



wwPDB EM Validation Summary Report ⓘ

Jun 16, 2022 – 01:33 pm BST

PDB ID : 7Z19
EMDB ID : EMD-14445
Title : E. coli C-P lyase bound to a single PhnK ABC domain
Authors : Amstrup, S.K.; Sofos, N.; Karlsen, J.L.; Skjerning, R.B.; Boesen, T.; Enghild, J.J.; Hove-Jensen, B.; Brodersen, D.E.
Deposited on : 2022-02-24
Resolution : 2.57 Å(reported)
Based on initial model : 4XB6

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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev8
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.28.1

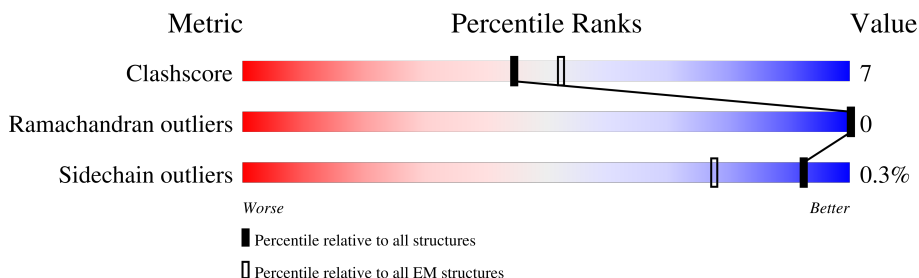
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.57 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	150	78% 16% 5%
1	E	150	79% 16% 5%
2	B	194	87% 12%
2	F	194	87% 12%
3	C	354	87% 12%
3	G	354	87% 13%
4	D	281	84% 14%
4	H	281	81% 16%

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Mol	Chain	Length	Quality of chain
5	I	258	<div> <div></div> <div>77%</div> <div>19%</div> <div></div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 34105 atoms, of which 16717 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 Alpha-D-ribose 1-methylphosphonate 5-triphosphate synthase subunit PhnG.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	142	Total	C	H	N	O	S	0	0
			2178	676	1080	209	207	6		
1	E	143	Total	C	H	N	O	S	0	0
			2194	681	1089	210	208	6		

- Molecule 2 is a protein called Alpha-D-ribose 1-methylphosphonate 5-triphosphate synthase subunit PhnH.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	192	Total	C	H	N	O	S	0	0
			2950	921	1489	257	276	7		
2	F	192	Total	C	H	N	O	S	0	0
			2955	923	1493	257	275	7		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	152	ARG	GLN	conflict	UNP P16686
F	152	ARG	GLN	conflict	UNP P16686

- Molecule 3 is a protein called Alpha-D-ribose 1-methylphosphonate 5-triphosphate synthase subunit PhnI.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	353	Total	C	H	N	O	S	0	0
			5408	1712	2677	478	530	11		
3	G	353	Total	C	H	N	O	S	0	0
			5408	1712	2677	478	530	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	322	VAL	ALA	conflict	UNP P16687
G	322	VAL	ALA	conflict	UNP P16687

- Molecule 4 is a protein called Alpha-D-ribose 1-methylphosphonate 5-phosphate C-P lyase.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	276	Total	C	H	N	O	S	0	0
			4331	1389	2134	375	419	14		
4	H	275	Total	C	H	N	O	S	0	0
			4317	1385	2128	373	417	14		

- Molecule 5 is a protein called Putative phosphonates utilization ATP-binding protein PhnK.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	I	248	Total	C	H	N	O	S	0	0
			3873	1208	1950	352	358	5		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	208	ALA	VAL	conflict	UNP P16678
I	253	HIS	-	expression tag	UNP P16678
I	254	HIS	-	expression tag	UNP P16678
I	255	HIS	-	expression tag	UNP P16678
I	256	HIS	-	expression tag	UNP P16678
I	257	HIS	-	expression tag	UNP P16678
I	258	HIS	-	expression tag	UNP P16678

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
6	C	1	Total	Zn	0
			1	1	
6	D	1	Total	Zn	0
			1	1	
6	G	1	Total	Zn	0
			1	1	
6	H	1	Total	Zn	0
			1	1	

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			AltConf
7	D	1	Total	O	P	0
			5	4	1	
7	H	1	Total	O	P	0
			5	4	1	

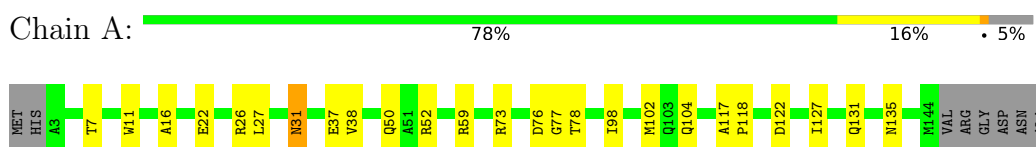
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		AltConf
8	A	35	Total	O	0
			35	35	
8	B	38	Total	O	0
			38	38	
8	C	110	Total	O	0
			110	110	
8	D	71	Total	O	0
			71	71	
8	E	20	Total	O	0
			20	20	
8	F	21	Total	O	0
			21	21	
8	G	114	Total	O	0
			114	114	
8	H	68	Total	O	0
			68	68	

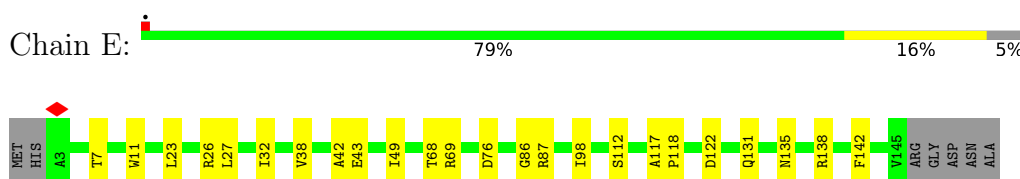
3 Residue-property plots

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.

