



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 04:49 PM UTC

PDB ID : 8SXB / pdb_00008sxb
EMDB ID : EMD-40830
Title : Bovine multidrug resistance protein 4 (MRP4) bound to prostaglandin E2 in MSP lipid nanodisc
Authors : Pourmal, S.; Stroud, R.M.
Deposited on : 2023-05-20
Resolution : 2.90 Å(reported)

This is a Full wwPDB EM Validation 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

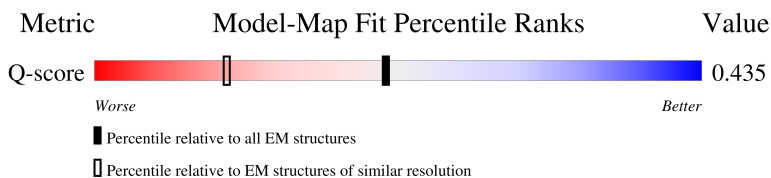
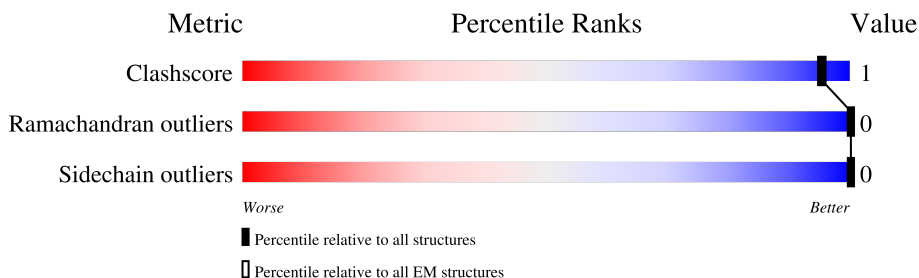
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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	1325	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 18635 atoms, of which 9436 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.

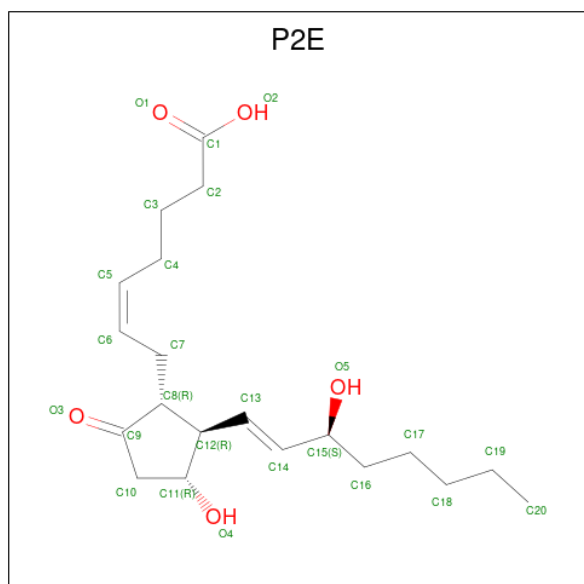
- Molecule 1 is a protein called Multidrug resistance-associated protein 4 isoform X1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	1152	18576	5951	9403	1544	1643	35	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1375	HIS	UNK	conflict	UNP A0A6P5CNW8
A	1864	ASN	UNK	conflict	UNP A0A6P5CNW8
A	2517	ILE	UNK	conflict	UNP A0A6P5CNW8
A	2600	GLU	UNK	conflict	UNP A0A6P5CNW8
A	2638	PHE	LEU	conflict	UNP A0A6P5CNW8

- Molecule 2 is (Z)-7-[(1R,2R,3R)-3-hydroxy-2-[(E,3S)-3-hydroxyoct-1-enyl]-5-oxo-cyclopentyl]hept-5-enoic acid (CCD ID: P2E) (formula: C₂₀H₃₂O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	H	O	0
			56	20	31	5	

- Molecule 3 is water.

Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	H	O	0
			3	2	1	

V2593	Q2594	Q2595	L2596	G2597	K2598	A2599	E2600	A2601	A2602	A2603	L2604	T2605	E2606	T2607	A2608	K2609	Q2610	V2611	Y2612	F2613	K2614	R2615	N2616	P2617	P2618	ASP	ILE	THR	HIS	ASN	GLY	HIS	VAL	VAL	MET	ASN	ALA	SER	SER	GLY	GLN	PRO	SER	ALA	PHE	THR	ILE	PHE	GLU	THR	ALA	LEU							
E2533	L2534	I2535	Q2536	K2537	K2538	I2539	R2540	E2541	K2542	F2543	A2544	H2545	C2546	T2547	V2548	L2549	T2550	I2551	A2552	H2553	R2554	L2555	N2556	T2557	I2558	I2559	D2560	S2561	D2562	K2563	I2564	M2565	V2566	L2567	D2568	S2569	Q2570	R2571	L2572	K2573	E2574	Y2575	D2576	E2577	P2578	Y2579	V2580	L2581	L2582	Q2583	N2584	R2585	D2586	S2587	L2588	F2589	Y2590	K2591	M2592
W2467	N2468	A2469	L2470	E2471	E2472	V2473	Q2474	L2475	K2476	E2477	A2478	I2479	E2480	D2481	L2482	P2483	G2484	K2485	M2486	D2487	T2488	E2489	L2490	A2491	E2492	S2493	G2494	S2495	N2496	F2497	S2498	V2499	G2500	Q2501	R2502	Q2503	L2504	V2505	C2506	A2510	R2513	F2514	I2517	D2521	E2522	A2523	T2524	A2525	N2526	V2527	D2528	P2529	R2530	T2531	D2532				
L2378	K2379	H2380	L2381	T2382	A2383	L2384	I2385	K2386	S2387	K2388	E2389	K2390	V2391	G2392	I2393	V2394	G2395	R2396	T2397	G2398	A2399	G2400	K2401	E2413	P2414	E2415	G2416	K2417	I2418	D2421	K2422	E2427	D2432	K2437	Q2442	E2443	L2446	F2447	T2448	G2449	R2452	K2453	N2459	E2460	H2461	S2462	D2463	E2464	E2465	L2466									

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	187047	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 ($e^-/\text{\AA}^2$)	66	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.115	Depositor
Minimum map value	-2.620	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.066	Depositor
Recommended contour level	0.55	Depositor
Map size (Å)	250.5, 250.5, 250.5	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.835, 0.835, 0.835	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P2E

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	0/9365	0.53	0/12693

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

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	9173	9403	9398	19	0
2	A	25	31	31	0	0
3	A	1	2	0	0	0
All	All	9199	9436	9429	19	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 1.

