



wwPDB EM Validation Summary Report ⓘ

Mar 28, 2026 – 04:29 PM UTC

PDB ID : 8V0G / pdb_00008v0g
EMDB ID : EMD-42854
Title : plasmodium falciparum Niemann-Pick type C1-related protein form I
Authors : Zhang, Z.; Lyu, M.
Deposited on : 2023-11-17
Resolution : 3.11 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

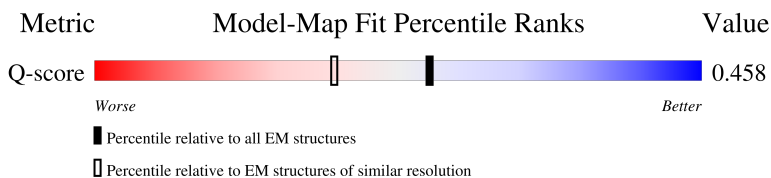
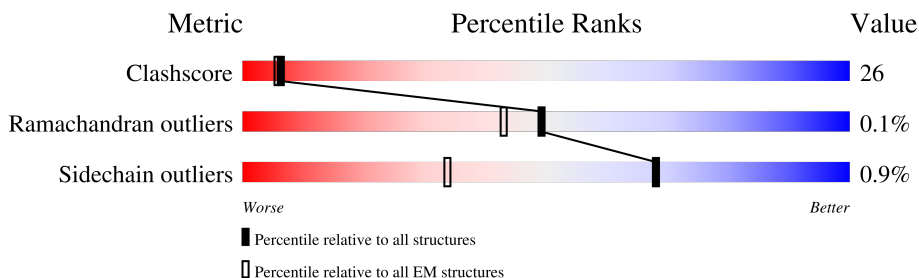
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.11 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	14465 (2.61 - 3.61)

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	1470	

2 Entry composition [i](#)

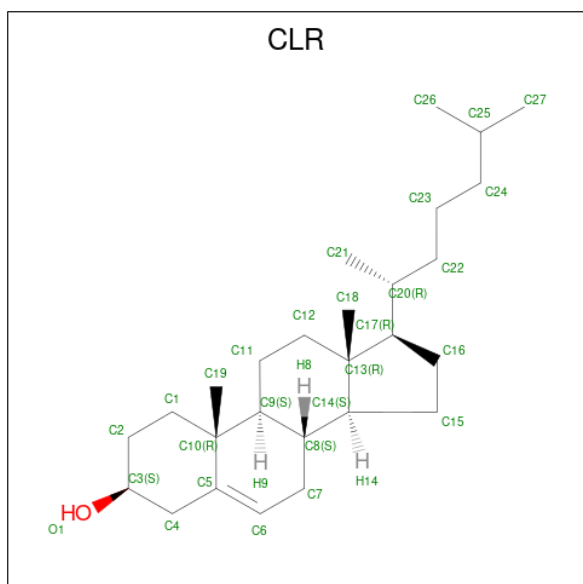
There are 3 unique types of molecules in this entry. The entry contains 8106 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Niemann-Pick type C1-related protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	985	8050	5285	1266	1454	45	0	0

- Molecule 2 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
2	A	1	28	27	1	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	

I1452	M1367	K1284	S1200	D1128	PHE	ASP	SER	ASN	ASP
T1453	I1368	Q1285	Q1201	F1129	THR	ILE	SER	ASP	ASP
	I1369	E1286	E1202		K1046	ILE	TYR	LYS	ASN
S1456	S1370		F1203	F1132	Y1047	ASN	ASN	LYS	LYS
M1457	M1371	L1289	V1204		I1048	SER	ASP	ASP	LYS
F1458	V1372	H1292	T1205	V1135	Y1049	ASN	LEU	GLY	LYS
L1459	I1373	H1293	S1206		E1050	ASN	GLN	ALA	ASP
P1460		V1207		F1138	E1051	LYS	SER	ILE	ASP
	L1376			D1139	P1052	ASN	SER	ILE	ILE
F1466		V1294	G1210	K1140	K1053	ASN	SER	ILE	ILE
G1467	G1379	Q1295	F1211	H1141	K1054	ILE	SER	ASN	GLY
P1468	M1296	M1296	F1212	F1142		LEU	LEU	ASN	LYS
L1469		F1213	F1212	I1143	N1055	LEU	PRO	ARG	LYS
H1470	I1382	L1301	F1214		I1056	SER	ASN	PRO	GLN
	D1383			Y1146	G1057	SER	PRO	SER	LYS
	H1384	I1304		R1147	K1058	ASN	SER	SER	LYS
	T1385	F1305	N1218	L1148	Y1059	GLU	SER	ASP	ASN
				G1149	F1060	ILE	ASN	GLU	ASN
V1389	V1390	T1308	L1222	E1150	R1061	ASN	GLU	GLU	ASN
Q1390	D1309	D1309		K1151	S1062	ASN	VAL	TYR	ASN
A1391			N1226	ASN	L1063	ASN	LEU	LYS	VAL
F1392		I1312	P1227	THR	V1064	SER	ASN	GLU	THR
S1393		I1313	Q1228	LYS		ASN	LYS	GLU	THR
H1394		E1314	E1229	GLU	Y1067	ASN	THR	LYS	VAL
S1395		V1315	F1230	ALA	Y1068	ASN	THR	LYS	VAL
M1396		T1316	Y1231	ALA	V1069	ASN	MET	LYS	SER
G1397		L1317	E1232	ALA	P1070	LYS	VAL	ASN	LYS
R1398		I1318	I1233	SER	F1071	PHE	TYR	LYS	GLY
T1399			F1234	PHE	L1072	ASN	GLU	ILE	GLY
R1400		I1322		LEU	F1076	ASN	THR	ILE	ASN
D1401		T1323	K1240	TYR	G1077	ASN	ASP	LEU	GLU
E1402		I1324	D1241	SER	K1078	GLU	GLU	ASN	LEU
K1403			F1242	LEU	I1079	ASP	LYS	VAL	VAL
M1404		I1327		THR	I1080	ALA	ASP	PHE	TYR
K1405			L1246	ASP		THR	LYS	ASN	TYR
		T1331	F1247	ARG	I1083	THR	LYS	ASP	GLY
L1410		A1332	K1248		M1084	LYS	LYS	ILE	ASN
M1411		Y1333	N1249	G1169	F1086	THR	GLU	THR	LEU
I1412		I1334		I1170	I1087	THR	ILE	ILE	ASP
G1413		I1335	L1254	M1171	I1088	GLN	LYS	ILE	ASP
P1414		K1336	G1256	N1172	I1089	GLN	SER	LYS	GLU
				S1173		PHE	SER	PRO	LYS
H1417		Y1339	W1261	P1174		ILE	LYS	ASN	THR
S1418		S1340		K1175	Y1094	ASN	LYS	GLU	THR
G1419		G1341		I1176		GLY	ASN	ASN	ASP
		V1342	Y1265	M1177	L1098	HIS	VAL	ILE	LYS
W1423		I1343	F1266	K1178		ASP	LYS	LEU	TYR
		I1344	Q1267		K1104	LYS	ASP	LEU	LEU
I1426						ASN	ILE	ASP	MET
S1427		I1347	V1270	M1184	K1107	ILE	LYS	ARG	ASN
			D1271	T1185		TYR	LYS	GLY	ASN
F1430		L1350	D1272	N1186		ASP	LYS	VAL	ILE
		I1351		L1187	D1112	LEU	SER	ASP	LYS
D1435		D1352	I1275	Q1188	S1113	LEU	VAL	VAL	LYS
			S1276	E1189		SER	MET	ILE	SER
V1438			S1277		R1116	SER	ILE	LYS	SER
		I1355	K1278	I1192		HIS	LYS	LYS	LYS
F1441		F1356	S1279	M1193	T1120	ASP	SER	SER	LEU
Q1442		M1359	L1280	M1194	F1126	GLY	TYR	GLY	LYS
			K1281	H1195	P1127	ALA	THR	TYR	ASP
		M1366				LEU	TYR	ASP	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	63097	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35.86	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.867	Depositor
Minimum map value	-0.535	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	321.00003, 321.00003, 321.00003	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.48	0/8239	0.68	1/11120 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	GLU	N-CA-C	-5.17	105.77	111.71