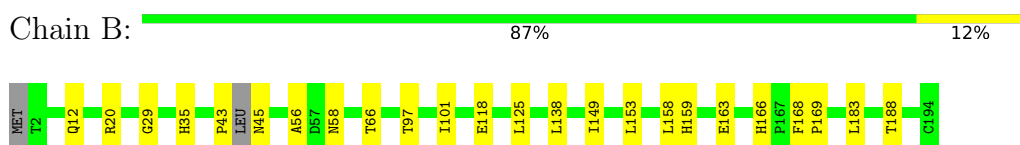
- Molecule 1: Alpha-D-ribose 1-methylphosphonate 5-triphosphate synthase subunit PhnG



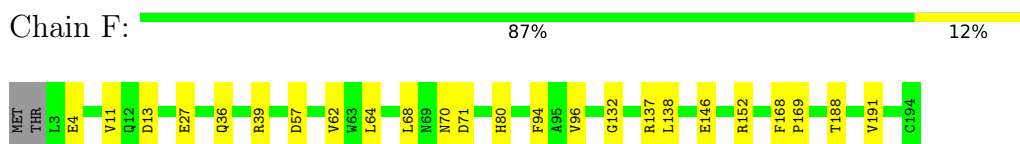
- Molecule 1: Alpha-D-ribose 1-methylphosphonate 5-triphosphate synthase subunit PhnG



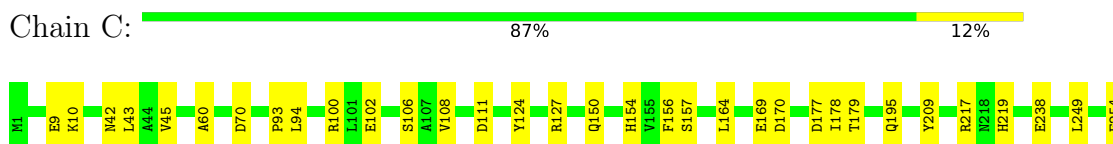
- Molecule 2: Alpha-D-ribose 1-methylphosphonate 5-triphosphate synthase subunit PhnH



- Molecule 2: Alpha-D-ribose 1-methylphosphonate 5-triphosphate synthase subunit PhnH



- Molecule 3: Alpha-D-ribose 1-methylphosphonate 5-triphosphate synthase subunit PhnI





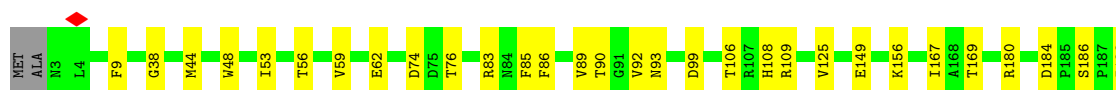
- Molecule 3: Alpha-D-ribose 1-methylphosphonate 5-triphosphate synthase subunit PhnI

Chain G: 87% 13%



- Molecule 4: Alpha-D-ribose 1-methylphosphonate 5-phosphate C-P lyase

Chain D: 84% 14%



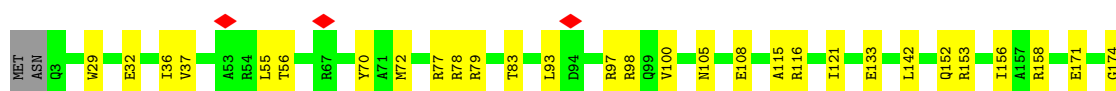
- Molecule 4: Alpha-D-ribose 1-methylphosphonate 5-phosphate C-P lyase

Chain H: 81% 16%



- Molecule 5: Putative phosphonates utilization ATP-binding protein PhnK

Chain I: 77% 19%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	50323	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 ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	0.7	Depositor
Maximum defocus (nm)	2	Depositor
Magnification	135000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.663	Depositor
Minimum map value	-0.647	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	325.36, 325.36, 325.36	wwPDB
Map dimensions	392, 392, 392	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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PO4

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	0.28	0/1114	0.56	0/1507
1	E	0.28	0/1121	0.55	0/1517
2	B	0.28	0/1488	0.51	0/2032
2	F	0.27	0/1490	0.50	0/2036
3	C	0.33	0/2785	0.51	0/3777
3	G	0.33	0/2785	0.54	1/3777 (0.0%)
4	D	0.34	0/2250	0.53	0/3059
4	H	0.35	0/2242	0.55	0/3048
5	I	0.28	0/1957	0.55	0/2657
All	All	0.31	0/17232	0.53	1/23410 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	346	ARG	NE-CZ-NH1	6.04	123.32	120.30

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	1098	1080	1079	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1105	1089	1088	20	0
2	B	1461	1489	1487	17	0
2	F	1462	1493	1492	18	0
3	C	2731	2677	2677	36	0
3	G	2731	2677	2677	40	0
4	D	2197	2134	2133	31	0
4	H	2189	2128	2127	40	0
5	I	1923	1950	1950	34	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
7	D	5	0	0	0	0
7	H	5	0	0	1	0
8	A	35	0	0	2	0
8	B	38	0	0	6	0
8	C	110	0	0	10	0
8	D	71	0	0	7	0
8	E	20	0	0	3	0
8	F	21	0	0	2	0
8	G	114	0	0	9	0
8	H	68	0	0	9	0
All	All	17388	16717	16710	228	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 7.

The worst 5 of 228 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:E:27:LEU:HD11	1:E:98:ILE:HD11	1.61	0.83
4:D:253:GLU:OE2	4:D:262:ARG:NH1	2.14	0.80
4:H:15:GLN:OE1	8:H:401:HOH:O	2.00	0.80
3:G:185:TYR:OH	8:G:501:HOH:O	2.00	0.80
4:H:268:ASP:OD1	8:H:402:HOH:O	2.01	0.78

