



wwPDB EM Validation Summary Report ⓘ

Sep 9, 2025 – 01:42 PM JST

PDB ID : 9JXE / pdb_00009jxe
EMDB ID : EMD-61860
Title : Cryo-EM structure of apo human XPR1, class 1, with one visible SPX domain
Authors : Wang, X.; Bai, Z.; Wallis, C.; Wang, H.; Han, Y.; Jin, R.; Lei, M.; Gu, C.;
Jessen, H.; Shears, S.; Sun, Y.; Corry, B.; Zhang, Y.
Deposited on : 2024-10-11
Resolution : 3.85 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
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

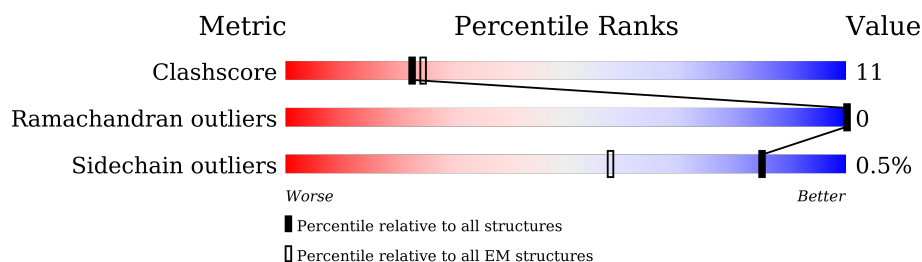
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.85 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	625	<div> <div>8%</div> <div>45%</div> <div>15%</div> <div>40%</div> </div>
1	B	625	<div> <div>23%</div> <div>64%</div> <div>21%</div> <div>15%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7577 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 Solute carrier family 53 member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	375	Total	C	N	O	S	0	0
			3132	2108	500	509	15		
1	B	531	Total	C	N	O	S	0	0
			4445	2960	717	749	19		

- Molecule 1: Solute carrier family 53 member 1



K68	I69	S74	E75	K76	L77	A78	E79	A80	Q81	R82	R83	F84	A85	T86	L87	Q88	N89	E90	L91	Q92	S93	SER	LEU	LEU	ASP	ALA	GLN	LYS	GLU	SER	THR	GLY	THR	VAL	THR	LEU	ARG	GLN	ARG	LYS	PRO	VAL	PHE	HIS	LEU	SER	HIS	GLU	GLU	ARG	VAL	GLN	HIS	ARG	ASN	I128	K129	D130
L131	K132	L133	A134	F135	S136	E137	F138	Y139	L140	S141	L142	I143	Y148	Q149	M150	Q88	L151	N152	F153	R157	K162	H163	D164	K165	I166	L167	E168	T169	S170	R171	G172	A173	D174	W175	R176	V177	A178	H179	V180	E181	V182	A183	P184	F185	Y186	T187	C188	K189	K190	I191	N192	Q193	L194	I195	S196	E197	T198	
E199	A200	V201	V202	T203	N204	E205	LEU	GLU	ASP	GLY	ASP	ARG	GLN	LYS	ALA	MET	LYS	ARG	LEU	VAL	PRO	PRO	GLY	ALA	ALA	GLN	PRO	A229	T233	V237	V246	L251	V256	L259	E260	T261	D262	R263	S264	P267	R270	I271	Y272	R273	G274	L277	L282											
F283	L284	N288	W292	V297	F303	E304	L305	N306	P307	R308	Q314	E318	I319	A320	L326	S330	L331	P338	I339	F354	F357	I360	Y367	F379	R380	V381	F382	T383	A384	P385	S402	L403	I406	L407	M408	D409	Y412	M413	S418	L419	E420																	
LEU	LYS	TRP	ASP	GLU	SER	LYS	GLY	LEU	LEU	PRO	ASN	ASN	SER	GLU	GLY	SER	GLY	ILE	CYS	HIS	LYS	Y443	T444	Y445	L458	I461	Q462	R468	R472	A473	L477	V478	G481	K482	T485	F488	M489	V490	T491	F492	H499	K500	E501	R502	G503	H504	S505	D506	T507	M508								
V509	Y512	L513	W514	I515	V516	F517	Y518	I519	I520	Y524	T525	L526	D529	W534	G535	L536	K539	N540	A541	G542	E543	F546	L547	R548	E549	E550	I551	Y559	Y560	C561	A562	I563	I564	V567	I568	T574	I577	T582	T583	L584	L585	P586	H587	D590	T591	I592												
V595	F596	A597	V601	R604	F605	W606	W607	W608	F609	L612	E613	H616	L617	G621	E622	F623	R624	A625																																								

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	94997	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 ($e^-/\text{\AA}^2$)	49.41	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	2.145	Depositor
Minimum map value	-1.462	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.052	Depositor
Recommended contour level	0.418	Depositor
Map size (\AA)	274.3, 274.3, 274.3	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.055, 1.055, 1.055	Depositor

5 Model quality

5.1 Standard geometry

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	0.22	0/3237	0.37	0/4406
1	B	0.20	0/4578	0.35	0/6206
All	All	0.21	0/7815	0.36	0/10612

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	3132	0	3122	74	0
1	B	4445	0	4424	97	0
All	All	7577	0	7546	168	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 11.

The worst 5 of 168 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:246:VAL:HG11	1:B:246:VAL:HG11	1.13	1.10
1:A:578:SER:O	1:A:581:SER:OG	1.91	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:PRO:O	1:A:268:LEU:HD13	1.79	0.83
1:B:563:ILE:O	1:B:567:VAL:HG23	1.81	0.80
1:A:251:LEU:HD21	1:A:331:LEU:HD23	1.65	0.78

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	371/625 (59%)	344 (93%)	27 (7%)	0	100	100
1	B	521/625 (83%)	494 (95%)	27 (5%)	0	100	100
All	All	892/1250 (71%)	838 (94%)	54 (6%)	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	332/556 (60%)	328 (99%)	4 (1%)	67	78
1	B	472/556 (85%)	472 (100%)	0	100	100
All	All	804/1112 (72%)	800 (100%)	4 (0%)	85	90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	316	LEU
1	A	406	ILE
1	A	579	ILE
1	A	605	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	576	GLN
1	A	616	HIS
1	B	462	GLN
1	A	499	HIS
1	A	399	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

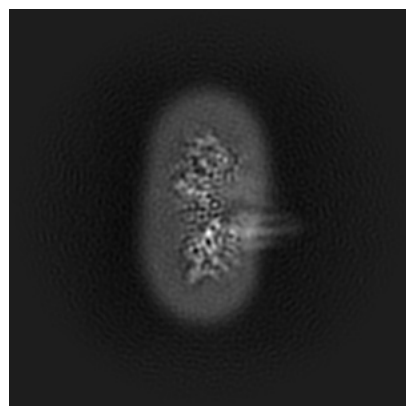
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61860. These allow visual inspection of the internal detail of the map and identification of artifacts.

