



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 01:43 PM UTC

PDB ID : 9SI1 / pdb_00009si1
EMDB ID : EMD-54923
Title : Mouse otoferlin (216-1931) in the lipid-free Ca²⁺-bound state, "closed-like" conformation
Authors : Cretu, C.; Moser, T.
Deposited on : 2025-08-28
Resolution : 3.10 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

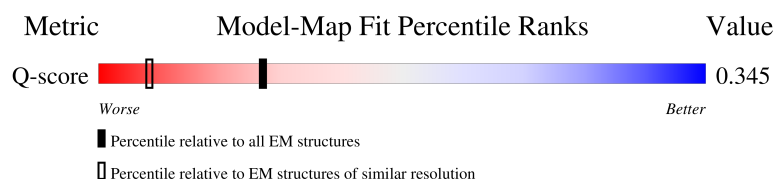
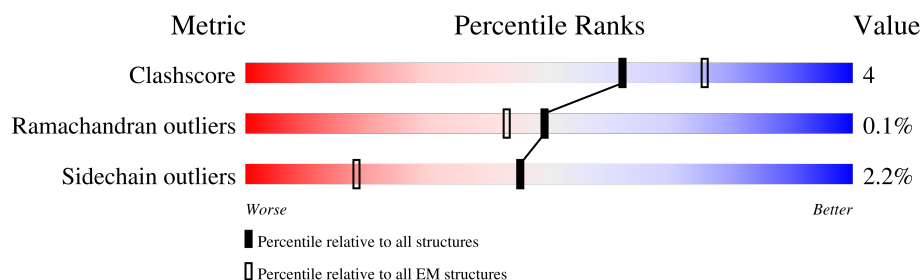
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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	1767	14% 73% 12% • 15%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12135 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 Otoferlin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1510	Total	C	N	O	S	0	0
			12126	7708	2079	2277	62		

There are 51 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	165	MET	-	initiating methionine	UNP A0A0R4J1K2
A	166	ALA	-	expression tag	UNP A0A0R4J1K2
A	167	SER	-	expression tag	UNP A0A0R4J1K2
A	168	TRP	-	expression tag	UNP A0A0R4J1K2
A	169	SER	-	expression tag	UNP A0A0R4J1K2
A	170	HIS	-	expression tag	UNP A0A0R4J1K2
A	171	PRO	-	expression tag	UNP A0A0R4J1K2
A	172	GLN	-	expression tag	UNP A0A0R4J1K2
A	173	PHE	-	expression tag	UNP A0A0R4J1K2
A	174	GLU	-	expression tag	UNP A0A0R4J1K2
A	175	LYS	-	expression tag	UNP A0A0R4J1K2
A	176	GLY	-	expression tag	UNP A0A0R4J1K2
A	177	GLY	-	expression tag	UNP A0A0R4J1K2
A	178	GLY	-	expression tag	UNP A0A0R4J1K2
A	179	SER	-	expression tag	UNP A0A0R4J1K2
A	180	GLY	-	expression tag	UNP A0A0R4J1K2
A	181	GLY	-	expression tag	UNP A0A0R4J1K2
A	182	GLY	-	expression tag	UNP A0A0R4J1K2
A	183	SER	-	expression tag	UNP A0A0R4J1K2
A	184	GLY	-	expression tag	UNP A0A0R4J1K2
A	185	GLY	-	expression tag	UNP A0A0R4J1K2
A	186	GLY	-	expression tag	UNP A0A0R4J1K2
A	187	SER	-	expression tag	UNP A0A0R4J1K2
A	188	TRP	-	expression tag	UNP A0A0R4J1K2
A	189	SER	-	expression tag	UNP A0A0R4J1K2
A	190	HIS	-	expression tag	UNP A0A0R4J1K2
A	191	PRO	-	expression tag	UNP A0A0R4J1K2
A	192	GLN	-	expression tag	UNP A0A0R4J1K2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	193	PHE	-	expression tag	UNP A0A0R4J1K2
A	194	GLU	-	expression tag	UNP A0A0R4J1K2
A	195	LYS	-	expression tag	UNP A0A0R4J1K2
A	196	LEU	-	expression tag	UNP A0A0R4J1K2
A	197	GLU	-	expression tag	UNP A0A0R4J1K2
A	198	VAL	-	expression tag	UNP A0A0R4J1K2
A	199	LEU	-	expression tag	UNP A0A0R4J1K2
A	200	PHE	-	expression tag	UNP A0A0R4J1K2
A	201	GLN	-	expression tag	UNP A0A0R4J1K2
A	202	GLY	-	expression tag	UNP A0A0R4J1K2
A	203	PRO	-	expression tag	UNP A0A0R4J1K2
A	204	GLY	-	expression tag	UNP A0A0R4J1K2
A	205	SER	-	expression tag	UNP A0A0R4J1K2
A	206	GLY	-	expression tag	UNP A0A0R4J1K2
A	207	ASP	-	expression tag	UNP A0A0R4J1K2
A	208	LYS	-	expression tag	UNP A0A0R4J1K2
A	209	ASP	-	expression tag	UNP A0A0R4J1K2
A	210	CYS	-	expression tag	UNP A0A0R4J1K2
A	211	GLU	-	expression tag	UNP A0A0R4J1K2
A	212	GLN	-	expression tag	UNP A0A0R4J1K2
A	213	SER	-	expression tag	UNP A0A0R4J1K2
A	214	ASN	-	expression tag	UNP A0A0R4J1K2
A	215	ALA	-	expression tag	UNP A0A0R4J1K2