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	8050	0	8078	417	0
2	A	28	0	46	7	0
3	A	28	0	26	1	0
All	All	8106	0	8150	418	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 26.

The worst 5 of 418 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:530:MET:HB3	1:A:646:PHE:HE1	1.22	1.05
1:A:1400:ARG:HD3	1:A:1467:GLY:H	1.34	0.92
1:A:1177:ASN:HD21	1:A:1295:GLN:H	1.15	0.91
1:A:80:THR:HA	1:A:1147:ARG:HH21	1.36	0.91
1:A:517:THR:HG22	1:A:523:SER:HB3	1.57	0.85

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	975/1470 (66%)	931 (96%)	43 (4%)	1 (0%)	48 77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	307	GLN

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	905/1371 (66%)	897 (99%)	8 (1%)	70 78

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1466	PHE
1	A	1342	VAL
1	A	733	PHE
1	A	450	VAL
1	A	1254	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1269	ASN
1	A	1442	GLN
1	A	1293	ASN
1	A	514	ASN
1	A	1267	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](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	1502	1	14,14,15	0.30	0	17,19,21	0.63	0
2	CLR	A	1501	-	31,31,31	0.88	2 (6%)	48,48,48	1.36	8 (16%)
3	NAG	A	1503	1	14,14,15	0.33	0	17,19,21	1.47	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1502	1	-	2/6/23/26	0/1/1/1
2	CLR	A	1501	-	-	0/10/68/68	0/4/4/4
3	NAG	A	1503	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1501	CLR	C13-C14	-2.17	1.51	1.55
2	A	1501	CLR	C10-C9	-2.14	1.52	1.56

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1503	NAG	C1-O5-C5	4.95	118.82	112.19
2	A	1501	CLR	C13-C14-C8	-3.16	109.92	114.41
2	A	1501	CLR	C11-C12-C13	-2.89	107.87	112.74
2	A	1501	CLR	C8-C7-C6	-2.86	108.79	112.76
2	A	1501	CLR	C17-C13-C14	2.85	103.37	100.10

There are no chirality outliers.

All (4) torsion outliers are listed below:

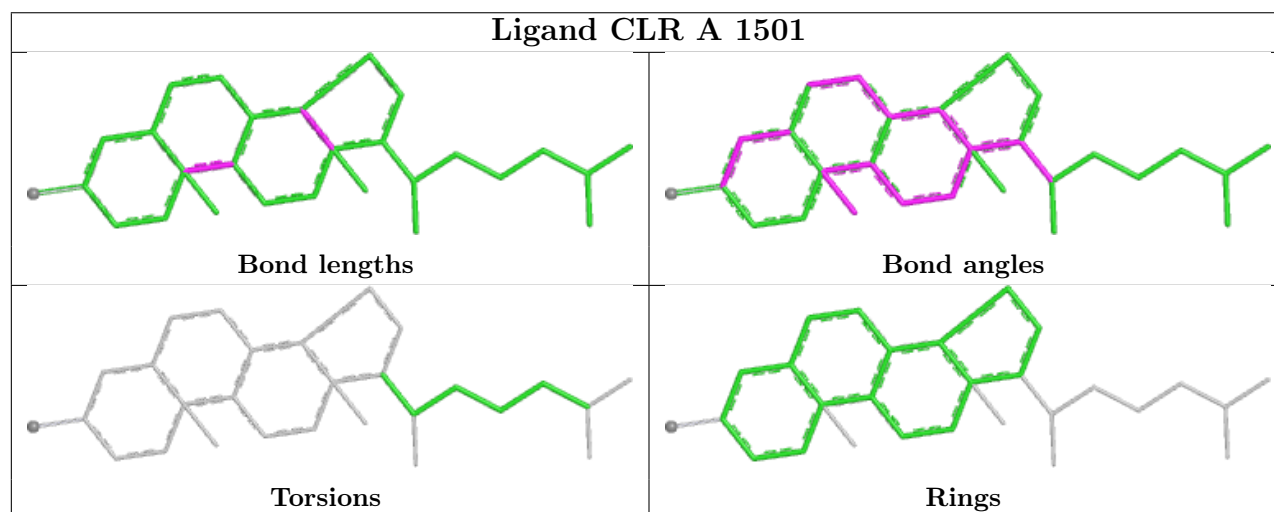
Mol	Chain	Res	Type	Atoms
3	A	1502	NAG	C8-C7-N2-C2
3	A	1502	NAG	O7-C7-N2-C2
3	A	1503	NAG	C8-C7-N2-C2
3	A	1503	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1502	NAG	1	0
2	A	1501	CLR	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

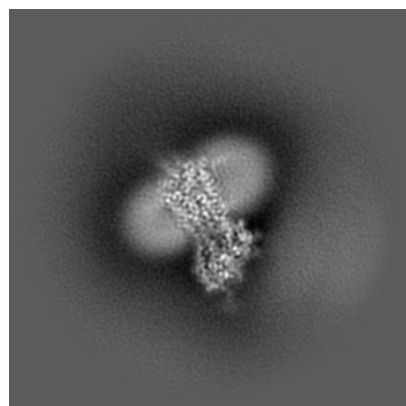
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42854. These allow visual inspection of the internal detail of the map and identification of artifacts.

