



wwPDB EM Validation Summary Report ⓘ

Jul 15, 2024 – 01:06 pm BST

PDB ID : 8BRJ
EMDB ID : EMD-16217
Title : Escherichia coli anaerobic fatty acid beta oxidation trifunctional enzyme (anEcTFE) trimeric complex
Authors : Sah-Teli, S.K.; Pinkas, M.; Novacek, J.; Venkatesan, R.
Deposited on : 2022-11-23
Resolution : 4.08 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

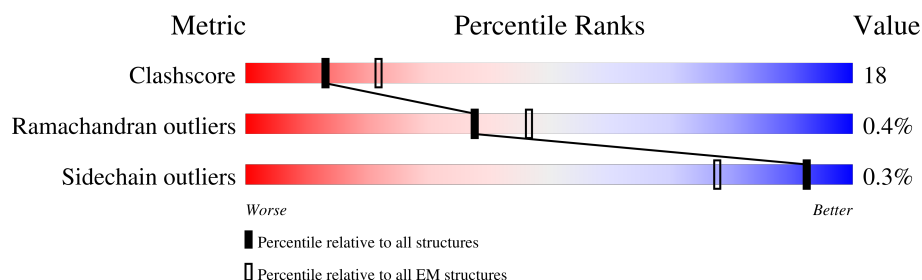
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.08 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	450	<div> <div>29%</div> <div>57%</div> <div>39%</div> <div>• •</div> </div>
1	B	450	<div> <div>45%</div> <div>60%</div> <div>37%</div> <div>•</div> </div>
2	C	714	<div> <div>50%</div> <div>60%</div> <div>39%</div> <div>•</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11627 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 3-ketoacyl-CoA thiolase FadI.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	436	Total	C	N	O	S	0	0
			3209	2018	581	593	17		
1	B	436	Total	C	N	O	S	0	0
			3214	2020	583	594	17		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP P76503
A	-12	GLY	-	expression tag	UNP P76503
A	-11	SER	-	expression tag	UNP P76503
A	-10	SER	-	expression tag	UNP P76503
A	-9	HIS	-	expression tag	UNP P76503
A	-8	HIS	-	expression tag	UNP P76503
A	-7	HIS	-	expression tag	UNP P76503
A	-6	HIS	-	expression tag	UNP P76503
A	-5	HIS	-	expression tag	UNP P76503
A	-4	HIS	-	expression tag	UNP P76503
A	-3	SER	-	expression tag	UNP P76503
A	-2	GLN	-	expression tag	UNP P76503
A	-1	ASP	-	expression tag	UNP P76503
A	0	PRO	-	expression tag	UNP P76503
B	-13	MET	-	initiating methionine	UNP P76503
B	-12	GLY	-	expression tag	UNP P76503
B	-11	SER	-	expression tag	UNP P76503
B	-10	SER	-	expression tag	UNP P76503
B	-9	HIS	-	expression tag	UNP P76503
B	-8	HIS	-	expression tag	UNP P76503
B	-7	HIS	-	expression tag	UNP P76503
B	-6	HIS	-	expression tag	UNP P76503
B	-5	HIS	-	expression tag	UNP P76503
B	-4	HIS	-	expression tag	UNP P76503
B	-3	SER	-	expression tag	UNP P76503
B	-2	GLN	-	expression tag	UNP P76503

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	ASP	-	expression tag	UNP P76503
B	0	PRO	-	expression tag	UNP P76503

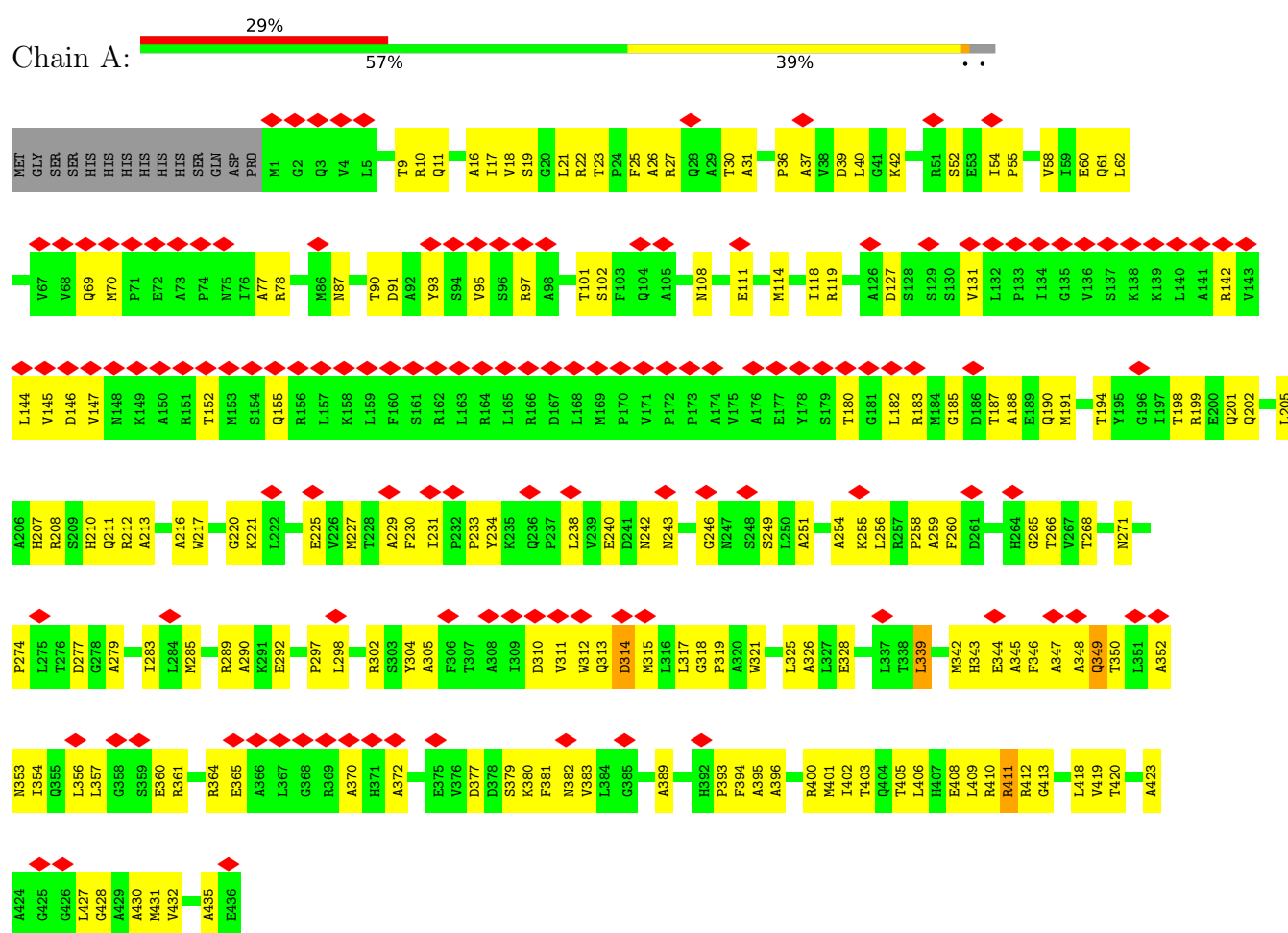
- Molecule 2 is a protein called Fatty acid oxidation complex subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	710	Total	C	N	O	S	0	0
			5204	3295	917	970	22		

