wwPDB EM Validation Summary Report (i)

Jul 1, 2024 – 12:39 PM EDT

PDB ID	:	8TEN
EMDB ID	:	EMD-41192
Title	:	Cryo-EM structure of Arabidopsis thaliana Bor1 mutant (R637E/E641R/R643E) in mixed occluded/inward-facing conformations in lauryl maltose neopentyl glycol (LMNG)
Authors	:	Jiang, Y.; Jiang, J.
Deposited on	:	2023-07-06
Resolution	:	2.98 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 (i) 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 (i)) were used in the production of this report:

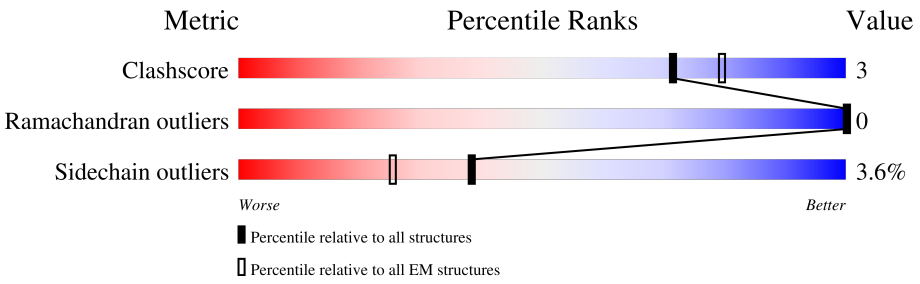
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.98 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 <=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	12% 62% 7% 31%
1	B	714	30% 61% 9% 30%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7872 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	P	S		
1	A	494	3903	2555	645	676	1	26	0	0
			Total	C	N	O	S			
1	B	502	3969	2632	643	665	29		0	0

There are 26 discrepancies between the modelled and reference sequences:

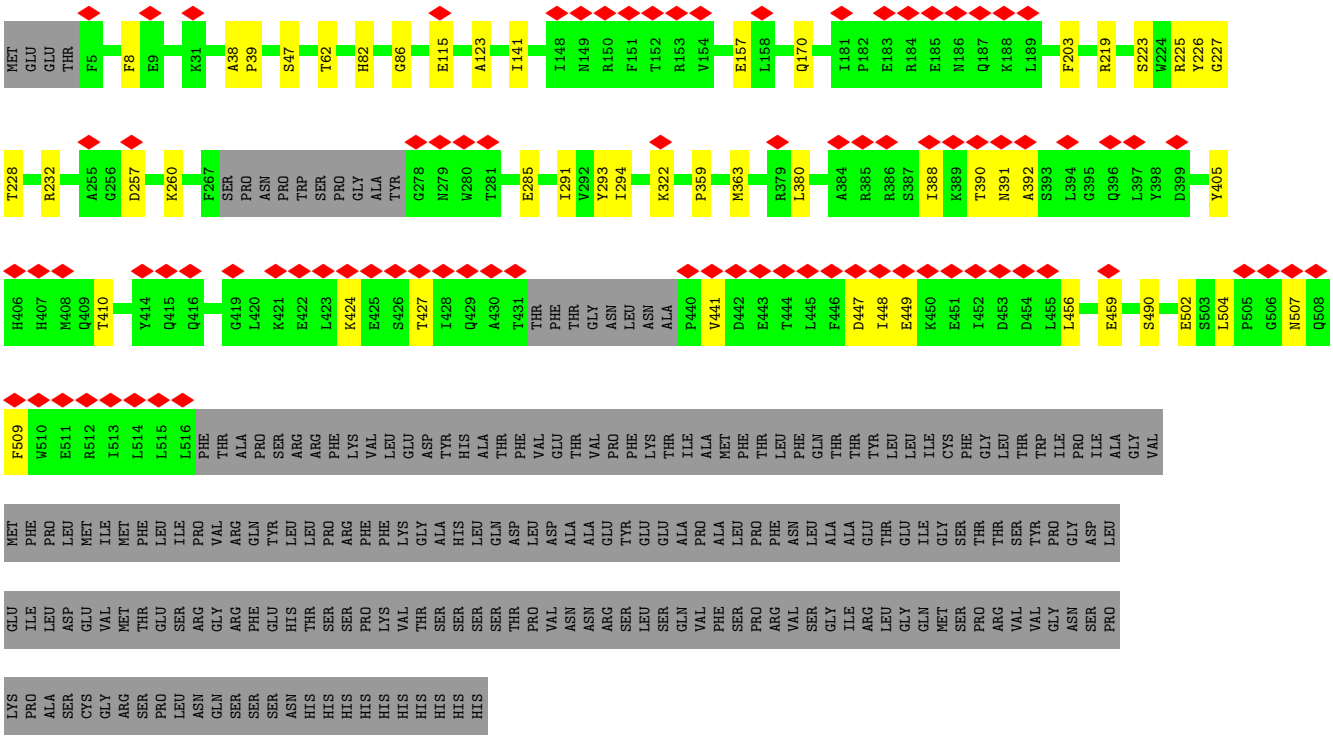
Chain	Residue	Modelled	Actual	Comment	Reference
A	637	GLU	ARG	engineered mutation	UNP Q8VYR7
A	641	ARG	GLU	engineered mutation	UNP Q8VYR7
A	643	GLU	ARG	engineered mutation	UNP Q8VYR7
A	705	HIS	-	expression tag	UNP Q8VYR7
A	706	HIS	-	expression tag	UNP Q8VYR7
A	707	HIS	-	expression tag	UNP Q8VYR7
A	708	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

