



wwPDB EM Validation Summary Report ⓘ

Aug 25, 2025 – 10:15 AM JST

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.dev126
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.45.1

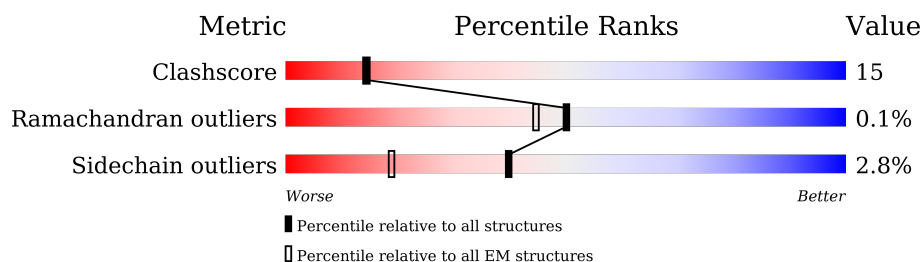
1 Overall quality at a glance

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1530	<div> <div>25%</div> <div>60%</div> <div>30%</div> <div>• 8%</div> </div>

2 Entry composition [i](#)

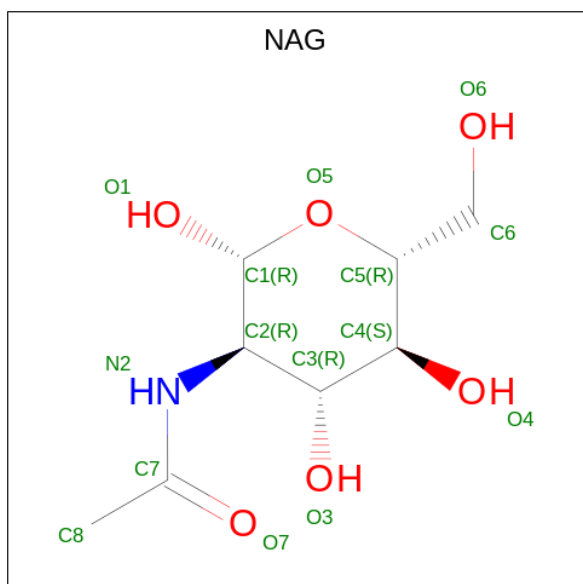
There are 2 unique types of molecules in this entry. The entry contains 11128 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	1406	Total	C	N	O	S	1	0
			11100	7195	1848	1998	59		

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

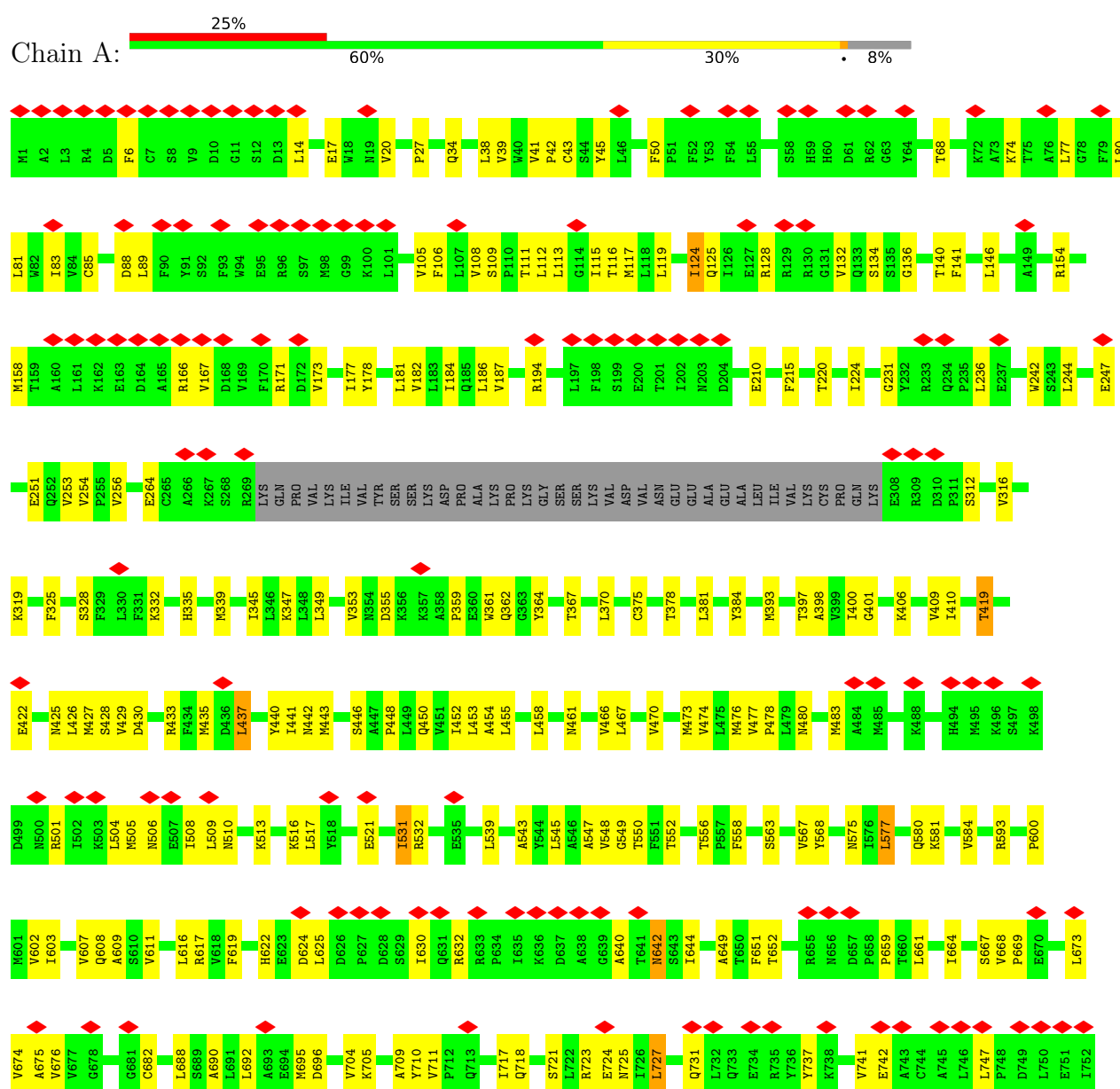


Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots [i](#)