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
2	A	9	Total Ca 9 9	0

VAL	VAL	SER	MET	GLU	PRO	GLU	GLU	PRO	VAL	VAL	LYS	LYS	LEU	GLU	THR	MET	LYS	LEU	ASP	ALA	VAL	VAL	LYS	VAL	ASP	VAL	LYS	LYS	LYS	LYS	GLY	PRO	ASN	SER	GLU	GLU	PRO	PRO	GLU	GLU	GLU	GLU	PRO	D1317	E1318	S1319					
V1324											E1336	GLN	LEU	GLN	HIS	GLU	THR	ASP	ALA	GLY	LEU	VAL	VAL	GLY	PRO	MET	LYS	LYS	LYS	LYS	LYS	LYS	ASN	GLN	PRO	GLY	PRO	GLY	GLY	GLN	GLY	SER	GLU	ALA	PRO						
GLU	LYS	LYS	LYS	A1398	K1399	K1408	S1412	E1413	F1414	D1415	S1416	F1417	E1418	L1426	L1427	R1428	G1429	K1430	T1431	G1432	D1433	D1434	E1435	D1436	G1437	S1438	T1439	E1440	E1441	E1442	R1443	T1444	V1445	G1446	R1447	F1448	K1449	V1457	E1461	D1462	V1463	S1464	R1465	E1466	A1467	G1468	Y1469	M1475	L1488	T1491	Y1492
V1493	V1494	R1495	T1504	N1505	G1506	K1507	A1508	I1512	A1513	I1514	K1515	L1516	G1517	K1518	T1519	D1520	I1521	E1525	L1532	V1535	S1539	F1540	D1541	I1542	E1543	A1544	S1550	M1551	L1552	V1562	G1563	T1564	G1569	K1572	L1575	E1576	T1586	C1587	G1588	I1589	A1590	Q1591	T1592	R1602	H1624						
F1625	G1626	R1630	V1631	R1632	N1635	R1636	V1637	F1638	T1639	R1651	T1654	D1655	E1656	L1663	V1672	E1679	H1680	L1686	L1687	M1688	P1689	D1690	K1691	Q1696	W1702	M1705	M1708	D1709	M1710	P1713	L1717	D1718	R1722	K1723	P1724	V1731	I1732	V1733	T1736	E1742	D1743										
D1744	D1745	F1746	F1747	T1748	G1749	A1750	K1751	S1752	S1753	F1756	L1761	Q1764	Q1765	E1766	D1767	K1768	Q1769	D1770	Y1788	D1793	Y1794	L1795	A1796	A1797	E1798	E1799	E1807	S1808	M1809	F1810	S1811	W1812	D1813	E1814	A1821	R1822	Q1826	T1827	H1832	F1833	S1834	E1843	L1846	N1847	R1848	F1849	P1850	R1851			
G1852	A1853	K1854	M1861	E1862	M1863	A1864	T1865	G1866	E1867	V1868	D1869	L1872	V1873	S1874	G1883	W1884	W1885	P1886	L1887	L1888	A1889	R1890	N1893	D1894	E1895	F1896	E1897	L1898	V1902	E1905	L1908	E1912	G1920	L1921	A1922	R1923	N1924	E1925	P1926	D1927	P1928	L1929	E1930	LYS							

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	66665	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 ($e^-/\text{\AA}^2$)	38.13	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.158	Depositor
Minimum map value	-0.094	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	259.2, 259.2, 259.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.72, 0.72, 0.72	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	2/12418 (0.0%)	0.59	3/16812 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1710	MET	C-N	5.53	1.40	1.33
1	A	1457	VAL	C-N	5.51	1.38	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1672	VAL	N-CA-C	-5.83	106.10	112.80
1	A	1162	VAL	CA-C-N	5.20	131.47	121.54
1	A	1162	VAL	C-N-CA	5.20	131.47	121.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1602	ARG	Sidechain

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	12126	0	11933	104	0
2	A	9	0	0	0	0
All	All	12135	0	11933	104	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 4.

The worst 5 of 104 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:280:LEU:HB2	1:A:285:MET:HE1	1.78	0.66
1:A:1051:TYR:HB3	1:A:1059:ALA:HB1	1.81	0.63
1:A:1732:ILE:HG23	1:A:1905:GLU:HB3	1.82	0.62
1:A:1495:ARG:HG2	1:A:1535:VAL:HA	1.82	0.62
1:A:1233:GLY:HA3	1:A:1426:LEU:HB3	1.82	0.61

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1498/1767 (85%)	1430 (96%)	67 (4%)	1 (0%)	48 78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1004	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	1335/1550 (86%)	1306 (98%)	29 (2%)	45 71

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1182	GLN
1	A	1795	LEU
1	A	1457	VAL
1	A	1732	ILE
1	A	1439	THR

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	A	1628	HIS
1	A	1765	GLN
1	A	1893	ASN
1	A	1847	ASN
1	A	1192	ASN

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](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

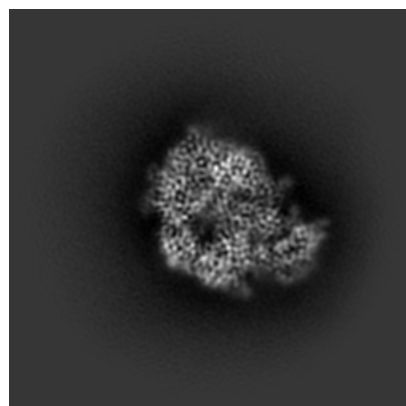
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54923. These allow visual inspection of the internal detail of the map and identification of artifacts.

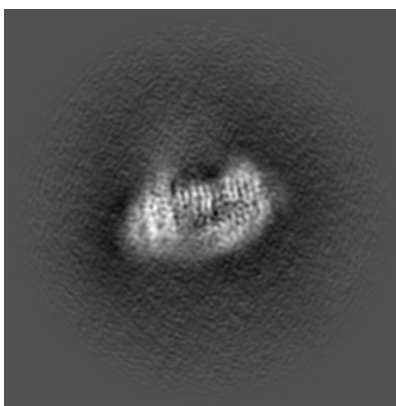
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