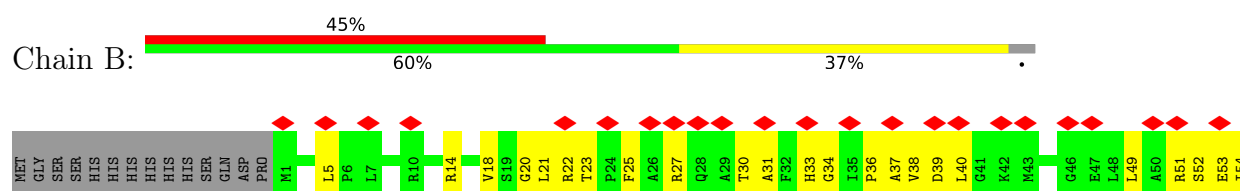
3 Residue-property plots

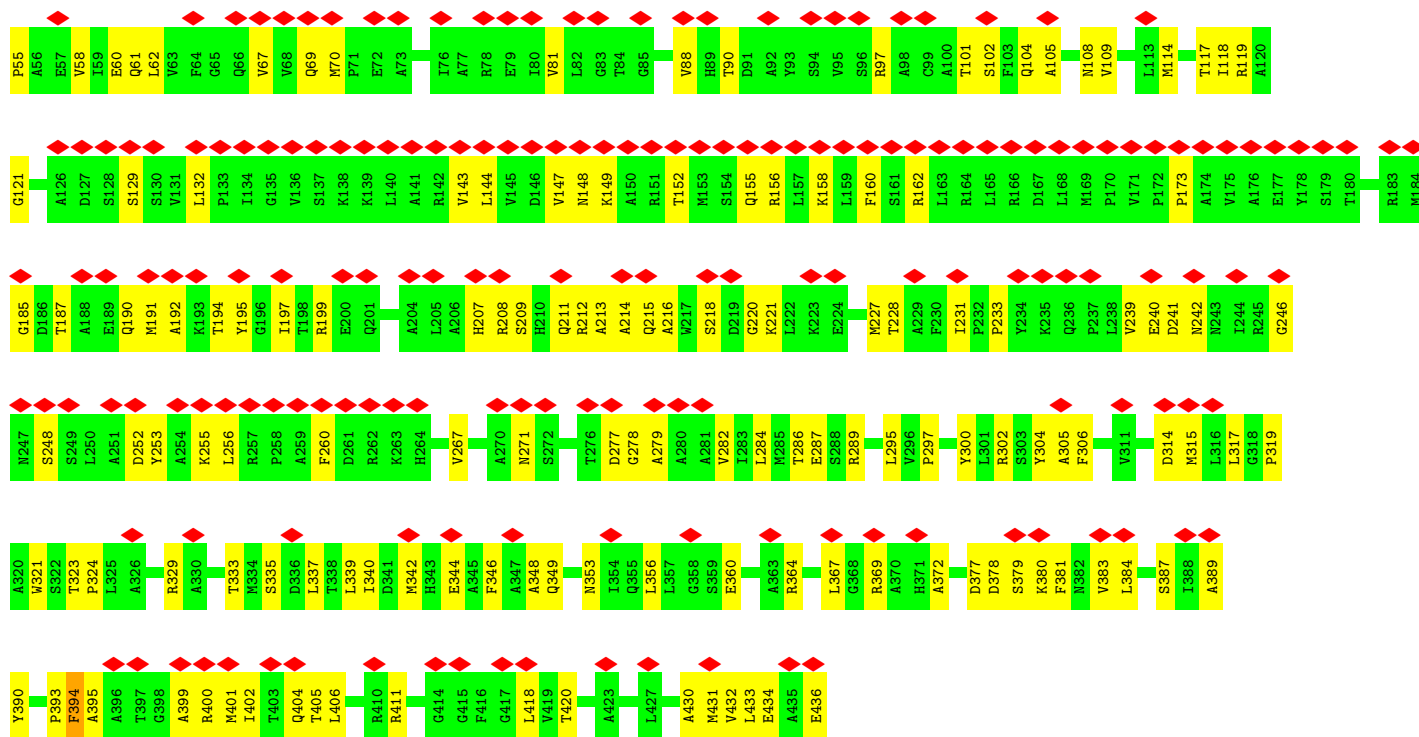
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 3-ketoacyl-CoA thiolase FadI

