wwPDB EM Validation Summary Report (i)

Oct 3, 2026 – 10:17 AM EDT

PDB ID	:	9ZFV / pdb_00009zfv
EMDB ID	:	EMD-74155
Title	:	Mitochondrial MDH and OSCP in the peripheral stalk of ATP synthase in Acanthamoeba castellanii
Authors	:	Fry, M.Y.; Luce, B.E.; Stefely, J.A.; Samuelson, J.; Mootha, V.K.; Chao, L.H.
Deposited on	:	2025-12-02
Resolution	:	4.21 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:

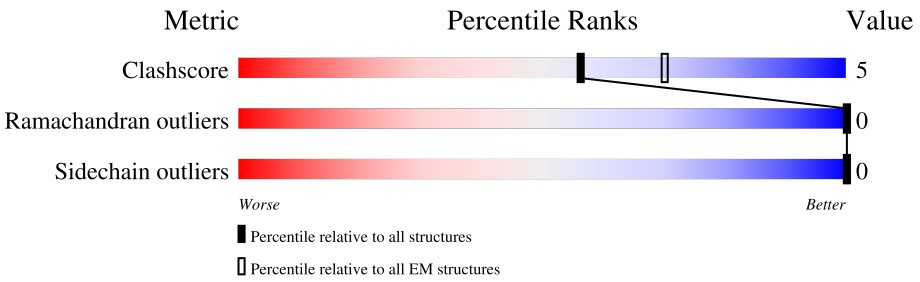
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

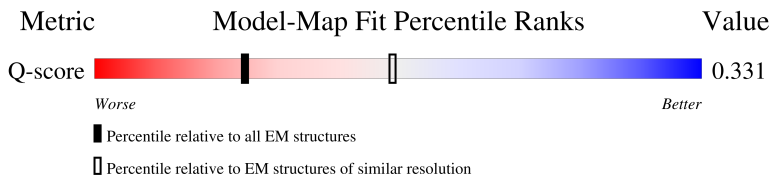
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.21 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4806 (3.71 - 4.71)

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	454	24% 75% 9% 16%
1	B	454	7% 77% 11% 12%
2	G	431	6% 42% • 55%
3	C	92	• 21% 7% 73%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15461 atoms, of which 7763 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 malate dehydrogenase.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	382	5823	1824	2919	514	552	14	0	0
1	B	398	6048	1891	3033	534	576	14	0	0

There are 82 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	217	VAL	SER	conflict	UNP L8HFT9
A	218	GLN	ARG	conflict	UNP L8HFT9
A	219	GLY	ALA	conflict	UNP L8HFT9
A	220	LYS	-	insertion	UNP L8HFT9
A	221	ALA	-	insertion	UNP L8HFT9
A	222	LEU	-	insertion	UNP L8HFT9
A	223	ASN	-	insertion	UNP L8HFT9
A	224	LYS	-	insertion	UNP L8HFT9
A	225	VAL	-	insertion	UNP L8HFT9
A	226	ALA	-	insertion	UNP L8HFT9
A	227	ASN	-	insertion	UNP L8HFT9
A	228	ARG	-	insertion	UNP L8HFT9
A	229	ASP	-	insertion	UNP L8HFT9
A	230	THR	-	insertion	UNP L8HFT9
A	231	LEU	-	insertion	UNP L8HFT9
A	232	ARG	-	insertion	UNP L8HFT9
A	233	VAL	-	insertion	UNP L8HFT9
A	234	CYS	-	insertion	UNP L8HFT9
A	235	VAL	-	insertion	UNP L8HFT9
A	236	VAL	-	insertion	UNP L8HFT9
A	237	GLY	-	insertion	UNP L8HFT9
A	238	ASN	-	insertion	UNP L8HFT9
A	239	PRO	-	insertion	UNP L8HFT9
A	240	ALA	-	insertion	UNP L8HFT9
A	241	ASN	-	insertion	UNP L8HFT9
A	242	THR	-	insertion	UNP L8HFT9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	243	ASN	-	insertion	UNP L8HFT9
A	244	ALA	-	insertion	UNP L8HFT9
A	245	LEU	-	insertion	UNP L8HFT9
A	246	ILE	-	insertion	UNP L8HFT9
A	247	ALA	-	insertion	UNP L8HFT9
A	248	SER	-	insertion	UNP L8HFT9
A	249	ALA	-	insertion	UNP L8HFT9
A	250	ASN	-	insertion	UNP L8HFT9
A	251	ALA	-	insertion	UNP L8HFT9
A	252	PRO	-	insertion	UNP L8HFT9
A	253	ASN	-	insertion	UNP L8HFT9
A	254	ILE	-	insertion	UNP L8HFT9
A	255	HIS	-	insertion	UNP L8HFT9
A	256	PRO	-	insertion	UNP L8HFT9
A	257	ARG	-	insertion	UNP L8HFT9
B	217	VAL	SER	conflict	UNP L8HFT9
B	218	GLN	ARG	conflict	UNP L8HFT9
B	219	GLY	ALA	conflict	UNP L8HFT9
B	220	LYS	-	insertion	UNP L8HFT9
B	221	ALA	-	insertion	UNP L8HFT9
B	222	LEU	-	insertion	UNP L8HFT9
B	223	ASN	-	insertion	UNP L8HFT9
B	224	LYS	-	insertion	UNP L8HFT9
B	225	VAL	-	insertion	UNP L8HFT9
B	226	ALA	-	insertion	UNP L8HFT9
B	227	ASN	-	insertion	UNP L8HFT9
B	228	ARG	-	insertion	UNP L8HFT9
B	229	ASP	-	insertion	UNP L8HFT9
B	230	THR	-	insertion	UNP L8HFT9
B	231	LEU	-	insertion	UNP L8HFT9
B	232	ARG	-	insertion	UNP L8HFT9
B	233	VAL	-	insertion	UNP L8HFT9
B	234	CYS	-	insertion	UNP L8HFT9
B	235	VAL	-	insertion	UNP L8HFT9
B	236	VAL	-	insertion	UNP L8HFT9
B	237	GLY	-	insertion	UNP L8HFT9
B	238	ASN	-	insertion	UNP L8HFT9
B	239	PRO	-	insertion	UNP L8HFT9
B	240	ALA	-	insertion	UNP L8HFT9
B	241	ASN	-	insertion	UNP L8HFT9
B	242	THR	-	insertion	UNP L8HFT9
B	243	ASN	-	insertion	UNP L8HFT9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	244	ALA	-	insertion	UNP L8HFT9
B	245	LEU	-	insertion	UNP L8HFT9
B	246	ILE	-	insertion	UNP L8HFT9
B	247	ALA	-	insertion	UNP L8HFT9
B	248	SER	-	insertion	UNP L8HFT9
B	249	ALA	-	insertion	UNP L8HFT9
B	250	ASN	-	insertion	UNP L8HFT9
B	251	ALA	-	insertion	UNP L8HFT9
B	252	PRO	-	insertion	UNP L8HFT9
B	253	ASN	-	insertion	UNP L8HFT9
B	254	ILE	-	insertion	UNP L8HFT9
B	255	HIS	-	insertion	UNP L8HFT9
B	256	PRO	-	insertion	UNP L8HFT9
B	257	ARG	-	insertion	UNP L8HFT9

- Molecule 2 is a protein called mitochondrial ATP synthase subunit oscp.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	G	196	3200	1022	1617	272	284	5	0	0

- Molecule 3 is a protein called ACANB14707.

