



wwPDB EM Validation Summary Report ⓘ

Feb 11, 2025 – 06:54 PM EST

PDB ID : 9CQ9
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.dev113
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) : 2.40

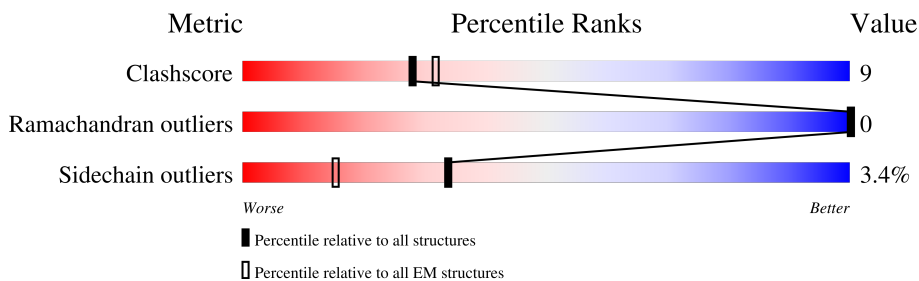
1 Overall quality at a glance

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)
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	2272	
1	B	2272	

2 Entry composition

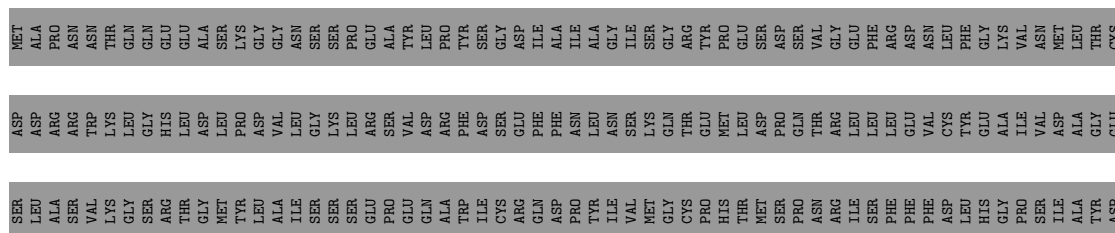
There is only 1 type of molecule in this entry. The entry contains 38874 atoms, of which 19370 are hydrogens and 0 are deuteriums.

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		

- Molecule 1: Polyketide synthase 1



E1598	F1469	M1343	SER	V1099	GLU	GLU	SER	VAL	VAL	GLY	SER	ASP	ASN	ALA	CYS	THR
T1604	L1470	D1344	SER	V1100	PHE	PHE	LEU	LYS	LEU	HIS	LEU	ALA	ASN	ILE	ALA	THR
L1613	L1471	D1345	SER	L1101	VAL	VAL	PRO	ILE	VAL	VAL	GLY	LEU	PRO	ALA	THR	CYS
E1633	E1474	T1353	F1218	D1110	PRO	PRO	GLY	PRO	ASN	HIS	ALA	SER	GLY	VAL	SER	SER
L1634	VAL	L1354	F1219	V1112	GLY	GLY	LEU	LYS	ALA	ALA	VAL	VAL	MET	ILE	GLU	LEU
V1637	GLU	A1358	A1224	S1113	THR	THR	LEU	PRO	GLU	ASP	GLY	VAL	PRO	LEU	VAL	VAL
Y1638	VAL	T1354	L1225	A1114	PRO	ARG	GLN	ARG	ASP	CYS	CYS	VAL	TYR	VAL	VAL	ALA
V1639	THR	E1226	R1227	G1115	LEU	ARG	SER	THR	SER	VAL	TYR	ASP	GLY	ASP	GLY	GLU
V1643	P1480	PRO	I1228	G1116	SER	ILE	LEU	ALA	THR	THR	CYS	ALA	SER	GLY	ALA	ALA
S1644	P1481	A1362	E1117	E1118	ASP	ASP	LYS	TRP	ILE	ILE	ASP	THR	SER	GLY	CYS	ALA
R1645	D1488	M1363	Q1231	I1119	MET	MET	ARG	LEU	SER	SER	GLY	ILE	SER	PHE	LEU	PHE
D1646	L1489	Q1368	T1232	T1124	VAL	VAL	THR	PRO	GLY	GLY	CYS	ASN	LYS	ILE	LEU	GLN
L1647	W1493	A1369	GLY	R1130	ALA	ALA	GLY	SER	VAL	ASP	ALA	ASN	PRO	PRO	THR	THR
D1657	L1494	HIS	H1238	E1139	TRP	ALA	GLU	VAL	ASP	VAL	GLU	ASP	GLN	ASN	SER	THR
E1658	V1497	L1372	F1243	E1140	ASP	ASP	SER	GLU	GLU	VAL	GLU	ASP	GLY	LEU	ALA	GLY
M1663	D1510	D1375	H1239	E1141	HIS	HIS	VAL	LEU	MET	VAL	VAL	PHE	GLY	GLY	ARG	ILE
G1671	D1515	Q1383	F1240	V1144	ALA	ALA	VAL	TRP	PHE	THR	THR	VAL	VAL	VAL	ASP	ASP
I1672	L1515	G1241	G1241	H1447	GLN	GLN	GLY	ASP	GLY	GLY	GLY	GLU	GLU	GLY	CYS	ALA
E1673	K1518	M1391	L1242	VAL	LEU	LEU	GLN	ALA	TRP	ASP	ASP	GLU	ASP	PHE	THR	THR
F1674	S1519	G1396	F1243	THR	GLU	GLU	LYS	PRO	VAL	GLU	GLU	GLU	THR	THR	VAL	VAL
D1678	D1520	F1397	L1248	GLY	VAL	VAL	ARG	ALA	PRO	LEU	LEU	LEU	THR	THR	VAL	VAL
T1679	G1523	V1410	L1254	ARG	LYS	LYS	ASN	GLN	ASP	GLY	GLY	GLY	ARG	GLY	ILE	ALA
K1680	M1524	ASP	L1254	ASP	ASN	ASN	ALA	SER	SER	ASP	ASP	ASP	THR	THR	THR	ASN
R1683	F1528	PRO	R1270	PRO	ASP	ASP	ASP	SER	SER	ASP	ASP	ASP	ARG	ARG	VAL	VAL
L1687	P1514	GLY	M1273	GLY	PHE	PHE	ASN	ALA	ALA	PHE	GLU	GLU	GLU	GLU	ASN	ASN
C1688	N1529	ALA	L1415	LYS	GLY	GLY	LEU	GLU	VAL	VAL	VAL	VAL	VAL	VAL	CYS	CYS
A1689	L1416	LYS	D1276	ARG	ARG	ARG	PHE	LEU	HIS	GLU	GLU	GLU	TRP	TRP	GLY	GLY
P1690	Q1533	L1417	G1277	PRO	VAL	VAL	LEU	ALA	VAL	VAL	VAL	VAL	ILE	ALA	ASP	ASP
P1691	E1534	L1427	L1278	GLY	GLN	GLN	PHE	ALA	ASN	ASN	ASN	ASN	THR	THR	LYS	LYS
A1692	S1537	F1428	M1279	ALA	ALA	ALA	PHE	ASN	ASN	ASN	ASN	ASN	ALA	ALA	VAL	VAL
V1697	V1540	R1429	S1280	T1162	SER	SER	SER	LEU	LEU	VAL	VAL	VAL	GLY	GLY	GLY	GLY
C1699	R1541	LYS	L1290	V1163	GLY	GLY	GLY	LEU	LEU	GLY	GLY	GLY	ILE	ILE	ALA	ALA
L1700	C1542	GLY	C1291	D1164	SER	SER	SER	LYS	PRO	PRO	PRO	PRO	ALA	ALA	ALA	ALA
S1702	F1560	D1433	H1302	Q1178	GLY	GLY	CYS	VAL	VAL	VAL	VAL	VAL	THR	THR	THR	THR
Q1709	R1561	L1436	V1306	V1191	ALA	ALA	PHE	LEU	LEU	LEU	LEU	LEU	ALA	ALA	ALA	ALA
H1710	Y1562	S1441	L1307	L1192	THR	THR	HIS	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
L1713	Y1562	S1441	E1308	K1195	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
P1720	M1566	A1442	A1311	L1198	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
V1721	D1567	A1443	A1311	L1198	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER
A1722	L1568	Q1444	F1328	L1204	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
R1733	H1583	R1446	D1332	Q1207	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS
G1734	T1587	H1452	Y1335	ASP	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
H1735	D1588	E1456	T1336	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
	Q1590	V1457	G1338	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER
		I1458		LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS

HIS	GLY	N2105	V1960	T1741
HIS	LEU	Y2106		
HIS	LYS		L1963	I1756
HIS	SER	N2110	F1966	
HIS	VAL	S2111	G1967	C1764
	SER		L1968	E1765
	GLY	D2114	E1969	I1766
	VAL	R2115		F1767
	ASP	L2116	V1979	I1768
	PRO			
	ASP	G2124	R1987	E1800
	ASP	L2125		
	LYS			V1803
	VAL	Q2131	I1990	T1807
	PHE		T1991	
	LEU	I2135	T1992	N1817
	ASP		G1993	
	LEU			R1829
	GLY	V2149	K1998	
	LEU	T2150		A1841
	ASP	E2151	V2010	SER
	SER		V2011	GLY
	LEU	W2154		ARG
	MET		D2031	GLY
	SER	N2158	L2032	SER
	VAL			ASP
	GLU	Y2167	L2035	ALA
	ILE	F2168		E1849
	LYS		L2041	D1859
	GLN	Q2171	N2044	T1860
	MET	N2172	L2045	S1861
	LEU	R2173	R2046	
	GLU		D2047	W1878
	ARG	V2176		
	ASP	A2177	Y2058	L1881
	LEU	C2178		L1897
	ASP			A1898
	LEU	K2184	T2061	R1899
	ALA	VAL		T1900
	LEU	LYS	K2065	V1901
	GLY	ALA	I2066	
	THR	VAL	VAL	V1908
	LYS	GLU	T2069	D1909
	ASP	GLY		
	ILE	GLY	L2072	E1915
	GLN	GLU	D2073	
	MET	GLU		K1926
	LEU	THR	S2076	I1927
	LEU	VAL		
	THR	GLY	L2081	E1930
	PHE	GLN		
	ALA	GLN	L2085	K1940
	GLN	GLN	D2086	K1941
	LEU	ILE		
	GLN	LYS	M2090	Y1957
	ALA	LYS		
	MET	ALA	P2091	
	VAL	VAL		
	GLN	GLY	S2092	
	HIS	ASN	S2093	
	VAL	VAL		
	LEU	LEU	T2104	
	HIS			

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

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	0.29	0/9950	0.51	0/13478
1	B	0.29	0/9950	0.51	0/13478
All	All	0.29	0/19900	0.51	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

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	186	0
1	B	9752	9685	9684	184	0
All	All	19504	19370	19368	365	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 365 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%)	1014 (97%)	36 (3%)	32	60
1	B	1050/1892 (56%)	1014 (97%)	36 (3%)	32	60
All	All	2100/3784 (56%)	2028 (97%)	72 (3%)	34	60

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1699	CYS
1	B	2178	CYS
1	B	1721	VAL
1	B	2031	ASP
1	A	1764	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1452	HIS
1	B	1452	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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.

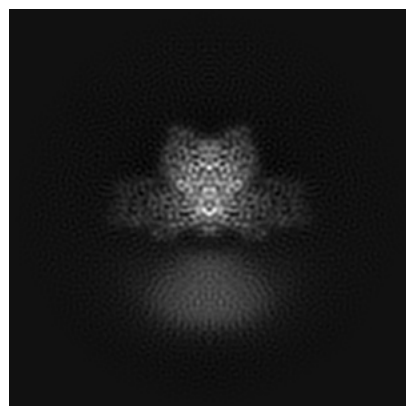
6 Map visualisation [i](#)

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.

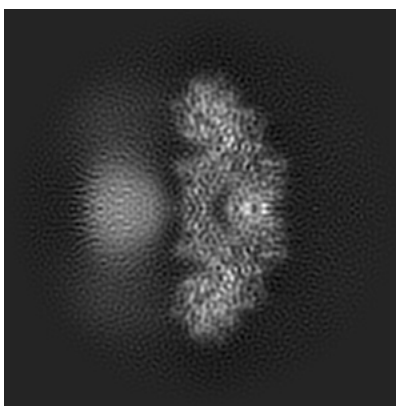
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

