



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 05:30 PM UTC

PDB ID : 9J9G / pdb_00009j9g
EMDB ID : EMD-61271
Title : Bovine ABCC1 conformation 2
Authors : Zhong, C.; Wang, F.; Liu, Z.; Yu, G.
Deposited on : 2024-08-22
Resolution : 3.18 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
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

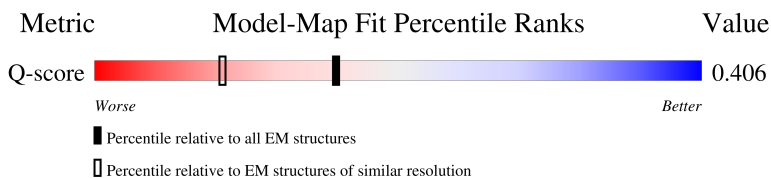
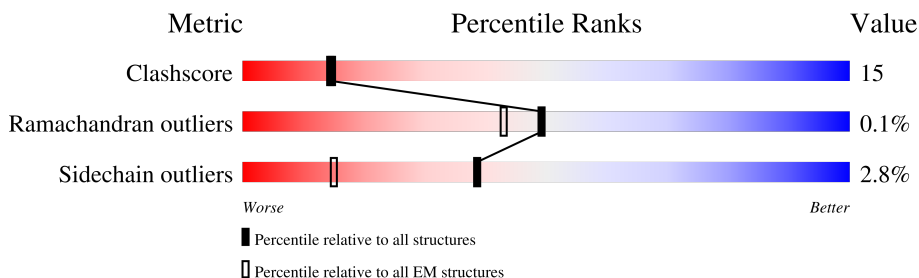
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.18 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	14470 (2.68 - 3.68)

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	1530	25% 60% 30% 8%

2 Entry composition [i](#)

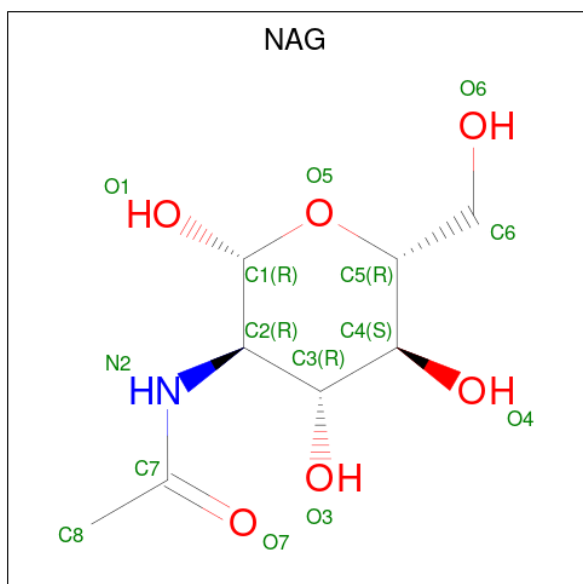
There are 2 unique types of molecules in this entry. The entry contains 11128 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Multidrug resistance-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1406	11100	7195	1848	1998	59	1	0

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

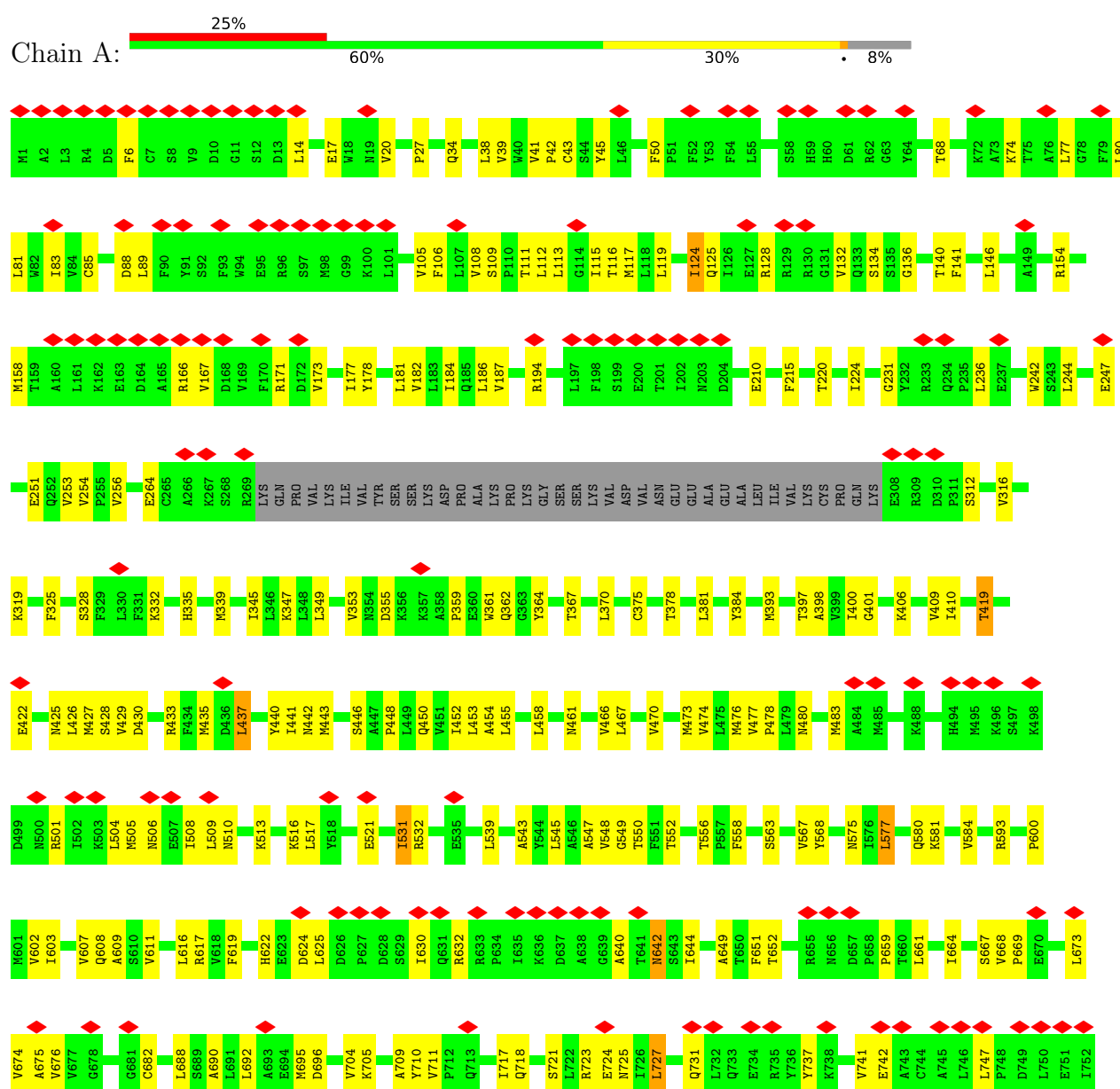


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
2	A	1	14	8	1	5	0
2	A	1	14	8	1	5	0