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
R1517	A1457	E1397	T1336	Q1276	K1180	V1072	ALA	PRO
G1518	A1458	V1398	L1337	I1277	N1073	N1073	ASP	GLY
L1519	V1459	W1399	G1338	I1278	R1074	F1075	LYS	LYS
F1520	D1460	T1400	L1339	Q1279	F1076	K1077	GLU	GLU
Y1521	L1461	S1401	F1340	D1279	S1076		VAL	VAL
S1522	E1462	L1402	R1341	M1280	D1080		LYS	LYS
M1523	T1463	L1404	I1342	A1281	G1083		GLN	GLN
A1524	D1464	A1405	K1343	P1282	S1084		GLN	GLN
D1526	D1465	H1406	A1346	P1283	M1085		MET	MET
K1529	L1466	L1407	E1347	K1284	I1086		GLY	GLY
D1526	I1467	K1408	G1348	M1286	M1086		LEU	LEU
SER	Q1468	G1409	E1349	P1287	I1086		VAL	VAL
LEU	S1469	F1410	I1350	Q1288	V1089		THR	THR
VAL	T1470	V1411	I1351	Q1289	I1090		ASP	ASP
	I1471	A1412	I1352	R1291	K1091		THR	THR
	R1472	A1413	D1353	G1290	K1091		ALA	ALA
	T1473	L1414	D1354	R1291	M1092		GLY	GLY
	Q1474	P1415	I1355	V1292	G1096		LYS	LYS
F1475	F1475	D1416	N1356	E1293	S1096		GLN	GLN
D1476	D1476	K1417	I1357	F1294	L1097		GLN	GLN
D1477	D1477	K1417	A1358	R1295	I1101		LEU	LEU
C1478	C1478	L1418	K1359	D1296	G1102		SER	SER
T1479	T1479	H1420	I1360	Y1297	I1105		SER	SER
V1480	V1480	E1421	G1361	G1297	L1109		SER	SER
L1481	L1481	C1422	L1362	G1298	A1110		SER	SER
T1482	T1482	A1423	H1363	L1299	T1111		TYR	TYR
T1483	T1483	E1424	D1364	R1300	A1114		SER	SER
H1485	H1485	G1425	L1365	Y1301	G1019		ARG	ARG
L1486	L1486	G1426	R1366	R1302	G1022		ASP	ASP
R1487	R1487	G1427	F1367	E1303	I1023		VAL	VAL
N1487	N1487	E1428	K1368	D1304	SER		SER	SER
L1489	L1489	L1429	I1369	L1305	V1029		GLN	GLN
I1490	I1490	S1430	T1370	D1306	H1118		HIS	HIS
M1491	M1491	V1431	I1371	L1307	P1119		HIS	HIS
D1492	D1492	G1432	P1372	V1308	P1120		THR	THR
Y1493	Y1493	Q1433	Q1373	L1309	S1033		SER	SER
T1494	T1494	R1434	D1375	K1310	V1036		THR	THR
R1495	R1495	Q1435	P1376	H1311	S1037		ALA	ALA
V1496	V1496	L1436	V1377	I1312	I1041		GLU	GLU
I1497	I1497	L1436	L1378	M1313	F1126		LEU	LEU
V1498	V1498	V1437	F1379	I1316	F1127		ARG	ARG
L1499	L1499	C1438	S1380	D1317	V1128		LYS	LYS
D1500	D1500	L1439	G1381	G1318			PRO	PRO
K1501	K1501	A1440	S1382	G1319	R1057		GLY	GLY
G1502	G1502	A1441	L1383	E1320	I1060		PRO	PRO
E1503	E1503	A1442	R1384	K1321	S1061		GLU	GLU
L1504	L1504	L1443	M1385	V1322	I1061		GLN	GLN
Q1505	Q1505	L1444	L1386	G1323	E1064		GLY	GLY
E1506	E1506	R1445	L1387	I1324	R1065		THR	THR
W1507	W1507	K1446	D1388	G1325	S1068		THR	THR
G1508	G1508	T1447	P1389	V1326	G1069		TRP	TRP
S1509	S1509	K1448	F1390	G1326	N1070		LYS	LYS
P1510	P1510	I1449	S1391	R1327			LEU	LEU
S1511	S1511	L1450	Q1392	T1328			GLY	GLY
D1512	D1512	V1451	Y1393	G1329			ALA	ALA
L1513	L1513	L1452	S1394	A1330			GLY	GLY
L1514	L1514	D1453	L1395	G1331			VAL	VAL
Q1515	Q1515	E1454	A1455	K1332			GLY	GLY
		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 (\AA)	265.6, 265.6, 265.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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

Continued on next page...

Continued from previous page...

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 78

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 65

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	2.32	5 (35%)	17,19,21	1.74	6 (35%)
2	NAG	A	1701	1	14,14,15	2.16	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	5.91	1.53	1.43
2	A	1701	NAG	O5-C1	5.37	1.52	1.43
2	A	1701	NAG	C7-N2	3.91	1.47	1.34
2	A	1702	NAG	C7-N2	3.83	1.47	1.34
2	A	1702	NAG	C2-N2	3.30	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	3.24	116.59	112.19
2	A	1702	NAG	C2-N2-C7	3.01	127.19	122.90
2	A	1702	NAG	C8-C7-N2	2.90	121.01	116.10
2	A	1702	NAG	C4-C3-C2	2.72	115.00	111.02
2	A	1702	NAG	C1-C2-N2	-2.26	106.63	110.49

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.

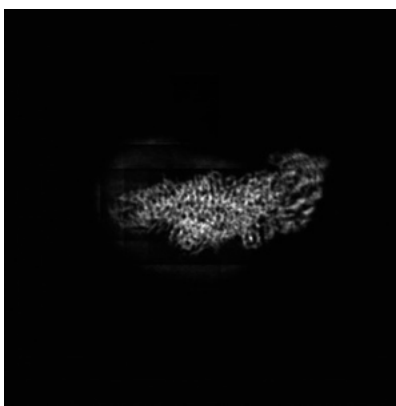
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