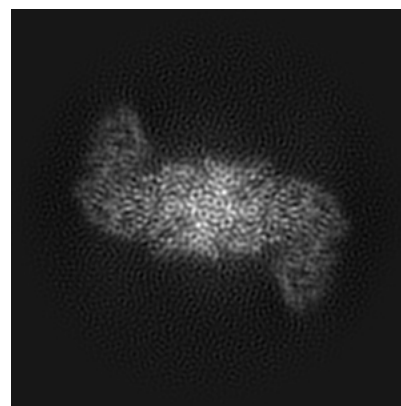
6.1.1 Primary map



X

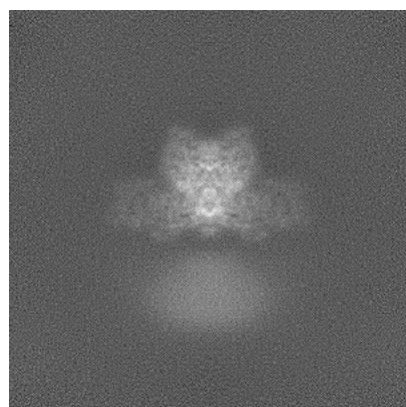


Y

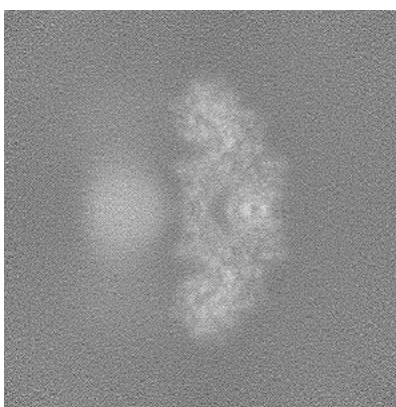


Z

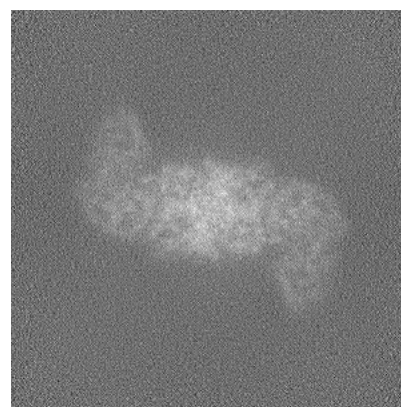
6.1.2 Raw map



X



Y

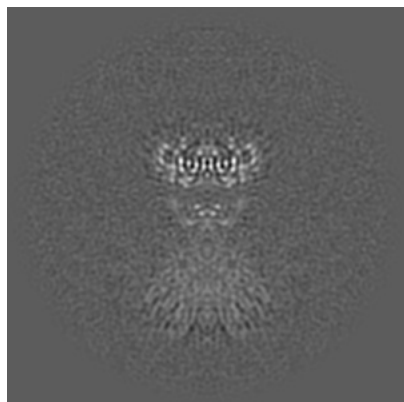


Z

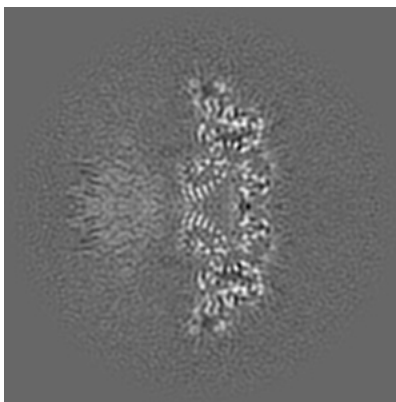
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

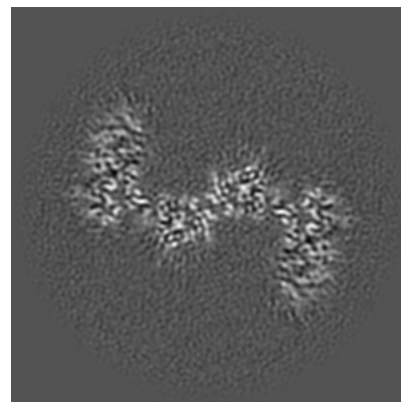
6.2.1 Primary map



X Index: 256

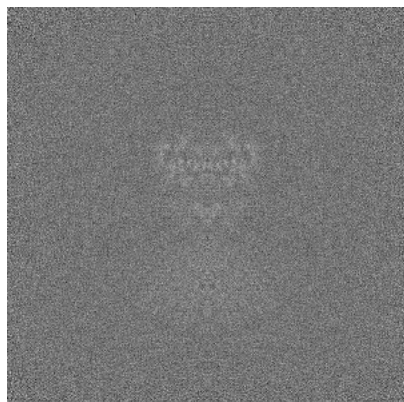


Y Index: 256

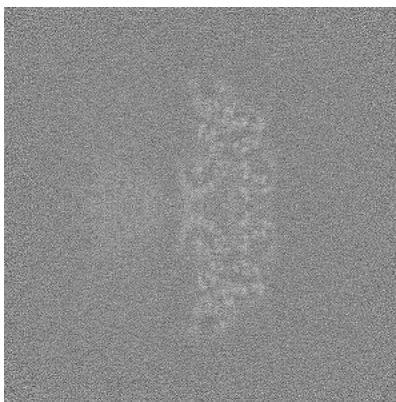


Z Index: 256

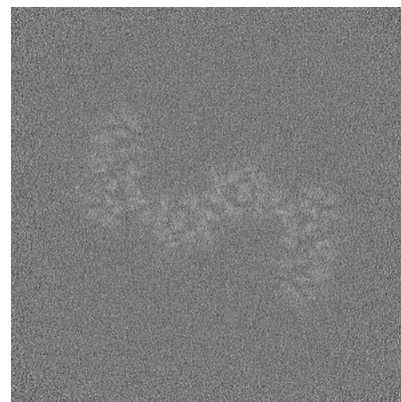
6.2.2 Raw map



X Index: 256



Y Index: 256

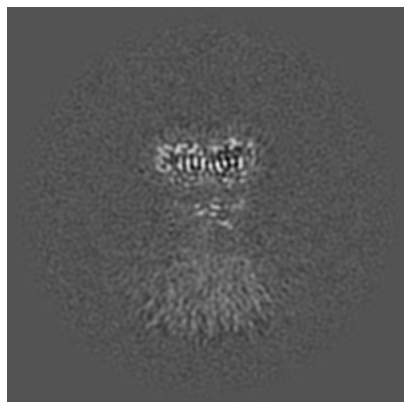


Z Index: 256

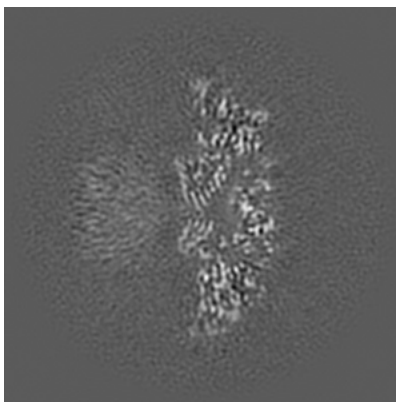
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