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: Multidrug resistance-associated protein 1



Q1516	T1456	E1396	L1335	E1272	Q1176	L1071	GLU	GLY	T821	L753
R1517	A1457	E1397	T1336	Q1276	K1180	V1072	ALA	PRO	R822	P754
G1518	A1458	V1398	L1337	I1277	N1073	N1073	ASP	GLY	L823	S755
L1519	V1459	W1399	G1338	I1278	R1074	F1075	LYS	LYS	L824	G756
F1520	D1460	T1400	L1339	Q1279	F1076	K1077	GLU	GLU	S830	D757
Y1521	L1461	S1401	F1340	D1279	S1076		GLN	VAL	Y831	R758
S1522	E1462	L1402	R1341	M1280	D1080			LYS	Y831	T759
M1523	T1463	L1404	I1342	A1281	D1083			GLN	Q834	E760
A1524	D1464	K1343	K1343	P1282	S1084			MET	M835	I761
K1525	H1406	A1346	A1346	P1283	D1085			ASN	D836	G762
D1526	L1407	E1347	E1347	M1285	M1086			GLY	V837	E763
SER	K1408	G1348	G1348	P1286	I1086			MET	I839	K764
GLY	G1409	E1349	E1349	W1287	V1089			LEU	I839	G765
LEU	F1410	I1350	I1350	Q1288	V1090			THR	S842	V766
VAL	V1411	I1351	I1351	Q1289	K1091			ASP	G843	
	S1412	I1352	I1352	G1290	K1091			THR	G844	L767
	A1413	D1353	D1353	R1291	M1092			ALA	G844	L768
	L1414	D1354	D1354	V1292	G1096			GLY	R845	
	P1415	I1355	I1355	E1293	L1097			LYS	S847	Q772
	D1416	N1356	N1356	F1294	I1101			GLN	E848	R775
	K1417	I1357	I1357	R1295	G1102			ARG	S849	V776
	L1418	A1358	A1358	D1296	L1105			GLN	S851	L778
	H1420	K1359	K1359	Y1297	T1109			GLN	Y852	
	E1421	I1360	I1360	G1298	L1109			GLN	Q853	V782
	C1422	G1361	G1361	L1299	A1110			SER	E854	Y783
	A1423	L1362	L1362	R1300	T1111			SER	L855	
	E1424	H1363	H1363	Y1301	G1019			SER	L856	D786
	G1425	D1364	D1364	R1302	A1114			ARG	Y857	V788
	G1426	L1365	L1365	E1303	A1115			ASP	R858	
	G1427	F1367	F1367	D1304	I1116			VAL	D859	L790
	N1428	K1368	K1368	L1305	T1117			SER	F862	L791
	L1429	I1369	I1369	D1306	I1118			GLN	T868	D792
	S1430	T1370	T1370	L1307	P1119			HIS	Y869	D793
	V1431	I1371	I1371	L1307	P1120			HIS	E864	P794
	G1432	F1372	F1372	V1308	Y1032			THR	F865	L795
	Q1433	Q1373	Q1373	L1309	S1033			SER	L866	
	R1434	D1375	D1375	K1310	V1036			THR	R867	D799
	Q1435	P1376	P1376	H1311	S1037			ALA	T868	A800
	L1436	V1377	V1377	I1312	I1041			GLU	H801	H801
	L1437	F1378	F1378	I1313	S1044			ARG	V802	V802
	C1438	F1379	F1379	I1316	R1057			LYS	G803	G803
	L1439	S1380	S1380	D1317	R1064			PRO	K804	K804
	A1440	G1381	G1381	G1318	E1068			GLY	H805	H805
	A1441	S1382	S1382	G1319	R1065			PRO	I806	I806
	A1442	L1383	L1383	E1261	I1060			THR	F807	F807
	A1443	R1384	R1384	E1262	S1061			GLU	E808	E808
	L1444	M1385	M1385	L1263	E1064			GLY	N809	N809
	R1445	L1386	L1386	I1321	S1146			GLN	V810	V810
	K1446	L1387	L1387	V1322	I1147			THR	I811	I811
	D1447	D1388	D1388	G1323	S1148			TRP	G812	G812
	T1447	P1389	P1389	I1325	L1159			LYS	P813	P813
	K1448	F1390	F1390	G1326				GLY	K814	K814
	I1449	S1391	S1391	R1327				LEU	G815	G815
	L1450	Q1392	Q1392	T1328				ALA	L816	L816
	V1451	Y1393	Y1393	G1329				GLY	L817	L817
	L1452	S1394	S1394	A1330				VAL	K818	K818
	D1453	D1395	D1395	G1331				GLY	N819	N819
	E1454			K1332				VAL	K820	K820
	A1455			S1333						
				S1334						

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	154111	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 ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.848	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	265.6, 265.6, 265.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83000004, 0.83000004, 0.83000004	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

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	0.19	0/11343	0.39	0/15404

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11100	0	11264	341	0
2	A	28	0	26	0	0
All	All	11128	0	11290	341	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 15.

The worst 5 of 341 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:1118:ILE:HG13	1:A:1119:PRO:HD3	1.44	0.99
1:A:675:ALA:HB2	1:A:835:MET:HE2	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1522:SER:HB2	1:A:1523:MET:HE2	1.64	0.78
1:A:1372:ILE:HG12	1:A:1450:LEU:HD12	1.66	0.77
1:A:501:ARG:HB2	1:A:531:ILE:HG21	1.66	0.77

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	1401/1530 (92%)	1354 (97%)	45 (3%)	2 (0%)	48 77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1289	VAL
1	A	1286	TRP

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	1219/1336 (91%)	1184 (97%)	35 (3%)	37 64

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1128	VAL
1	A	1252	GLU
1	A	1359	LYS
1	A	642	ASN
1	A	624	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	834	GLN
1	A	1238	GLN
1	A	442	ASN
1	A	480	ASN
1	A	494	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](#)

2 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
2	NAG	A	1702	1	14,14,15	2.33	5 (35%)	17,19,21	1.78	6 (35%)
2	NAG	A	1701	1	14,14,15	2.17	4 (28%)	17,19,21	1.20	1 (5%)