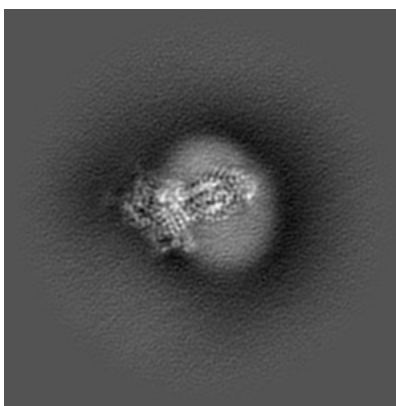
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

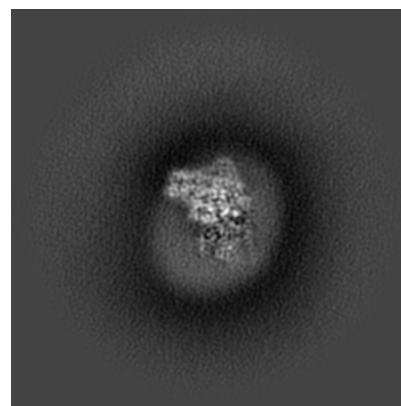
6.1.1 Primary map



X

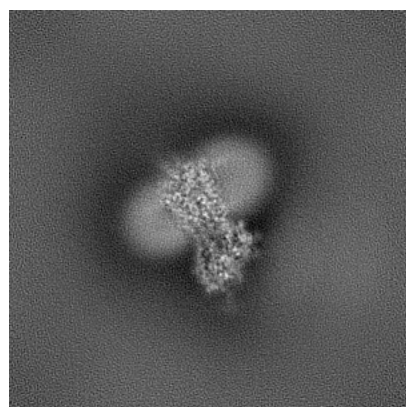


Y

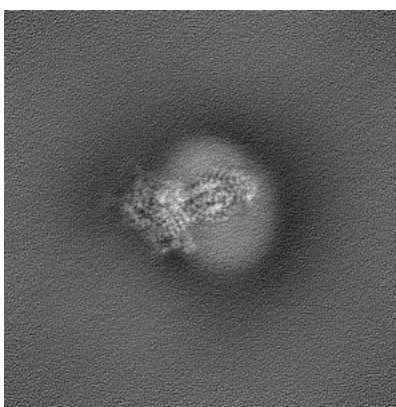


Z

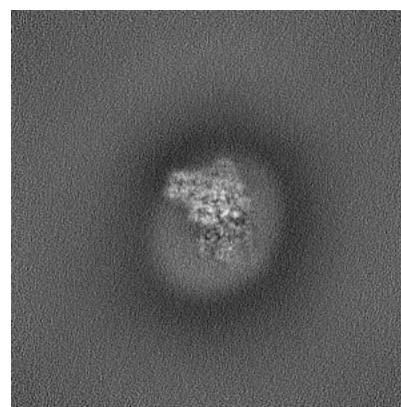
6.1.2 Raw map



X



Y

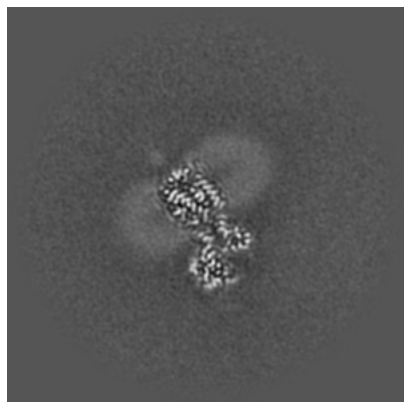


Z

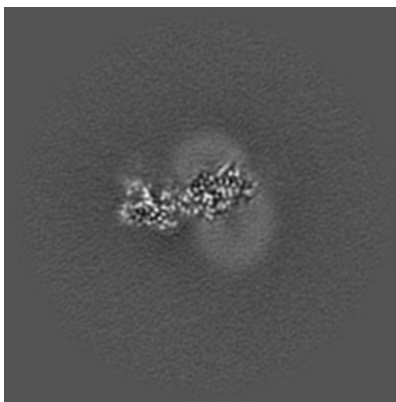
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

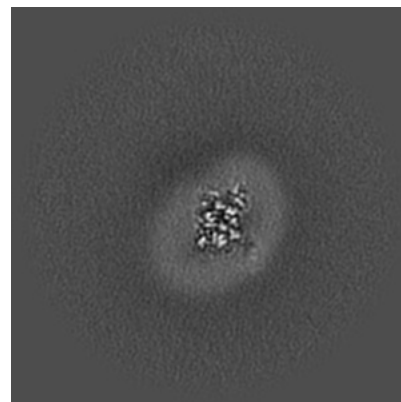
6.2.1 Primary map



X Index: 150

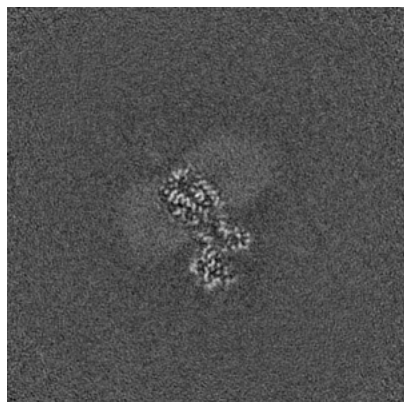


Y Index: 150

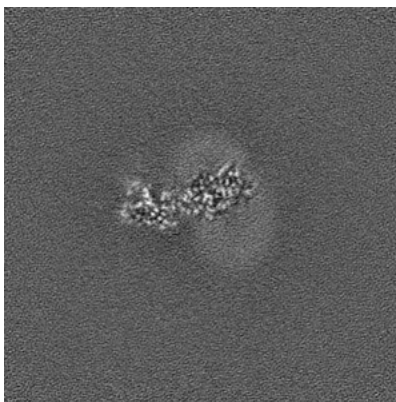


Z Index: 150

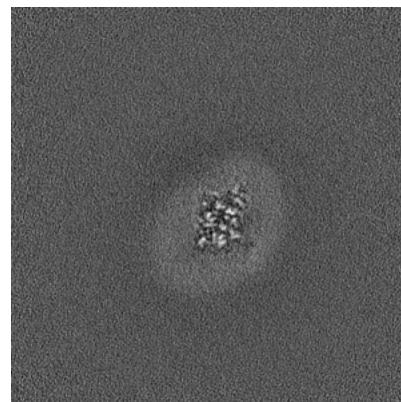
6.2.2 Raw map



X Index: 150



Y Index: 150

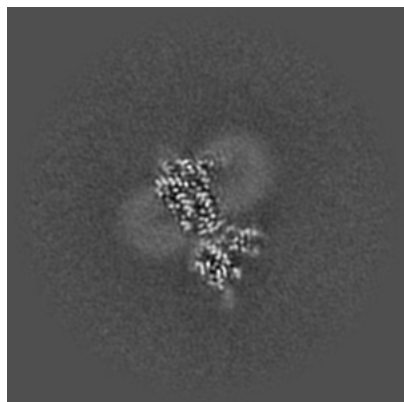


Z Index: 150

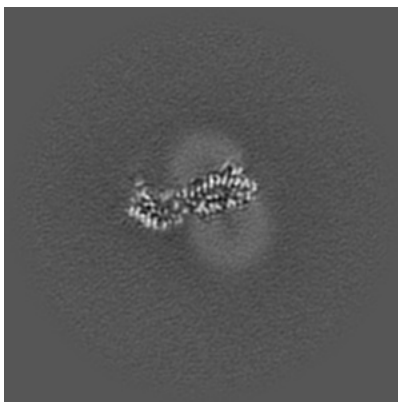
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

