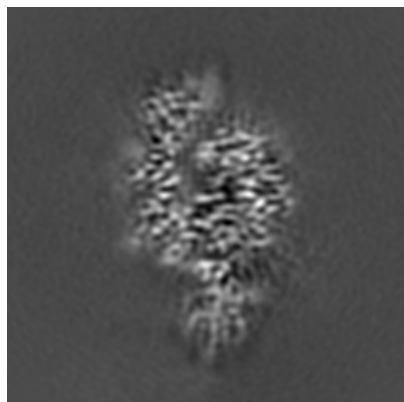


Z Index: 78

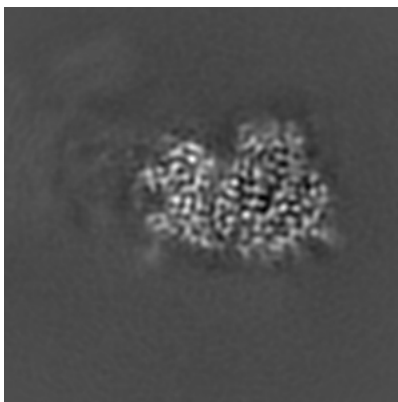
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

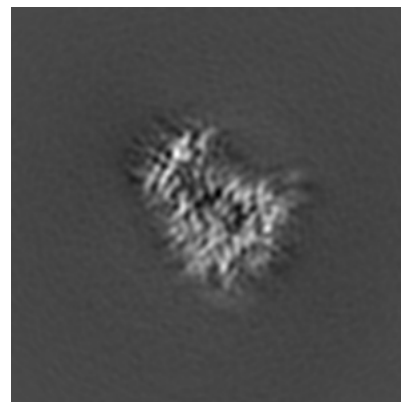
6.3.1 Primary map



X Index: 73

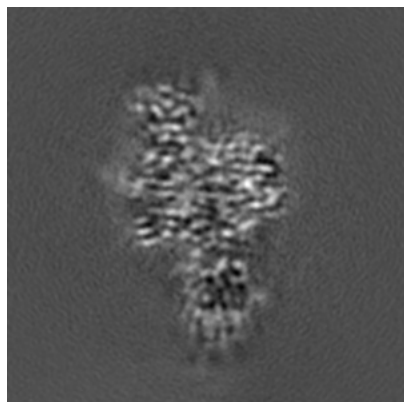


Y Index: 64

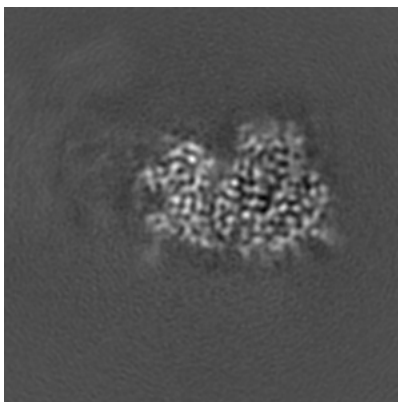


Z Index: 76

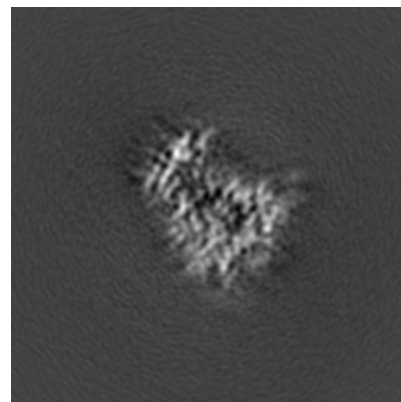
6.3.2 Raw map



X Index: 78



Y Index: 64

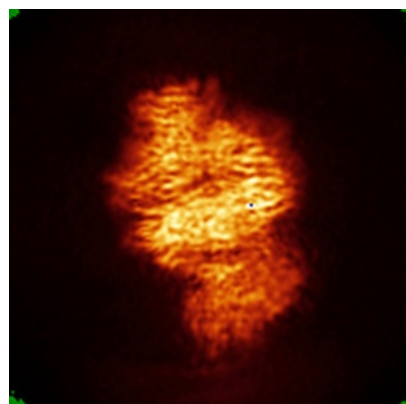


Z Index: 76

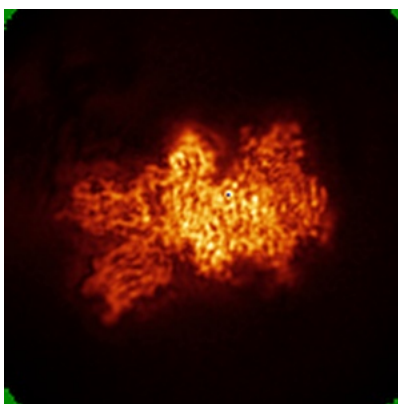
The images above show the largest variance slices of the map in three orthogonal directions.