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
2	NAG	A	1702	1	-	3/6/23/26	0/1/1/1
2	NAG	A	1701	1	-	0/6/23/26	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1702	NAG	O5-C1	5.64	1.53	1.43
2	A	1701	NAG	O5-C1	5.12	1.52	1.43
2	A	1701	NAG	C7-N2	4.17	1.47	1.34
2	A	1702	NAG	C7-N2	4.08	1.47	1.34
2	A	1702	NAG	C2-N2	3.42	1.51	1.46

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1702	NAG	C1-O5-C5	3.28	116.59	112.19
2	A	1702	NAG	C2-N2-C7	3.20	127.19	122.90
2	A	1702	NAG	C8-C7-N2	2.95	121.01	116.12
2	A	1702	NAG	C4-C3-C2	2.72	115.00	111.02
2	A	1702	NAG	C1-C2-N2	-2.41	106.63	110.43

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1702	NAG	C8-C7-N2-C2
2	A	1702	NAG	O7-C7-N2-C2
2	A	1702	NAG	O5-C5-C6-O6

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-61271. These allow visual inspection of the internal detail of the map and identification of artifacts.

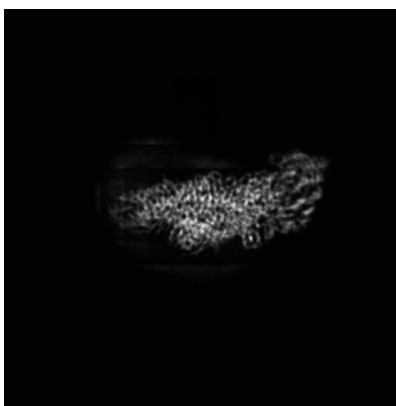
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