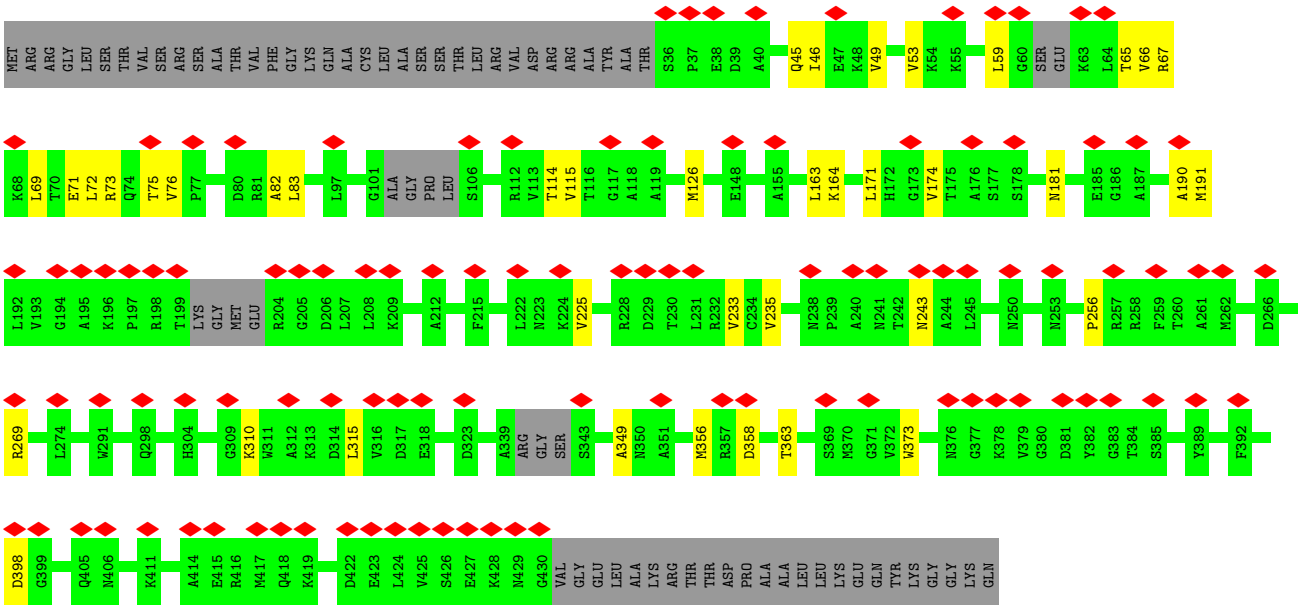
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
3	C	25	390	121	194	35	40	0	0

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.

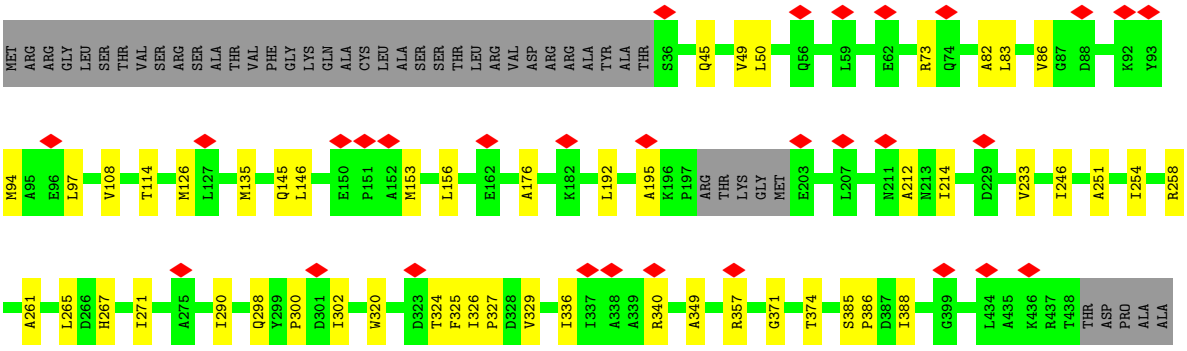
- Molecule 1: malate dehydrogenase

Chain A:



- Molecule 1: malate dehydrogenase

Chain B:



LEU LEU LYS GLU GLN TYR LYS GLY GLY LYS GLN

- Molecule 2: mitochondrial ATP synthase subunit oscp

Chain G:

MET TYR ALA SER ARG SER SER GLY MET ALA CYS ARG SER ARG LEU ALA SER ARG VAL ALA PRO ARG MET GLY ASN ALA ALA ARG LEU VAL SER ALA ARG GLY PHE SER GLN THR LEU VAL THR GLN GLN LYS LYS GLY GLU ALA THR THR ALA ALA PRO VAL PHE LYS ILE ASP GLU GLU

PHE ASP ASP TYR LYS ASP VAL THR ALA SER ASN GLU GLN VAL GLU K41 V48 Q49 S52 G53 K54 H55 V68 L69 N70 A71 V72 A85 P90 N91 F92 Q93 L96 D102 R107 L114 K115 G116 A117 D118 F119 H120 R121 L122 T123 Q124 K125 F126 L127 V128

L131 L132 E133 L137 H154 A165 R175 K182 E186 A187 D188 F195 L201 I202 V207 GLU VAL GLY SER ASN Y213 S220 R241 PRO LYS GLU LEU HIS ILE ASN SER PHE ASP THR SER SER LEU PHE ALA PRO LEU SER GLY VAL LYS ILE THR ALA ALA

ASP LEU ASP LYS THR LEU ALA ASP VAL LEU GLY SER LYS LYS GLU ALA PHE GLN ALA ALA ASP LEU ASP ARG THR LEU LYS GLN ALA LEU GLU ASP ALA GLN ARG ASP ALA GLY PHE SER GLY ASP TYR GLU LYS ASN VAL LEU GLU GLN THR ARG ASN LEU ASP PHE GLU LYS LEU LYS

THR VAL LYS GLN LEU ASP LEU ALA GLN HIS GLU LYS HIS LEU MET GLN LYS HIS ASN ILE ALA ASP ASN ASP ALA GLU GLY LYS ARG LYS VAL LYS ALA LYS ILE GLU GLU LEU LYS ARG PHE LYS GLU LEU ASP THR SER PHE ILE GLY GLU VAL LEU LYS LYS HIS GLN PRO GLU THR

TYR LYS LYS TYR GLN SER VAL PHE GLN

- Molecule 3: ACANB14707

Chain C:

MET SER LYS ARG LEU ILE THR ARG ALA THR LEU LEU ASN GLY ARG LEU ALA THR ALA TRP ALA PRO SER ARG SER TYR ALA GLU ALA ALA VAL PRO LYS LEU GLY LYS ASP ILE GLN PRO LYS ASN TYR ARG ARG PRO ASP GLY THR TYR GLU PRO CYS ASP GLU ILE LEU PHE LEU SER VAL

ILE GLY Y38 L42 K49 T53 N54 T55 L56 V57 L58 N62 LYS THR ALA SER GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10863	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	0.99	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.430	Depositor
Minimum map value	-0.277	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.125	Depositor
Map size (Å)	361.68002, 361.68002, 361.68002	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	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	0.11	0/2952	0.24	0/3995
1	B	0.13	0/3067	0.26	0/4154
2	G	0.11	0/1616	0.23	0/2179
3	C	0.13	0/197	0.22	0/266
All	All	0.12	0/7832	0.24	0/10594

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	2904	2919	2919	34	0
1	B	3015	3033	3033	32	0
2	G	1583	1617	1617	10	0
3	C	196	194	194	7	0
All	All	7698	7763	7763	75	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 5.