All (19) 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:2088:TYR:O	1:A:2092:THR:HG23	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2127:ARG:NH2	1:A:2342:GLU:O	2.29	0.64
1:A:2522:GLU:HG2	1:A:2552:ALA:HA	1.89	0.54
1:A:1423:GLU:OE1	1:A:1537:ALA:HB1	2.09	0.52
1:A:1698:GLU:O	1:A:1701:VAL:HG22	2.13	0.48
1:A:2186:ILE:HB	1:A:2187:PRO:HD3	1.94	0.48
1:A:2522:GLU:OE2	1:A:2551:ILE:HG22	2.13	0.48
1:A:2551:ILE:HD12	1:A:2551:ILE:H	1.79	0.48
1:A:2189:VAL:HB	1:A:2190:PRO:HD3	1.98	0.45
1:A:2522:GLU:CG	1:A:2551:ILE:HG22	2.47	0.45
1:A:1436:ILE:HD12	1:A:1461:LEU:HD22	1.99	0.44
1:A:1689:PHE:HB3	1:A:1690:PRO:HD3	1.98	0.44
1:A:1497:LYS:NZ	1:A:1714:GLU:OE1	2.40	0.44
1:A:2560:ASP:OD1	1:A:2560:ASP:N	2.51	0.44
1:A:1368:LEU:HD23	1:A:1368:LEU:H	1.85	0.42
1:A:1655:THR:O	1:A:1658:THR:HG22	2.19	0.42
1:A:1475:TYR:CZ	1:A:1479:VAL:HG11	2.54	0.41
1:A:1774:LEU:C	1:A:1774:LEU:HD23	2.46	0.41
1:A:2237:TYR:N	1:A:2237:TYR:CD1	2.89	0.41

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	1144/1325 (86%)	1121 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	999/1156 (86%)	999 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1386	GLN
1	A	1749	GLN
1	A	1871	GLN
1	A	2254	HIS
1	A	2442	GLN
1	A	2503	GLN
1	A	2526	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	P2E	A	2701	-	25,25,25	0.73	1 (4%)	25,31,31	1.10	3 (12%)

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	P2E	A	2701	-	-	4/19/35/35	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2701	P2E	O2-C1	-2.76	1.21	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2701	P2E	C16-C15-C14	-2.49	107.18	111.94
2	A	2701	P2E	O2-C1-C2	2.23	121.03	114.00
2	A	2701	P2E	C11-C10-C9	-2.15	102.65	105.56

There are no chirality outliers.

All (4) torsion outliers are listed below:

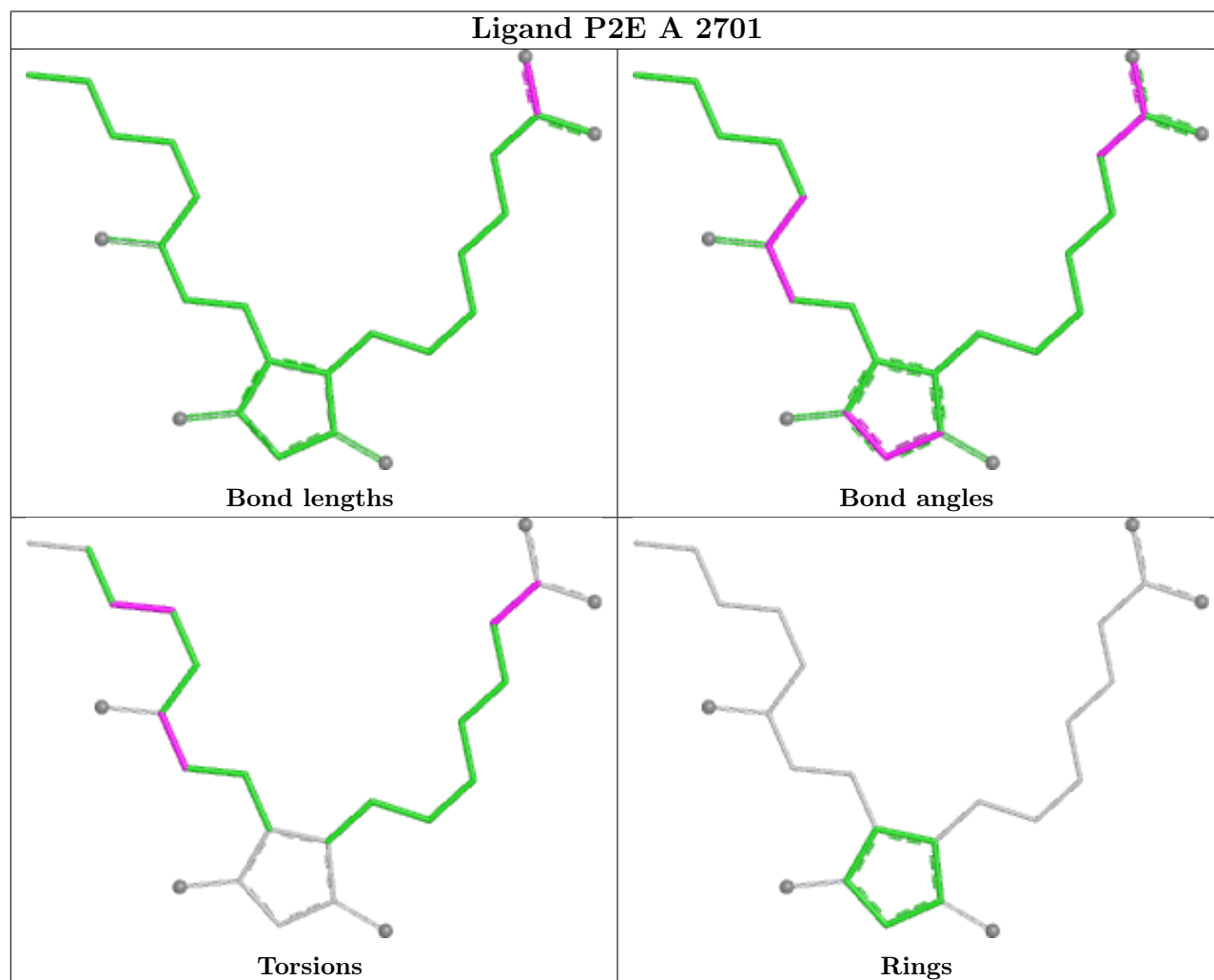
Mol	Chain	Res	Type	Atoms
2	A	2701	P2E	C13-C14-C15-O5
2	A	2701	P2E	C13-C14-C15-C16
2	A	2701	P2E	C16-C17-C18-C19
2	A	2701	P2E	O2-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

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.

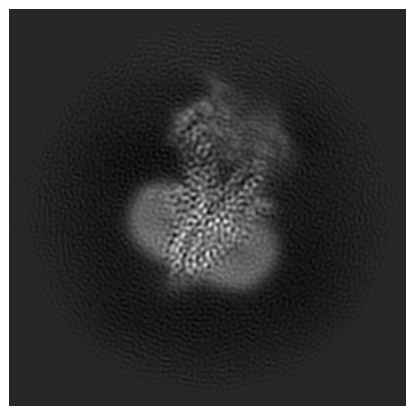
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40830. These allow visual inspection of the internal detail of the map and identification of artifacts.

