



Full wwPDB EM Validation Report ⓘ

Jul 1, 2024 – 12:21 PM EDT

PDB ID : 8TEM
EMDB ID : EMD-41191
Title : Cryo-EM structure of Arabidopsis thaliana Bor1 mutant (R637E/E641R/R643E) in the inward-facing conformation in lauryl maltose neopentyl glycol (LMNG)
Authors : Jiang, Y.; Jiang, J.
Deposited on : 2023-07-06
Resolution : 3.02 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.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

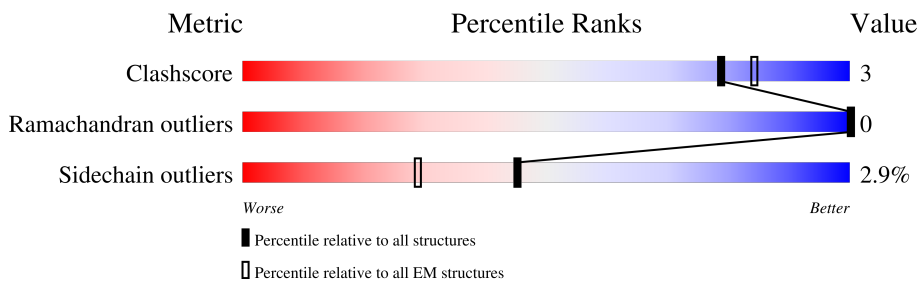
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.02 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	714	
1	B	714	

2 Entry composition i

There is only 1 type of molecule in this entry. The entry contains 7992 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 Boron transporter 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	505	3996	2651	647	669	29	0	0
1	B	505	3996	2651	647	669	29	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	637	GLU	ARG	engineered mutation	UNP Q8VYR7
A	641	ARG	GLU	engineered mutation	UNP Q8VYR7
A	643	GLU	ARG	engineered mutation	UNP Q8VYR7
A	705	HIS	-	expression tag	UNP Q8VYR7
A	706	HIS	-	expression tag	UNP Q8VYR7
A	707	HIS	-	expression tag	UNP Q8VYR7
A	708	HIS	-	expression tag	UNP Q8VYR7
A	709	HIS	-	expression tag	UNP Q8VYR7
A	710	HIS	-	expression tag	UNP Q8VYR7
A	711	HIS	-	expression tag	UNP Q8VYR7
A	712	HIS	-	expression tag	UNP Q8VYR7
A	713	HIS	-	expression tag	UNP Q8VYR7
A	714	HIS	-	expression tag	UNP Q8VYR7
B	637	GLU	ARG	engineered mutation	UNP Q8VYR7
B	641	ARG	GLU	engineered mutation	UNP Q8VYR7
B	643	GLU	ARG	engineered mutation	UNP Q8VYR7
B	705	HIS	-	expression tag	UNP Q8VYR7
B	706	HIS	-	expression tag	UNP Q8VYR7
B	707	HIS	-	expression tag	UNP Q8VYR7
B	708	HIS	-	expression tag	UNP Q8VYR7
B	709	HIS	-	expression tag	UNP Q8VYR7
B	710	HIS	-	expression tag	UNP Q8VYR7
B	711	HIS	-	expression tag	UNP Q8VYR7
B	712	HIS	-	expression tag	UNP Q8VYR7
B	713	HIS	-	expression tag	UNP Q8VYR7
B	714	HIS	-	expression tag	UNP Q8VYR7

MET	GLU	GLU	THR	F5	V6	P7	F8	E9	G10	I11	K12	M13	D14	L15	K16	G17	R18	L19	M20	C21	Y22	K23	Q24	D25	W26	T27	G28	G29	F30	K31	A32	G33	F34	R35	I36	L37	A38	P39	I43	A46	L58	T62	A76	M80	I81	H82	S83	I84	I85	C86	G87	Q88	P89
L90	A112	R113	P114	E115	D119	L120	V130	C142	G143	A144	C145	S146	I147	I148	M149	R150	F151	T152	R153	V154	A155	G156	E157	L161	M165	D177	E178	F179	R180	E183	R184	E185	M186	Q187	K188	L189	K190	F203	R219	S223	W224	R225	W230	S231	Y332	D237	A255						
G256	D257	K260	R264	F267	N270	P271	W272	S273	PRO	GLY	ALA	THR	GLY	TRP	T281	K284	L287	D288	I291	G296	A297	F298	Y309	F310	D311	H312	S313	S316	Q317	L318	A319	Q320	Q321	K322	E323	F324	M325	L326	K327	K328	F329	S330	S331	Y332	H333	Y334	D335						
L344	G356	V357	I358	P359	Q360	S361	P362	M363	H364	T365	K366	S367	L368	A369	THR	LEU	LYS	TYR	GLN	LEU	PRO	ARG	ASN	ARG	LEU	VAL	ALA	THR	ALA	ARG	SER	ILE	LYS	ILE	LYS	THR	ASN	ALA	LEU	GLY	LEU	LEU	GLN	TRP	LEU	VAL							
TYR	GLN	GLN	PRO	GLN	GLY	LEU	LYS	GLU	LYS	GLU	THR	GLN	ALA	THR	PHE	THR	GLY	ASN	LEU	ASN	ALA	PRO	VAL	ASP	GLU	THR	LEU	PHE	ILE	GLY	LYS	ILE	GLU	ILE	LEU	PRO	VAL	GLU	V460	K461	E462	Q463	L469	Q470	S471	T472	M473	T489	Y495				
M499	L516	F517	T518	A519	R522	RE23	F524	K525	V526	L527	E528	D529	Y530	H531	A532	V535	E536	T537	F540	K541	I565	F570	P571	L572	M573	L574	M575	F576	Q582	Y583	L584	R587	F588	F589	K590	G591	A592	H593	L594	Q595	D596	L597	D598	A599	E601	Y602	E603	E604	A605				
P606	ALA	LEU	PRO	PHE	ASN	LEU	ALA	ALA	GLU	THR	GLU	ILE	ARG	LEU	THR	THR	THR	GLY	ASP	PRO	LEU	GLU	ILE	ASP	GLU	CYS	GLY	VAL	ARG	SER	THR	GLU	LEU	SER	ARG	GLN	SER	SER	SER	PHE	GLY	THR	HIS	HIS	HIS	HIS	HIS	HIS	HIS				
VAL	PHE	SER	PRO	ARG	VAL	SER	GLY	ILE	ARG	LEU	THR	GLU	ILE	ARG	LEU	THR	THR	THR	THR	GLY	ASP	PRO	LEU	GLU	ILE	ASP	GLU	CYS	GLY	VAL	ARG	SER	THR	GLU	LEU	SER	ARG	GLN	SER	SER	SER	PHE	GLY	THR	HIS	HIS	HIS	HIS	HIS	HIS			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	80443	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 ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.060	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.015	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](#)

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	0/4109	0.47	0/5582
1	B	0.26	0/4109	0.47	0/5582
All	All	0.26	0/8218	0.47	0/11164

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	3996	0	4096	24	0
1	B	3996	0	4096	23	0
All	All	7992	0	8192	45	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 3.