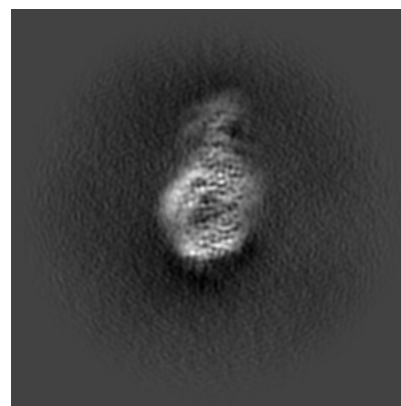
6.1.1 Primary map



X

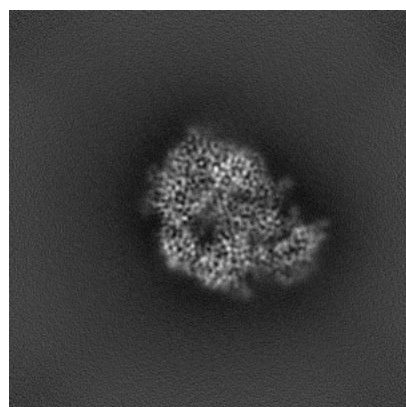


Y

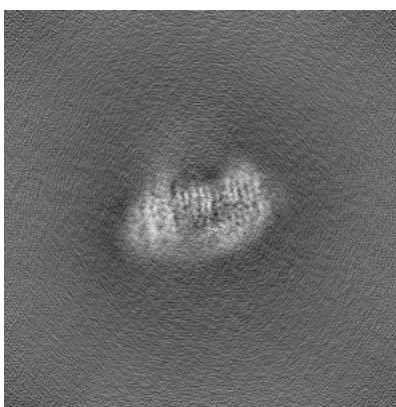


Z

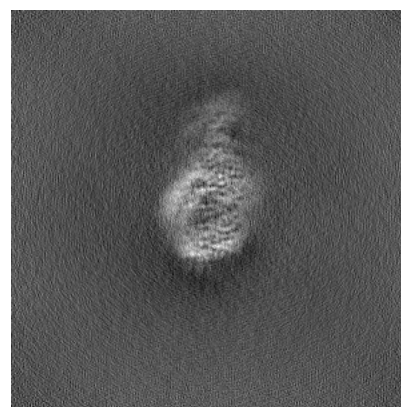
6.1.2 Raw map



X



Y

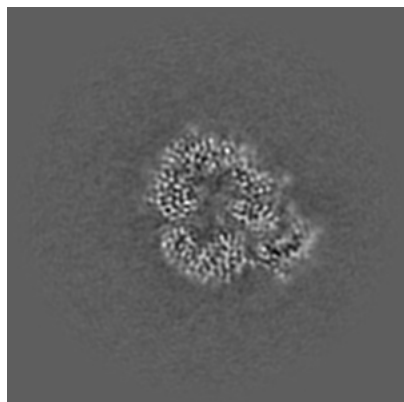


Z

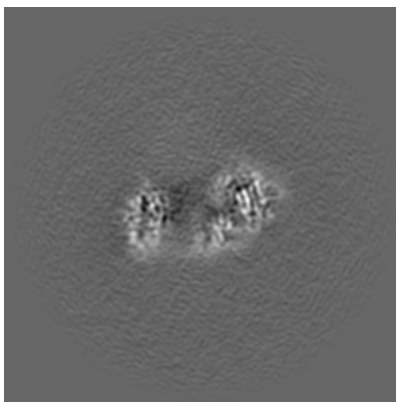
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

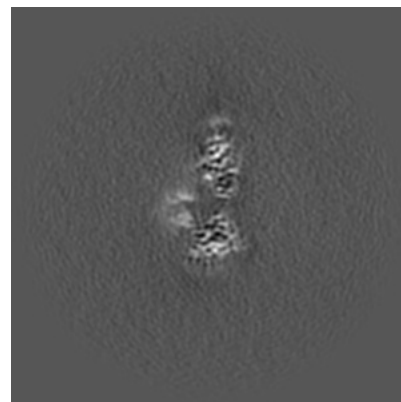
6.2.1 Primary map



X Index: 180

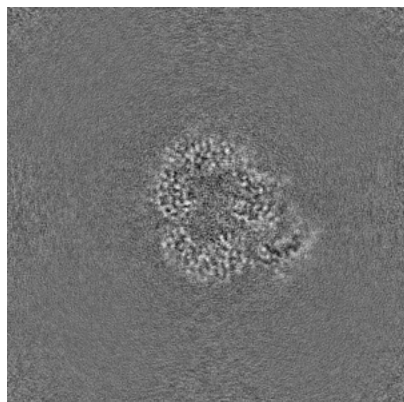


Y Index: 180

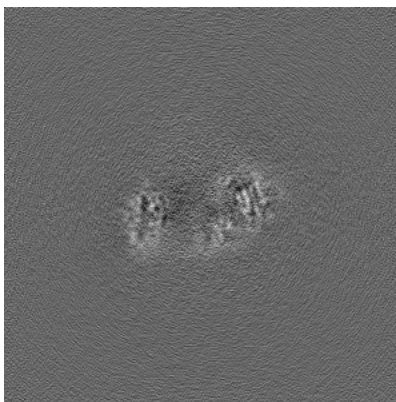


Z Index: 180

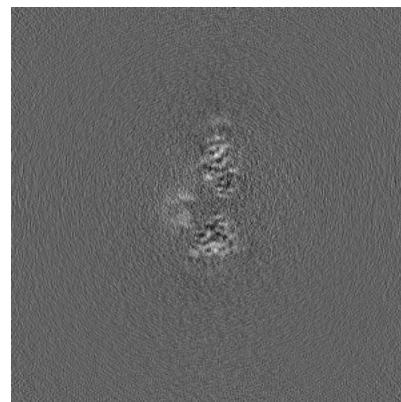
6.2.2 Raw map



X Index: 180



Y Index: 180

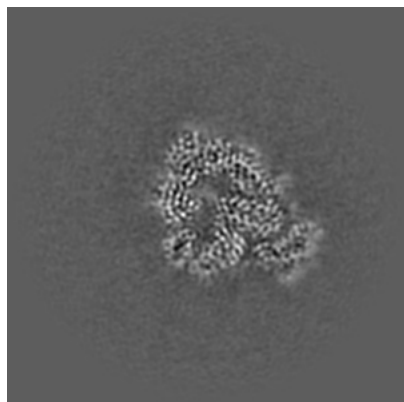


Z Index: 180

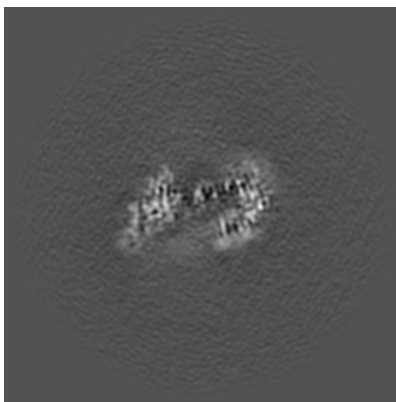
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