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	140/150 (93%)	138 (99%)	2 (1%)	0	100	100
1	E	141/150 (94%)	140 (99%)	1 (1%)	0	100	100
2	B	188/194 (97%)	181 (96%)	7 (4%)	0	100	100
2	F	190/194 (98%)	180 (95%)	10 (5%)	0	100	100
3	C	351/354 (99%)	343 (98%)	8 (2%)	0	100	100
3	G	351/354 (99%)	346 (99%)	5 (1%)	0	100	100
4	D	274/281 (98%)	270 (98%)	4 (2%)	0	100	100
4	H	273/281 (97%)	266 (97%)	7 (3%)	0	100	100
5	I	246/258 (95%)	234 (95%)	12 (5%)	0	100	100
All	All	2154/2216 (97%)	2098 (97%)	56 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	109/115 (95%)	108 (99%)	1 (1%)	78	90
1	E	110/115 (96%)	110 (100%)	0	100	100
2	B	162/164 (99%)	161 (99%)	1 (1%)	86	94
2	F	162/164 (99%)	162 (100%)	0	100	100
3	C	286/286 (100%)	285 (100%)	1 (0%)	92	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	286/286 (100%)	285 (100%)	1 (0%)	92	97
4	D	240/244 (98%)	239 (100%)	1 (0%)	91	97
4	H	239/244 (98%)	239 (100%)	0	100	100
5	I	209/219 (95%)	209 (100%)	0	100	100
All	All	1803/1837 (98%)	1798 (100%)	5 (0%)	92	97

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

Mol	Chain	Res	Type
1	A	31	ASN
2	B	58	ASN
3	C	328	HIS
4	D	180	ARG
3	G	328	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	108	HIS
5	I	239	HIS

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](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
7	PO4	H	302	-	4,4,4	1.07	0	6,6,6	0.44	0
7	PO4	D	302	-	4,4,4	1.10	0	6,6,6	0.43	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	302	PO4	1	0

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.

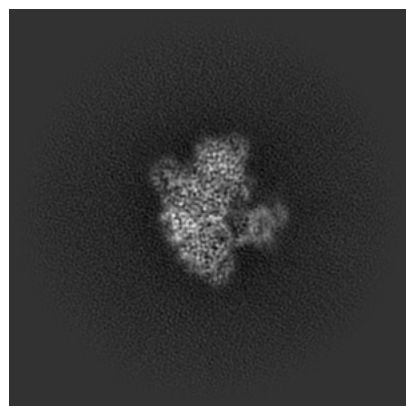
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14445. These allow visual inspection of the internal detail of the map and identification of artifacts.

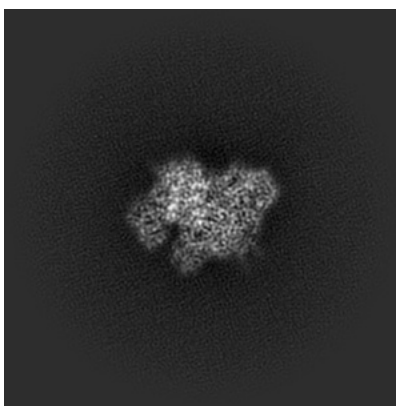
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

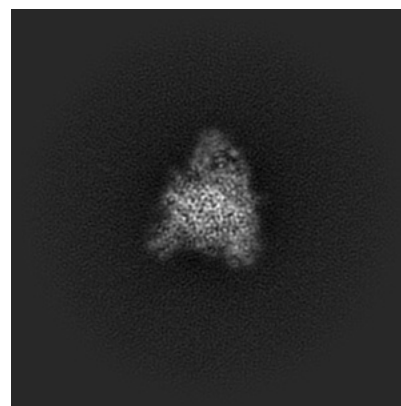
6.1.1 Primary map



X

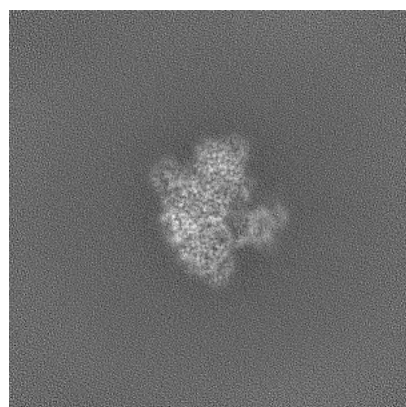


Y

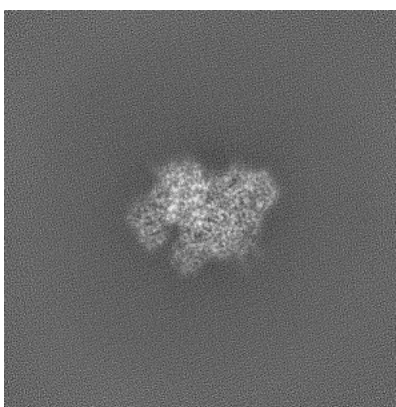


Z

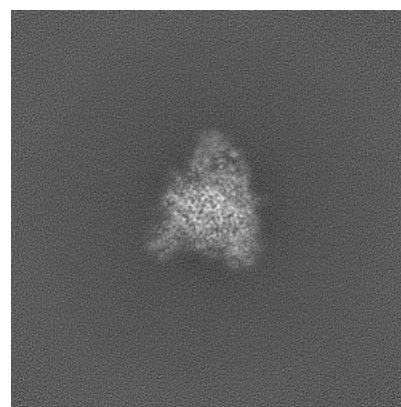
6.1.2 Raw map



X



Y

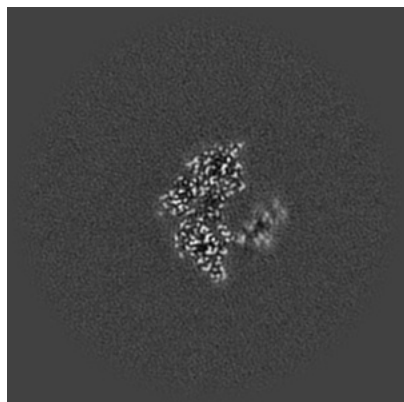


Z

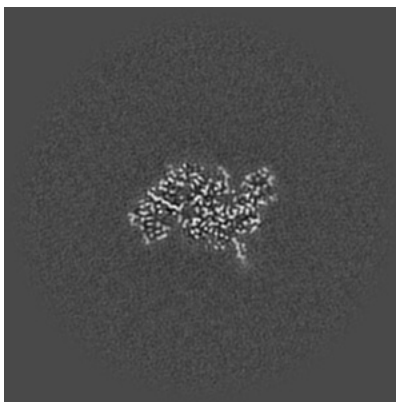
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