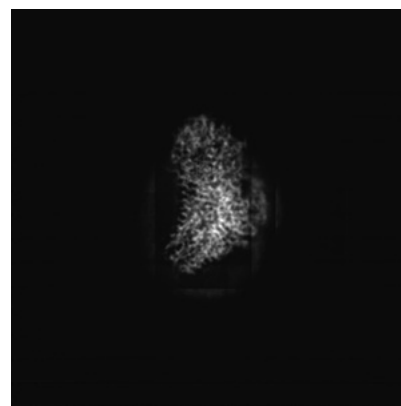
6.1.1 Primary map



X

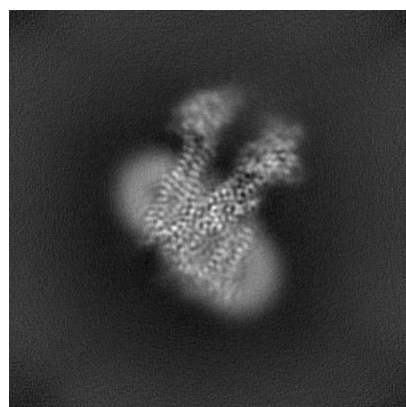


Y

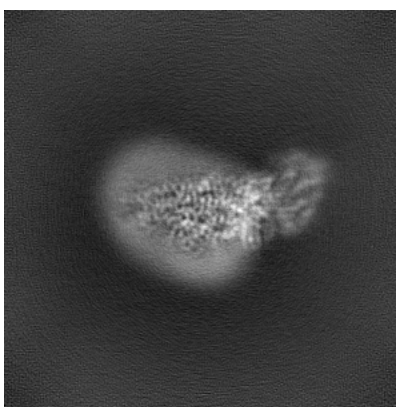


Z

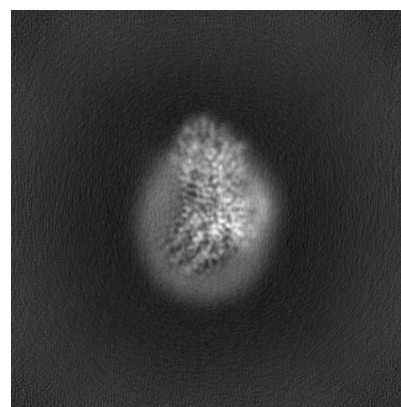
6.1.2 Raw map



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: 160

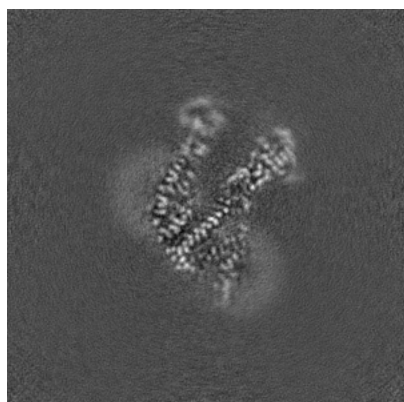


Y Index: 160

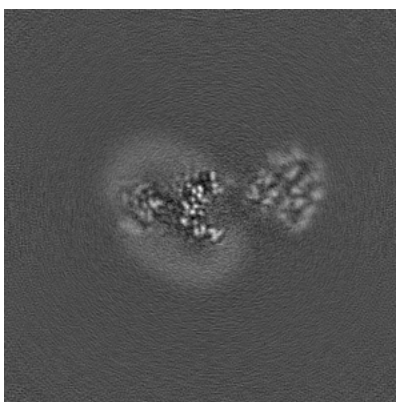


Z Index: 160

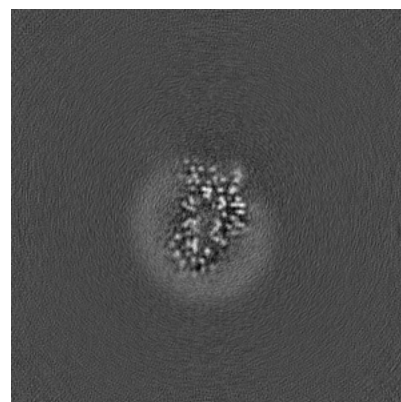
6.2.2 Raw map



X Index: 160



Y Index: 160



Z Index: 160

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: 167

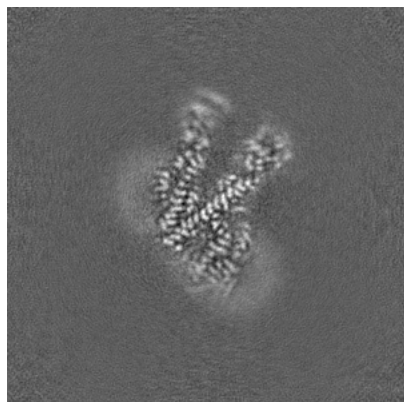


Y Index: 141

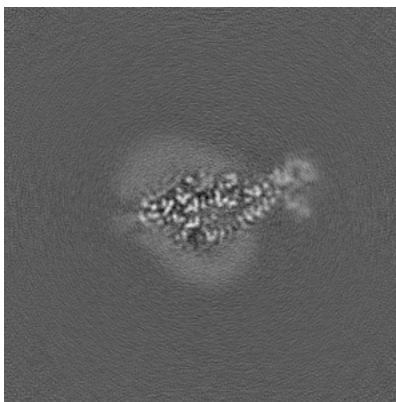


Z Index: 153

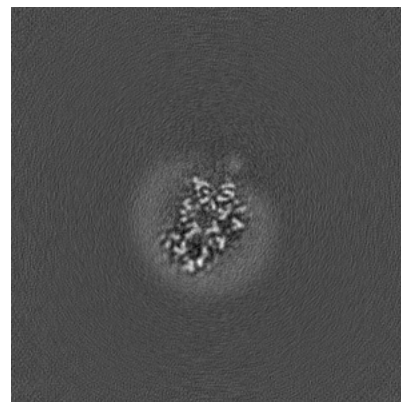
6.3.2 Raw map



X Index: 167



Y Index: 141

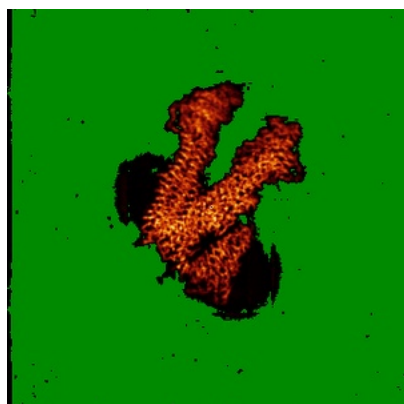


Z Index: 153

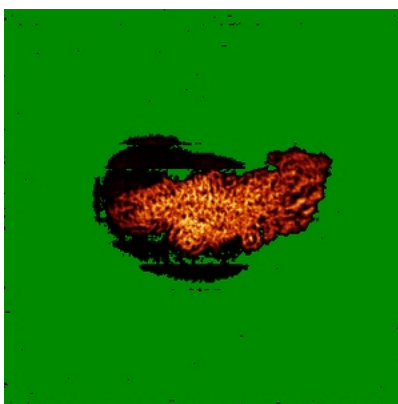
The images above show the largest variance slices of the map in three orthogonal directions.

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

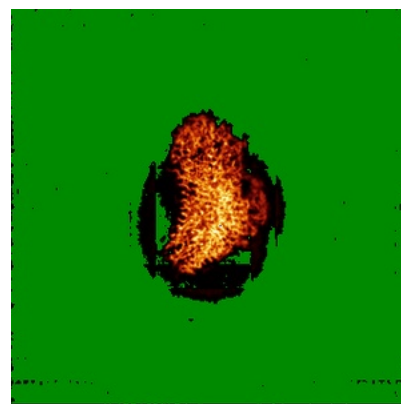
6.4.1 Primary map



X

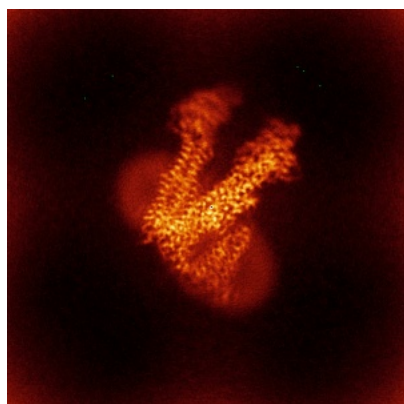


Y

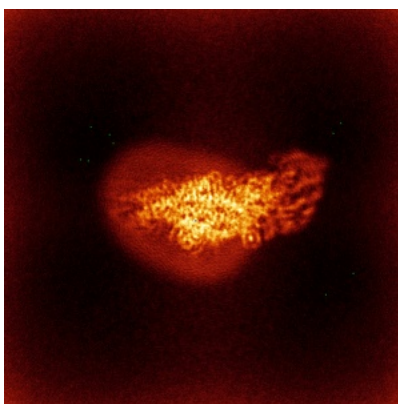


Z

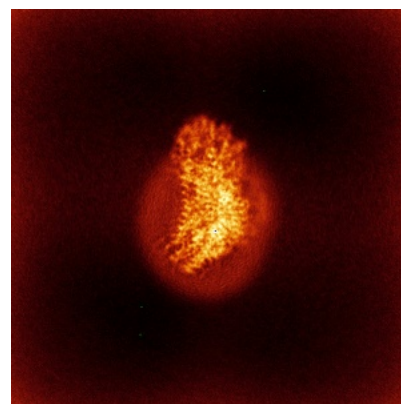
6.4.2 Raw map



X



Y

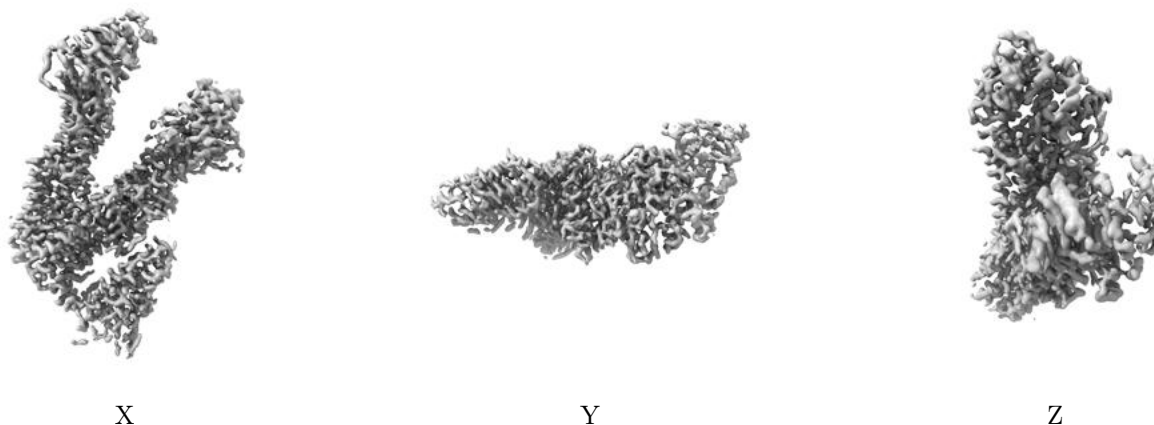


Z

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.