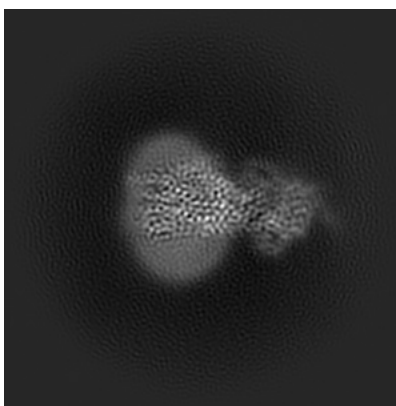
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

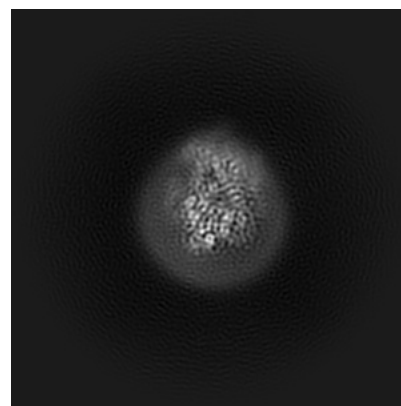
6.1.1 Primary map



X

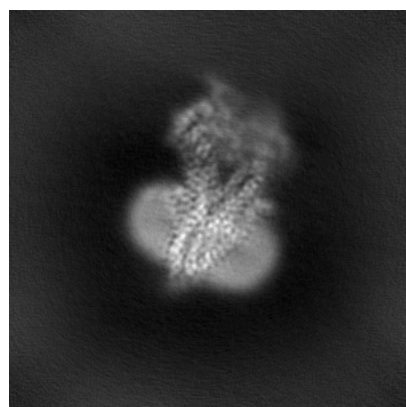


Y

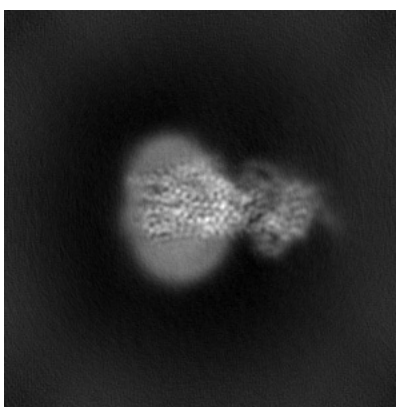


Z

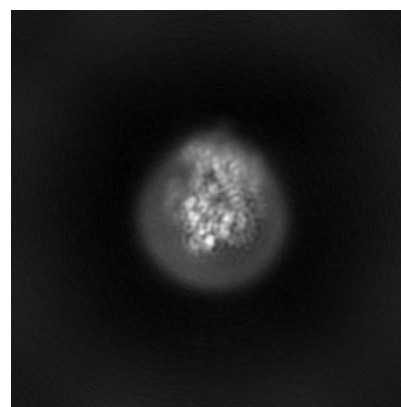
6.1.2 Raw map



X



Y

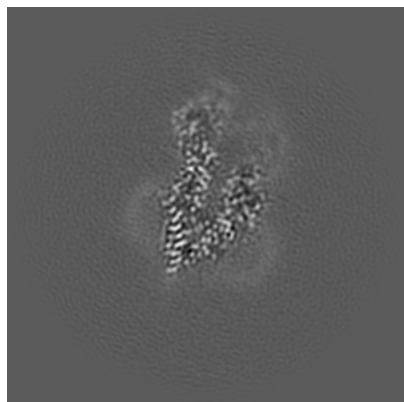


Z

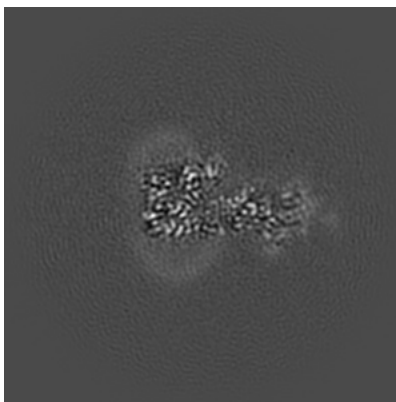
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

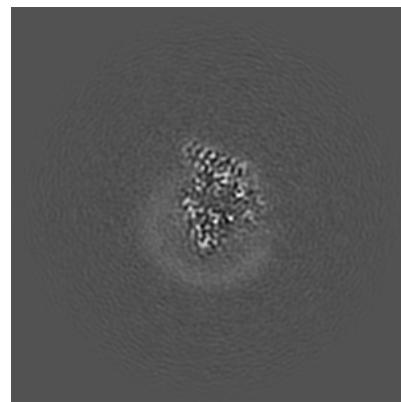
6.2.1 Primary map



X Index: 150

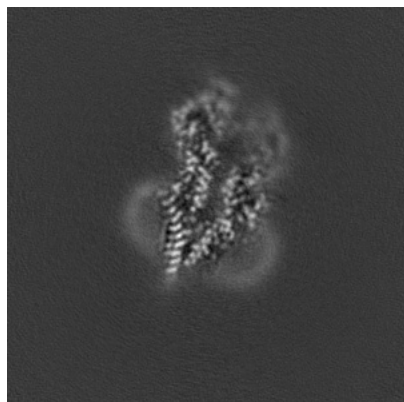


Y Index: 150

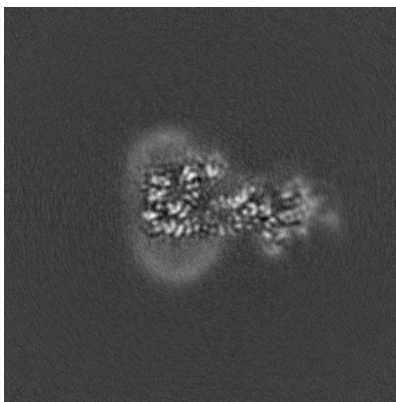


Z Index: 150

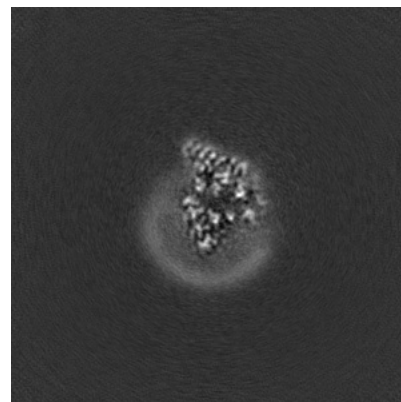
6.2.2 Raw map



X Index: 150



Y Index: 150

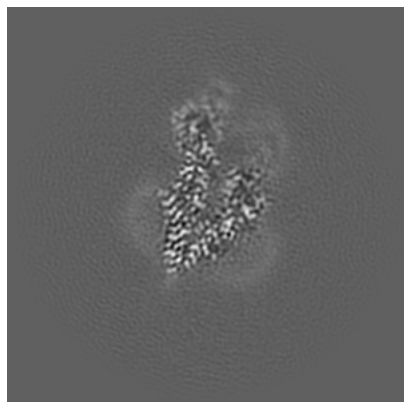


Z Index: 150

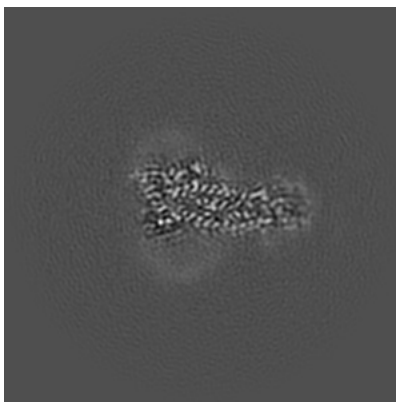
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