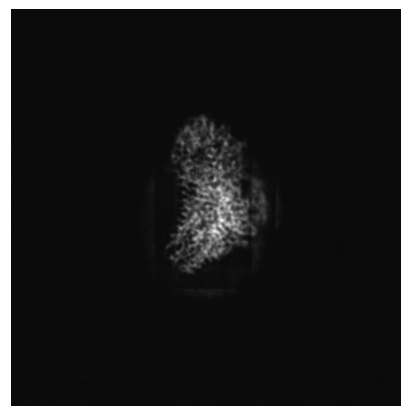
6.1.1 Primary map



X

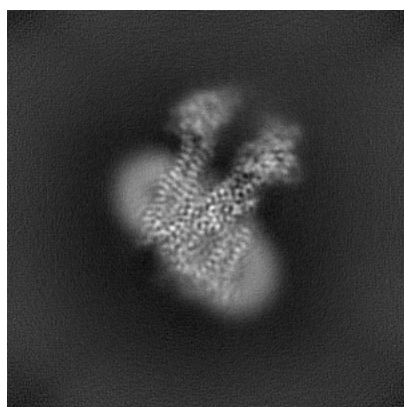


Y

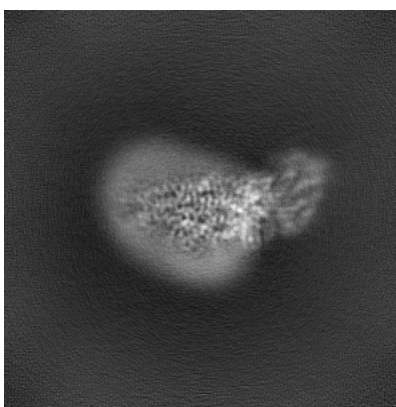


Z

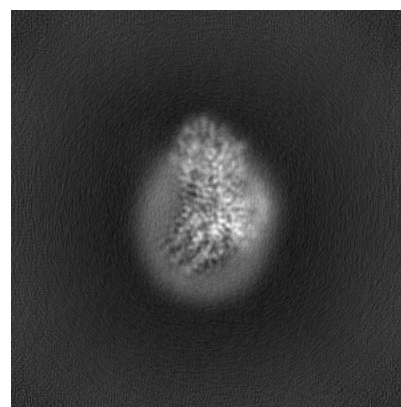
6.1.2 Raw map



X



Y



Z

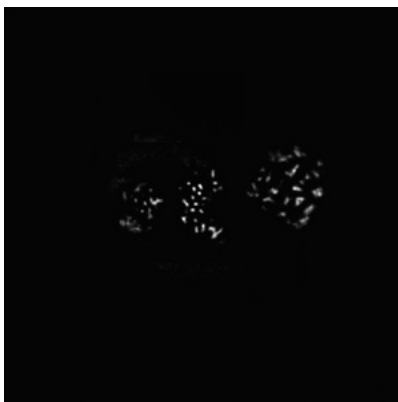
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 160

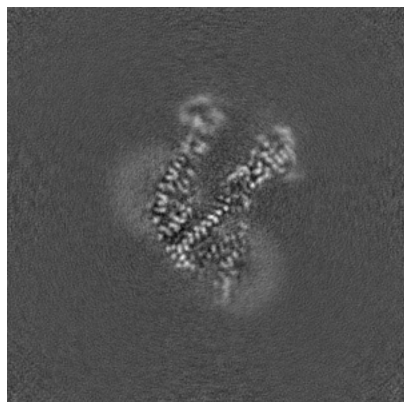


Y Index: 160

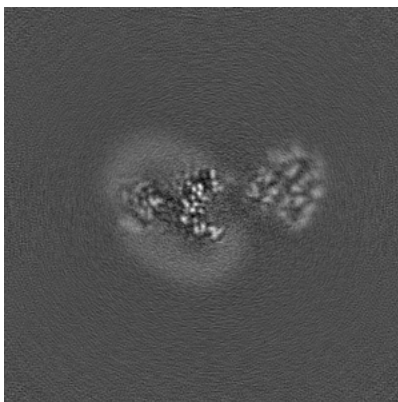


Z Index: 160

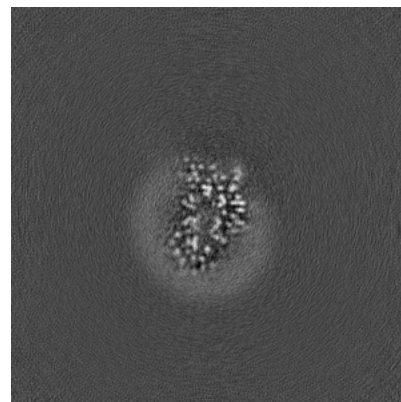
6.2.2 Raw map



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

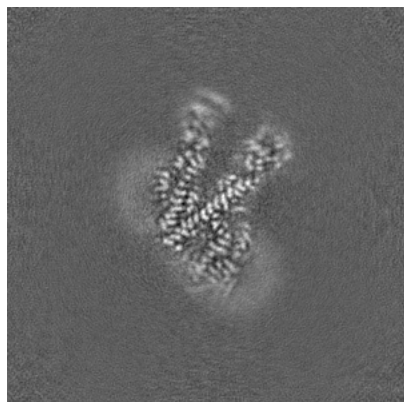


Y Index: 141

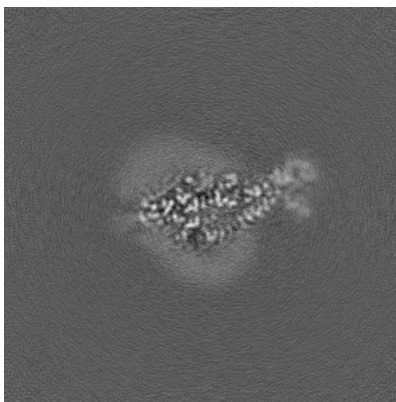


Z Index: 153

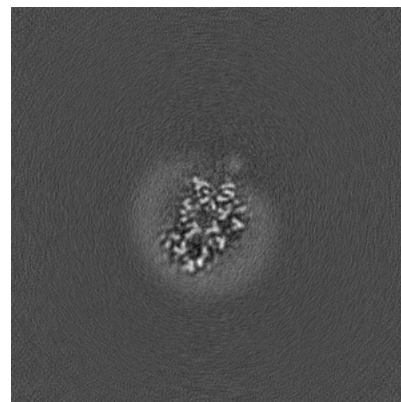
6.3.2 Raw map



X Index: 167



Y Index: 141

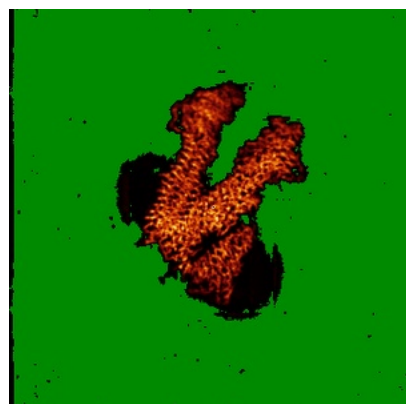


Z Index: 153

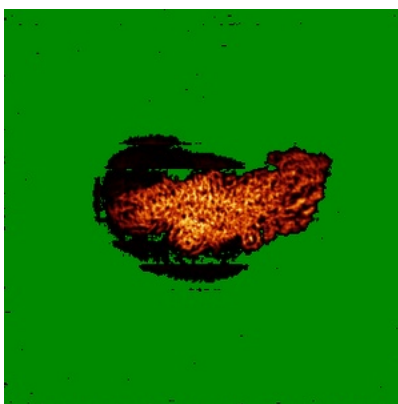
The images above show the largest variance slices of the map in three orthogonal directions.