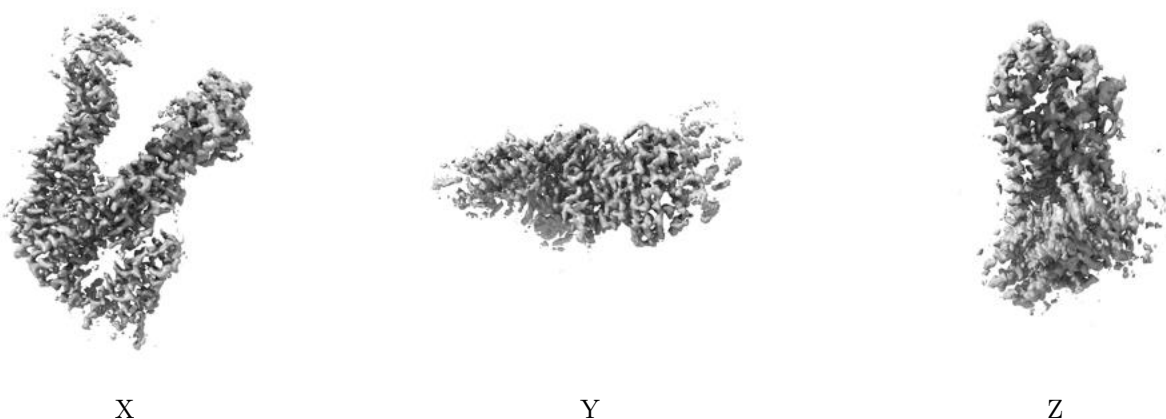
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. 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.

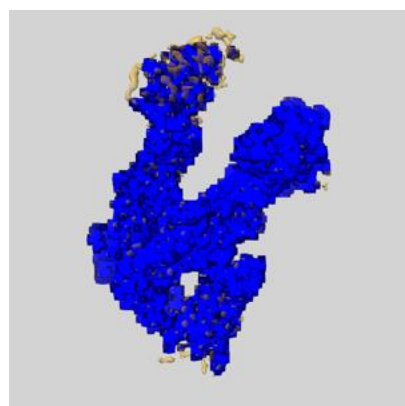
6.6 Mask visualisation [i](#)

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

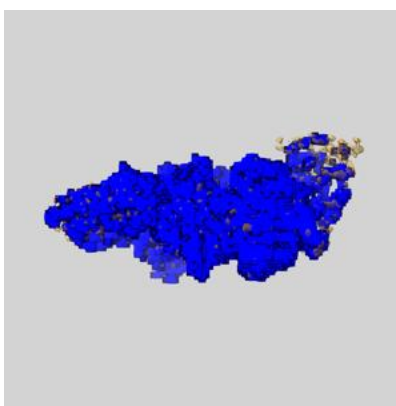
A mask typically either:

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

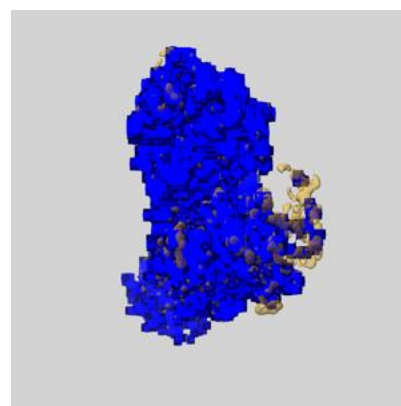
6.6.1 emd_61271_msk_1.map [i](#)



