



# wwPDB EM Validation Summary Report ⓘ

Feb 22, 2025 – 03:08 PM EST

PDB ID : 9E9R  
EMDB ID : EMD-47801  
Title : The Structure of ApoB100 from Human Low-Density Lipoprotein  
Authors : Berndsen, Z.T.; Cassidy, C.K.  
Deposited on : 2024-11-08  
Resolution : 9.00 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](mailto: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.dev117  
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) : 2.41.4

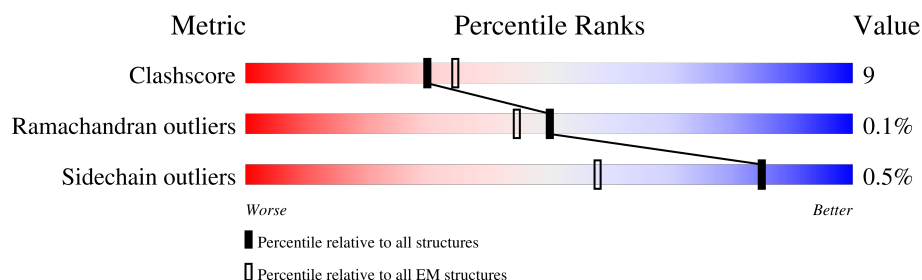
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 9.00 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  $\geq 3$ , 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	4563	<div> <div>21%</div> <div>64%</div> <div>17%</div> <div>19%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 58841 atoms, of which 29424 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.

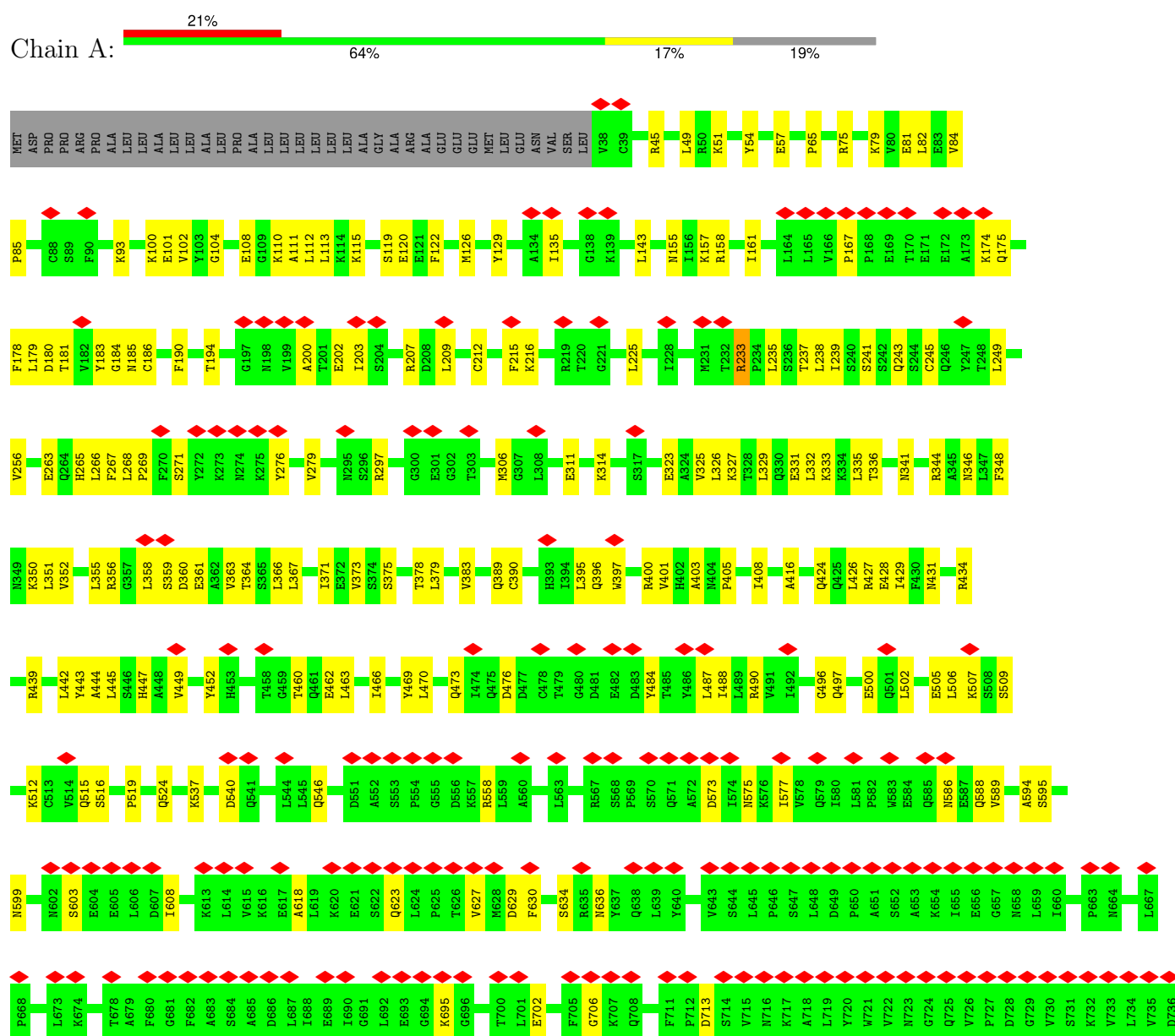
- Molecule 1 is a protein called Apolipoprotein B 100.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	3715	58841	18700	29424	4951	5679	87	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