The worst 5 of 75 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:66:VAL:HG12	3:C:56:LEU:HD13	1.69	0.75
1:A:358:ASP:HB3	1:A:363:THR:HG22	1.83	0.60
1:A:235:VAL:HG21	1:A:243:ASN:HB2	1.84	0.60
1:B:50:LEU:HD21	1:B:82:ALA:HB3	1.83	0.58
1:B:192:LEU:HD13	1:B:233:VAL:HG13	1.87	0.55

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	372/454 (82%)	367 (99%)	5 (1%)	0	100	100
1	B	394/454 (87%)	381 (97%)	13 (3%)	0	100	100
2	G	192/431 (44%)	184 (96%)	8 (4%)	0	100	100
3	C	23/92 (25%)	23 (100%)	0	0	100	100
All	All	981/1431 (69%)	955 (97%)	26 (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	307/362 (85%)	307 (100%)	0	100	100
1	B	318/362 (88%)	318 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	170/369 (46%)	170 (100%)	0	100	100
3	C	21/76 (28%)	21 (100%)	0	100	100
All	All	816/1169 (70%)	816 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	A	56	GLN
1	B	418	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

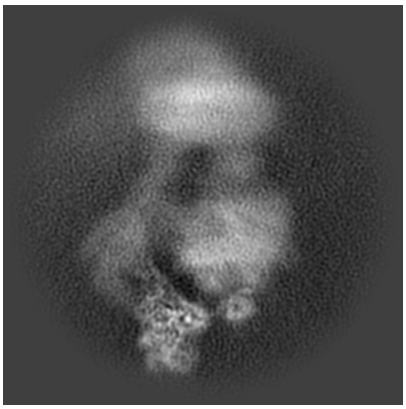
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-74155. These allow visual inspection of the internal detail of the map and identification of artifacts.

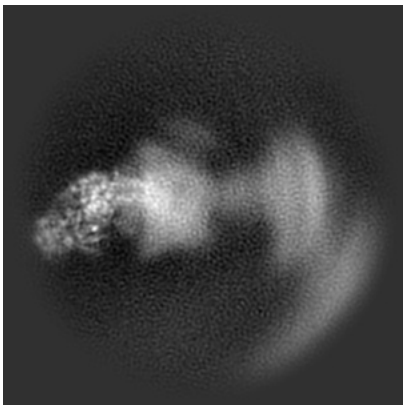
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map



X



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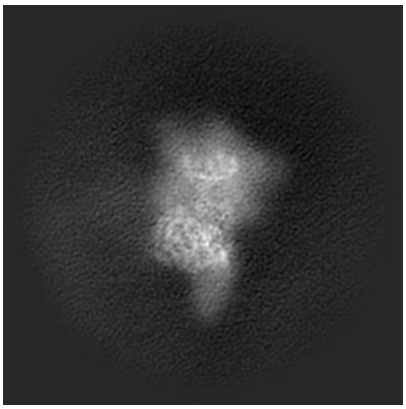
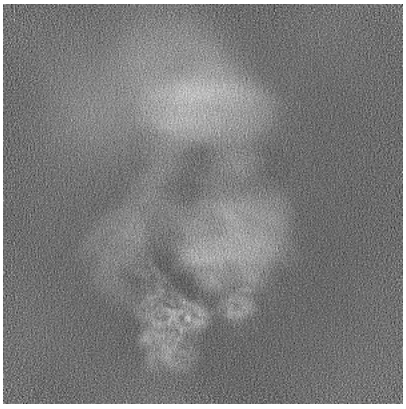


Z

6.1.2 Raw map



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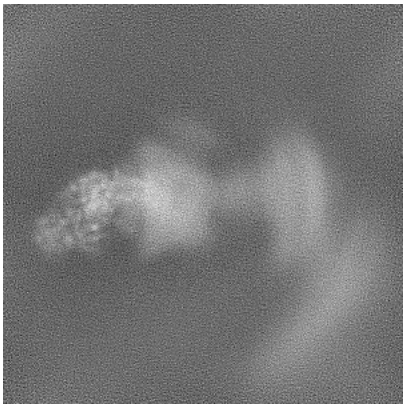

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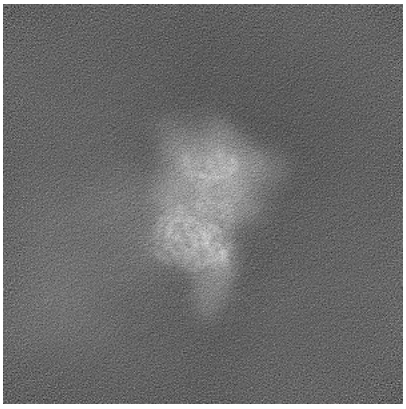
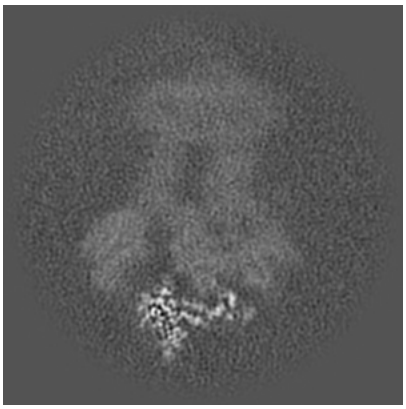


