



Full wwPDB EM Validation Report ⓘ

Jan 15, 2025 – 10:13 AM EST

PDB ID : 8TEG
EMDB ID : EMD-41185
Title : Cryo-EM structure of Arabidopsis thaliana Bor1 in lipid nanodiscs (protomer-focused refinement)
Authors : Jiang, Y.; Jiang, J.
Deposited on : 2023-07-06
Resolution : 2.15 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.dev113
MolProbity : 4.02b-467
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) : 2.40

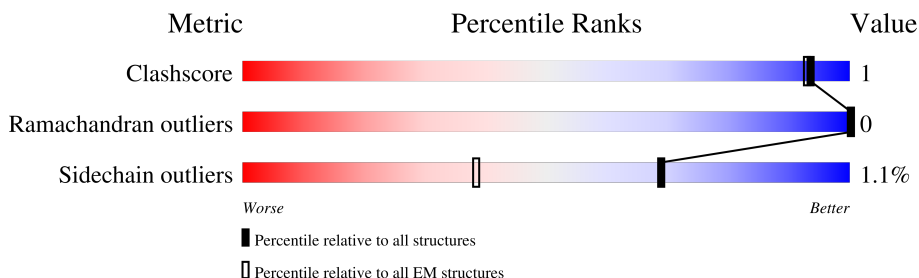
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.15 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	714	
1	B	714	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4518 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
1	A	539	Total	C	N	O	S	0	0
			4247	2813	683	722	29		
1	B	22	Total	C	N	O	S	0	0
			183	113	33	36	1		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	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

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		AltConf
2	A	81	Total	O	0
			81	81	

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Mol	Chain	Residues	Atoms		AltConf
2	B	7	Total	O	0
			7	7	

GLN	GLU	LYS	MET	LYS	MET	LYS	SER	ALA
MET	GLU	THR	THR	THR	ILE	PRO	PRO	SER
SER	GLU	ILE	ILE	ILE	LYS	ILE	MET	MET
PRO	GLU	ALA	ALA	LYS	LEV	THR	HIS	ILE
ARG	ALA	MET	MET	LEV	LEV	GLU	THR	ALA
VAL	PRO	PHE	THR	MET	THR	SER	LYS	VAL
GLY	ALA	THR	LEV	ILE	THR	THR	LEV	LEV
ASN	PRO	LEV	LEV	PRO	THR	GLN	LEV	TTR
SER	PRO	PHE	GLN	THR	THR	ALA	ALA	THR
PRO	ALA	TTR	LEV	VAL	THR	LEV	LYS	HIS
ALA	ALA	LEV	LEV	THR	PHE	THR	LYS	ASN
SER	GLU	LEV	LEV	GLY	GLY	THR	GLN	SER
GLY	GLU	ILE	ILE	PHE	ALA	ASN	LEV	ALA
THR	GLU	THR	THR	ALA	LEV	ARG	GLN	GLN
CYS	GLU	PHE	PHE	CYS	ALA	ASN	ASN	LEV
ARG	ILE	GLY	GLY	THR	MET	ALA	ARG	ALA
SER	GLY	LEV	LEV	THR	ALA	PRO	ARG	ALA
PRO	SER	THR	THR	LEV	ILE	VAL	LEV	GLN
LEV	THR	TTR	TTR	ILE	THR	VAL	VAL	GLN
ASN	THR	TTR	TTR	THR	GLU	ASP	VAL	LYS
GLN	SER	ILE	ILE	SER	LEV	THR	THR	GLU
SER	SER	ILE	ILE	PRO	LEV	PRO	THR	THR
SER	SER	ALA	ALA	GLY	ASN	GLY	ARG	ALA
ASN	D632	GLY	GLY	ASN	GLN	ASP	ARG	ASN
HIS	Y624	VAL	VAL	GLN	GLN	ILE	ILE	LYS
HIS	+	MET	MET	PHE	PHE	GLU	THR	SER
HIS	+	PRO	PRO	PHE	PRO	GLU	ASN	SER
HIS	T645	LEV	LEV	LEV	LEV	ILE	ALA	TTR
HIS	SER	THR	THR	THR	THR	ASP	SER	HIS
HIS	VAL	ILE	ILE	ILE	ILE	ASP	LEV	TTR
HIS	THR	MET	MET	LEV	LEV	GLY	GLY	ASP
HIS	SER	PHE	PHE	LEV	LEV	LEV	LEV	LEV
HIS	SER	LEV	LEV	THR	THR	LEV	TTR	LEV
HIS	SER	THR	THR	ALA	ALA	ASP	ASP	LEV
	SER	PRO	VAL	PRO	GLU	GLY	ASN	GLY
	THR	ARG	ARG	LYS	VAL	VAL	LYS	PHE
	VAL	GLN	GLN	THR	ARG	GLN	GLN	PHE
	ASN	TTR	TTR	ARG	ARG	GLN	GLU	THR
	ASN	LEV	LEV	LEV	PHE	ARG	ALA	LEV
	ARG	LEV	LEV	VAL	VAL	VAL	MET	LEV
	SER	ARG	ARG	PRO	VAL	VAL	THR	CYS
	LEV	THR	THR	THR	THR	THR	HIS	GLY
	LEV	THR	THR	THR	THR	THR	ASN	GLY
	PRO	ALA	ALA	ALA	ALA	LEV	PRO	LEV
	ARG	ALA	ALA	HIS	HIS	THR	VAL	PRO
	VAL	LEV	LEV	LEV	LEV	PHE	TTR	PRO
	SER	ASN	ASN	ASN	ASN	GLY	GLN	ASN
	GLN	THR	THR	THR	THR	GLY	GLN	GLN
	GLY	ILE	ILE	ASP	ASP	VAL	VAL	ILE
	ARG	ALA	ALA	ALA	ALA	PRO	GLY	GLN
	LEV	ALA	ALA	ALA	ALA	LEV	GLY	GLN

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	853837	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	0.203	Depositor
Minimum map value	-0.123	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	318.72, 318.72, 318.72	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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	0.32	1/4367 (0.0%)	0.56	2/5937 (0.0%)
1	B	0.24	0/186	0.56	0/249
All	All	0.32	1/4553 (0.0%)	0.56	2/6186 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	114	PRO	CG-CD	-12.22	1.10	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	PRO	N-CD-CG	-16.69	78.16	103.20
1	A	114	PRO	CA-CB-CG	-12.80	79.68	104.00