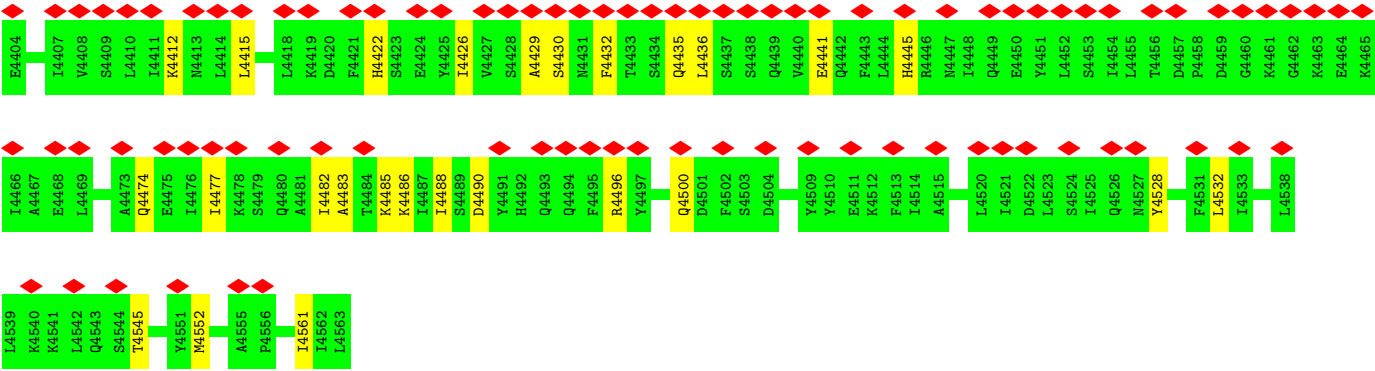
#### • Molecule 1: Apolipoprotein B 100



R2012	L1890	K1778	G1635	M1523	H1390	LEU	V1232	T1114	G997	A895	V816	H737
T2013	F1896	Y1780	I1636	N1524	M1391	LYS	A1233	K1115	R1000	R896	I817	F738
L2014						LEU	M1234	E1116				
A2015						GLU	S1235	E1117			G820	Y740
D2016	V1899	L1786	G1639	M1531	V1396	THR	S1236	P1127	L1003	T903	N823	T741
L2017	M1900	Q1787	A1640	G1534	D1397	VAL	L1237	R1128	E1004	N904	D824	K742
L2018	A1901	Q1789	H1641	R1536	L1399	ARG	L1238	L1129	L1005	P905		
T2019	P1902	Y1644	T1644	D1539	L1400	THR	Q1239	E1136	R1006	F906	F826	D744
L2019	F1903	L1645	L1645	S1543	V1404	ALA	K1240		P1007	H907		
L2020		R1646	R1646			LEU	A1241		T1008	G910	K745	
D2021	G1915	D1807	I1647	S1543	T1411	LEU	A1241	W1141	G1009	L911	Y829	K745
S2022	K9316	L1808	T1657	T1647		PHE	S1242		E1010	L911	H746	
P2023	L1917					LYS	G1243	R1164	I1011	H914	E747	
I2024	A1918	M1811	L1664	L1550	K1415	SER	S1244	V1165	Q1013	E833	Q748	
K2025			L1665		N1416	VAL	L1245	A1166	S1015	K921	D749	
V2026	H1923	L1821	V1666	M1557	L1420	GLY	P1246	E1172	F924	M750	M750	
P2027	T1924	V1822	L1667	T1558	S1421	PHE			I925	E837	V751	
G1925			E1668		C1422	HIS			V1016	L838	M752	
L2028	G1926	N1826	E1674	K1562		LEU	Q1249	E1175	E1021	T840	G753	
L2029	L1927	L1827	L1675	M1665	R1427	PRO	T1250	F1176	R1024	G841		
L2030			L1676			ARG	L1251	E1177				
S2031	G1948	M1833	S1677	S1572	M1434	GLU	D1253	M1183	R1027	G839	L844	
E2032			S1678		H1439	GLN	P1257	V1184				
P2033	V1955	Y1840	K1683	M1585	V1440	VAL	H1254	N1192	T1037	H843	Q847	
I2034	S1956	A1841	T1685	K1586	E1441	PRO	L1255		Q1038	L844		
N2035	I1957	I1942	L1684	M1587		THR	M1256	V1195	A1039	S946	S850	
L2036	K1958		T1686	D1588	G1444	PHE	S1257				S851	
S1959						THR					G852	
I2037	I1960	A1845	N1687	M1595	N1445	ILE	F1261	S1198	A1042	K949		
D2038		A1846	G1688	A1596	N1446	PRO	N1262	D1199	K1043	T950	G857	K763
L2039		L1847	R1689	L1597	P1447	LYS	L1263	Y1200	Q1044	F951	D764	
A2039	L1964	S1848		R1599	V1448	LEU	Q1264	P1201	T1045	V952	K359	L765
L2040			S1698	S1600	D1456		N1265	K1202	N1054	Q861	G861	K766
E2041	V1968	K1852	G1701	E1601			M1266	S1203	M1058	K967	V862	S767
M2042	L1971	A1853	K1702	Y1602	P1463	V1350	G1267	L1204			K863	E769
R2043	L1972	D1854		Q1603	Q1464	P1351	L1268	H1205	I1066	G972		
L2044	T1973		L1705	A1604	K1474	L1352	P1269	M1206		L974	V866	A772
A2045	P1974	G1861	L1710	D1605	K1475	L1353	D1270	Y1207	V1071	Y875	E872	R774
V2046	Q1977	E1863	Q1715	S1608	K1476	L1356	F1271		L1077	Y981		
E2047	T1978	R1867		L1609	Q1477	D1357	H1272	R1210	R1078		K876	L777
K2048	M1981	L1868	V1731	R1610	H1478	L1358	I1273	L1211			V879	E778
P2049		N1869	L1736	F1611	L1479	L1366		L1212	E1082	A984	S880	I779
F2052	F1987	T1870	Y1746	L1614	F1480		L1277	H1214	S1083	S985	V881	L780
		D1871		L1619	V1492	V1369	Y1287	R1215	T1084	S986		
V2055						A1371		V1216	G1085	T987	V884	E783
K2059		G1874	G1761	H1622	R1507		K1291		G1086	D988	T885	L784
Y2060	A1988	L1875	L1762		D1508	S1370	M1292		D1095	S989	N886	F786
N2063	N2000	A1876		E1625	P1509	L1378	S1293	T1219	I1096	S991	M887	
Q2064	T2001	S1877	Y1774	D1629	N1510	S1384		D1220	Y992	G988	I889	D791
D2065	K2002	S1775		L1630	T1511	L1385	I1298	F1223	Q1097	S993		
		S1776	D1777	L1631	G1512	R1386	PRO	R1224	M1098	I890	I891	L794
V2066	T2005	D1777		G1632	E1517	Y1389	LEU	H1225	K1099	L995		
H2067	E2008				R1521		PRO	V1226	K1100	T996	F894	
S2068		S1887			F1522		PHE	G1227	D1113			M801
I2069							GLY					R804
N2070							LYS					
L2071							SER					Q807
P2072							ARG					
F2073							ASP					I813
F2074												
F2075												









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	52843	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)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.148	Depositor
Minimum map value	-0.560	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.182	Depositor
Map size (Å)	490.5, 490.5, 490.5	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	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	0.26	0/29997	0.47	0/40579

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2820	ASN	Peptide

### 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	29417	29424	29417	524	0
All	All	29417	29424	29417	524	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 524 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:500:GLU:OE2	1:A:537:LYS:NZ	1.96	0.98
1:A:325:VAL:HG13	1:A:351:LEU:HD11	1.46	0.95
1:A:323:GLU:OE1	1:A:327:LYS:NZ	2.03	0.92
1:A:3632:ARG:NH1	1:A:3633:TRP:O	2.03	0.92
1:A:3482:SER:OG	1:A:3484:GLU:OE2	1.90	0.89

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	3703/4563 (81%)	3543 (96%)	156 (4%)	4 (0%)	48 83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3828	PRO
1	A	1477	GLN
1	A	3906	ALA
1	A	1804	ASN

### 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	3299/4080 (81%)	3283 (100%)	16 (0%)	86 89

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4071	LYS
1	A	3886	ARG
1	A	2418	LYS
1	A	3638	ARG
1	A	1702	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	255	HIS
1	A	1013	GLN
1	A	1478	HIS
1	A	3051	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](#)

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 ⓘ

There are no chain breaks in this entry.

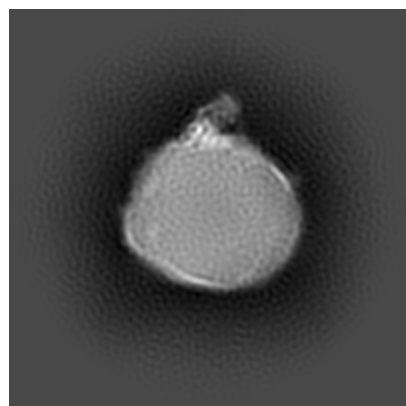
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47801. These allow visual inspection of the internal detail of the map and identification of artifacts.