Z

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

6.2 Central slices (i)

6.2.1 Primary map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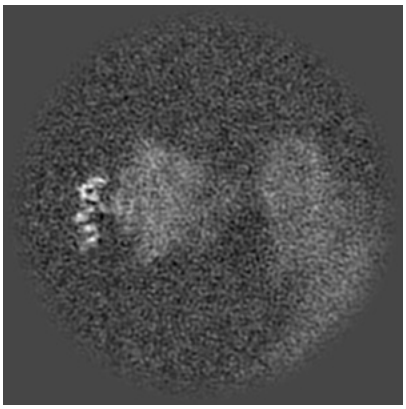
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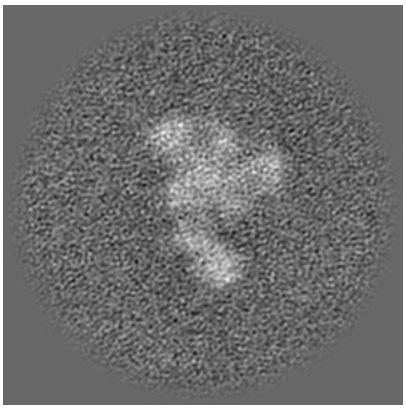
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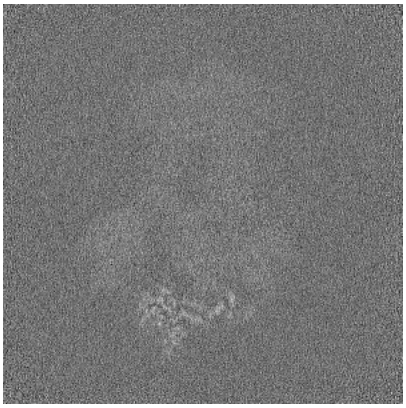
6.2.2 Raw map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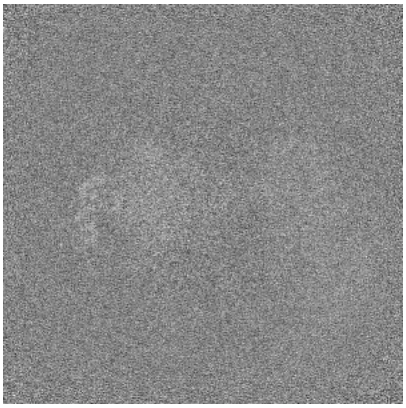
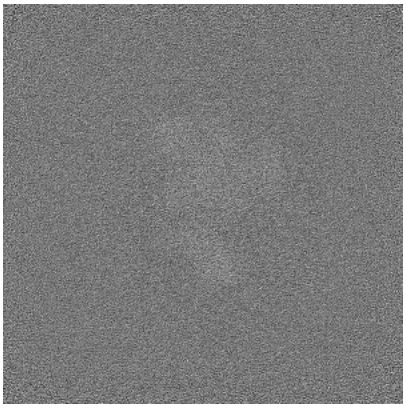
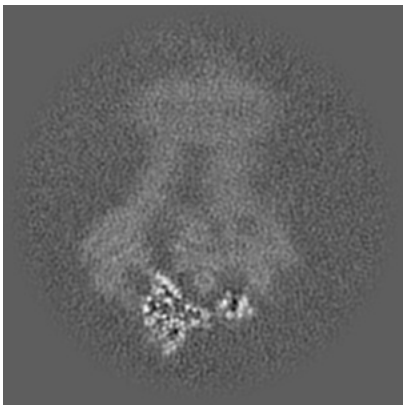

Y Index: 220


Z Index: 220

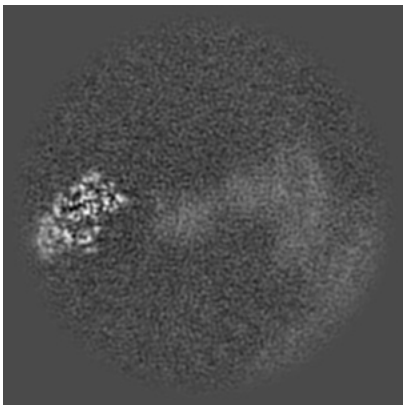
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

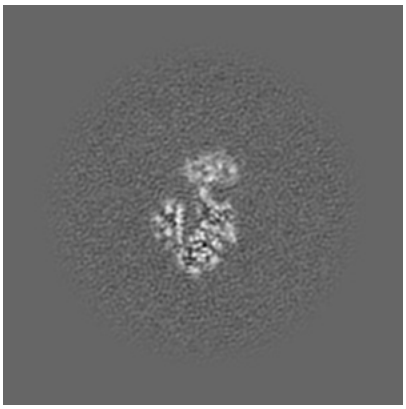
6.3.1 Primary map



X Index: 226

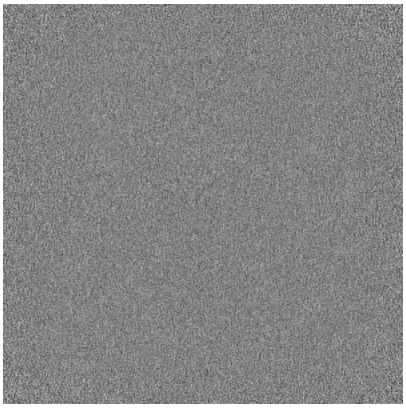


Y Index: 184

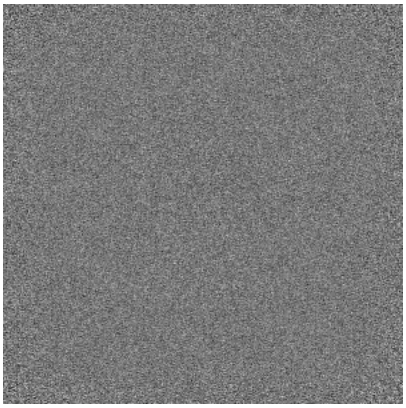


Z Index: 100

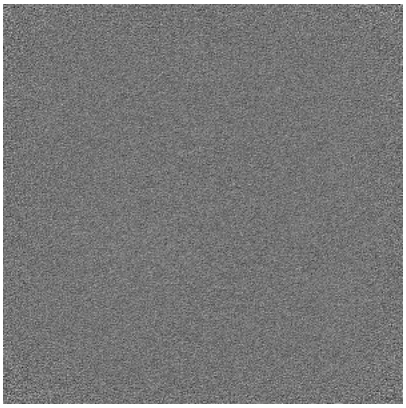
6.3.2 Raw map



X Index: 0



Y Index: 0

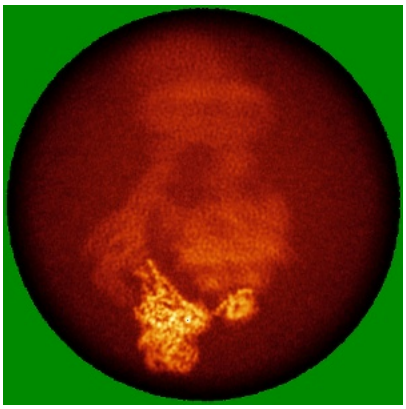


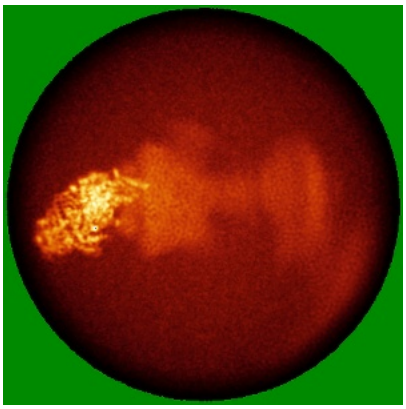
Z Index: 0

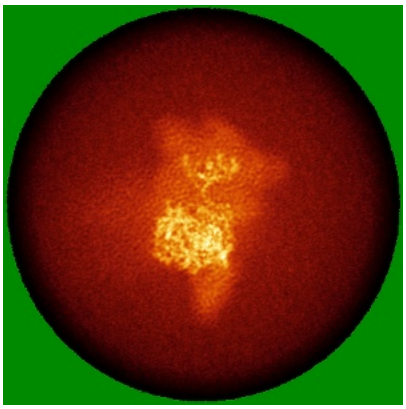
The images above show the largest variance slices of the map in three orthogonal directions.