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	4247	0	4341	11	0
1	B	183	0	172	0	0
2	A	81	0	0	0	0
2	B	7	0	0	0	0
All	All	4518	0	4513	11	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 (11) 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	2.19	0.57
1:A:357:VAL:HG23	1:A:360:GLN:HB2	1.91	0.53
1:A:609:PRO:HD2	1:A:612:LEU:HD12	1.89	0.52
1:A:541:LYS:O	1:A:545:MET:HG2	2.10	0.51
1:A:281:THR:HG22	1:A:283:VAL:H	1.78	0.48
1:A:38:ALA:HB3	1:A:39:PRO:HD3	1.94	0.48
1:A:180:ARG:O	1:A:264:ARG:NH2	2.48	0.44
1:A:323:GLU:OE1	1:A:323:GLU:N	2.41	0.44
1:A:25:ASP:OD1	1:A:328:LYS:NZ	2.32	0.41
1:A:627:ASP:OD1	1:A:627:ASP:N	2.53	0.41
1:A:214:THR:HB	1:A:243:MET:SD	2.62	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	533/714 (75%)	525 (98%)	8 (2%)	0	100	100
1	B	20/714 (3%)	20 (100%)	0	0	100	100
All	All	553/1428 (39%)	545 (99%)	8 (1%)	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	454/613 (74%)	449 (99%)	5 (1%)	70	75
1	B	20/613 (3%)	20 (100%)	0	100	100
All	All	474/1226 (39%)	469 (99%)	5 (1%)	69	75

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	PHE
1	A	217	ARG
1	A	260	LYS
1	A	287	LEU
1	A	541	LYS

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 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 ⓘ

There are no chain breaks in this entry.

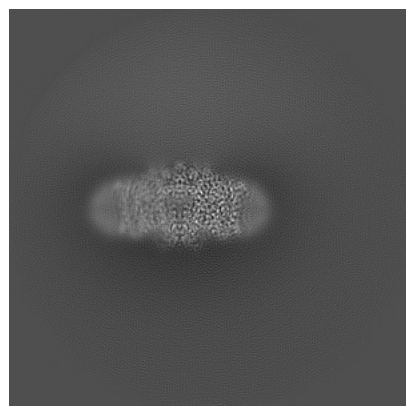
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41185. These allow visual inspection of the internal detail of the map and identification of artifacts.

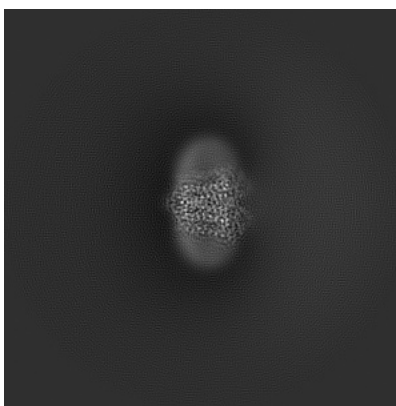
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

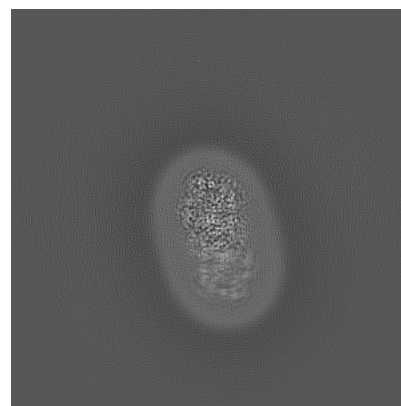
6.1.1 Primary map



X

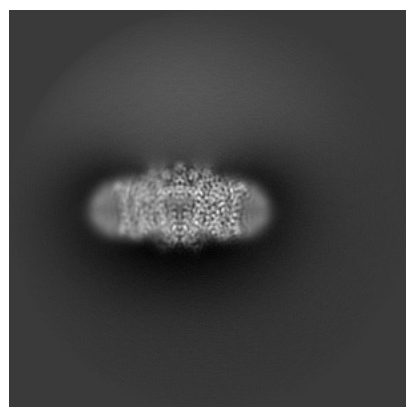


Y

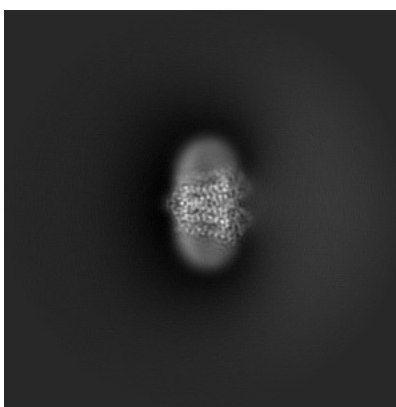


Z

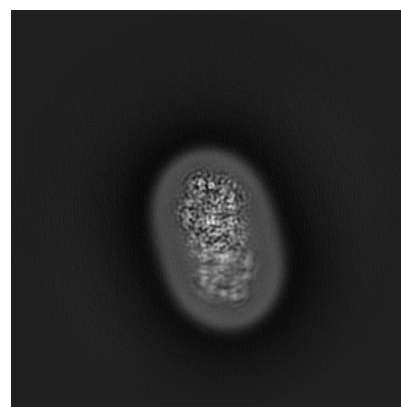
6.1.2 Raw map



X



Y

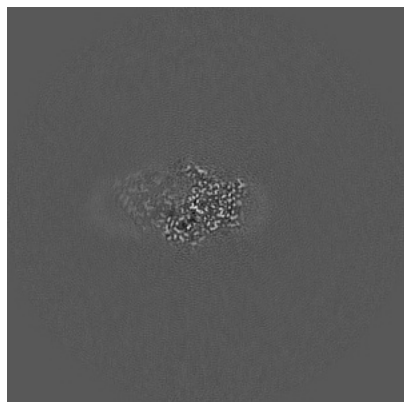


Z

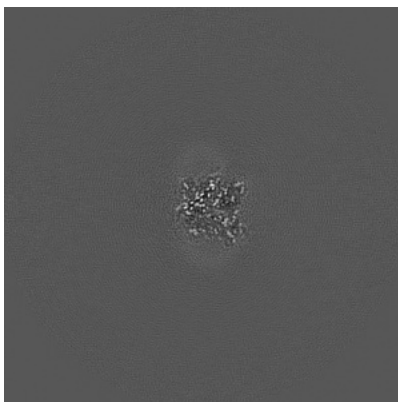
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