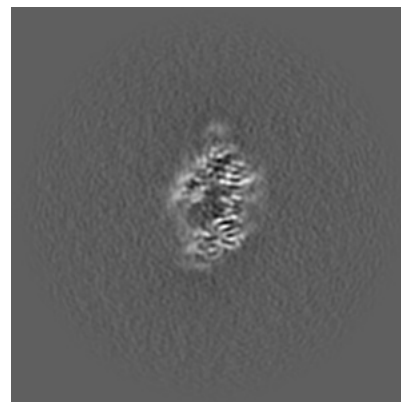
6.3.1 Primary map



X Index: 187

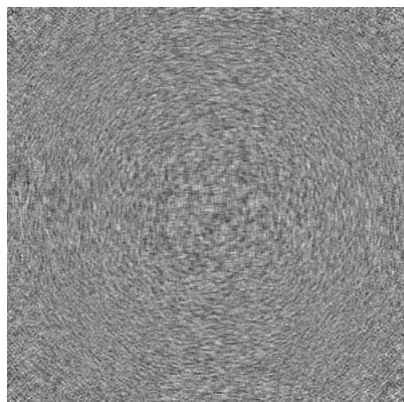


Y Index: 198

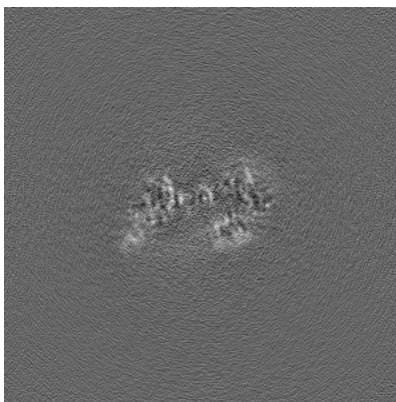


Z Index: 207

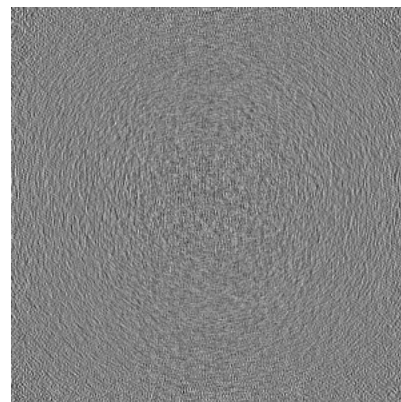
6.3.2 Raw map



X Index: 0



Y Index: 195

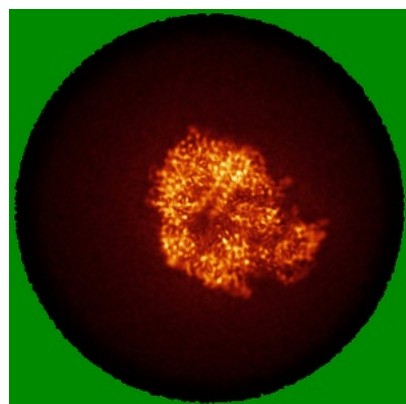


Z Index: 0

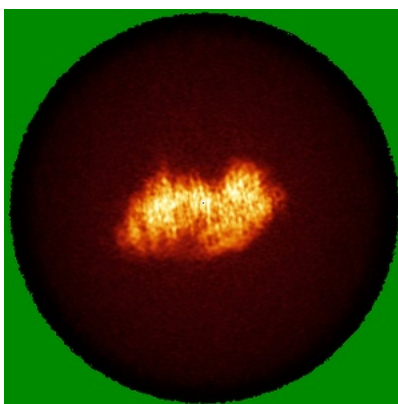
The images above show the largest variance slices of the map in three orthogonal directions.

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

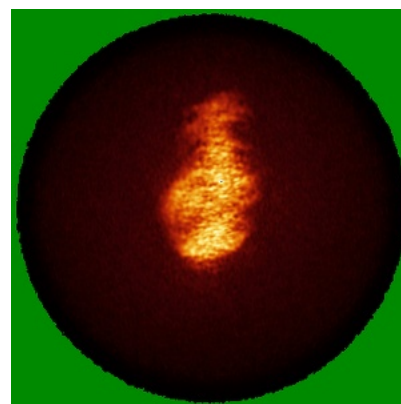
6.4.1 Primary map



X

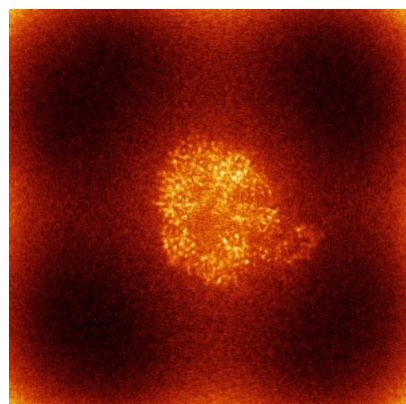


Y

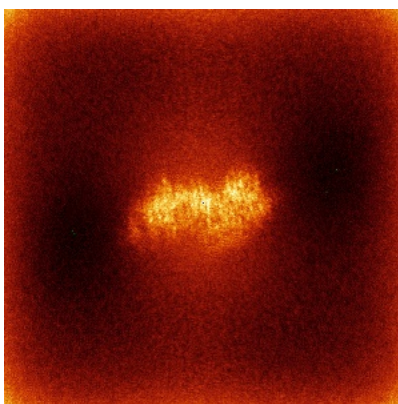


Z

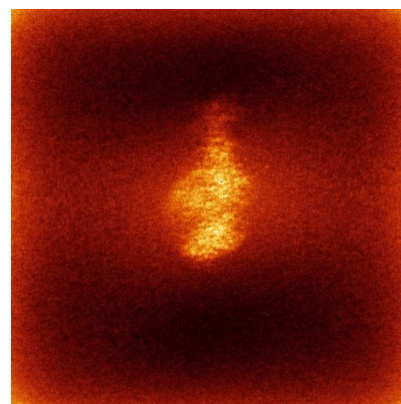
6.4.2 Raw map



X



Y

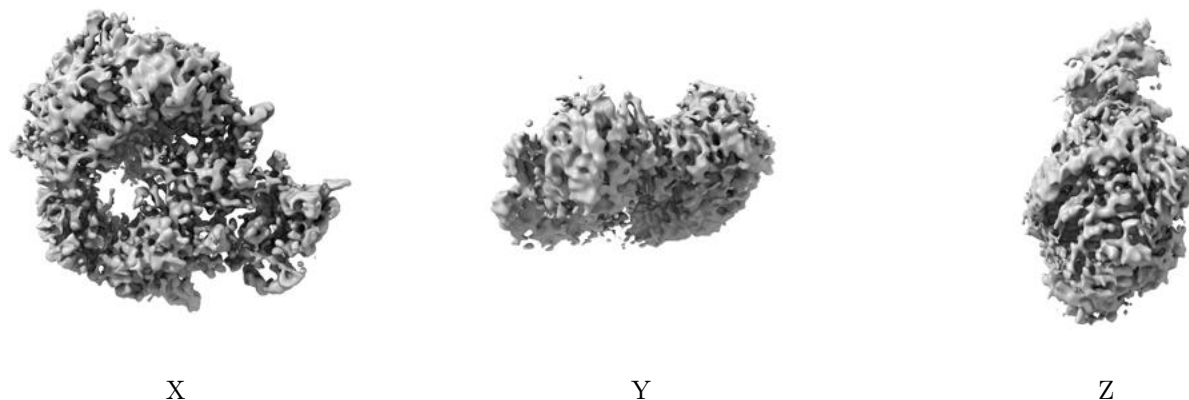


Z

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.

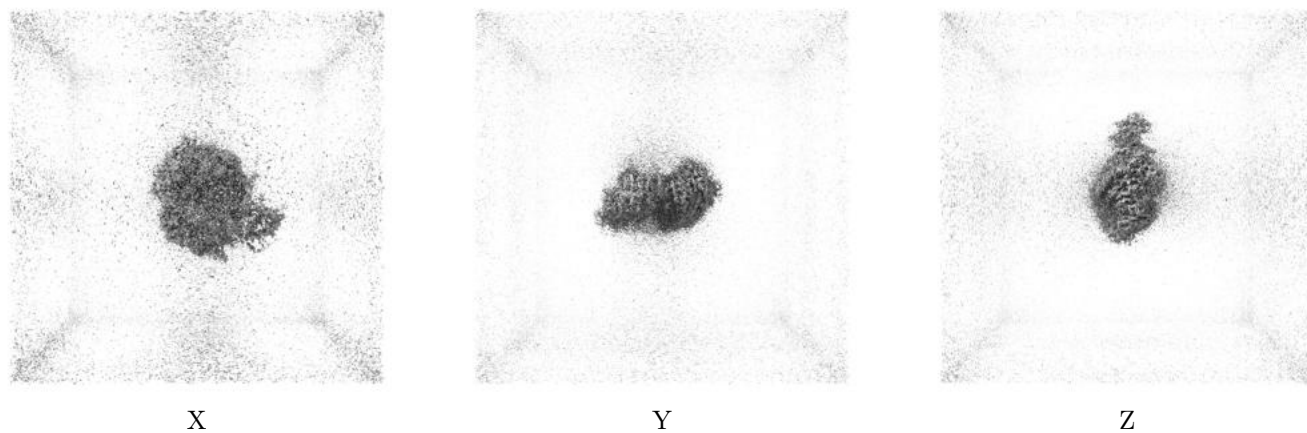
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