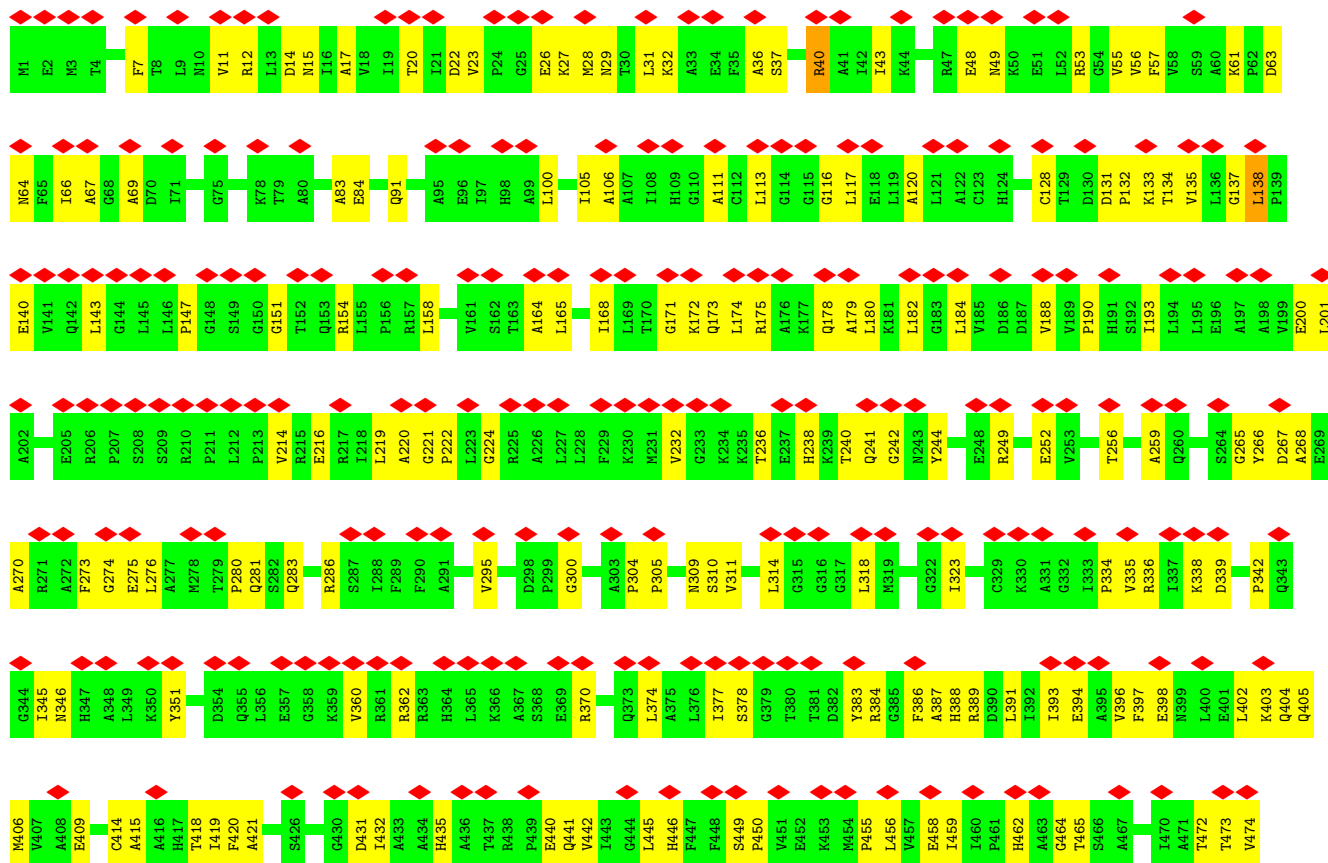


• Molecule 1: 3-ketoacyl-CoA thiolase FadI





• Molecule 2: Fatty acid oxidation complex subunit alpha



S668	L669	G670	A671	G672	E673	V674	V675	A676	I677	M678	Q679	R680	L681	A682	T683	Q684	Y685	G686	S687	R688	F689	T690	P691	C692	E693	R694	L695	V696	E697	M698	G699	A700	R701	Q702	G703	E703	S704	F705	T708	T709	A710	THR	ASP	LEU	GLN												
I601	Y602	P603	L604	I605	G606	T607	Q608	G609	Q610	G611	R612	I613	S614	Q617	E620	R621	C622	V623	M624	L625	M626	L627	N628	E629	A630	V631	R632	D635	E636	Q637	V638	I639	R640	S641	V642	G645	D646	A649	V650	I653	G654	F655	P656	P657	F658	L659	G660	F663	R664	Y665	I666	D667					
E538	V539	G540	I541	D542	T543	G544	T545	K546	I547	I548	P549	V550	L551	E552	A553	E557	R558	F559	S560	A561	P562	A563	N564	V565	V566	S567	S568	I569	L570	N571	D572	D573	R574	K575	G576	R577	K578	N579	G580	R581	G582	F583	Y584	G587	Q588	K589	G590	R591	K592	S593	K594	K595	Q596	V597	D598	P599	A600
K475	L476	A477	K478	K479	Q480	G481	K482	T483	F484	I485	V486	V487	A491	G492	F493	Y494	N496	R497	I498	L499	A500	P501	Y502	I503	N504	E505	A506	I507	R508	M509	L510	T511	Q512	G513	E514	R515	V516	E517	H518	I519	D520	A521	A522	L523	F526	G527	F528	P529	V530	G531	P532	I533	Q534	L535	L536	D537	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	37357	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 ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.542	Depositor
Minimum map value	-0.214	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	298.08002, 298.08002, 298.08002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82800007, 0.82800007, 0.82800007	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.26	0/3263	0.54	0/4427
1	B	0.25	0/3268	0.53	0/4433
2	C	0.26	0/5293	0.50	0/7193
All	All	0.26	0/11824	0.52	0/16053

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	3209	0	3238	128	0
1	B	3214	0	3245	108	0
2	C	5204	0	5197	199	0
All	All	11627	0	11680	427	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 18.

The worst 5 of 427 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:243:ASN:HD21	1:A:274:PRO:HG2	1.34	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ILE:HG22	1:A:233:PRO:HD2	1.60	0.80
1:B:27:ARG:H	1:B:242:ASN:HD21	1.35	0.75
1:A:60:GLU:HB2	1:A:118:ILE:HG23	1.69	0.75
1:B:197:ILE:HG21	1:B:348:ALA:HA	1.68	0.74

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	434/450 (96%)	400 (92%)	31 (7%)	3 (1%)	22	61
1	B	434/450 (96%)	406 (94%)	26 (6%)	2 (0%)	29	67
2	C	708/714 (99%)	655 (92%)	51 (7%)	2 (0%)	41	75
All	All	1576/1614 (98%)	1461 (93%)	108 (7%)	7 (0%)	38	71

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	349	GLN
1	A	389	ALA
1	B	389	ALA
2	C	530	VAL
2	C	613	ILE

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	320/347 (92%)	318 (99%)	2 (1%)	86	92
1	B	321/347 (92%)	321 (100%)	0	100	100
2	C	524/570 (92%)	522 (100%)	2 (0%)	91	94
All	All	1165/1264 (92%)	1161 (100%)	4 (0%)	92	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	314	ASP
1	A	411	ARG
2	C	40	ARG
2	C	138	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	64	ASN
2	C	679	GLN
1	B	190	GLN
1	B	343	HIS
1	B	349	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 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.

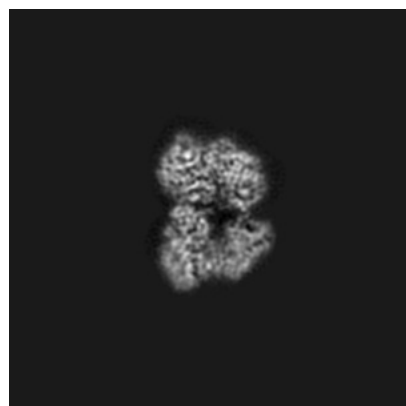
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16217. These allow visual inspection of the internal detail of the map and identification of artifacts.

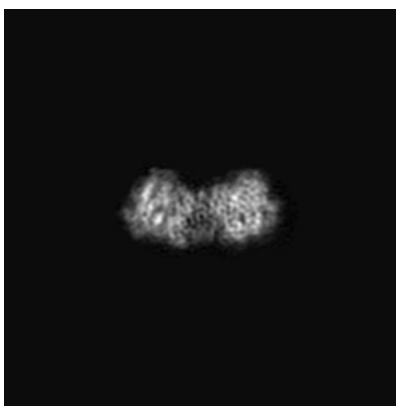
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