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

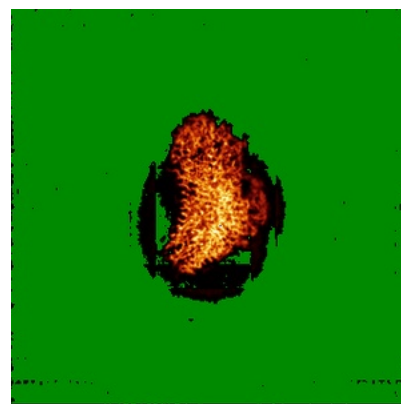
6.4.1 Primary map



X

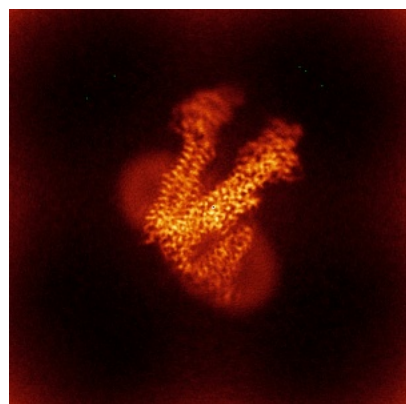


Y

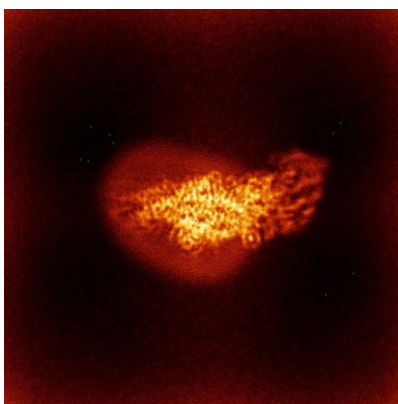


Z

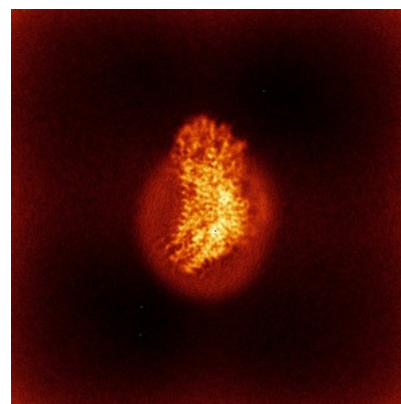
6.4.2 Raw map



X



Y

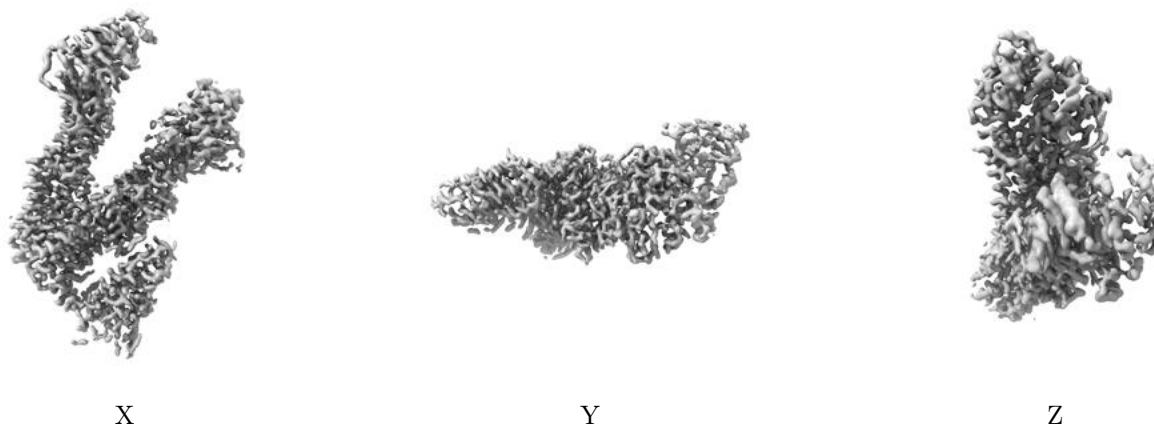


Z

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.

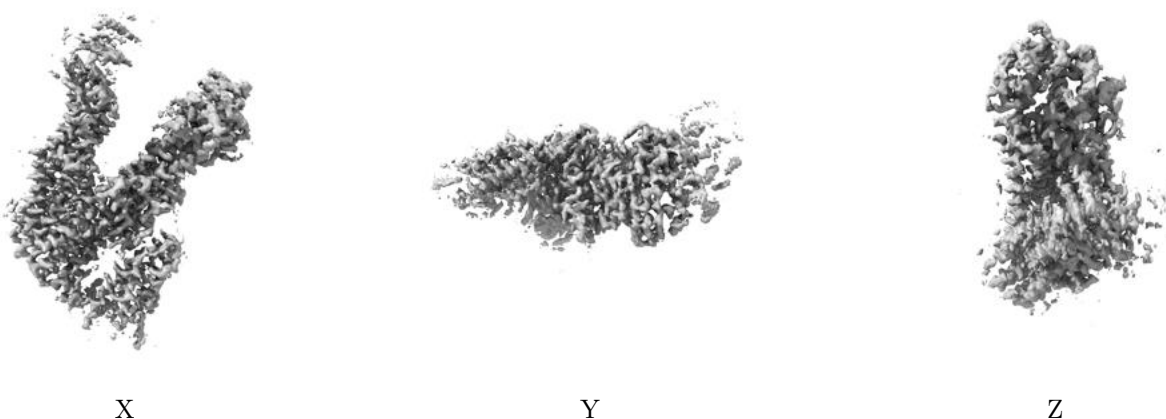
6.5 Orthogonal surface views [i](#)

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.