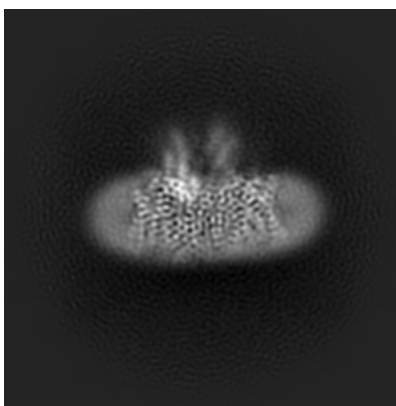
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

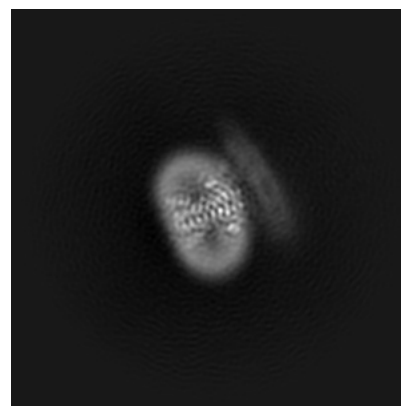
6.1.1 Primary map



X

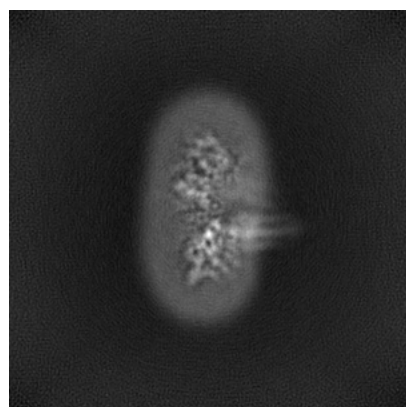


Y

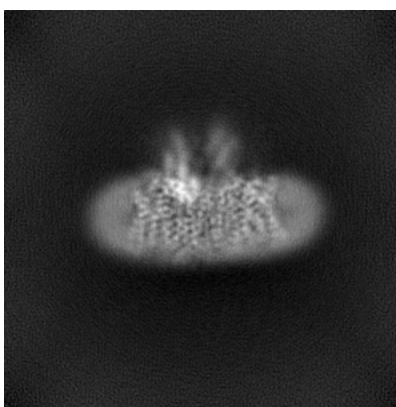


Z

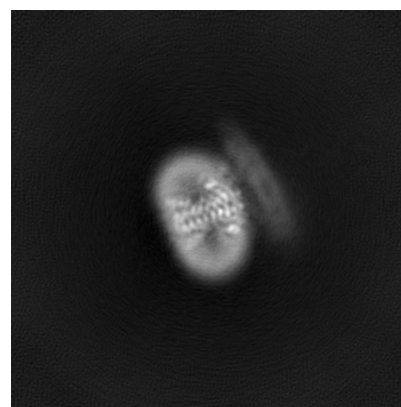
6.1.2 Raw map



X



Y

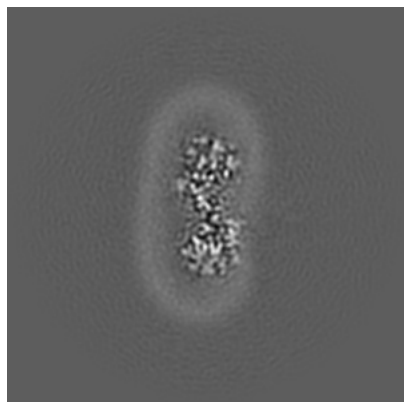


Z

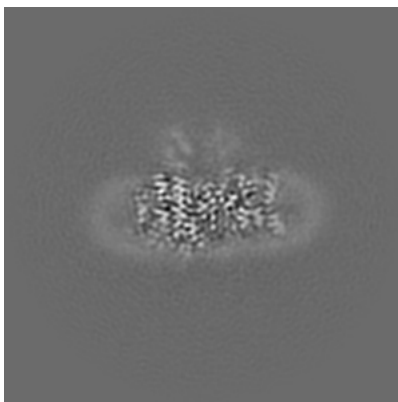
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