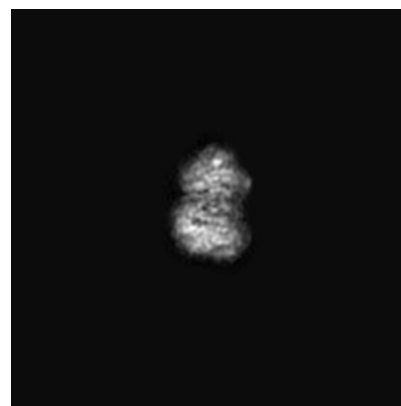
6.1.1 Primary map



X

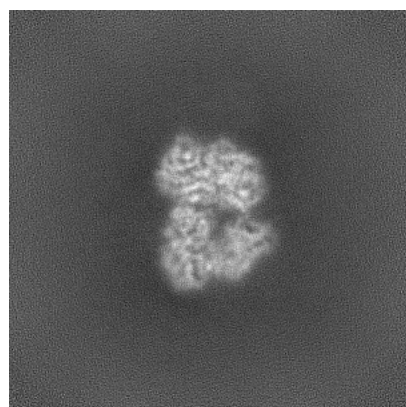


Y

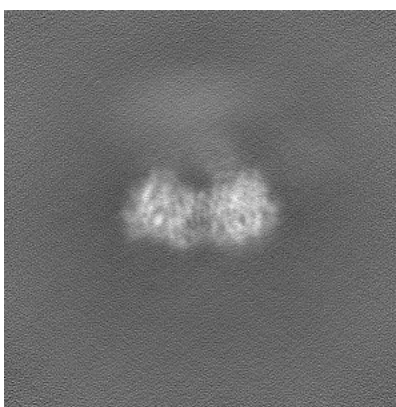


Z

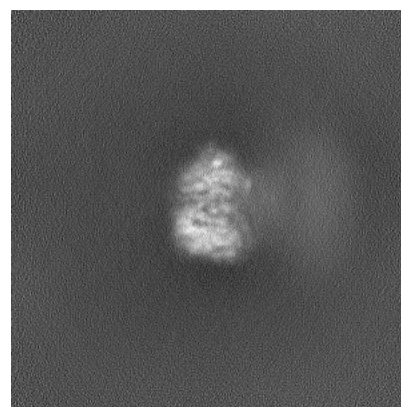
6.1.2 Raw map



X



Y

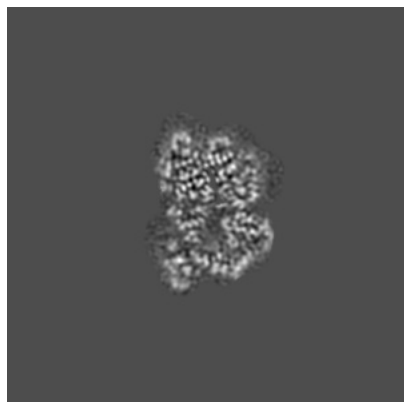


Z

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

6.2 Central slices [i](#)

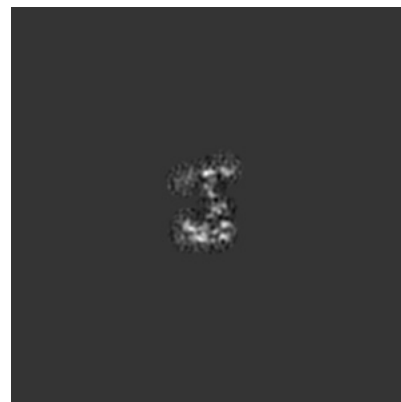
6.2.1 Primary map



X Index: 180

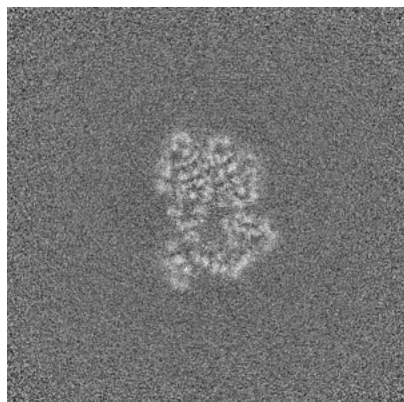


Y Index: 180

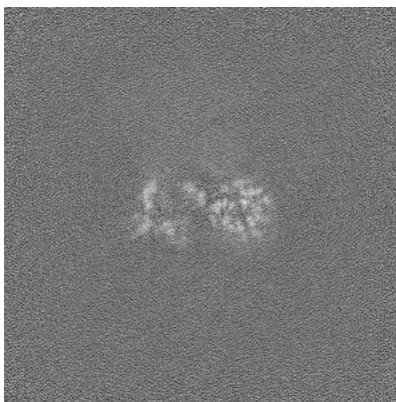


Z Index: 180

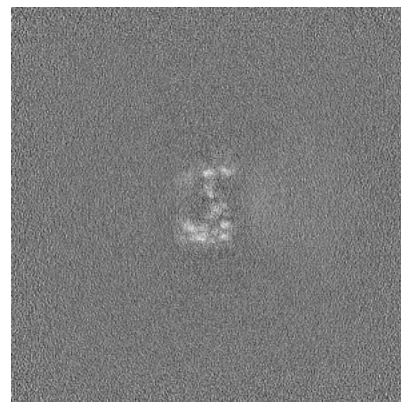
6.2.2 Raw map



X Index: 180



Y Index: 180

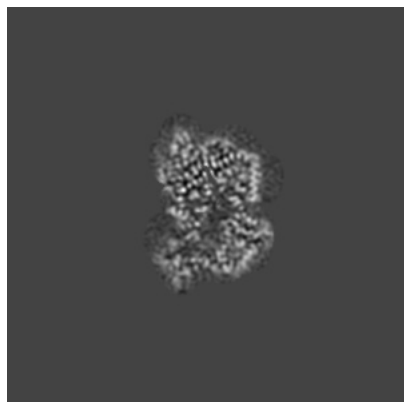


Z Index: 180

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

6.3 Largest variance slices [i](#)

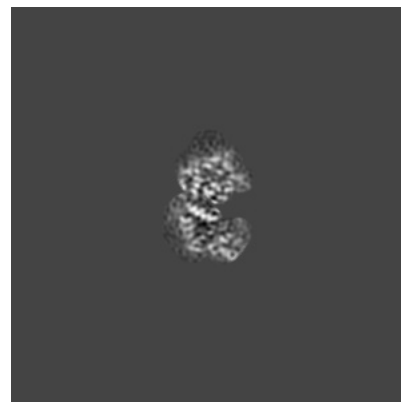
6.3.1 Primary map



X Index: 183

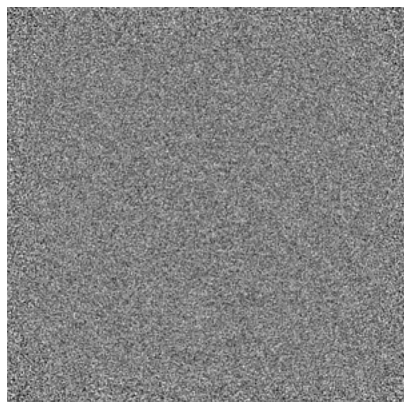


Y Index: 161

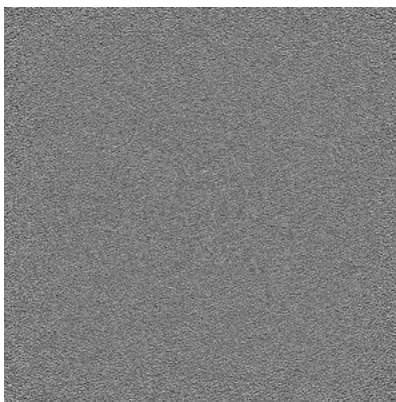


Z Index: 211

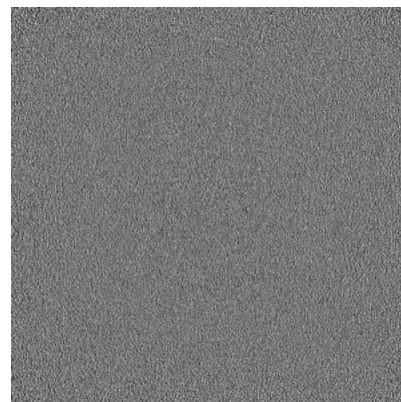
6.3.2 Raw map



X Index: 0



Y Index: 0

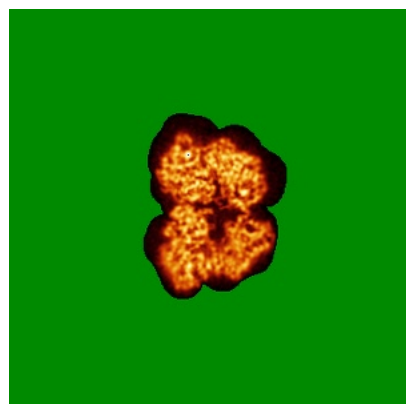


Z Index: 359

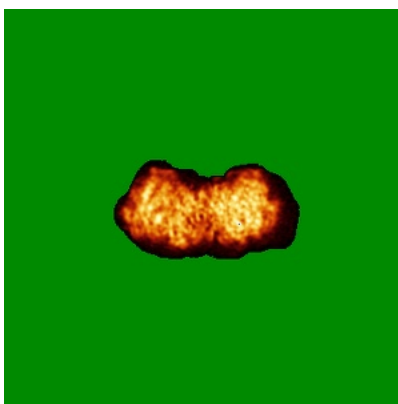
The images above show the largest variance slices of the map in three orthogonal directions.