All (45) 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:144:ALA:O	1:A:309:TYR:OH	2.09	0.70
1:B:144:ALA:O	1:B:309:TYR:OH	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:GLU:OE2	1:B:489:THR:OG1	2.18	0.61
1:A:178:GLU:OE2	1:A:489:THR:OG1	2.18	0.61
1:B:260:LYS:HD2	1:B:260:LYS:H	1.69	0.57
1:A:260:LYS:H	1:A:260:LYS:HD2	1.69	0.57
1:A:260:LYS:HD2	1:A:260:LYS:N	2.21	0.56
1:B:260:LYS:HD2	1:B:260:LYS:N	2.21	0.55
1:A:76:ALA:O	1:A:80:MET:HG3	2.06	0.55
1:B:76:ALA:O	1:B:80:MET:HG3	2.06	0.54
1:A:469:LEU:O	1:A:473:MET:HG3	2.10	0.52
1:B:469:LEU:O	1:B:473:MET:HG3	2.10	0.51
1:B:38:ALA:HB3	1:B:39:PRO:HD3	1.94	0.49
1:A:153:ARG:O	1:A:157:GLU:HG2	2.13	0.49
1:B:58:LEU:O	1:B:62:THR:OG1	2.11	0.48
1:A:522:ARG:HG2	1:B:225:ARG:O	2.12	0.48
1:B:153:ARG:O	1:B:157:GLU:HG2	2.13	0.48
1:A:38:ALA:HB3	1:A:39:PRO:HD3	1.94	0.48
1:A:225:ARG:O	1:B:522:ARG:HG2	2.16	0.46
1:A:598:ASP:CG	1:A:598:ASP:O	2.55	0.46
1:B:598:ASP:CG	1:B:598:ASP:O	2.55	0.45
1:A:58:LEU:O	1:A:62:THR:OG1	2.11	0.45
1:A:570:PHE:N	1:A:571:PRO:CD	2.80	0.45
1:B:161:LEU:O	1:B:165:MET:HG3	2.18	0.44
1:B:570:PHE:N	1:B:571:PRO:CD	2.80	0.44
1:A:23:LYS:O	1:A:27:THR:OG1	2.32	0.44
1:A:161:LEU:O	1:A:165:MET:HG3	2.18	0.44
1:B:495:TYR:O	1:B:499:MET:HG3	2.18	0.44
1:A:154:VAL:HG13	1:A:155:ALA:N	2.33	0.44
1:A:495:TYR:O	1:A:499:MET:HG3	2.18	0.43
1:B:10:GLY:O	1:B:14:ASP:OD2	2.36	0.43
1:B:154:VAL:HG13	1:B:155:ALA:N	2.33	0.43
1:B:357:VAL:HG23	1:B:360:GLN:HB2	2.01	0.43
1:A:357:VAL:HG23	1:A:360:GLN:HB2	2.01	0.43
1:A:130:VAL:HG22	1:A:344:LEU:CD1	2.49	0.42
1:A:180:ARG:O	1:A:264:ARG:NH2	2.42	0.42
1:A:10:GLY:O	1:A:14:ASP:OD2	2.37	0.42
1:B:130:VAL:HG22	1:B:344:LEU:CD1	2.49	0.42
1:B:25:ASP:OD1	1:B:328:LYS:NZ	2.47	0.41
1:B:82:HIS:O	1:B:86:GLY:N	2.54	0.41
1:B:180:ARG:O	1:B:264:ARG:NH2	2.42	0.41
1:A:84:ILE:HG22	1:A:85:ILE:HG23	2.03	0.41
1:A:25:ASP:OD1	1:A:328:LYS:NZ	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:ILE:HG22	1:B:85:ILE:HG23	2.03	0.41
1:A:504:LEU:N	1:A:505:PRO:CD	2.85	0.40

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	499/714 (70%)	481 (96%)	18 (4%)	0	100	100
1	B	499/714 (70%)	481 (96%)	18 (4%)	0	100	100
All	All	998/1428 (70%)	962 (96%)	36 (4%)	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	427/612 (70%)	415 (97%)	12 (3%)	43	76
1	B	427/612 (70%)	414 (97%)	13 (3%)	41	74
All	All	854/1224 (70%)	829 (97%)	25 (3%)	45	75

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	24	GLN
1	A	27	THR
1	A	187	GLN
1	A	203	PHE
1	A	219	ARG
1	A	223	SER
1	A	260	LYS
1	A	327	ARG
1	A	471	SER
1	A	524	PHE
1	A	598	ASP
1	B	23	LYS
1	B	24	GLN
1	B	27	THR
1	B	177	ASP
1	B	187	GLN
1	B	203	PHE
1	B	219	ARG
1	B	223	SER
1	B	260	LYS
1	B	327	ARG
1	B	471	SER
1	B	524	PHE
1	B	598	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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.

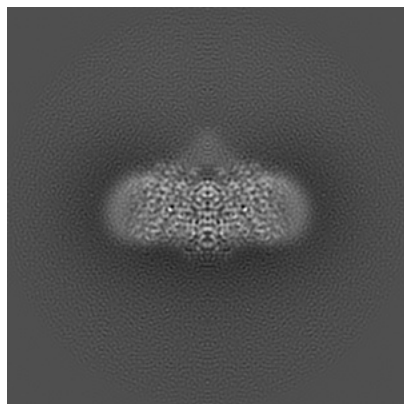
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41191. These allow visual inspection of the internal detail of the map and identification of artifacts.

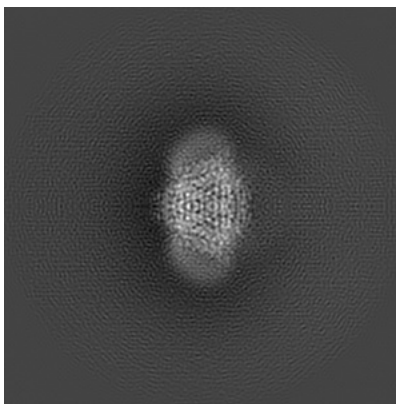
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

