



wwPDB EM Validation Summary Report ⓘ

Jun 20, 2024 – 06:58 AM JST

PDB ID : 7WXF
EMDB ID : EMD-32877
Title : GPR domain of Drosophila P5CS filament with glutamate
Authors : Liu, J.L.; Zhong, J.; Guo, C.J.; Zhou, X.
Deposited on : 2022-02-14
Resolution : 3.60 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

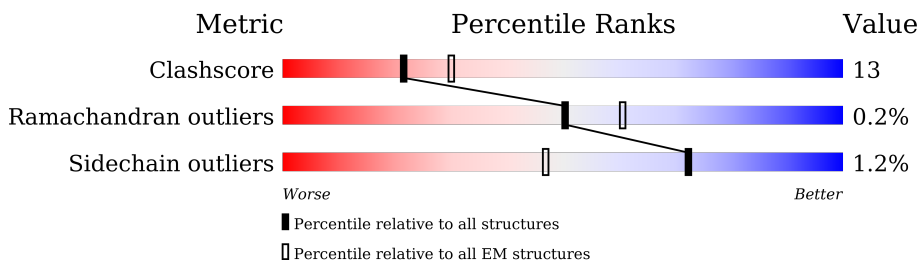
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	776	 39% 16% 45%
1	B	776	 38% 17% 45%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6494 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.

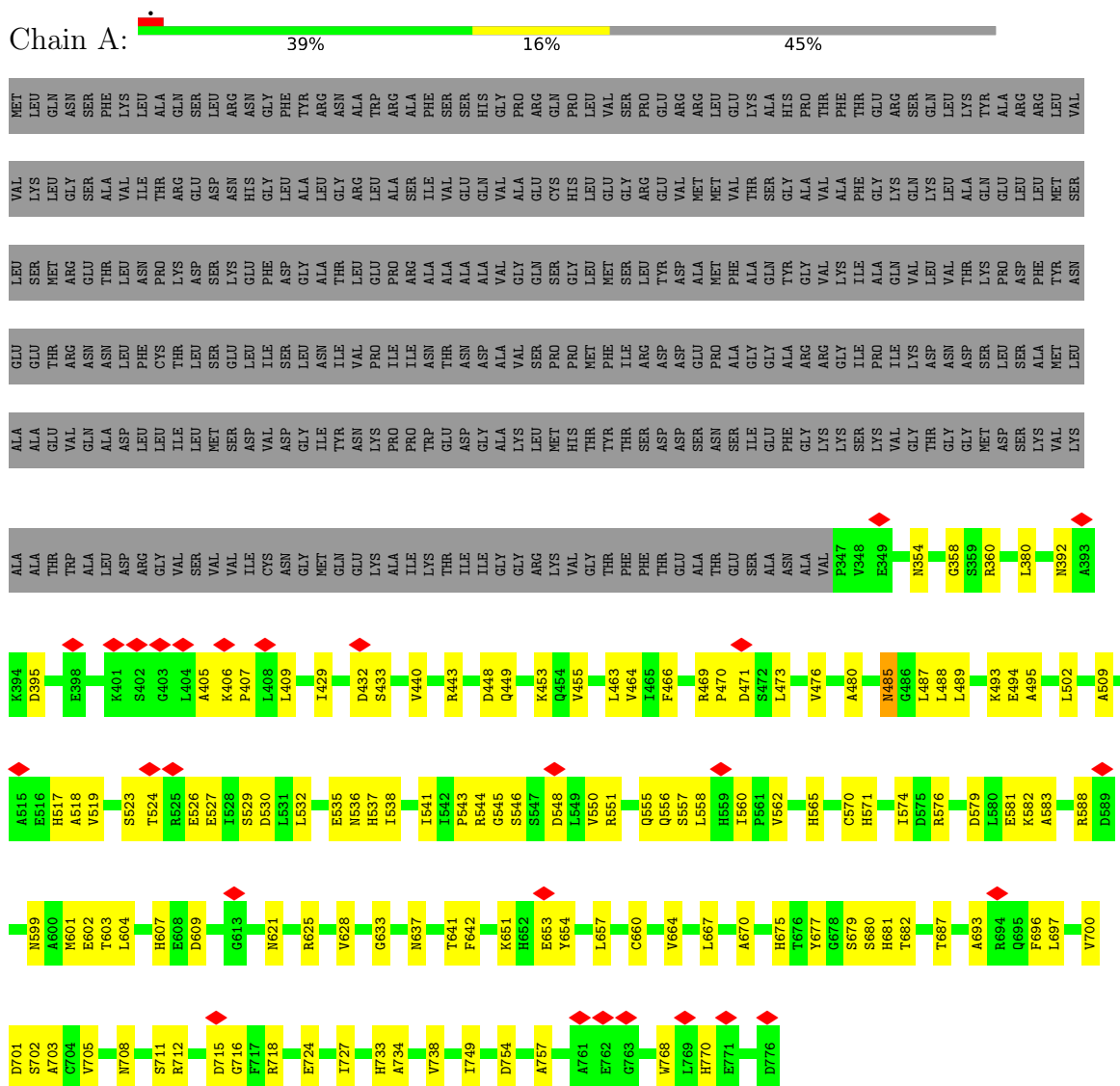
- Molecule 1 is a protein called Delta-1-pyrroline-5-carboxylate synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	430	Total	C	N	O	S	0	0
			3247	2027	586	619	15		
1	B	430	Total	C	N	O	S	0	0
			3247	2027	586	619	15		

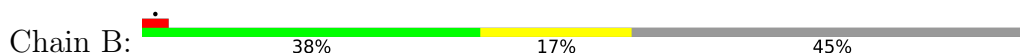
3 Residue-property plots

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: Delta-1-pyrroline-5-carboxylate synthase