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

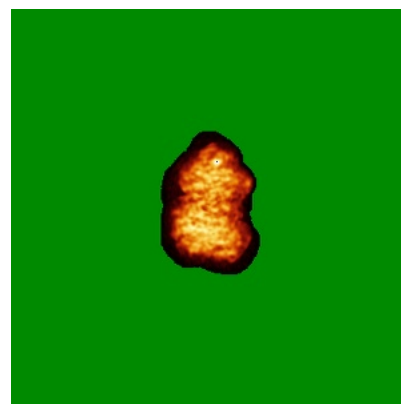
6.4.1 Primary map



X

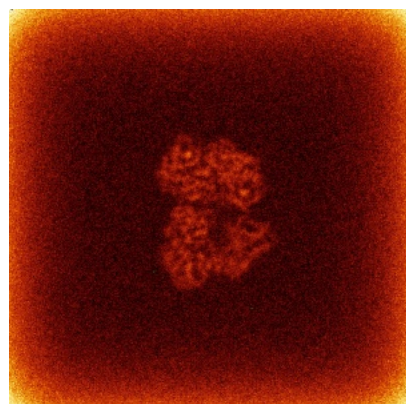


Y

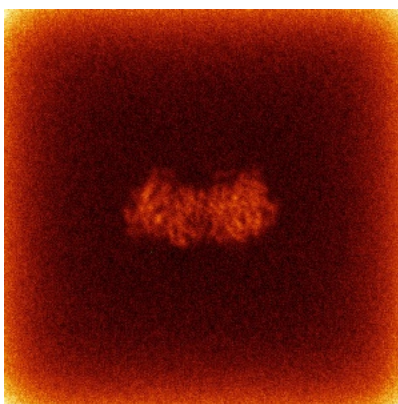


Z

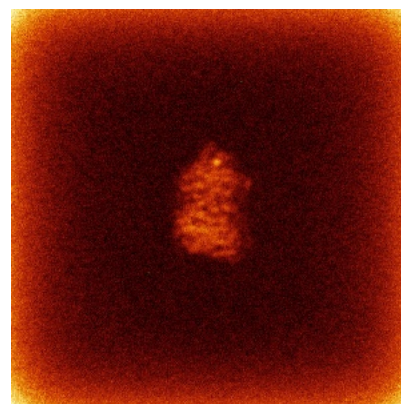
6.4.2 Raw map



X



Y

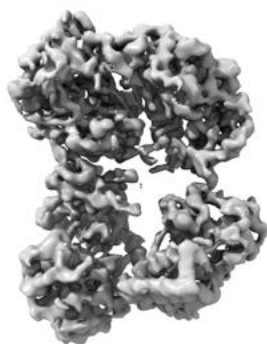


Z

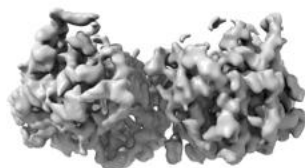
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

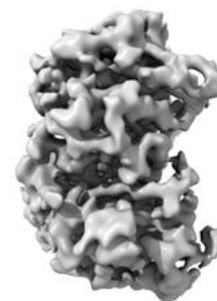
6.5.1 Primary map



X



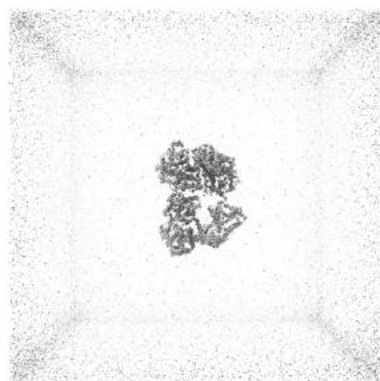
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

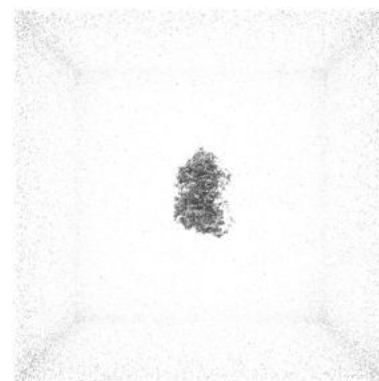
6.5.2 Raw map



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.

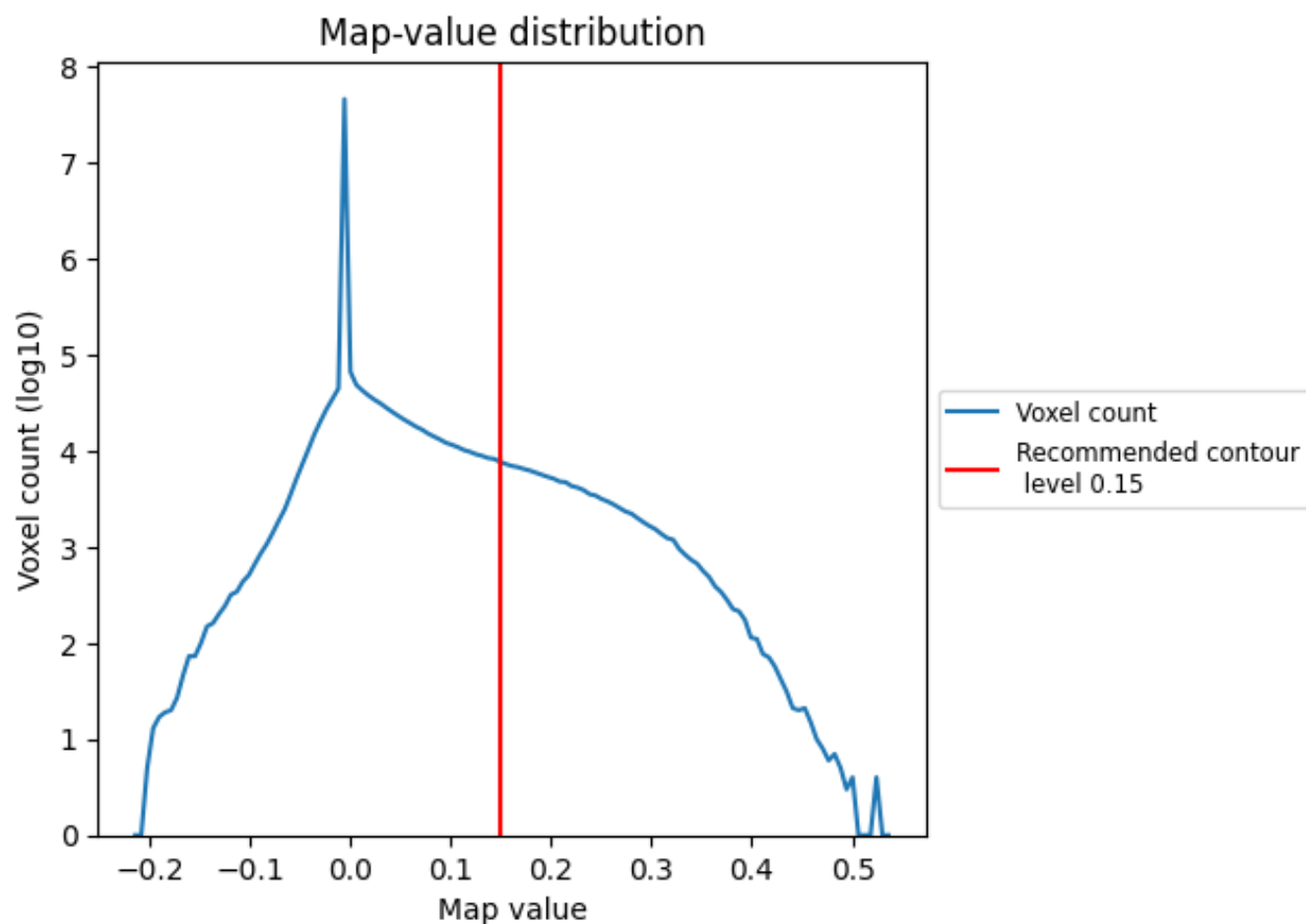
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