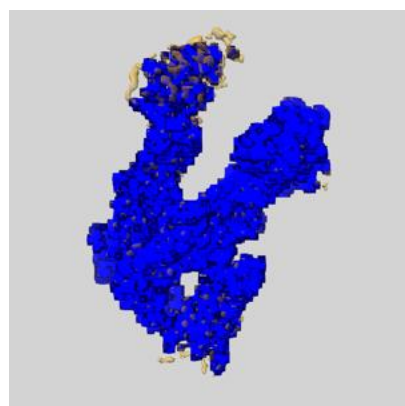
6.6 Mask visualisation [i](#)

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

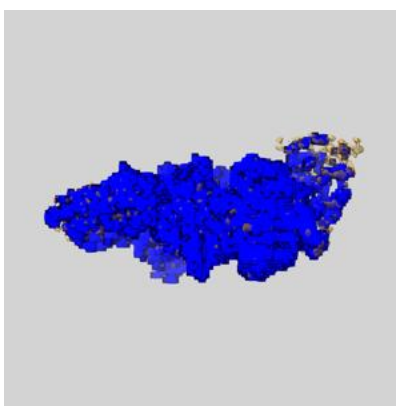
A mask typically either:

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

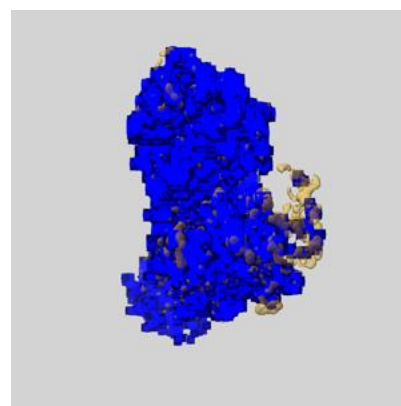
6.6.1 emd_61271_msk_1.map [i](#)