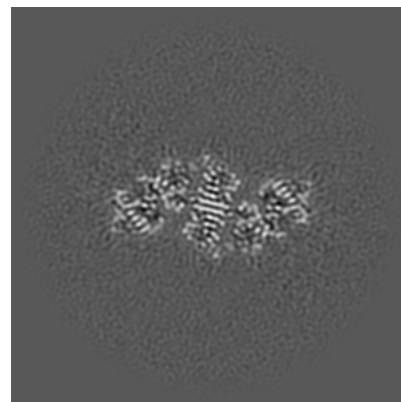
6.3.1 Primary map



X Index: 259

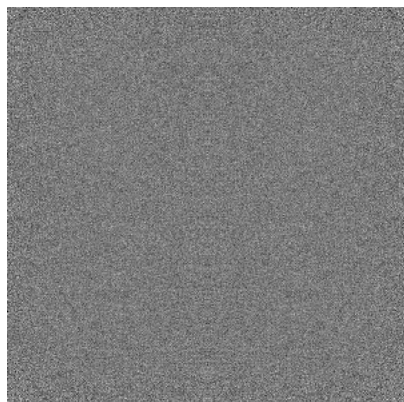


Y Index: 261

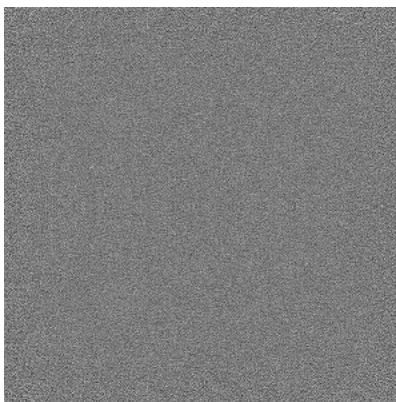


Z Index: 309

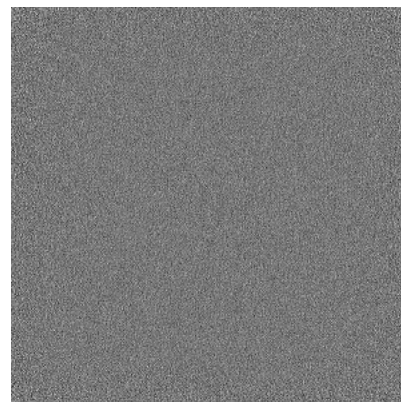
6.3.2 Raw map



X Index: 0



Y Index: 0

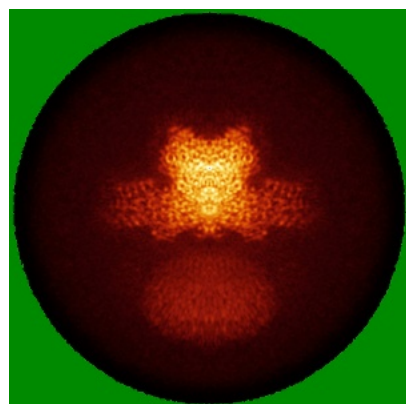


Z Index: 0

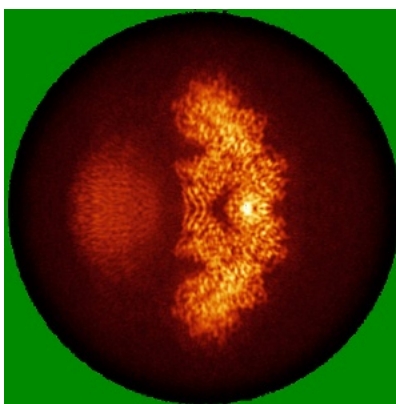
The images above show the largest variance slices of the map in three orthogonal directions.

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

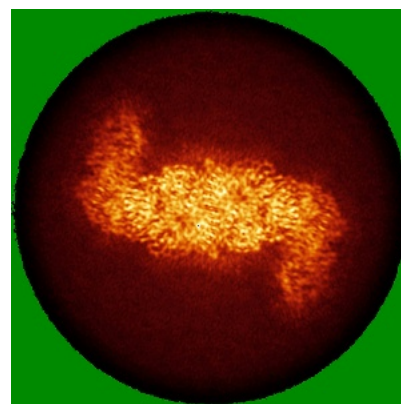
6.4.1 Primary map



X

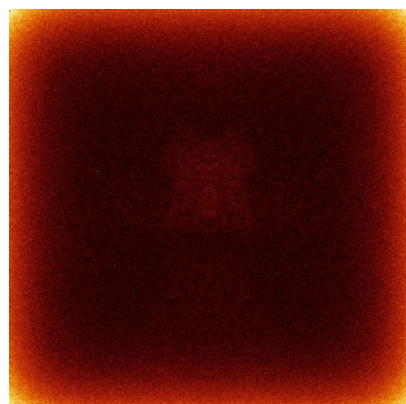


Y

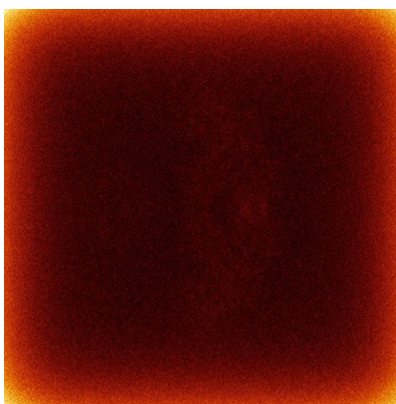


Z

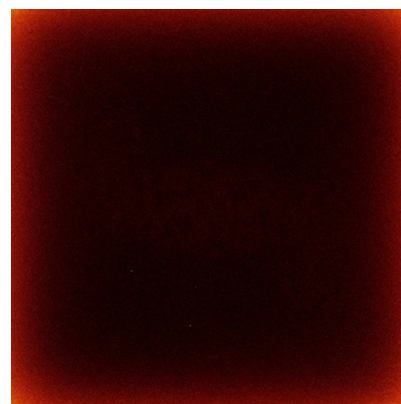
6.4.2 Raw map



X



Y

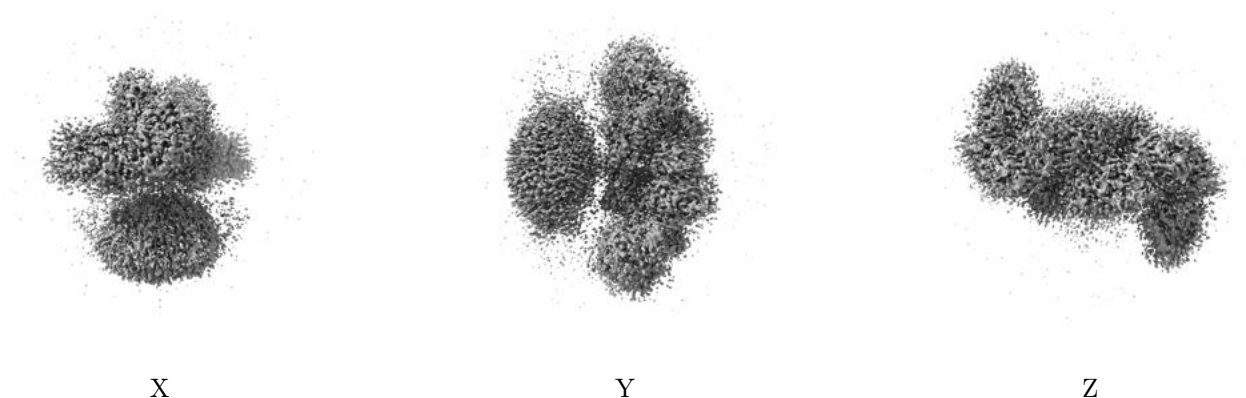


Z

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.