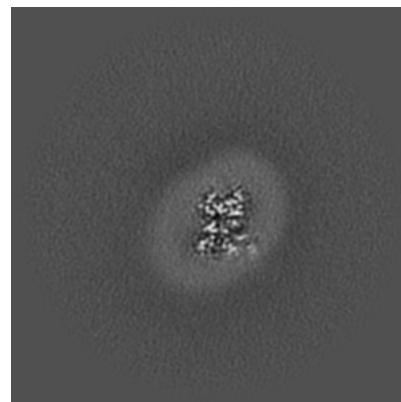
6.3.1 Primary map



X Index: 158

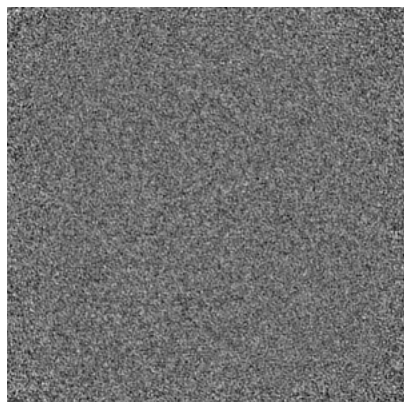


Y Index: 145

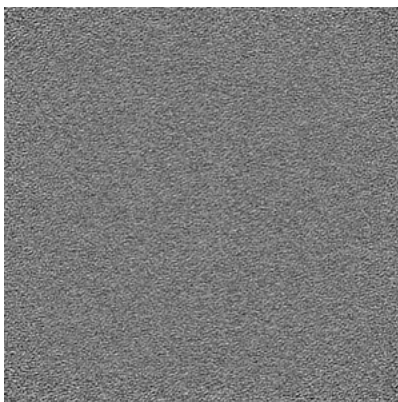


Z Index: 155

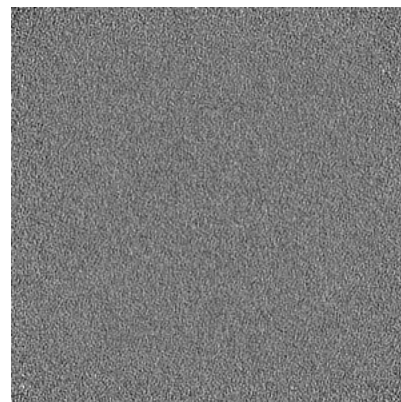
6.3.2 Raw map



X Index: 0



Y Index: 0

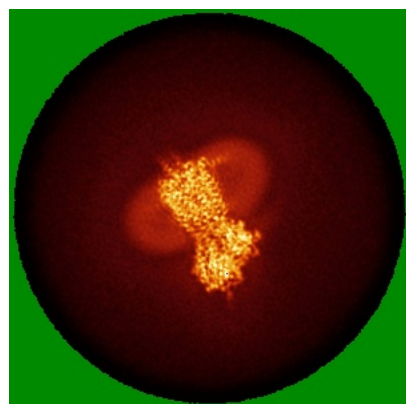


Z Index: 0

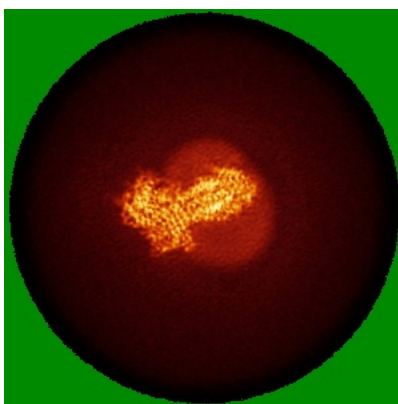
The images above show the largest variance slices of the map in three orthogonal directions.

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

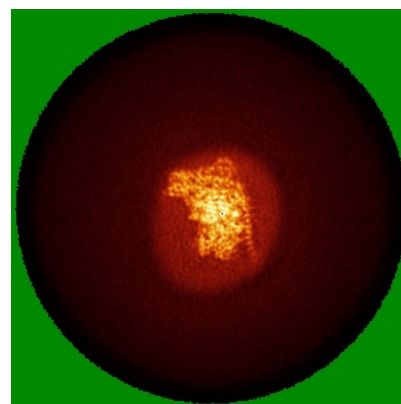
6.4.1 Primary map



X

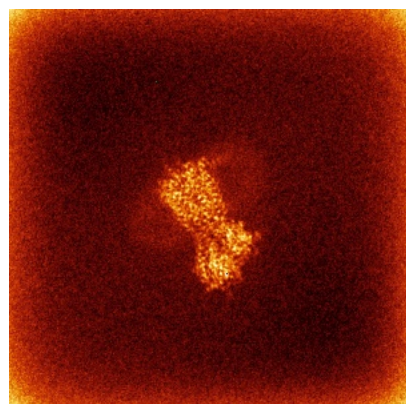


Y

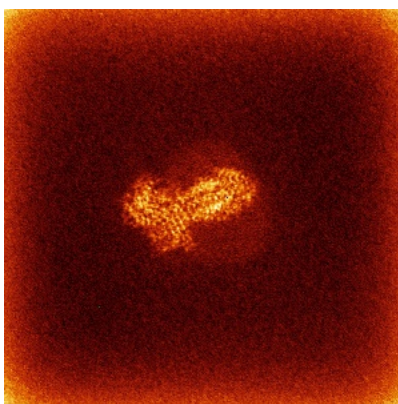


Z

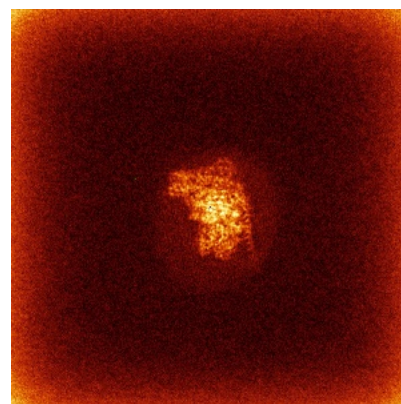
6.4.2 Raw map



X



Y



Z

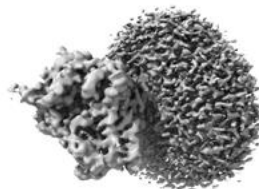
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