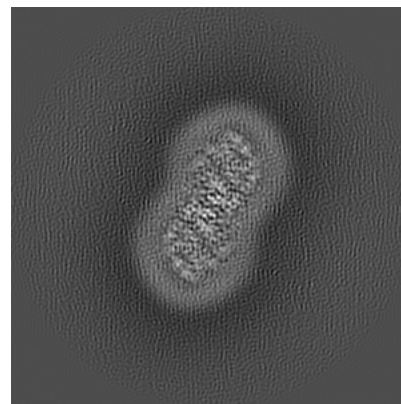
6.1.1 Primary map



X

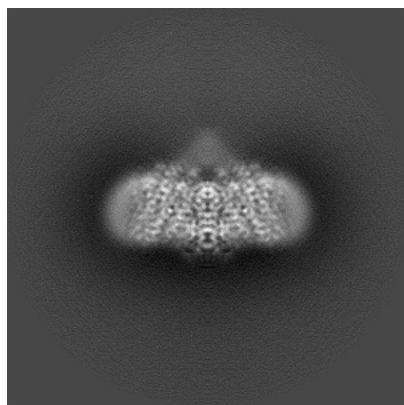


Y

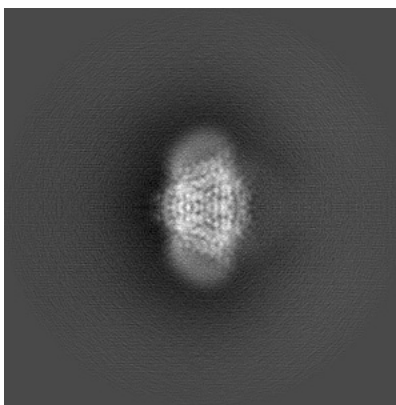


Z

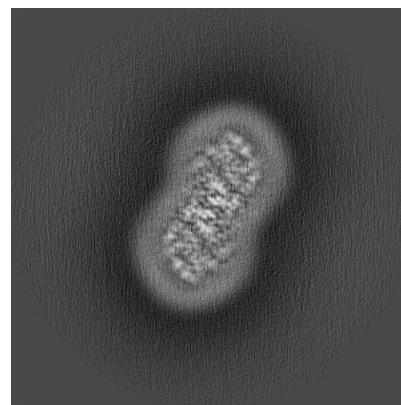
6.1.2 Raw map



X



Y

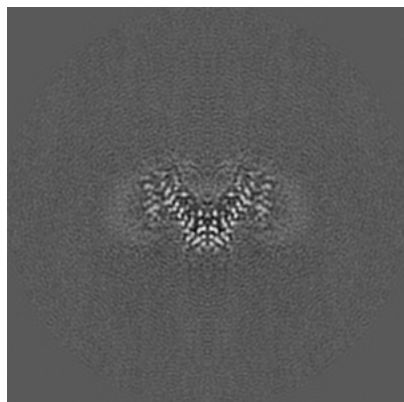


Z

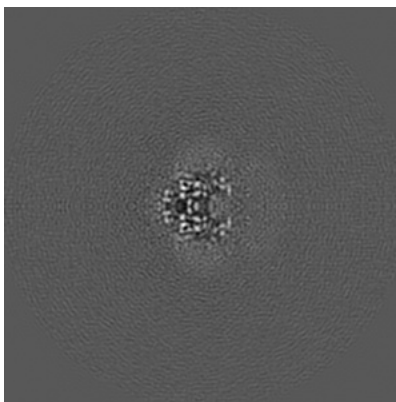
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

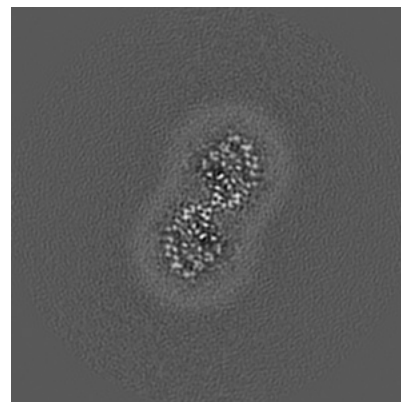
6.2.1 Primary map



X Index: 160

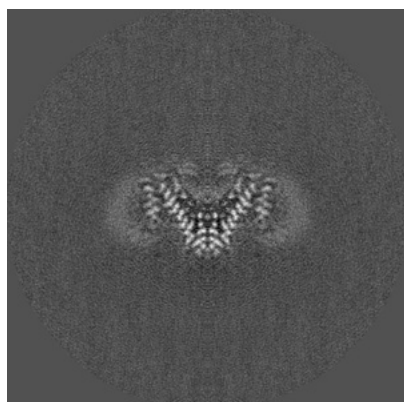


Y Index: 160

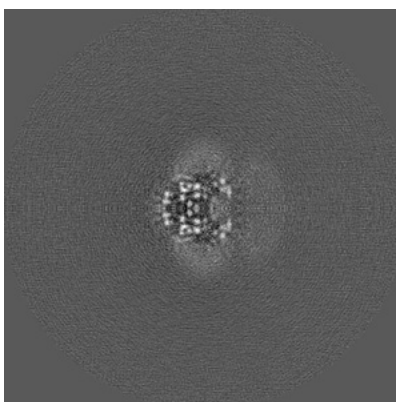


Z Index: 160

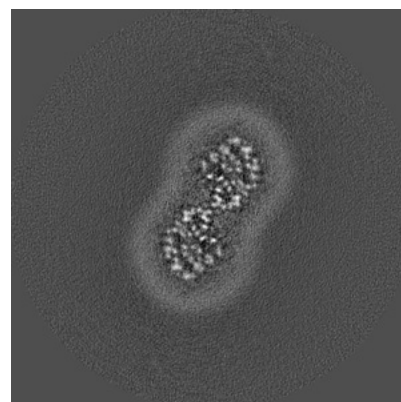
6.2.2 Raw map



X Index: 160



Y Index: 160

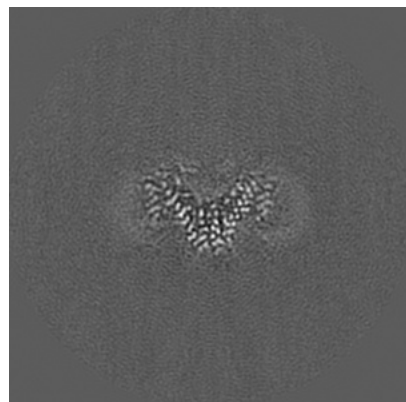


Z Index: 160

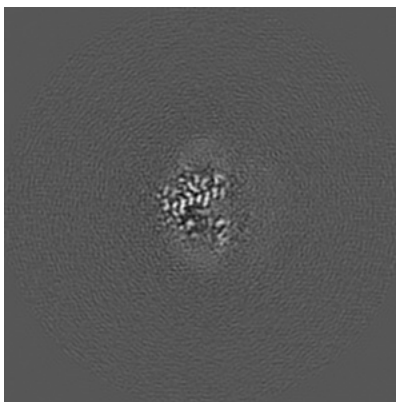
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