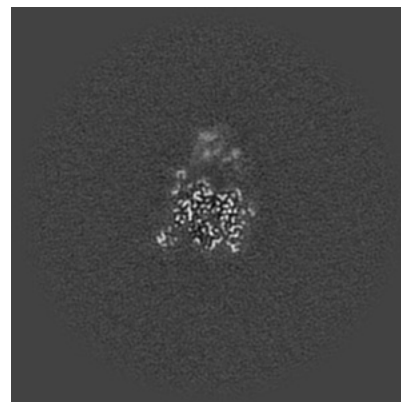
6.2.1 Primary map



X Index: 196

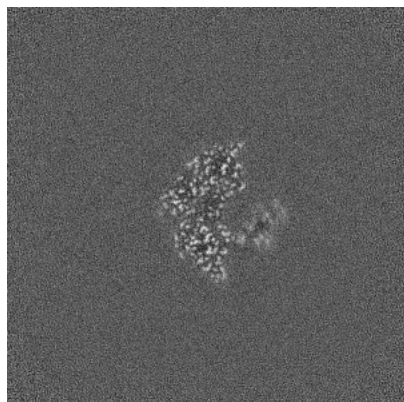


Y Index: 196

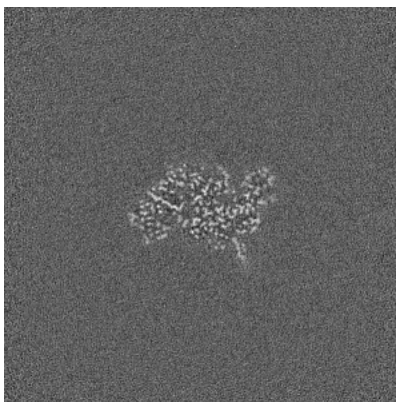


Z Index: 196

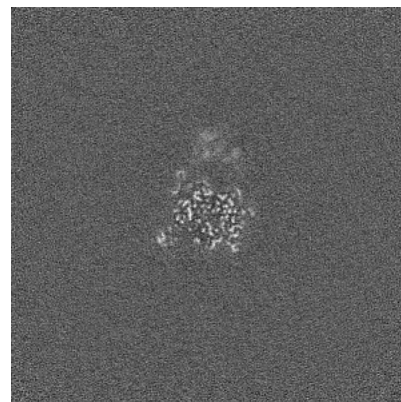
6.2.2 Raw map



X Index: 196



Y Index: 196

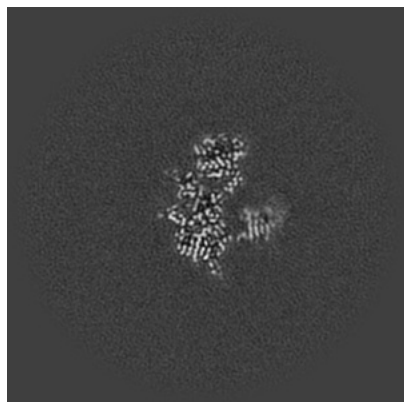


Z Index: 196

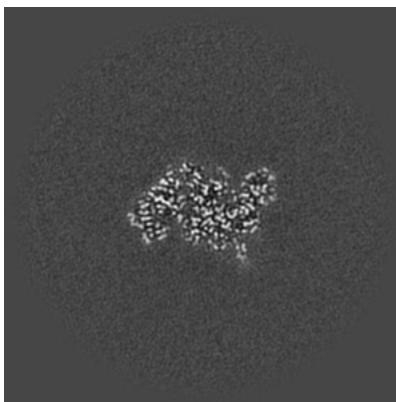
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