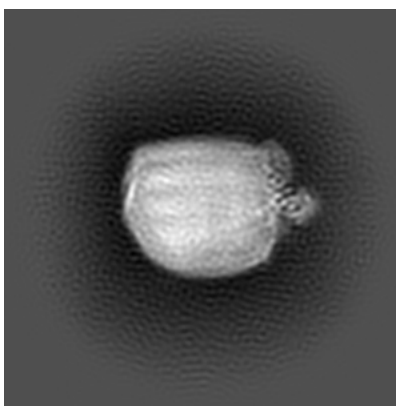
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

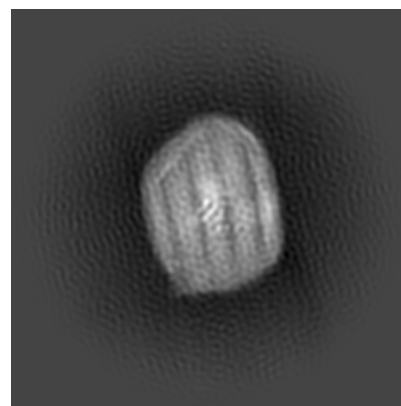
#### 6.1.1 Primary map



X

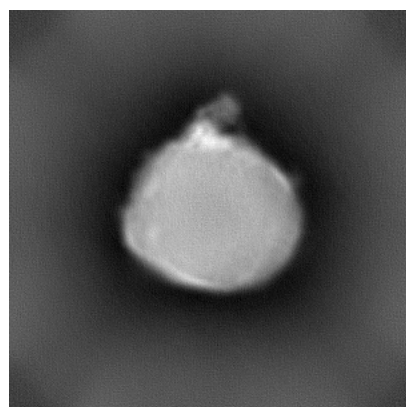


Y

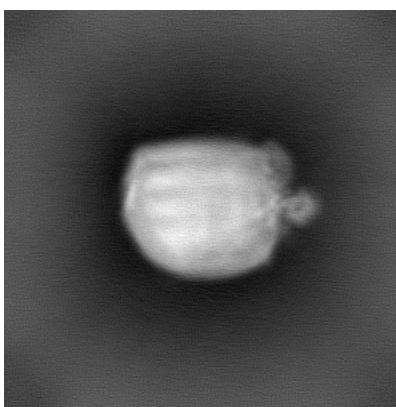


Z

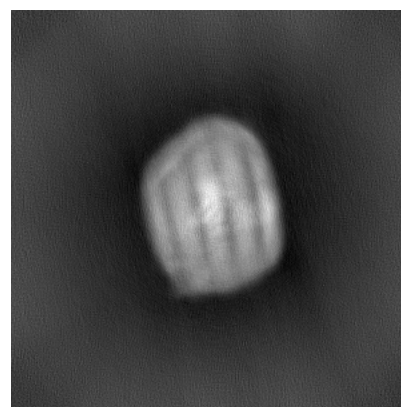
#### 6.1.2 Raw map



X



Y

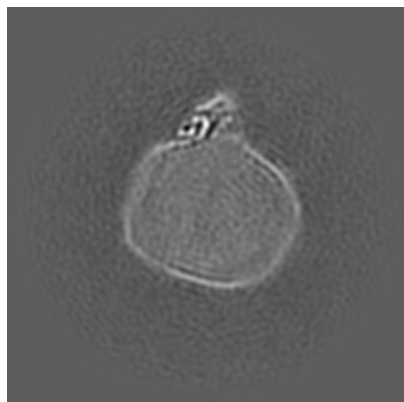


Z

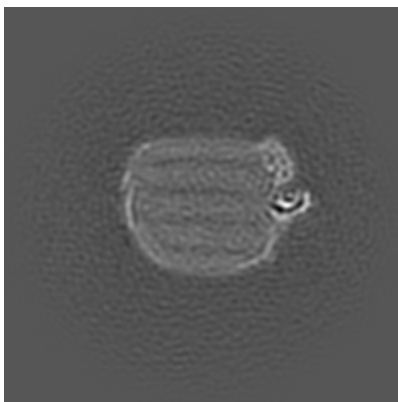
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