• Molecule 1: Delta-1-pyrroline-5-carboxylate synthase



Q695	F696	L697	V700	D701	S702	K703	V705	N708	S711	R712	D715	G716	F717	R718	E724	I727	H733	A734	V738	I749	D754	A757	A761	E762	G763	V768	L769	H770	E771	D776																						
5586	A587	R588	D589	N599	A600	N601	E602	T603	L604	H607	E608	D609	L610	G613	N621	R625	V628	G633	N637	T641	F642	K651	H652	E653	Y654	L657	C660	V664	L667	A670	H675	T676	Y677	S680	H681	T682	T687	A693														
E516	H517	A518	V519	S523	T524	R525	E526	E527	I528	S529	D530	L531	L532	E535	N536	H537	I538	D539	L540	I541	P543	R544	G545	S546	S547	D548	L549	V550	R551	S552	I553	Q554	Q555	Q556	S557	L558	H559	I560	P561	V562	H565	C570	H571	V572	Y573	I574	D575	R576	D579	L580	E581	K582
N392	A393	K394	D395	E398	K401	S402	G403	L404	A405	K406	L408	L409	I429	D432	S433	V440	R443	D448	Q449	K453	Q454	V455	L463	V464	I465	F466	R469	P470	D471	S472	L473	V476	A480	W485	G486	L487	L488	L489	E494	A495	A509	A515										
ALA	ALA	TRP	ALA	LEU	ASP	ARG	GLY	VAL	VAL	VAL	ILE	CYS	ASN	ASN	MET	GLN	GLU	LYS	ALA	ILE	PRO	TRP	THR	ILE	ILE	GLY	ARG	LYS	VAL	GLY	THR	ALA	ASN	ALA	VAL	P347	V348	E349	N354	G358	S359	R360	L380	L389								
ALA	ALA	TRP	VAL	GLN	ALA	ASP	LEU	PHE	LEU	CYS	THR	LEU	ILE	ASP	ASP	GLY	TYR	ASN	VAL	PRO	ILE	PRO	ALA	THR	ASN	ASP	GLY	VAL	LEU	SER	PRO	ILE	LYS	ASP	LEU	VAL	THR	GLY	ASN	THR	GLY	ASP	SER	LEU	SER	ALA	VAL	LYS				
GLU	GLU	THR	ARG	ASN	ASN	LEU	PHE	LEU	ASP	LEU	ILE	ASP	ASP	GLY	LEU	ILE	ASN	ILE	TYR	ASN	VAL	PRO	GLU	THR	LEU	ILE	ASN	ASP	GLU	PRO	MET	MET	PHE	ALA	GLN	VAL	THR	GLY	ILE	ALA	GLY	VAL	GLN	LYS	ARG	GLU	ARG	SER	GLN	SER		
LEU	SER	MET	ARG	GLU	GLU	THR	ASN	PRO	LYS	ASP	GLY	ASP	THR	LEU	THR	ASN	VAL	GLU	PRO	ILE	ARG	SER	ALA	VAL	ALA	VAL	MET	SER	LEU	ARG	GLY	VAL	PHE	THR	GLY	ALA	ILE	ALA	GLN	VAL	LEU	VAL	GLN	LYS	ARG	GLU	ARG	SER	GLN	SER		
VAL	LEU	GLY	GLY	SER	ALA	ALA	VAL	THR	ARG	GLU	LEU	THR	ALA	GLY	LEU	ASN	VAL	ARG	LEU	PRO	ALA	SER	ALA	VAL	GLN	VAL	GLY	MET	VAL	VAL	VAL	THR	THR	GLY	SER	ALA	THR	GLY	ALA	ILE	ALA	GLN	VAL	GLN	LYS	ARG	GLU	ARG	SER	GLN	SER	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	286291	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 ($e^-/\text{\AA}^2$)	72	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.251	Depositor
Minimum map value	-0.147	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	317.99997, 317.99997, 317.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	0.36	0/3297	0.50	0/4462
1	B	0.36	0/3297	0.50	0/4462
All	All	0.36	0/6594	0.50	0/8924

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	3247	0	3285	87	0
1	B	3247	0	3285	91	0
All	All	6494	0	6570	170	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 13.

The worst 5 of 170 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:532:LEU:HD21	1:A:557:SER:HA	1.58	0.85
1:B:532:LEU:HD21	1:B:557:SER:HA	1.58	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:681:HIS:HD1	1:B:682:THR:HG1	1.37	0.72
1:A:681:HIS:HD1	1:A:682:THR:HG1	1.36	0.71
1:B:570:CYS:O	1:B:571:HIS:ND1	2.24	0.70

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	428/776 (55%)	373 (87%)	54 (13%)	1 (0%)	47	79
1	B	428/776 (55%)	373 (87%)	54 (13%)	1 (0%)	47	79
All	All	856/1552 (55%)	746 (87%)	108 (13%)	2 (0%)	50	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	526	GLU
1	B	526	GLU

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	345/630 (55%)	341 (99%)	4 (1%)	71	87

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	345/630 (55%)	341 (99%)	4 (1%)	71	87
All	All	690/1260 (55%)	682 (99%)	8 (1%)	72	87

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	588	ARG
1	B	485	ASN
1	B	360	ARG
1	A	588	ARG
1	B	432	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	708	ASN
1	B	652	HIS
1	B	354	ASN
1	B	708	ASN
1	B	565	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](#)

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.

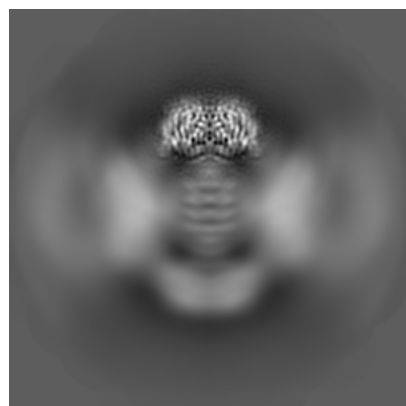
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32877. These allow visual inspection of the internal detail of the map and identification of artifacts.

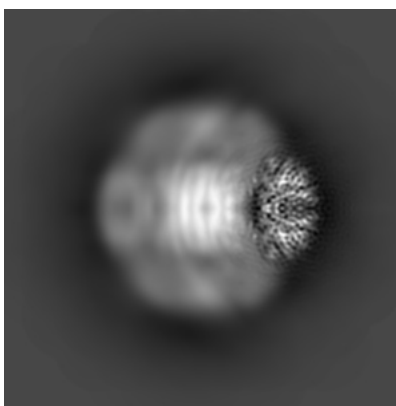
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