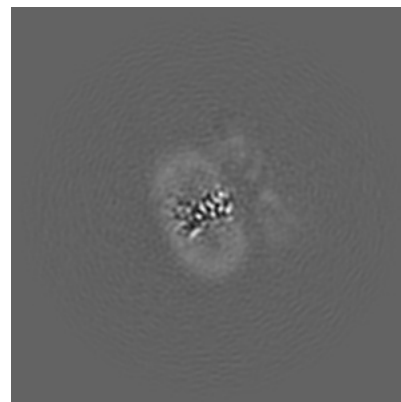
6.2.1 Primary map



X Index: 130

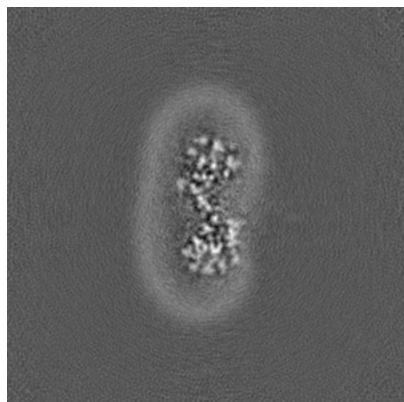


Y Index: 130

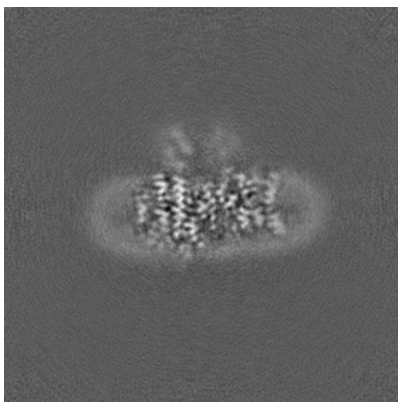


Z Index: 130

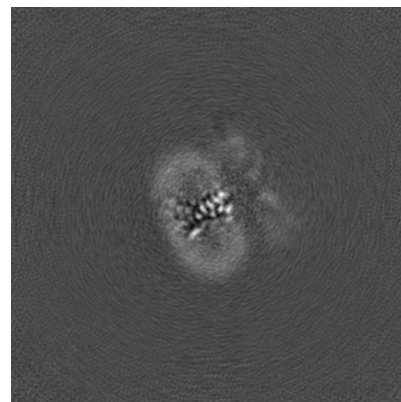
6.2.2 Raw map



X Index: 130



Y Index: 130

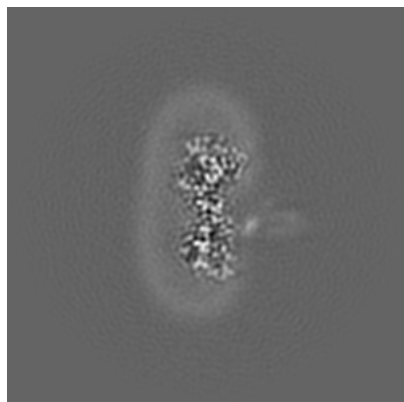


Z Index: 130

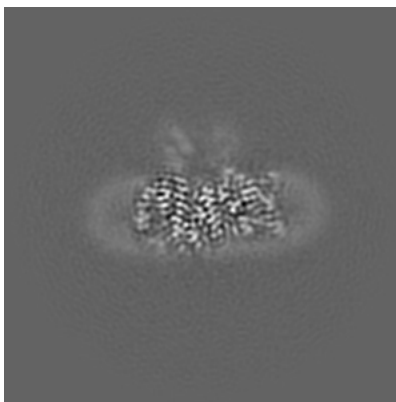
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

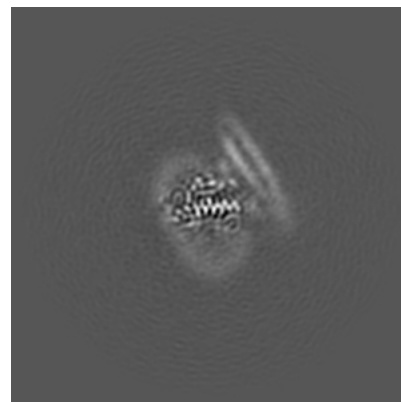
6.3.1 Primary map



X Index: 136

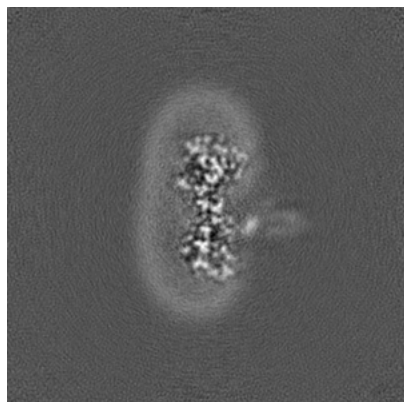


Y Index: 128

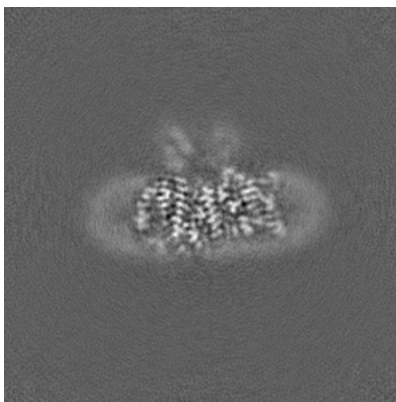


Z Index: 114

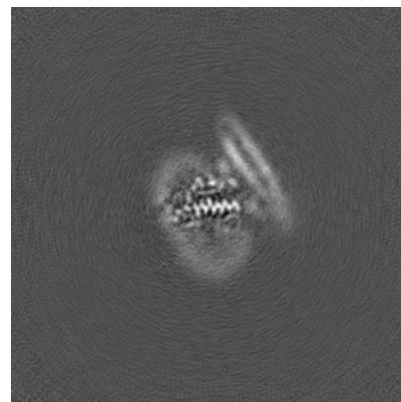
6.3.2 Raw map



X Index: 136



Y Index: 128

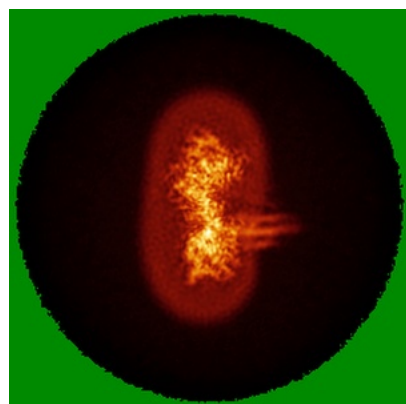


Z Index: 114

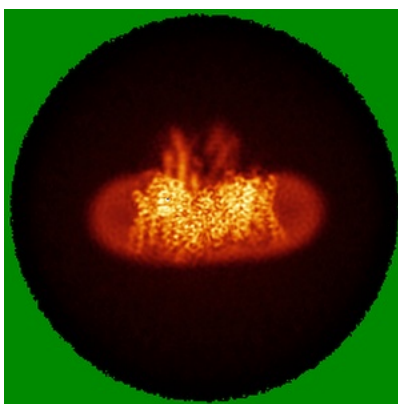
The images above show the largest variance slices of the map in three orthogonal directions.