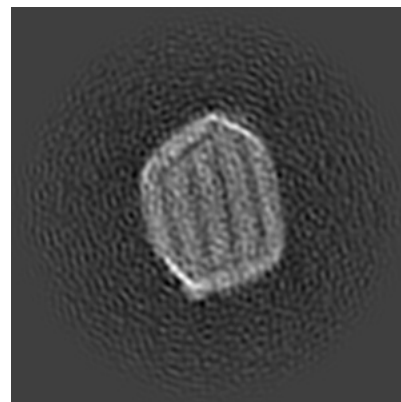
### 6.2.1 Primary map



X Index: 225

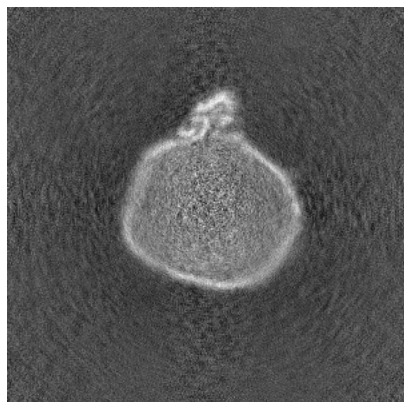


Y Index: 225

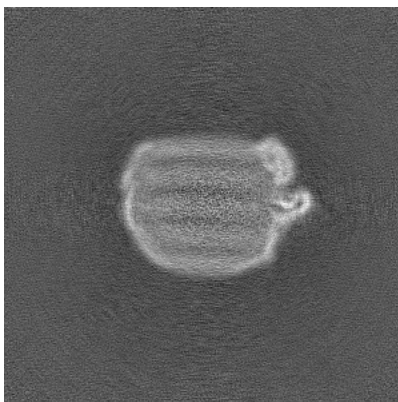


Z Index: 225

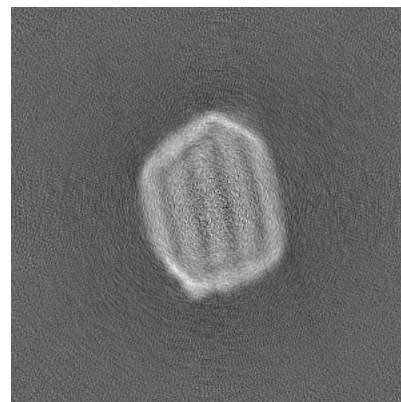
### 6.2.2 Raw map



X Index: 225



Y Index: 225



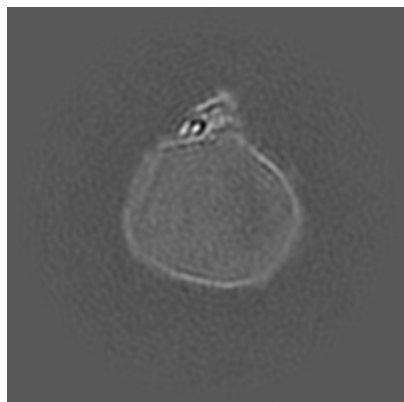
Z Index: 225

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

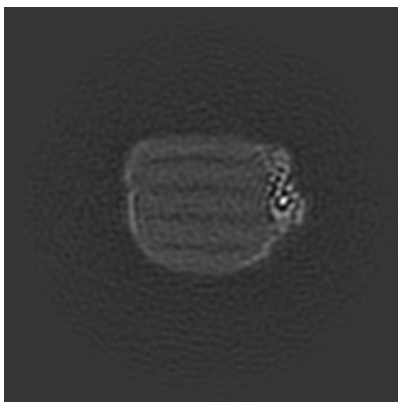


## 6.3 Largest variance slices [i](#)

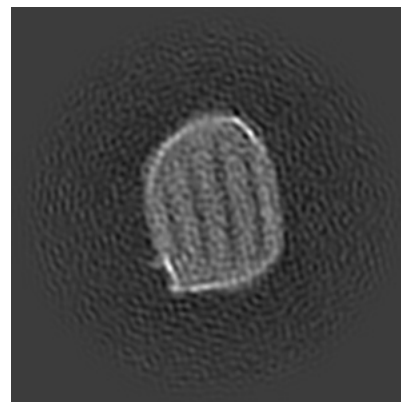
### 6.3.1 Primary map



X Index: 230

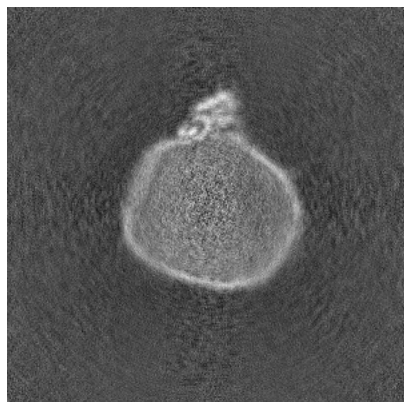


Y Index: 213

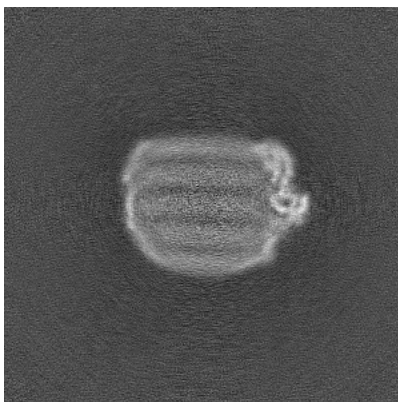


Z Index: 196

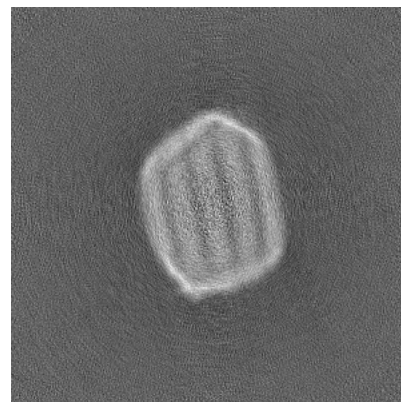
### 6.3.2 Raw map



X Index: 227



Y Index: 219



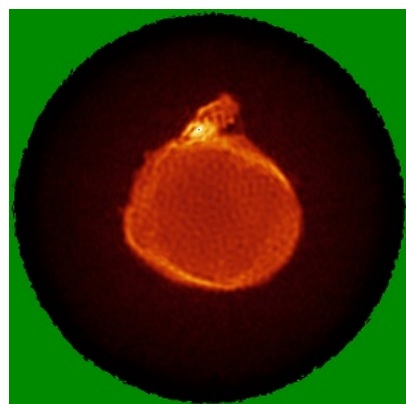
Z Index: 219

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

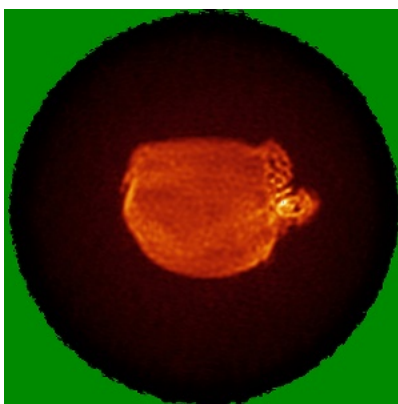


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

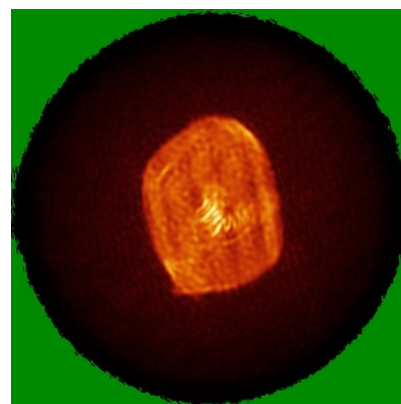
### 6.4.1 Primary map



X

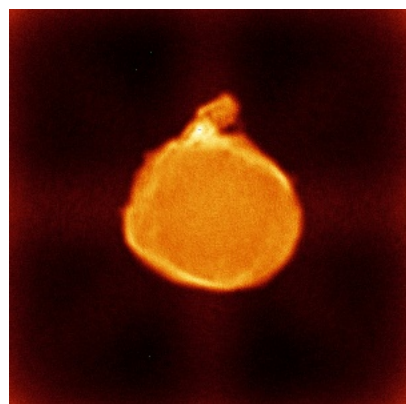


Y

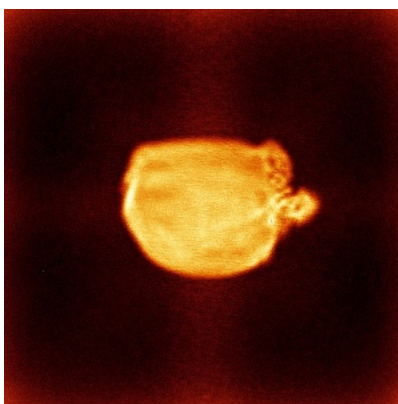


Z

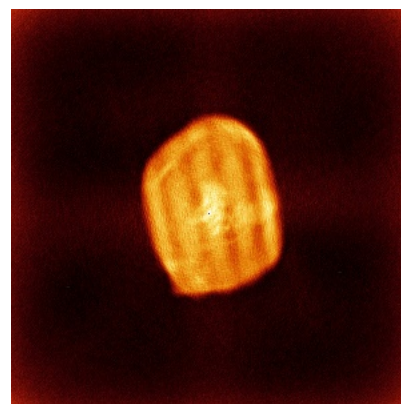
### 6.4.2 Raw map



X



Y

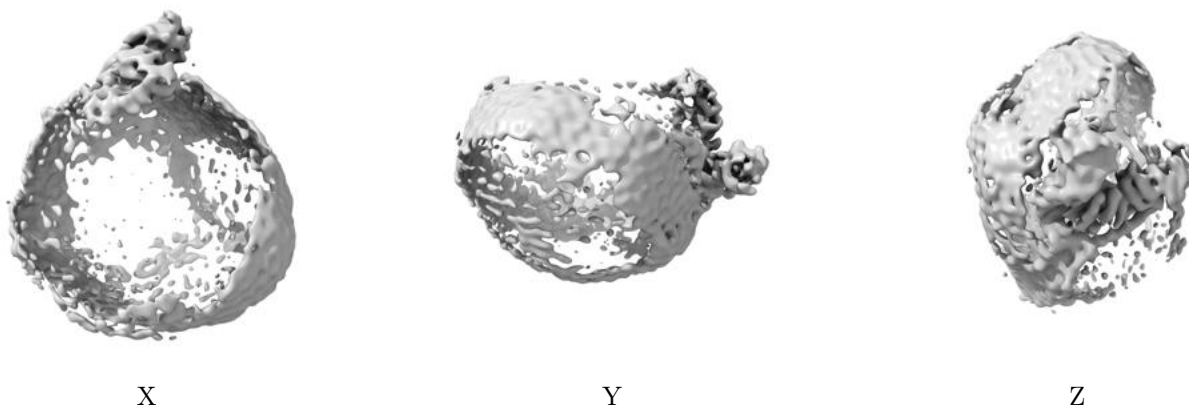


Z

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.