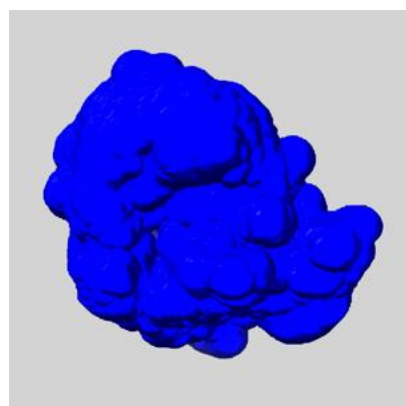
6.6 Mask visualisation [i](#)

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

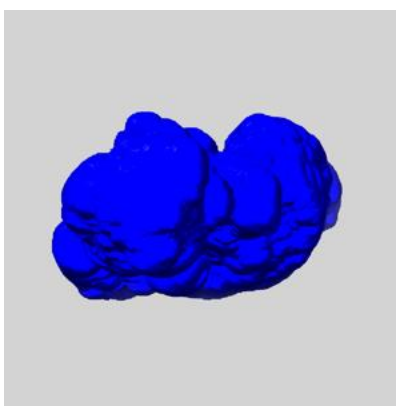
A mask typically either:

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

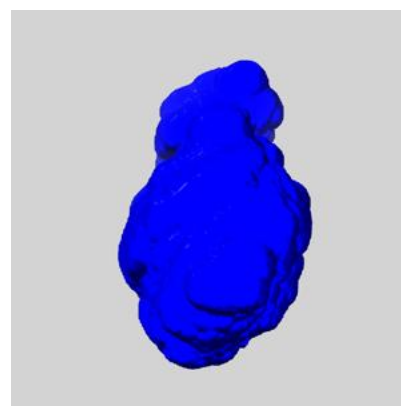
6.6.1 emd_54923_msk_1.map [i](#)