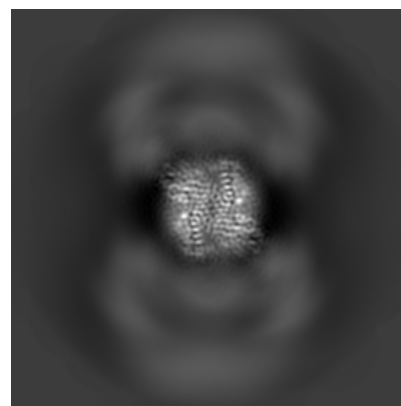
6.1.1 Primary map



X

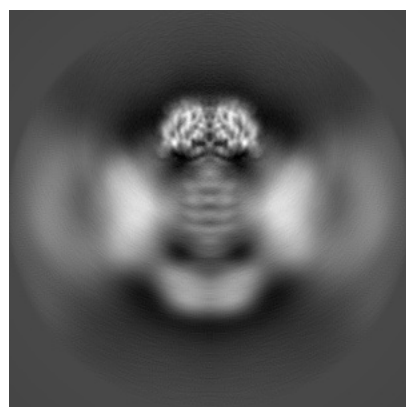


Y

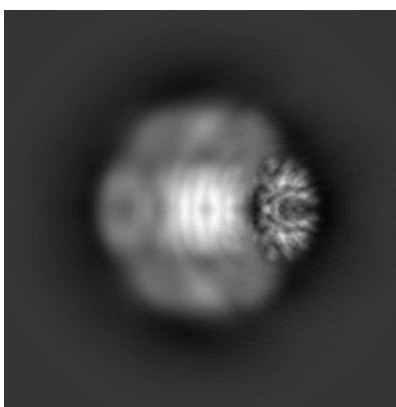


Z

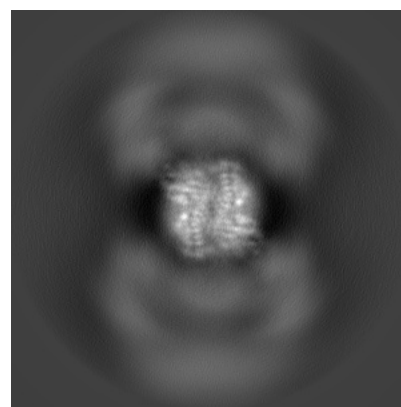
6.1.2 Raw map



X



Y

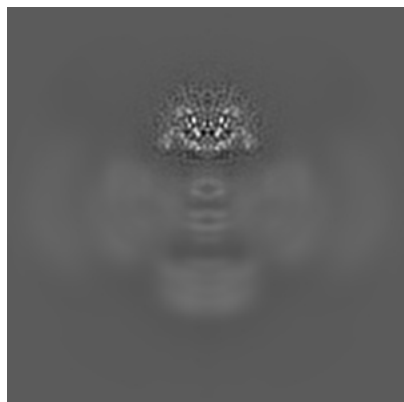


Z

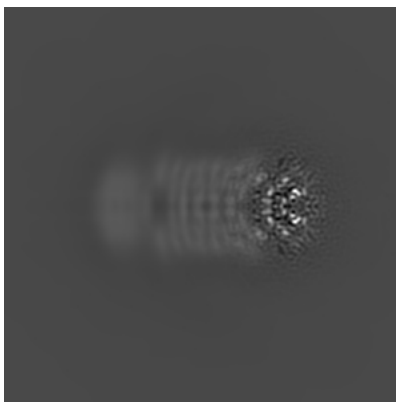
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

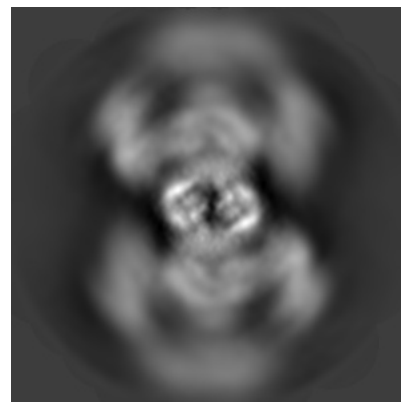
6.2.1 Primary map



X Index: 150

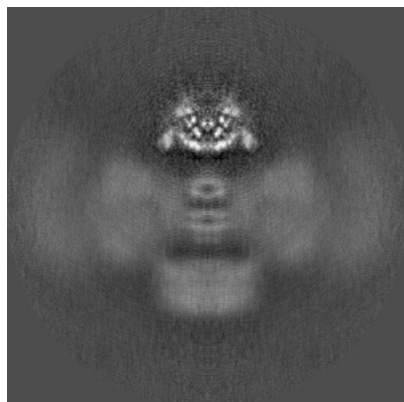


Y Index: 150

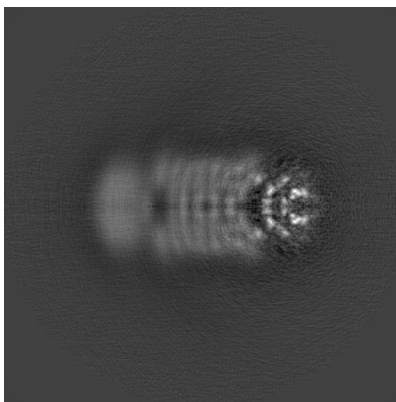


Z Index: 150

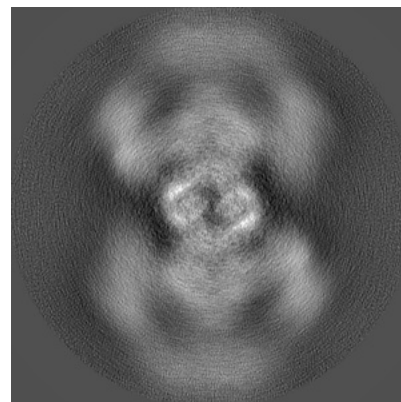
6.2.2 Raw map



X Index: 150



Y Index: 150

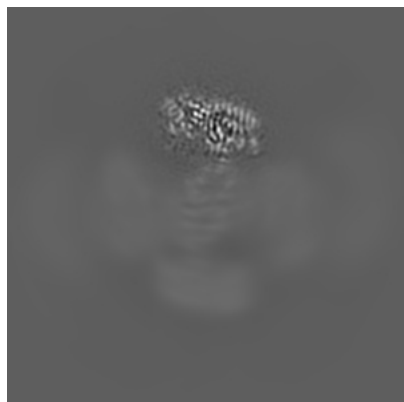


Z Index: 150

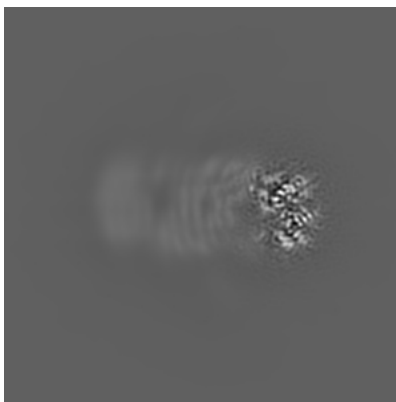
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