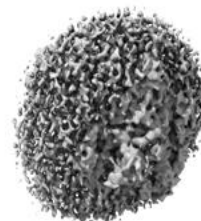
6.5.1 Primary map



X



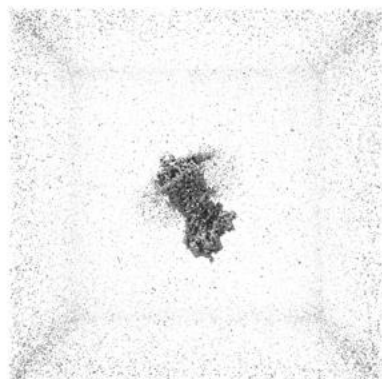
Y



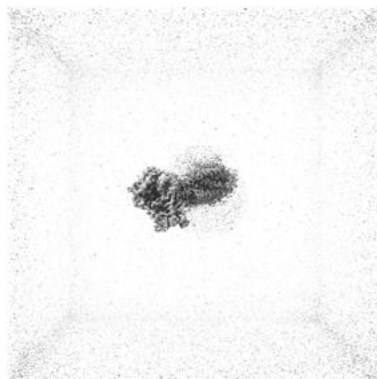
Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

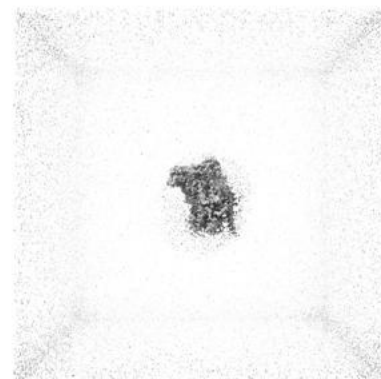
6.5.2 Raw map



X



Y



Z

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.

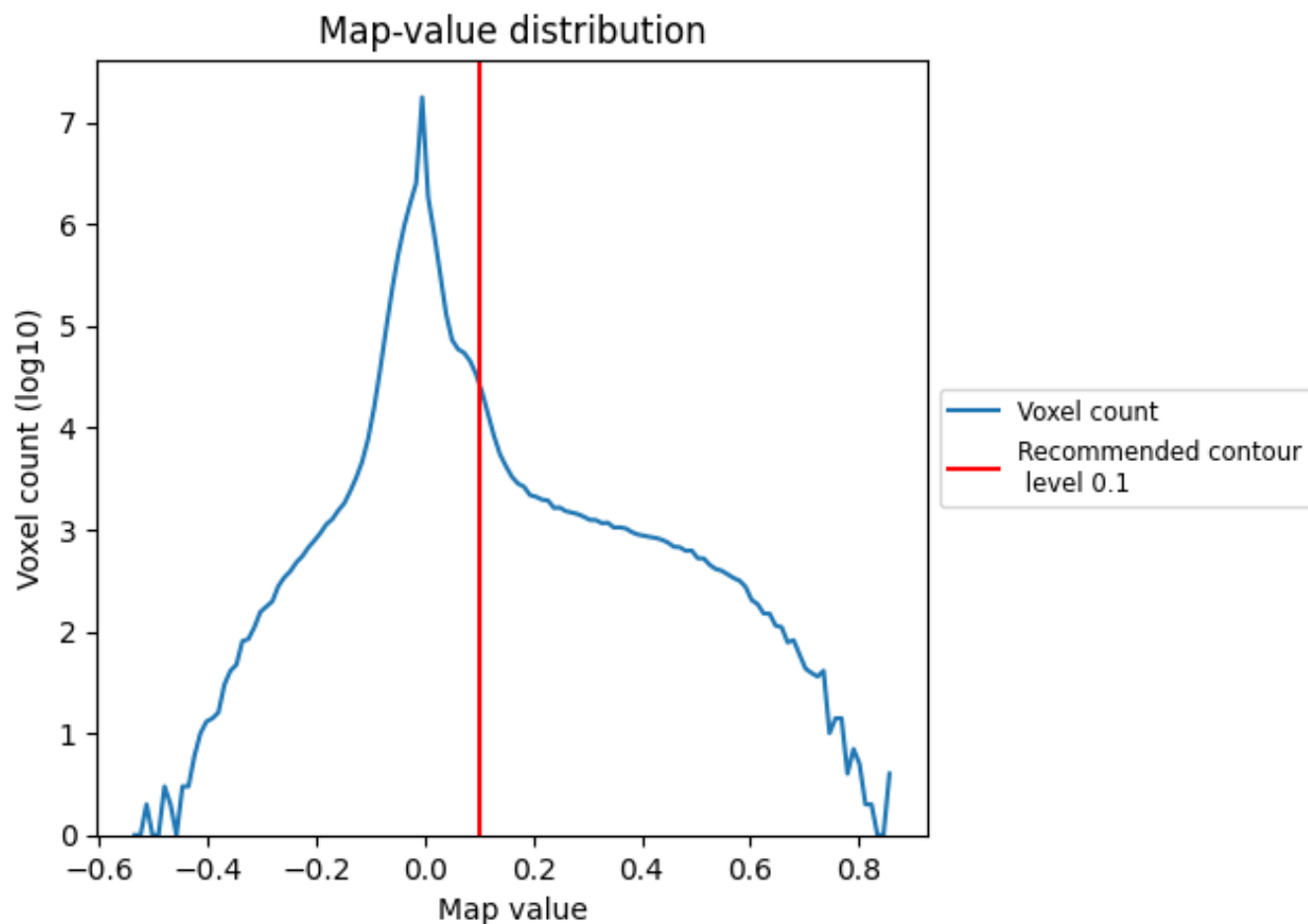
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