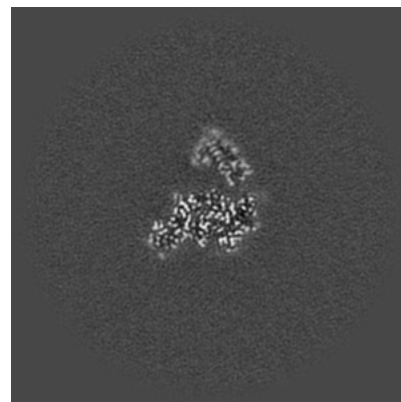
6.3.1 Primary map



X Index: 205

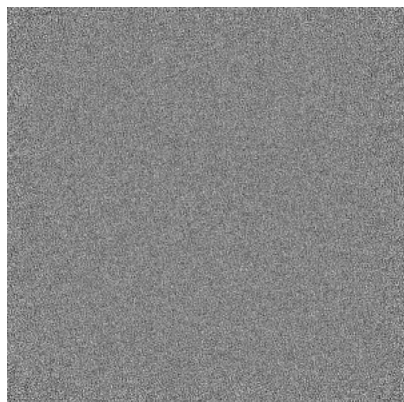


Y Index: 197

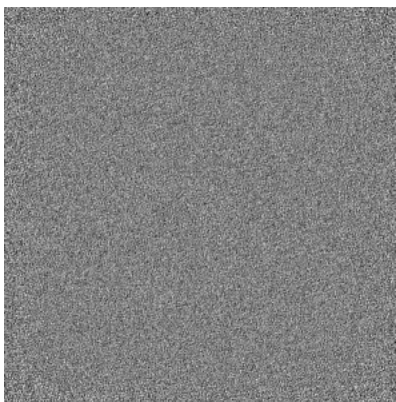


Z Index: 184

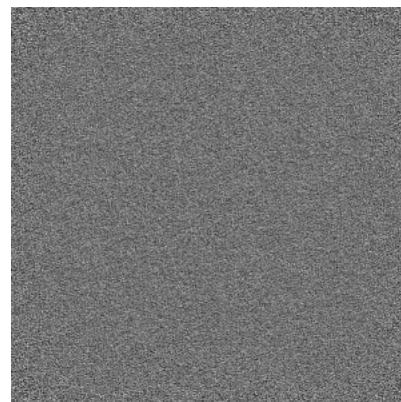
6.3.2 Raw map



X Index: 0



Y Index: 0

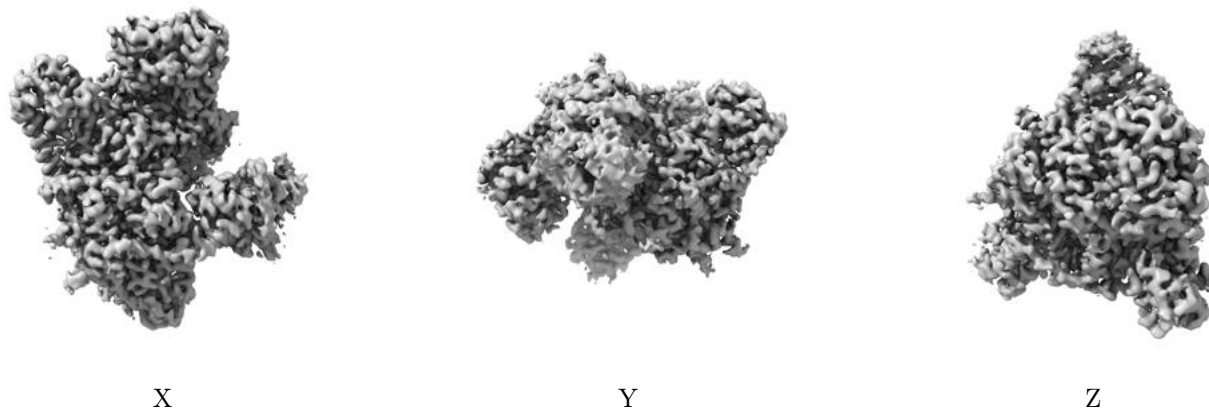


Z Index: 0

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

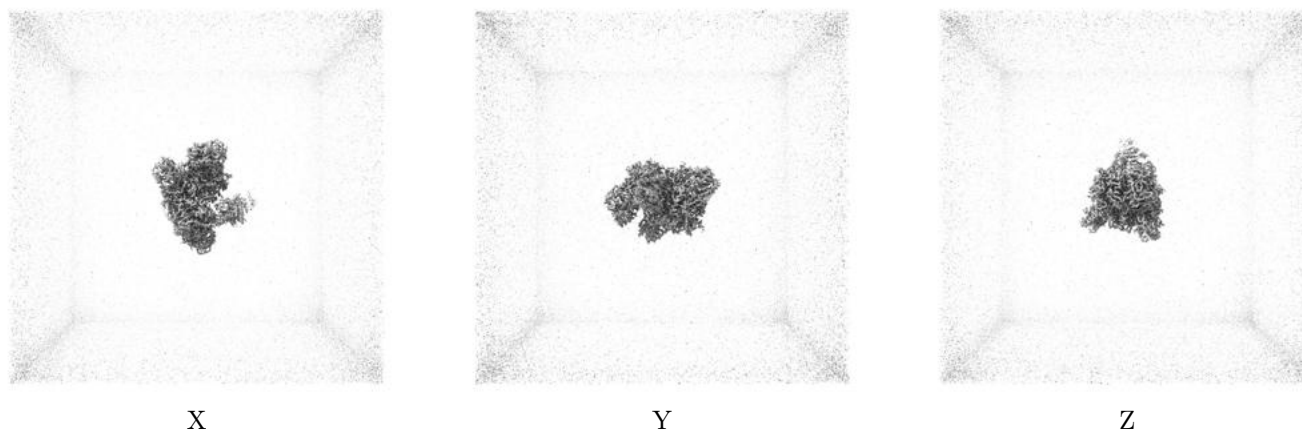
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

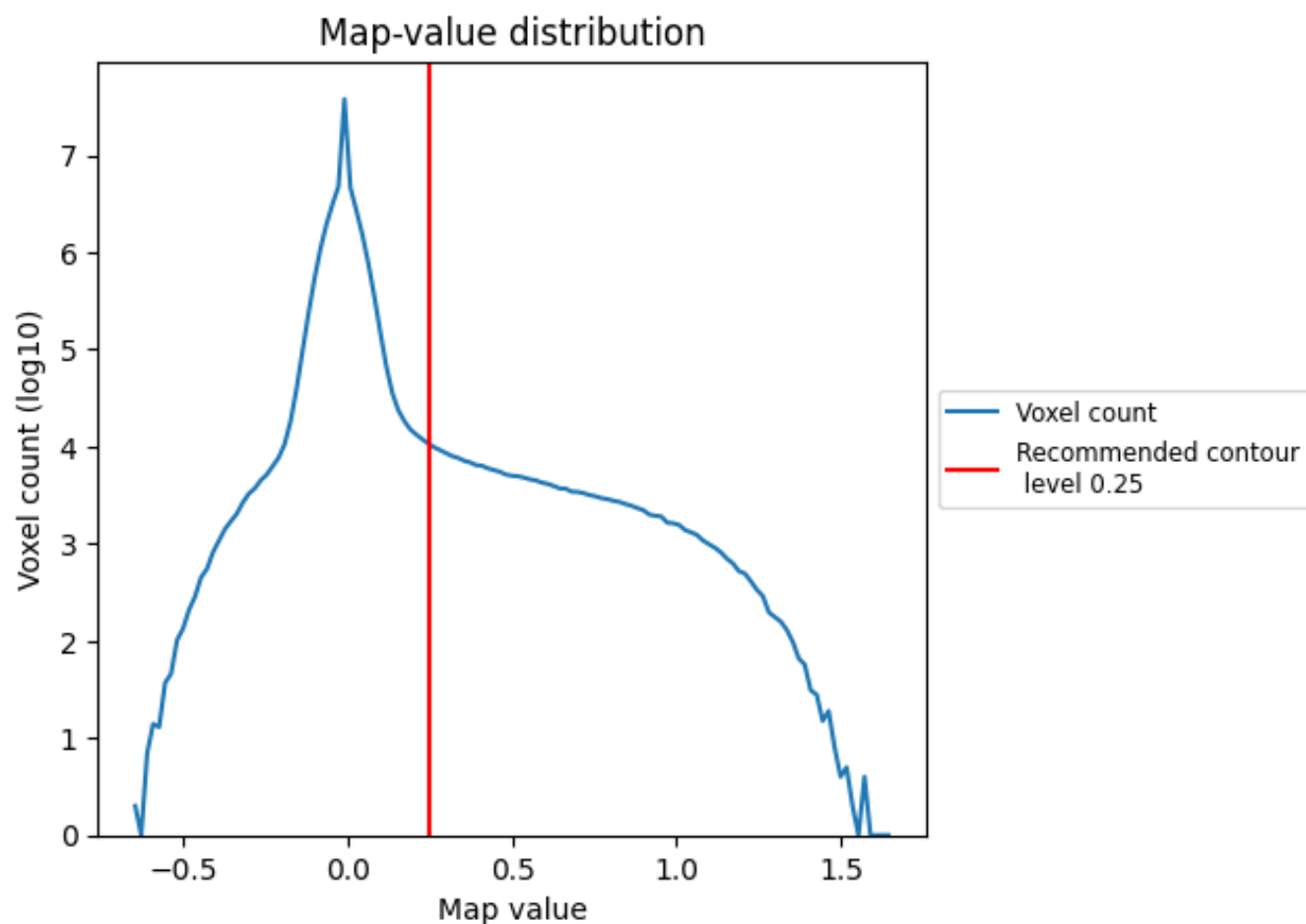
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