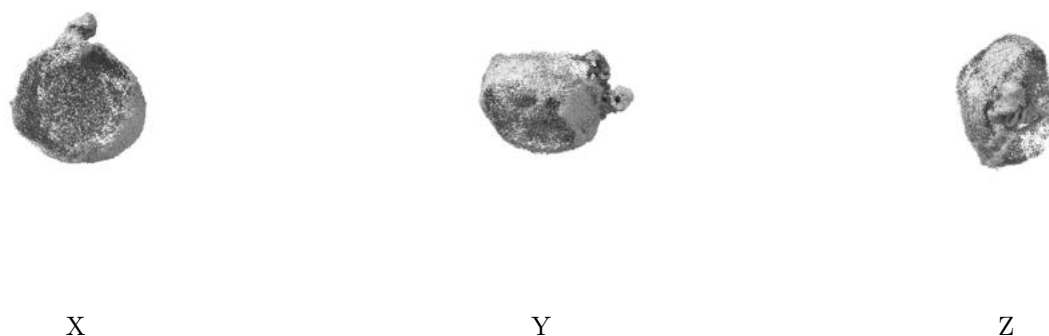
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.182. 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.

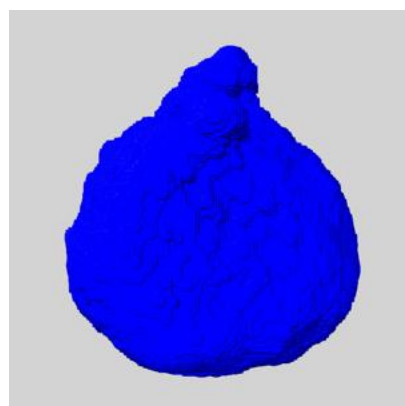
## 6.6 Mask visualisation [i](#)

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

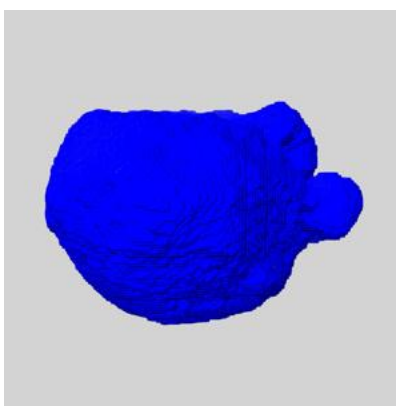
A mask typically either:

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

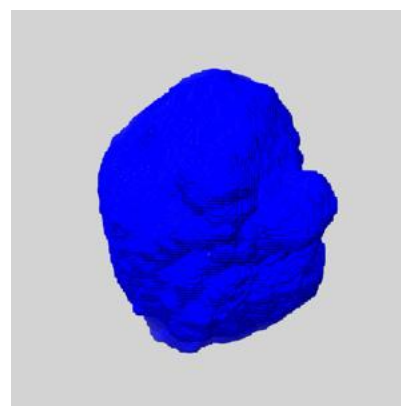
### 6.6.1 emd\_47801\_msk\_1.map [i](#)