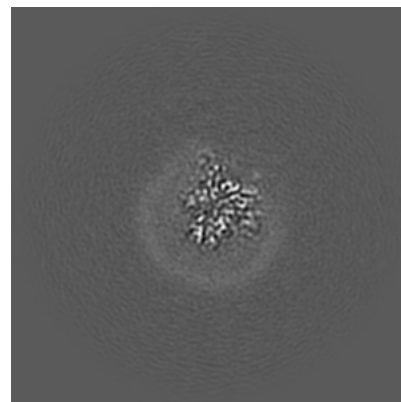
6.3.1 Primary map



X Index: 149

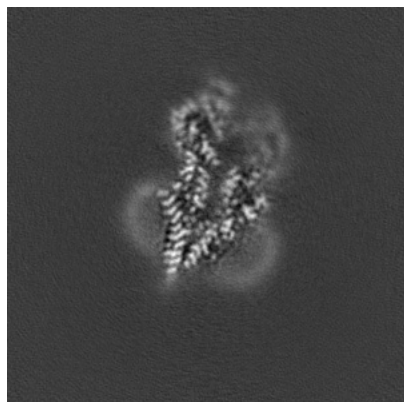


Y Index: 142

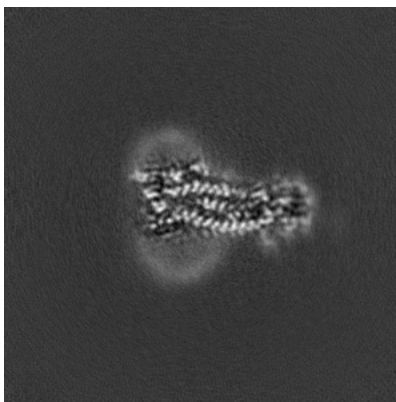


Z Index: 140

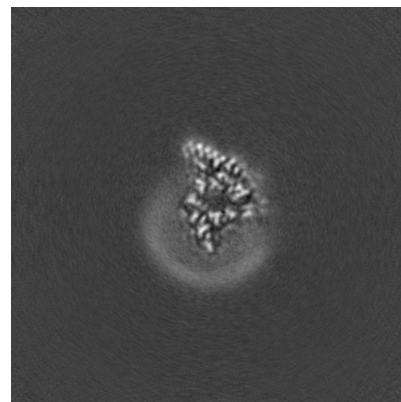
6.3.2 Raw map



X Index: 149



Y Index: 143

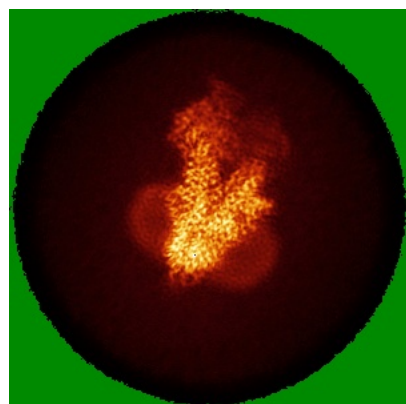


Z Index: 152

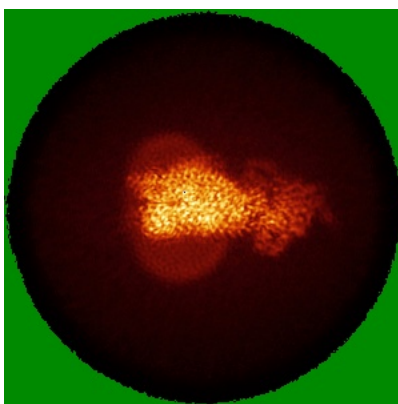
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