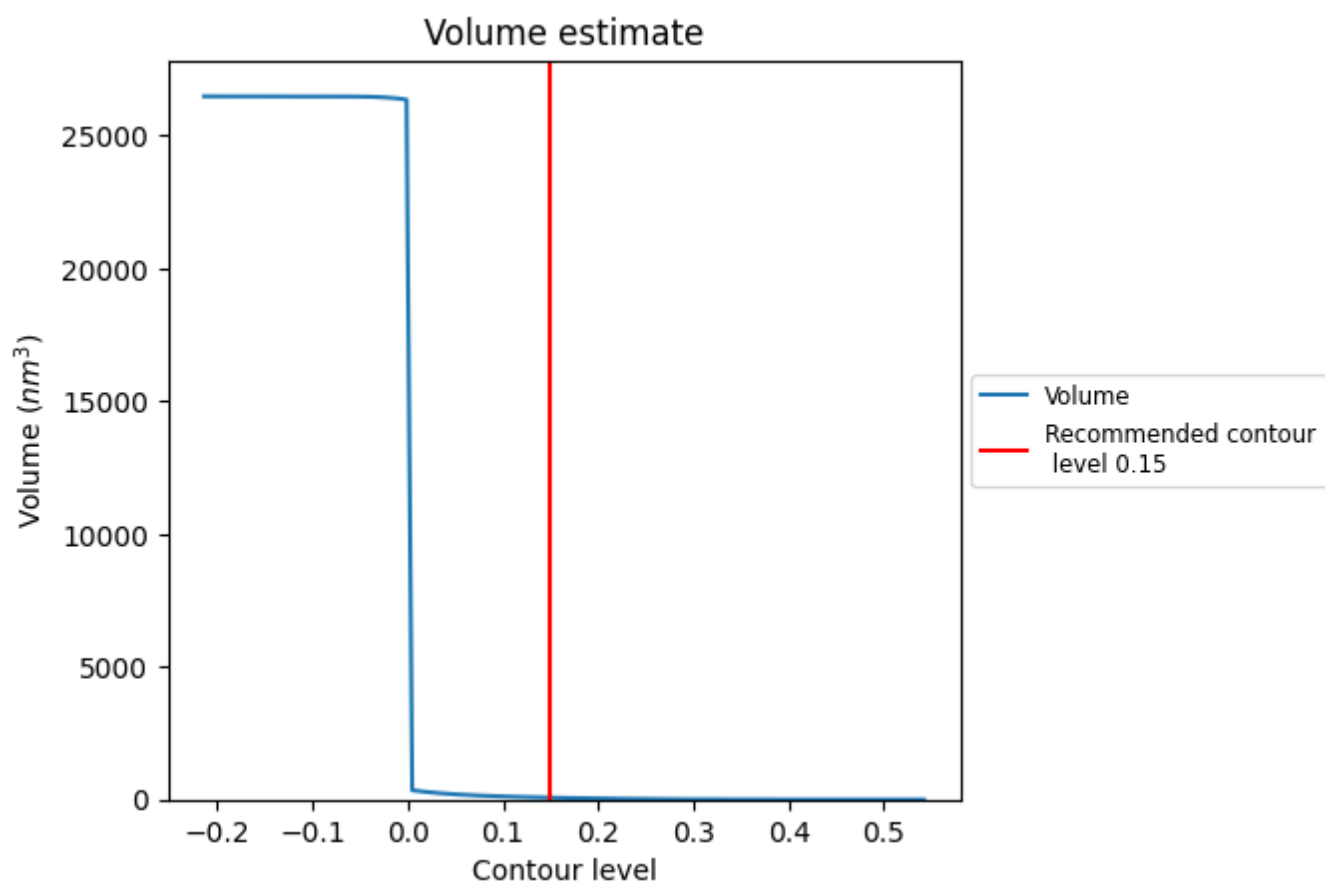
This section contains the results of statistical analysis of the map.

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.

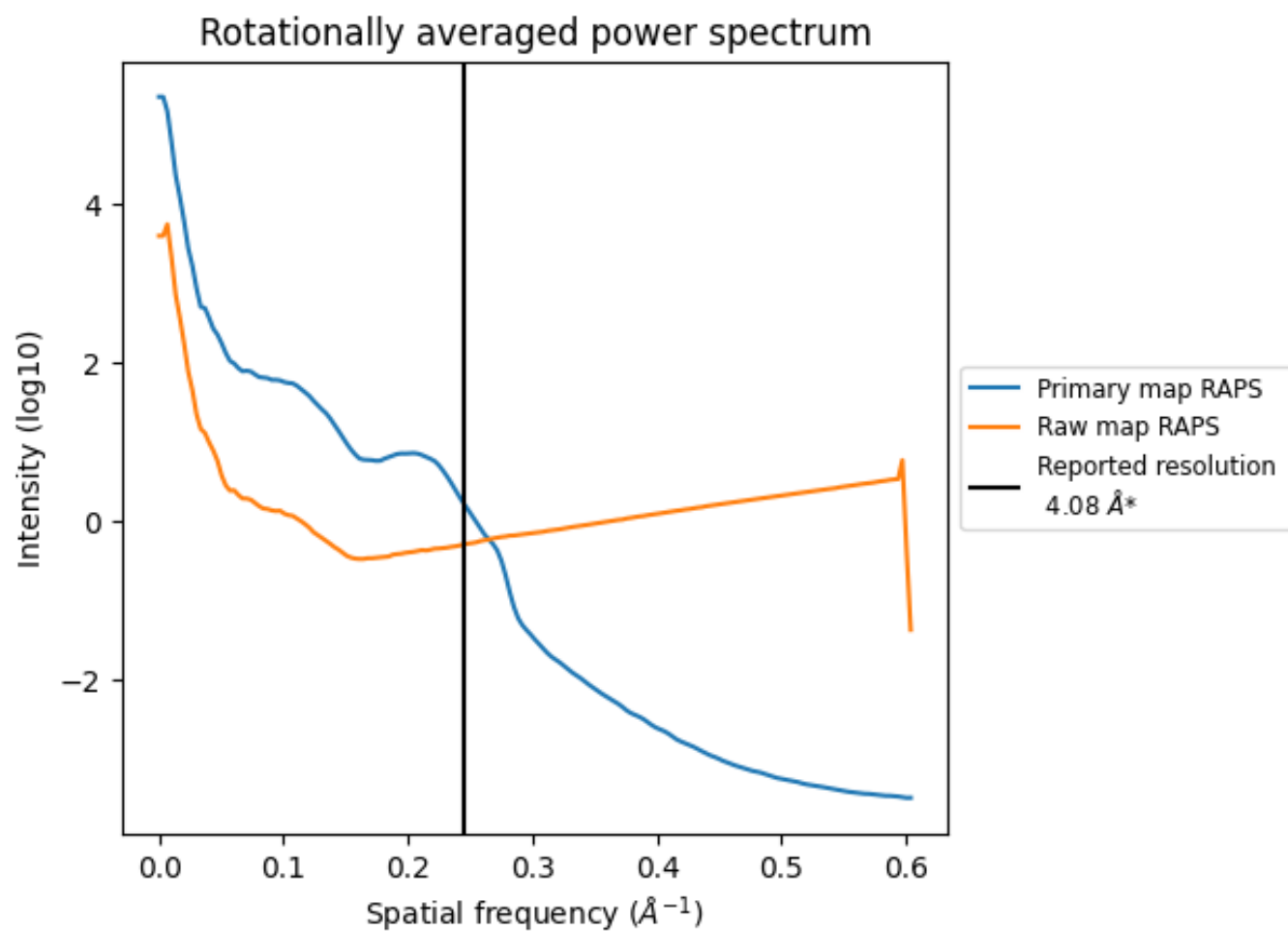
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 71 nm^3 ; this corresponds to an approximate mass of 64 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 ⓘ