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

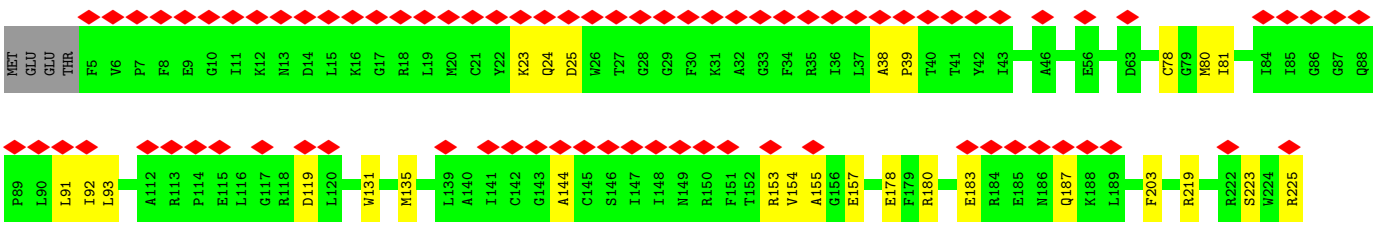
• Molecule 1: Boron transporter 1

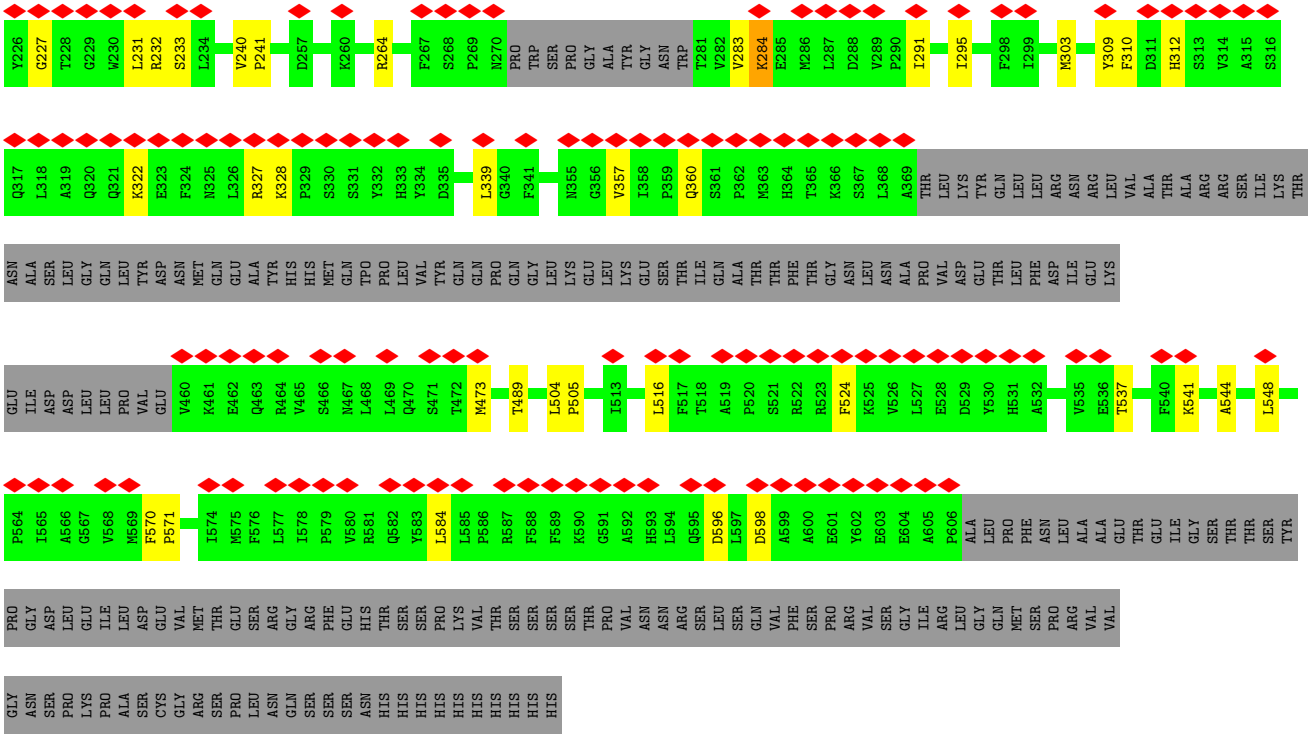
Chain A:



• Molecule 1: Boron transporter 1

Chain B:




Y226 G227 T228 G229 W230 L231 R232 S233 L234 V240 P241 D257 K260 R264 F267 S268 P269 N270 PRO TRP SER PRO GLY ALA TYR GLY ASN TRP T281 V282 V283 K284 E285 M286 L287 D288 V289 P290 I291 I295 F298 I299 M303 Y309 F310 D311 H312 S313 V314 A315 S316
Q317 L318 A319 Q320 Q321 K322 E323 F324 N325 L326 R327 K328 P329 S330 S331 Y332 H333 Y334 D335 L339 G340 F341 N355 G356 V357 I358 P359 Q360 S361 P362 M363 H364 T365 K366 S367 L368 A369 THR LEU LYS TYR GLN LEU LEU ARG ASN ARG LEU VAL ALA THR ALA ARG ARG SER ILE LYS THR
ASN ALA SER LEU GLY GLN LEU TYR ASP ASN MET GLN GLU ALA TYR HIS HIS MET GLN TPO PRO LEU VAL TYR GLN GLN PRO GLN GLY LEU LYS GLU LEU LYS GLU SER THR ILE GLN ALA THR THR PHE THR GLY ASN LEU ASN ALA PRO VAL ASP GLU THR LEU PHE ASP ILE GLU LYS
GLU ILE ASP ASP LEU LEU PRO VAL GLU V460 K461 E462 Q463 R464 V465 S466 M467 L468 L469 Q470 S471 T472 M473 T489 L504 P505 I513 L516 F517 T518 A519 P520 S521 R522 R523 F524 K525 V526 L527 E528 D529 Y530 H531 A532 V535 E536 T537 F540 K541 A544 L548
P564 I565 A566 G567 V568 M569 F570 P571 I574 M575 F576 L577 I578 P579 V580 R581 Q582 Y583 L584 L585 P586 R587 F588 F589 K590 G591 A592 H593 L594 Q595 D596 L597 D598 A599 A600 E601 Y602 E603 E604 A605 P606 ALA LEU PRO PHE ASN LEU ALA ALA GLU THR GLU ILE GLY SER THR THR SER TYR
PRO GLY ASP LEU GLU ILE LEU ASP GLU VAL MET THR GLU SER ARG GLY ARG PHE GLU HIS THR SER SER PRO LYS VAL THR SER SER SER SER THR PRO VAL ASN ASN ARG SER LEU SER GLN VAL PHE SER PRO ARG VAL SER GLY ILE ARG LEU GLY GLN MET SER PRO ARG VAL VAL
GLY ASN SER PRO LYS PRO ALA SER CYS GLY ARG SER PRO LEU ASN GLN SER SER SER ASN HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	132093	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 ($e^-/Å^2$)	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	0.078	Depositor
Minimum map value	-0.042	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)

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

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	0.25	0/3987	0.46	0/5405
1	B	0.26	0/4079	0.47	0/5539
All	All	0.25	0/8066	0.47	0/10944

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	3903	0	3999	24	0
1	B	3969	0	4074	31	0
All	All	7872	0	8073	55	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.

