



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 11:58 PM UTC

PDB ID : 9CQ9 / pdb_00009cq9
EMDB ID : EMD-45812
Title : Modifying region of EcPKS1
Authors : Schubert, H.L.; Hill, C.P.
Deposited on : 2024-07-19
Resolution : 3.50 Å(reported)
Based on initial model : .

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

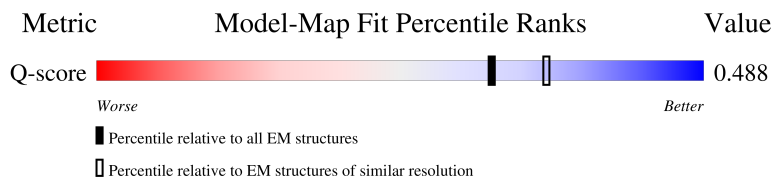
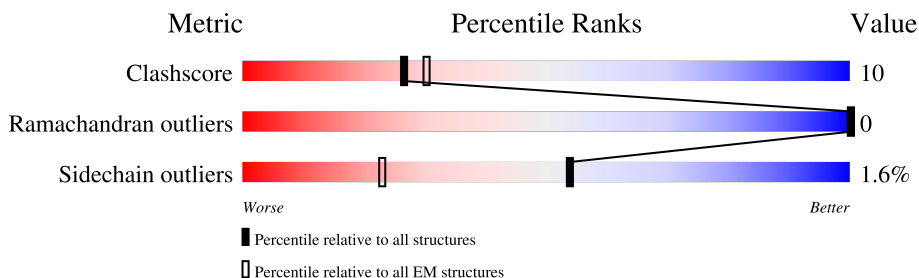
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	13950 (3.00 - 4.00)

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	2272	 43% 12% 45%
1	B	2272	 43% 12% 45%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 38874 atoms, of which 19370 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 Polyketide synthase 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1256	Total	C	H	N	O	S	0	0
			19437	6164	9685	1709	1825	54		
1	B	1256	Total	C	H	N	O	S	0	0
			19437	6164	9685	1709	1825	54		

Y1638	VAL	T1563	D1217	V1100	L923	GLU	GLU	VAL	GLY	SER	ASP	ASN	ALA	CYS	ASN	THR
V1643	THR	L1354	F1218	L1101	M947	PHE	PHE	PRO	HIS	LEU	ALA	GLY	ILE	CYS	GLY	ALA
S1644	P1480	A1224	A1224	D1110	I1111	VAL	VAL	ILE	CYS	GLU	THR	ALA	THR	THR	ALA	THR
R1645	D1488	T1568	E1226	V1112	V957	PRO	PRO	SER	HIS	SER	GLY	VAL	VAL	PRO	SER	SER
L1647	L1489	ASP	R1227	S1113	M962	GLY	GLY	GLY	ASN	ALA	ALA	VAL	ILE	GLU	SER	VAL
D1657	A1362	PRO	I1228	A1114	Q969	LEU	LEU	LEU	GLU	VAL	PRO	GLY	LEU	ILE	ILE	GLU
E1658	A1369	Q1231	Q1232	G1115	L976	GLN	GLN	ARG	ASP	ASP	TYR	TYR	ALA	VAL	VAL	VAL
M1663	V1497	H1372	GLY	V1117	L977	VAL	VAL	ALA	THR	THR	ALA	TYR	HIS	GLY	GLY	ALA
T1669	D1510	D1373	HIS	E1118	A978	LYS	LYS	TRP	ASP	GLY	THR	ILE	SER	CYS	THR	ALA
L1670	L1515	L1374	GLN	I1119	V982	ARG	ARG	LEU	LEU	CYS	VAL	CYS	ASP	GLY	LEU	PHE
I1672	K1518	Q1383	H1238	T1124	D986	LEU	LEU	THR	ALA	THR	ALA	ALA	LEU	LYS	LYS	GLN
F1674	G1523	M1391	L1242	R1130	K987	ASN	ASN	GLY	ASP	GLU	VAL	ASP	ASN	GLN	THR	THR
D1678	M1524	G1396	F1243	E1139	V989	SER	SER	GLU	GLU	GLU	MET	ASP	ALA	PRO	ALA	SER
T1679	F1528	F1397	L1248	V1144	L990	VAL	VAL	GLU	CYS	LEU	LEU	PHE	GLY	GLY	ARG	VAL
K1680	N1529	V1410	L1254	H1147	E991	VAL	VAL	TRP	VAL	TRP	PHE	GLU	VAL	VAL	ILE	ASP
R1683	C1530	L1413	R1270	VAL	T992	GLY	GLY	ASP	GLY	GLY	MET	THR	THR	LYS	ALA	CYS
L1687	Q1533	P1414	M1273	THR	S1000	LEU	LEU	SER	ALA	ASP	GLU	GLU	PHE	THR	THR	THR
A1689	E1534	T1415	M1273	GLY	S1001	GLN	GLN	ALA	PRO	GLU	GLU	GLU	THR	CYS	VAL	VAL
P1690	S1537	L1416	V1274	ARG	Q1003	LYS	LYS	ALA	ALA	LEU	LYS	LYS	ARG	LYS	ILE	ALA
P1691	L1417	L1416	V1275	ASP	L1022	ASN	ASN	GLN	GLN	THR	THR	LYS	SER	ASP	VAL	VAL
A1692	L1427	L1427	G1276	GLY	E1026	ALA	ASP	SER	SER	ILE	ALA	ALA	ARG	GLY	LYS	ASN
V1697	P1428	P1428	L1278	ALA	R1036	ASP	ASN	SER	ALA	LEU	LEU	VAL	THR	ARG	VAL	THR
C1699	R1429	R1429	L1279	LYS	R1036	ASN	ASN	ALA	GLU	GLU	GLU	VAL	THR	GLY	GLY	ASN
L1700	LYS	LYS	S1280	ARG	GLY	LEU	LEU	PHE	PHE	GLY	GLY	THR	THR	THR	GLN	GLN
R1701	SER	SER	S1280	GLY	I1046	ARG	ARG	GLY	GLY	THR	THR	VAL	THR	THR	THR	THR
R1701	GLY	D1433	L1290	ALA	VAL	GLN	GLN	ALA	ASN	ILE	ILE	ALA	ALA	LYS	ASN	ASN
S1702	D1567	L1436	C1291	T1162	M1056	PHE	PHE	ASN	ASN	LEU	LEU	VAL	VAL	VAL	VAL	VAL
S1703	L1568	L1436	H1302	Q1178	D1057	ALA	ALA	ASN	ASN	SER	SER	ILE	ILE	ARG	GLY	GLY
Q1709	H1583	Y1440	V1306	V1191	V1059	GLY	GLY	VAL	VAL	GLY	GLY	ILE	ILE	GLY	GLY	GLY
H1710	T1586	S1441	L1307	L1192	L1061	LYS	LYS	PRO	ALA	THR	THR	GLN	GLN	LEU	LEU	LEU
L1713	T1587	A1442	E1308	K1195	M1062	CYS	CYS	VAL	TYR	ALA	ALA	ALA	ALA	THR	THR	THR
P1720	Q1590	Q1444	A1311	L1198	R1067	PHE	PHE	LEU	HIS	SER	VAL	SER	SER	PRO	PRO	PRO
V1721	E1598	H1452	Y1317	L1318	M1073	ALA	ALA	ALA	THR	GLY	THR	GLY	GLY	GLY	GLY	GLY
A1722	T1604	E1456	R1318	L1204	T1081	SER	SER	LEU	GLY	TRP	TRP	ALA	ALA	ILE	ILE	ILE
R1733	T1613	V1457	D1332	Q1207	N1082	LEU	LEU	GLN	ASN	SER	CYS	GLY	GLY	GLY	GLY	GLY
G1734	L1613	I1458	Y1335	ASP	I1083	PRO	PRO	LYS	LYS	MET	LEU	ILE	ILE	GLY	GLY	GLY
H1735	T1336	F1469	T1336	LEU	P1092	LEU	LEU	ILE	TYR	GLY	GLY	GLY	GLY	GLY	GLY	GLY
D1740	S1625	L1470	G1338	GLY	D1095	ALA	ALA	PRO	ALA	ARG	GLN	GLN	GLN	GLY	GLY	GLY
T1741	L1471	L1471	G1338	SER	D1096	LYS	LYS	THR	SER	PRO	ASP	GLY	GLY	THR	THR	THR
E1693	E1633	R1474	M1343	SER	E1096	TYR	TYR	ALA	ALA	ASP	VAL	GLN	GLN	GLY	GLY	GLY
L1694	L1634	VAL	D1344	SER	D1097	PRO	PRO	ILE	ASP	PHE	PHE	ALA	ALA	ALA	ALA	ALA
V1637	V1637	GLU	D1345	SER	V1099	VAL	VAL	ILE	ILE	ILE	HIS	ARG	ARG	ASP	ASP	ASP