X



Y

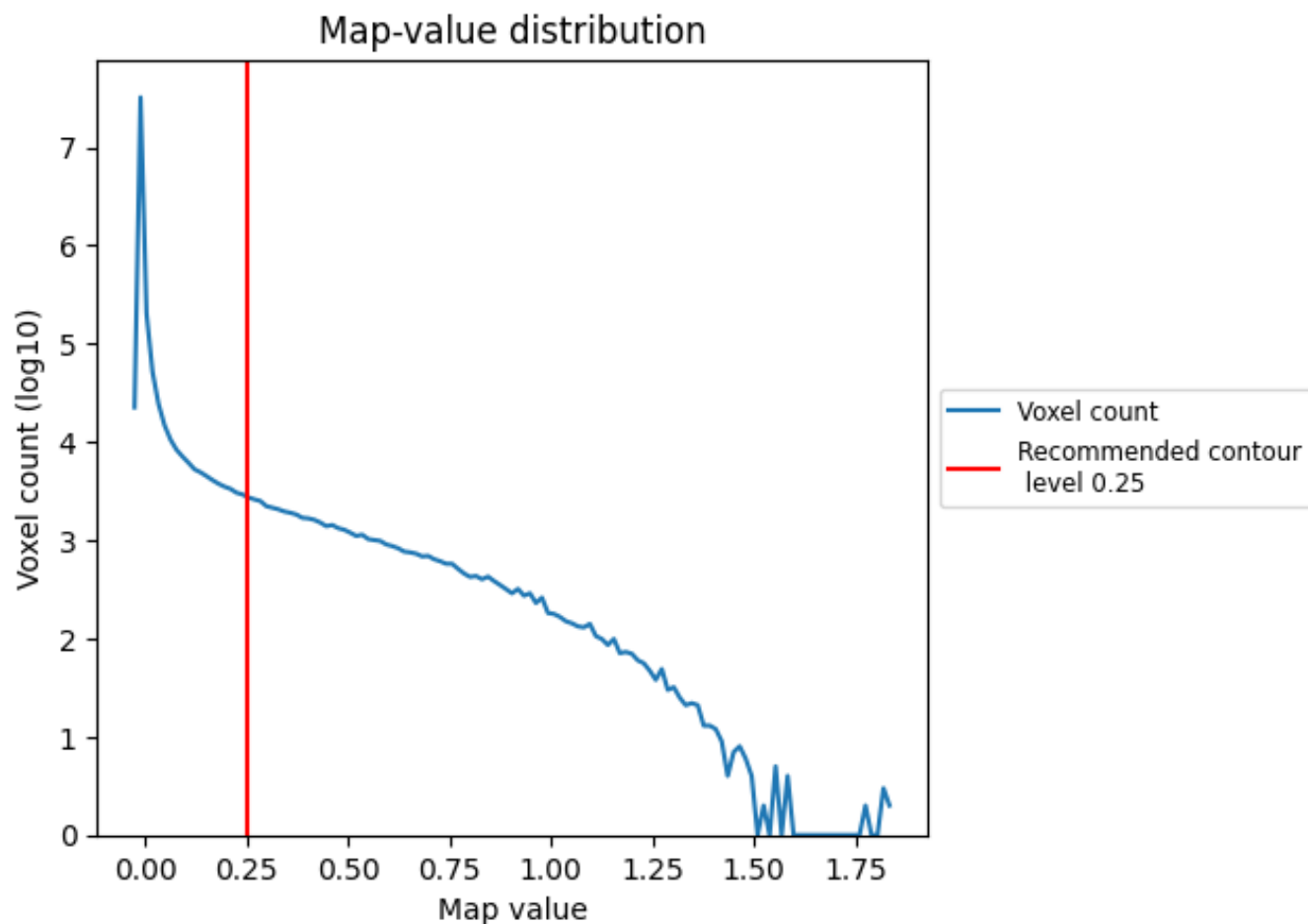


Z

7 Map analysis [i](#)

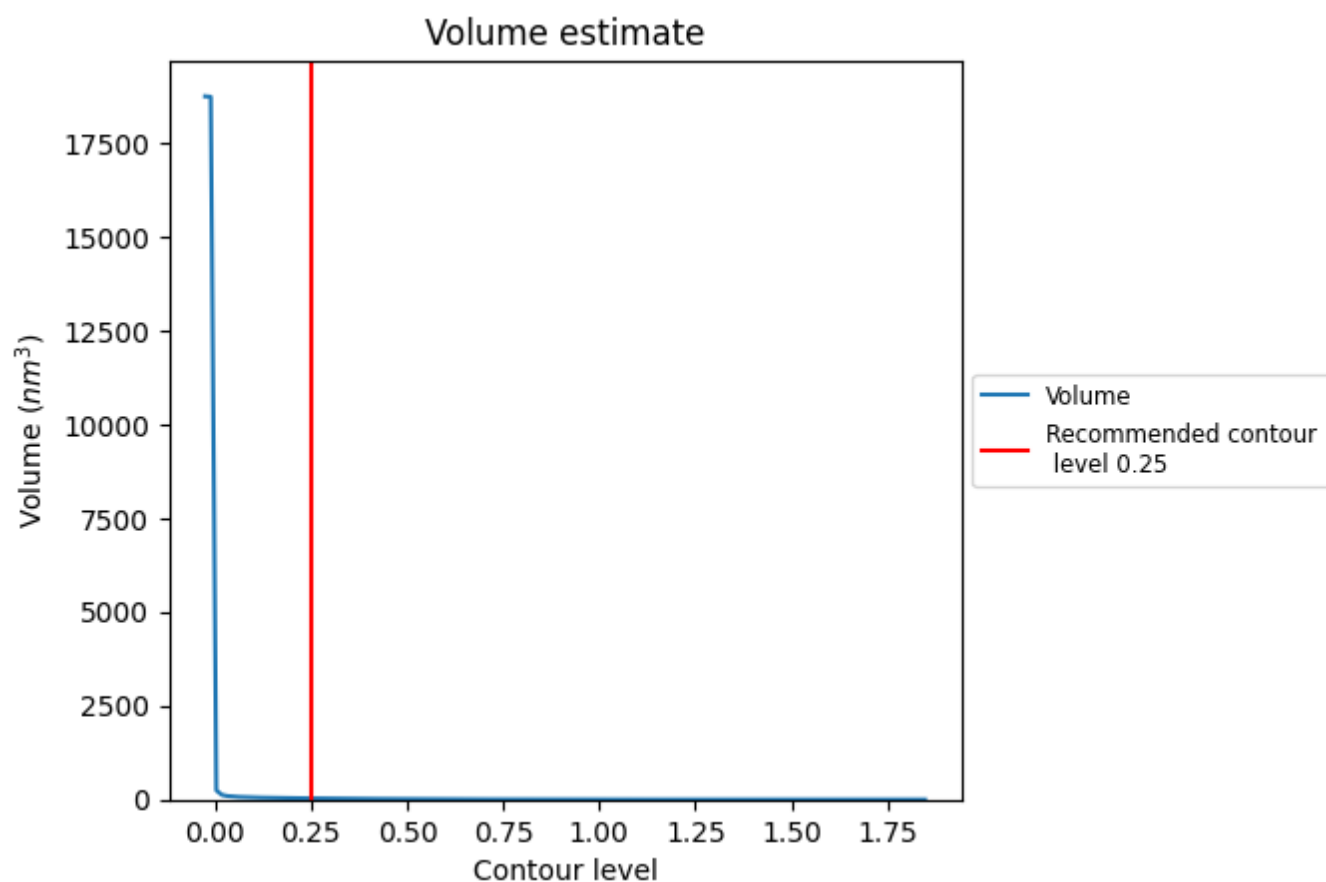
This section contains the results of statistical analysis of the map.

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.

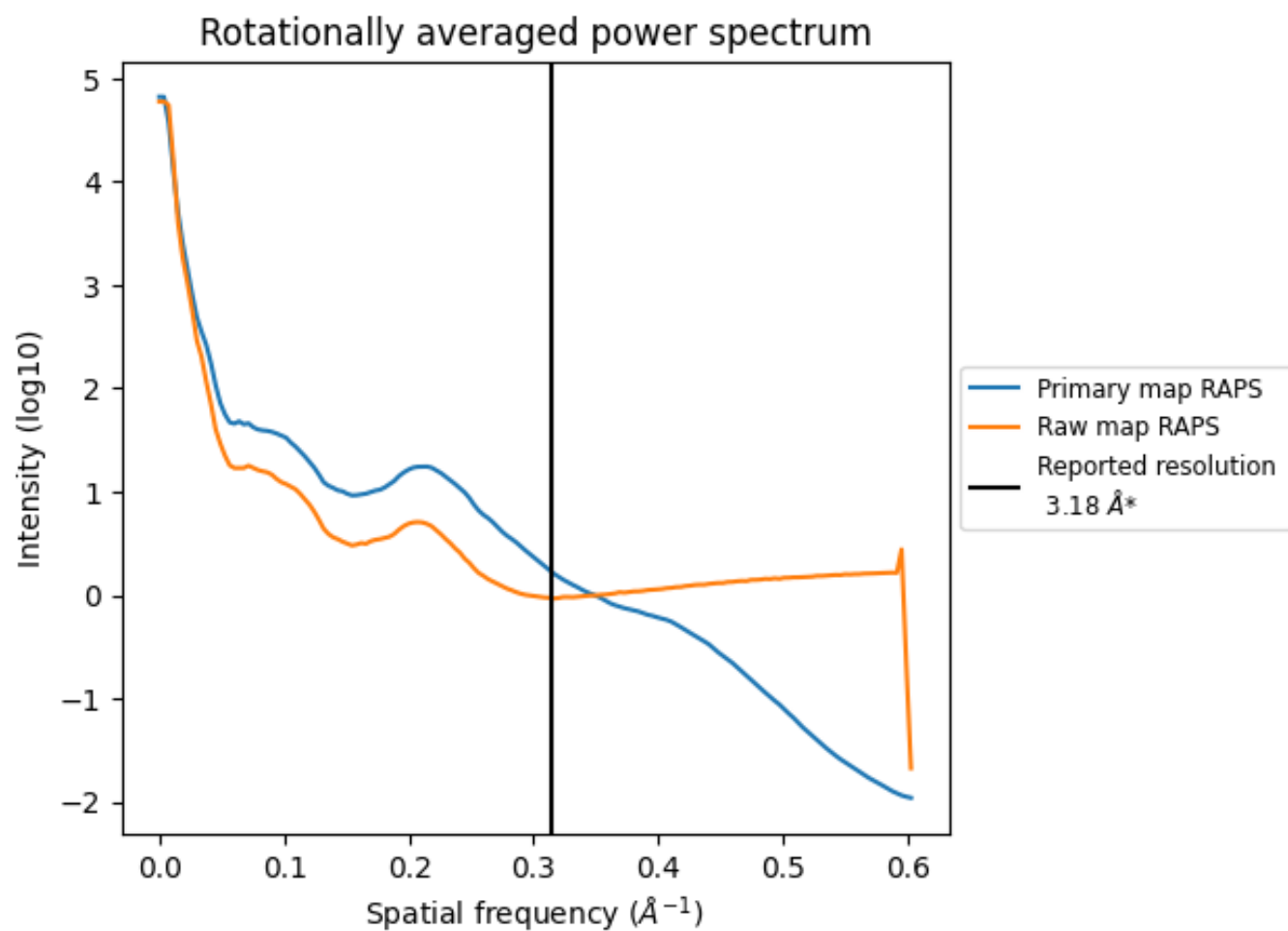
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 32 nm³; this corresponds to an approximate mass of 29 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 ⓘ