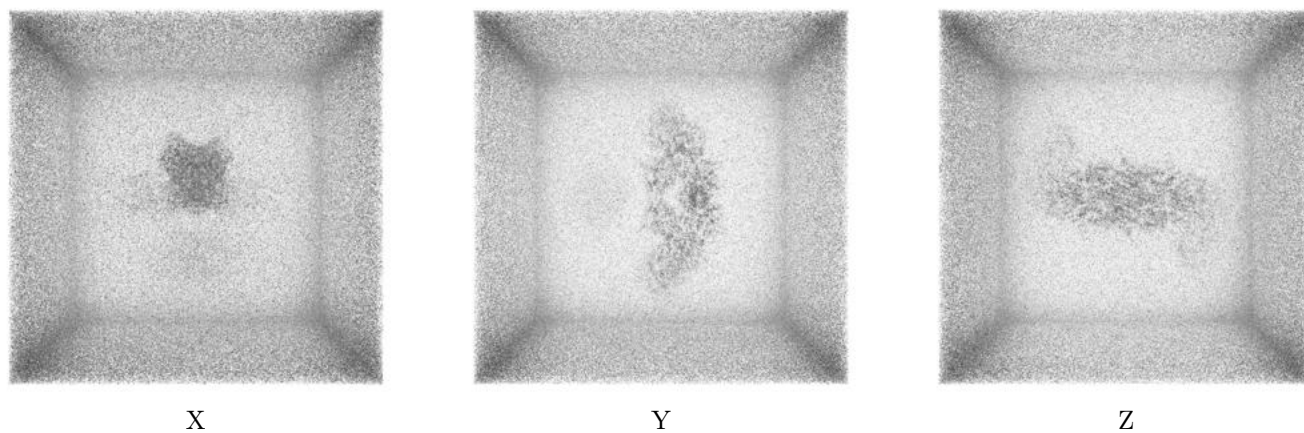
6.5 Orthogonal surface views [i](#)

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.

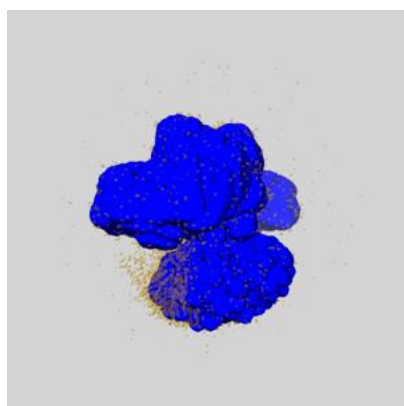
6.6 Mask visualisation [i](#)

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

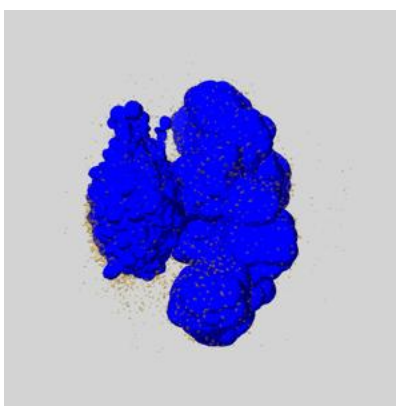
A mask typically either:

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

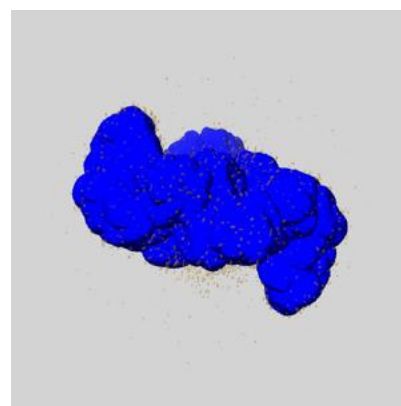
6.6.1 emd_45812_msk_1.map [i](#)