X



Y

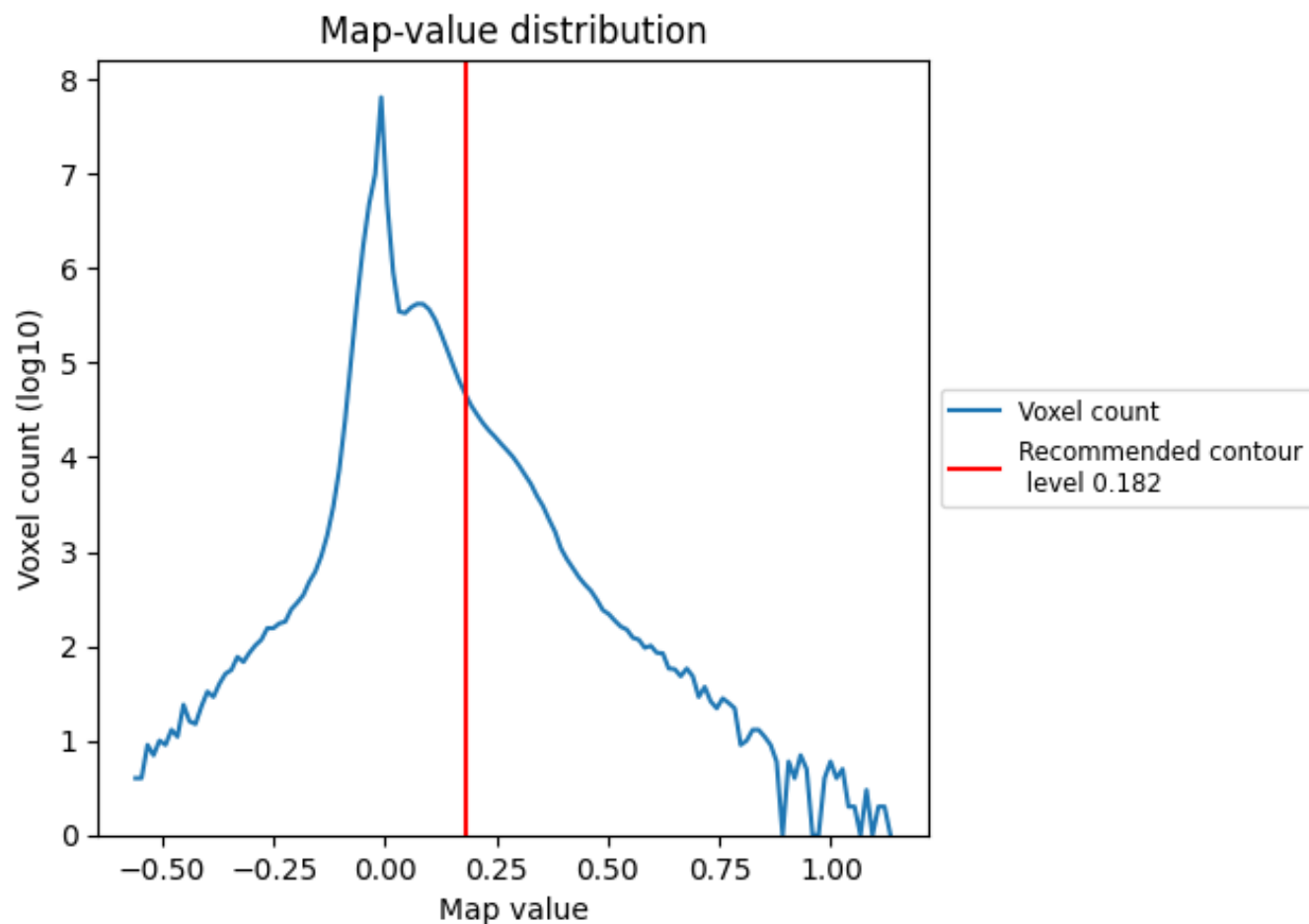


Z

## 7 Map analysis [i](#)

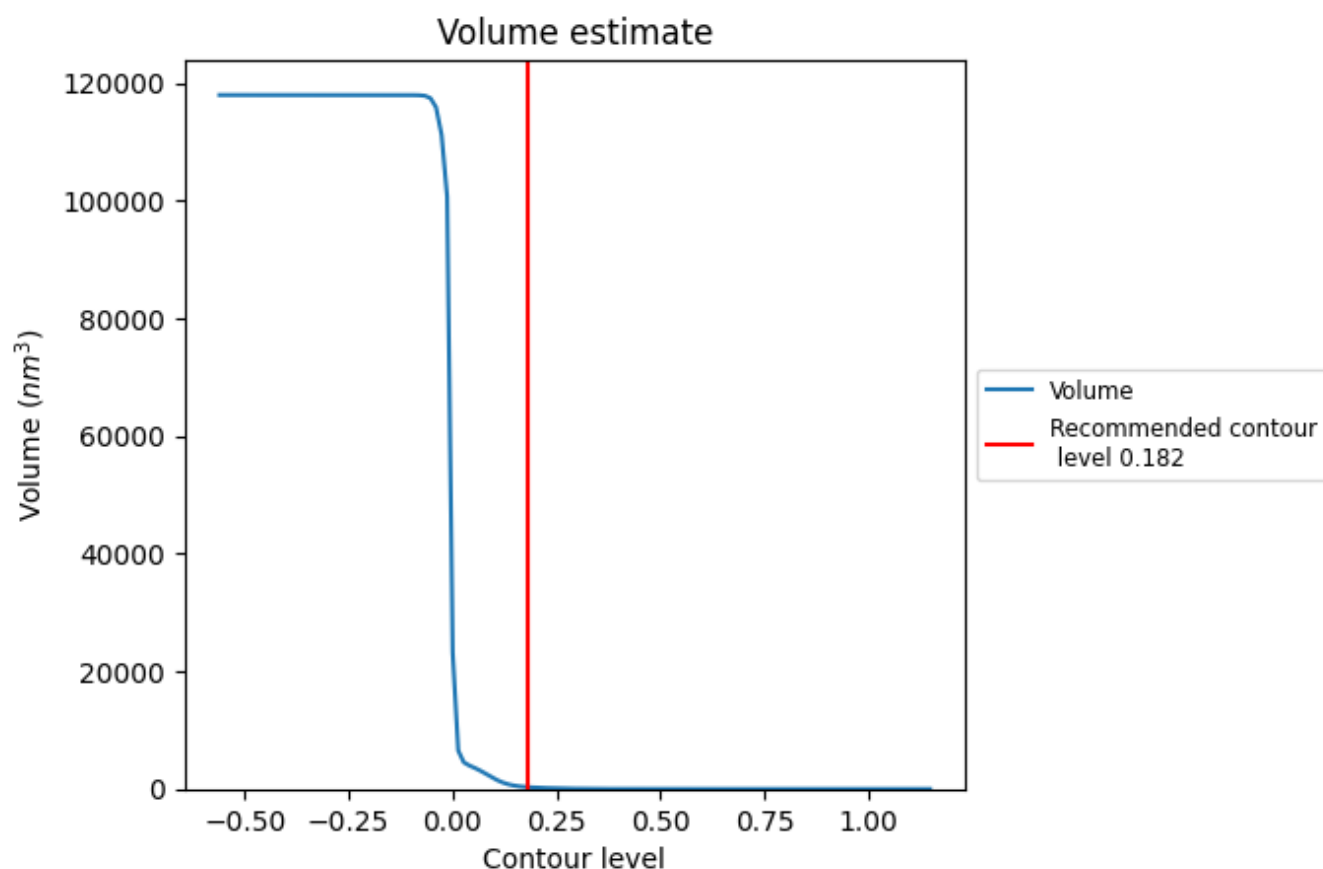
This section contains the results of statistical analysis of the map.

### 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.

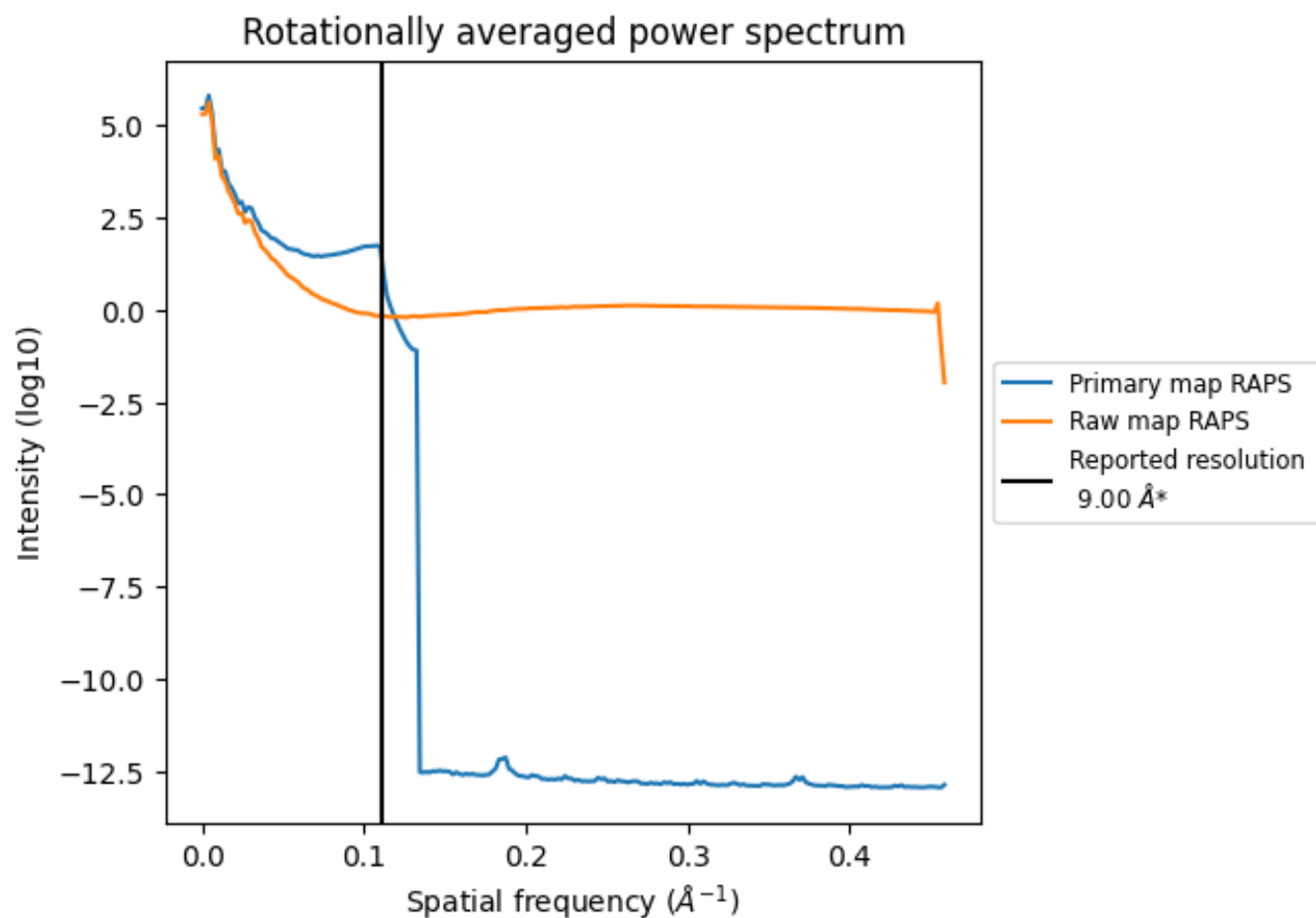
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 304 nm<sup>3</sup>; this corresponds to an approximate mass of 275 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 ⓘ