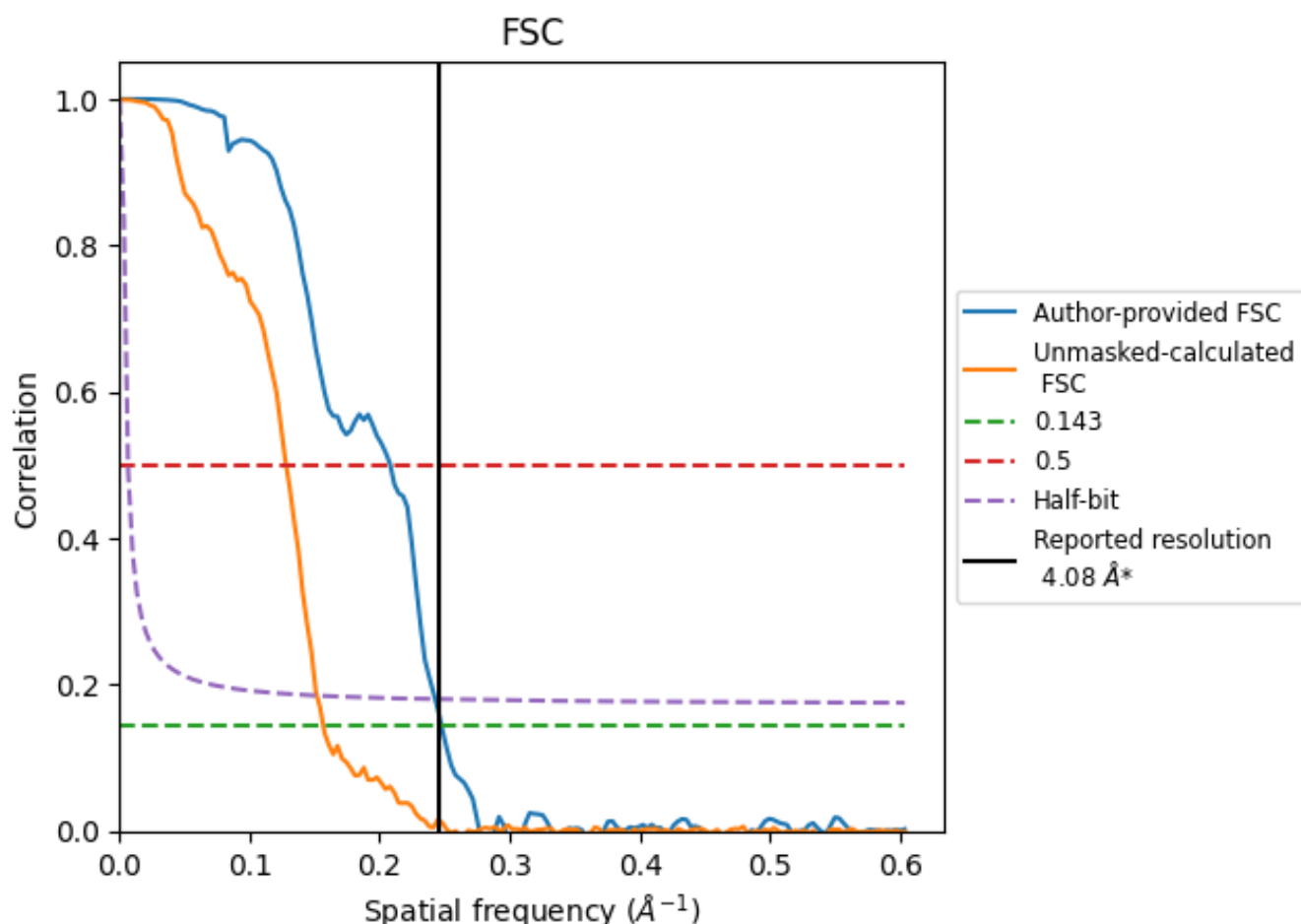


*Reported resolution corresponds to spatial frequency of 0.245 Å⁻¹

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 0.245 Å⁻¹

8.2 Resolution estimates [i](#)

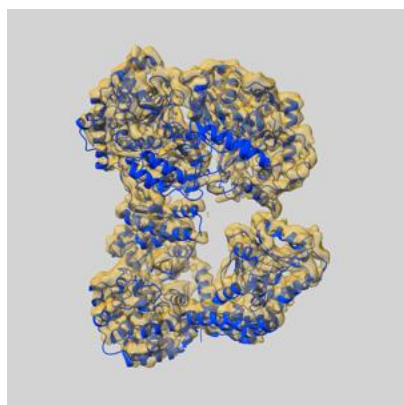
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.08	-	-
Author-provided FSC curve	4.04	4.80	4.12
Unmasked-calculated*	6.38	7.81	6.59

*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 6.38 differs from the reported value 4.08 by more than 10 %

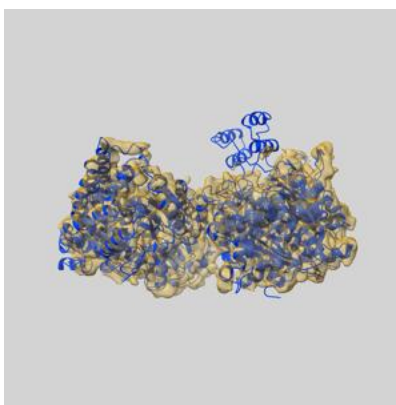
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16217 and PDB model 8BRJ. Per-residue inclusion information can be found in section [3](#) on page [5](#).