X



Y

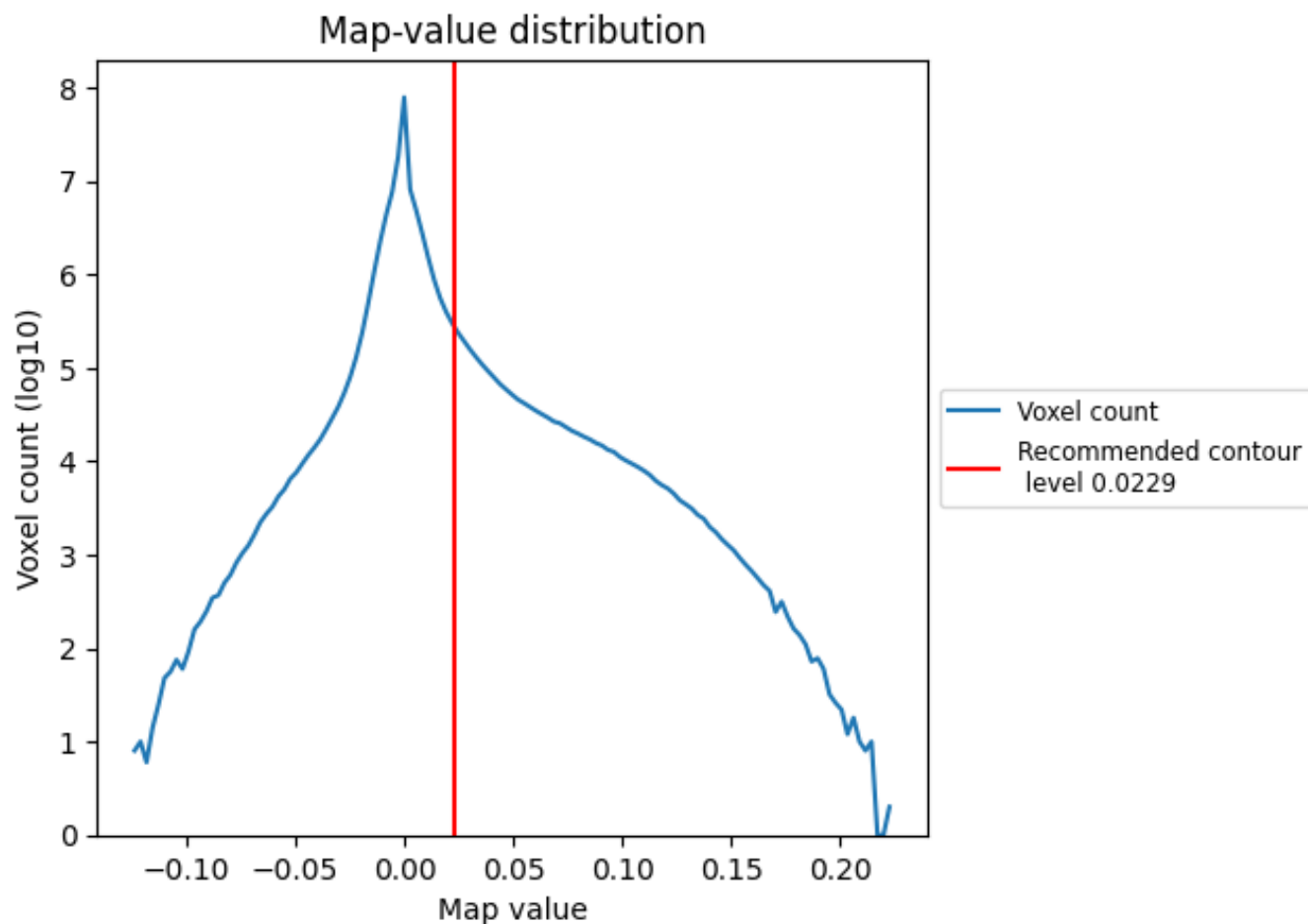


Z

7 Map analysis [i](#)

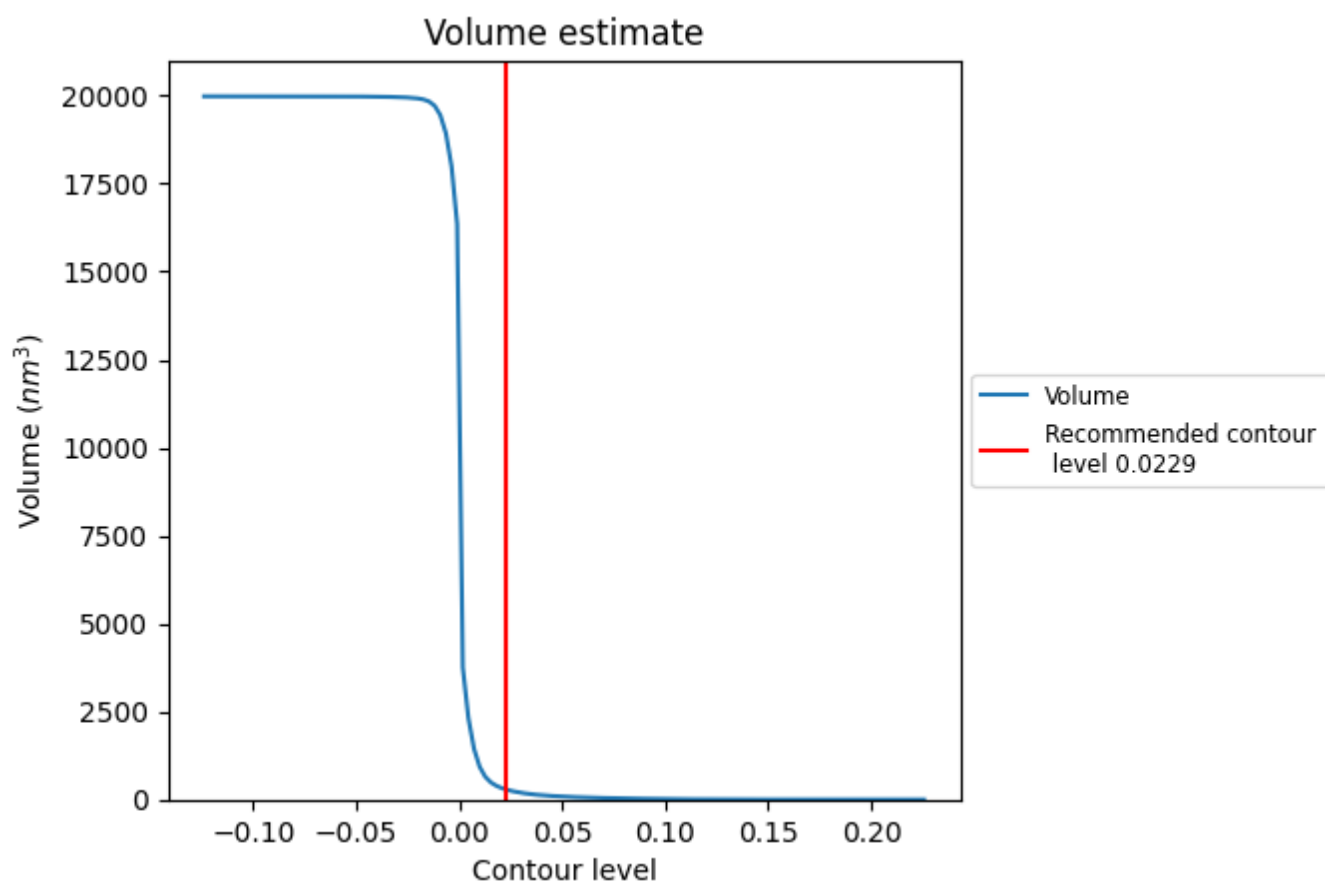
This section contains the results of statistical analysis of the map.

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.

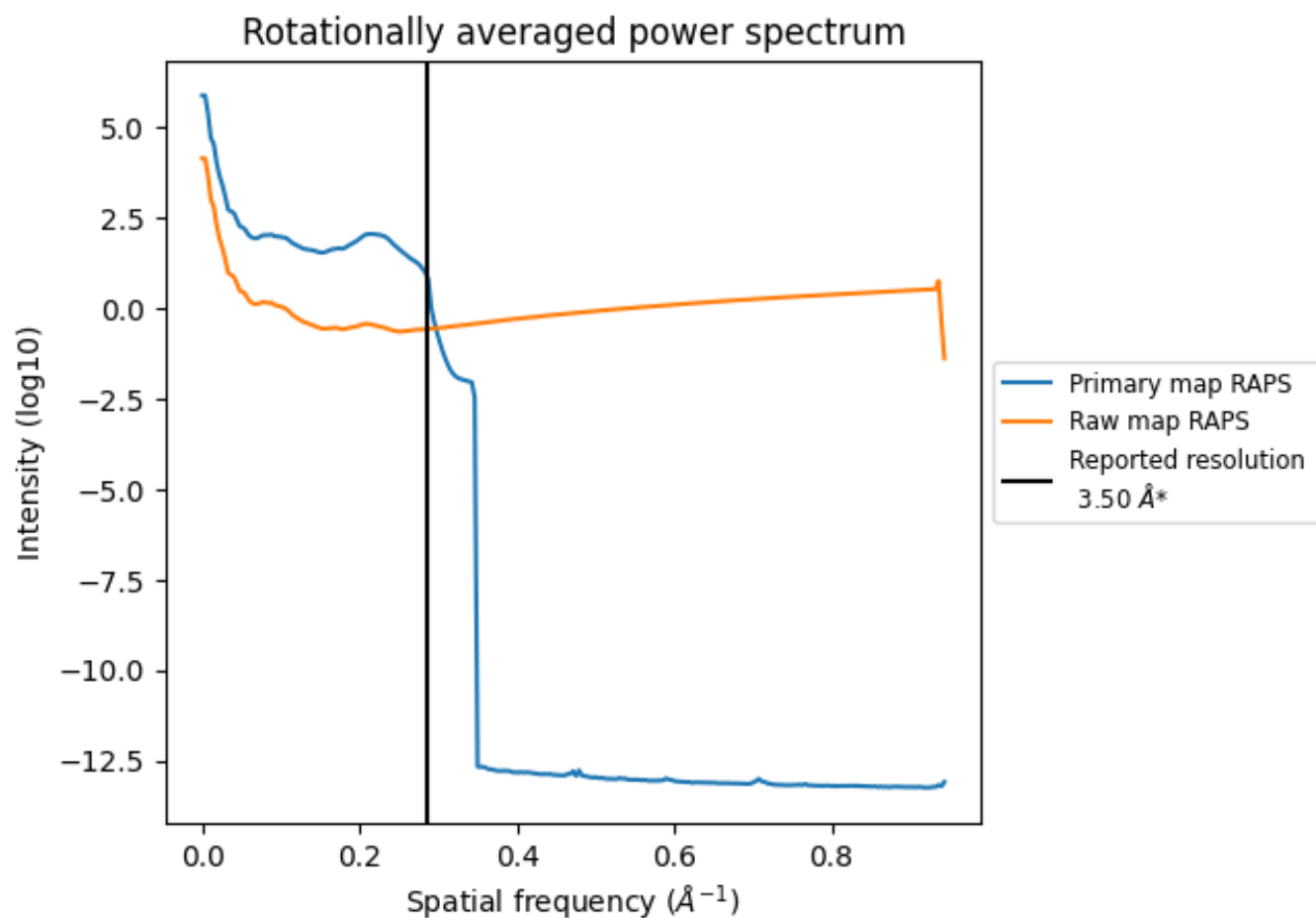
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 284 nm^3 ; 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 ⓘ