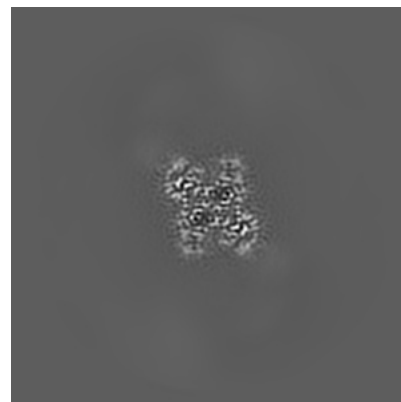
6.3.1 Primary map



X Index: 160

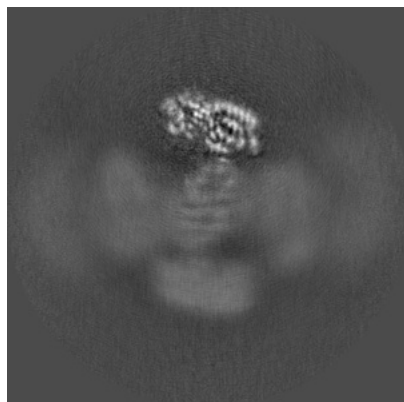


Y Index: 158

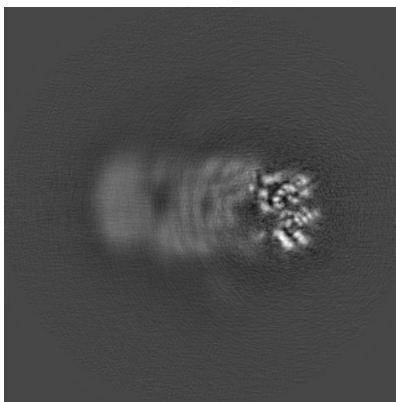


Z Index: 210

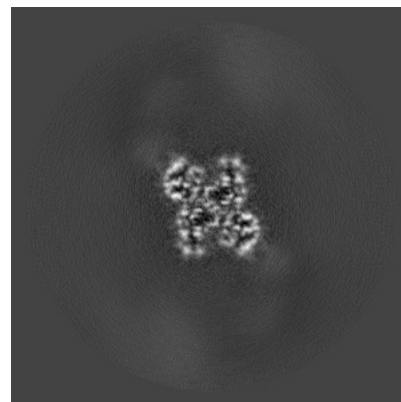
6.3.2 Raw map



X Index: 160



Y Index: 158



Z Index: 211

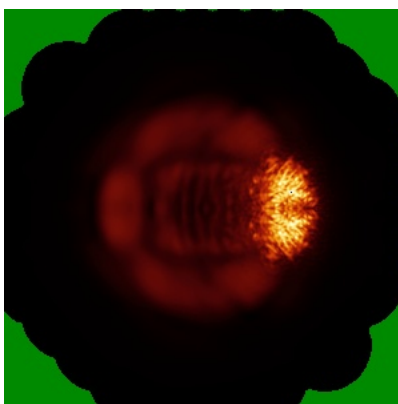
The images above show the largest variance slices of the map in three orthogonal directions.

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

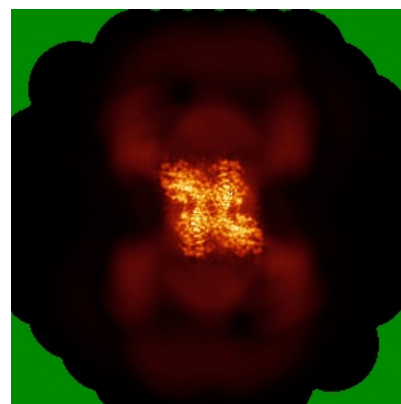
6.4.1 Primary map



X

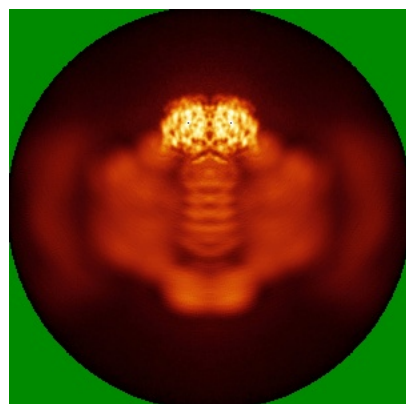


Y

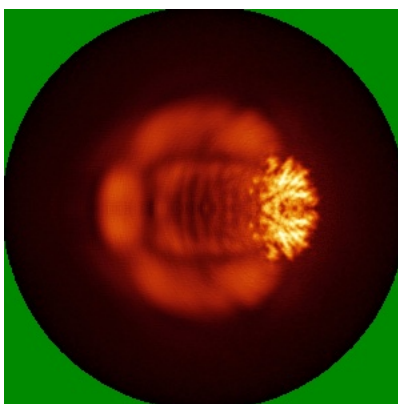


Z

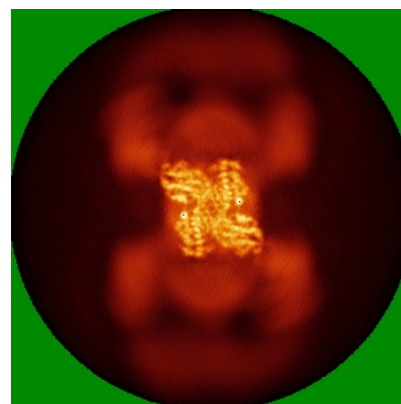
6.4.2 Raw map



X



Y

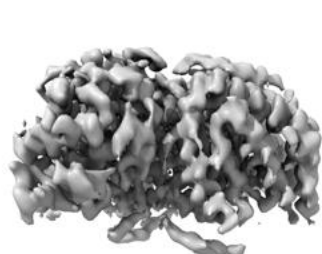


Z

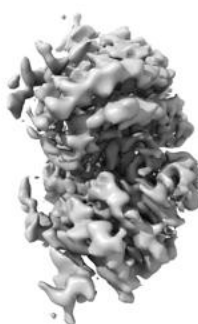
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

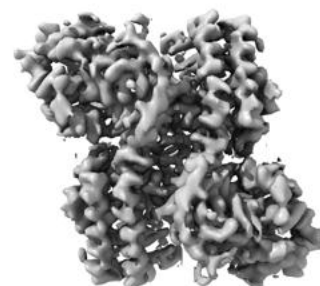
6.5.1 Primary map



X



Y



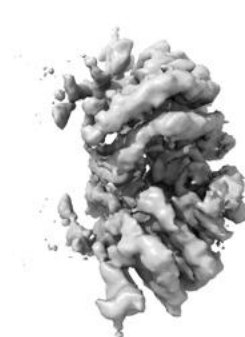
Z

The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

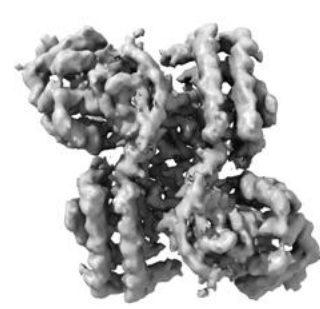
6.5.2 Raw map



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 shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