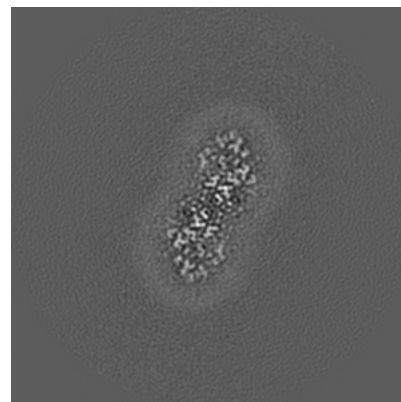
6.3.1 Primary map



X Index: 161

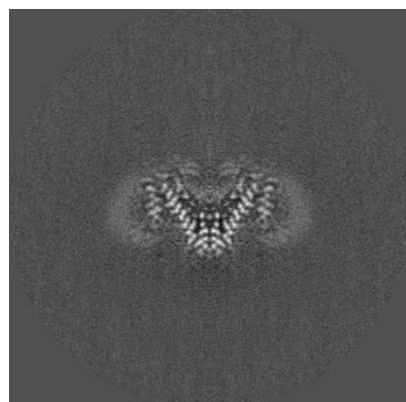


Y Index: 163

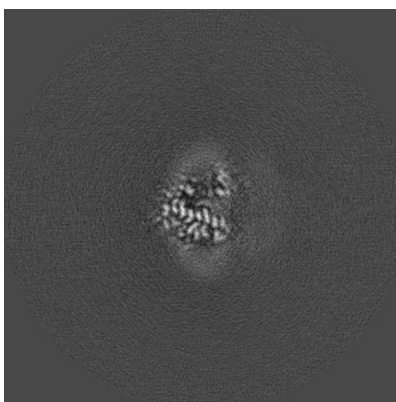


Z Index: 151

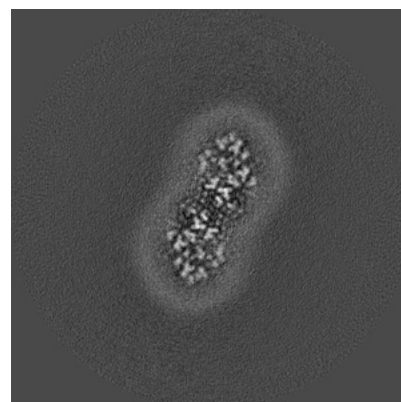
6.3.2 Raw map



X Index: 160



Y Index: 157

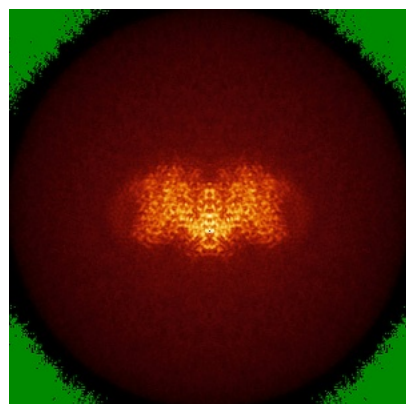


Z Index: 151

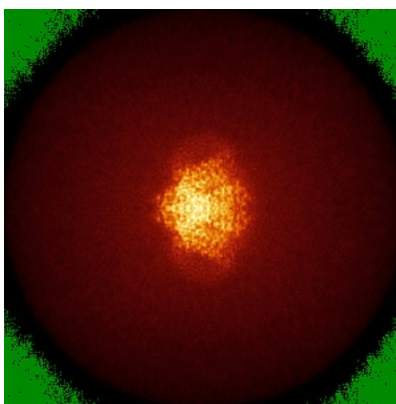
The images above show the largest variance slices of the map in three orthogonal directions.

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

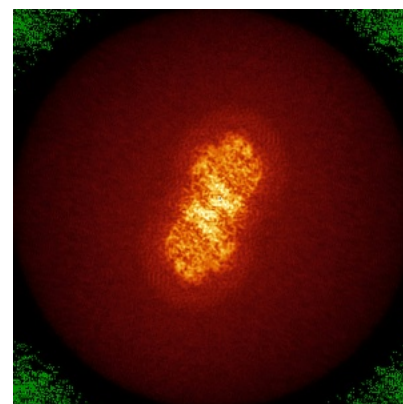
6.4.1 Primary map



X

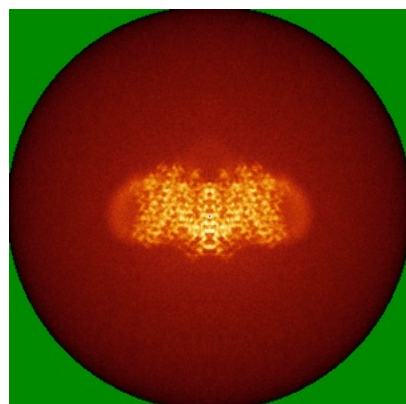


Y

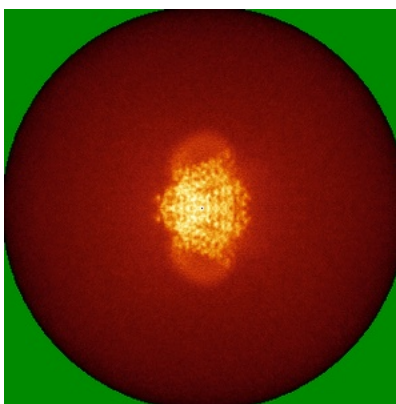


Z

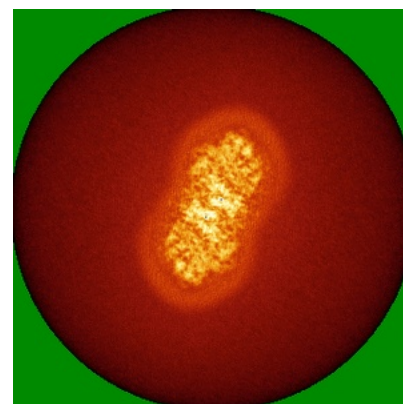
6.4.2 Raw map



X



Y

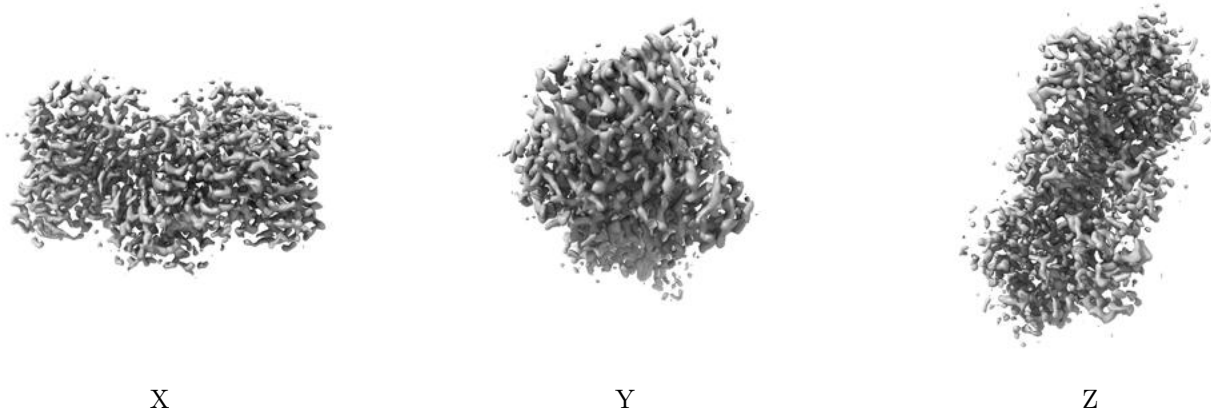


Z

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.