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

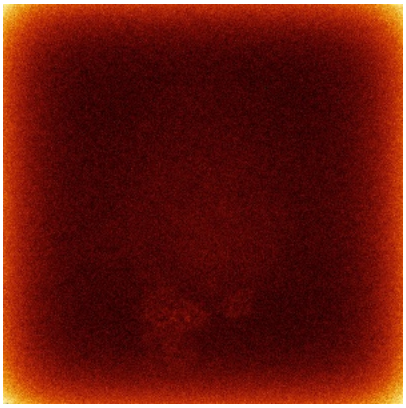
6.4.1 Primary map

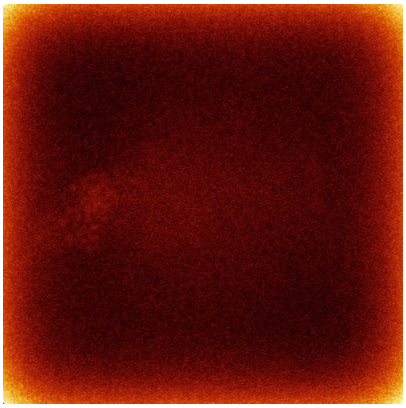

X

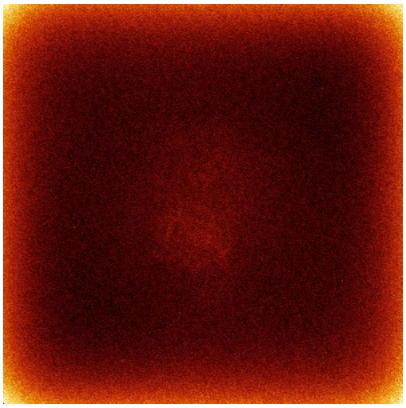

Y


Z

6.4.2 Raw map


X

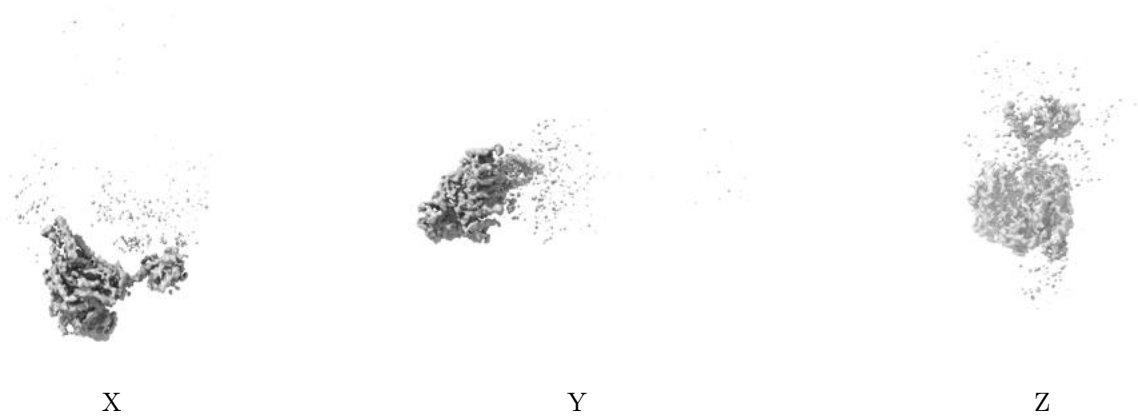

Y


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 0.125. 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.

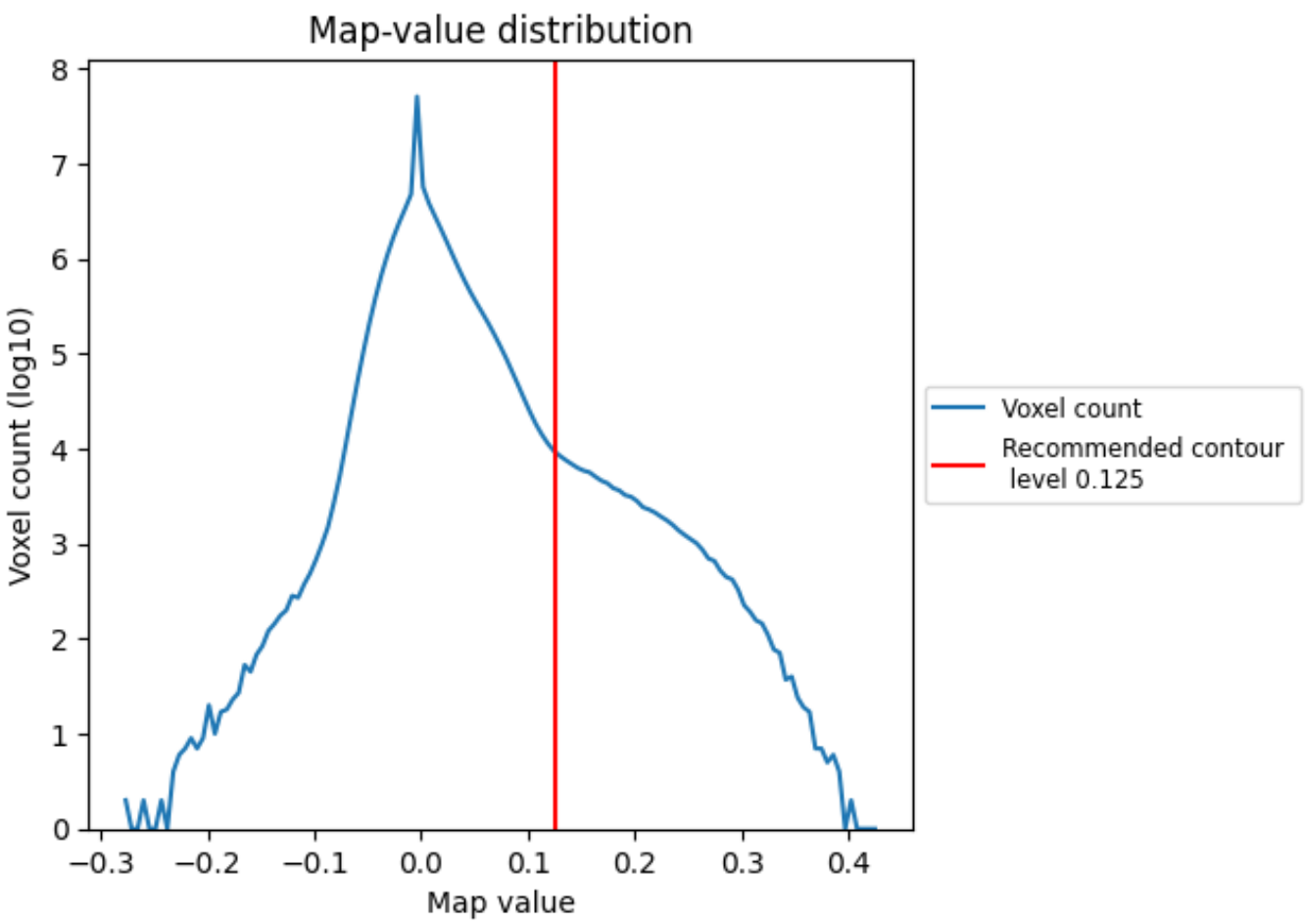
6.6 Mask visualisation (i)