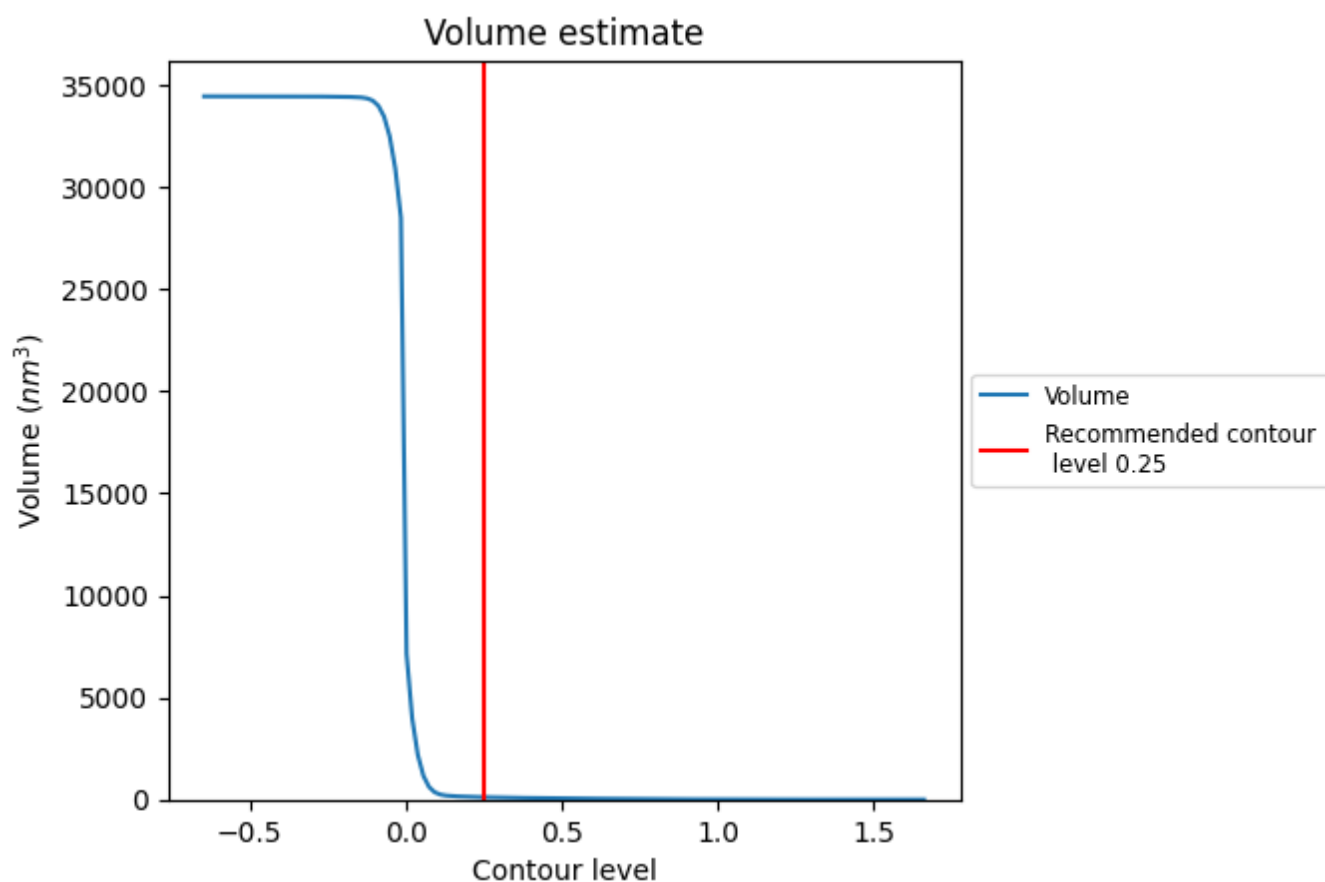
This section contains the results of statistical analysis of the map.

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.