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

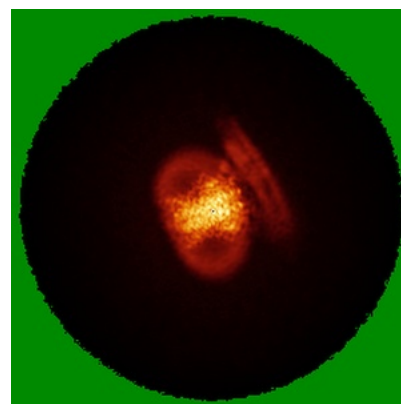
6.4.1 Primary map



X

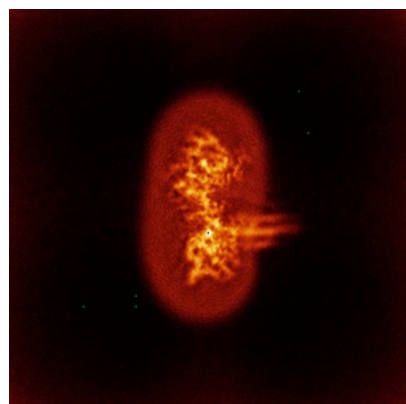


Y

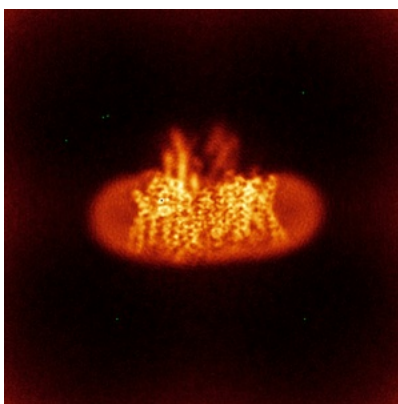


Z

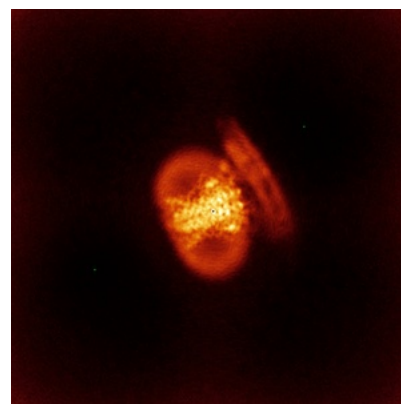
6.4.2 Raw map



X



Y

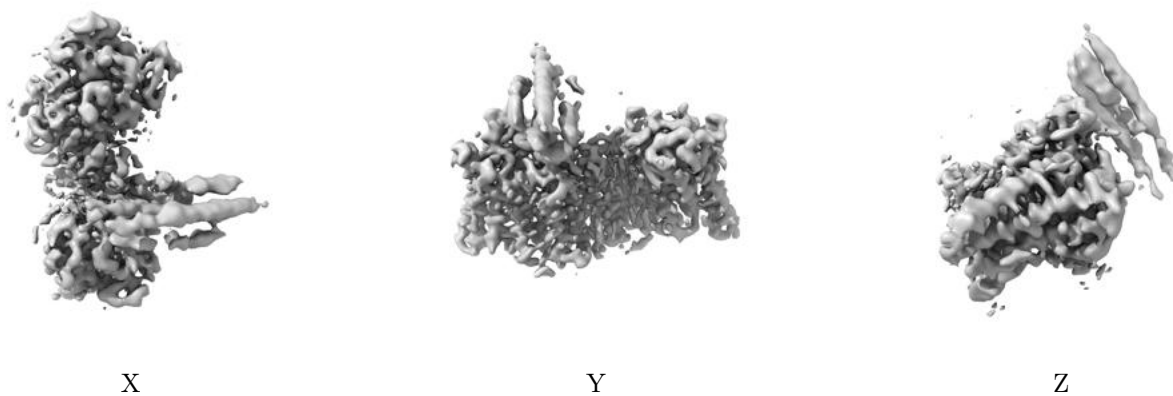


Z

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.

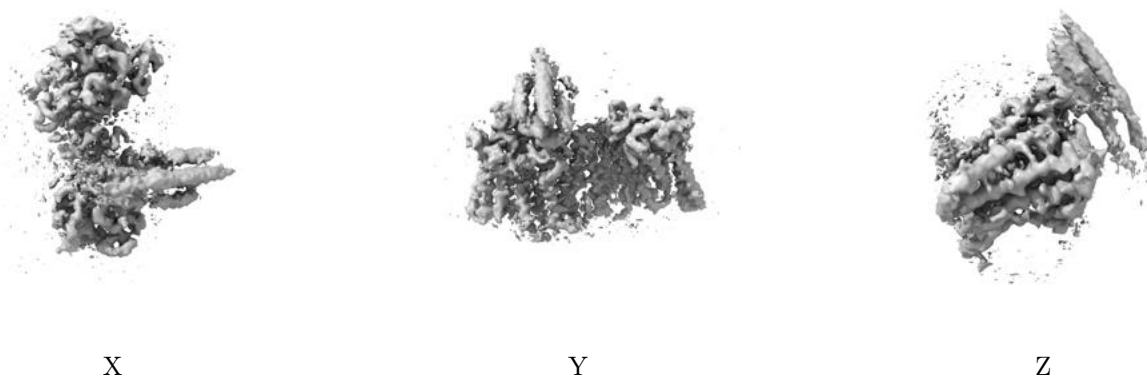
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.418. 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.