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

7 Map analysis (i)

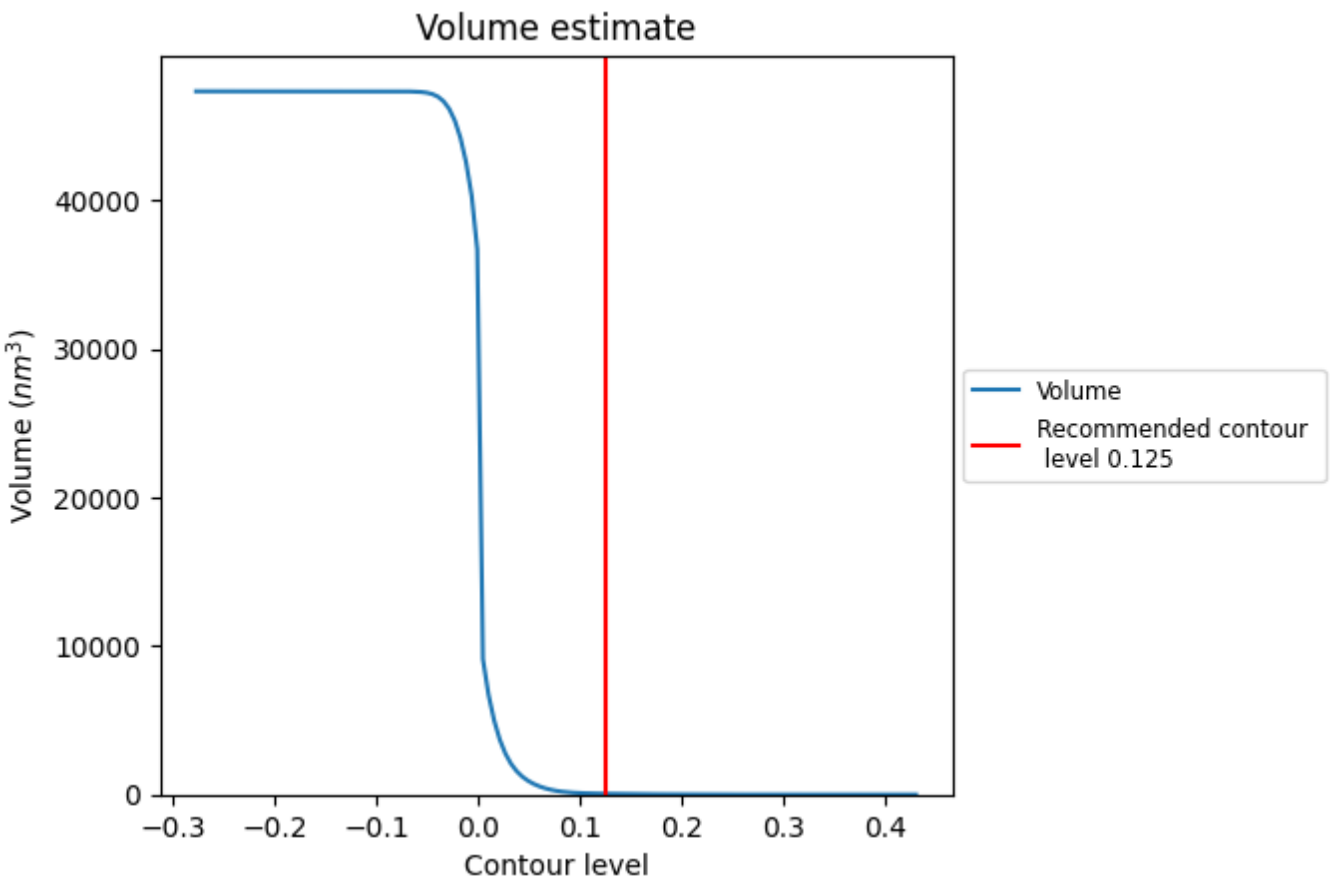
This section contains the results of statistical analysis of the map.

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.

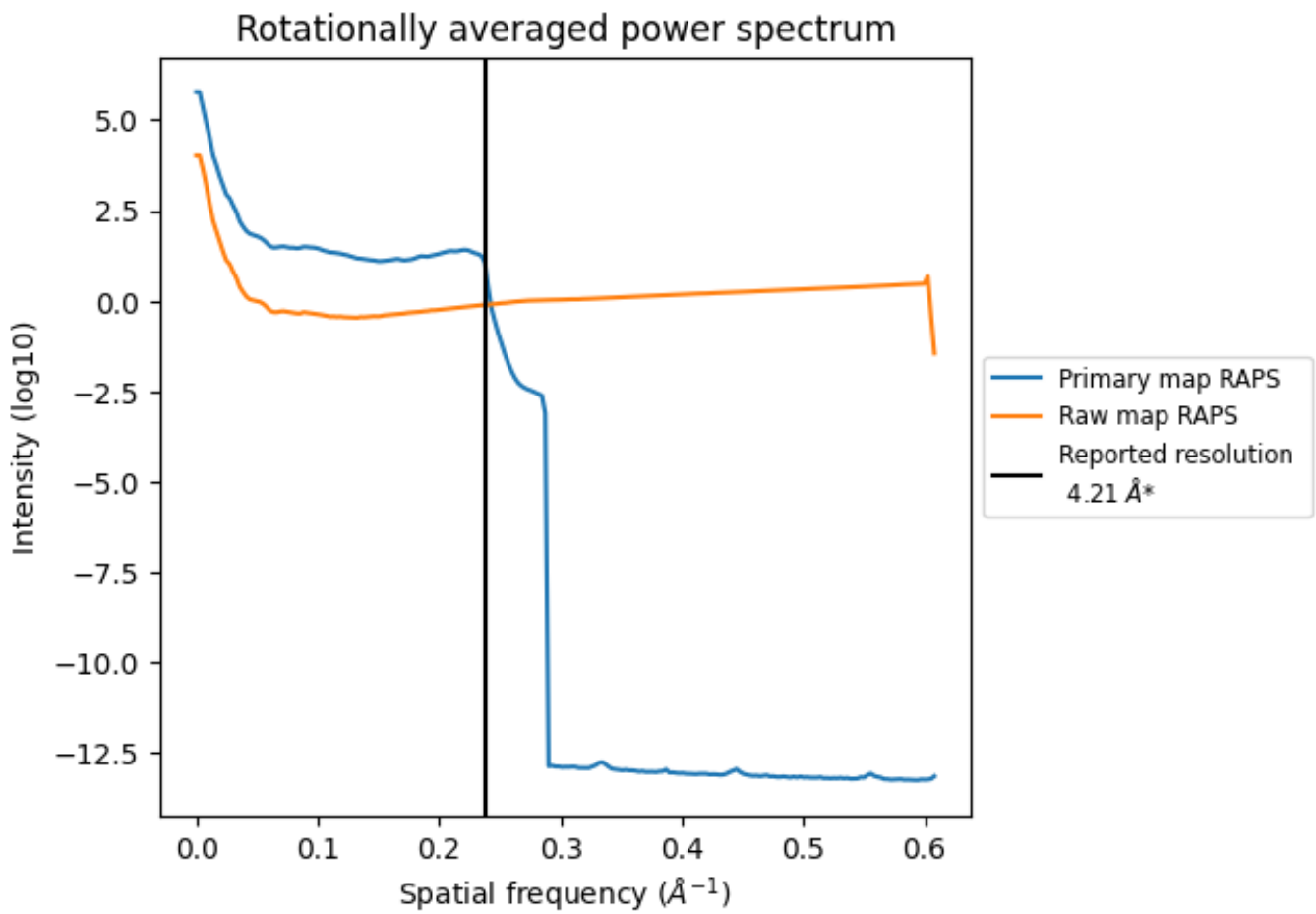
7.2 Volume estimate (i)