The worst 5 of 55 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:227:GLY:O	1:A:232:ARG:NH1	2.17	0.77
1:A:405:TYR:OH	1:A:459:GLU:OE2	2.08	0.72
1:A:388:ILE:HA	1:A:392:ALA:HB2	1.73	0.70
1:B:144:ALA:O	1:B:309:TYR:OH	2.10	0.70
1:A:392:ALA:HB1	1:A:441:VAL:HG12	1.74	0.69

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	487/714 (68%)	470 (96%)	17 (4%)	0	100	100
1	B	496/714 (70%)	482 (97%)	14 (3%)	0	100	100
All	All	983/1428 (69%)	952 (97%)	31 (3%)	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	418/612 (68%)	404 (97%)	14 (3%)	38	71
1	B	424/612 (69%)	408 (96%)	16 (4%)	33	67
All	All	842/1224 (69%)	812 (96%)	30 (4%)	38	68

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	23	LYS
1	B	473	MET
1	B	187	GLN
1	B	584	LEU
1	B	303	MET

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)

1 non-standard protein/DNA/RNA residue 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	$\#\|Z\| > 2$
1	TPO	A	410	1	8,10,11	1.08	0	10,14,16	1.70	1 (10%)

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
1	TPO	A	410	1	-	0/9/11/13	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	410	TPO	P-OG1-CB	-4.62	109.24	123.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

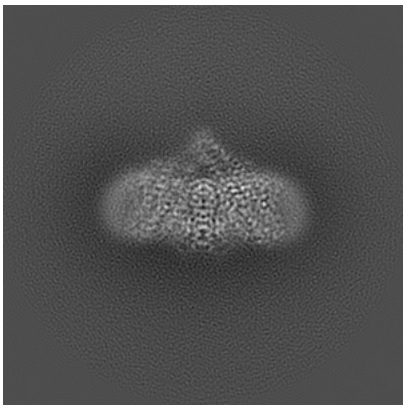
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-41192. These allow visual inspection of the internal detail of the map and identification of artifacts.

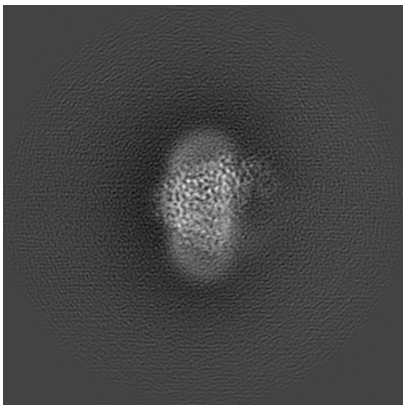
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map



X



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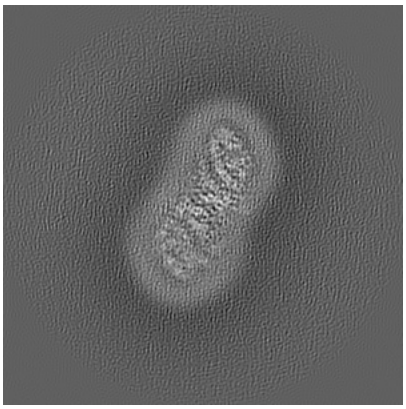
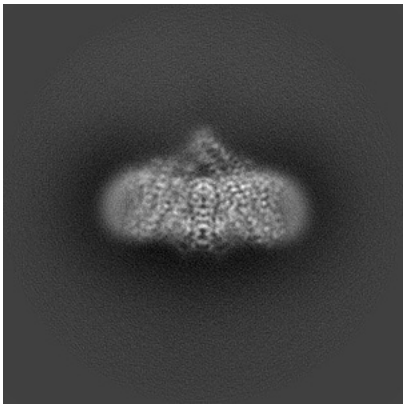


Z

6.1.2 Raw map



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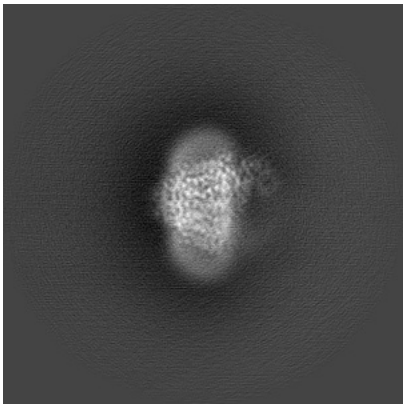
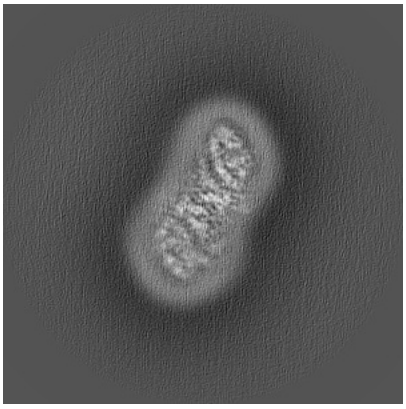