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

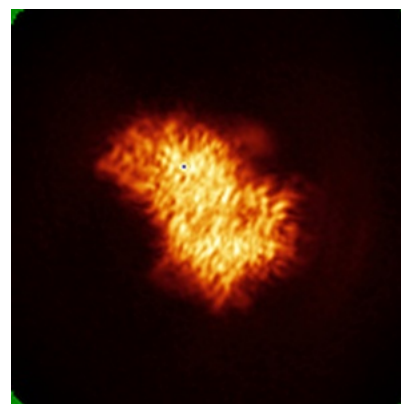
6.4.1 Primary map



X

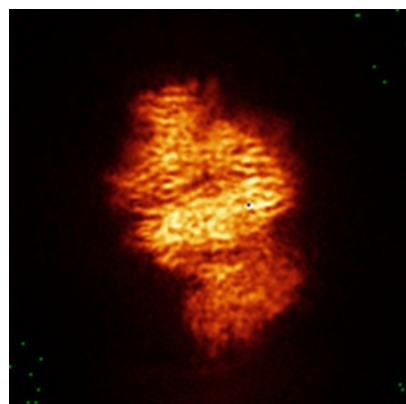


Y

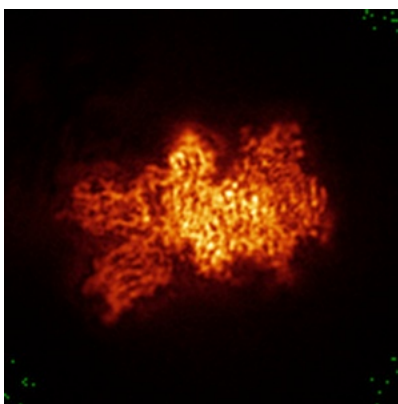


Z

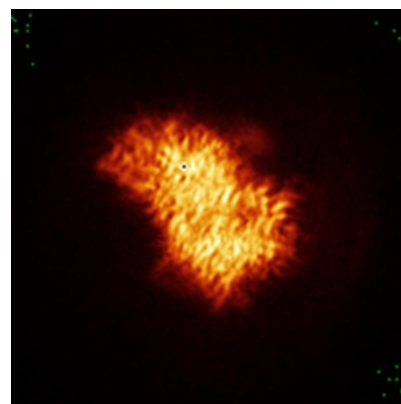
6.4.2 Raw map



X



Y

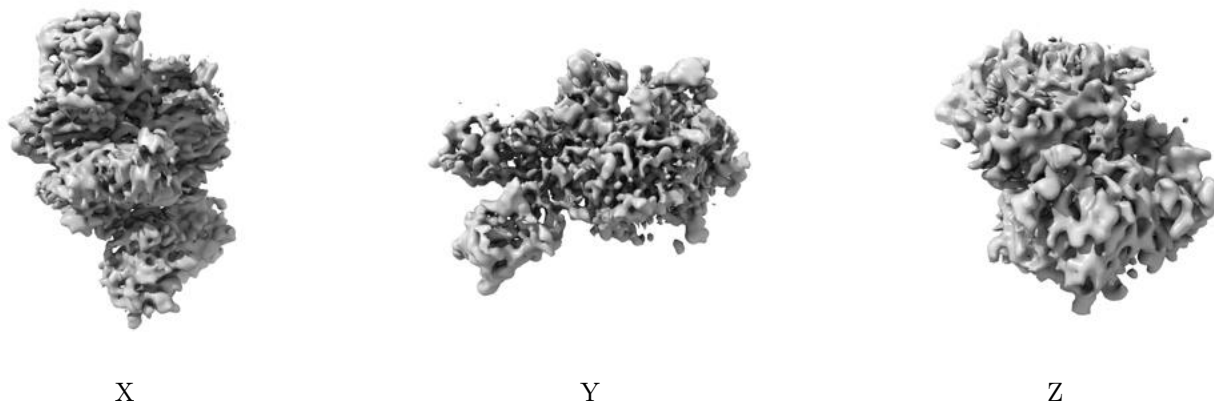


Z

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.