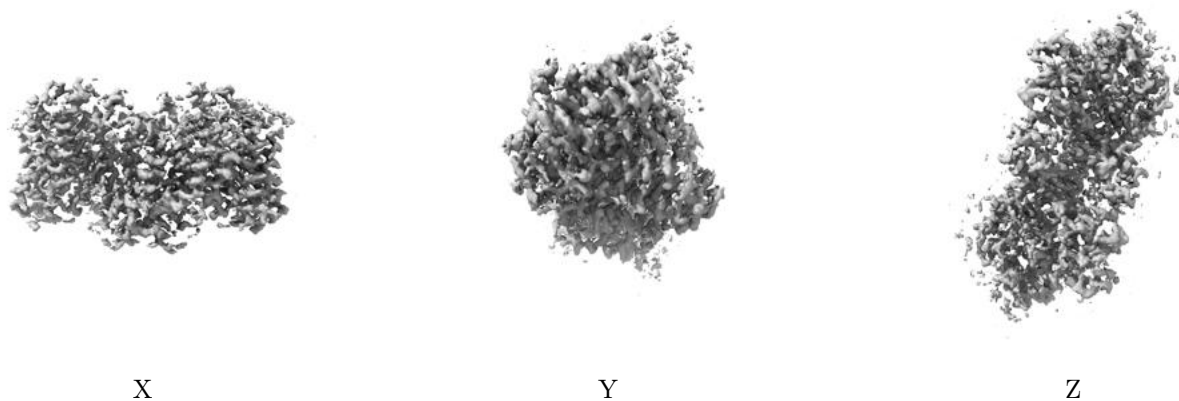
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. 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.

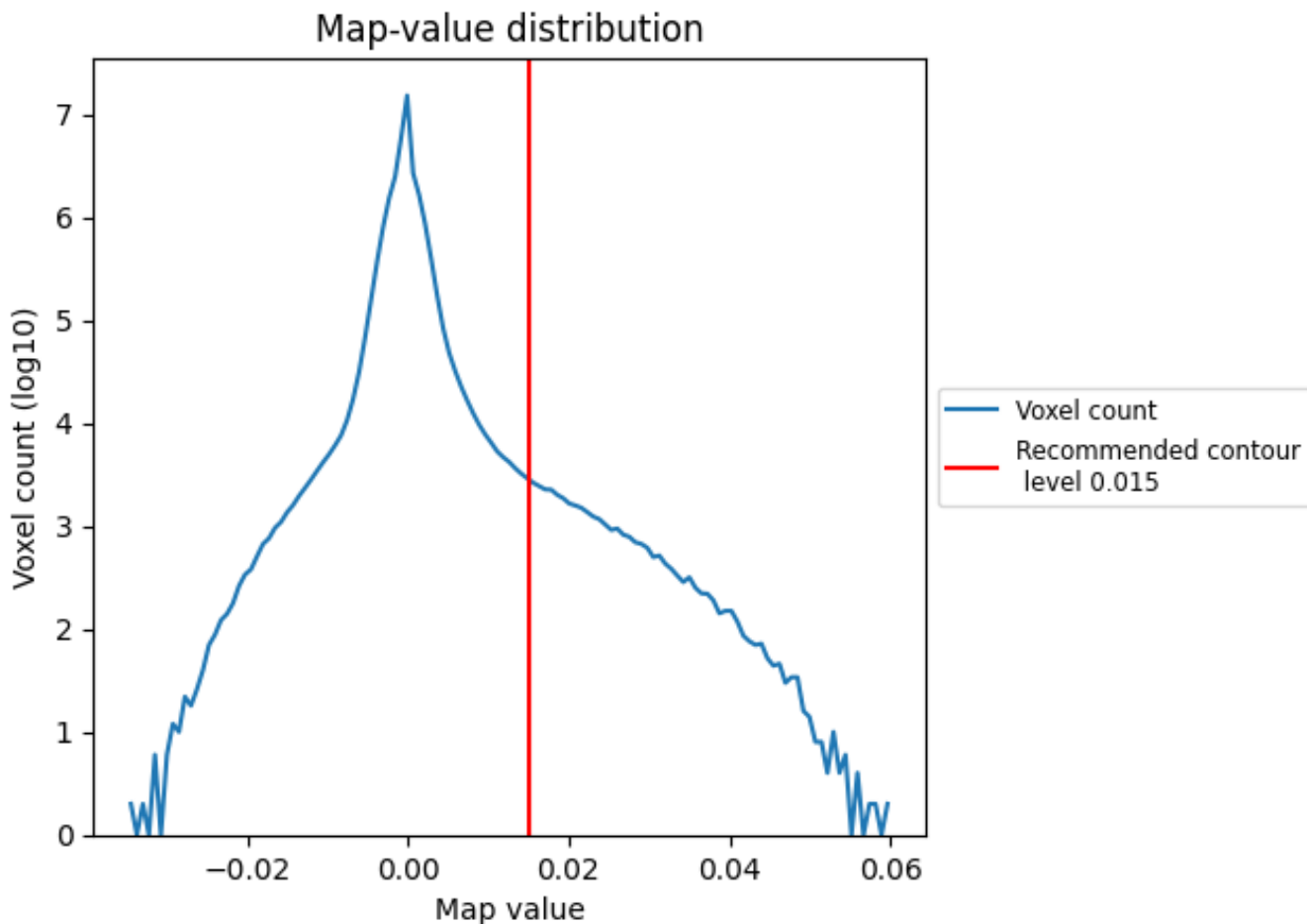
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