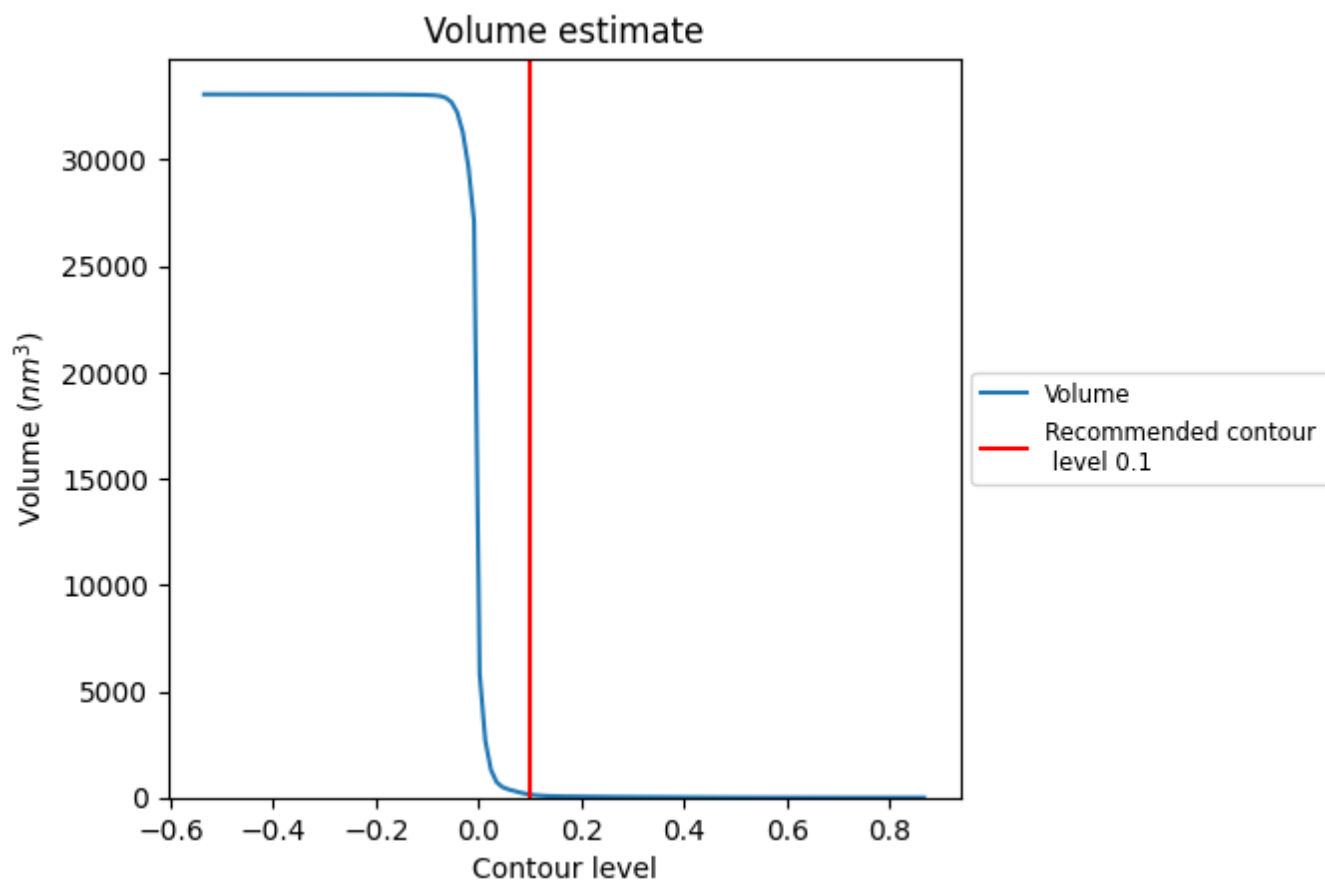
This section contains the results of statistical analysis of the map.

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.

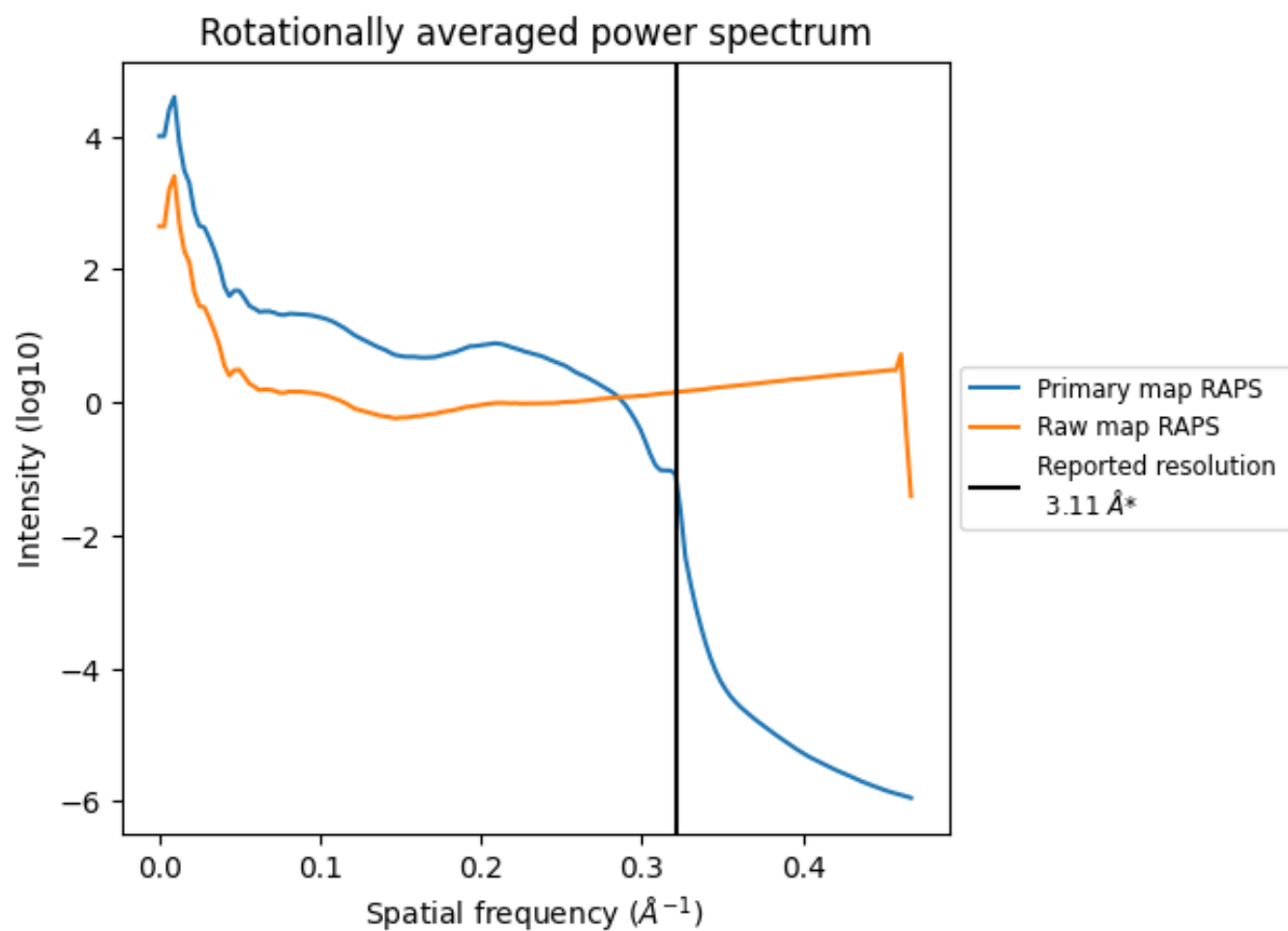
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 144 nm^3 ; this corresponds to an approximate mass of 130 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 ⓘ