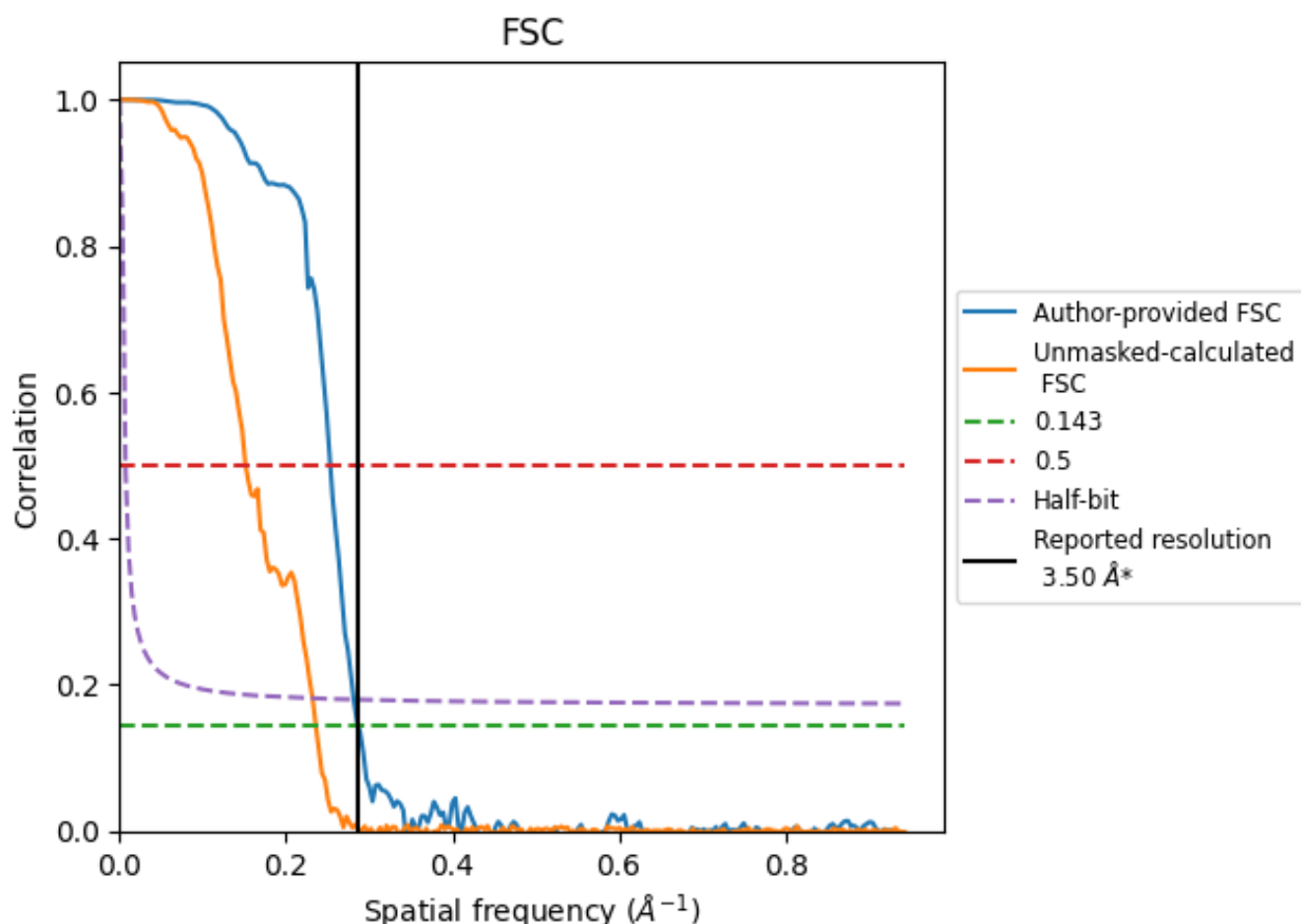


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 Å⁻¹

8.2 Resolution estimates [i](#)

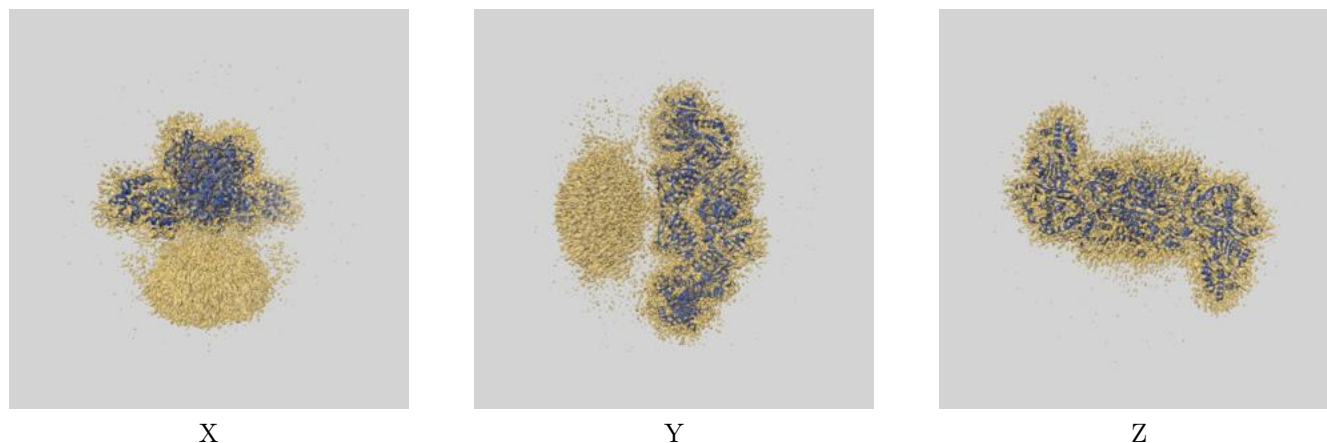
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.49	3.95	3.55
Unmasked-calculated*	4.24	6.60	4.31

*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](#)