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	143694	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.226	Depositor
Minimum map value	-0.124	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0229	Depositor
Map size (Å)	271.36, 271.36, 271.36	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.53, 0.53, 0.53	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	0.20	0/9950	0.36	0/13478
1	B	0.20	0/9950	0.36	0/13478
All	All	0.20	0/19900	0.36	0/26956

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	9752	9685	9684	198	0
1	B	9752	9685	9684	198	0
All	All	19504	19370	19368	389	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 10.

The worst 5 of 389 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:1311:ALA:HB2	1:A:1337:VAL:HG13	1.23	1.11
1:B:1311:ALA:HB2	1:B:1337:VAL:HG13	1.23	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1311:ALA:CB	1:A:1337:VAL:HG13	1.84	1.08
1:B:1311:ALA:CB	1:B:1337:VAL:HG13	1.84	1.05
1:A:1308:GLU:OE1	1:A:1335:TYR:OH	1.83	0.96

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	1240/2272 (55%)	1137 (92%)	103 (8%)	0	100	100
1	B	1240/2272 (55%)	1137 (92%)	103 (8%)	0	100	100
All	All	2480/4544 (55%)	2274 (92%)	206 (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	1050/1892 (56%)	1033 (98%)	17 (2%)	55	70
1	B	1050/1892 (56%)	1034 (98%)	16 (2%)	57	71
All	All	2100/3784 (56%)	2067 (98%)	33 (2%)	54	70

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1740	ASP
1	B	1766	ILE
1	B	2175	VAL
1	A	1740	ASP
1	A	1721	VAL

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

Mol	Chain	Res	Type
1	B	1571	ASN
1	B	1874	GLN
1	B	2103	GLN
1	B	1972	HIS
1	A	2103	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.

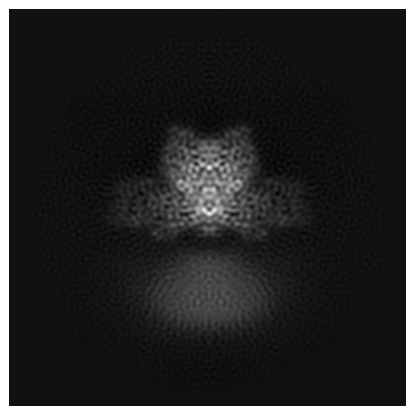
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45812. These allow visual inspection of the internal detail of the map and identification of artifacts.

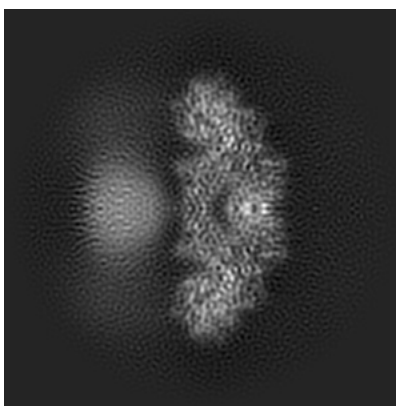
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