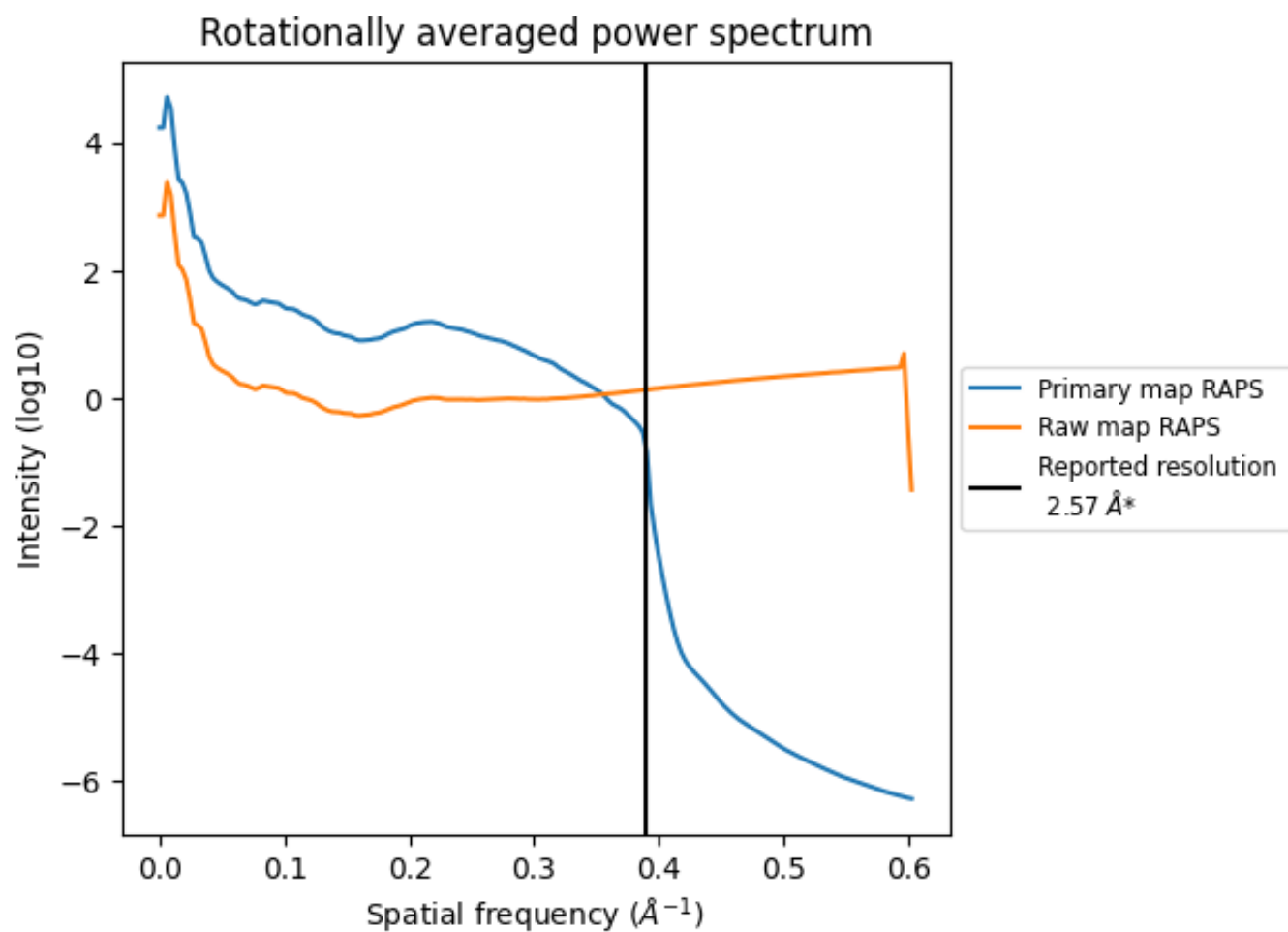
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 116 nm³; this corresponds to an approximate mass of 105 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 ⓘ