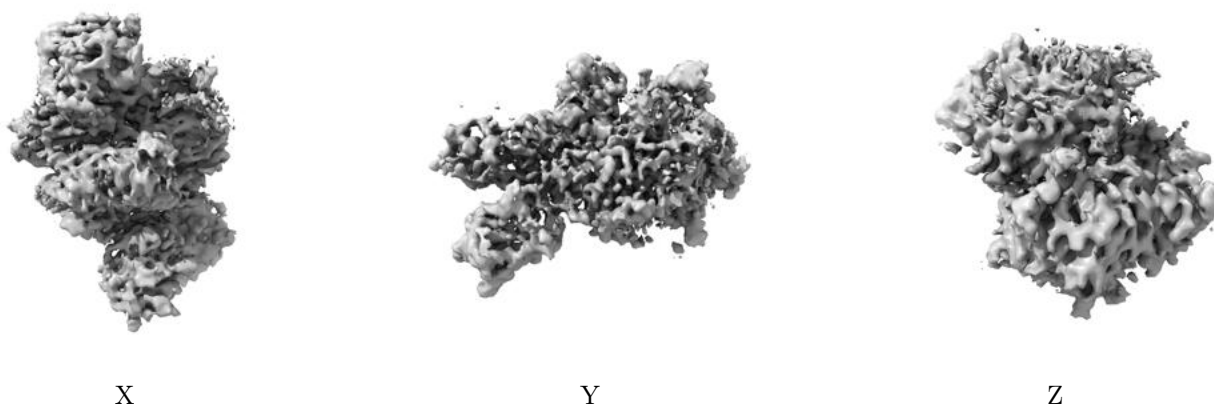
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.035. 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.

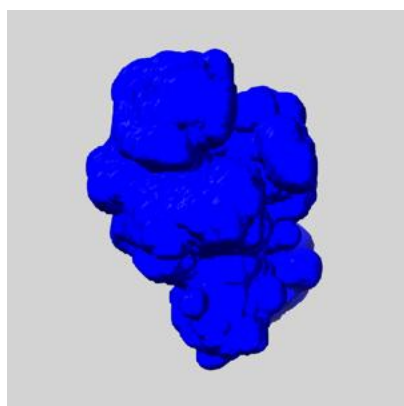
6.6 Mask visualisation [i](#)

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

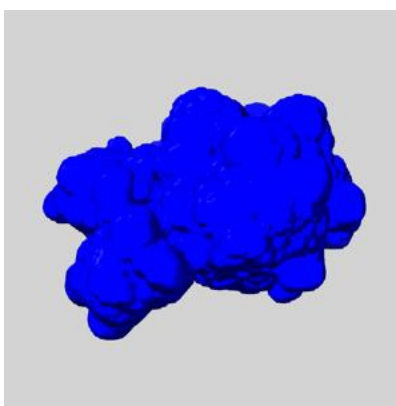
A mask typically either:

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

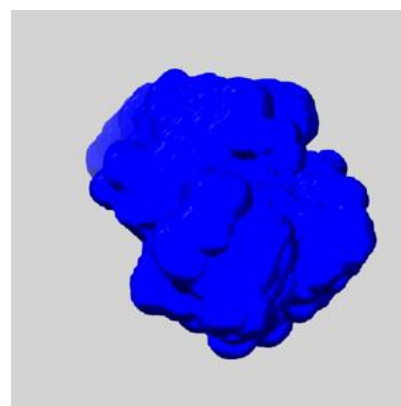
6.6.1 emd_61327_msk_1.map [i](#)



