



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 12:35 AM UTC

PDB ID : 8POE / pdb_00008poe
EMDB ID : EMD-17789
Title : Structure of tissue-specific lipid scramblase ATG9B homotrimer, refined with C3 symmetry applied
Authors : Chiduza, G.N.; Pye, V.E.; Tooze, S.A.; Cherepanov, P.
Deposited on : 2023-07-04
Resolution : 4.20 Å(reported)
Based on initial model : .

This is a Full wwPDB EM Validation 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:

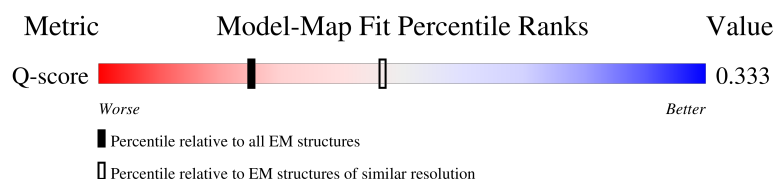
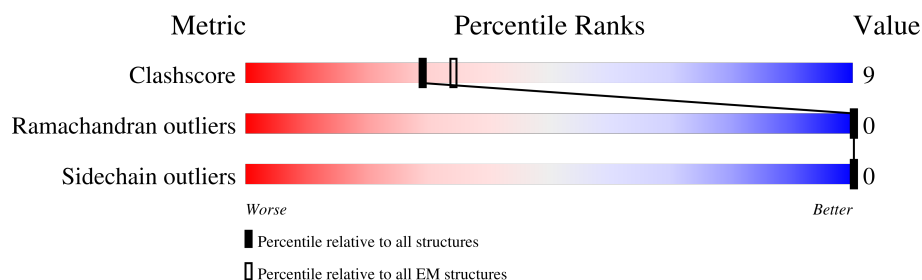
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 4.20 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	5410 (3.70 - 4.70)

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	960	 5% 37% 10% 52%
1	B	960	 5% 36% 12% 52%
1	C	960	 5% 36% 11% 52%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10947 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 Autophagy-related protein 9B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	457	Total	C	N	O	S	0	0
			3649	2395	643	601	10		
1	B	457	Total	C	N	O	S	0	0
			3649	2395	643	601	10		
1	C	457	Total	C	N	O	S	0	0
			3649	2395	643	601	10		