X



Y

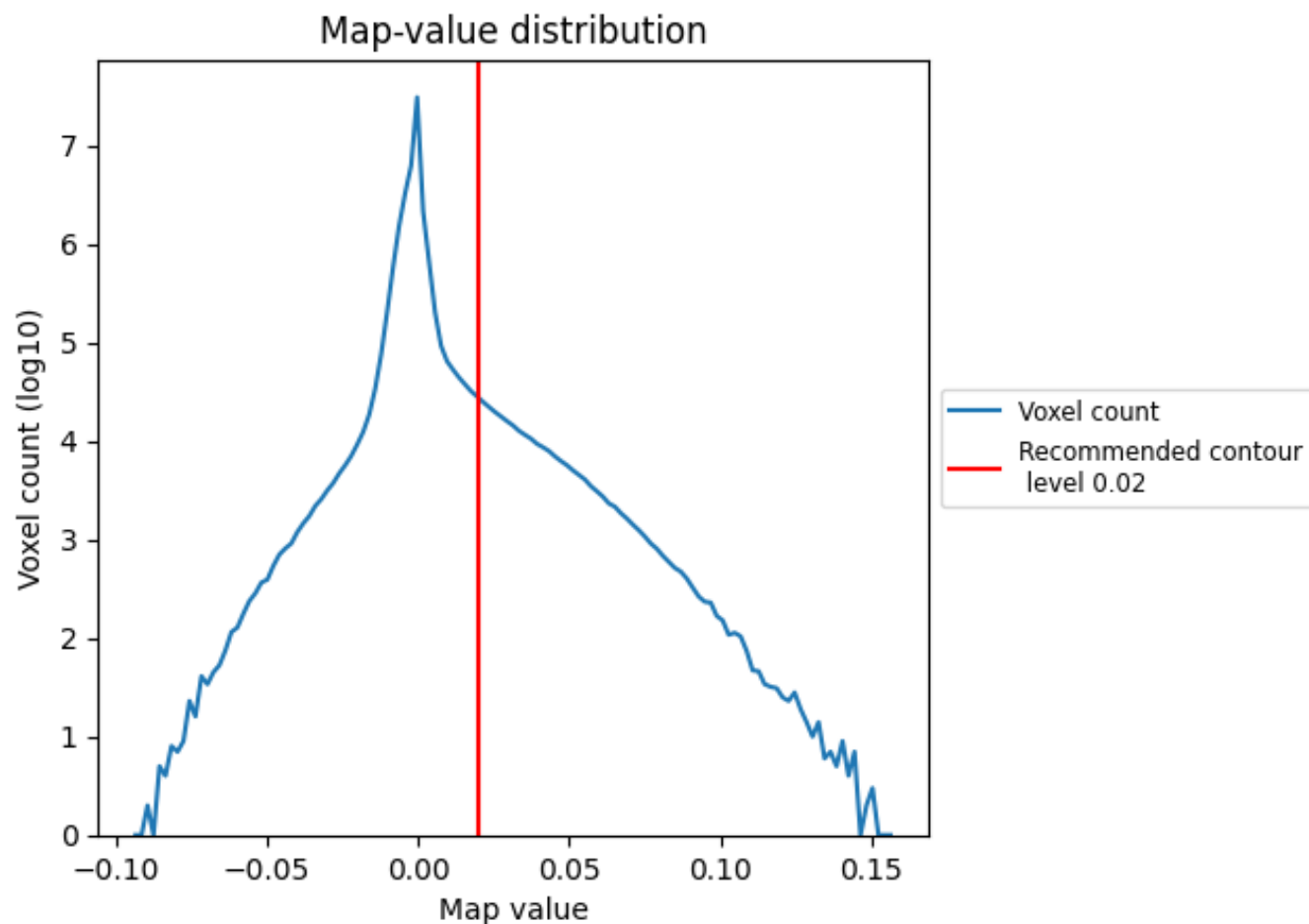


Z

7 Map analysis [i](#)

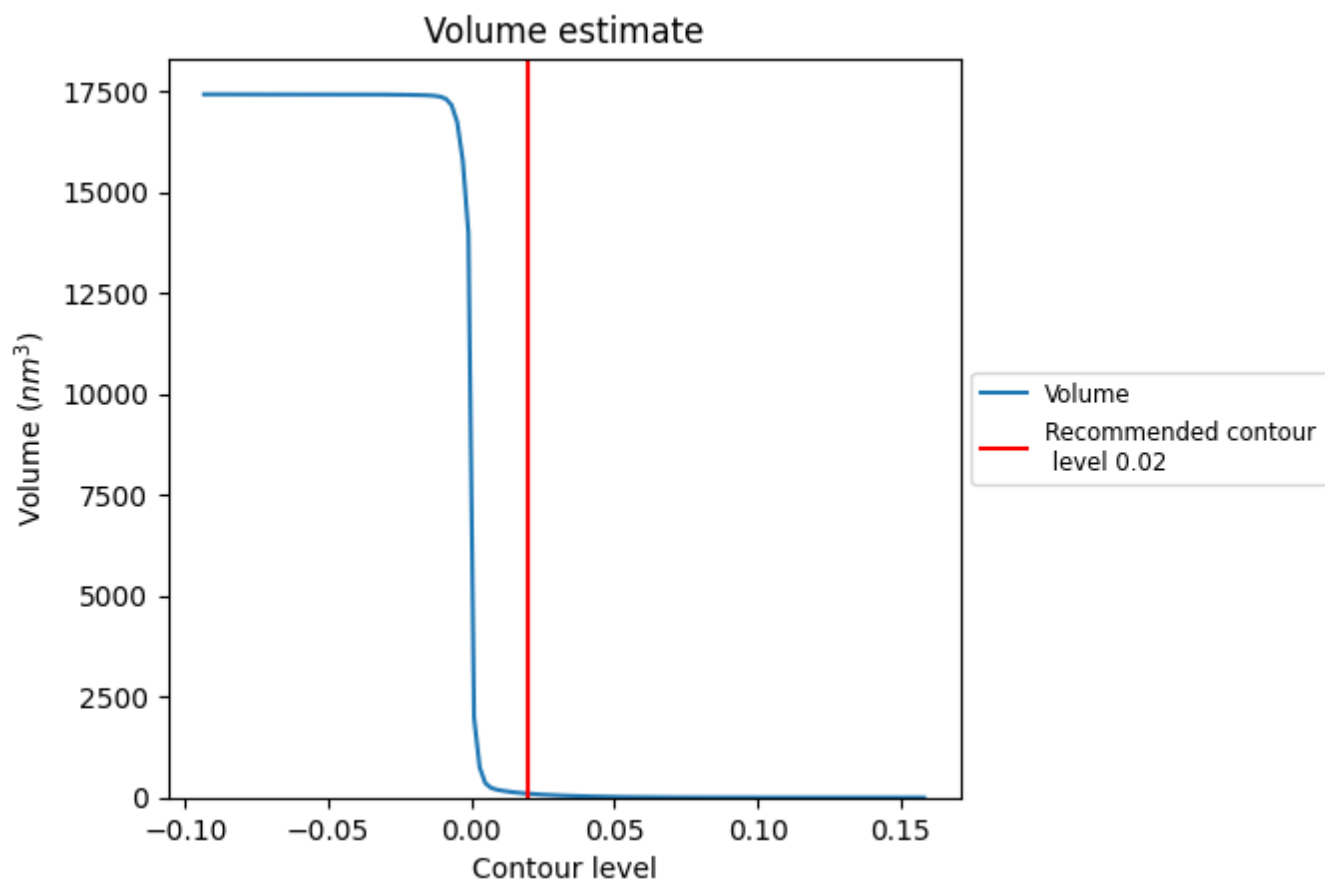
This section contains the results of statistical analysis of the map.

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.

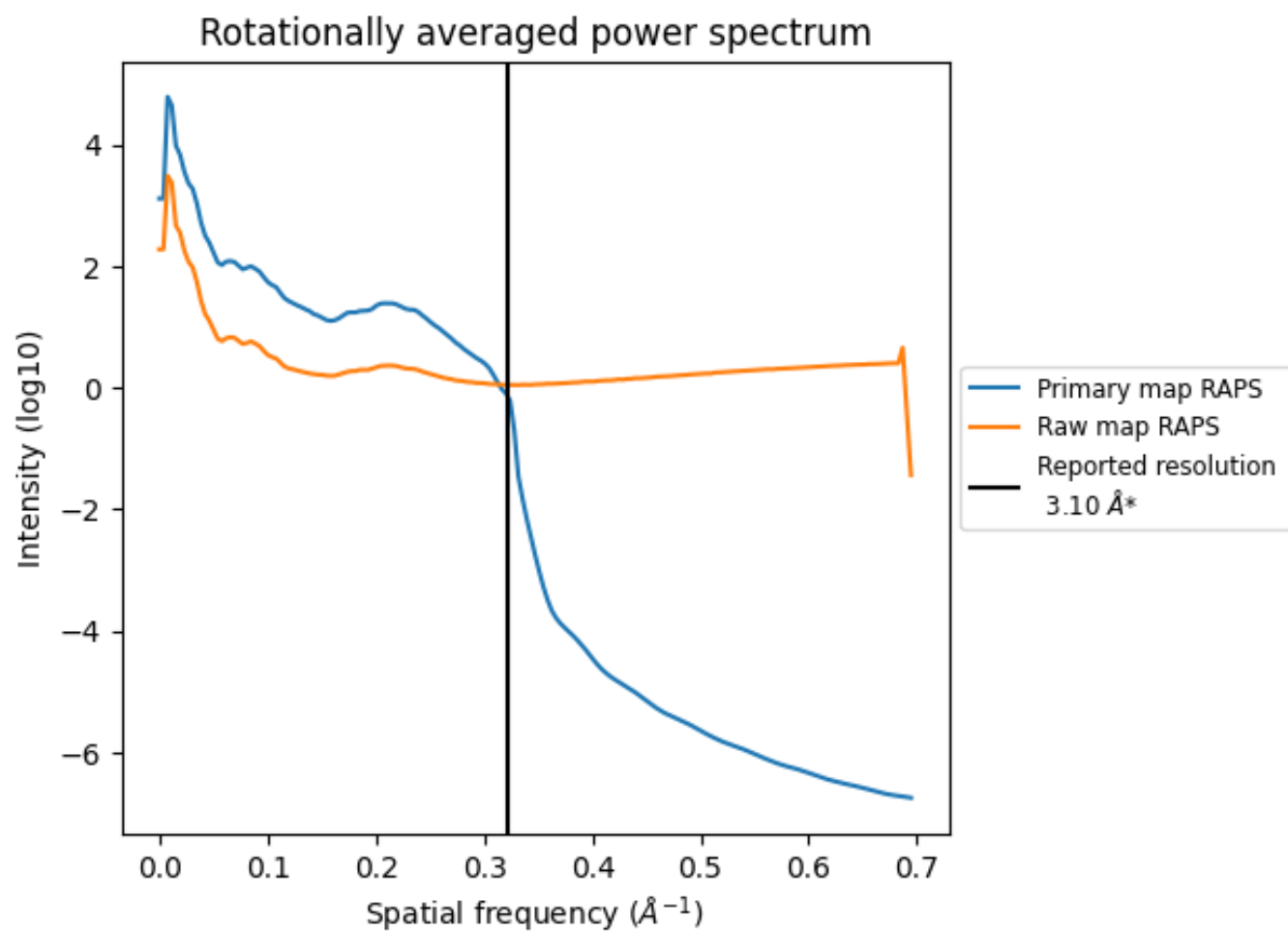
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 96 nm³; this corresponds to an approximate mass of 87 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 ⓘ