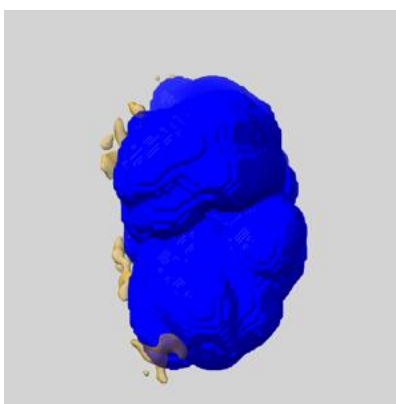
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

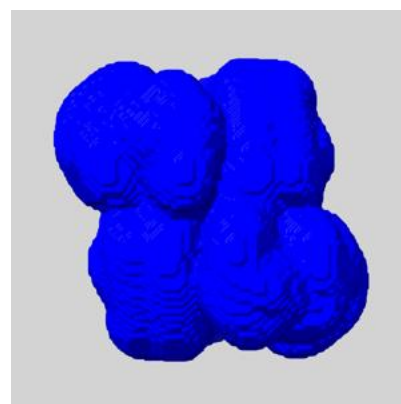
6.6.1 emd_32877_msk_1.map [i](#)



X



Y

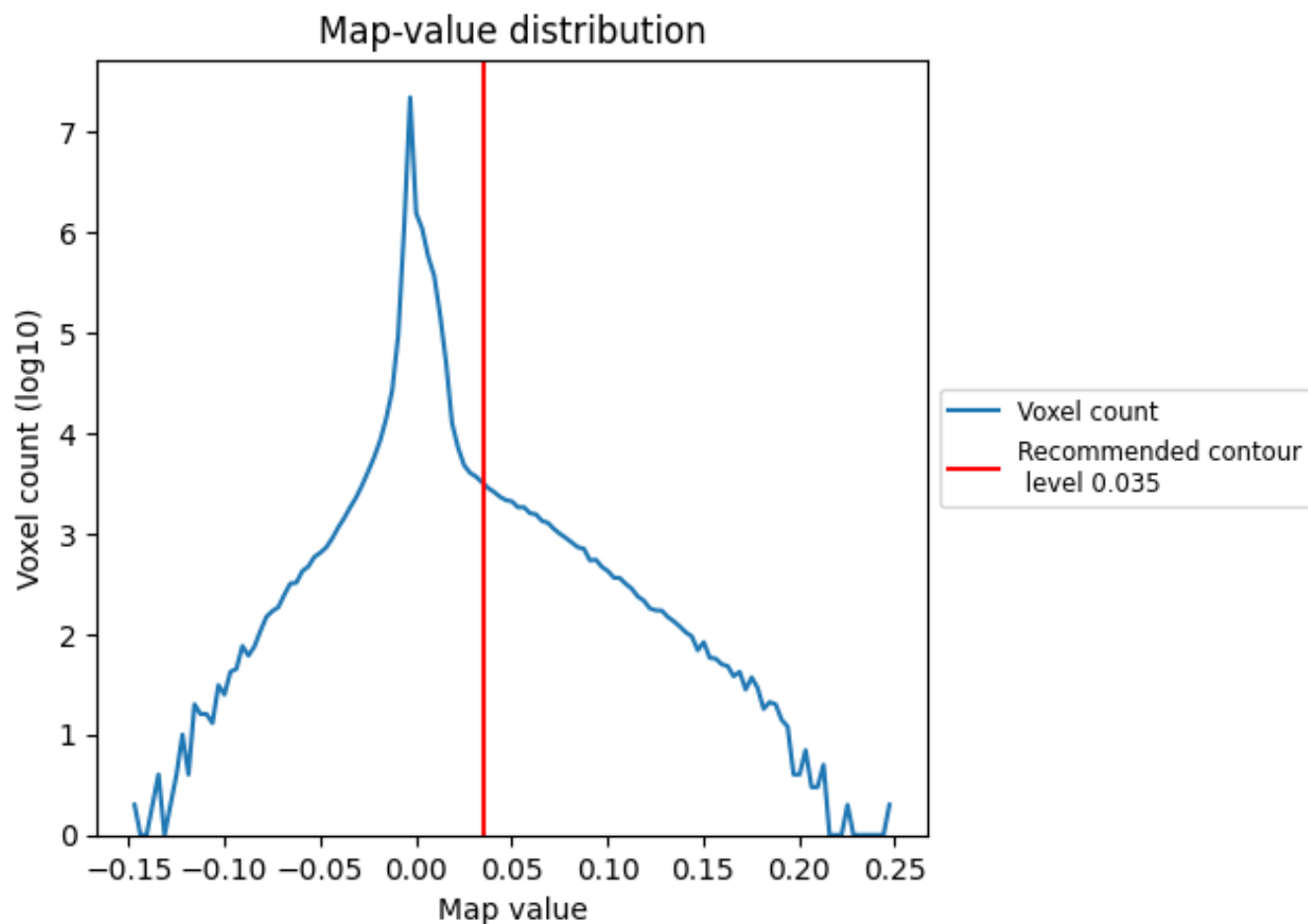


Z

7 Map analysis [i](#)

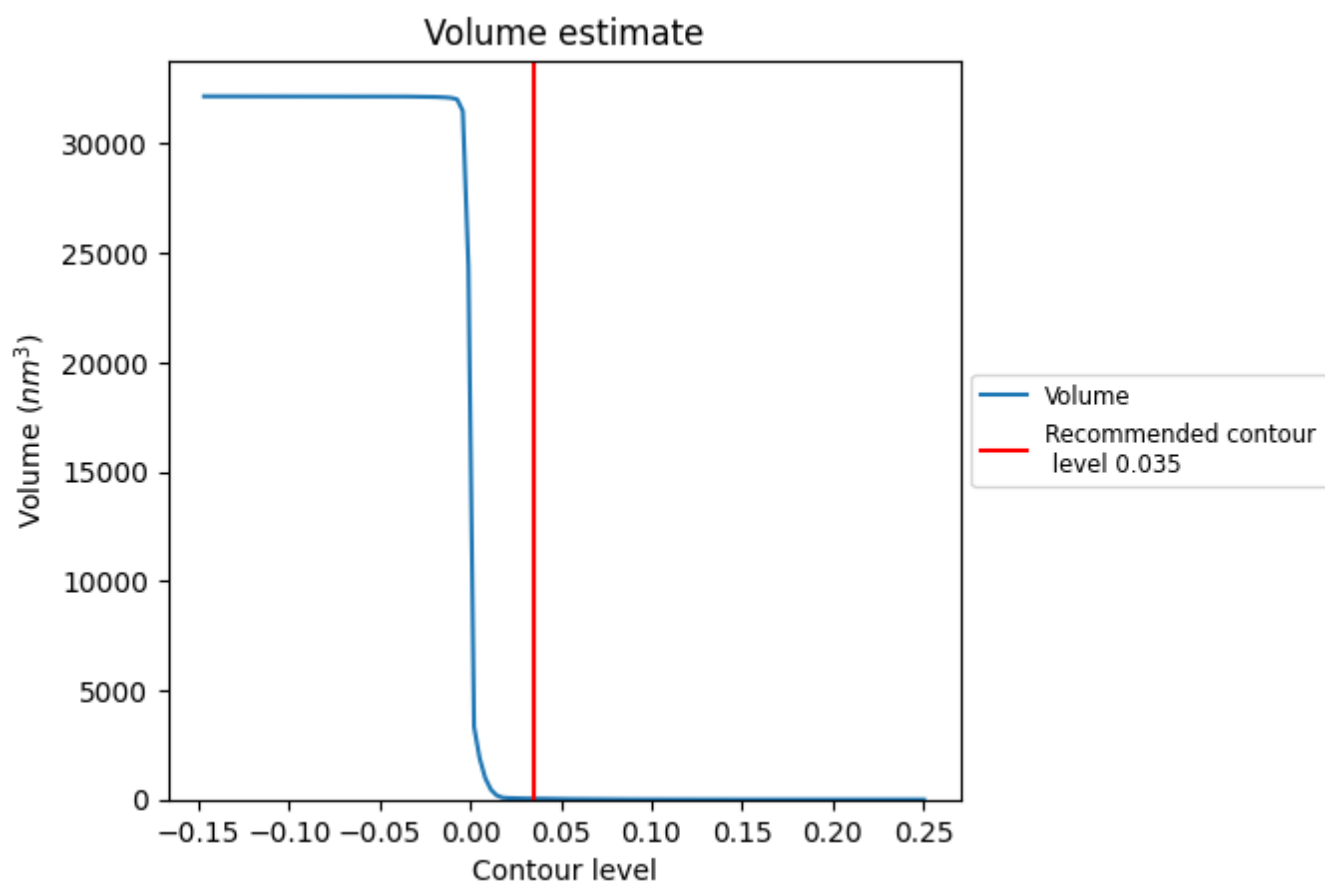