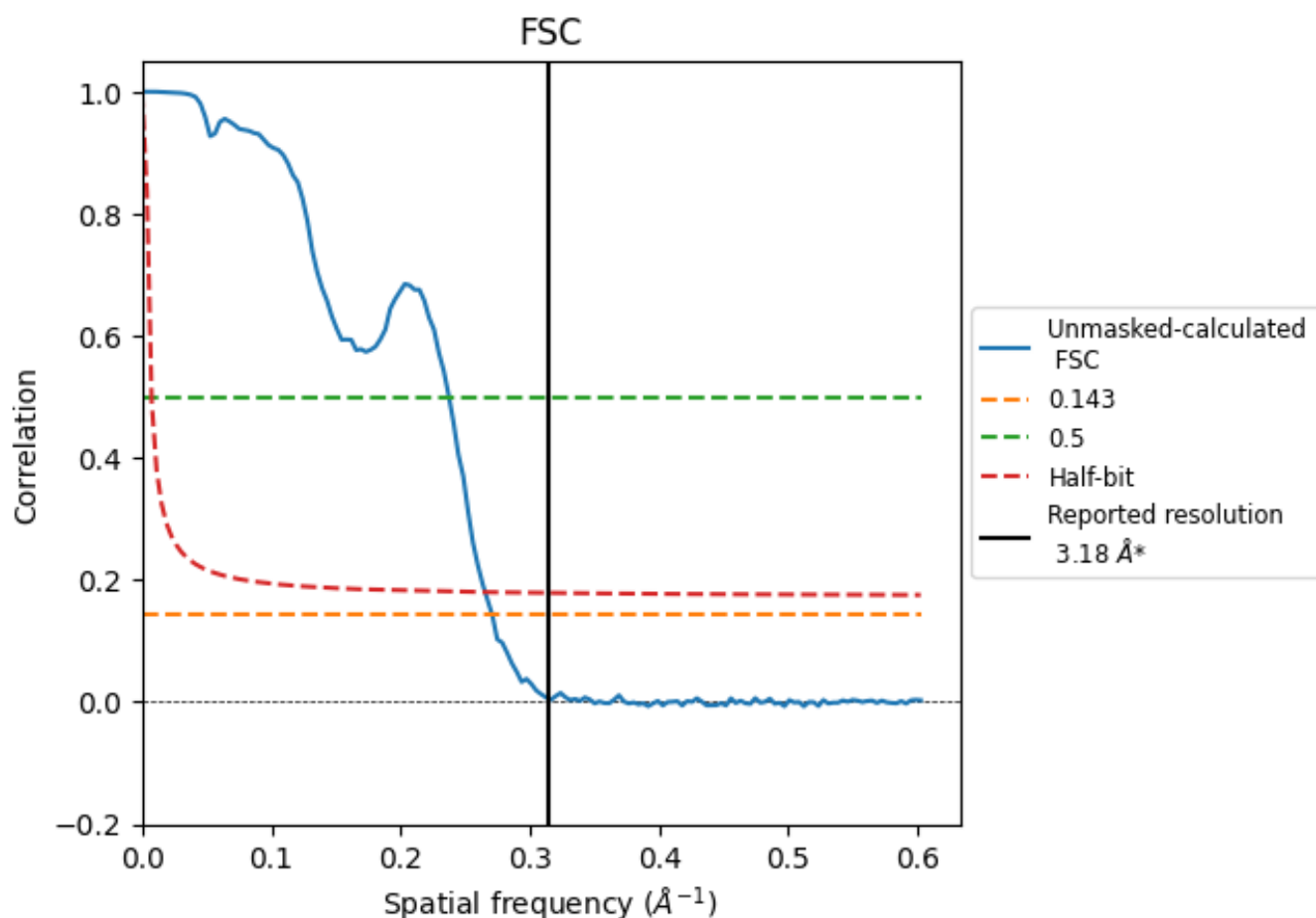


*Reported resolution corresponds to spatial frequency of 0.314 Å⁻¹

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 $0.314 \text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

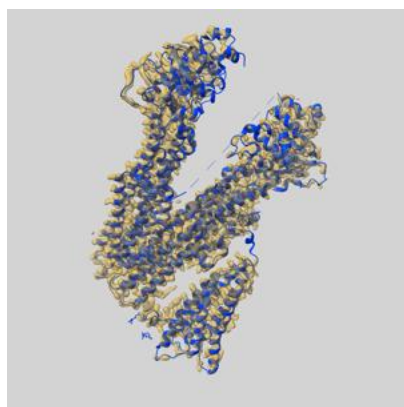
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.18	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.69	4.21	3.77

*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 3.69 differs from the reported value 3.18 by more than 10 %

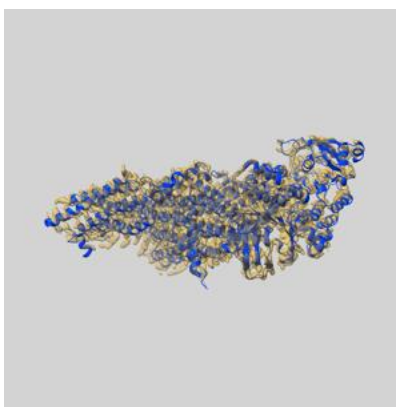
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-61271 and PDB model 9J9G. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