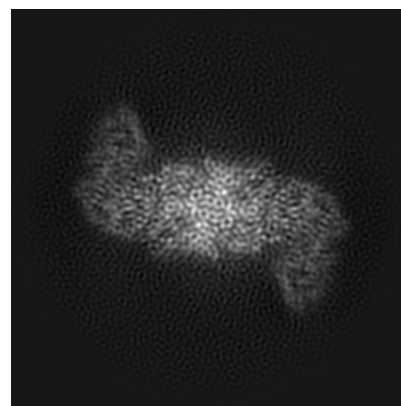
6.1.1 Primary map



X

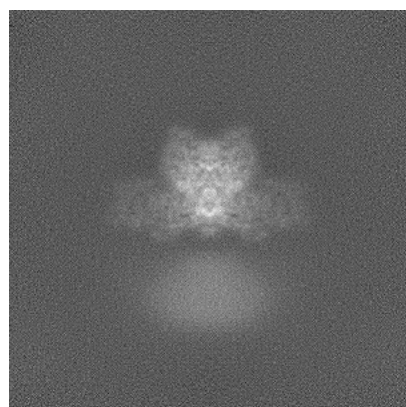


Y

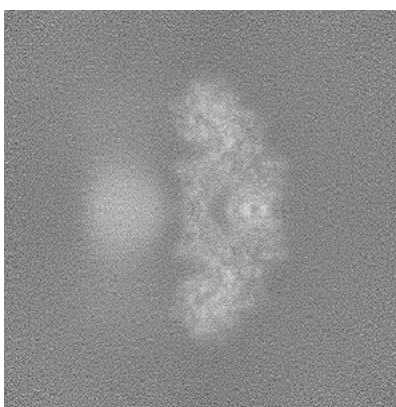


Z

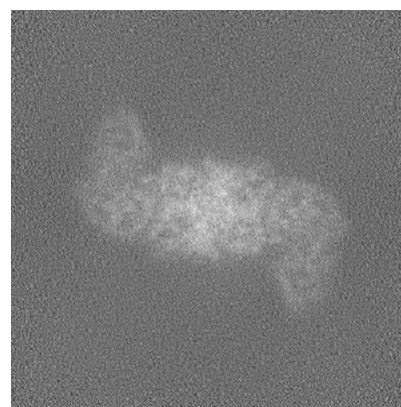
6.1.2 Raw map



X



Y

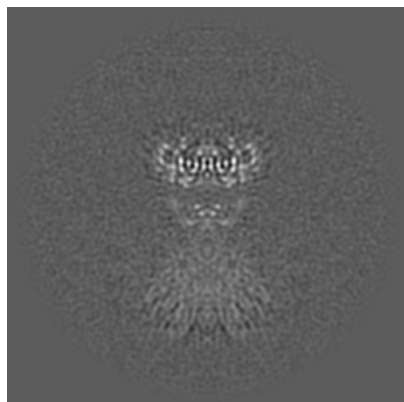


Z

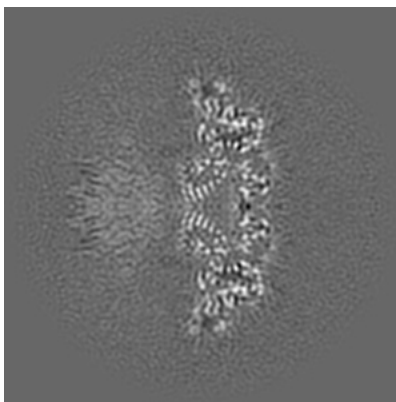
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

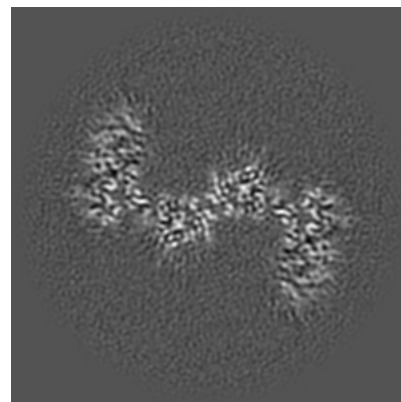
6.2.1 Primary map



X Index: 256

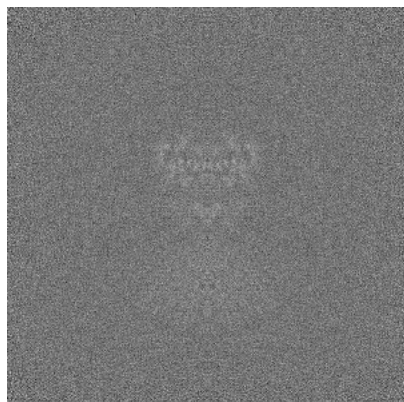


Y Index: 256

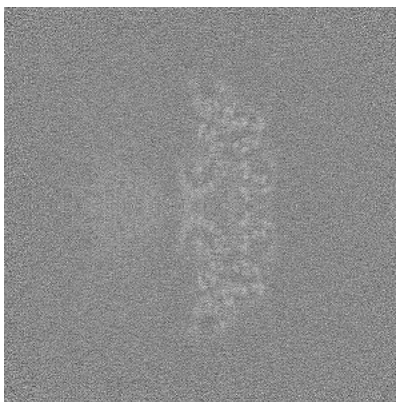


Z Index: 256

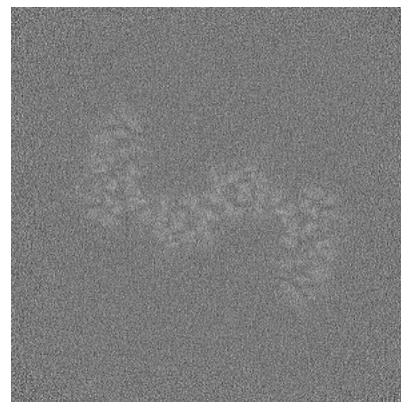
6.2.2 Raw map



X Index: 256



Y Index: 256

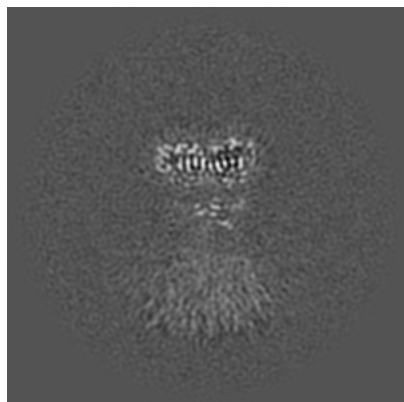


Z Index: 256

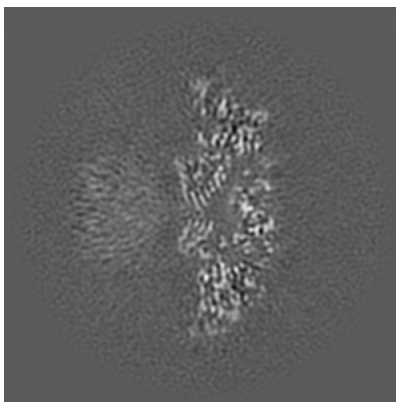
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