X



Y

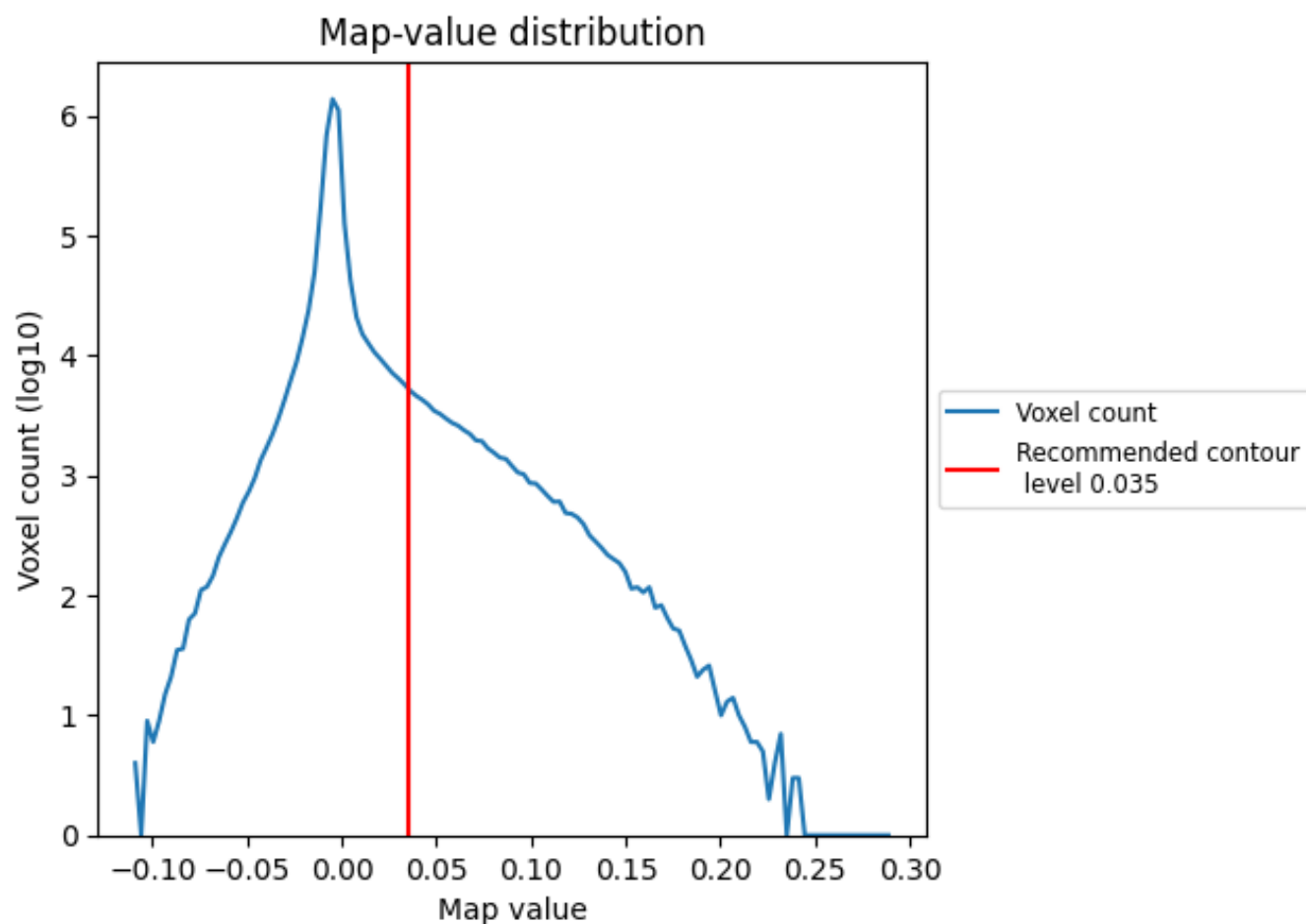


Z

7 Map analysis [i](#)

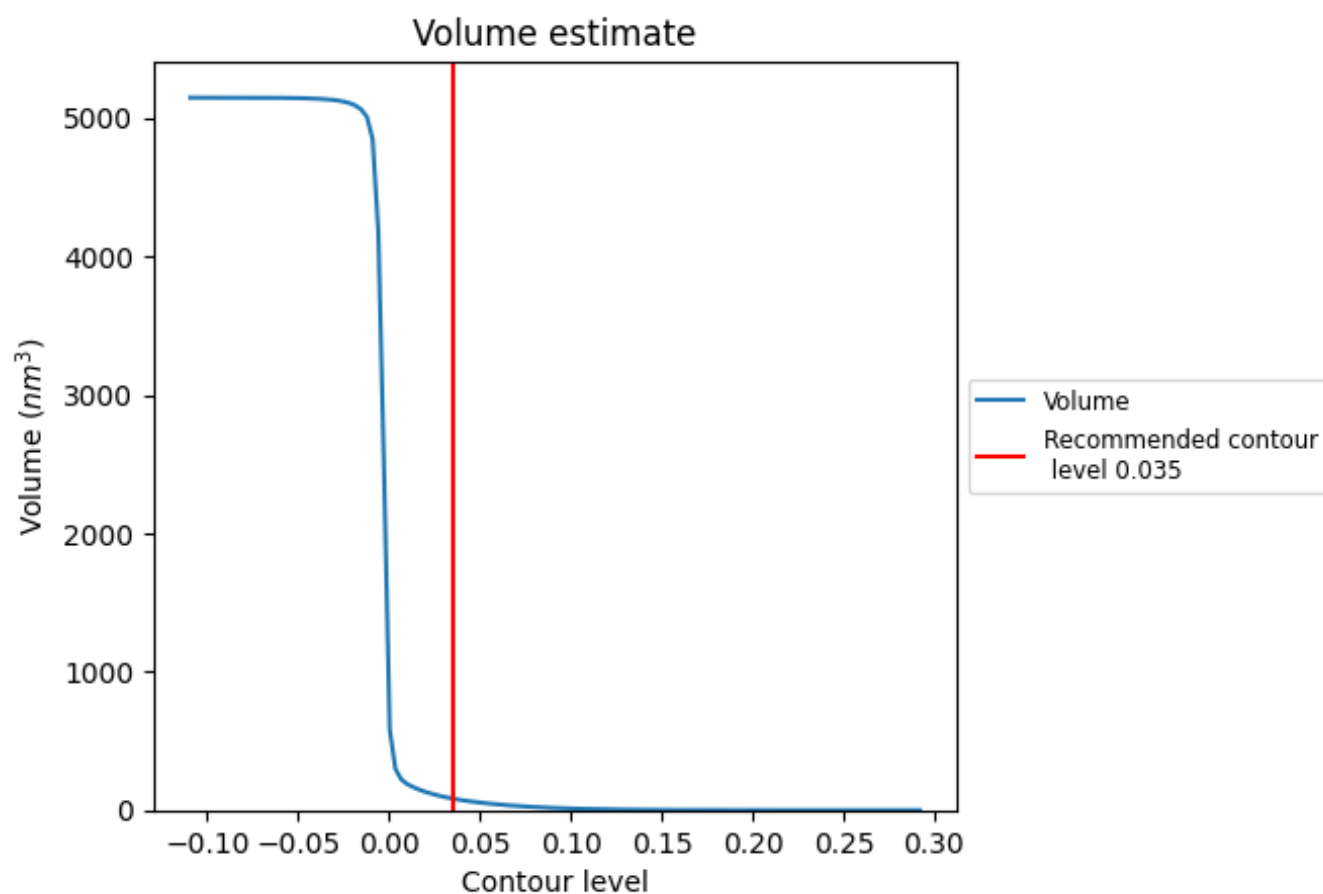
This section contains the results of statistical analysis of the map.