X



Y

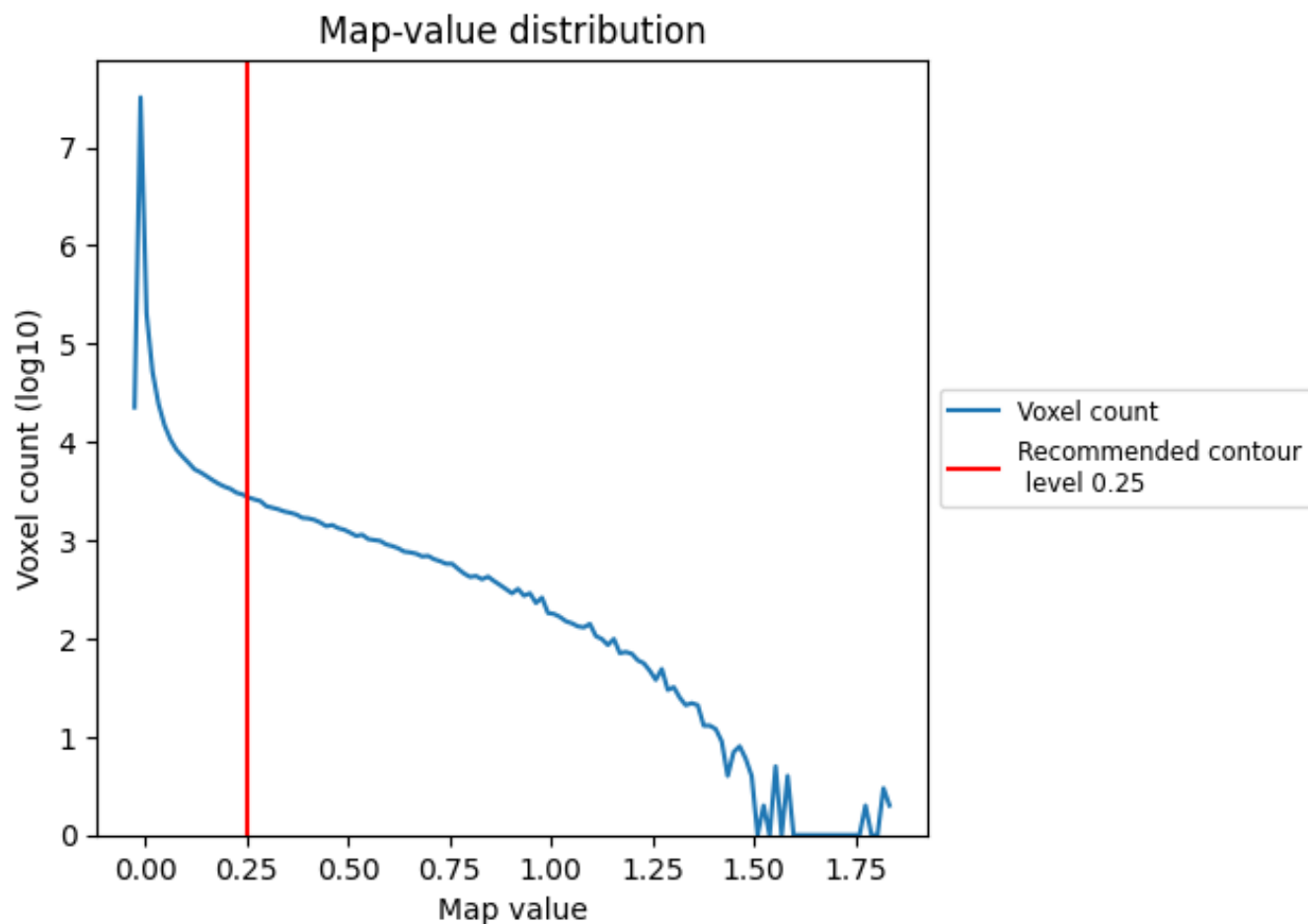


Z

7 Map analysis [i](#)

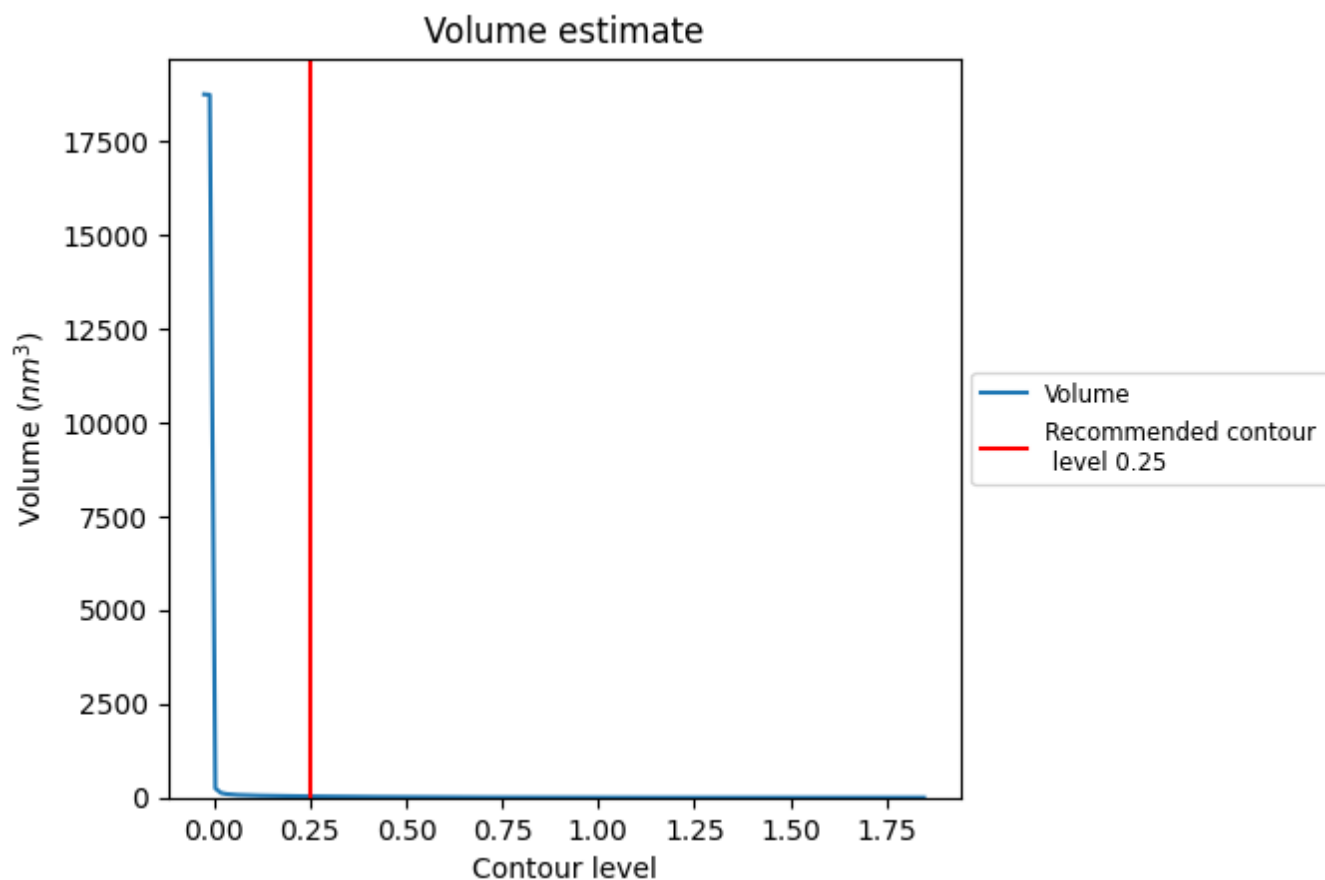
This section contains the results of statistical analysis of the map.

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.

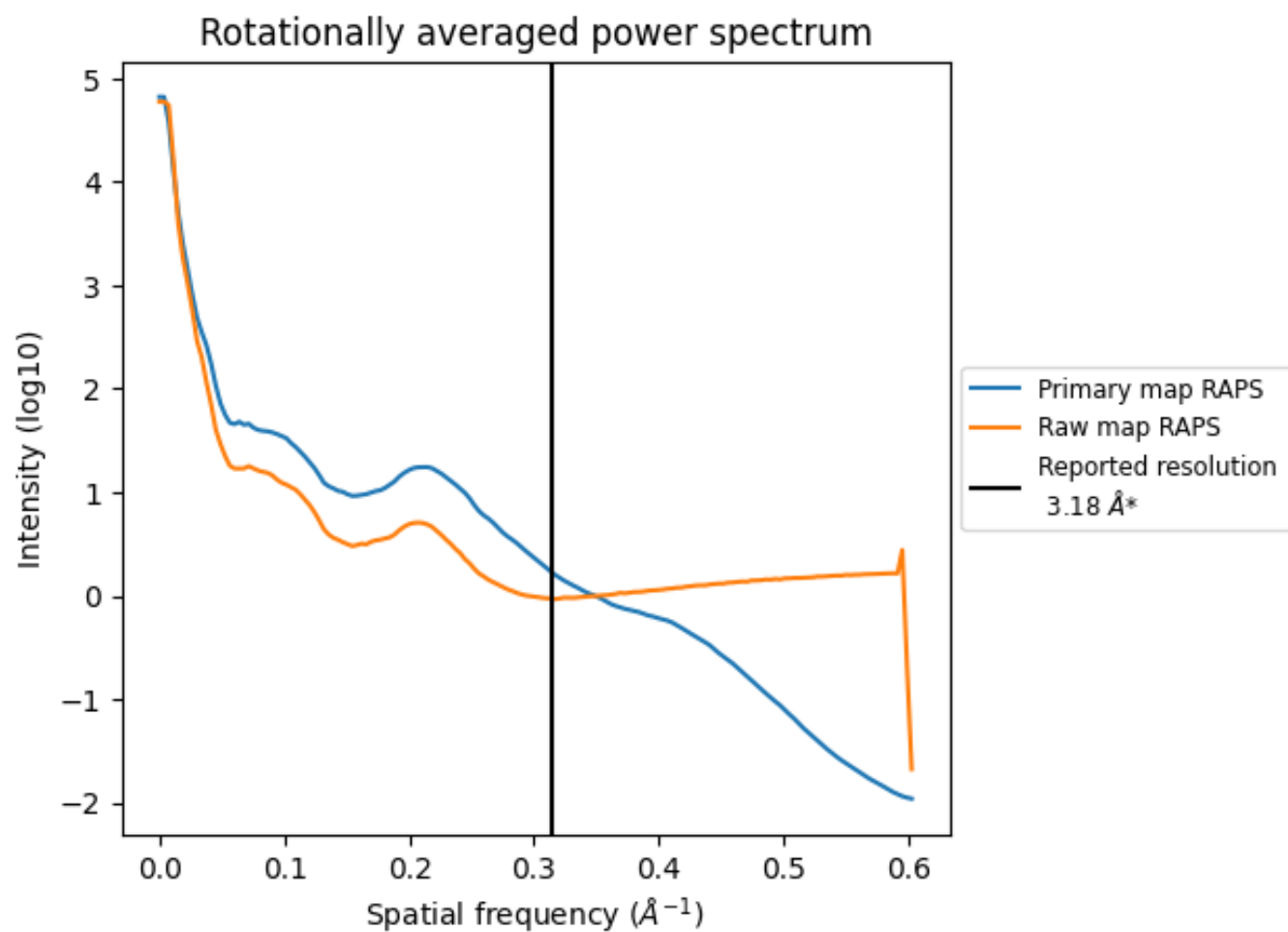
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 32 nm^3 ; 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 ⓘ