Y

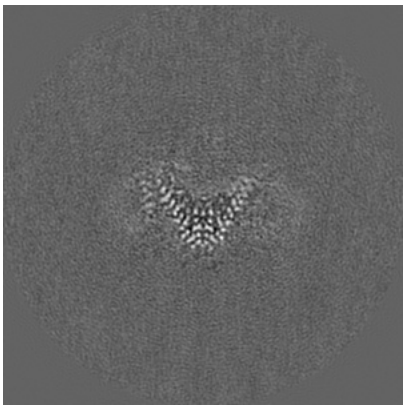


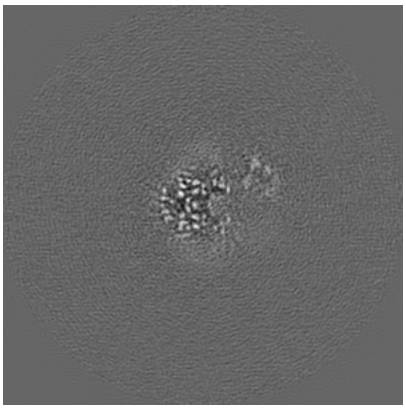
Z

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

6.2 Central slices (i)

6.2.1 Primary map


X Index: 160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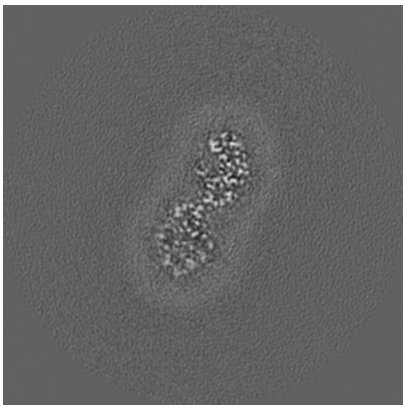
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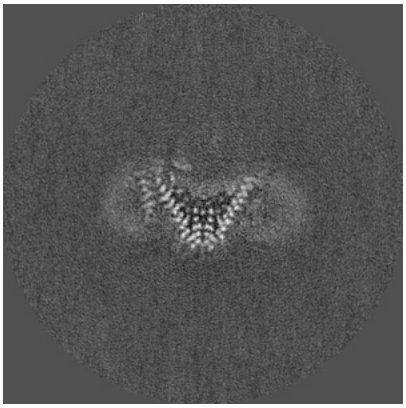
6.2.2 Raw map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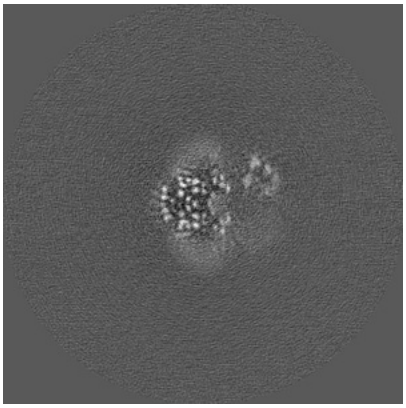
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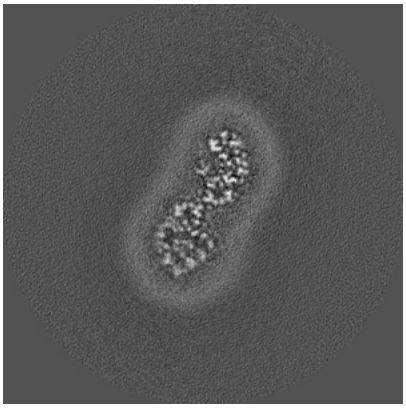
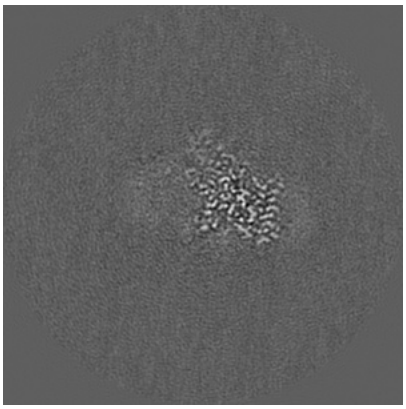

Z Index: 160

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

6.3 Largest variance slices (i)

6.3.1 Primary map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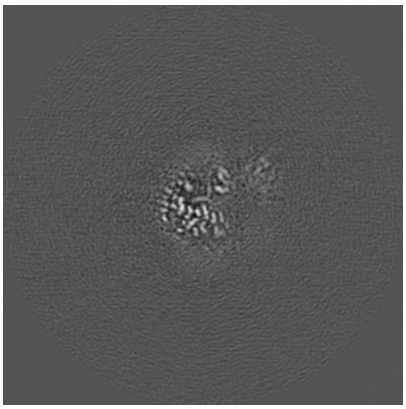
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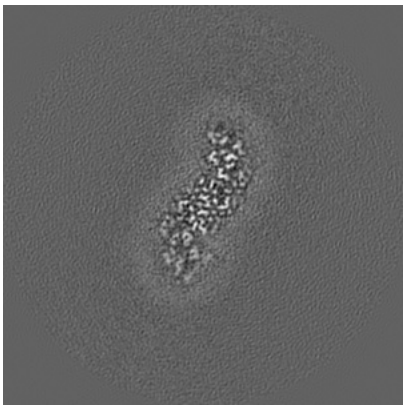
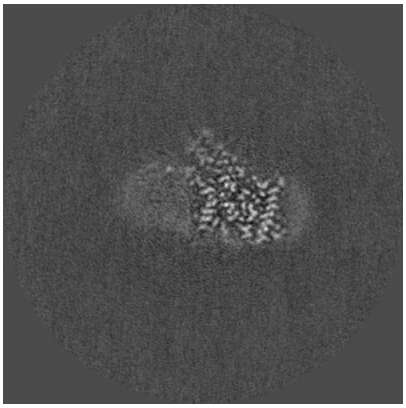
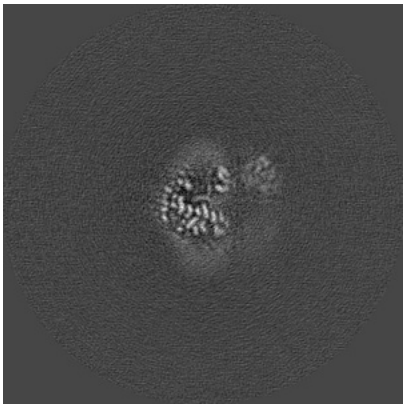
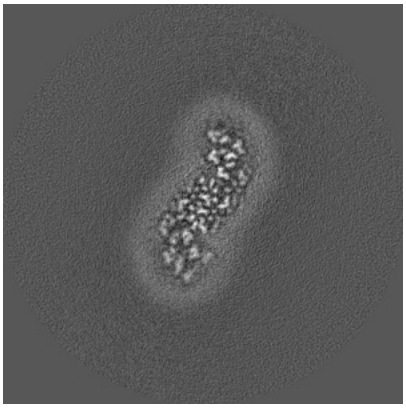

Z Index: 147

6.3.2 Raw map


X Index: 179

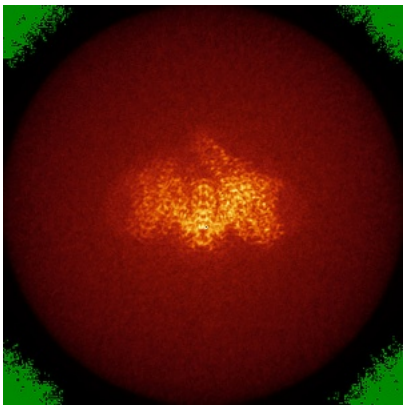

Y Index: 157

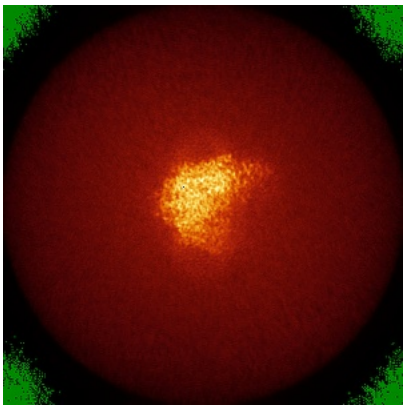

Z Index: 147

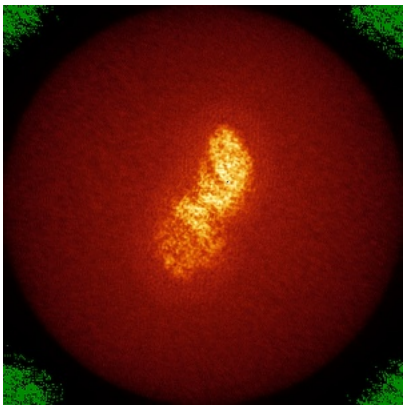
The images above show the largest variance slices of the map in three orthogonal directions.