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.

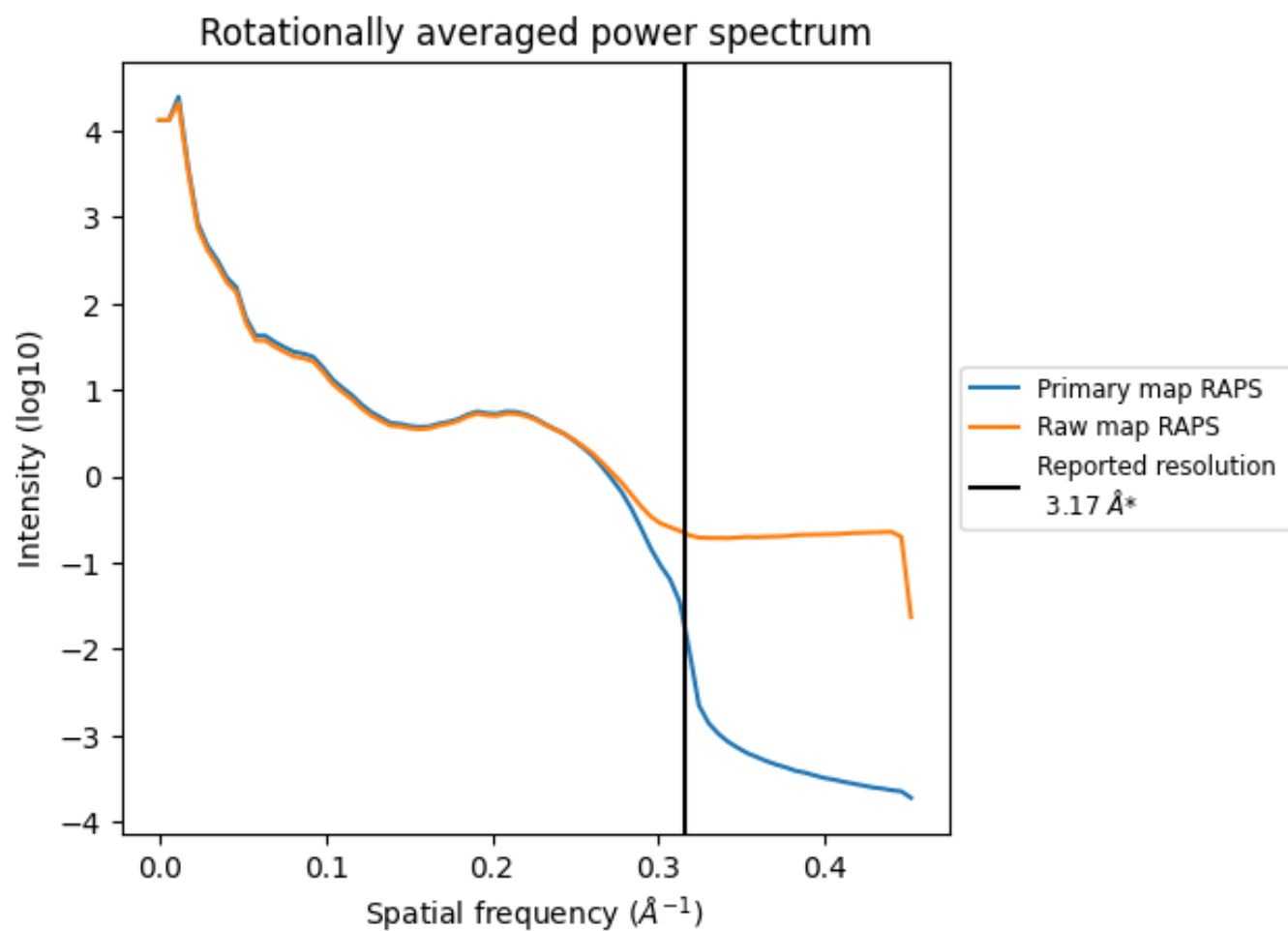
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 84 nm^3 ; 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 ⓘ