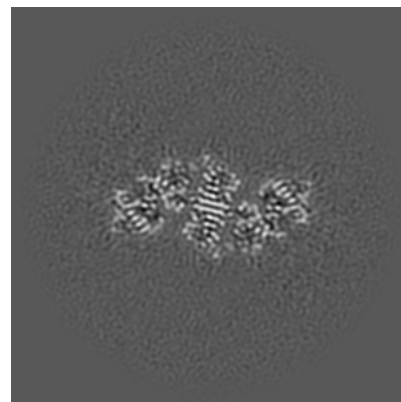
6.3.1 Primary map



X Index: 259

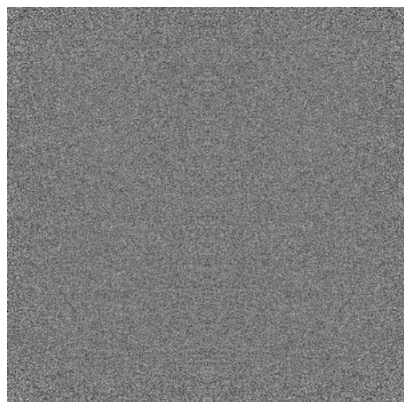


Y Index: 261

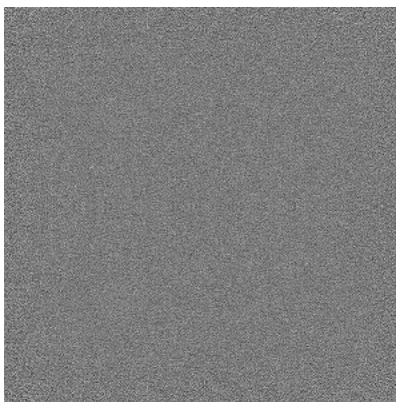


Z Index: 309

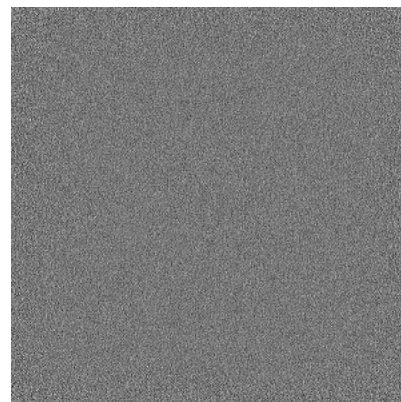
6.3.2 Raw map



X Index: 0



Y Index: 0

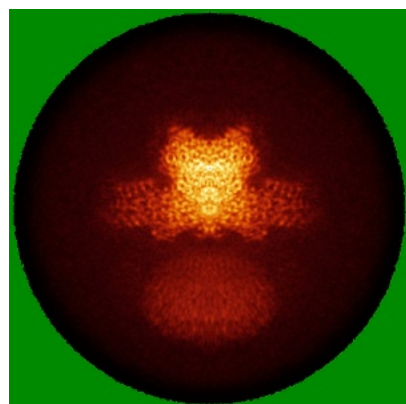


Z Index: 0

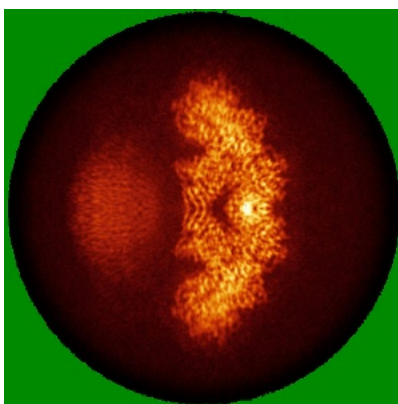
The images above show the largest variance slices of the map in three orthogonal directions.

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

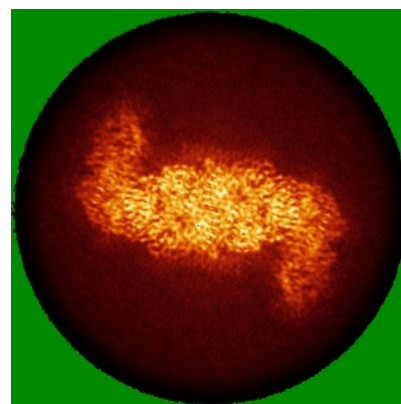
6.4.1 Primary map



X

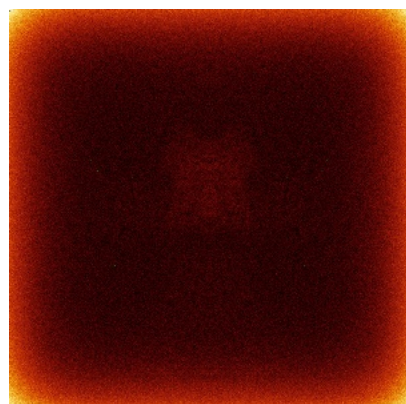


Y

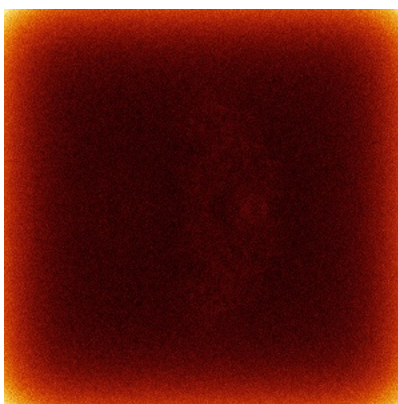


Z

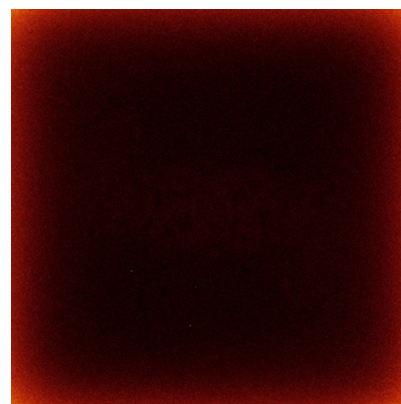
6.4.2 Raw map



X



Y

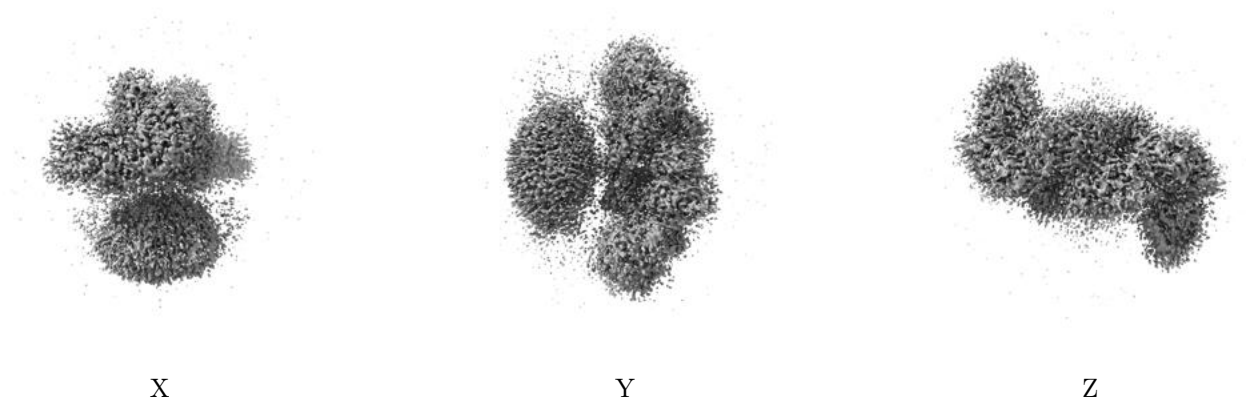


Z

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.

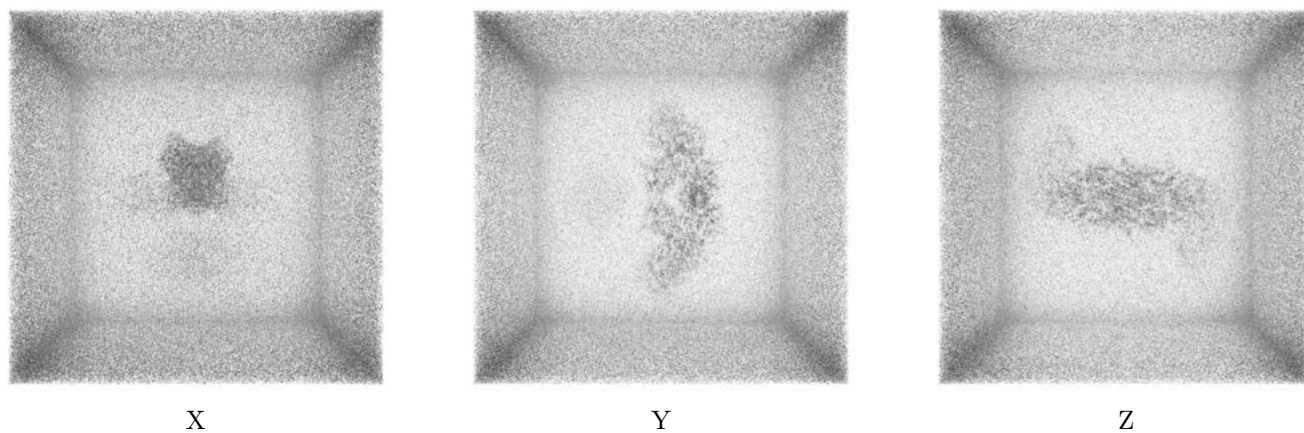
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0229. 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.