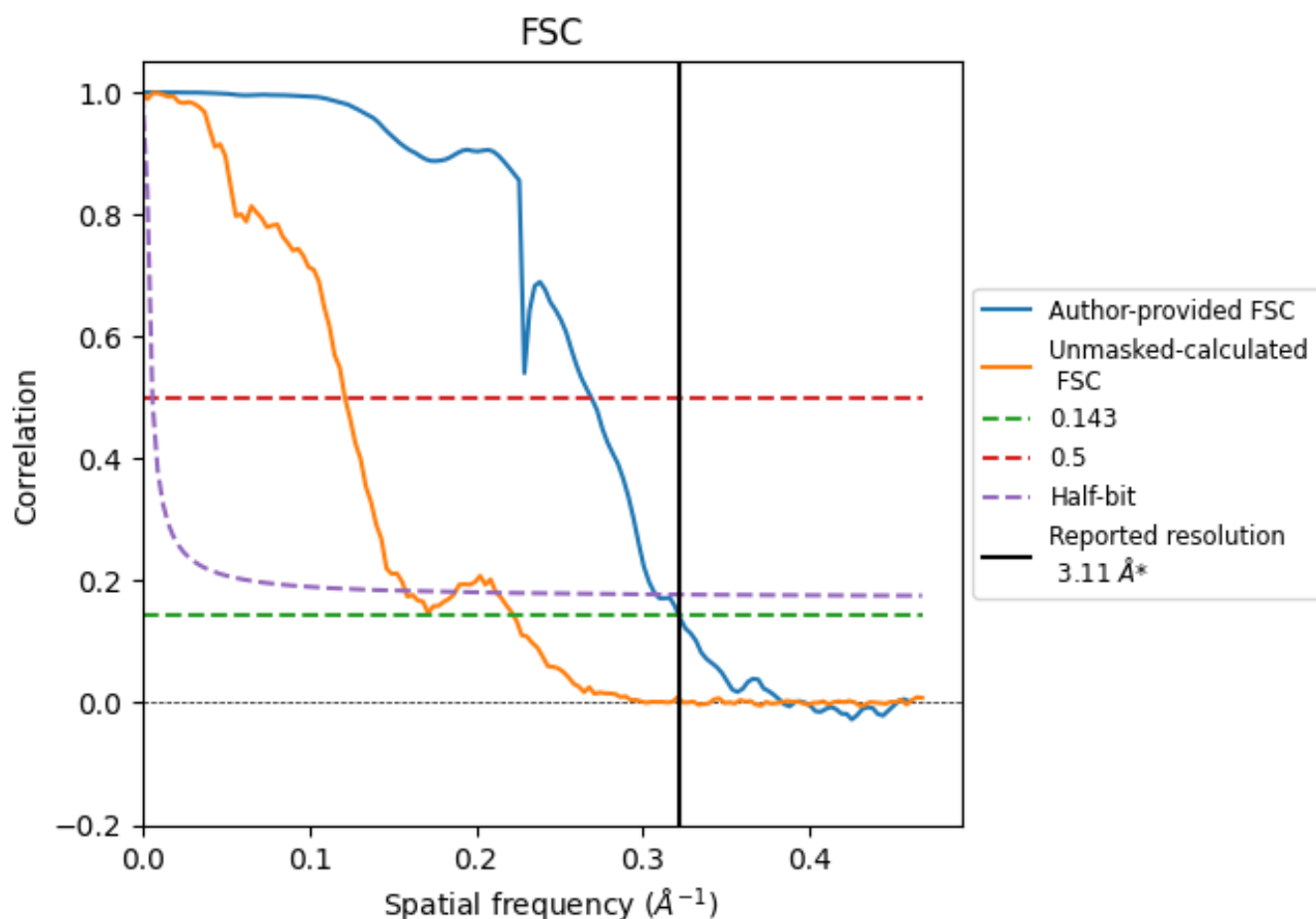


*Reported resolution corresponds to spatial frequency of 0.322 Å⁻¹

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 0.322 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

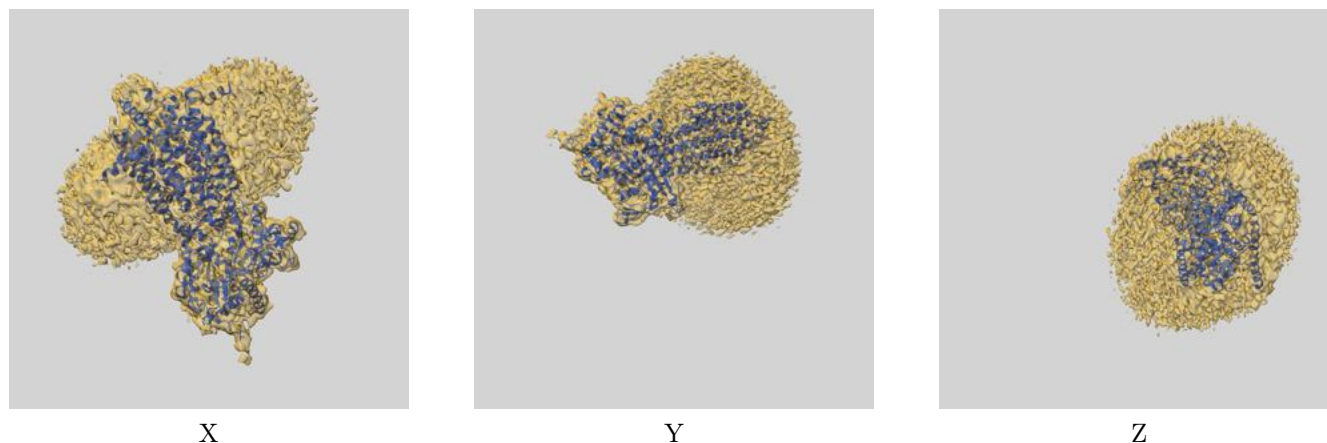
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.11	-	-
Author-provided FSC curve	3.11	3.72	3.25
Unmasked-calculated*	4.50	8.24	6.34

*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 4.50 differs from the reported value 3.11 by more than 10 %