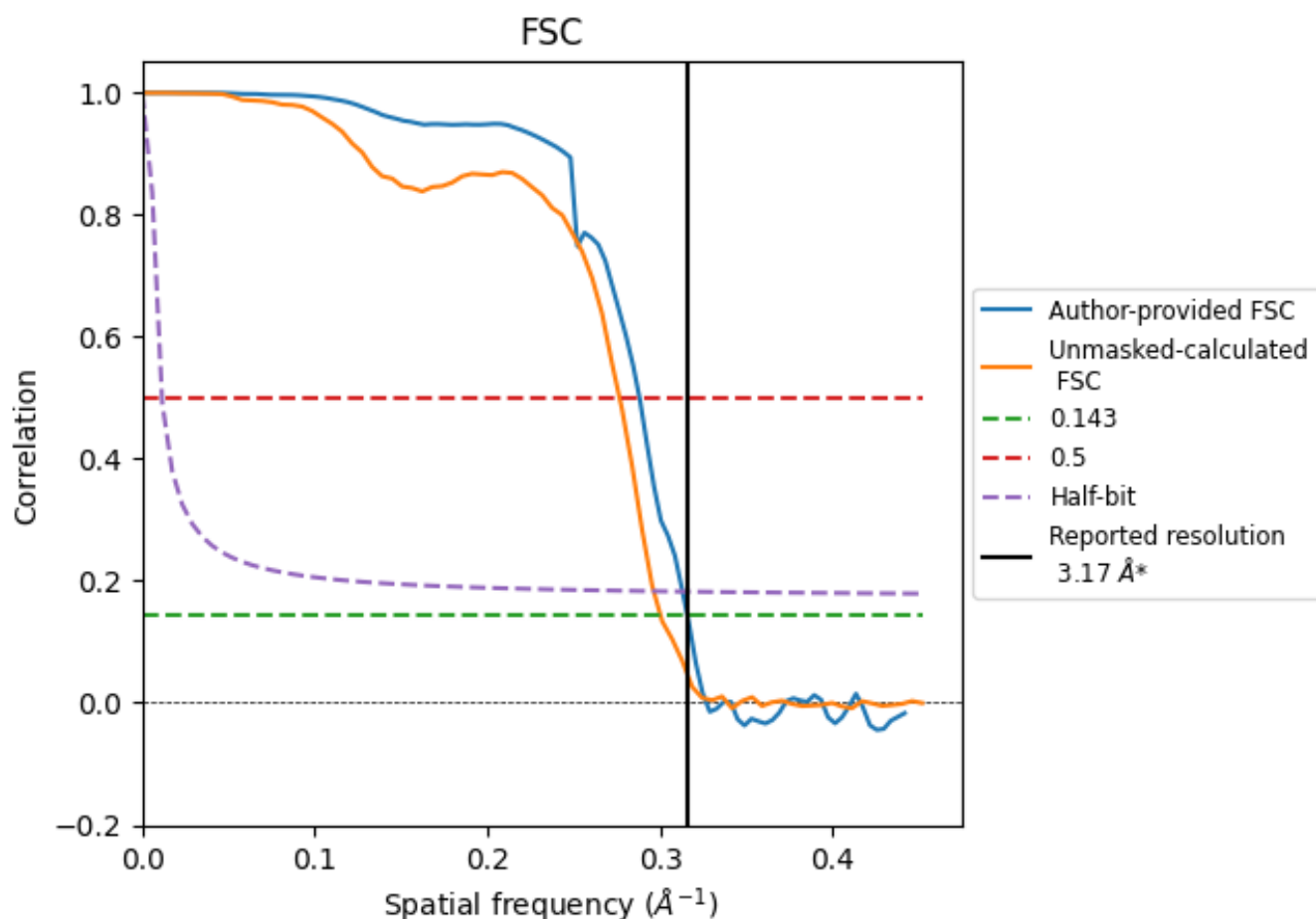


*Reported resolution corresponds to spatial frequency of 0.315 \AA^{-1}

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 0.315 \AA^{-1}

8.2 Resolution estimates [i](#)

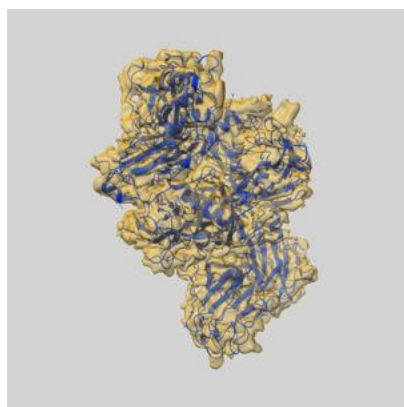
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.17	-	-
Author-provided FSC curve	3.17	3.47	3.19
Unmasked-calculated*	3.33	3.62	3.37