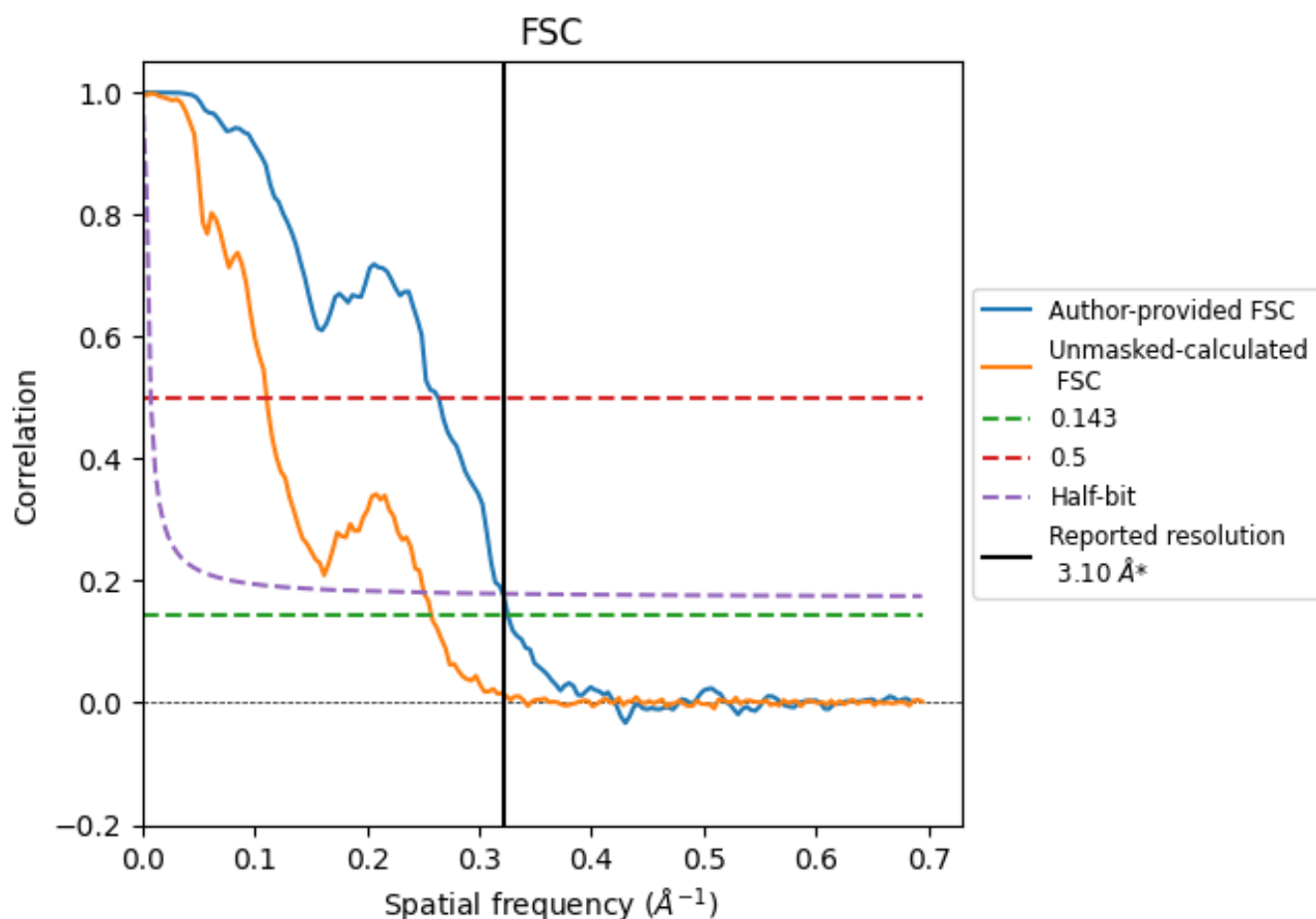


*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

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 $0.323 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

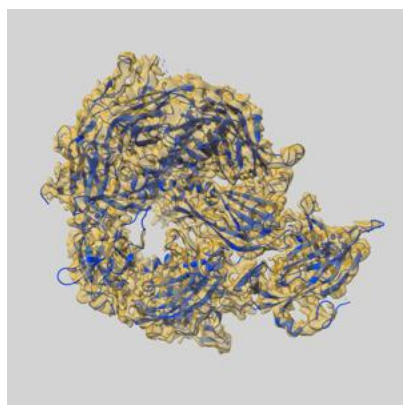
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.07	3.80	3.11
Unmasked-calculated*	3.88	9.03	3.99

*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 3.88 differs from the reported value 3.1 by more than 10 %

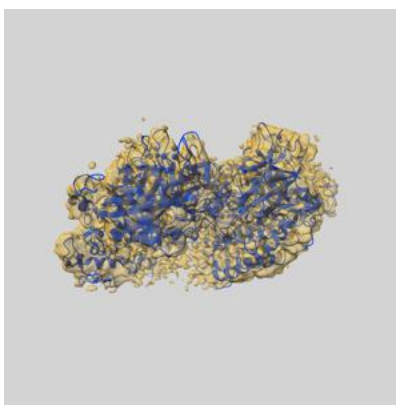
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54923 and PDB model 9SI1. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

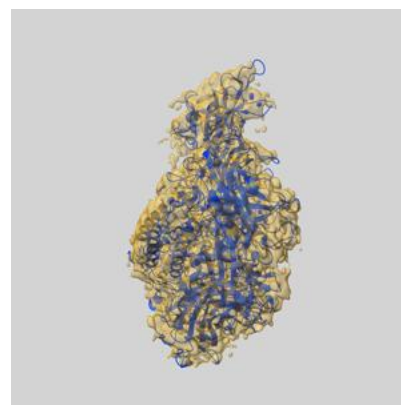
9.1 Map-model overlay [i](#)