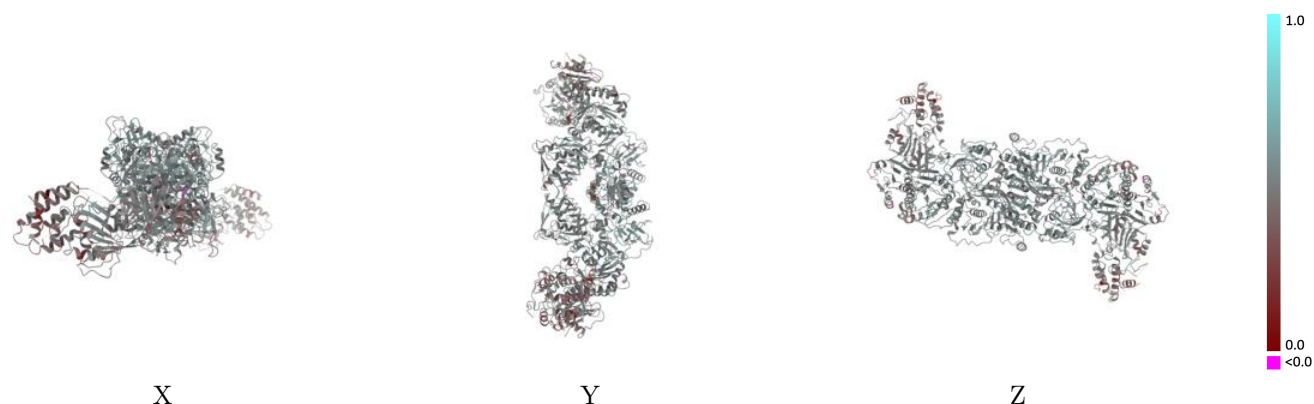
This section contains information regarding the fit between EMDB map EMD-45812 and PDB model 9CQ9. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



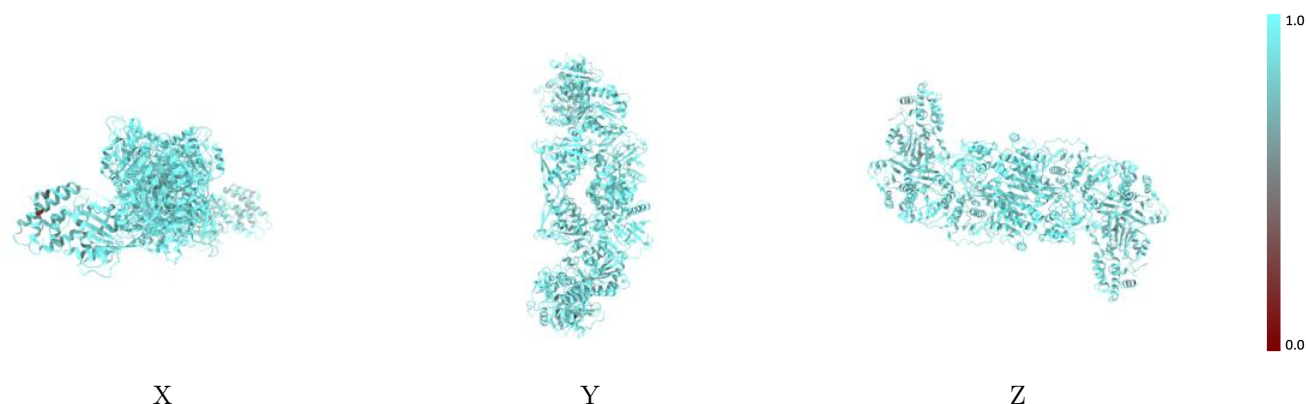
The images above show the 3D surface view of the map at the recommended contour level 0.0229 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



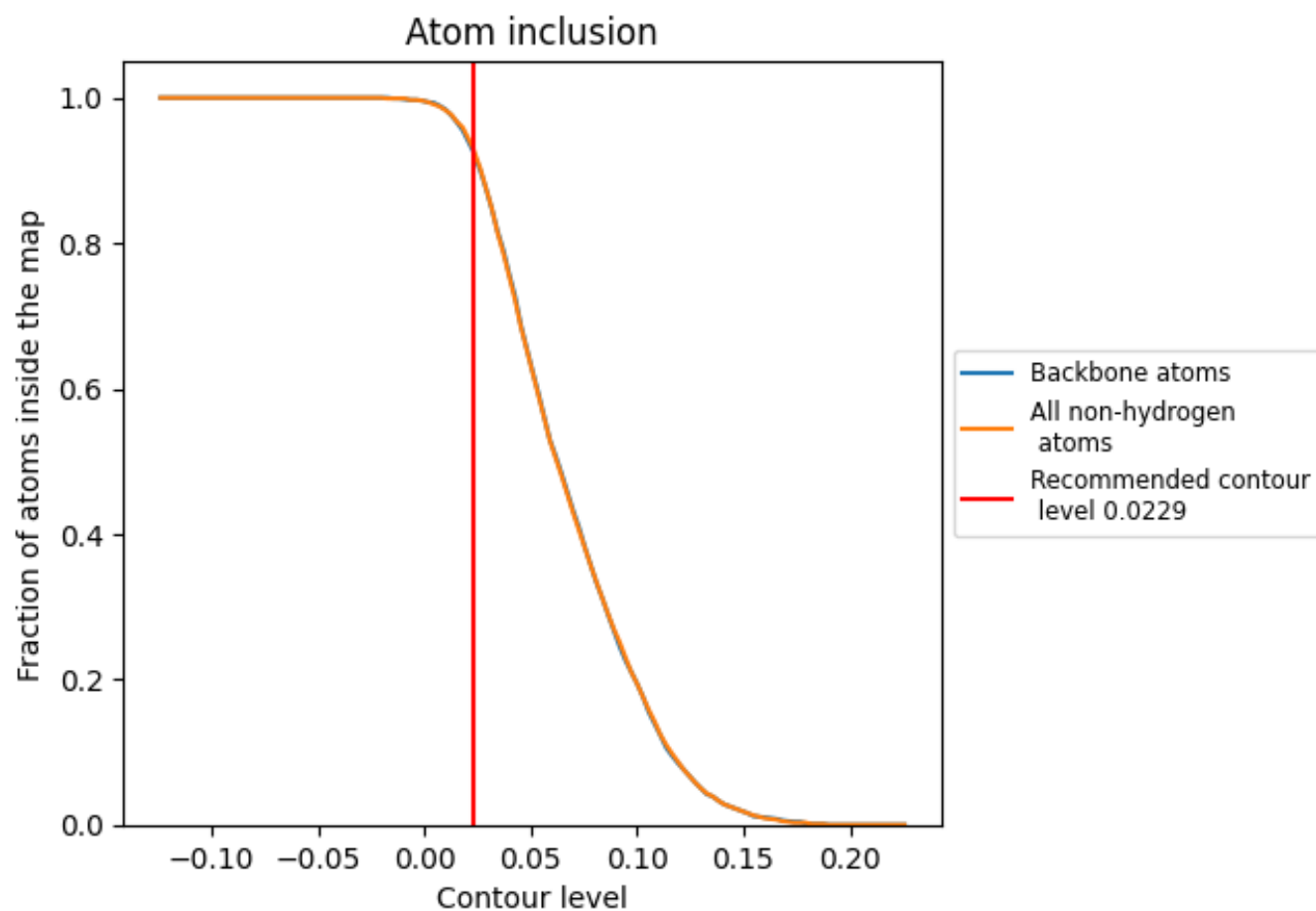
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	<div></div> 0.9310	<div></div> 0.4880
A	<div></div> 0.9290	<div></div> 0.4880
B	<div></div> 0.9290	<div></div> 0.4890