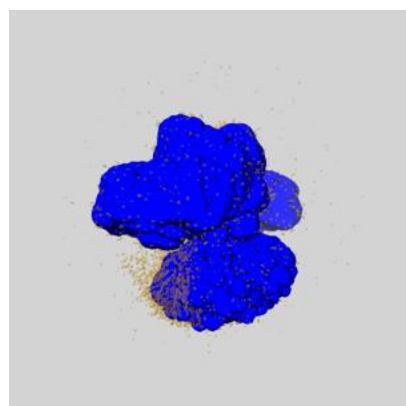
6.6 Mask visualisation [i](#)

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

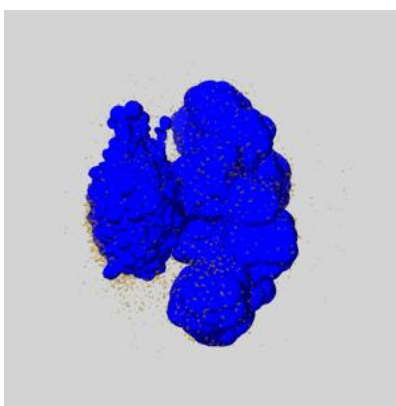
A mask typically either:

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

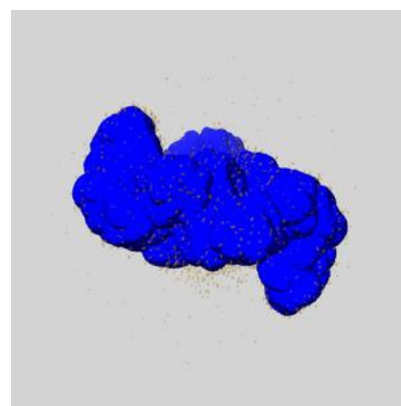
6.6.1 emd_45812_msk_1.map [i](#)