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

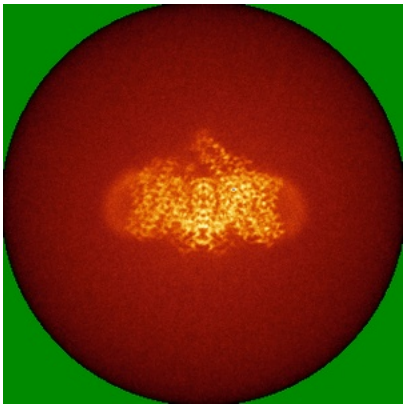
6.4.1 Primary map

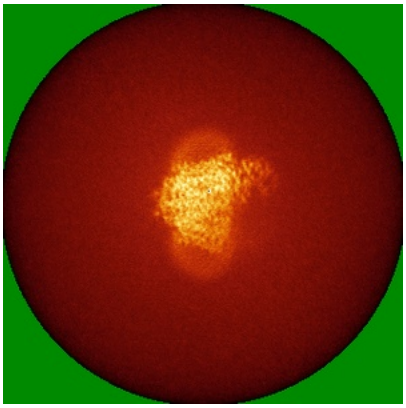

X

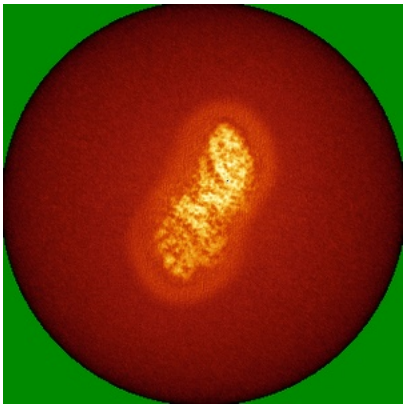

Y


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

X Y Z

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

X Y Z

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.

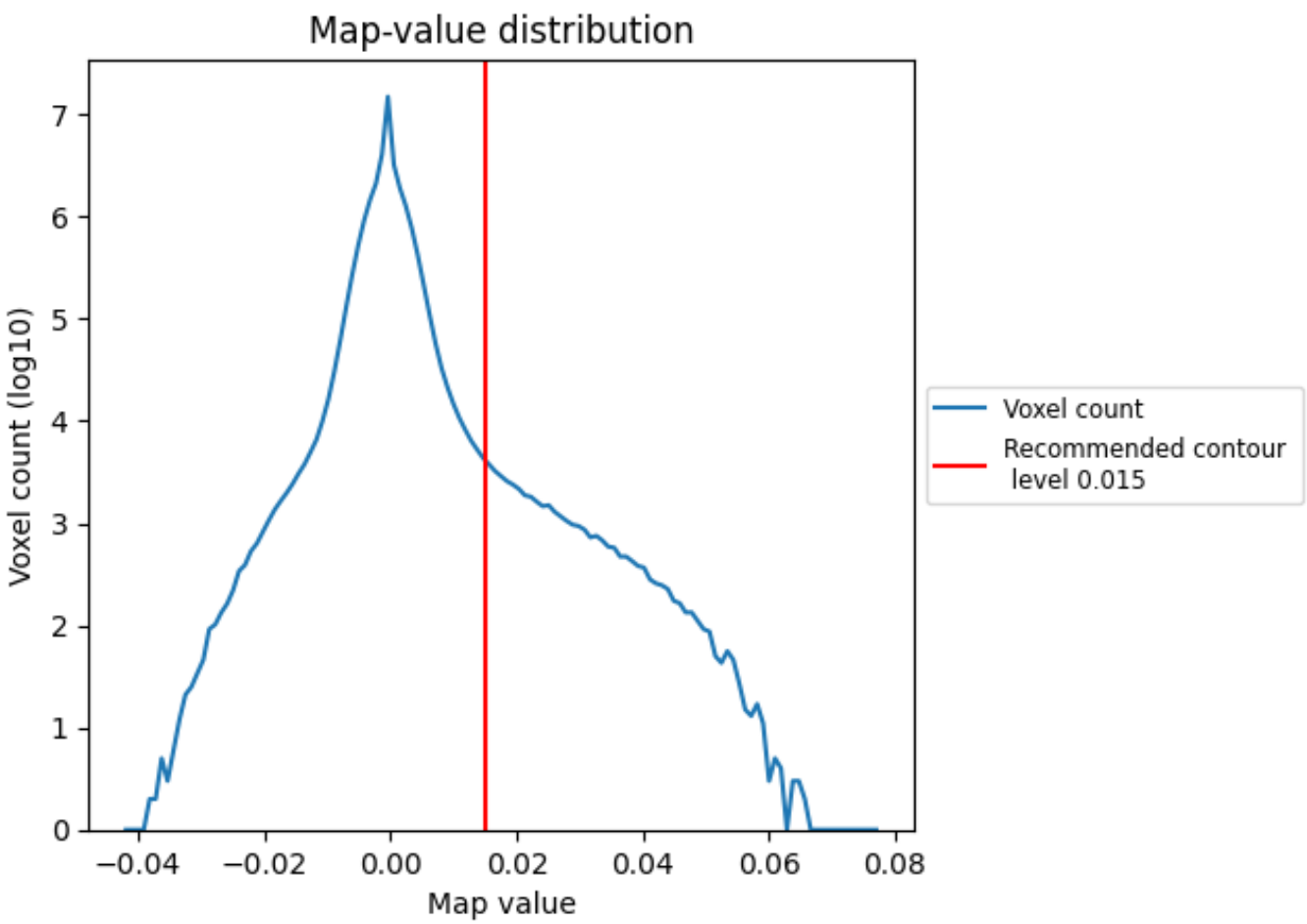
6.6 Mask visualisation (i)