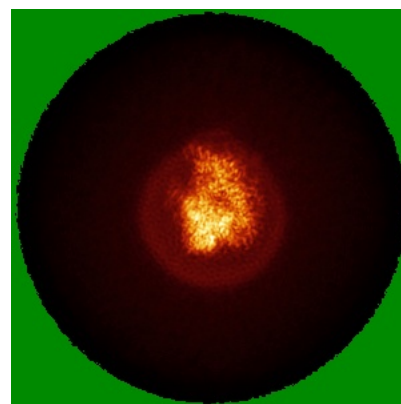
6.4.1 Primary map



X

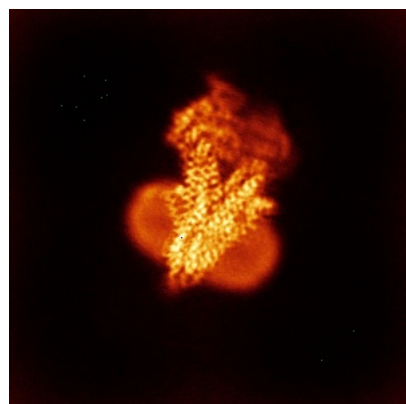


Y

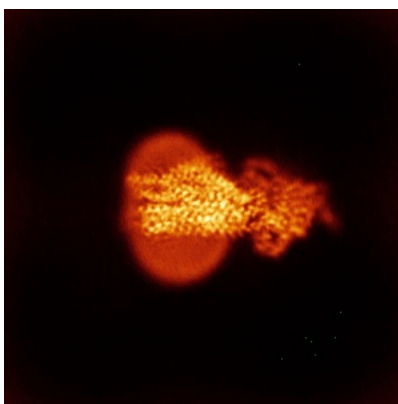


Z

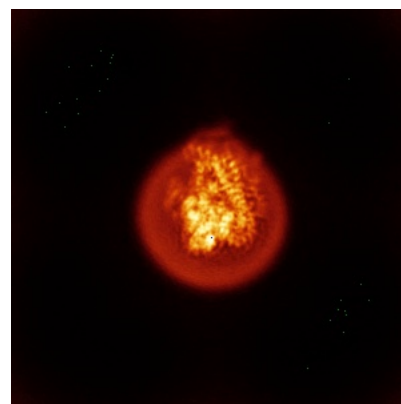
6.4.2 Raw map



X



Y

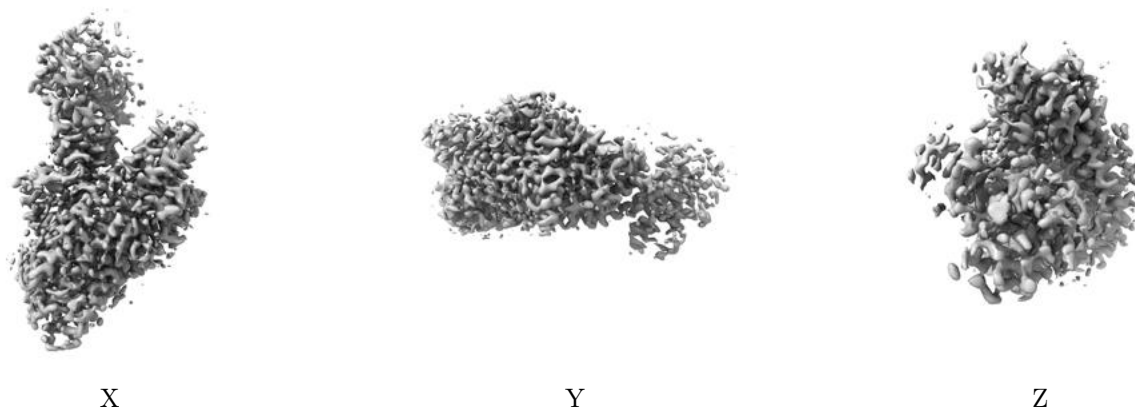


Z

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.

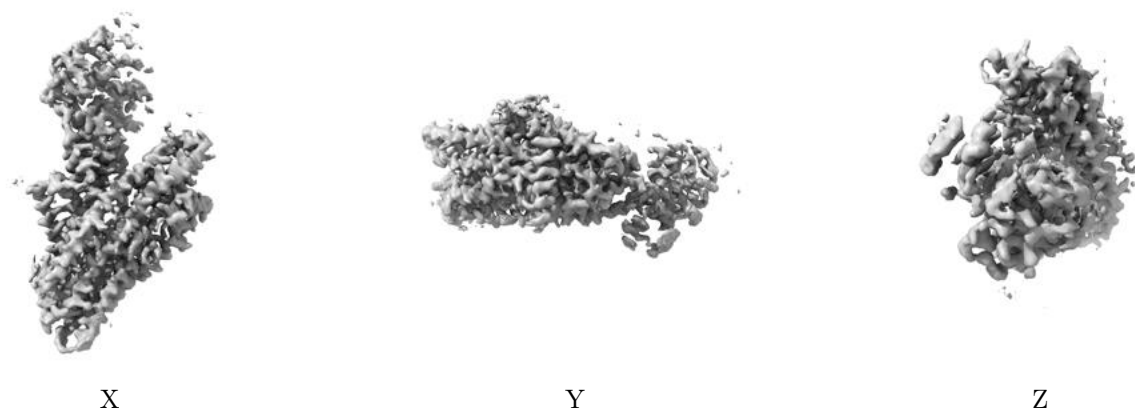
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.55. 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.

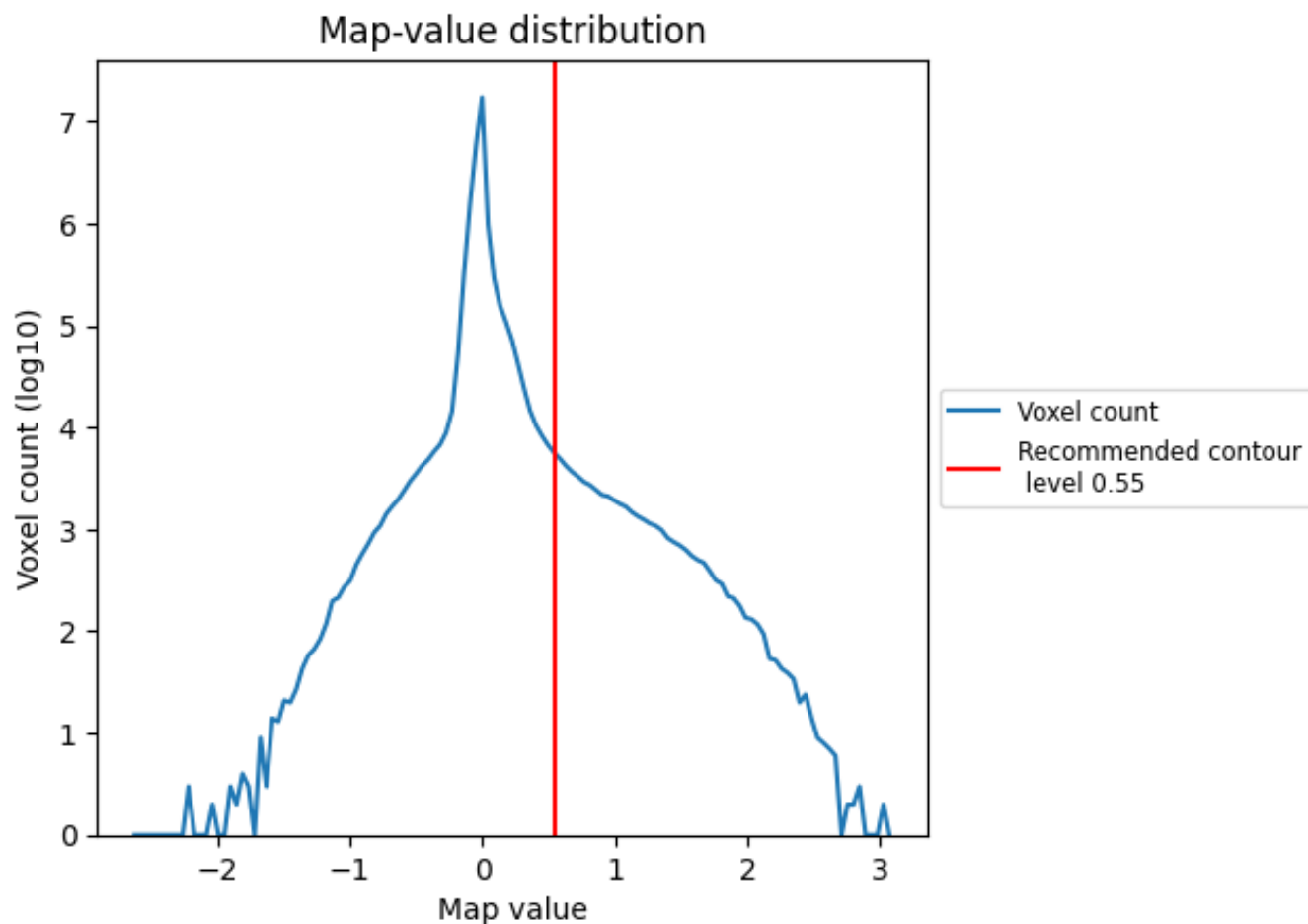
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