X



Y

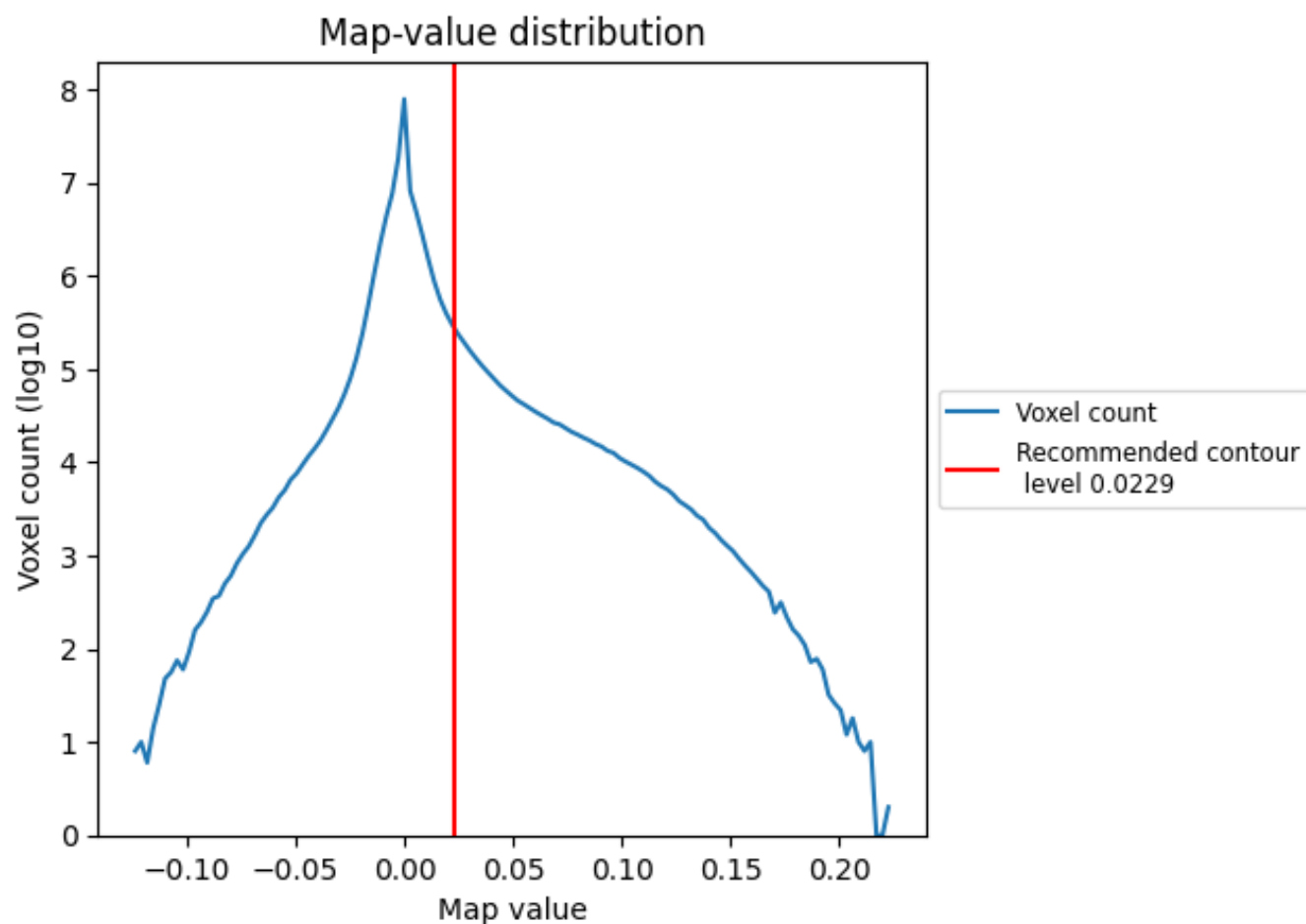


Z

7 Map analysis [i](#)

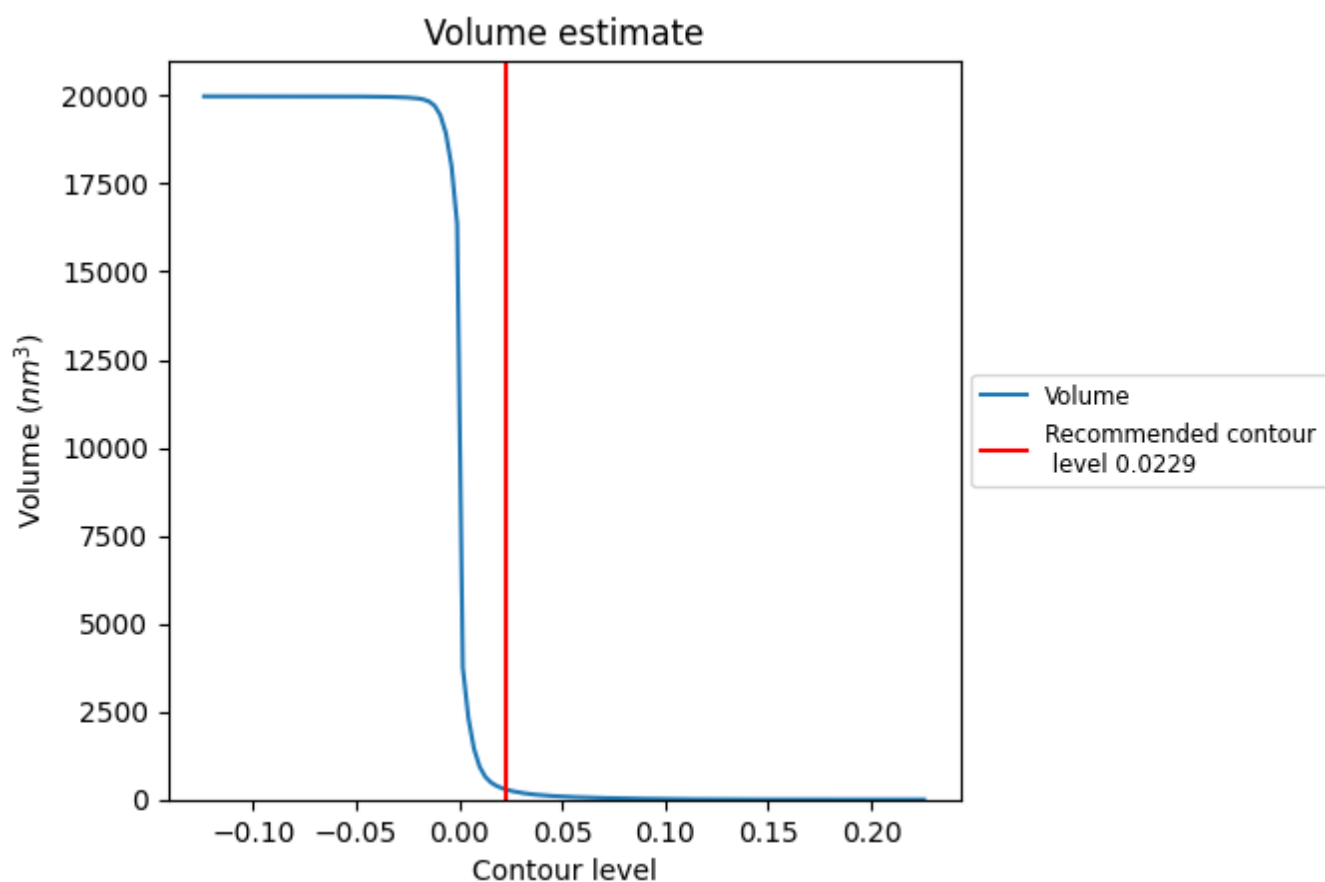
This section contains the results of statistical analysis of the map.

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.

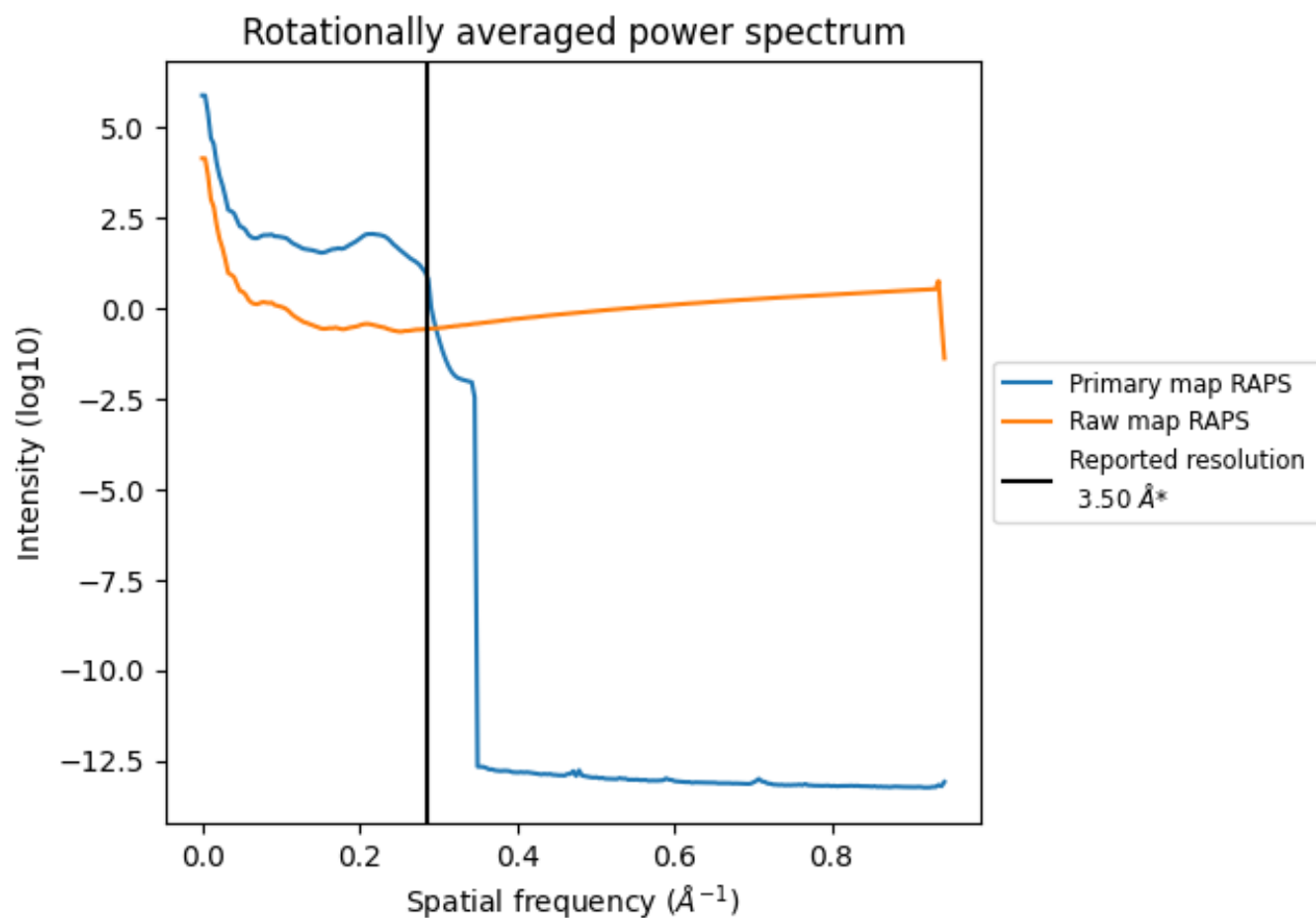
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 284 nm³; this corresponds to an approximate mass of 256 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 ⓘ