X



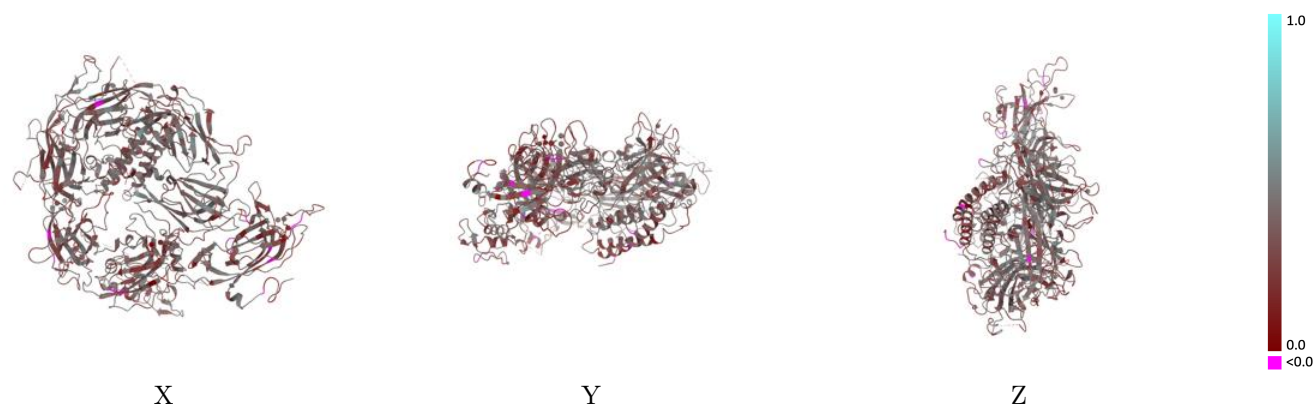
Y



Z

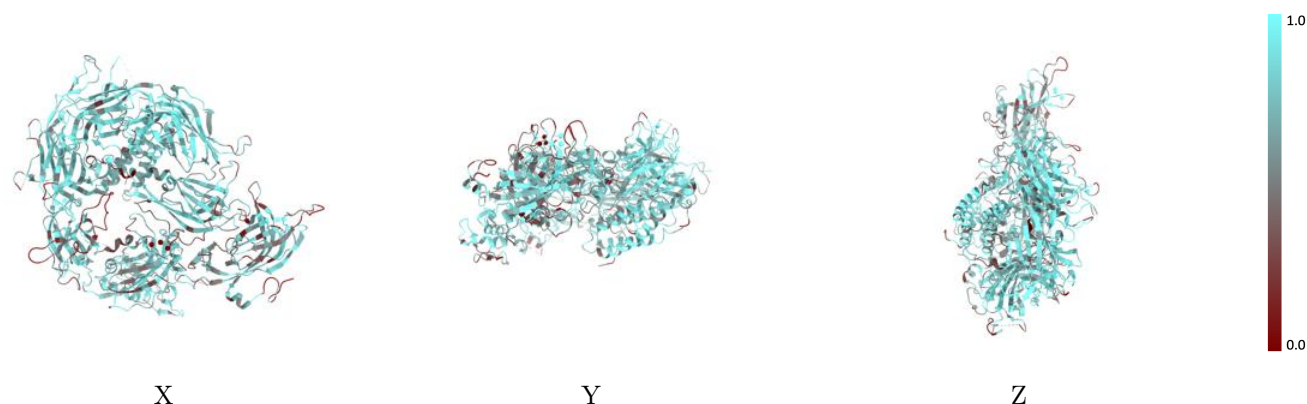
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



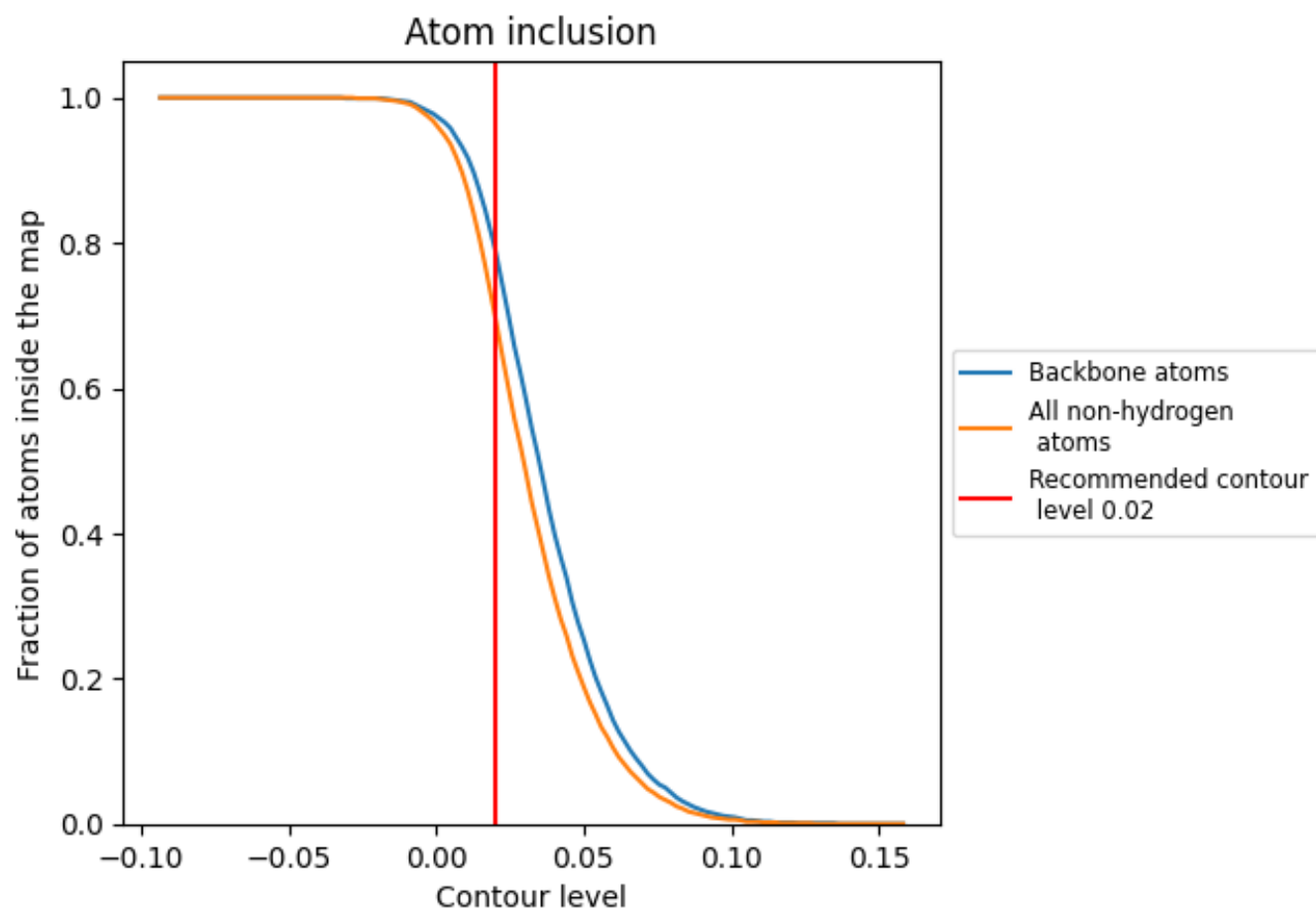
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 70% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6980	0.3450
A	0.6980	0.3450