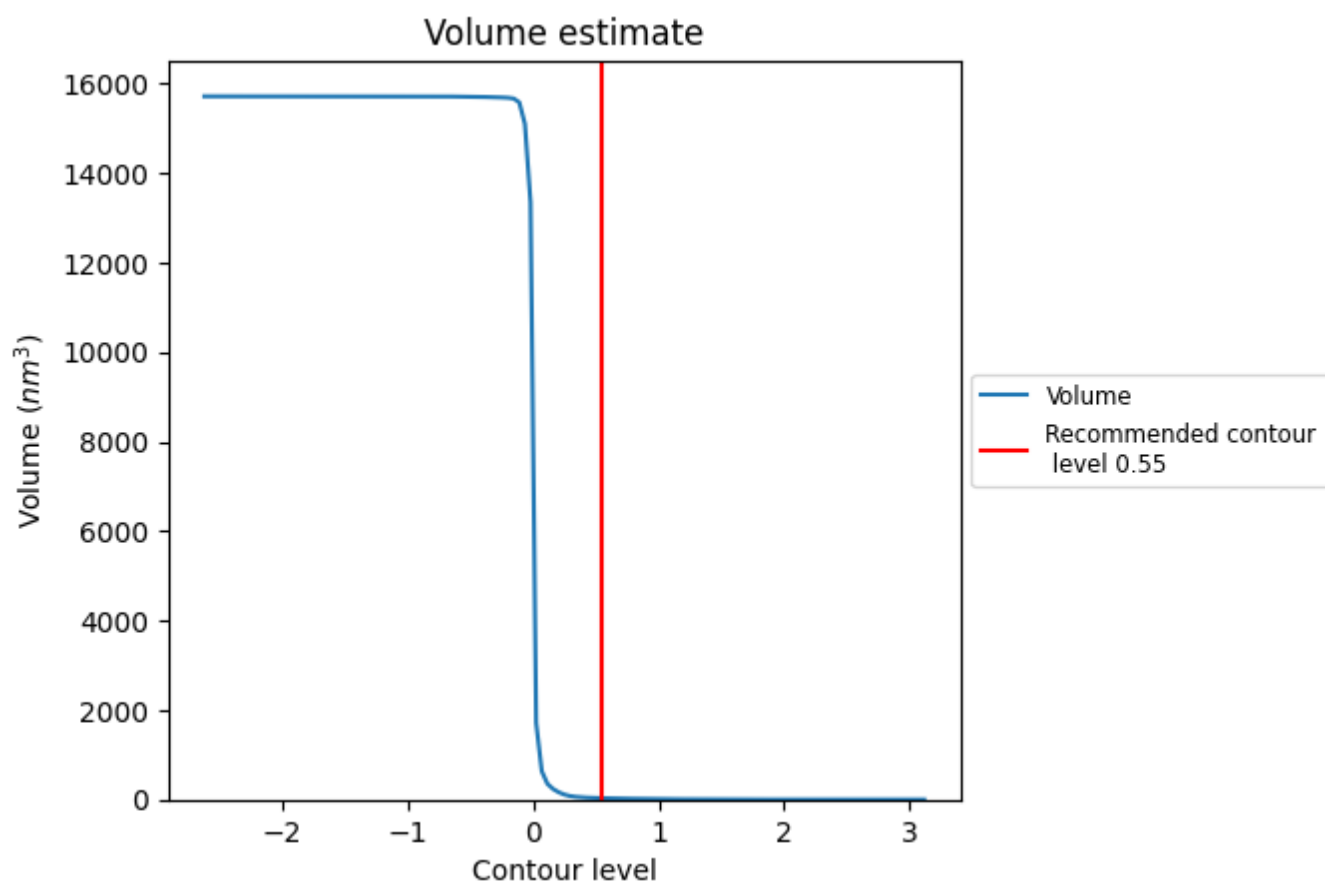
This section contains the results of statistical analysis of the map.

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.

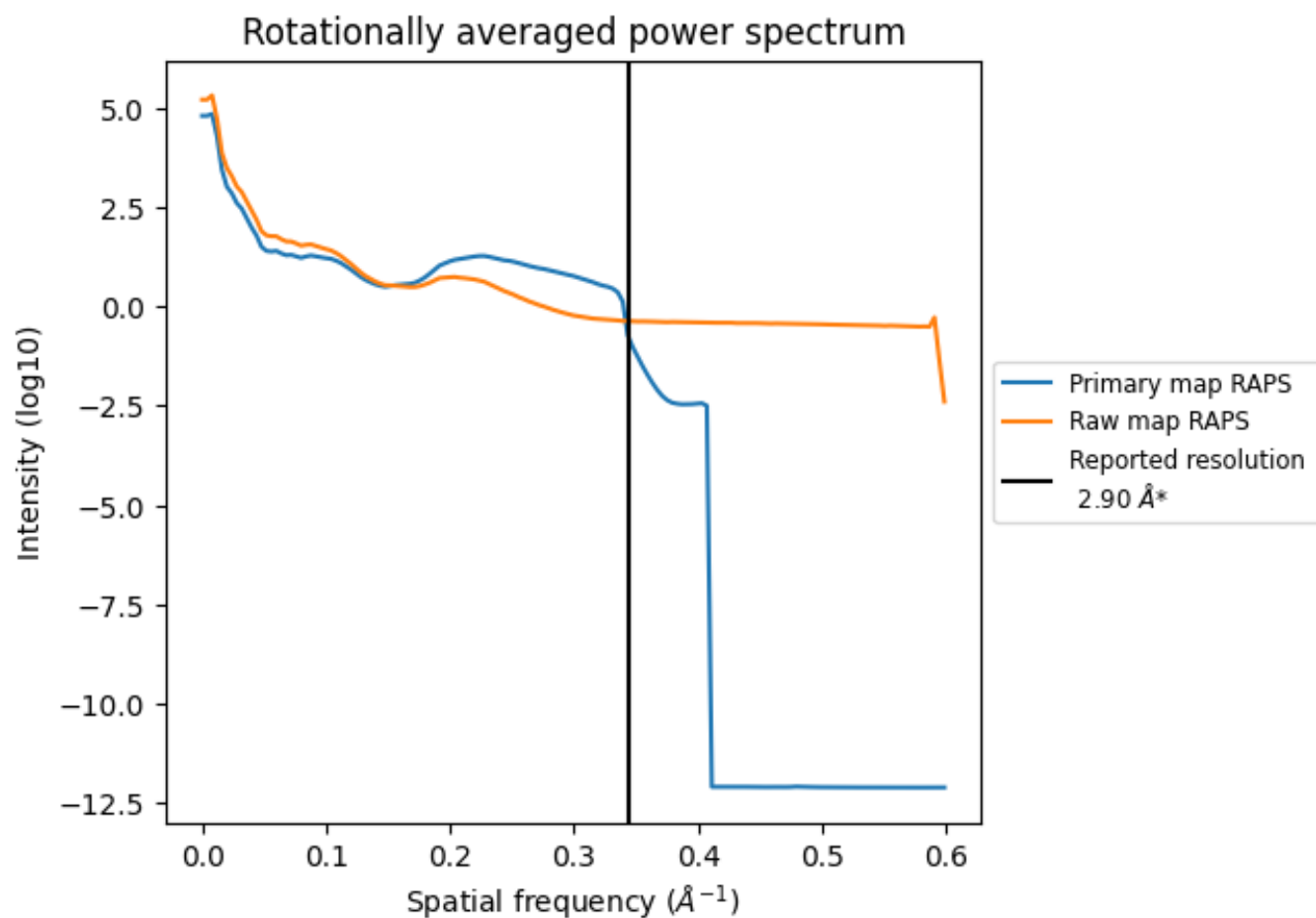
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 31 nm^3 ; this corresponds to an approximate mass of 28 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 ⓘ