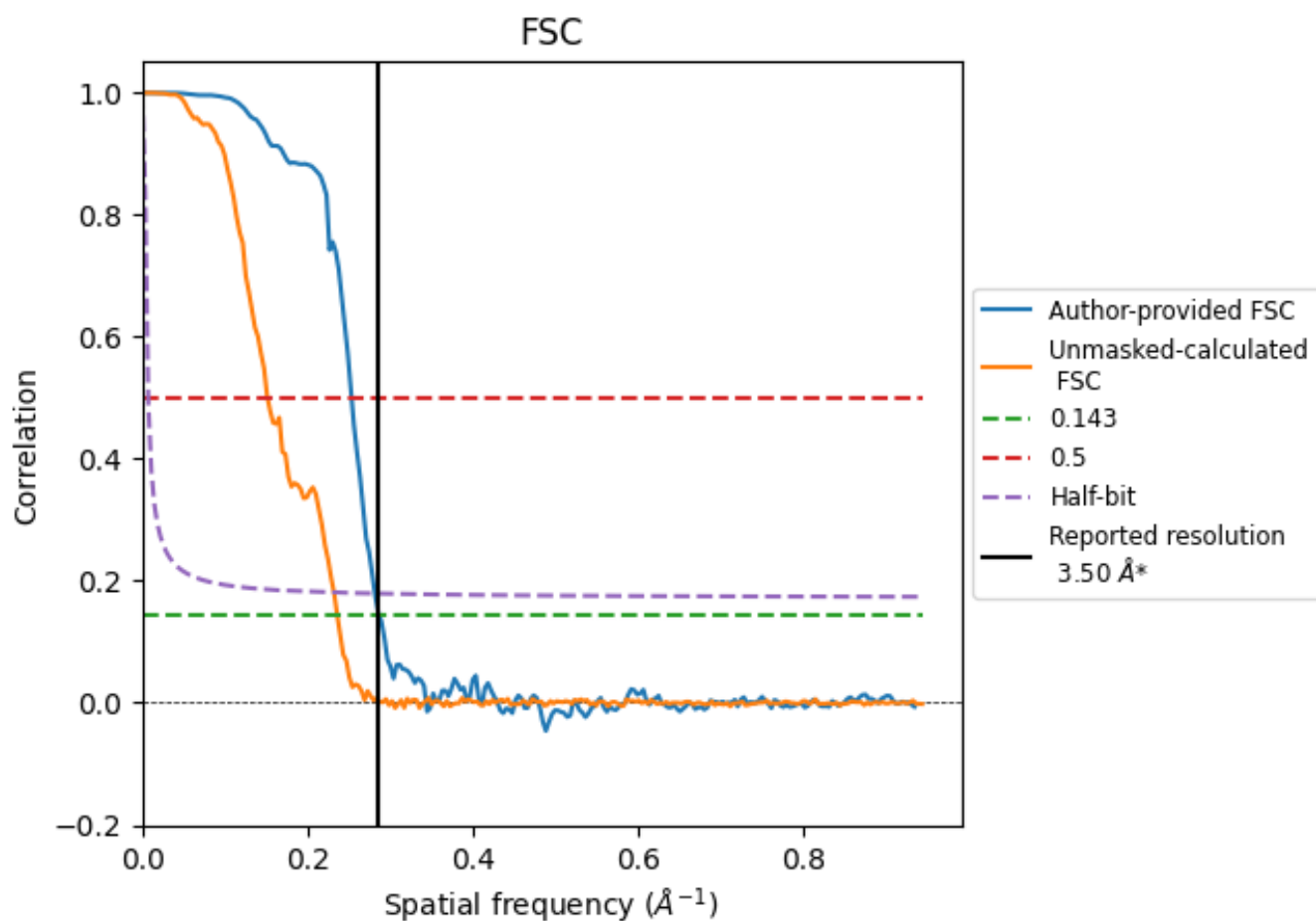


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

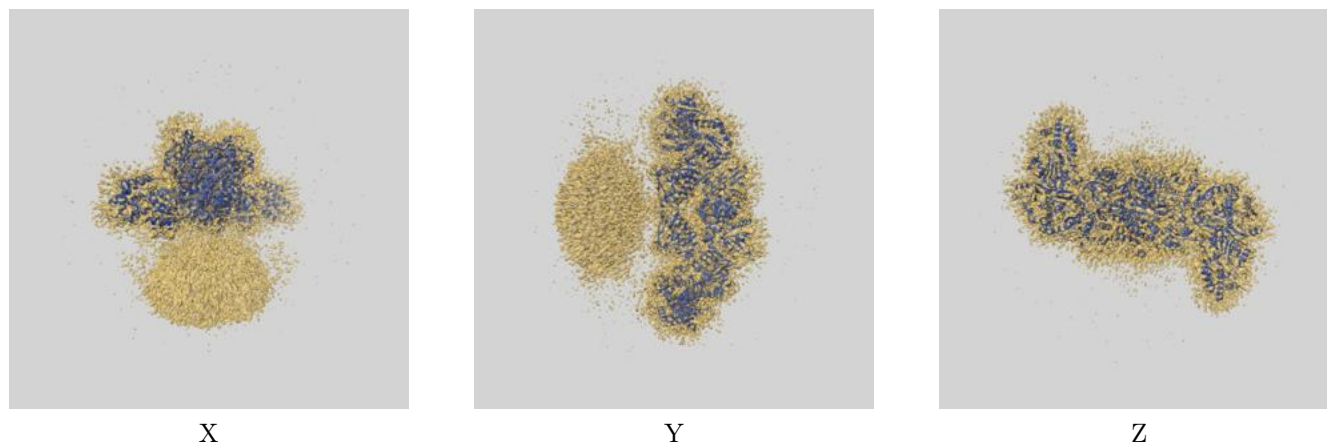
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.49	3.95	3.55
Unmasked-calculated*	4.24	6.60	4.31

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.24 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