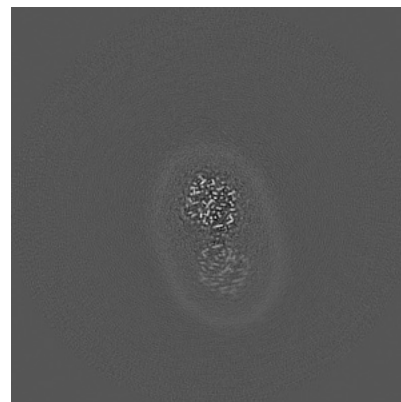
6.2.1 Primary map



X Index: 192

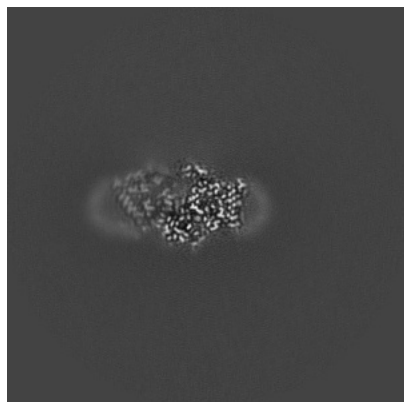


Y Index: 192

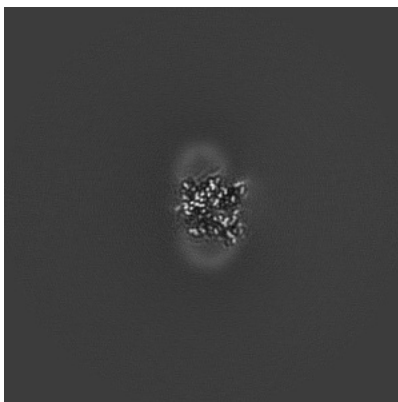


Z Index: 192

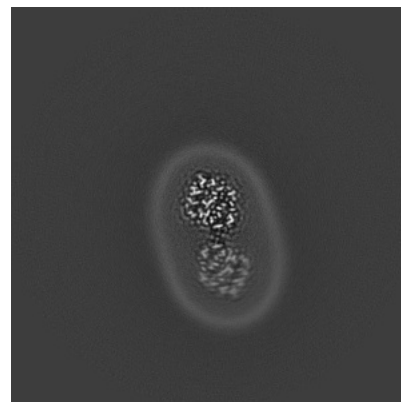
6.2.2 Raw map



X Index: 192



Y Index: 192

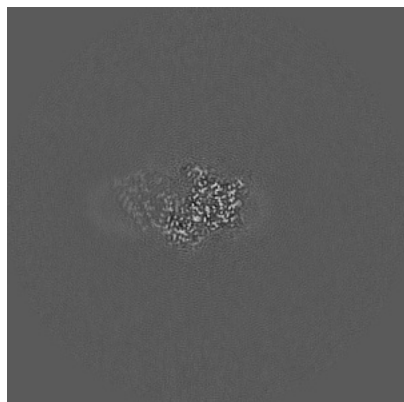


Z Index: 192

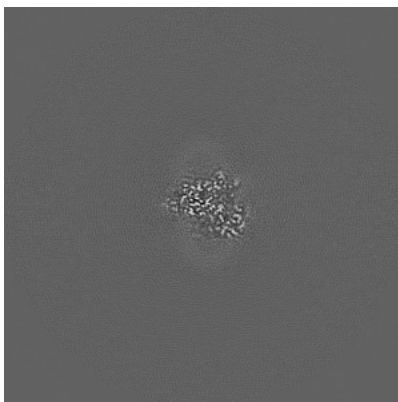
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