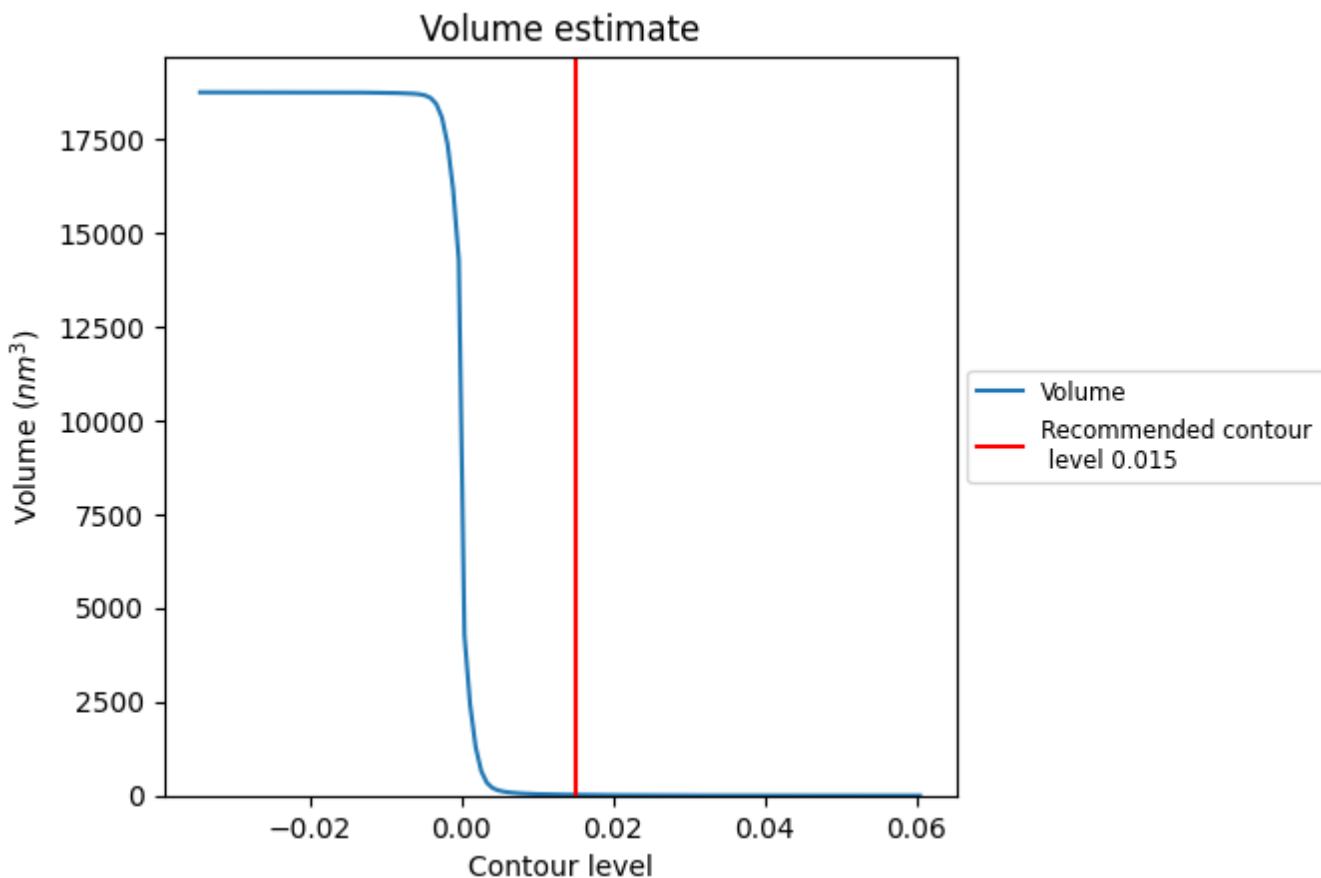
This section contains the results of statistical analysis of the map.

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.

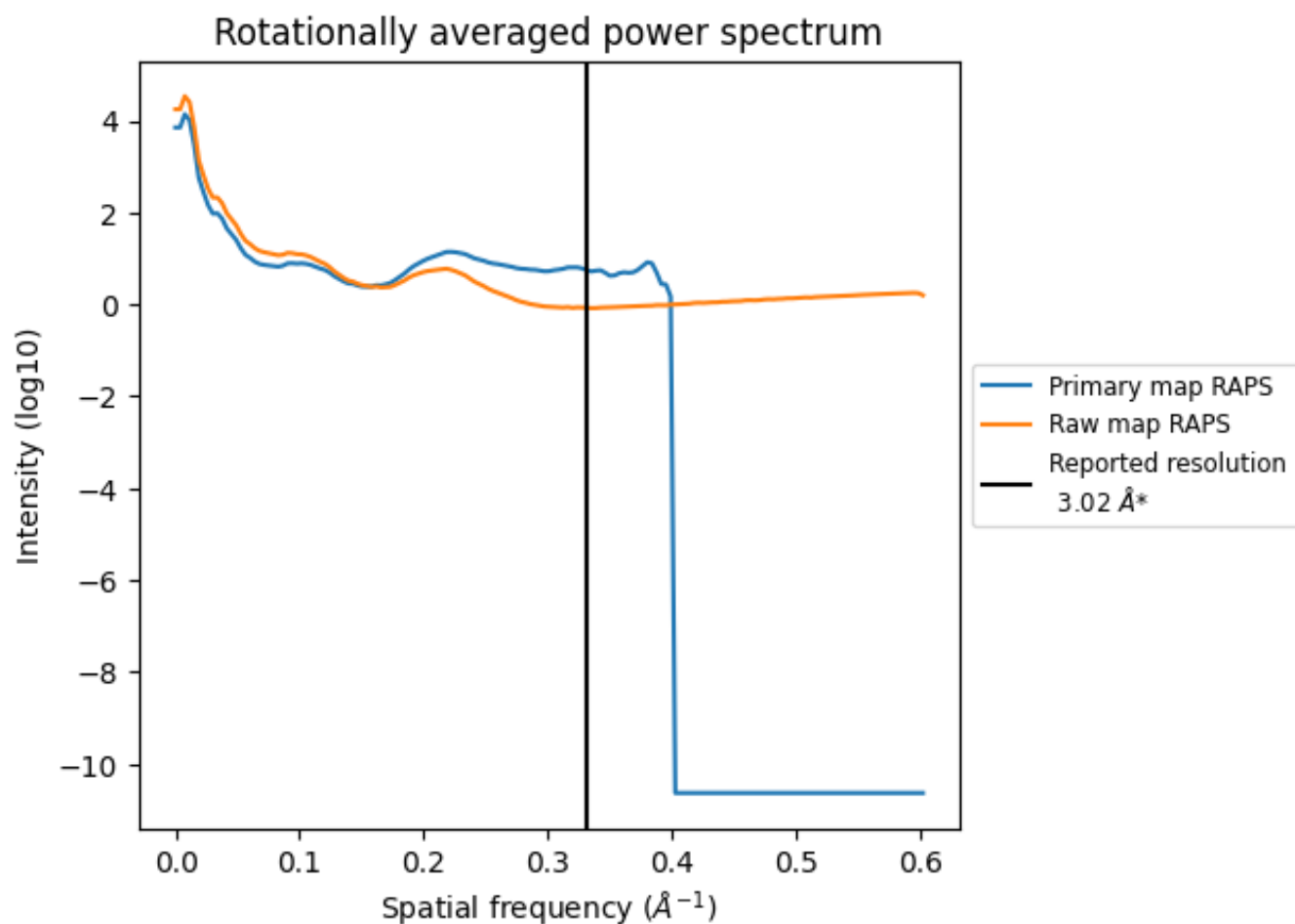
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 20 nm^3 ; this corresponds to an approximate mass of 18 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 [i](#)