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

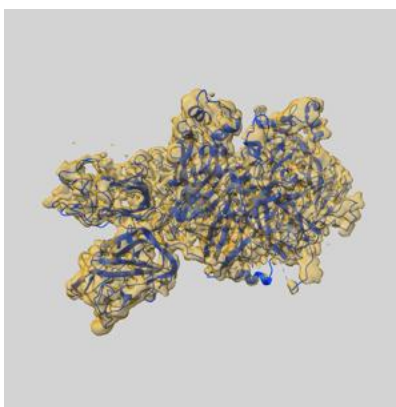
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-61327 and PDB model 9JBV. Per-residue inclusion information can be found in section [3](#) on page [5](#).

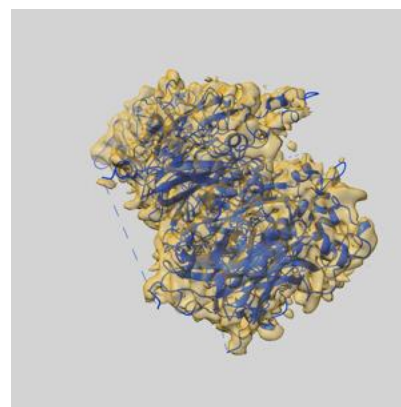
9.1 Map-model overlay [i](#)



X



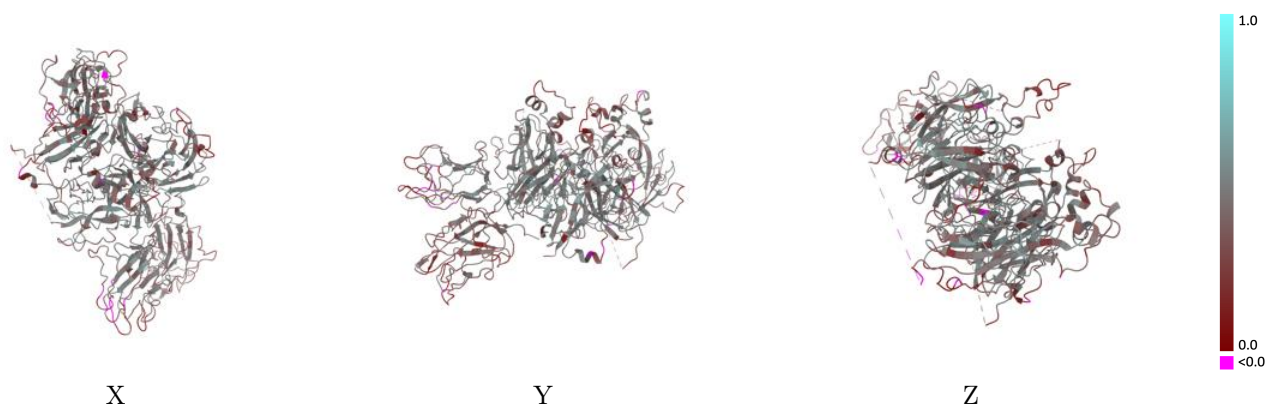
Y



Z

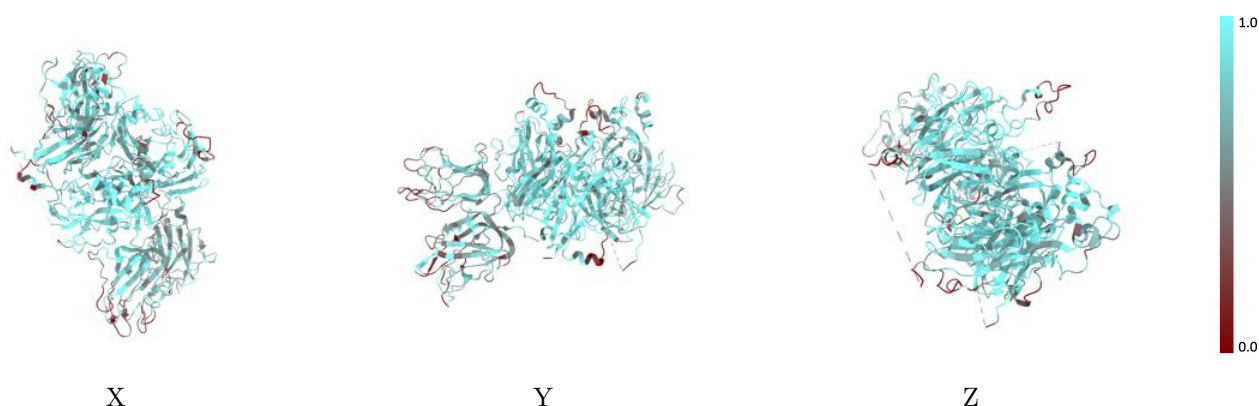
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