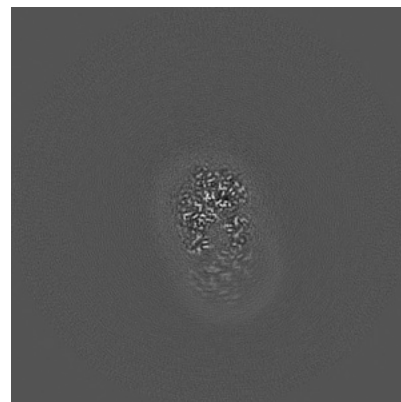
6.3.1 Primary map



X Index: 193

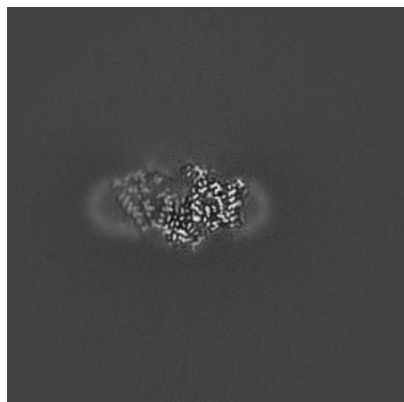


Y Index: 179

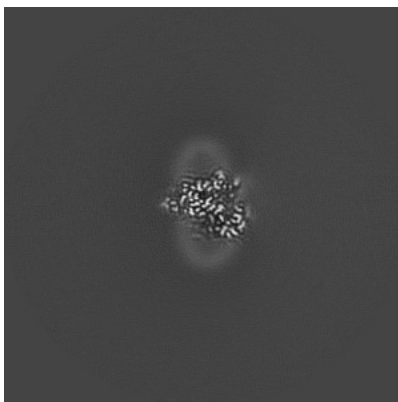


Z Index: 208

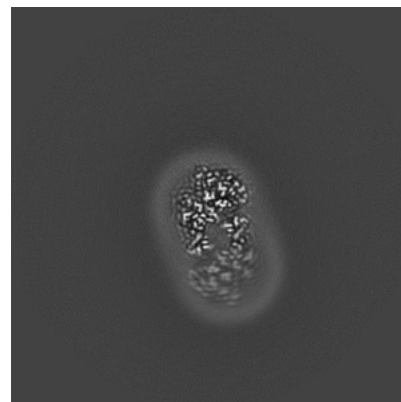
6.3.2 Raw map



X Index: 193



Y Index: 179

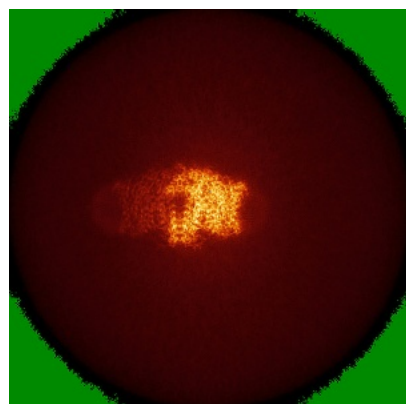


Z Index: 208

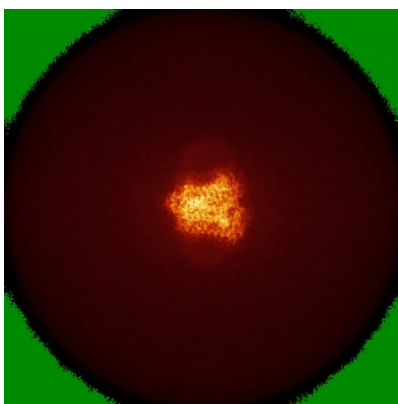
The images above show the largest variance slices of the map in three orthogonal directions.

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

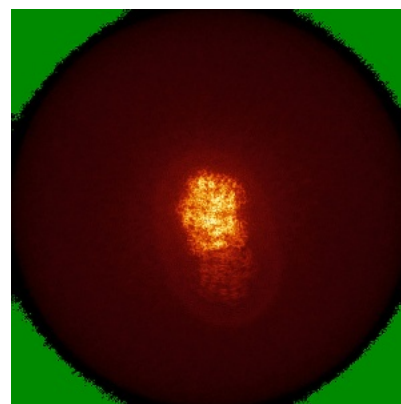
6.4.1 Primary map



X



Y

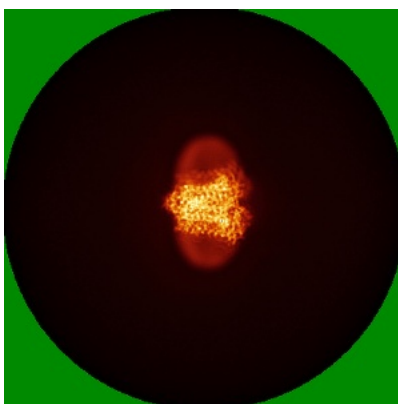


Z

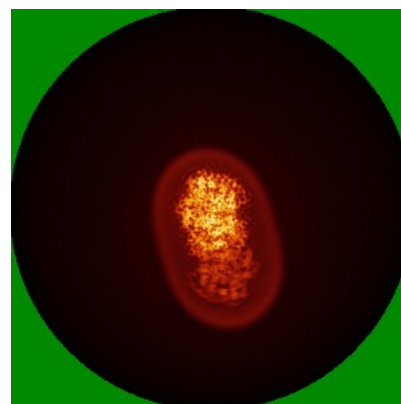
6.4.2 Raw map



X



Y

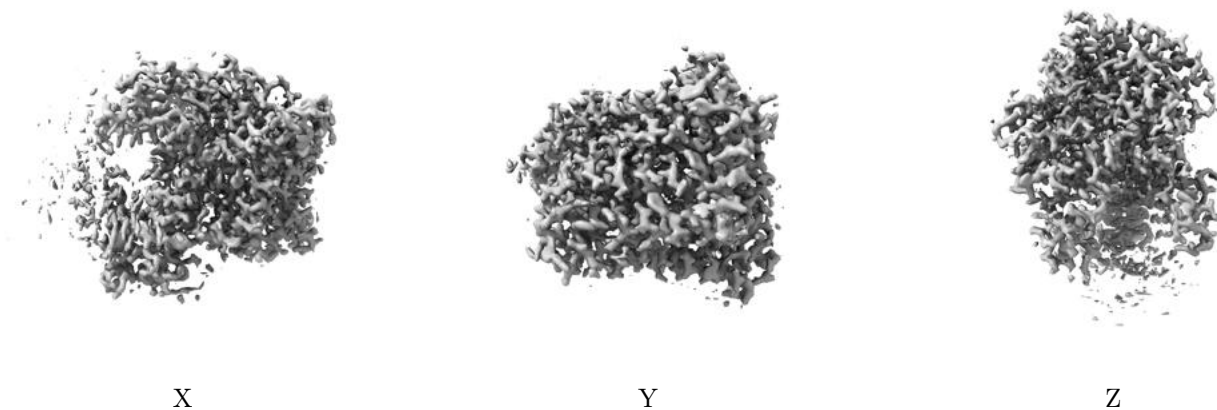


Z

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.

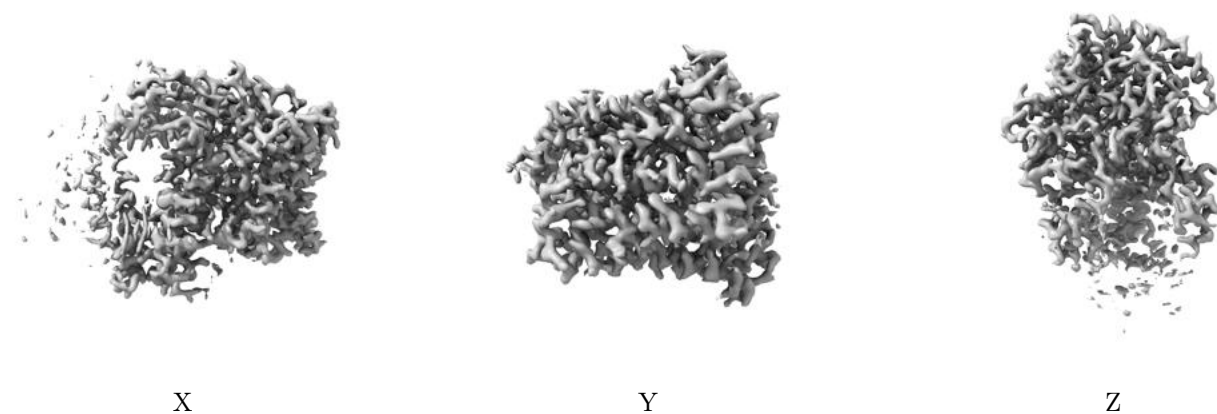
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. 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.