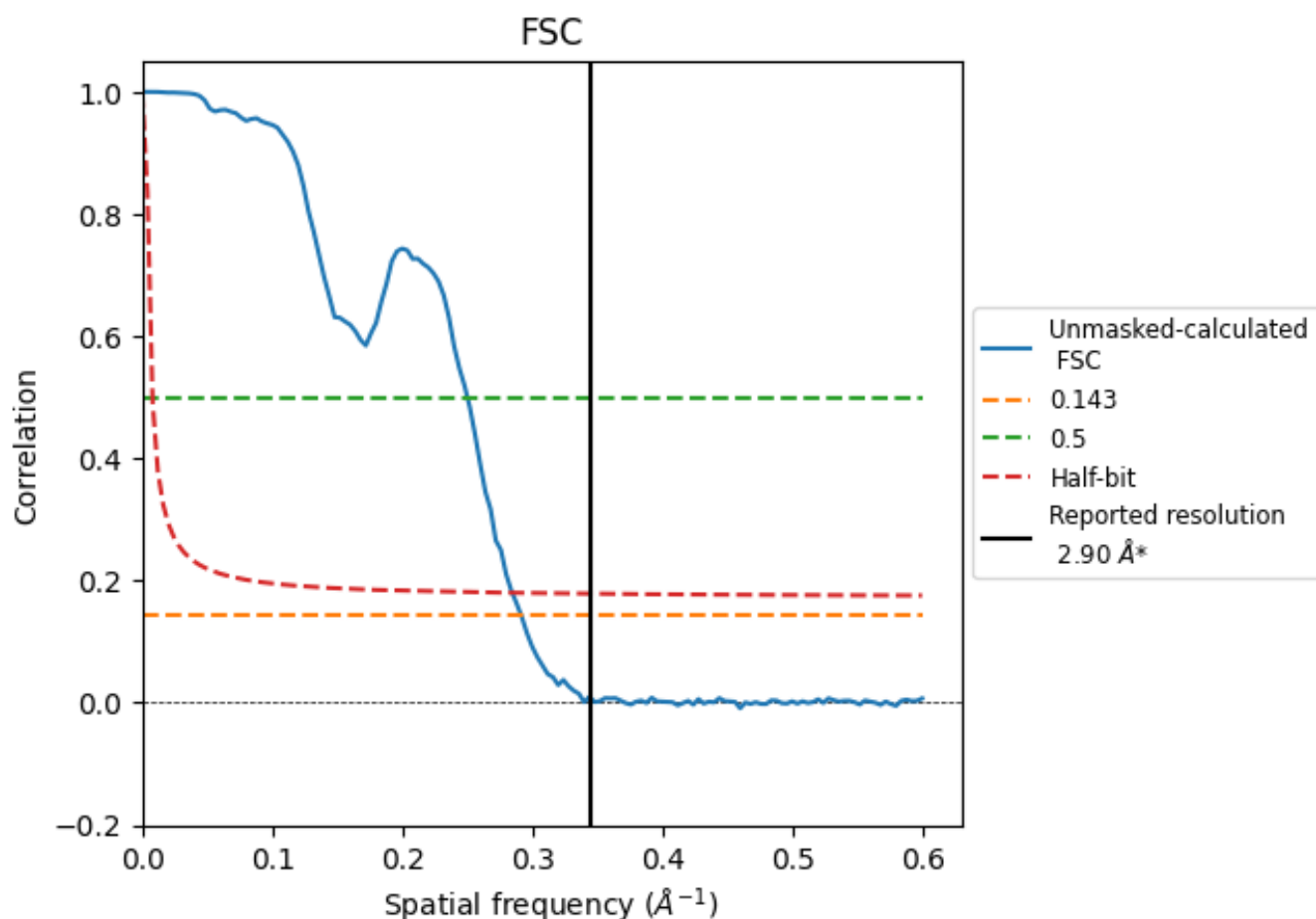


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

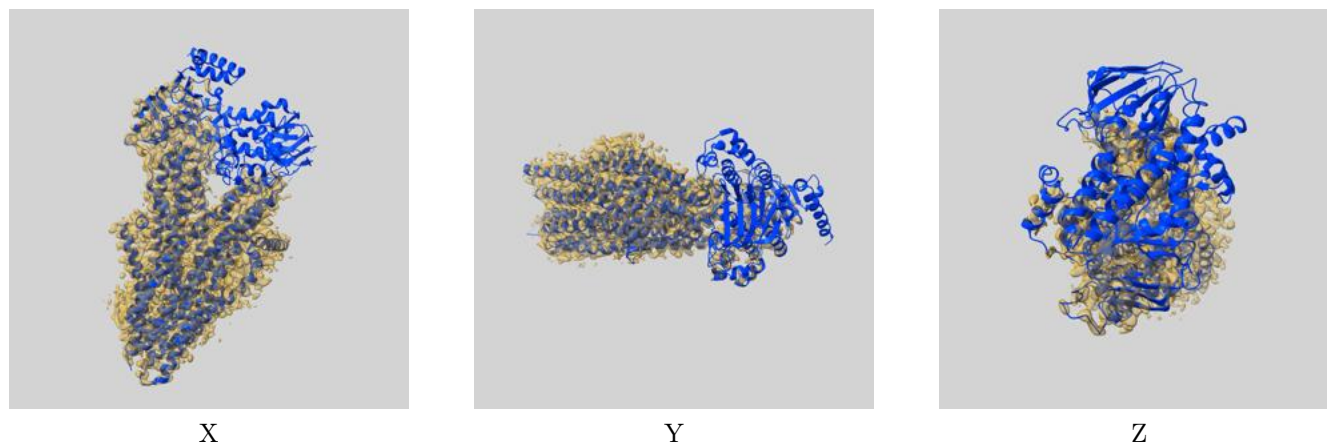
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.44	4.01	3.52

*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 3.44 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