The volume at the recommended contour level is 56 nm^3; this corresponds to an approximate mass of 51 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)

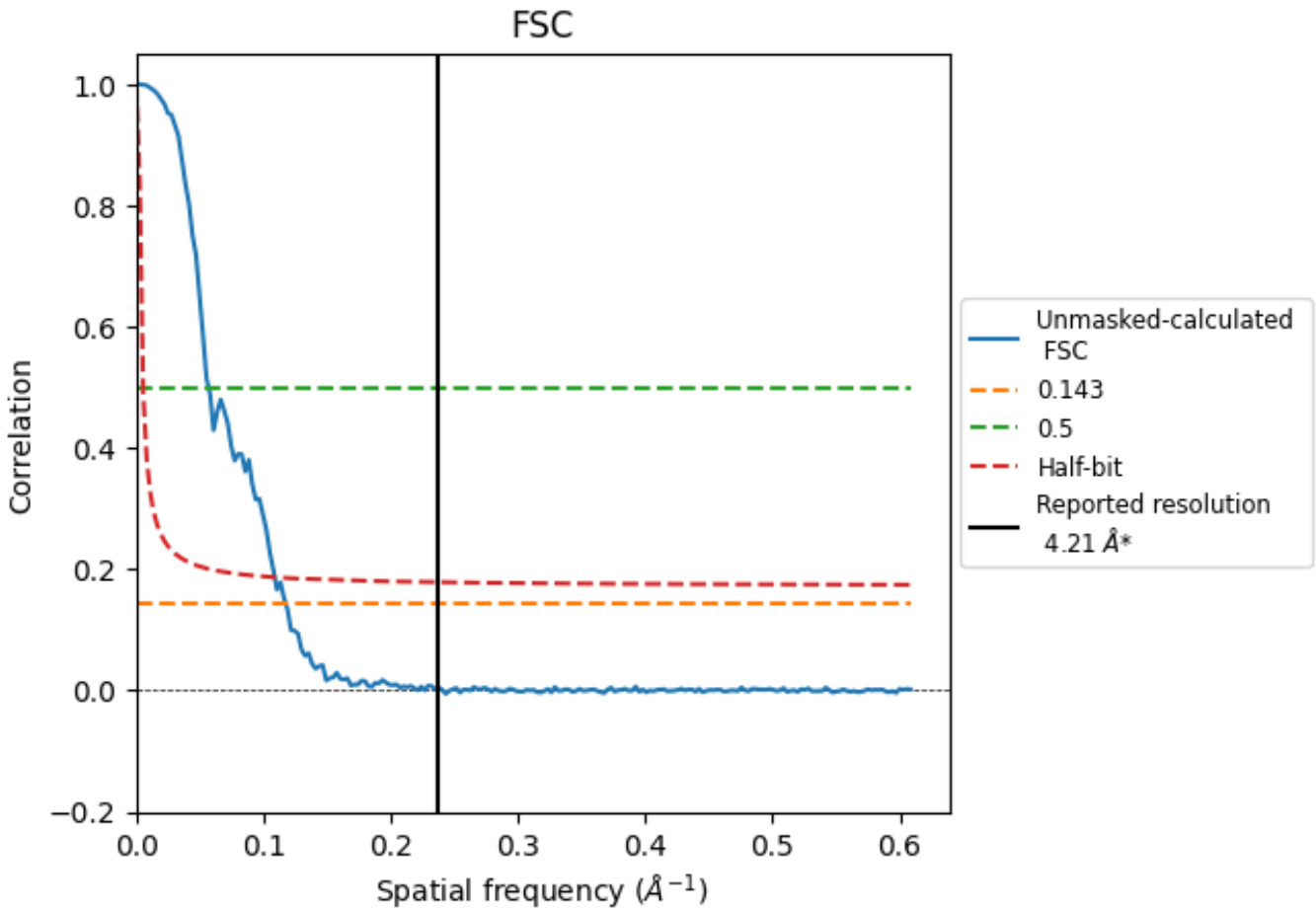


*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

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 0.238 Å^{-1}

8.2 Resolution estimates (i)

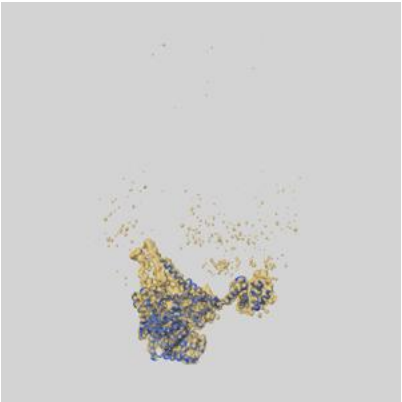
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.21	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.51	17.61	9.18

*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 8.51 differs from the reported value 4.21 by more than 10 %

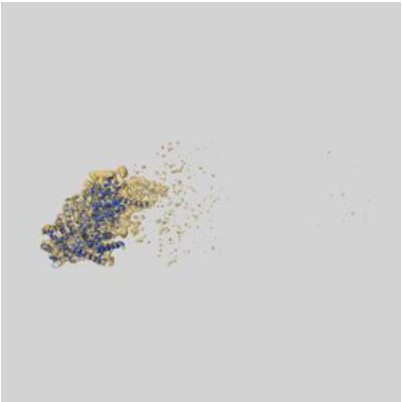
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-74155 and PDB model 9ZFV. Per-residue inclusion information can be found in section 3 on page 6.