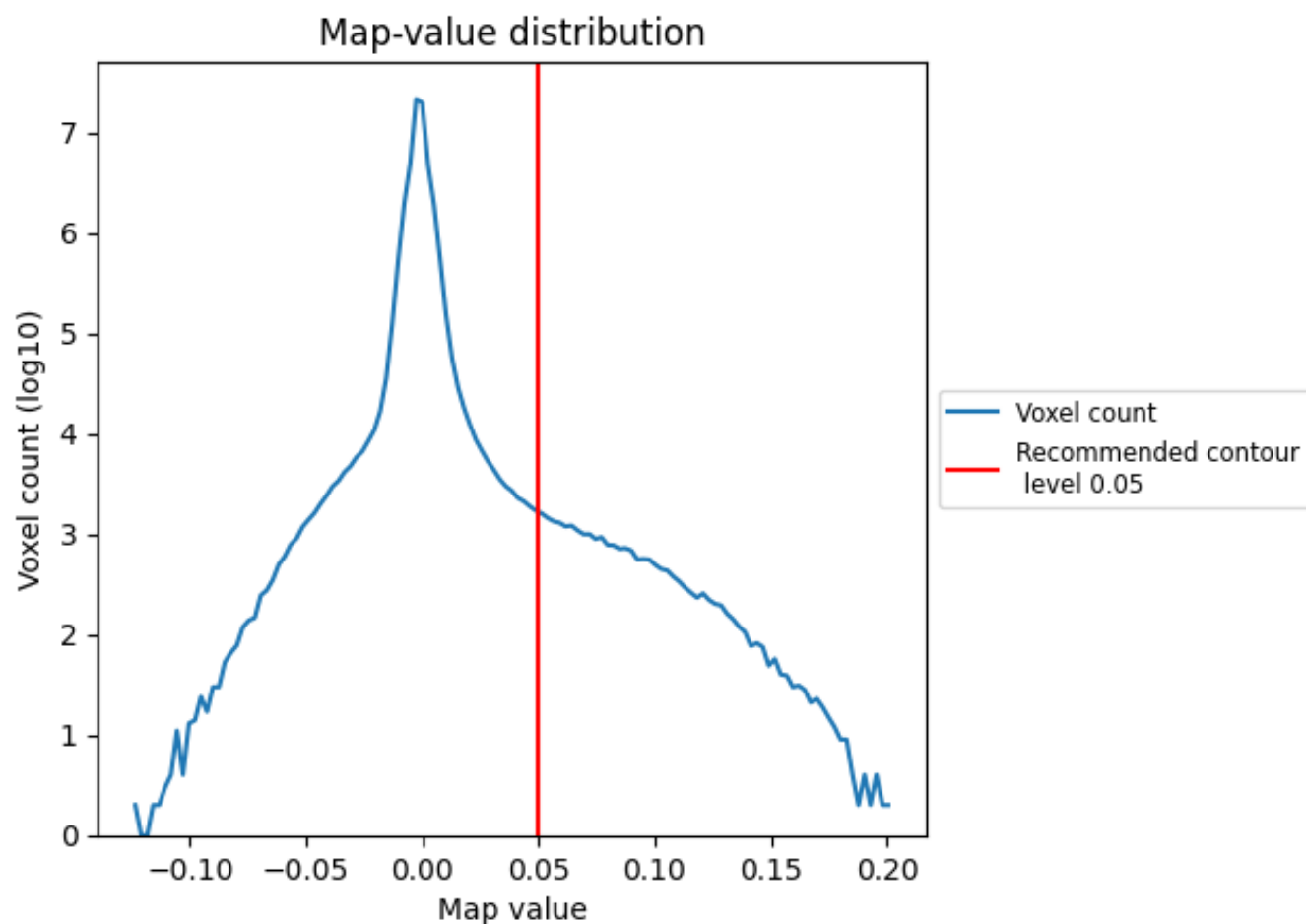
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

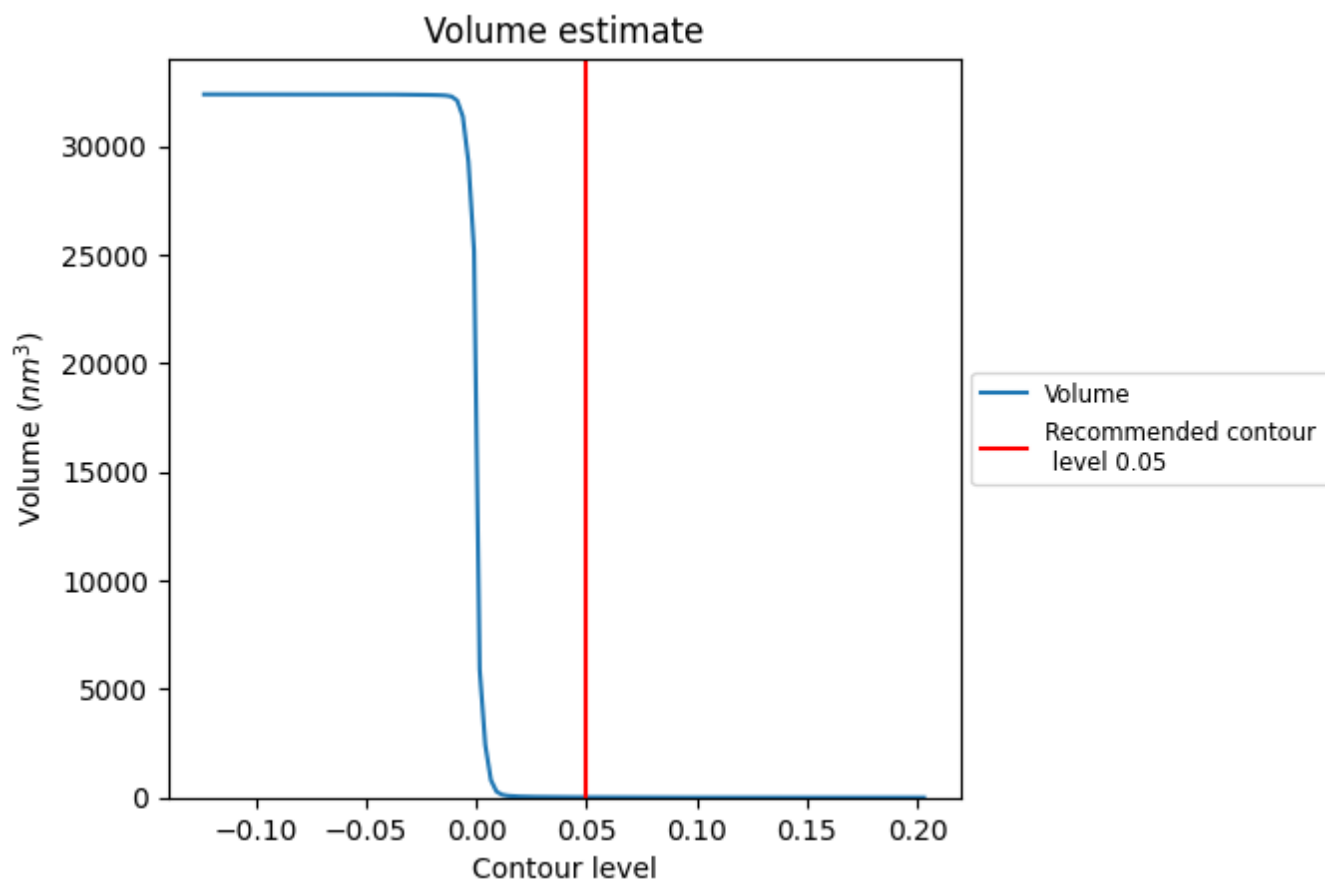
This section contains the results of statistical analysis of the map.