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

7 Map analysis (i)

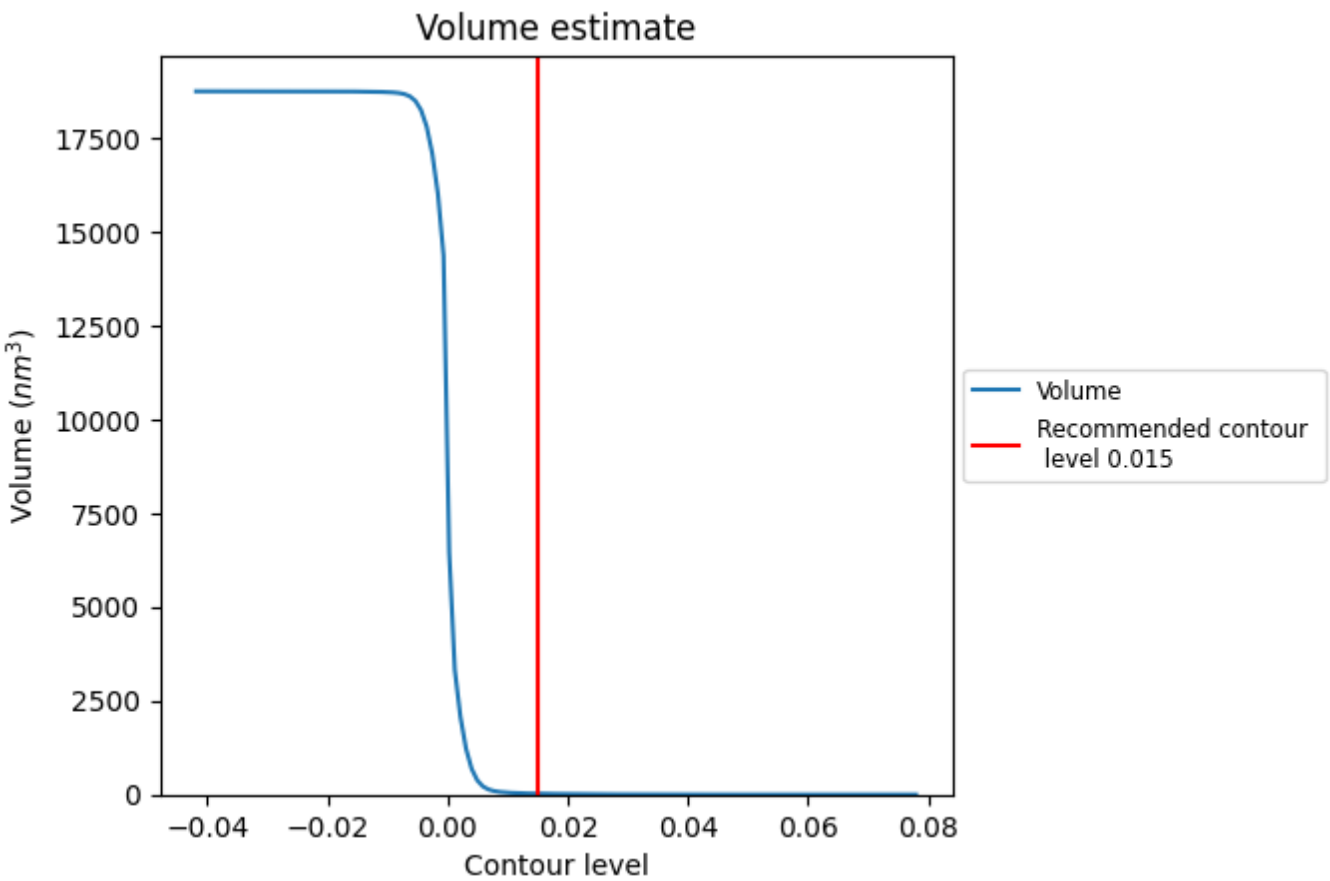
This section contains the results of statistical analysis of the map.

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.

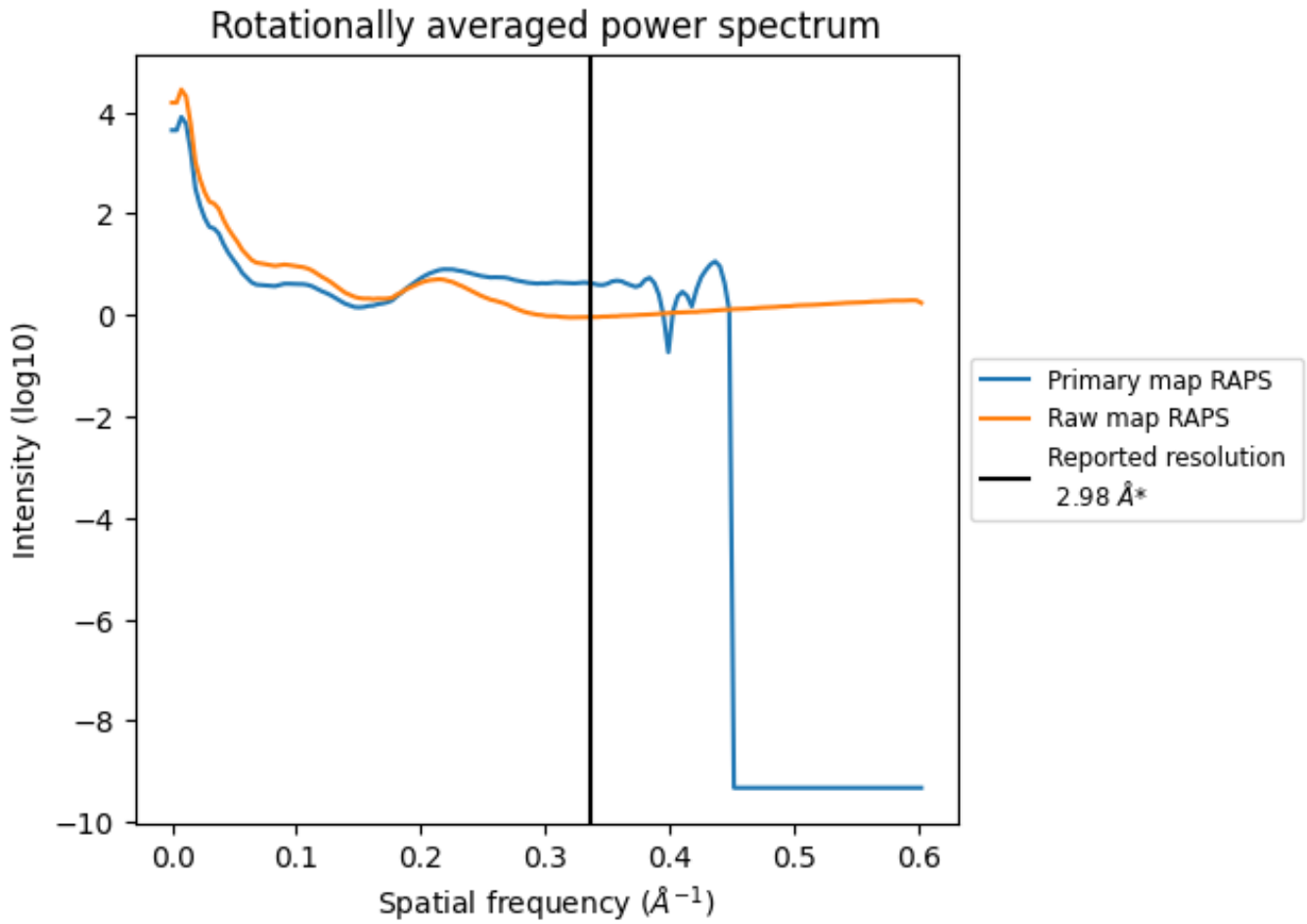
7.2 Volume estimate (i)