This section contains the results of statistical analysis of the map.

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.

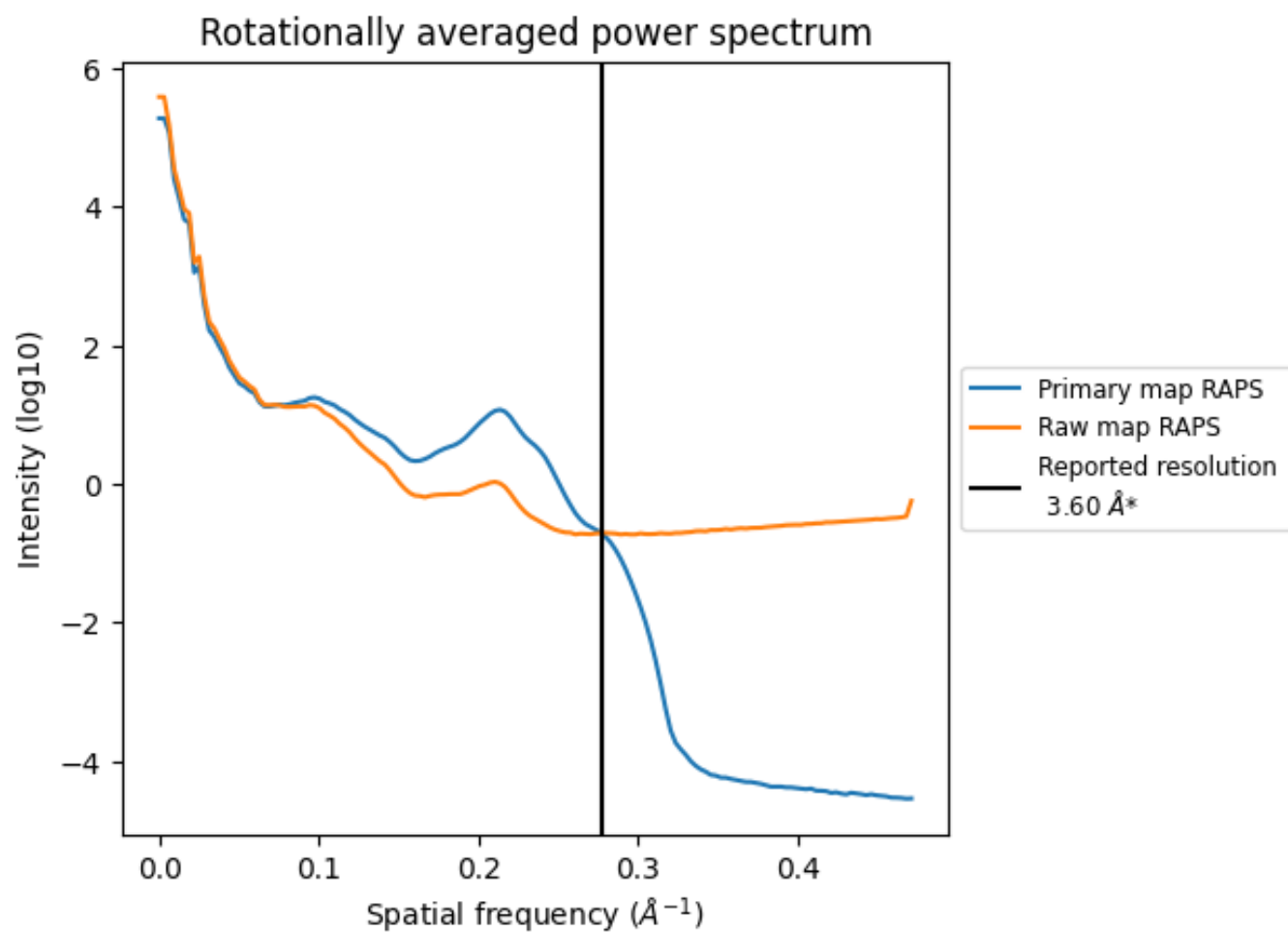
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 42 nm^3 ; this corresponds to an approximate mass of 38 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 ⓘ