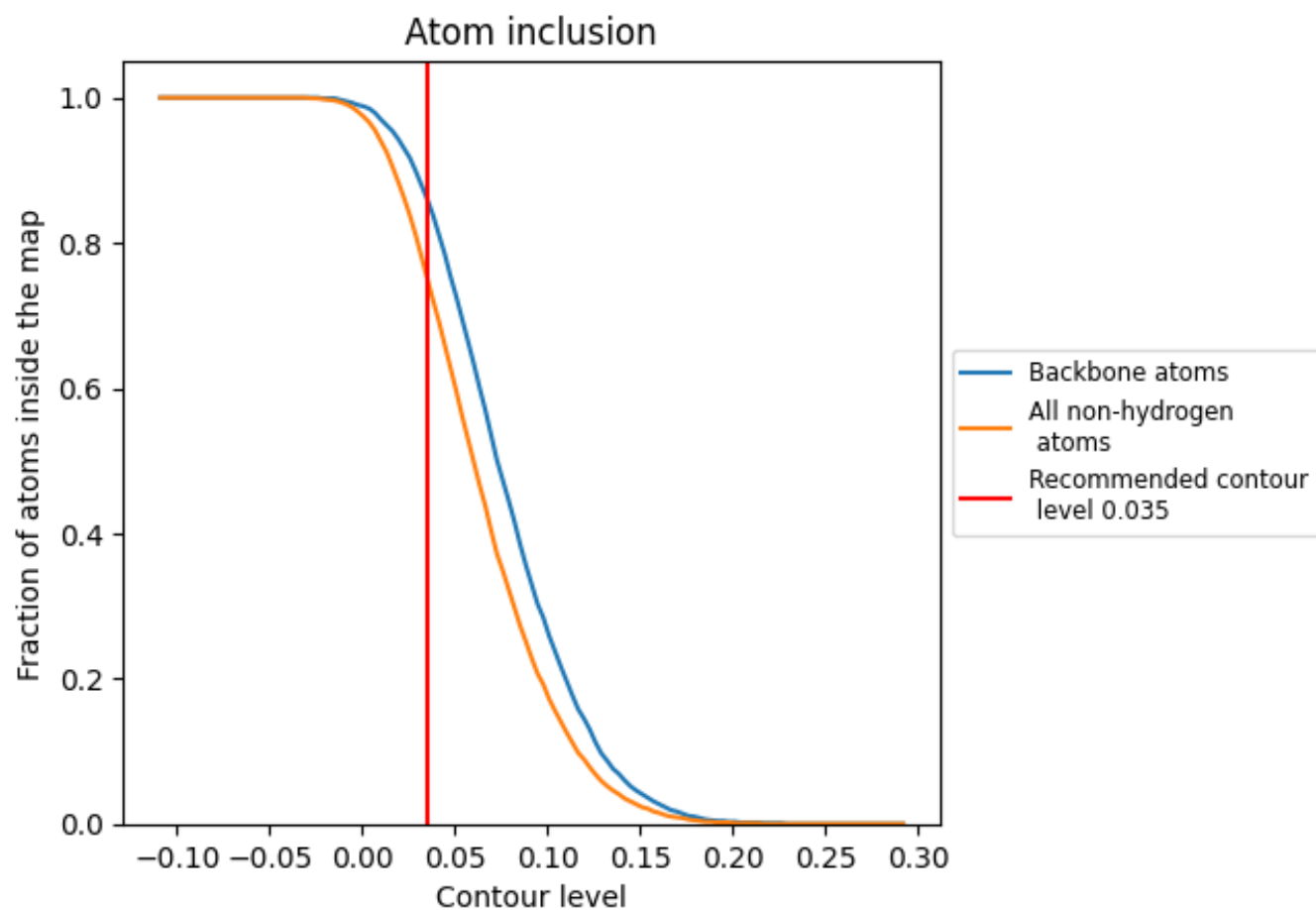
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).

9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 75% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7510	<div><div></div></div> 0.4000
A	<div><div></div></div> 0.7510	<div><div></div></div> 0.4000