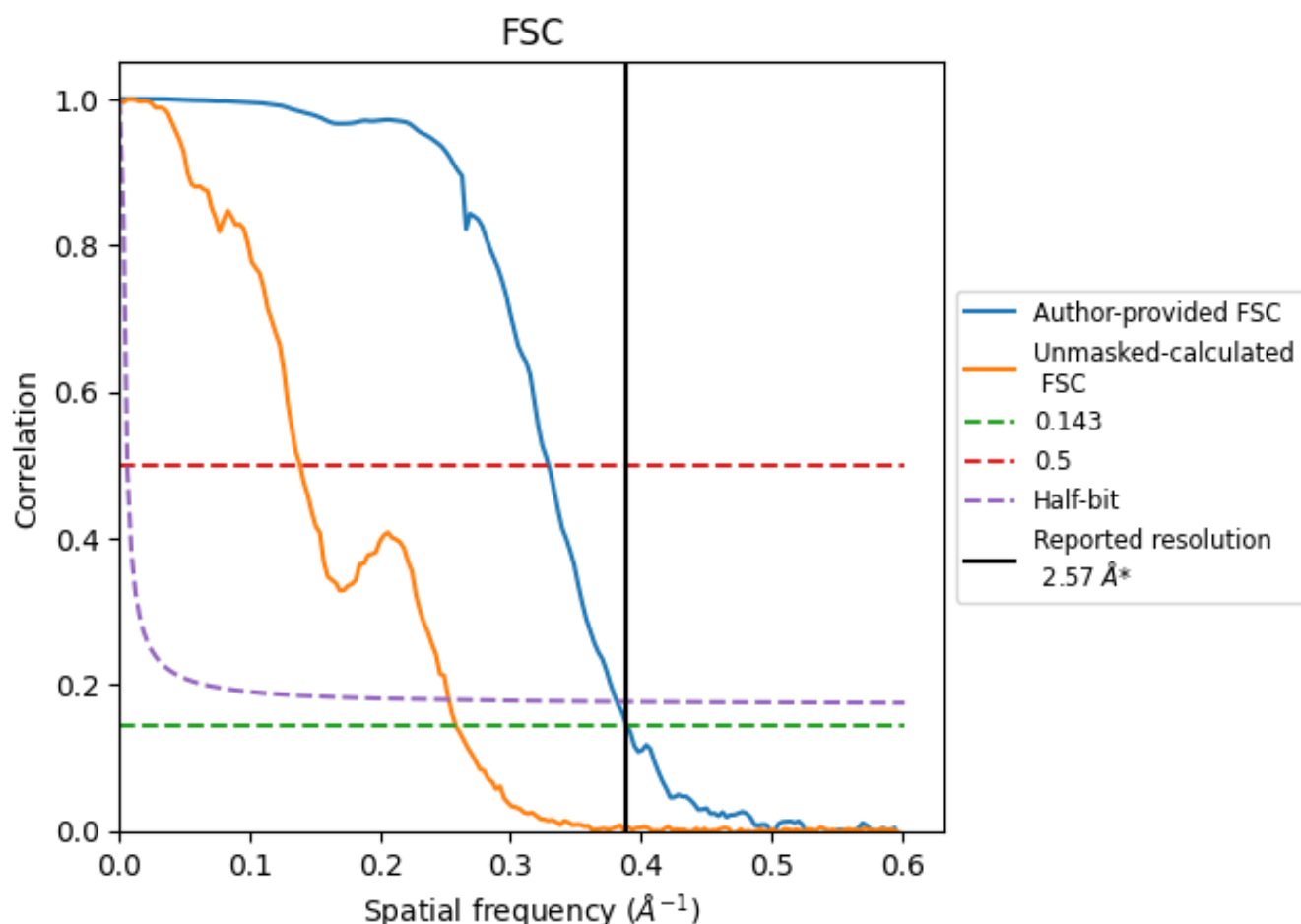


*Reported resolution corresponds to spatial frequency of 0.389 Å⁻¹

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 0.389 \AA^{-1}

8.2 Resolution estimates [i](#)

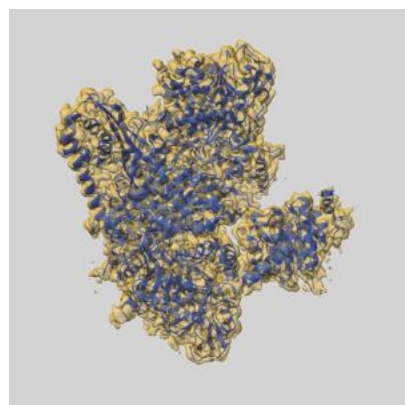
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.57	-	-
Author-provided FSC curve	2.57	3.04	2.62
Unmasked-calculated*	3.87	7.23	3.96

*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 3.87 differs from the reported value 2.57 by more than 10 %

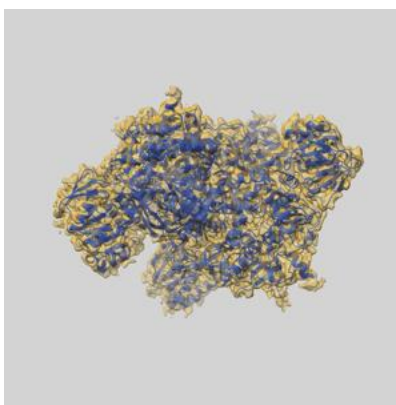
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14445 and PDB model 7Z19. Per-residue inclusion information can be found in section 3 on page 7.

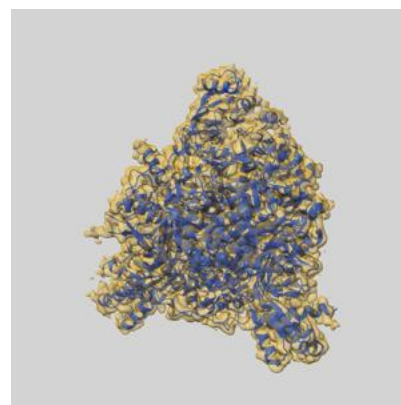
9.1 Map-model overlay [i](#)



X



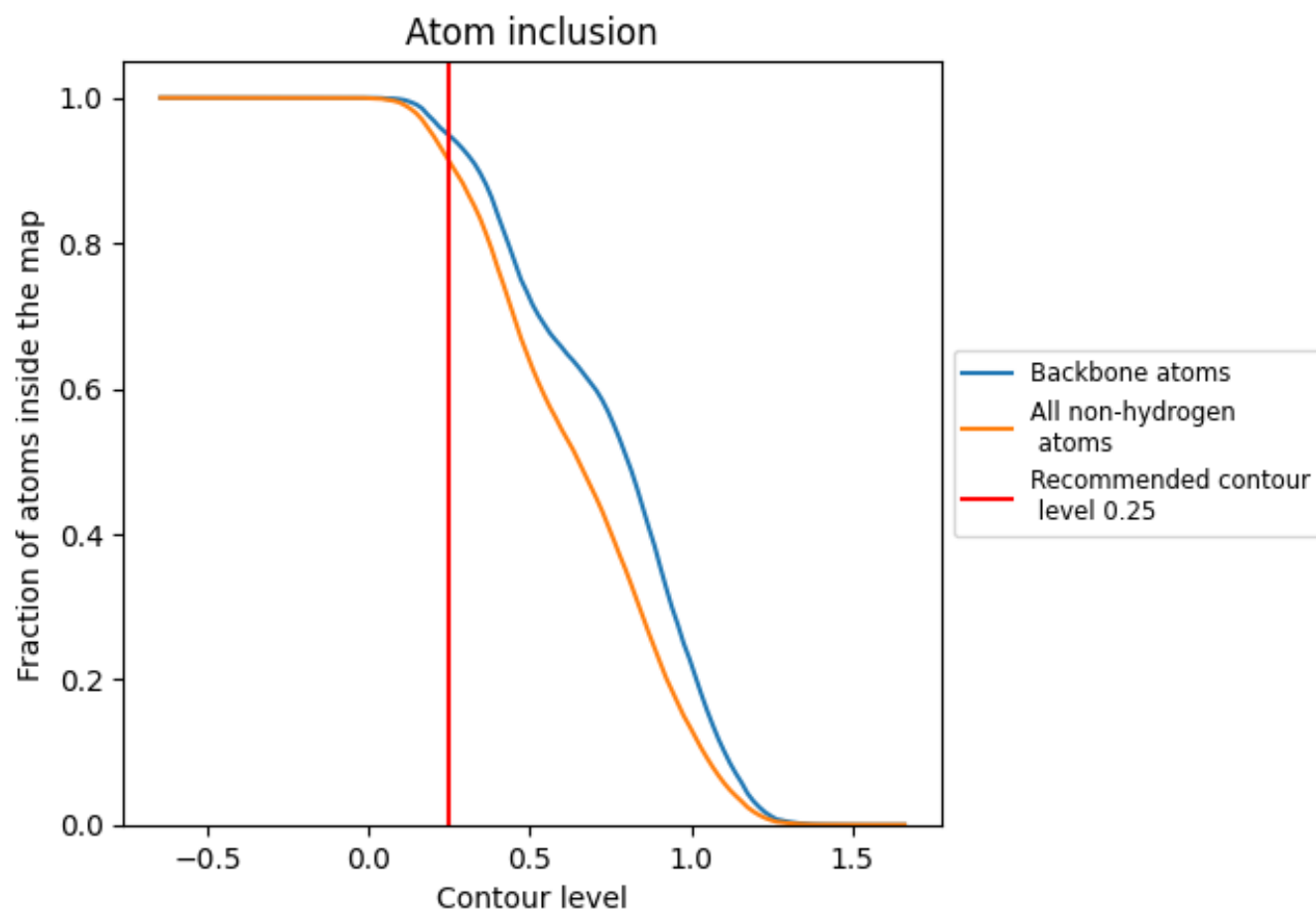
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25 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 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.