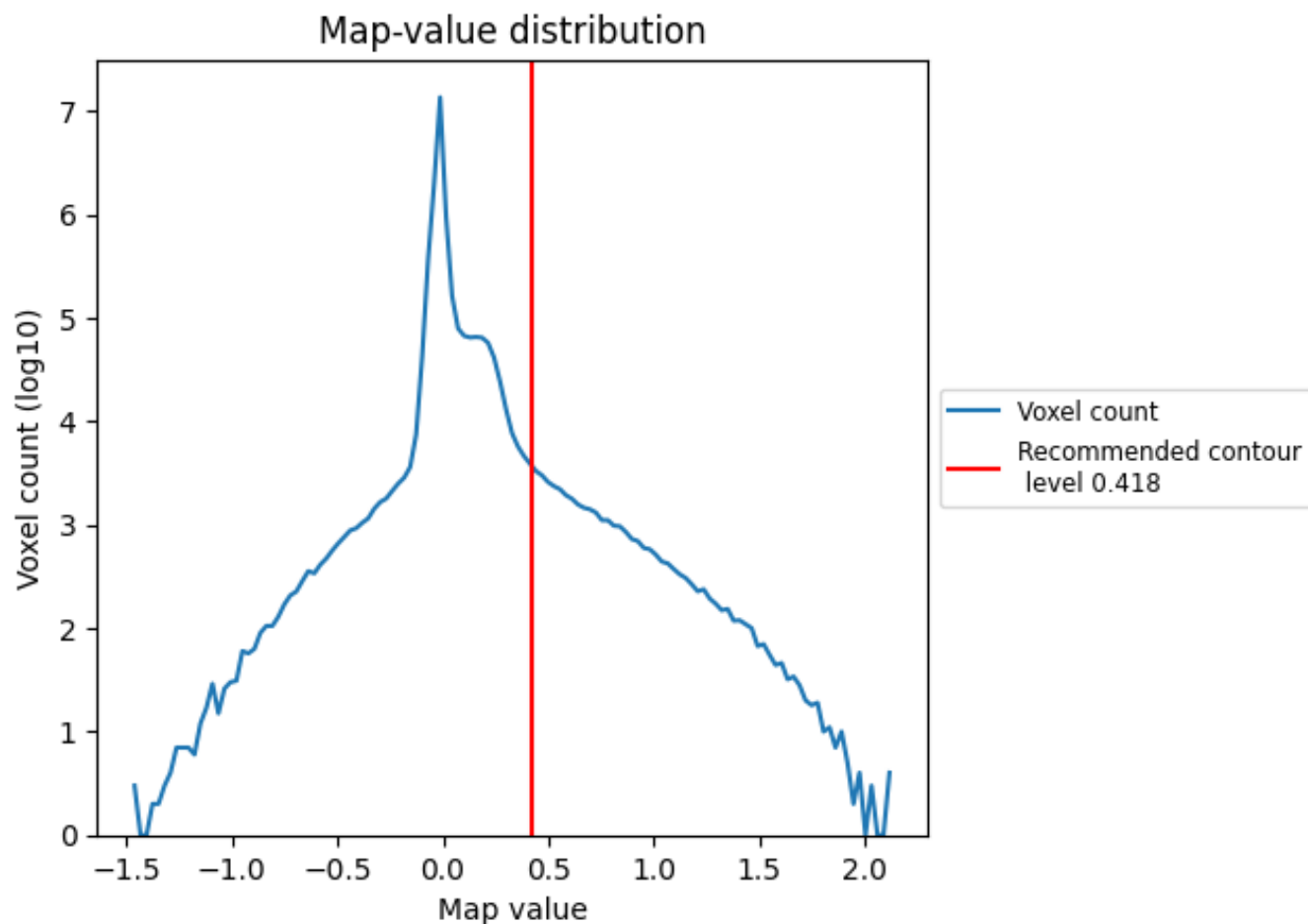
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

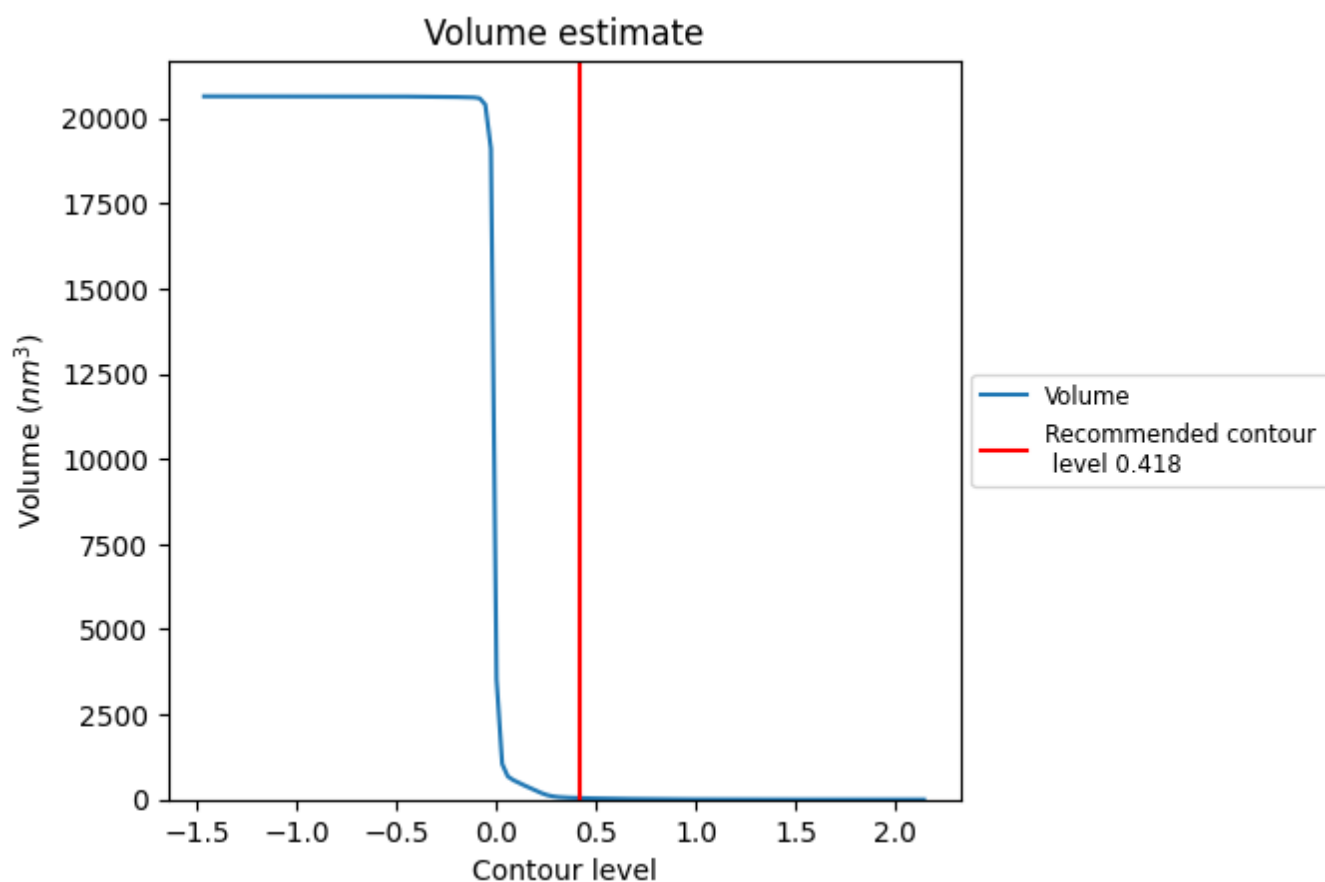
This section contains the results of statistical analysis of the map.