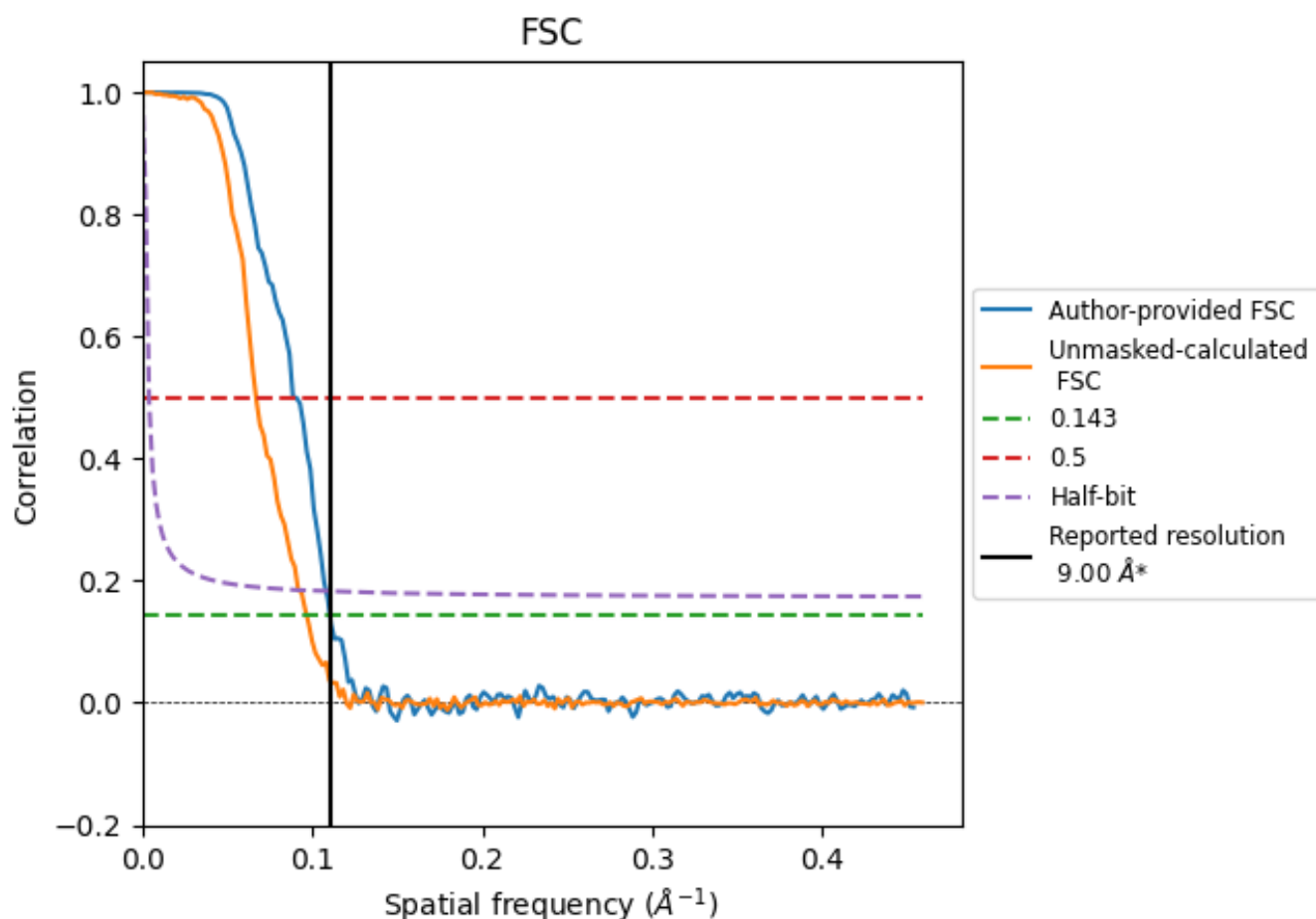


\*Reported resolution corresponds to spatial frequency of 0.111 Å<sup>-1</sup>

## 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 0.111  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.00	-	-
Author-provided FSC curve	9.06	11.27	9.24
Unmasked-calculated*	10.34	14.93	10.85

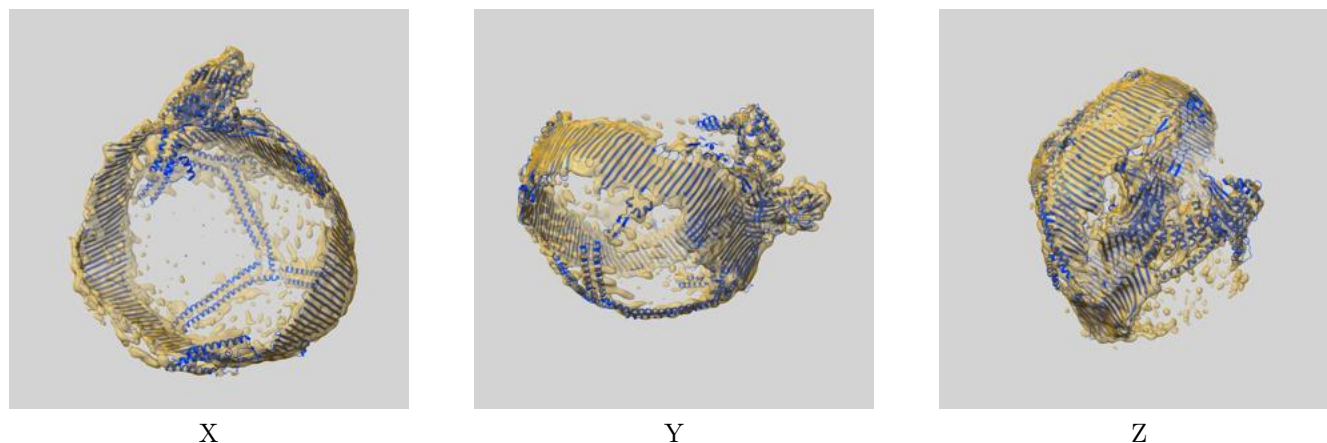
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 10.34 differs from the reported value 9.0 by more than 10 %