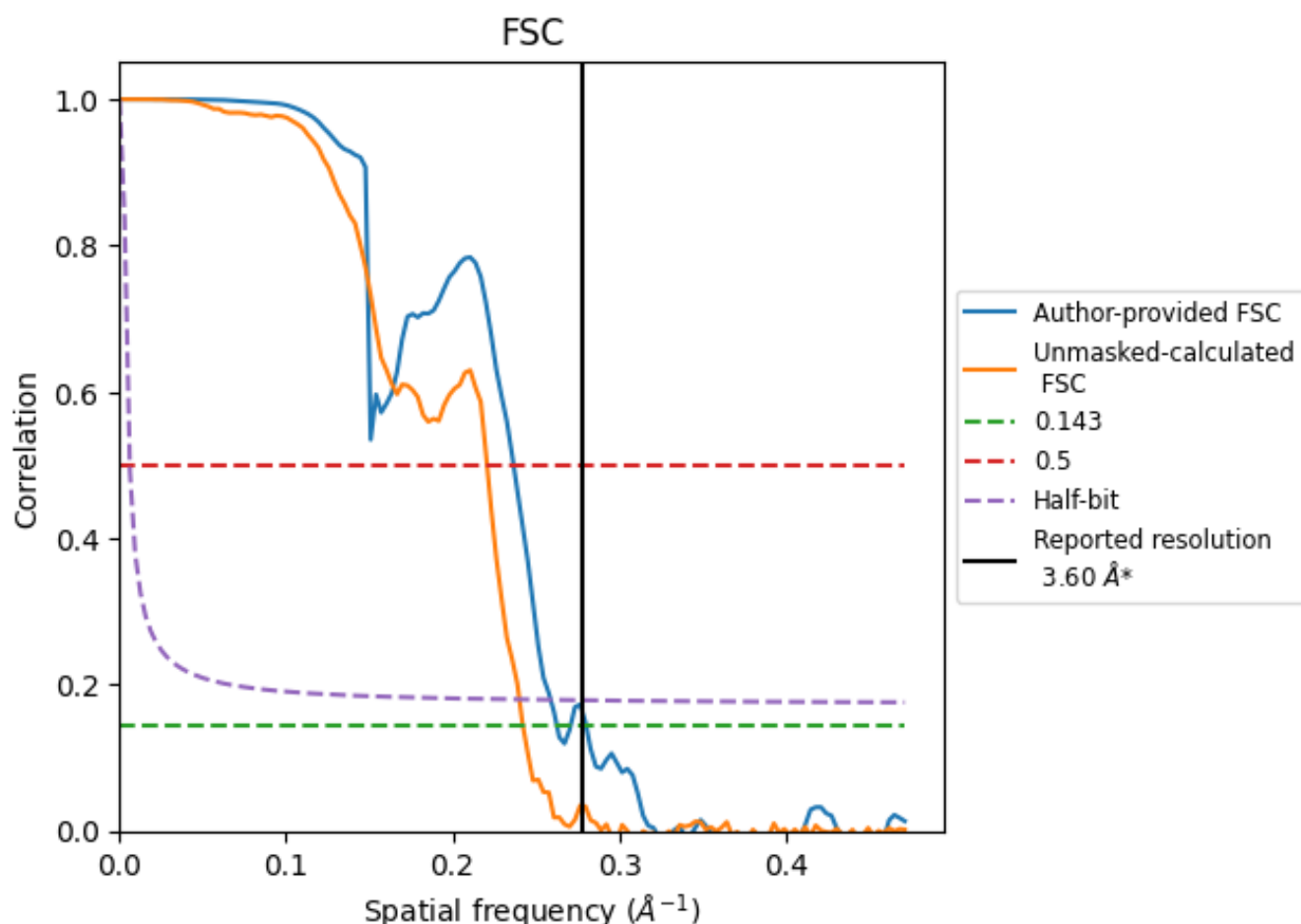


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

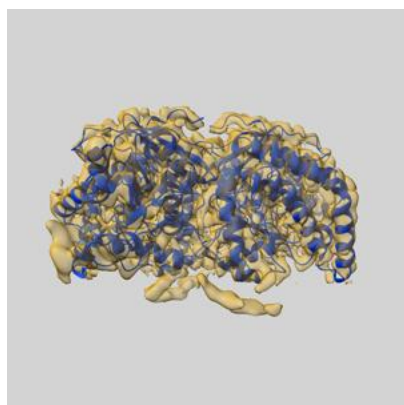
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.81	4.22	3.86
Unmasked-calculated*	4.13	4.53	4.16

*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 4.13 differs from the reported value 3.6 by more than 10 %

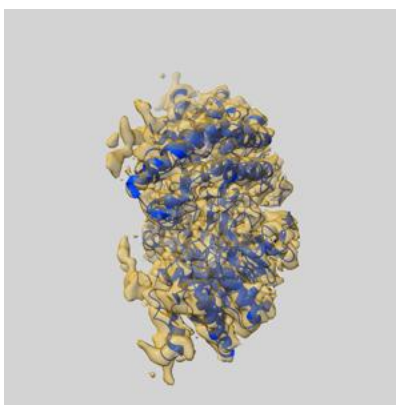
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32877 and PDB model 7WXF. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

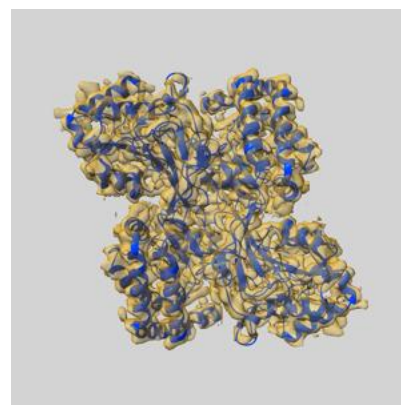
9.1 Map-model overlay [i](#)