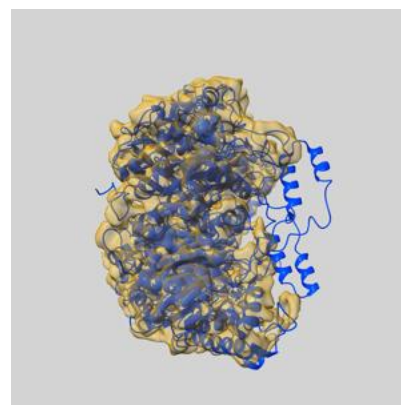
9.1 Map-model overlay [i](#)



X



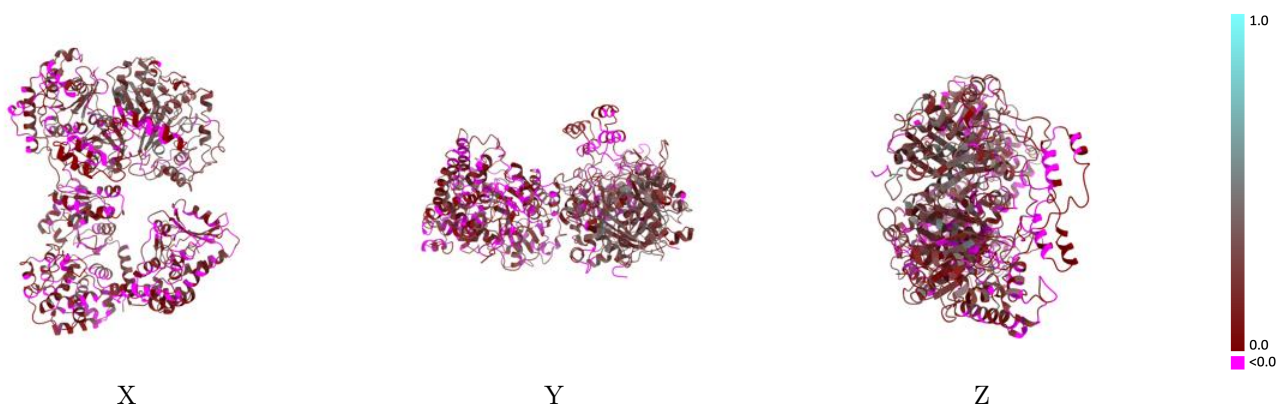
Y



Z

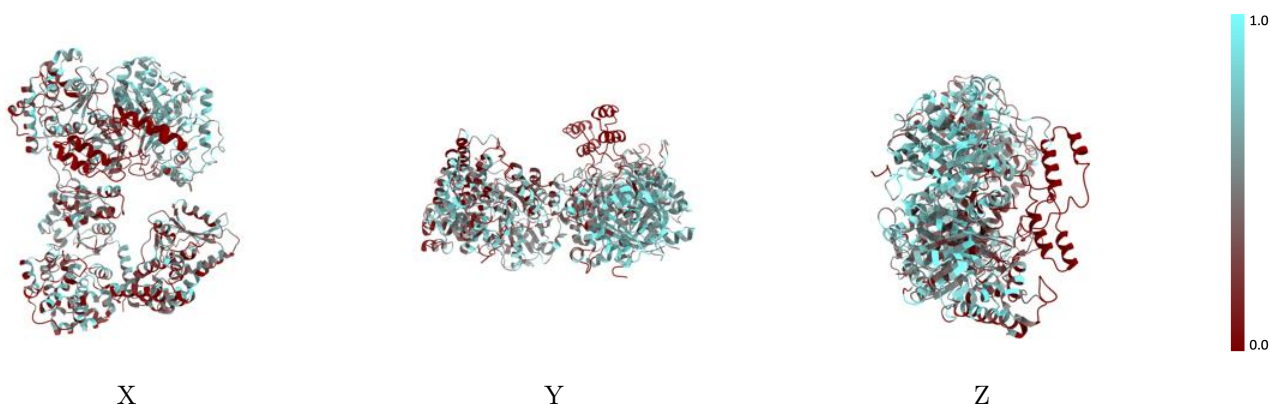
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



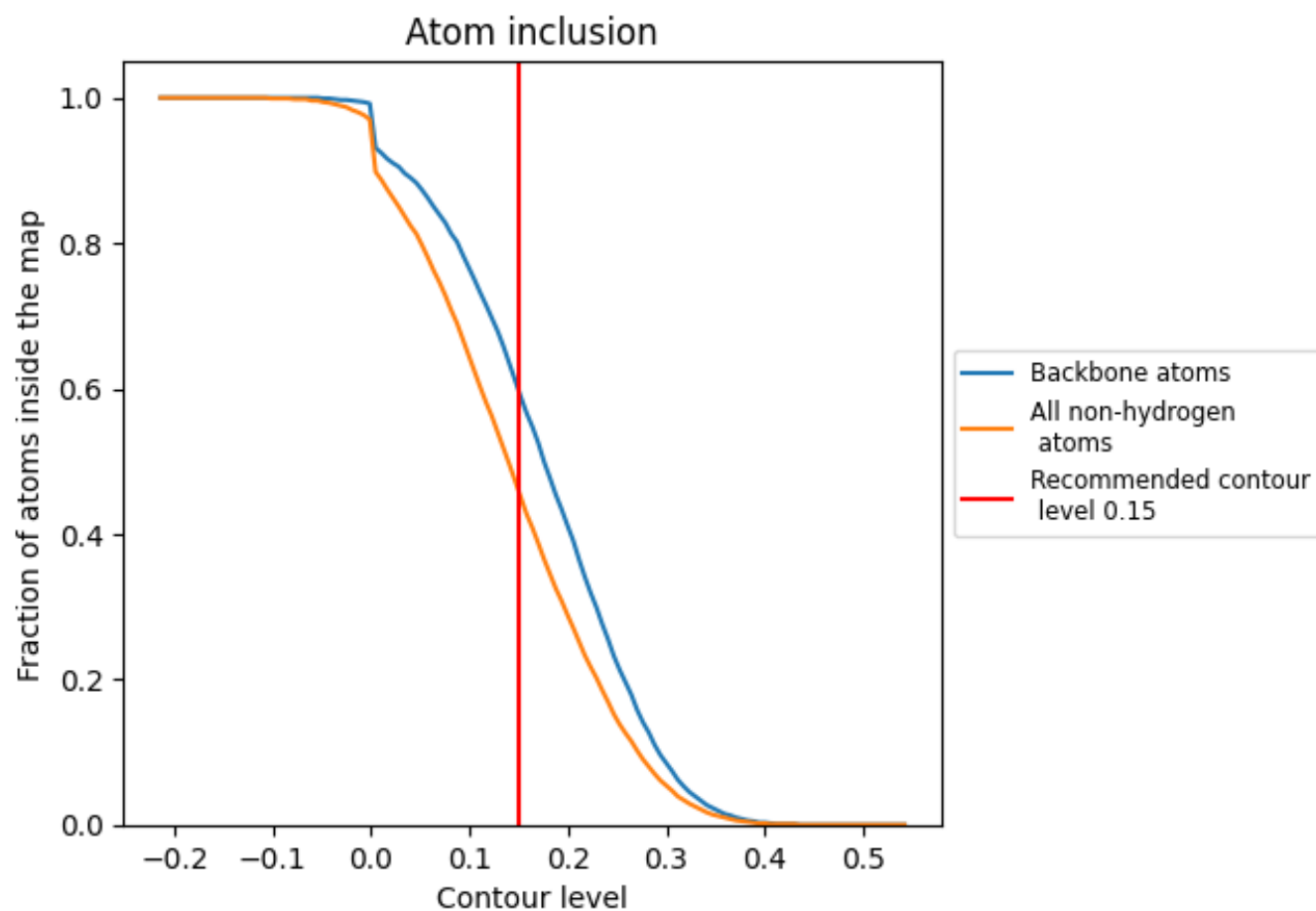
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 46% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4590	<div></div> 0.1320
A	<div></div> 0.5280	<div></div> 0.2150
B	<div></div> 0.4340	<div></div> 0.1320
C	<div></div> 0.4310	<div></div> 0.0800