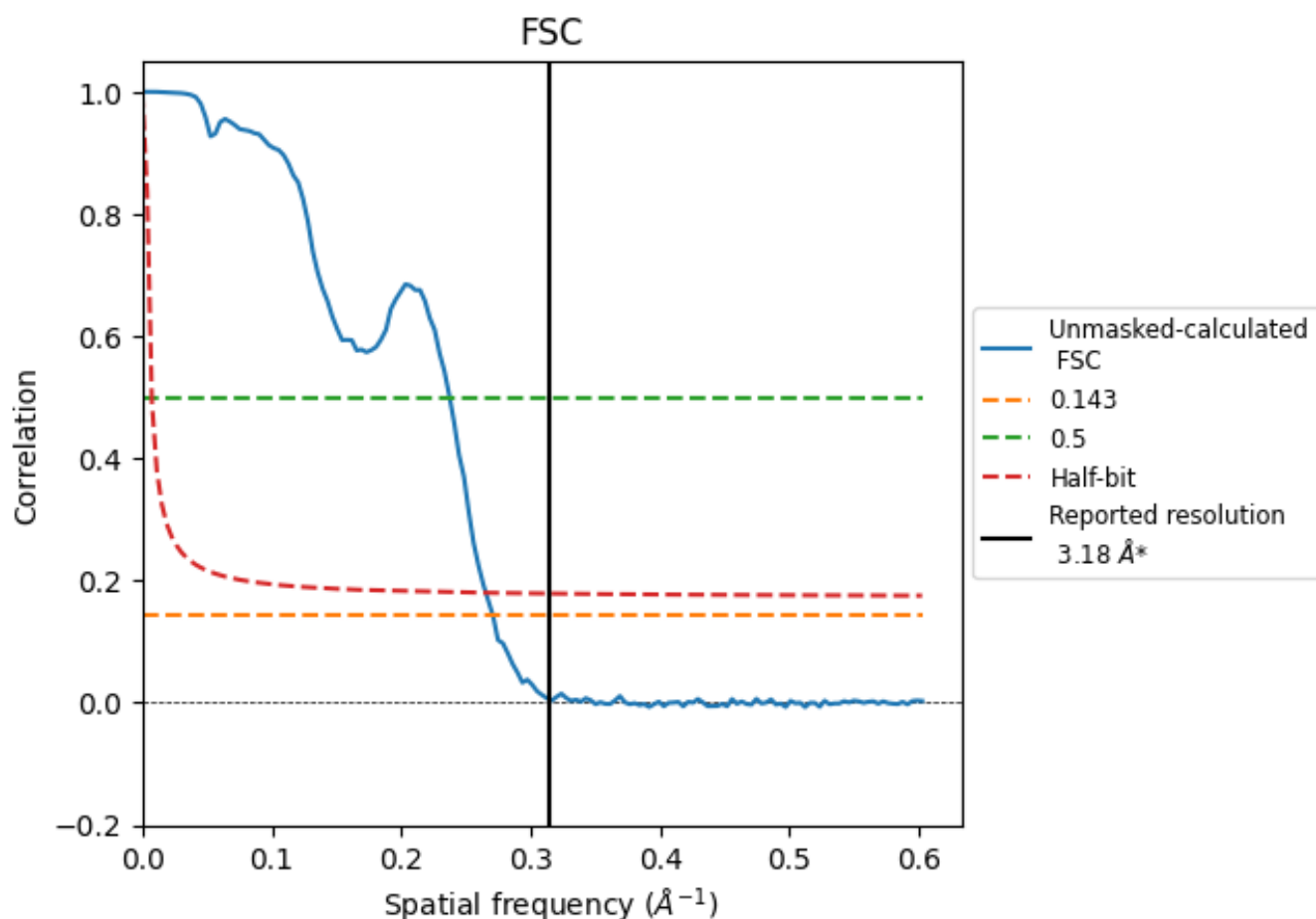


*Reported resolution corresponds to spatial frequency of 0.314 Å⁻¹

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 \AA^{-1}

8.2 Resolution estimates [i](#)

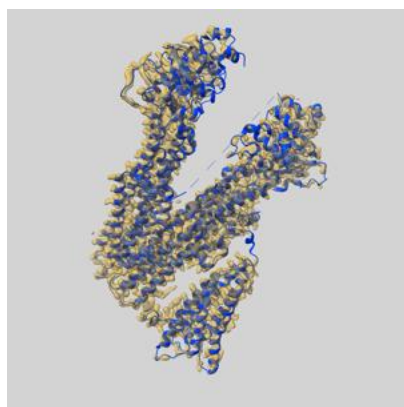
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.18	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.69	4.21	3.77

*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 %

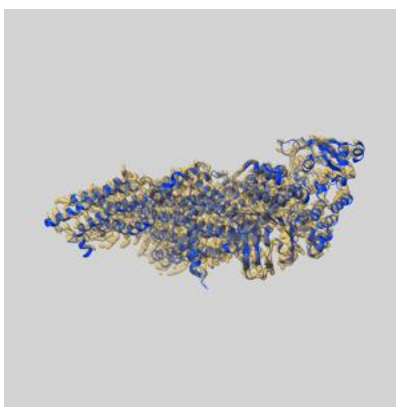
9 Map-model fit [i](#)

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](#).

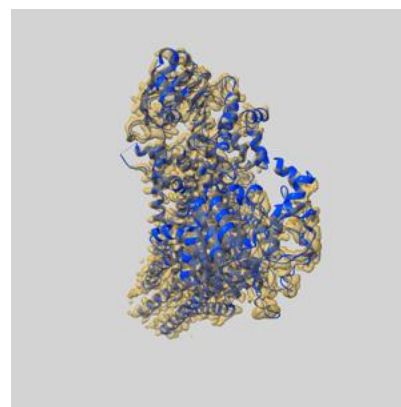
9.1 Map-model overlay [i](#)