The volume at the recommended contour level is 24 nm^3; this corresponds to an approximate mass of 22 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)

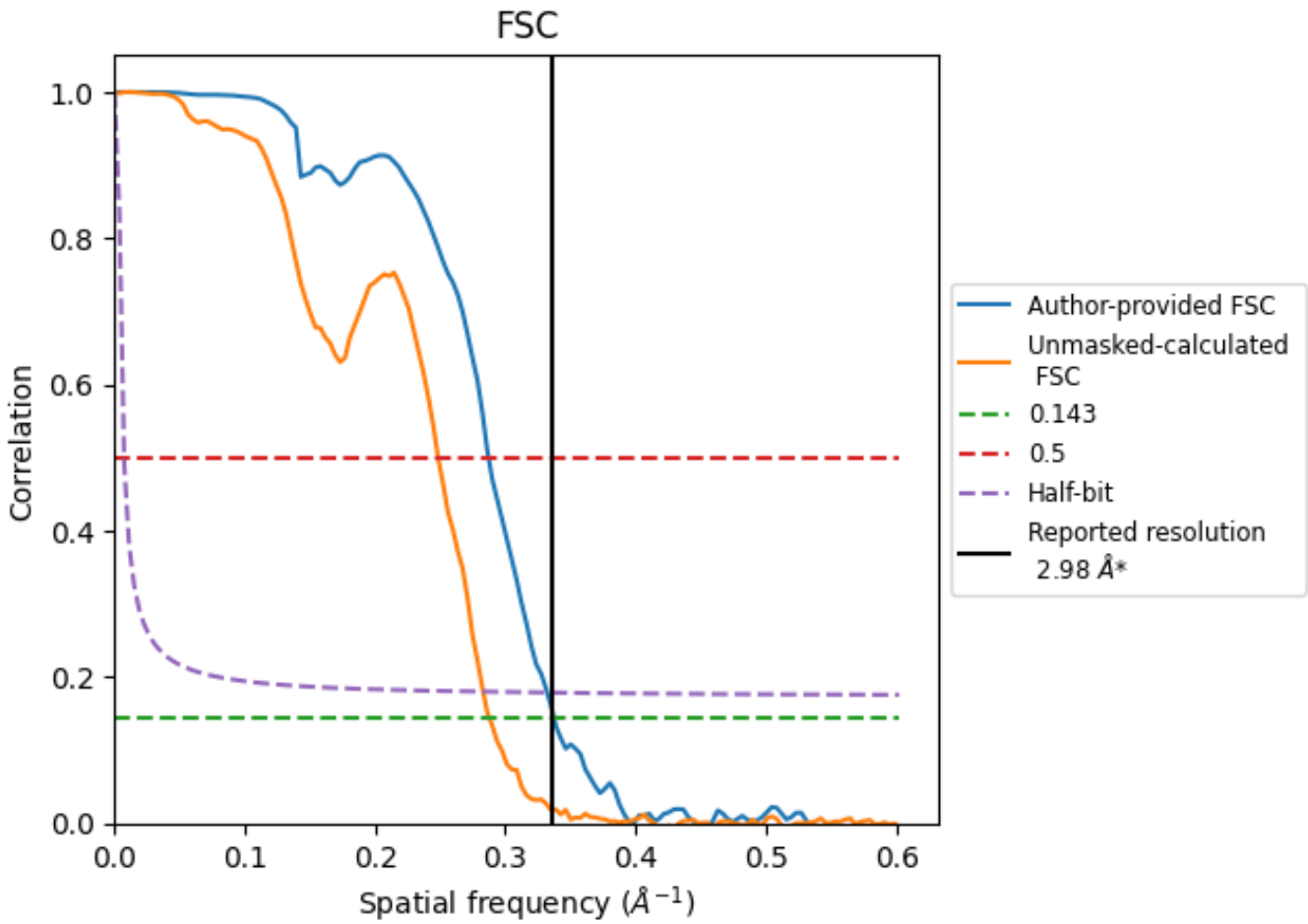


*Reported resolution corresponds to spatial frequency of 0.336 Å^{-1}

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 0.336 Å^{-1}

8.2 Resolution estimates (i)

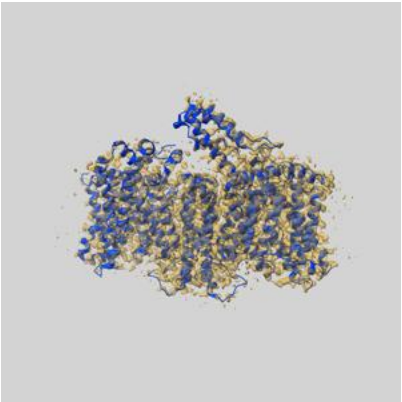
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.98	-	-
Author-provided FSC curve	2.96	3.48	3.01
Unmasked-calculated*	3.47	4.03	3.53

*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 3.47 differs from the reported value 2.98 by more than 10 %

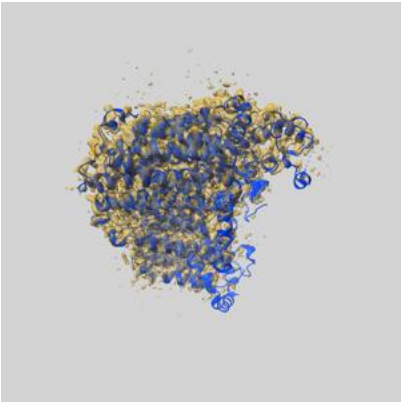
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-41192 and PDB model 8TEN. Per-residue inclusion information can be found in section 3 on page 4.

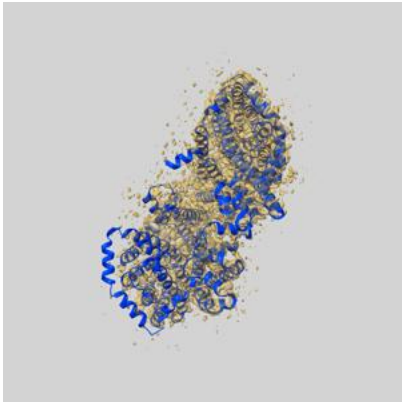
9.1 Map-model overlay (i)