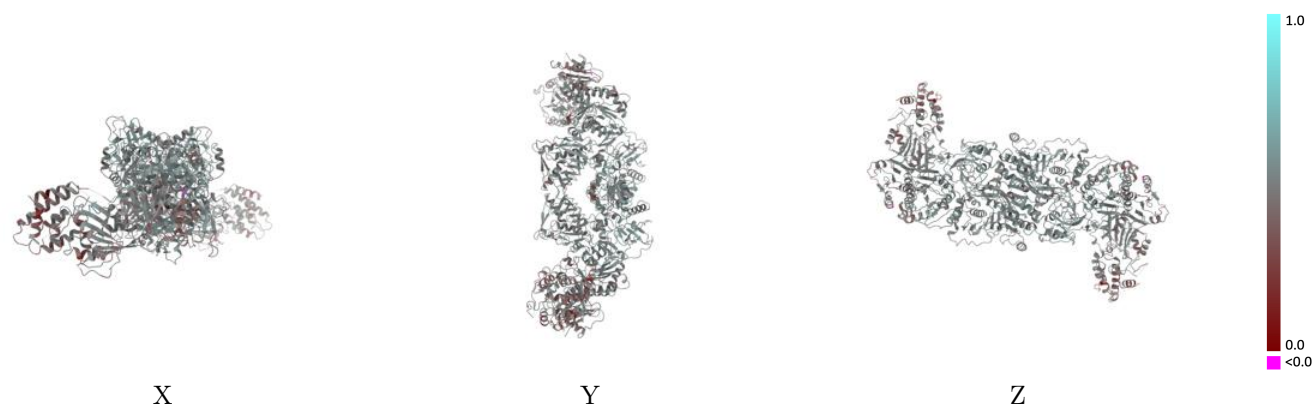
This section contains information regarding the fit between EMDB map EMD-45812 and PDB model 9CQ9. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



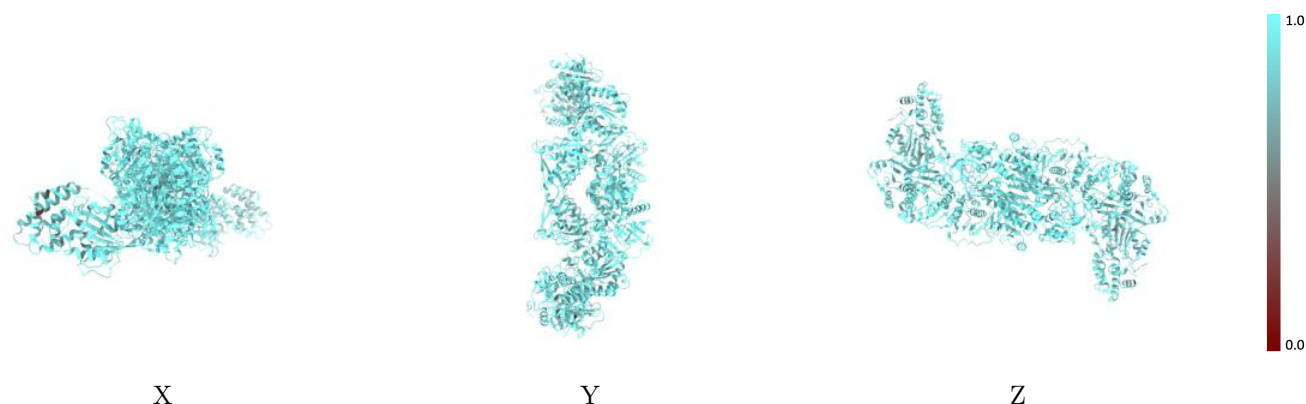
The images above show the 3D surface view of the map at the recommended contour level 0.0229 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



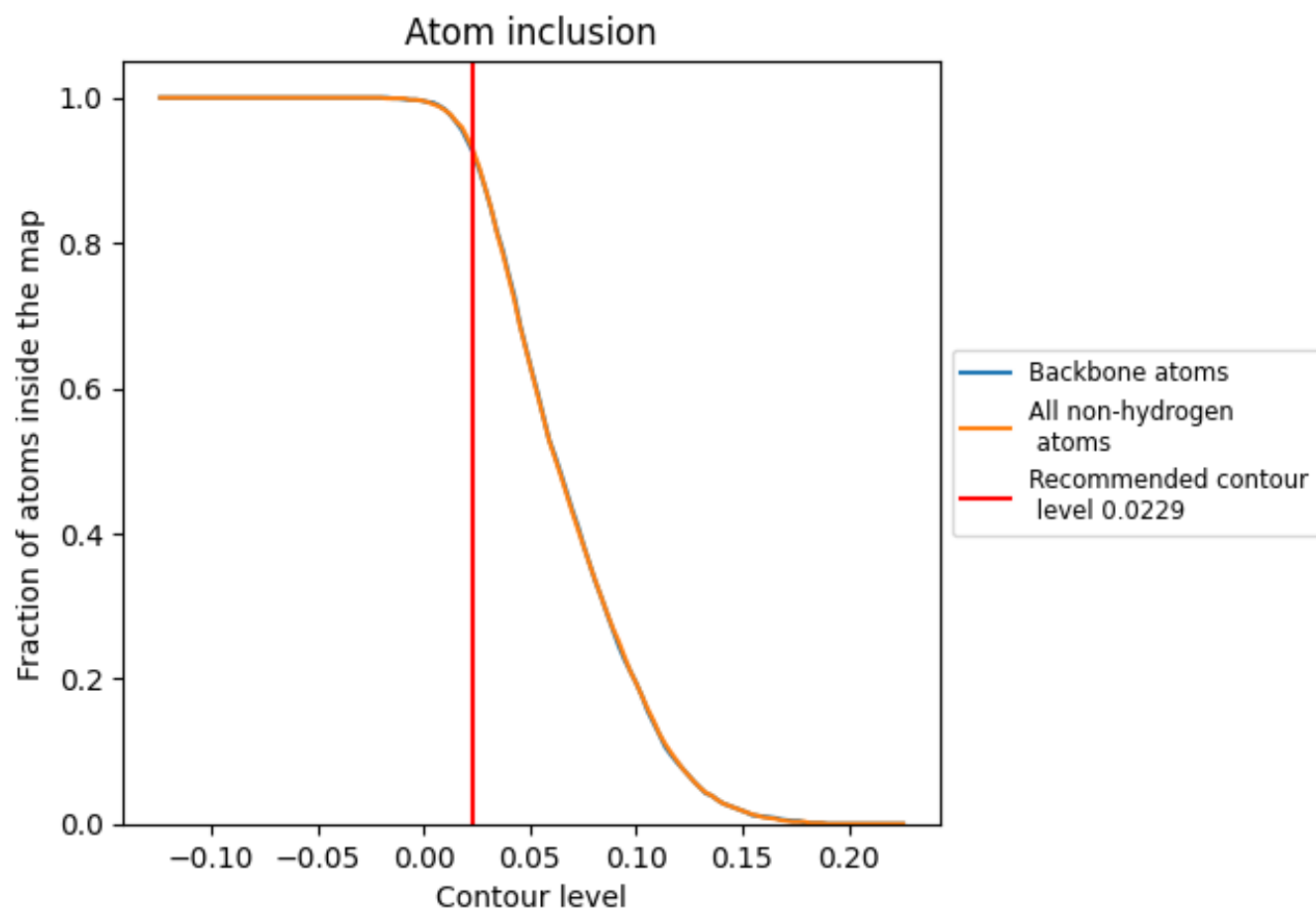
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0229).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 93% 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 (0.0229) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9310	0.4880
A	0.9290	0.4880
B	0.9290	0.4890