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.

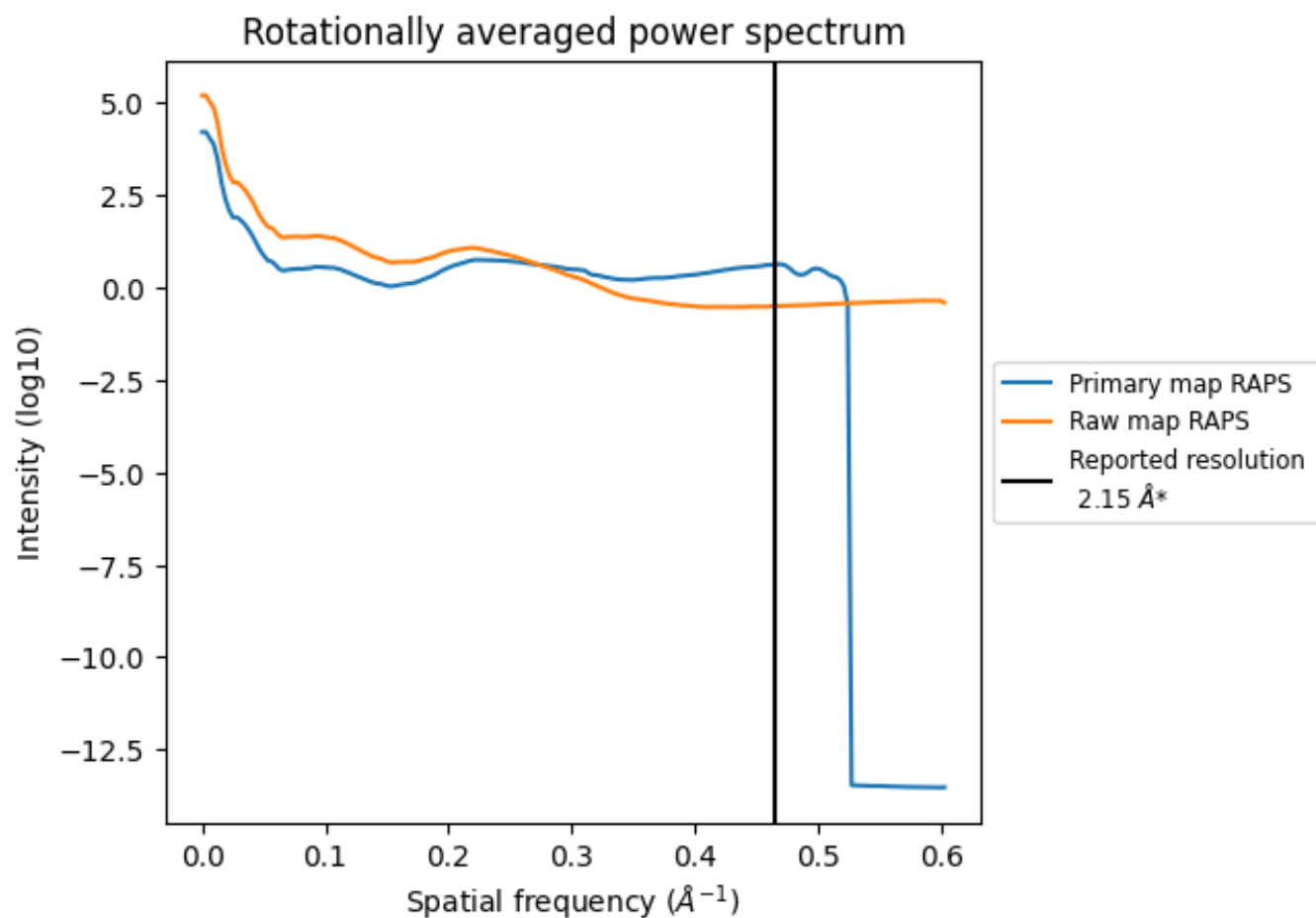
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 14 nm³; this corresponds to an approximate mass of 12 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 ⓘ