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.

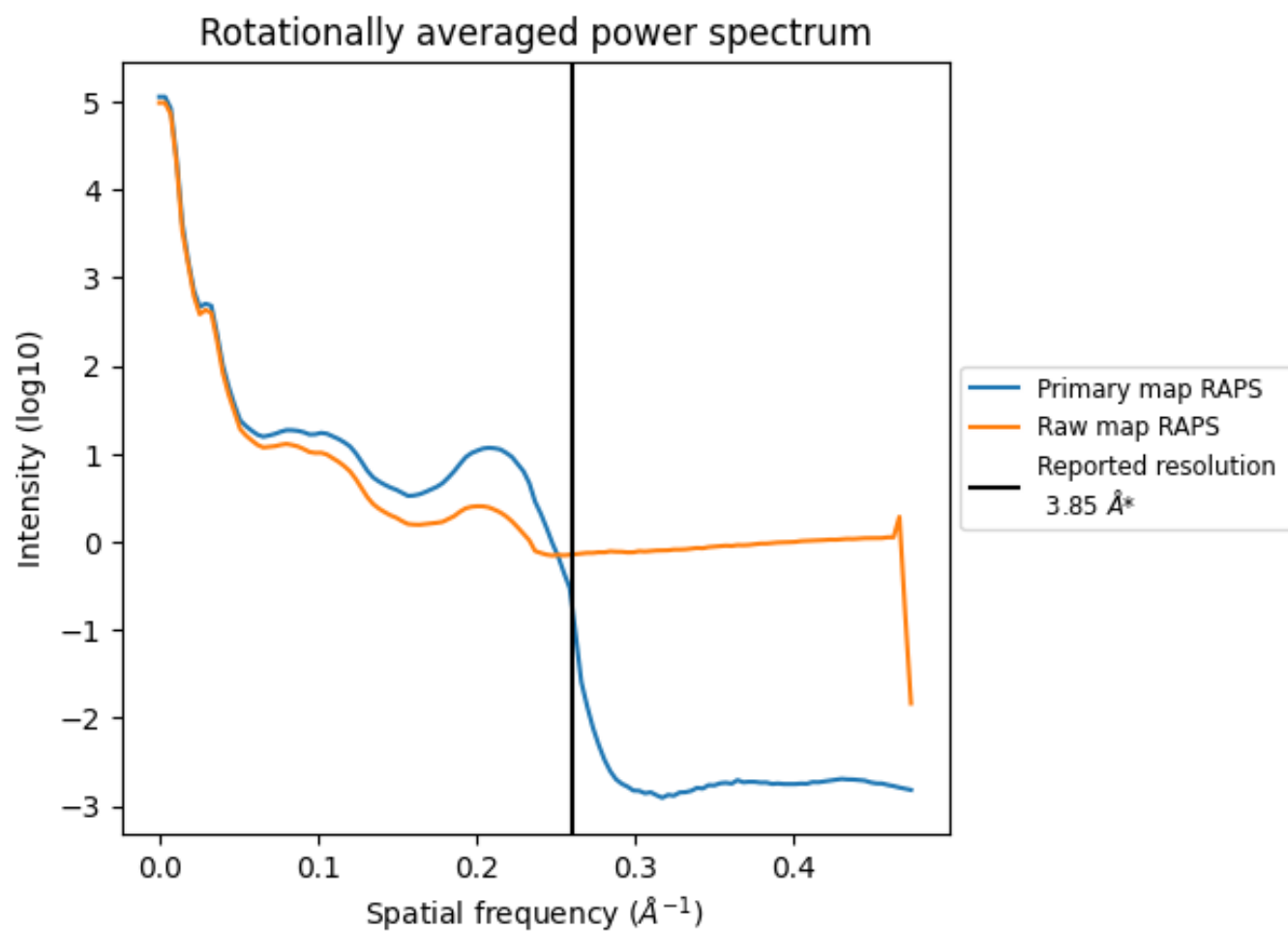
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 45 nm^3 ; this corresponds to an approximate mass of 41 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 ⓘ