9 Map-model fit [i](#)

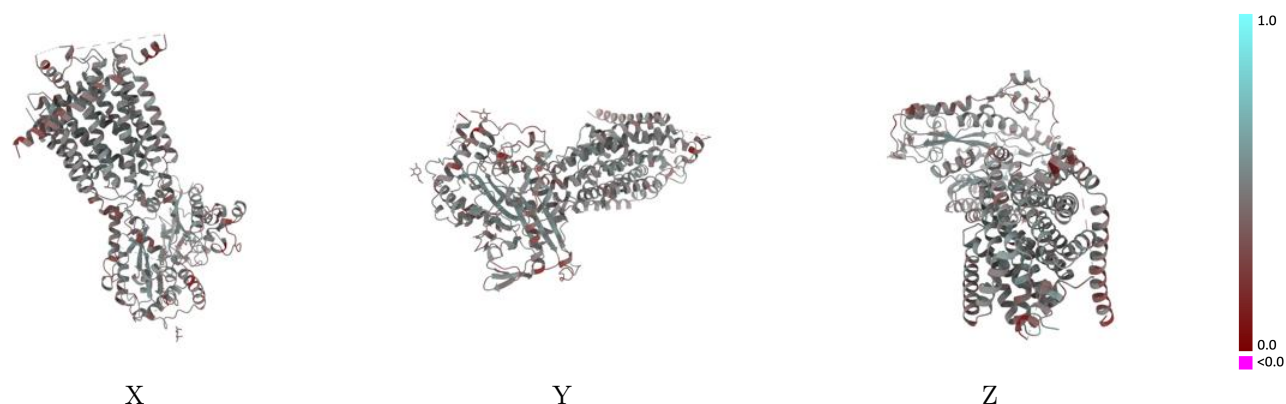
This section contains information regarding the fit between EMDB map EMD-42854 and PDB model 8V0G. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



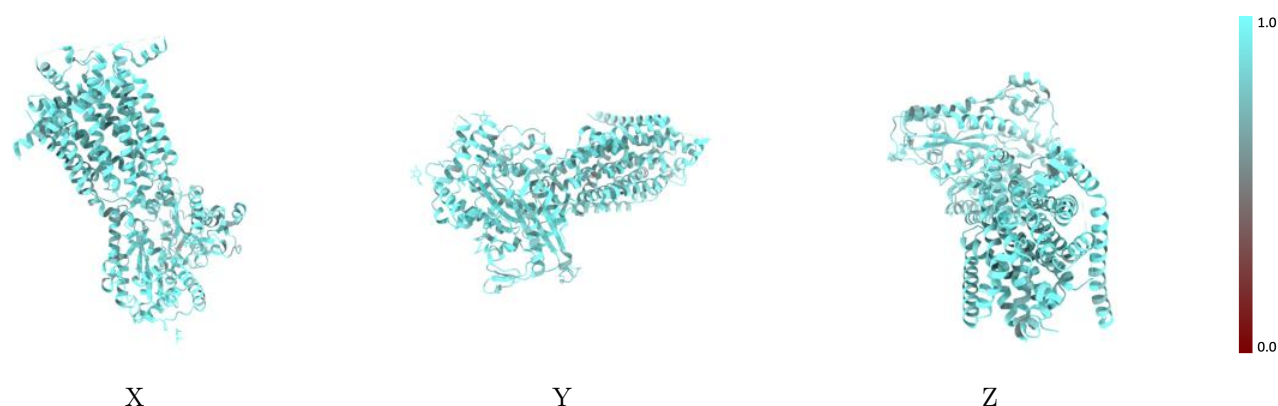
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



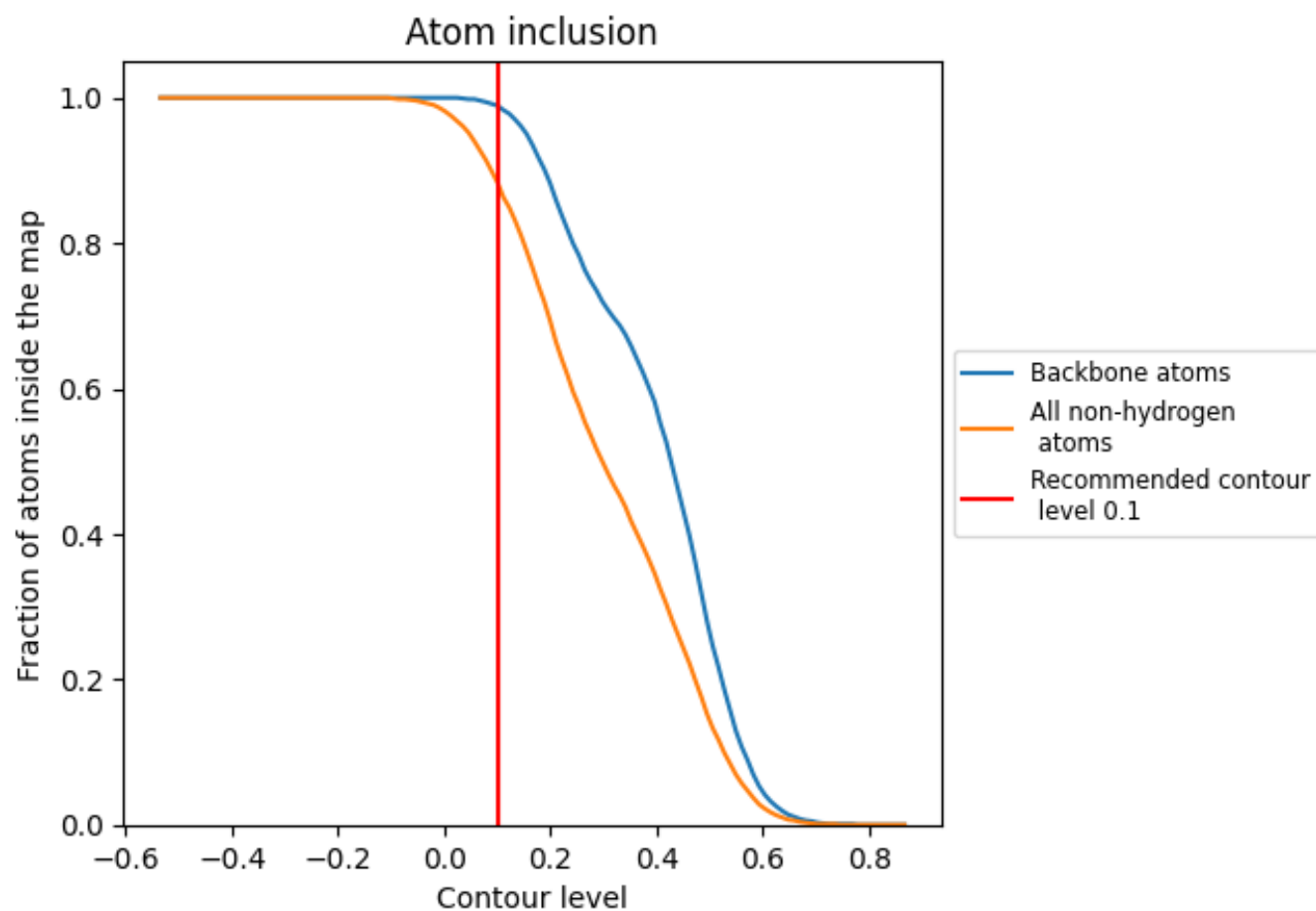
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 88% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8840	0.4580
A	0.8840	0.4580