X



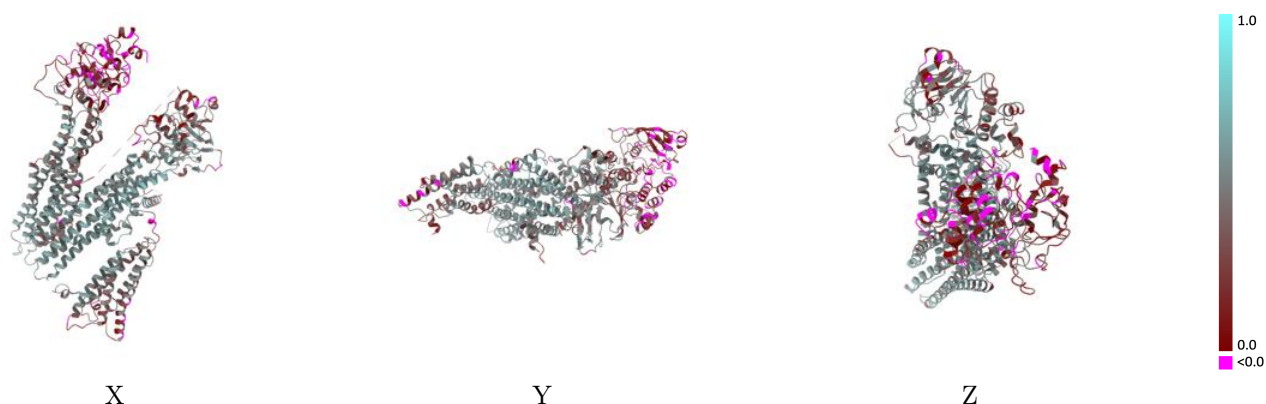
Y



Z

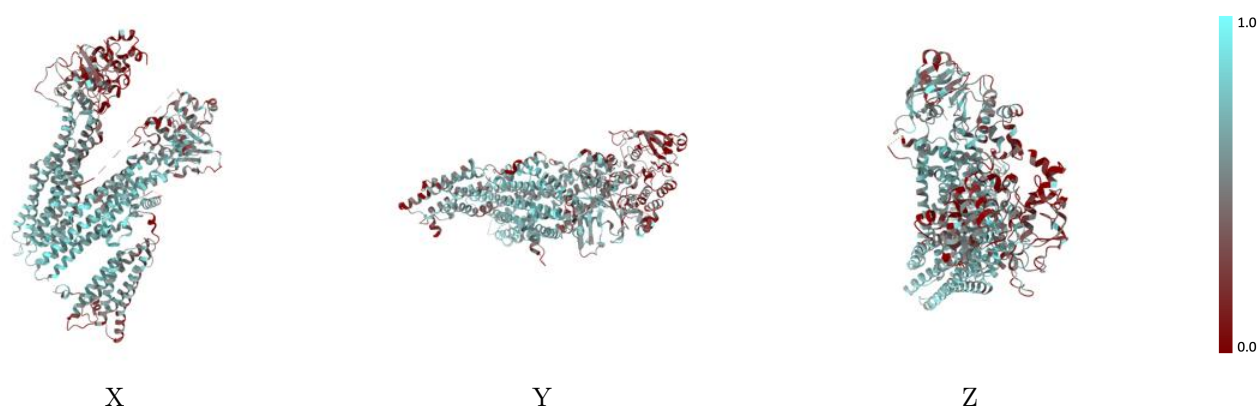
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



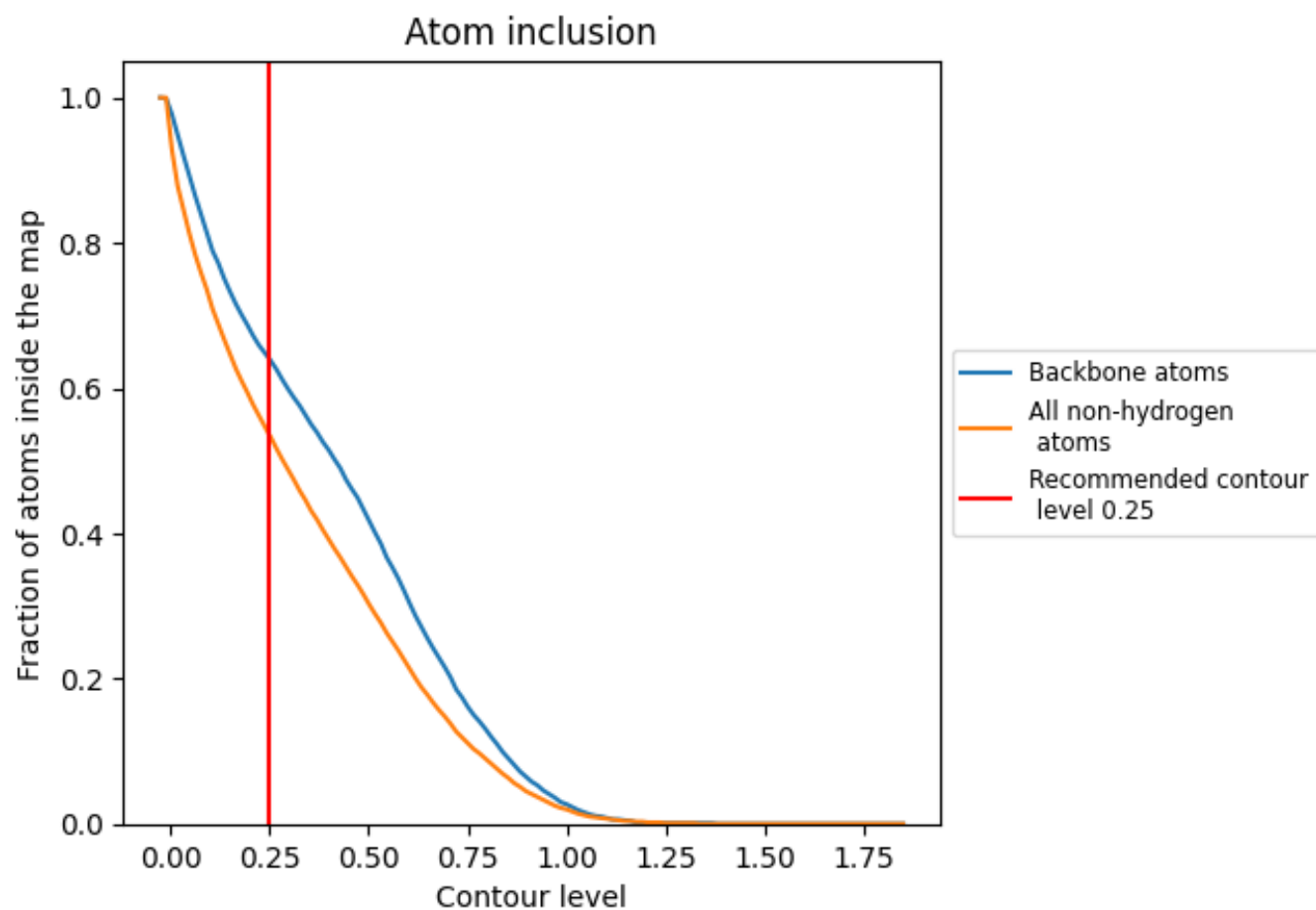
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

9.4 Atom inclusion [i](#)



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	<div></div> 0.5350	<div></div> 0.4060
A	<div></div> 0.5350	<div></div> 0.4060