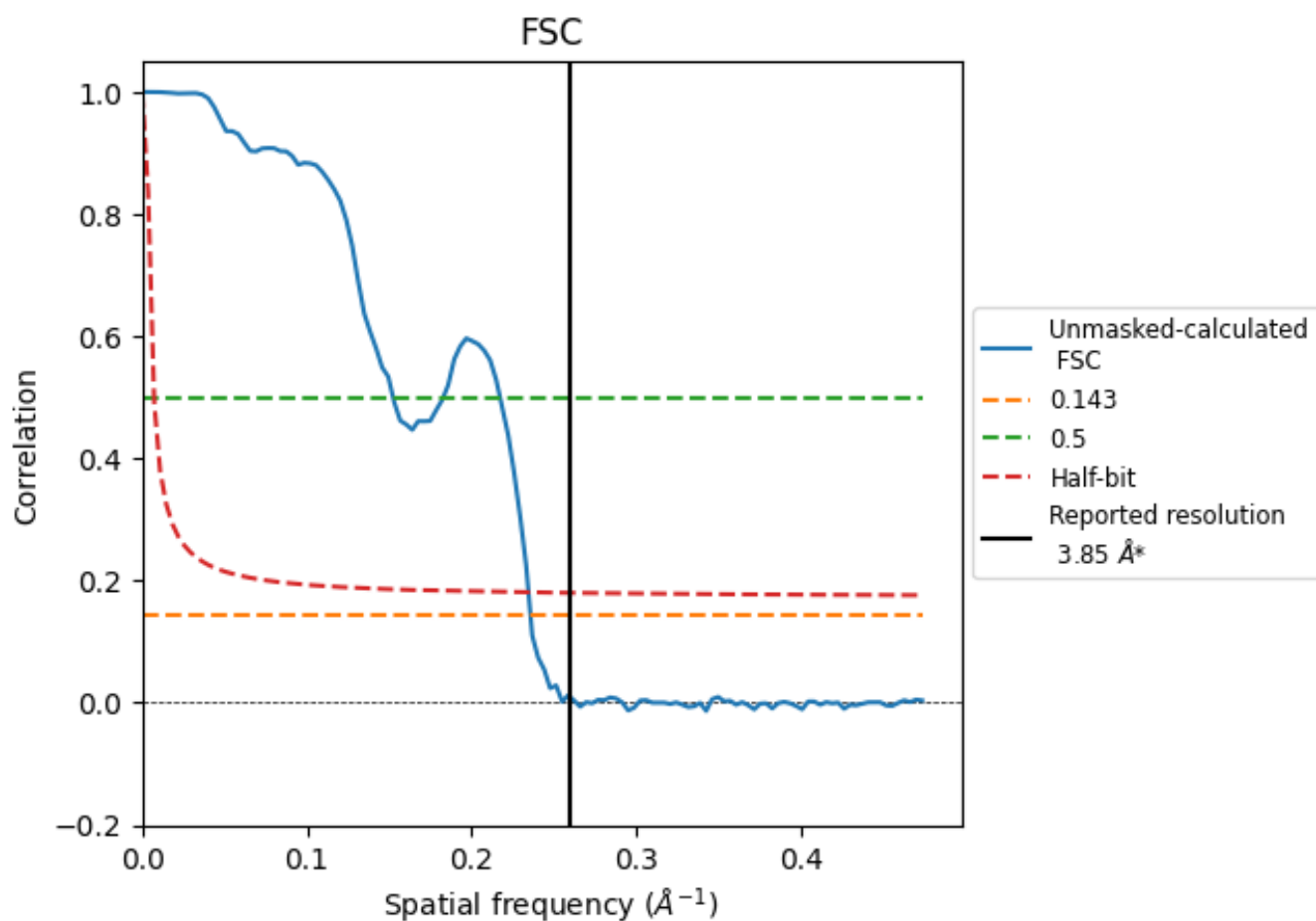


*Reported resolution corresponds to spatial frequency of 0.260 \AA^{-1}

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 0.260 Å⁻¹

8.2 Resolution estimates [i](#)

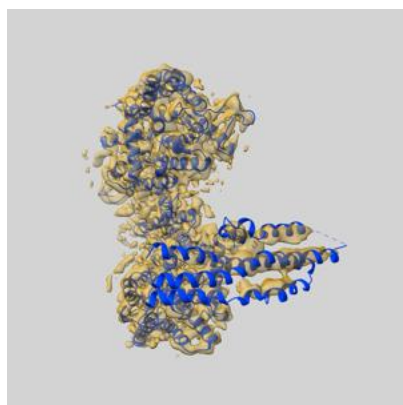
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.85	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.24	6.56	4.26

*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 4.24 differs from the reported value 3.85 by more than 10 %

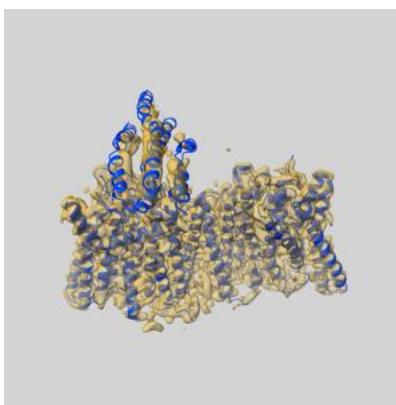
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-61860 and PDB model 9JXE. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

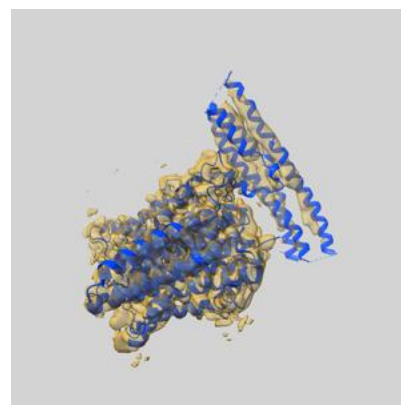
9.1 Map-model overlay [i](#)