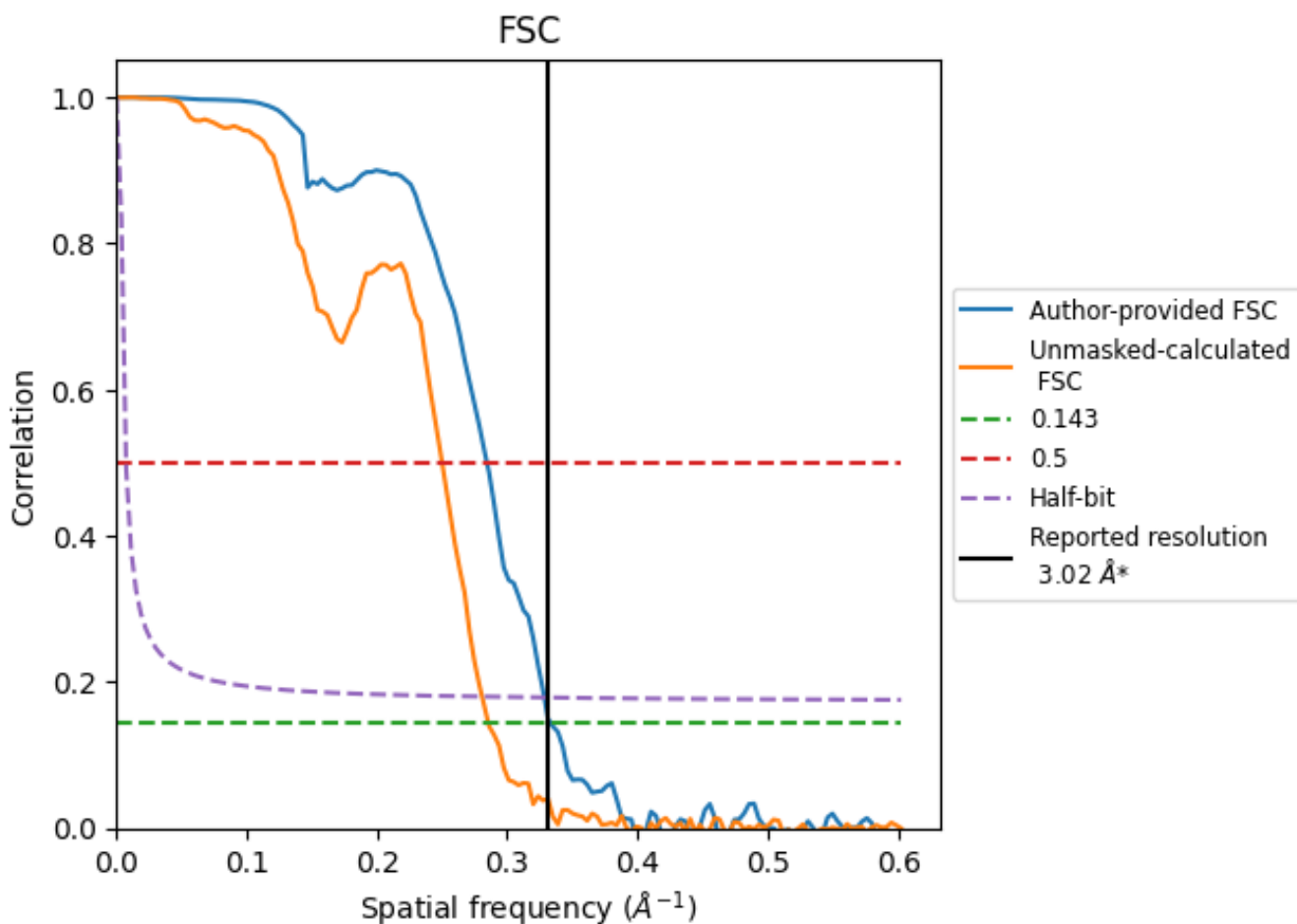


*Reported resolution corresponds to spatial frequency of 0.331 Å⁻¹

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 0.331 \AA^{-1}

8.2 Resolution estimates [i](#)

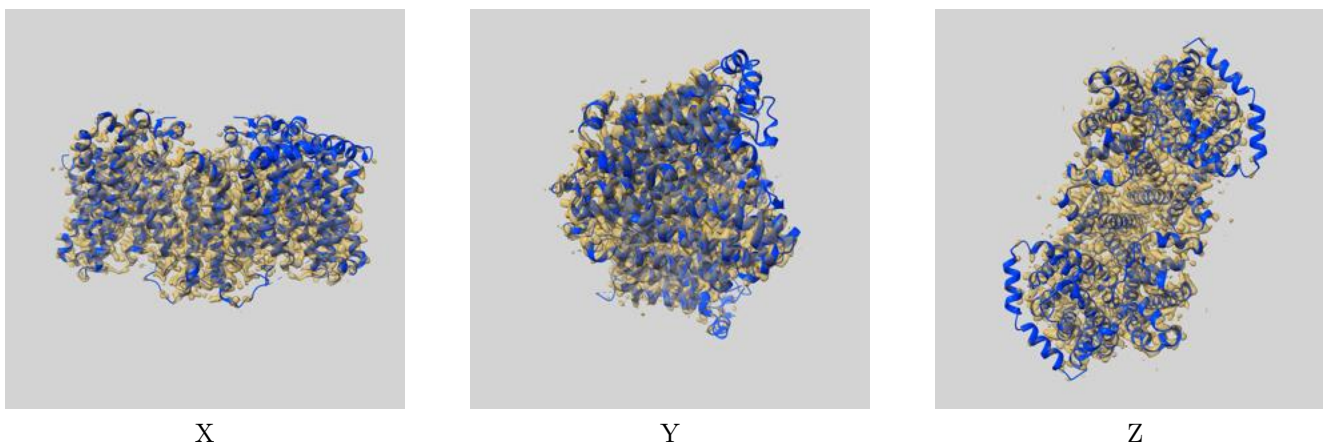
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.02	-	-
Author-provided FSC curve	3.00	3.51	3.04
Unmasked-calculated*	3.50	4.00	3.56

*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 3.50 differs from the reported value 3.02 by more than 10 %