X



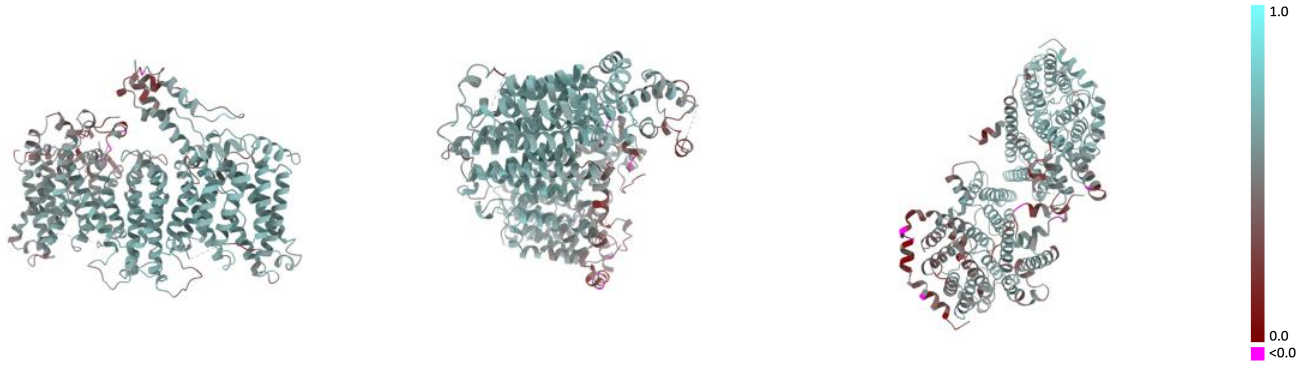
Y



Z

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

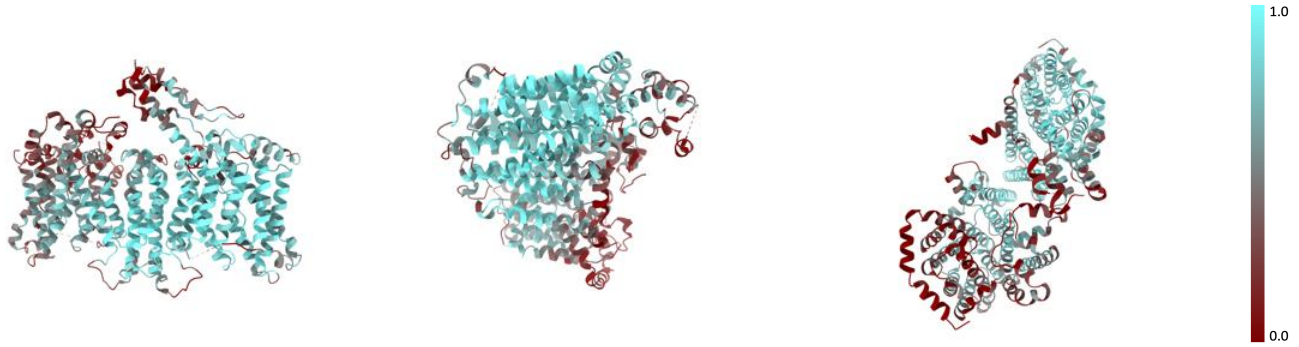
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

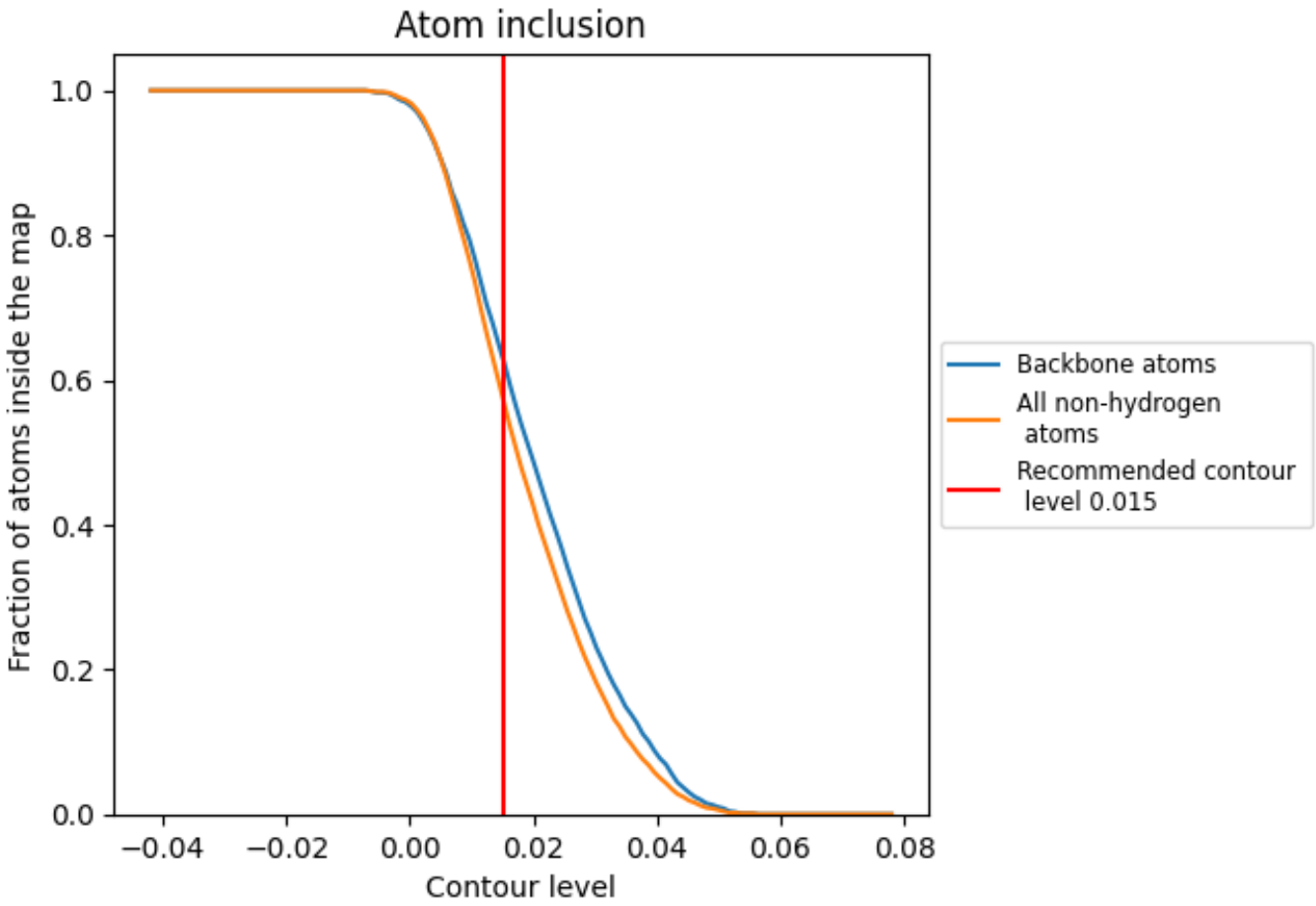
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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, 63% of all backbone atoms, 58% 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	0.5760	0.5450
A	0.6860	0.5820
B	0.4680	0.5100