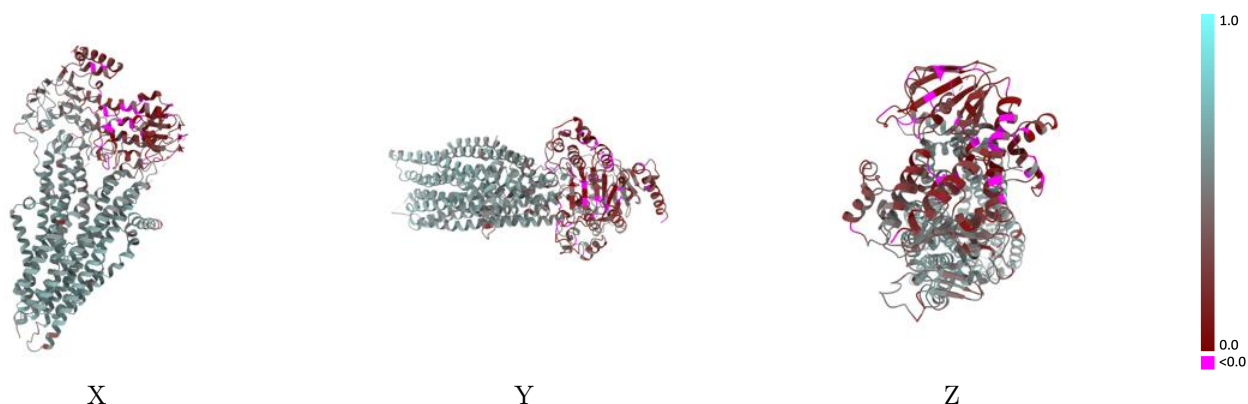
This section contains information regarding the fit between EMDB map EMD-40830 and PDB model 8SXB. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



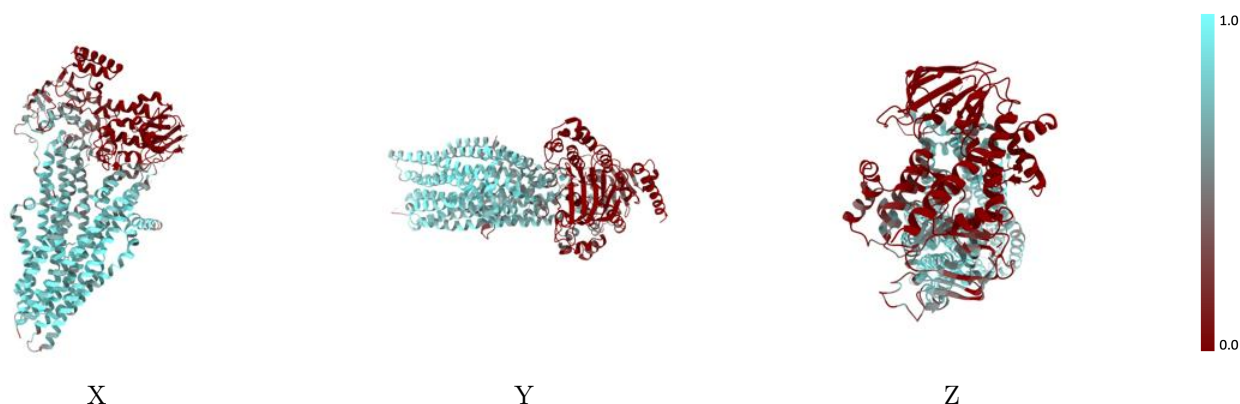
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



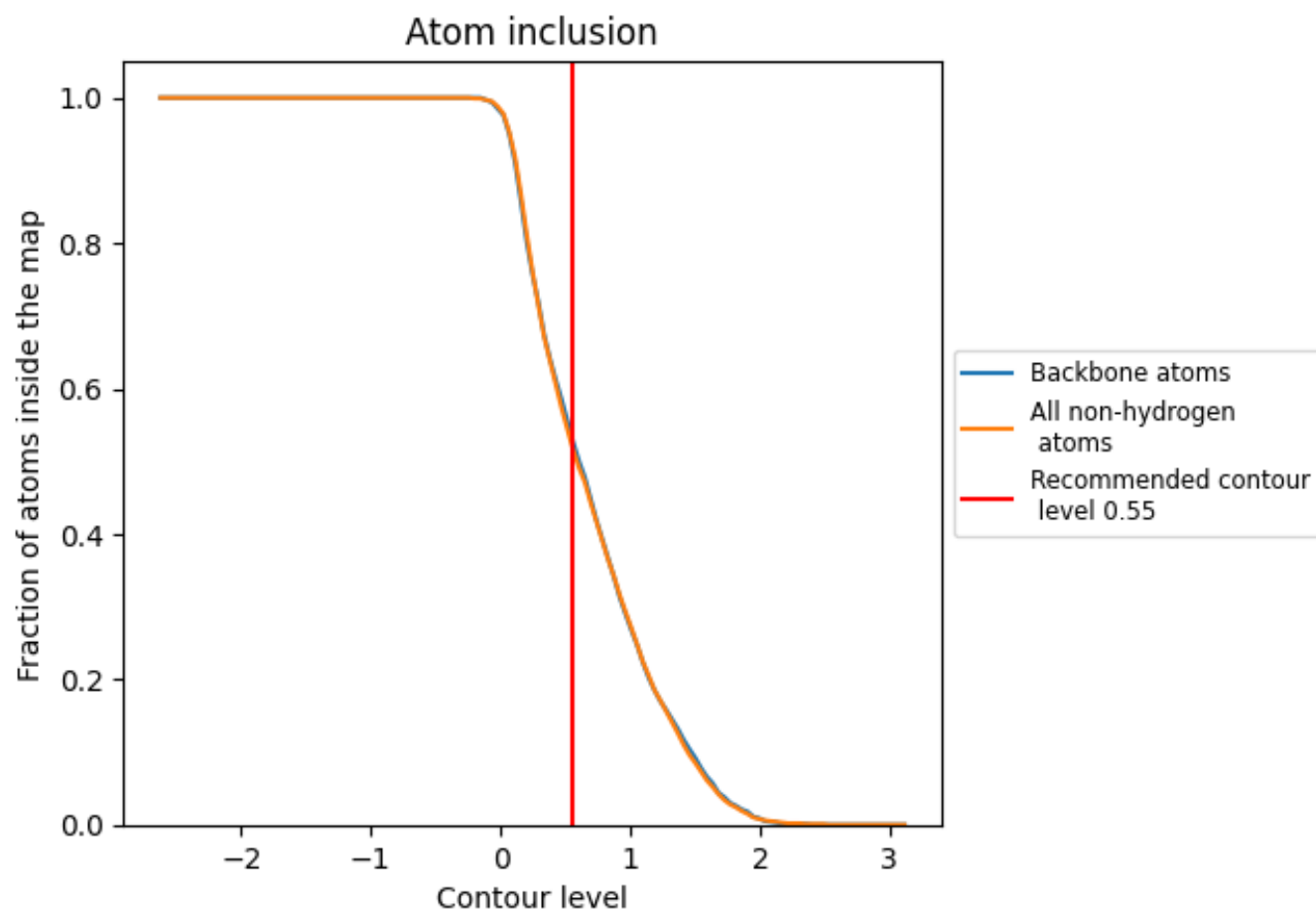
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.55).

9.4 Atom inclusion [i](#)



At the recommended contour level, 53% of all backbone atoms, 52% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5220	0.4350
A	0.5190	0.4350