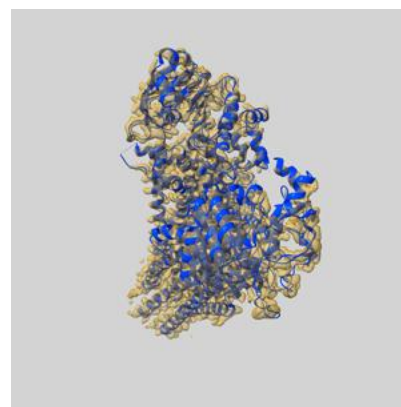
9.1 Map-model overlay [i](#)



X



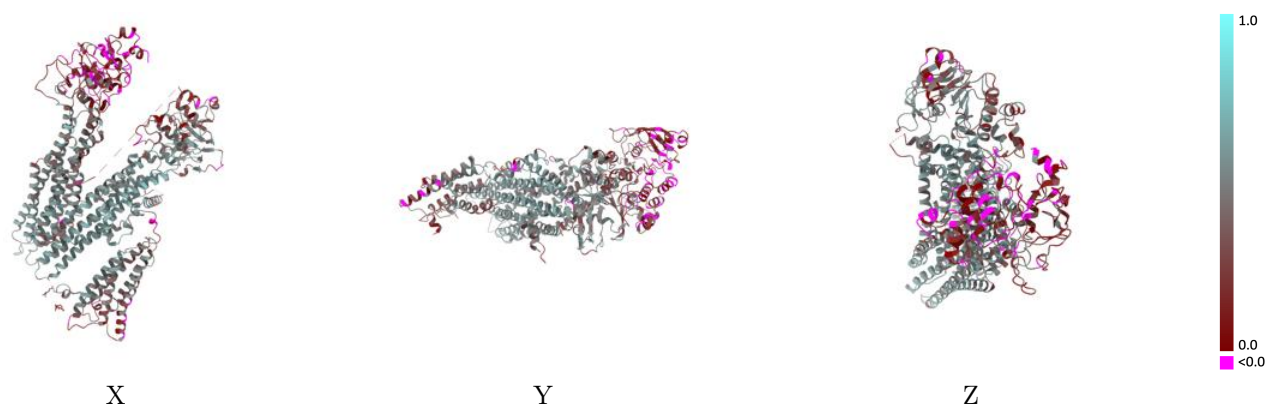
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25 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](#)

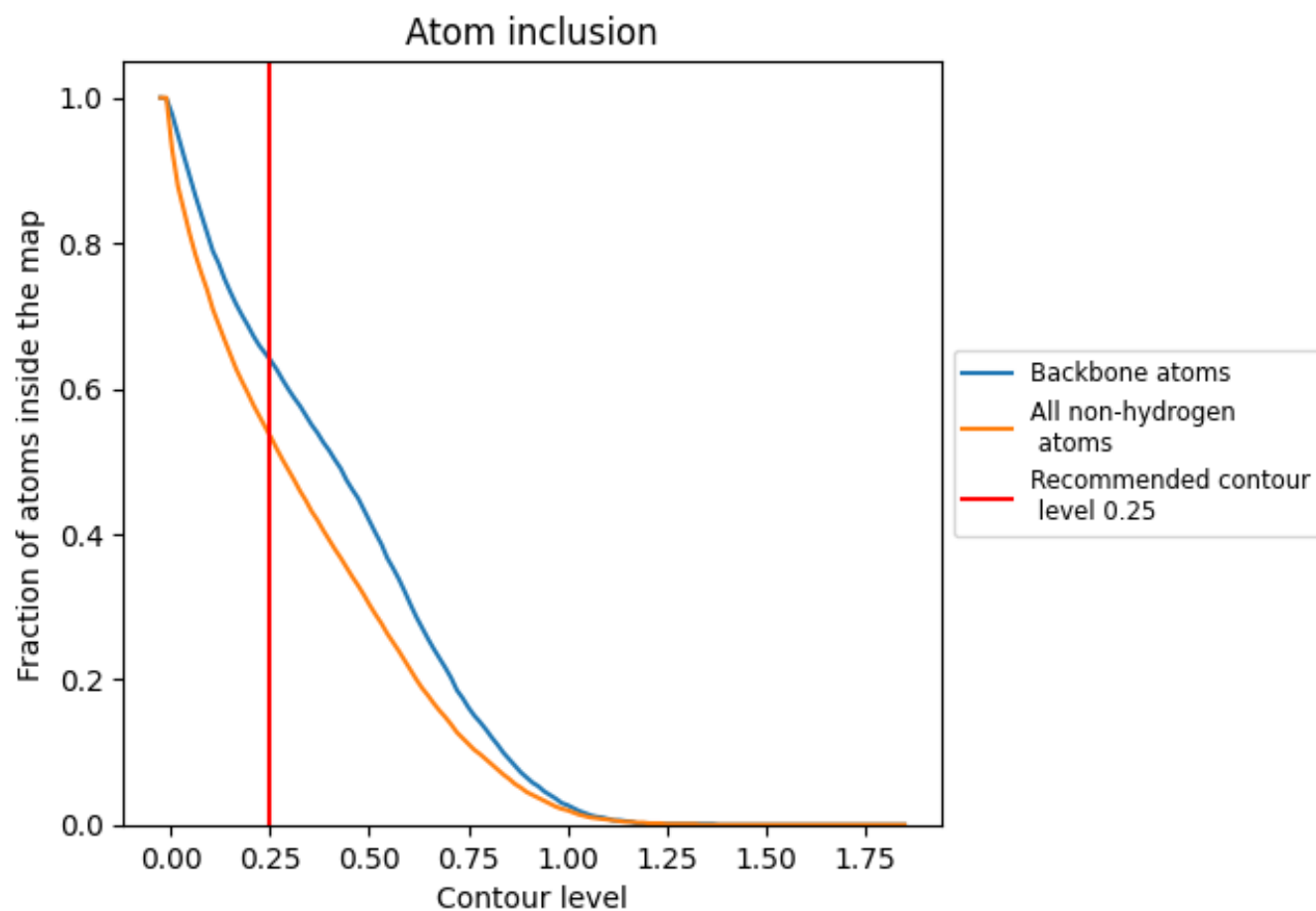


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 64% of all backbone atoms, 54% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5350	0.4060
A	0.5350	0.4060