9 Map-model fit [i](#)

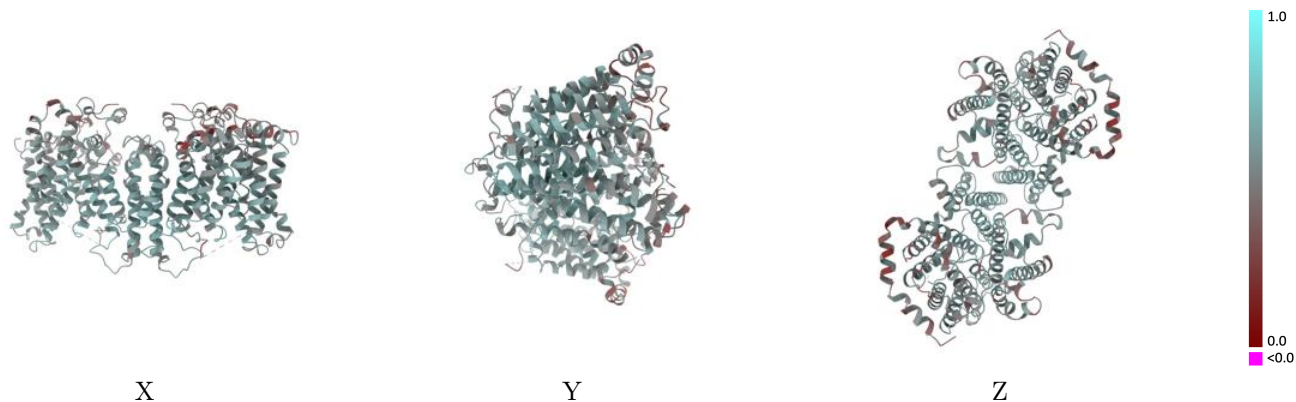
This section contains information regarding the fit between EMDB map EMD-41191 and PDB model 8TEM. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



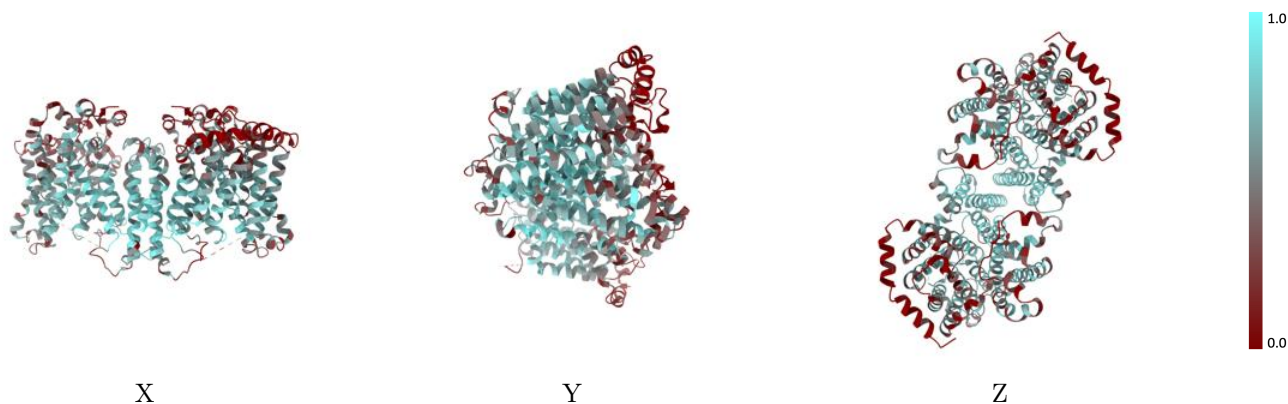
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



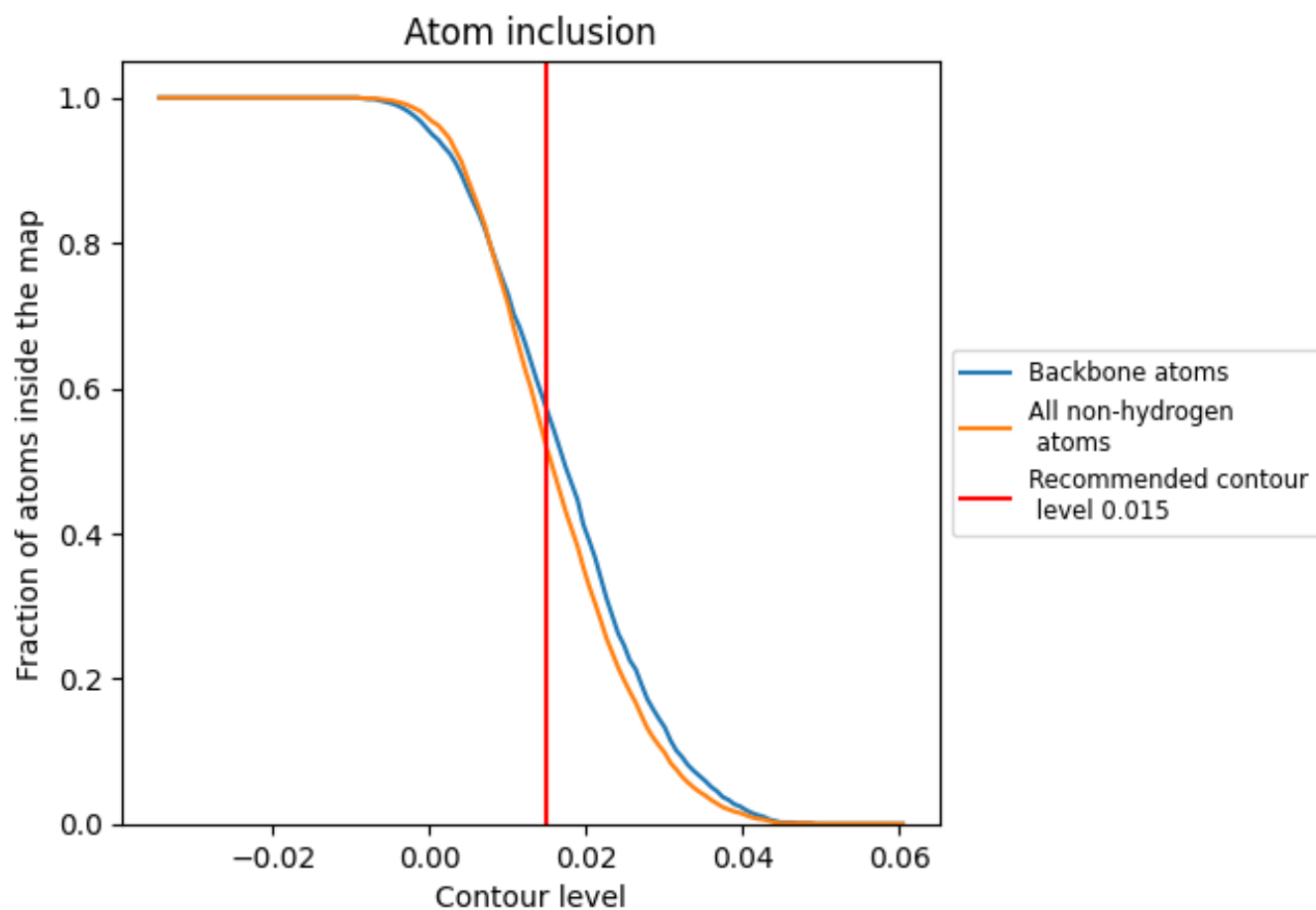
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 57% of all backbone atoms, 52% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	█ 0.5160	█ 0.5400
A	█ 0.5160	█ 0.5390
B	█ 0.5160	█ 0.5400