## 9 Map-model fit [i](#)

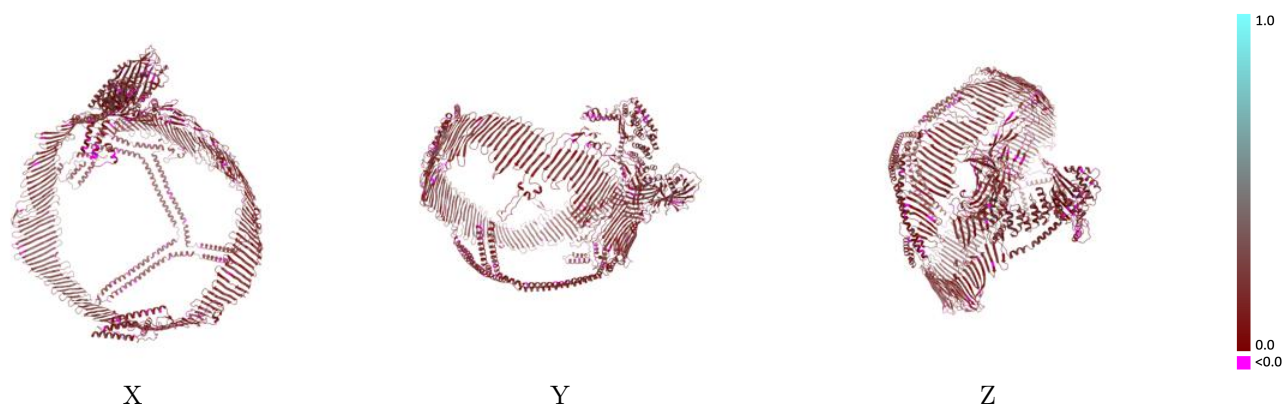
This section contains information regarding the fit between EMDB map EMD-47801 and PDB model 9E9R. Per-residue inclusion information can be found in section [3](#) on page [4](#).

### 9.1 Map-model overlay [i](#)



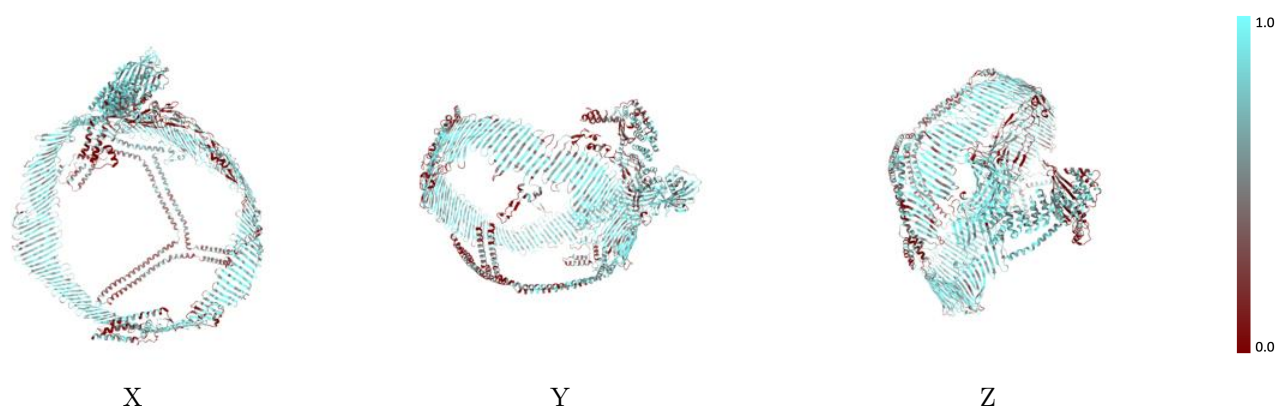
The images above show the 3D surface view of the map at the recommended contour level 0.182 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



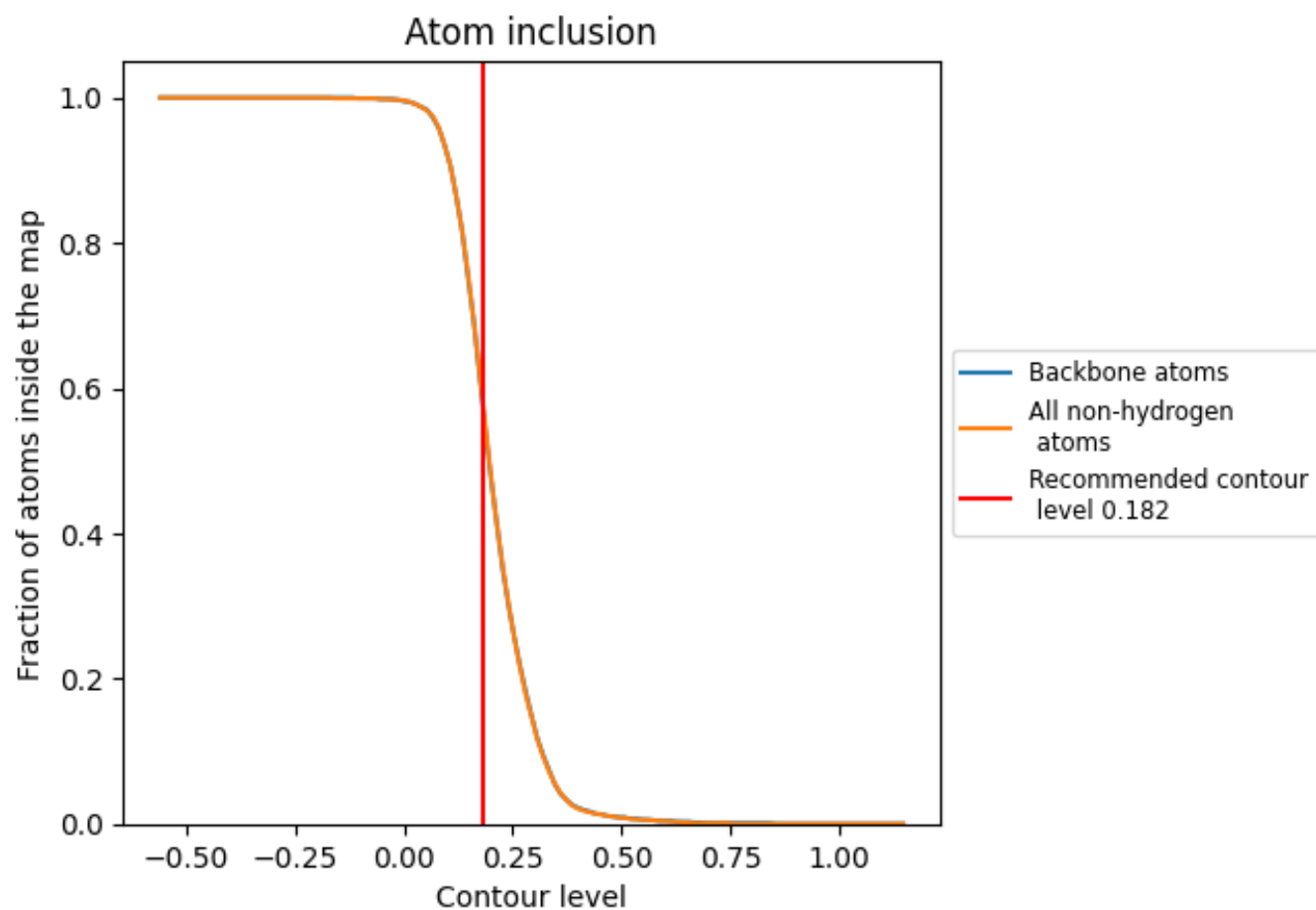
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.182).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 57% of all backbone atoms, 58% 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 (0.182) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5760	<div></div> 0.1710
A	<div></div> 0.5800	<div></div> 0.1710