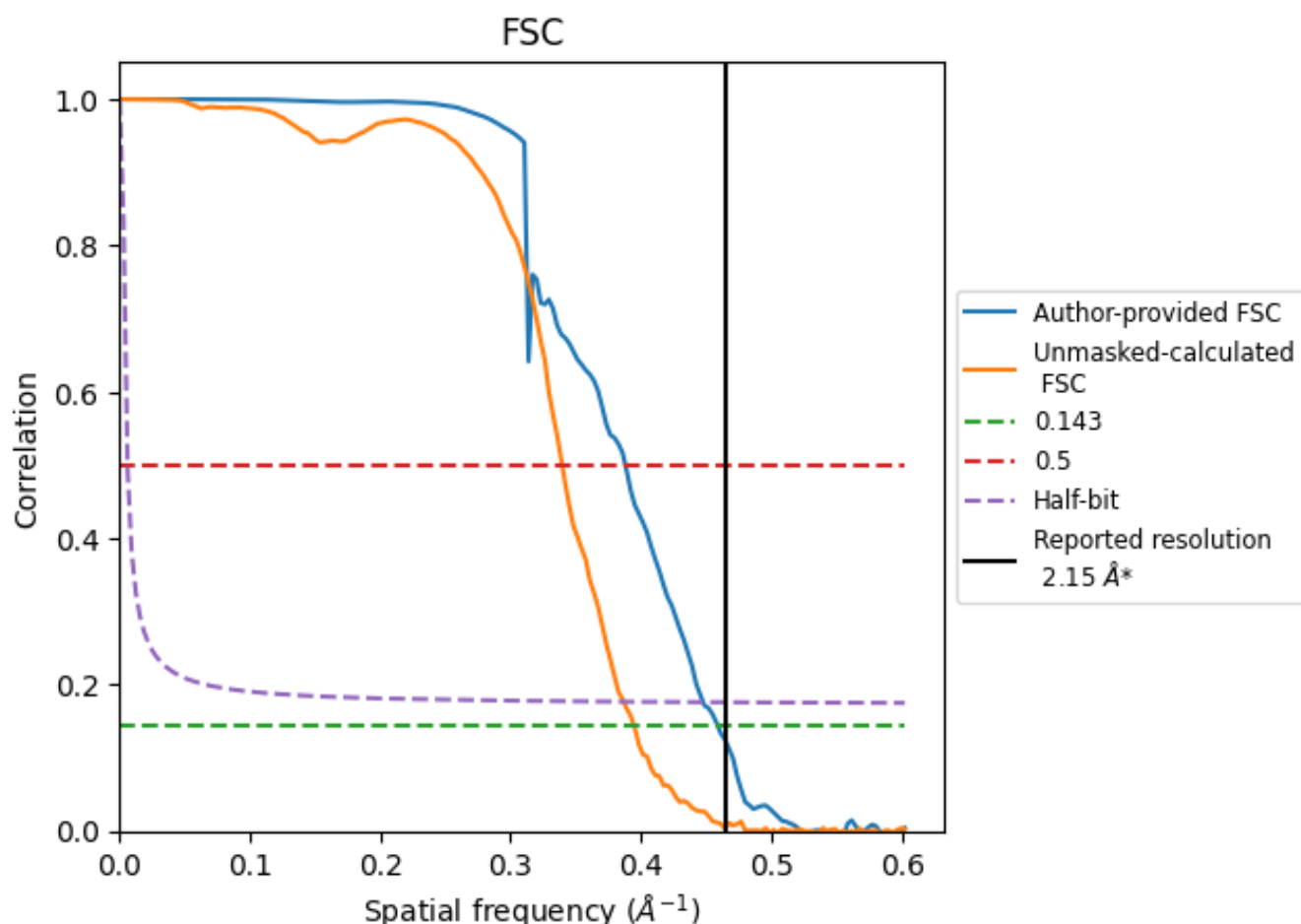


*Reported resolution corresponds to spatial frequency of 0.465 Å⁻¹

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 0.465 Å⁻¹

8.2 Resolution estimates [i](#)

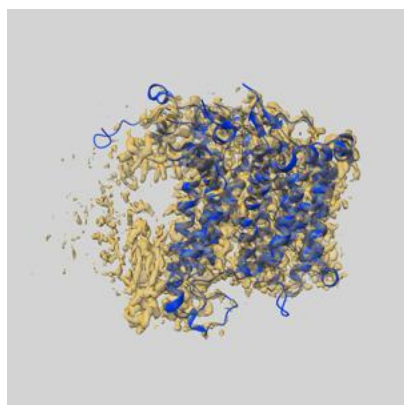
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.15	-	-
Author-provided FSC curve	2.18	2.58	2.23
Unmasked-calculated*	2.53	2.95	2.59

*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 2.53 differs from the reported value 2.15 by more than 10 %

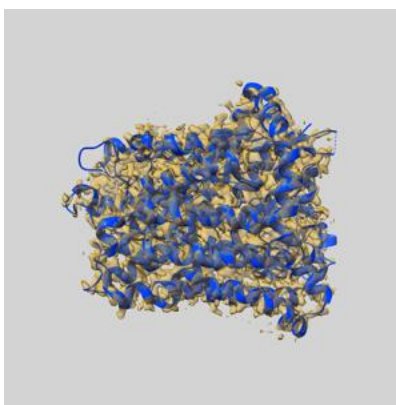
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41185 and PDB model 8TEG. Per-residue inclusion information can be found in section [3](#) on page [5](#).

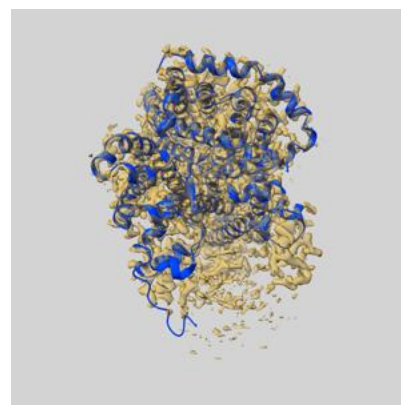
9.1 Map-model overlay [i](#)