X



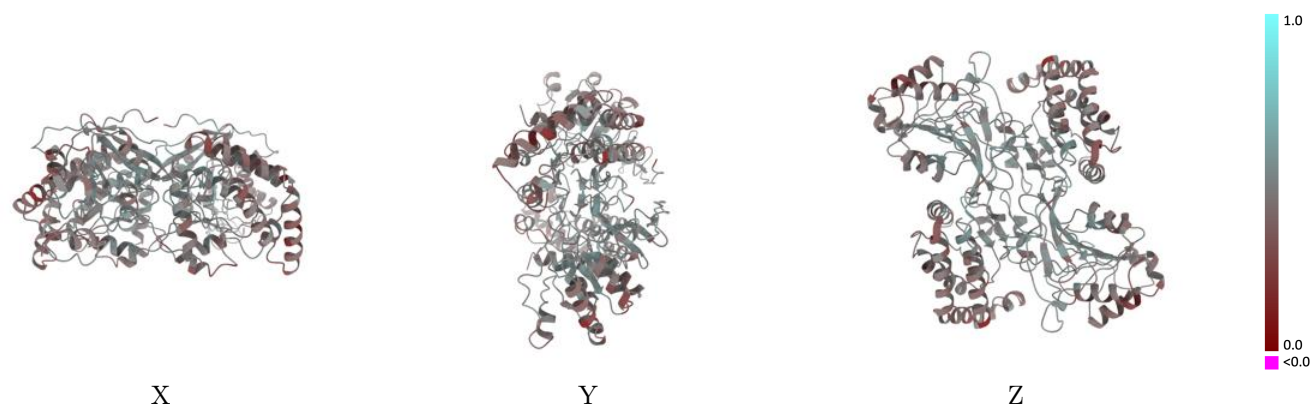
Y



Z

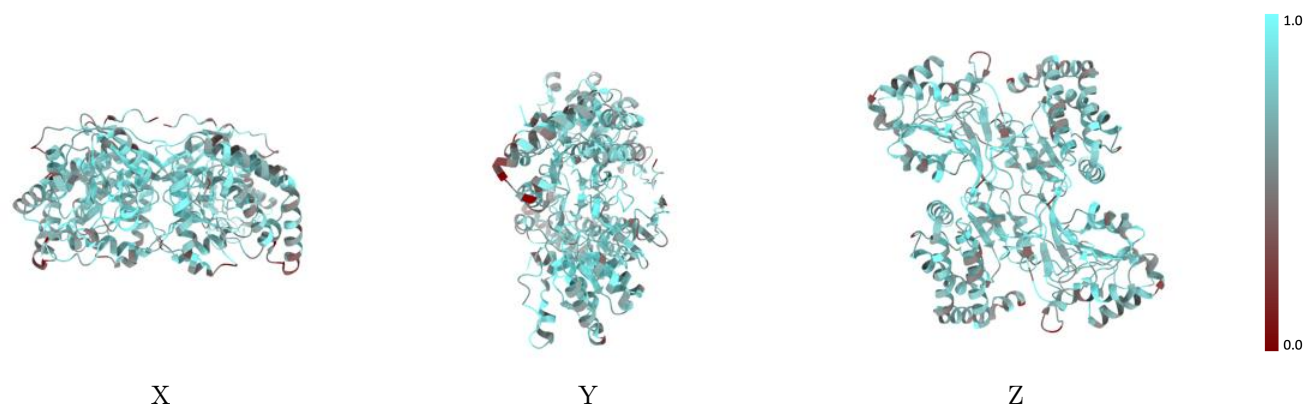
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



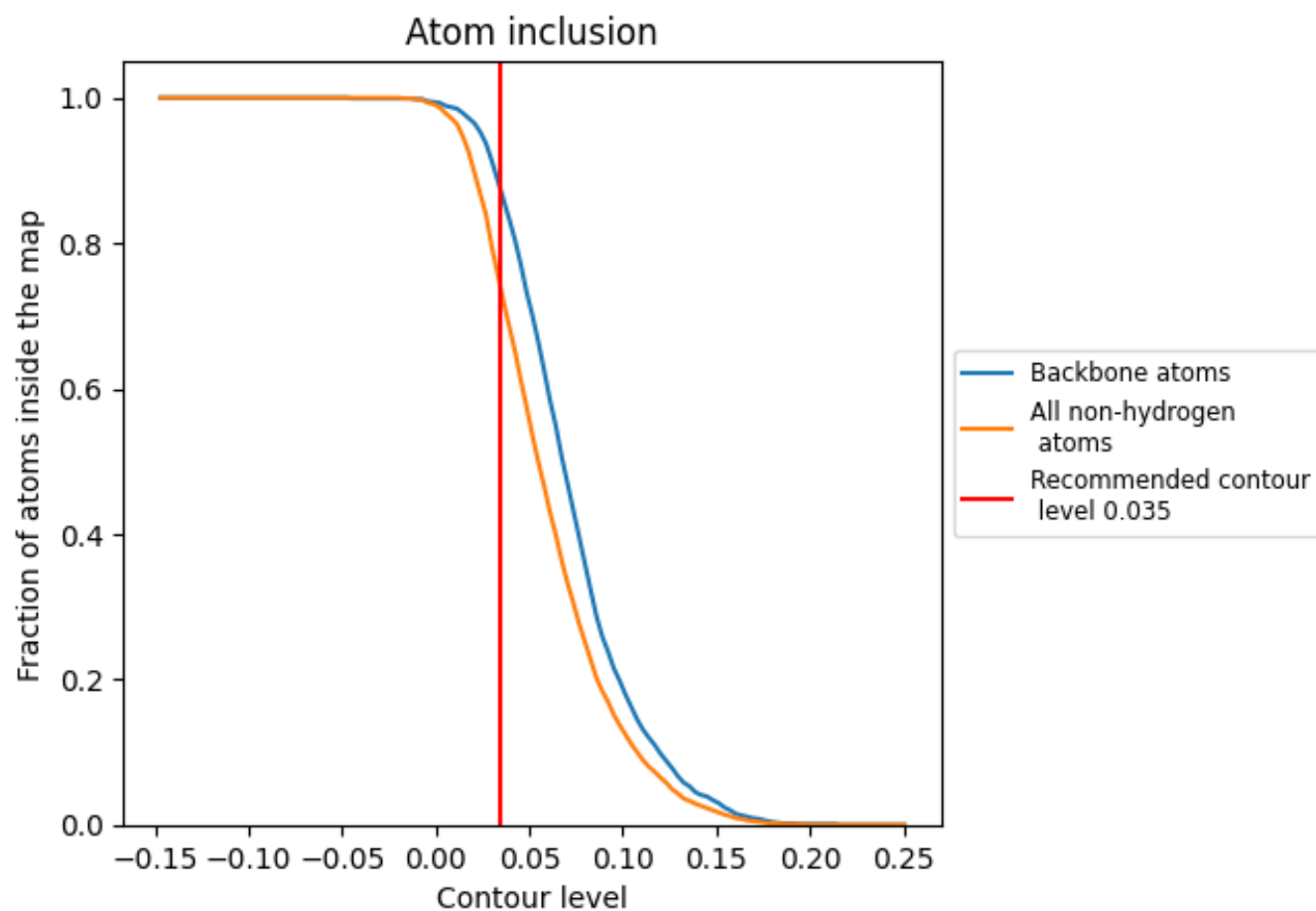
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 74% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7350	<div></div> 0.4570
A	<div></div> 0.7350	<div></div> 0.4560
B	<div></div> 0.7350	<div></div> 0.4580