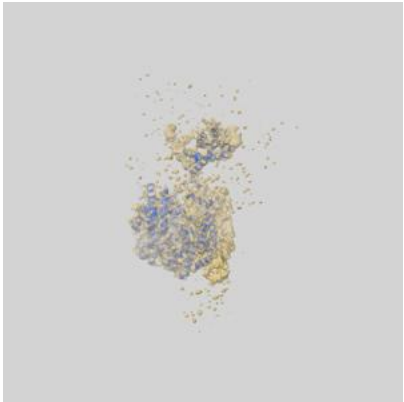
9.1 Map-model overlay (i)



X



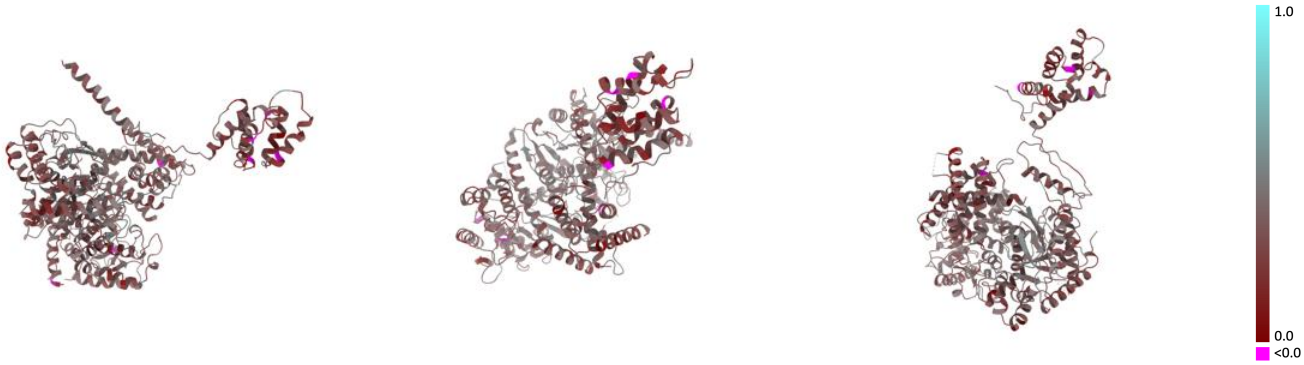
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.125 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.

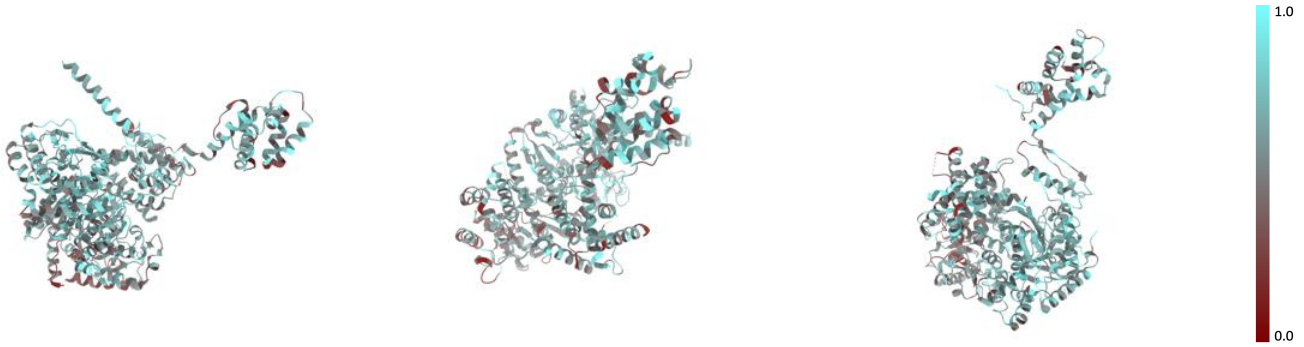
9.2 Q-score mapped to coordinate model (i)



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.

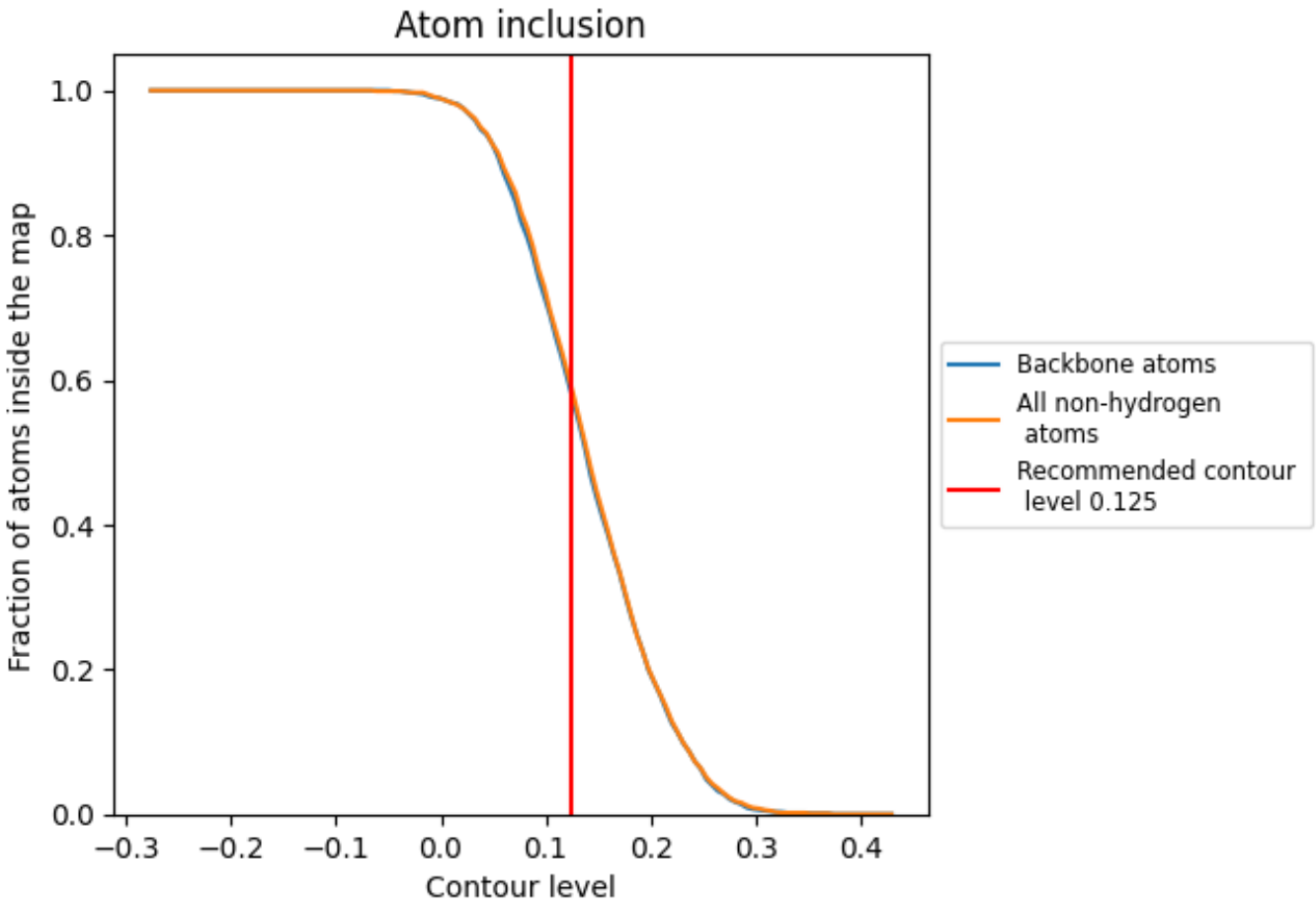
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.125).

9.4 Atom inclusion (i)



At the recommended contour level, 58% of all backbone atoms, 59% 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 (0.125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5890	0.3310
A	0.5230	0.3130
B	0.6520	0.3570
C	0.6210	0.3240
G	0.6230	0.3130