X



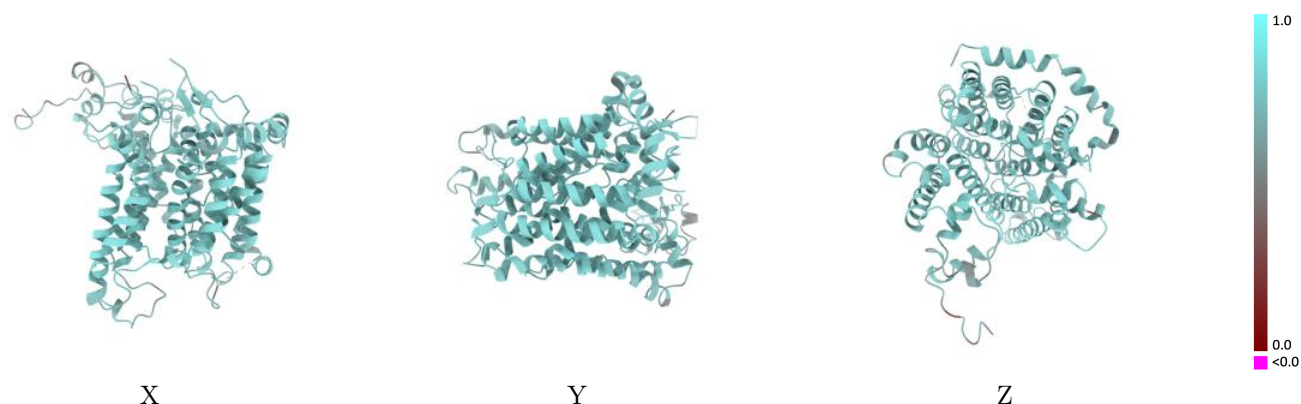
Y



Z

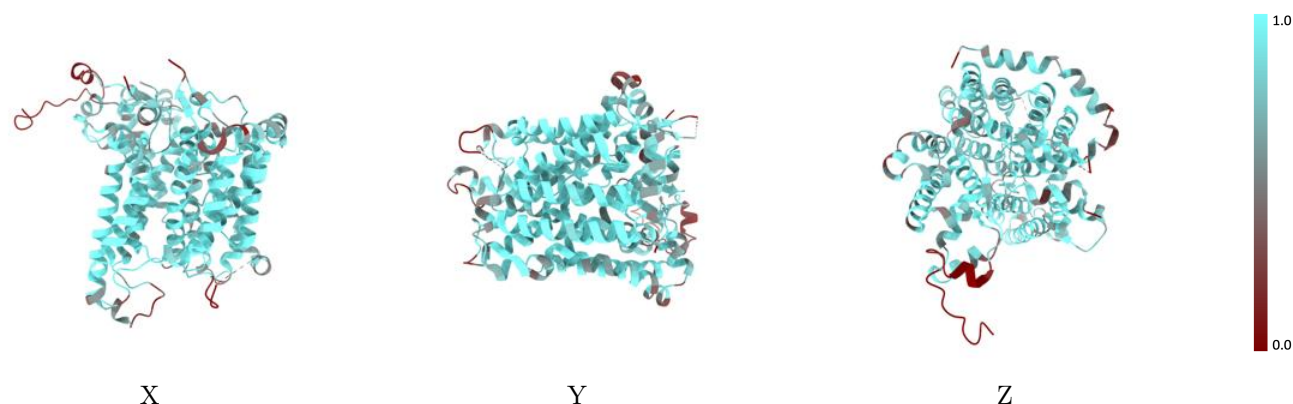
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



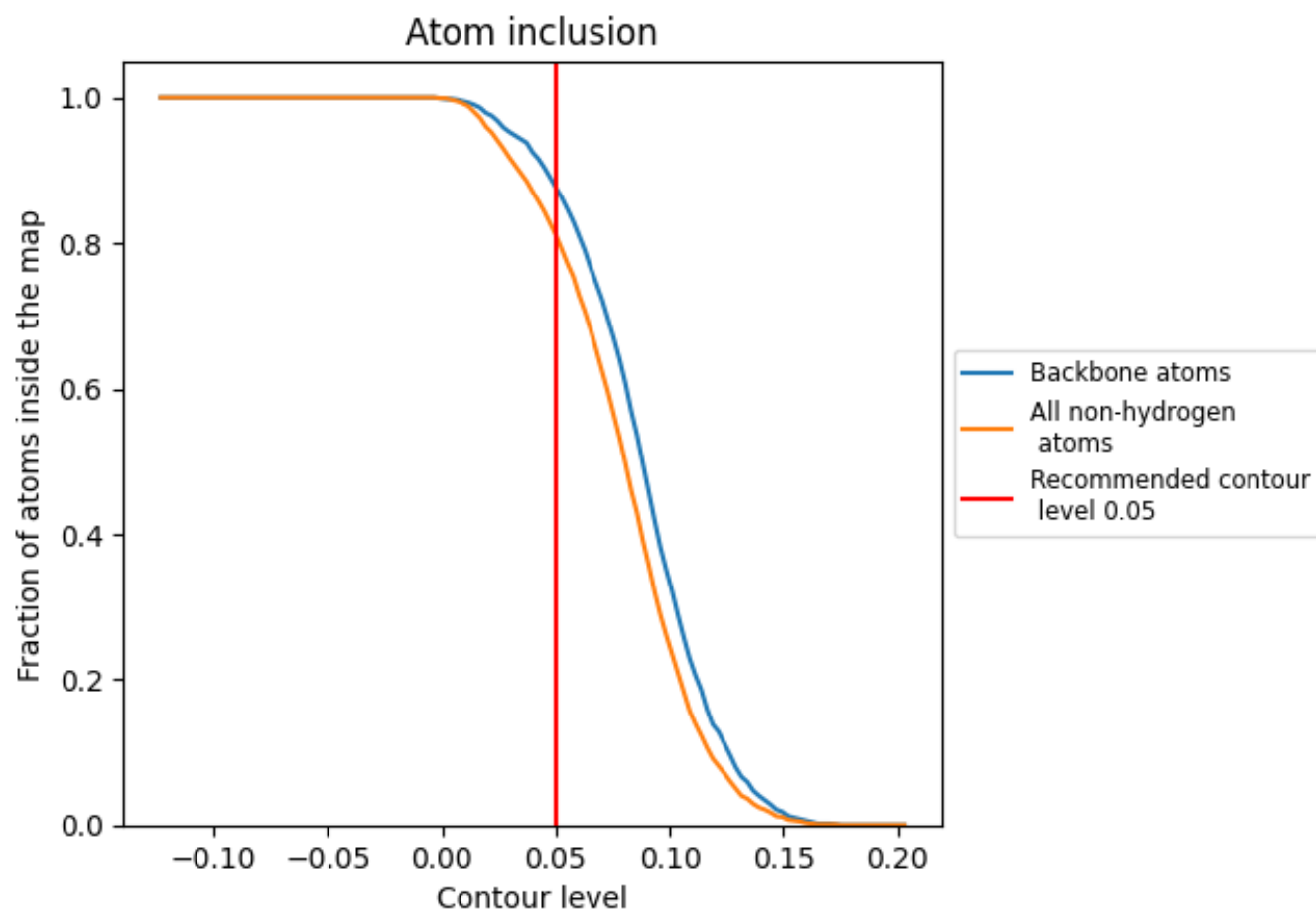
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 81% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8120	<div></div> 0.7300
A	<div></div> 0.8180	<div></div> 0.7310
B	<div></div> 0.6930	<div></div> 0.7040