X



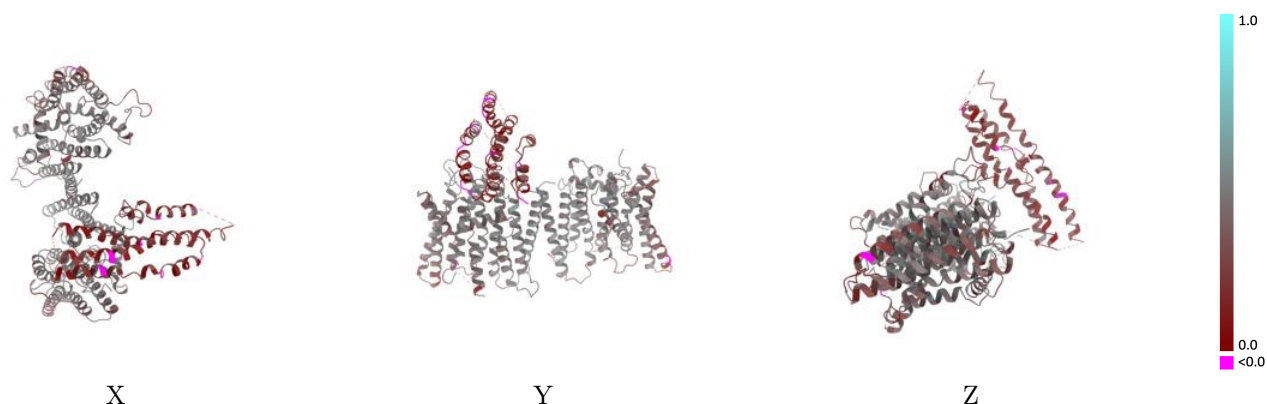
Y



Z

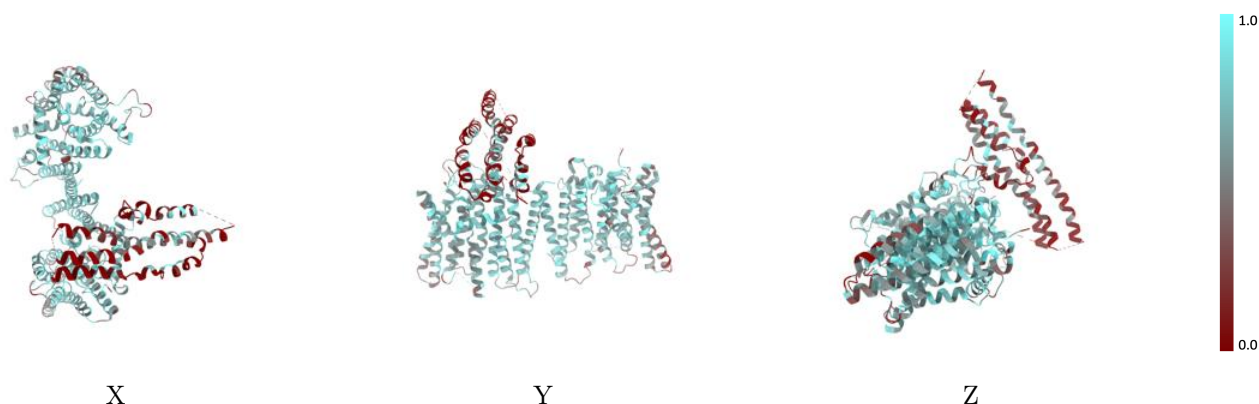
The images above show the 3D surface view of the map at the recommended contour level 0.418 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



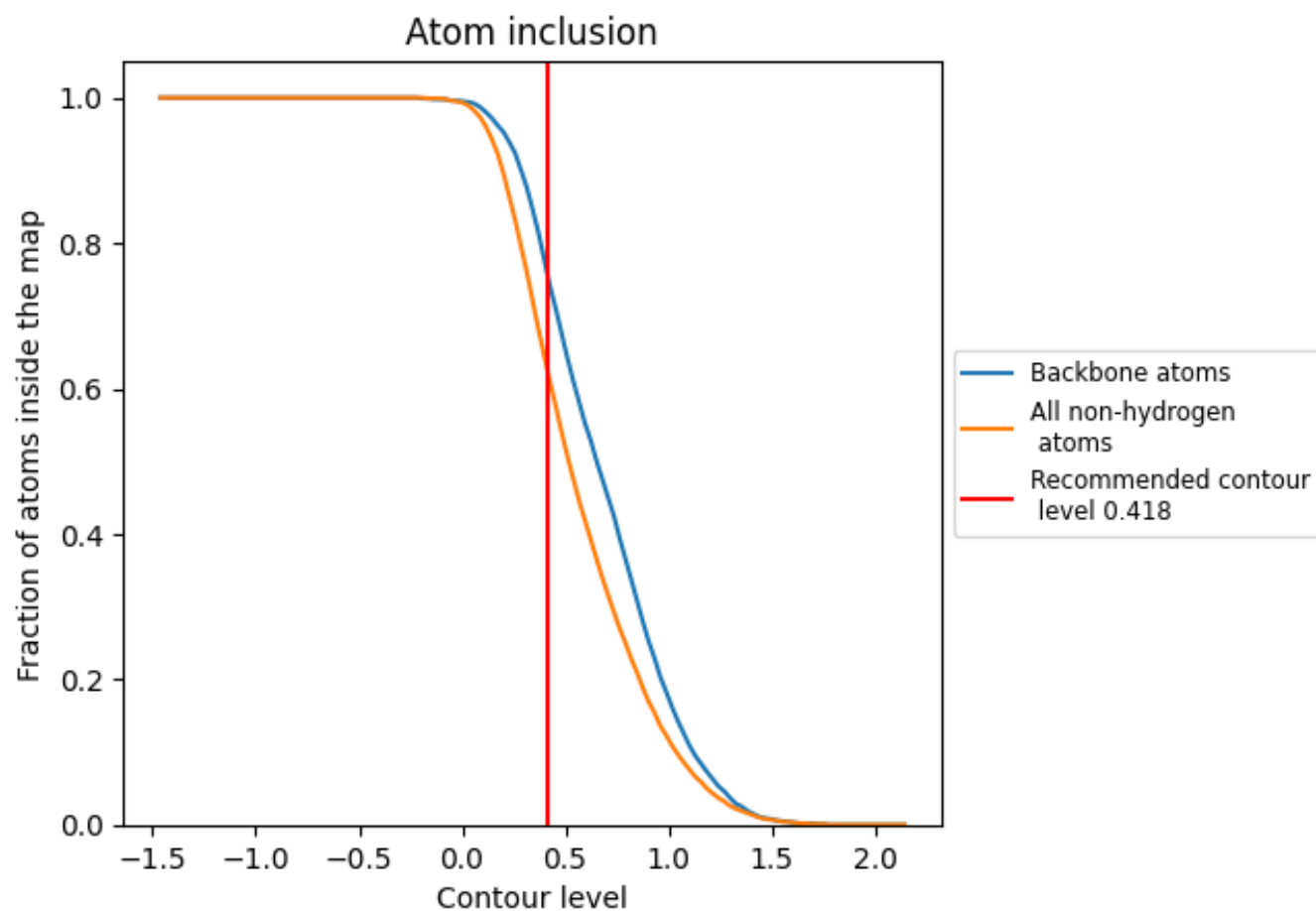
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.418).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 62% 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 (0.418) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6190	<div></div> 0.3770
A	<div></div> 0.6830	<div></div> 0.4120
B	<div></div> 0.5730	<div></div> 0.3510