There are 111 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	ASP	-	expression tag	UNP Q674R7
A	-34	TYR	-	expression tag	UNP Q674R7
A	-33	LYS	-	expression tag	UNP Q674R7
A	-32	ASP	-	expression tag	UNP Q674R7
A	-31	ASP	-	expression tag	UNP Q674R7
A	-30	ASP	-	expression tag	UNP Q674R7
A	-29	ASP	-	expression tag	UNP Q674R7
A	-28	LYS	-	expression tag	UNP Q674R7
A	-27	ASP	-	expression tag	UNP Q674R7
A	-26	TYR	-	expression tag	UNP Q674R7
A	-25	LYS	-	expression tag	UNP Q674R7
A	-24	ASP	-	expression tag	UNP Q674R7
A	-23	ASP	-	expression tag	UNP Q674R7
A	-22	ASP	-	expression tag	UNP Q674R7
A	-21	ASP	-	expression tag	UNP Q674R7
A	-20	LYS	-	expression tag	UNP Q674R7
A	-19	ASP	-	expression tag	UNP Q674R7
A	-18	TYR	-	expression tag	UNP Q674R7
A	-17	LYS	-	expression tag	UNP Q674R7
A	-16	ASP	-	expression tag	UNP Q674R7
A	-15	ASP	-	expression tag	UNP Q674R7
A	-14	ASP	-	expression tag	UNP Q674R7
A	-13	ASP	-	expression tag	UNP Q674R7
A	-12	LYS	-	expression tag	UNP Q674R7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	HIS	-	expression tag	UNP Q674R7
A	-10	HIS	-	expression tag	UNP Q674R7
A	-9	HIS	-	expression tag	UNP Q674R7
A	-8	HIS	-	expression tag	UNP Q674R7
A	-7	HIS	-	expression tag	UNP Q674R7
A	-6	HIS	-	expression tag	UNP Q674R7
A	-5	GLU	-	expression tag	UNP Q674R7
A	-4	ASN	-	expression tag	UNP Q674R7
A	-3	LEU	-	expression tag	UNP Q674R7
A	-2	TYR	-	expression tag	UNP Q674R7
A	-1	PHE	-	expression tag	UNP Q674R7
A	0	GLN	-	expression tag	UNP Q674R7
A	1	GLY	-	expression tag	UNP Q674R7
B	-35	ASP	-	expression tag	UNP Q674R7
B	-34	TYR	-	expression tag	UNP Q674R7
B	-33	LYS	-	expression tag	UNP Q674R7
B	-32	ASP	-	expression tag	UNP Q674R7
B	-31	ASP	-	expression tag	UNP Q674R7
B	-30	ASP	-	expression tag	UNP Q674R7
B	-29	ASP	-	expression tag	UNP Q674R7
B	-28	LYS	-	expression tag	UNP Q674R7
B	-27	ASP	-	expression tag	UNP Q674R7
B	-26	TYR	-	expression tag	UNP Q674R7
B	-25	LYS	-	expression tag	UNP Q674R7
B	-24	ASP	-	expression tag	UNP Q674R7
B	-23	ASP	-	expression tag	UNP Q674R7
B	-22	ASP	-	expression tag	UNP Q674R7
B	-21	ASP	-	expression tag	UNP Q674R7
B	-20	LYS	-	expression tag	UNP Q674R7
B	-19	ASP	-	expression tag	UNP Q674R7
B	-18	TYR	-	expression tag	UNP Q674R7
B	-17	LYS	-	expression tag	UNP Q674R7
B	-16	ASP	-	expression tag	UNP Q674R7
B	-15	ASP	-	expression tag	UNP Q674R7
B	-14	ASP	-	expression tag	UNP Q674R7
B	-13	ASP	-	expression tag	UNP Q674R7
B	-12	LYS	-	expression tag	UNP Q674R7
B	-11	HIS	-	expression tag	UNP Q674R7
B	-10	HIS	-	expression tag	UNP Q674R7
B	-9	HIS	-	expression tag	UNP Q674R7
B	-8	HIS	-	expression tag	UNP Q674R7
B	-7	HIS	-	expression tag	UNP Q674R7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	expression tag	UNP Q674R7
B	-5	GLU	-	expression tag	UNP Q674R7
B	-4	ASN	-	expression tag	UNP Q674R7
B	-3	LEU	-	expression tag	UNP Q674R7
B	-2	TYR	-	expression tag	UNP Q674R7
B	-1	PHE	-	expression tag	UNP Q674R7
B	0	GLN	-	expression tag	UNP Q674R7
B	1	GLY	-	expression tag	UNP Q674R7
C	-35	ASP	-	expression tag	UNP Q674R7
C	-34	TYR	-	expression tag	UNP Q674R7
C	-33	LYS	-	expression tag	UNP Q674R7
C	-32	ASP	-	expression tag	UNP Q674R7
C	-31	ASP	-	expression tag	UNP Q674R7
C	-30	ASP	-	expression tag	UNP Q674R7
C	-29	ASP	-	expression tag	UNP Q674R7
C	-28	LYS	-	expression tag	UNP Q674R7
C	-27	ASP	-	expression tag	UNP Q674R7
C	-26	TYR	-	expression tag	UNP Q674R7
C	-25	LYS	-	expression tag	UNP Q674R7
C	-24	ASP	-	expression tag	UNP Q674R7
C	-23	ASP	-	expression tag	UNP Q674R7
C	-22	ASP	-	expression tag	UNP Q674R7
C	-21	ASP	-	expression tag	UNP Q674R7
C	-20	LYS	-	expression tag	UNP Q674R7
C	-19	ASP	-	expression tag	UNP Q674R7
C	-18	TYR	-	expression tag	UNP Q674R7
C	-17	LYS	-	expression tag	UNP Q674R7
C	-16	ASP	-	expression tag	UNP Q674R7
C	-15	ASP	-	expression tag	UNP Q674R7
C	-14	ASP	-	expression tag	UNP Q674R7
C	-13	ASP	-	expression tag	UNP Q674R7
C	-12	LYS	-	expression tag	UNP Q674R7
C	-11	HIS	-	expression tag	UNP Q674R7
C	-10	HIS	-	expression tag	UNP Q674R7
C	-9	HIS	-	expression tag	UNP Q674R7
C	-8	HIS	-	expression tag	UNP Q674R7
C	-7	HIS	-	expression tag	UNP Q674R7
C	-6	HIS	-	expression tag	UNP Q674R7
C	-5	GLU	-	expression tag	UNP Q674R7
C	-4	ASN	-	expression tag	UNP Q674R7
C	-3	LEU	-	expression tag	UNP Q674R7
C	-2	TYR	-	expression tag	UNP Q674R7

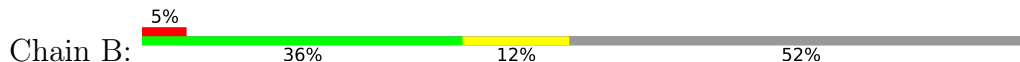
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	PHE	-	expression tag	UNP Q674R7
C	0	GLN	-	expression tag	UNP Q674R7
C	1	GLY	-	expression tag	UNP Q674R7

[illegible]

- Molecule 1: Autophagy-related protein 9B

[illegible][illegible]

GLN	SER	CYS	HIS	SER	ALA	LEU	PRO	PRO	ILE	PRO	ALA	ALA	THR	ALA	PRO	PRO	THR	GLN	GLN	ALA	ALA	PRO	ALA	THR	MET	THR	PRO	PRO	ALA	ALA	SER	SER	SER	THR	PRO	PRO	PRO	LEU	ALA	PRO	PRO	ALA	ALA	THR	THR	PRO	PRO	ASP	GLN	CYS	PRO	GLN	GLN	SER	PRO	PRO	LEU	GLY	VAL	ARG	LEU	GLY	PRO
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[illegible][illegible]

H318	P321	E322	V327	P328	V329	A330	E331	L337	Q340	R341	L345	R350	T353	E354	L355	D356	I357	R360	T361	L362	R363	V364	T365	R366	V367	L371	L377	P378	A379	G386	G387	S388	L403	L411	L418	P419	Y422	R423	R424	S425	D426	Q427	R428
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L431	A432	A433	R434	V435	G436	R437	T438	V439	L440	L441	L442	A443	L454	Q457	V461	H465	V466	E467	L468	L469	R470	R471	E472	P473	G474	A475	L476	G477	R483	L484	A485	L489	R490	L495	R502	R505	A511	A512	F513	L514	R515	T516	A517	L526	L527	Q530	L531
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L542 L543 L544 L545 L546 L547 L548 L549 L550 L551 L552 L553 L554 L555 L556 L557 L558 L559 L560 L561 L562 L563 L564 L565 L566 L567 L568 L569 L570 L571 L572 L573 L574 L575 L576 L577 L578 L579 L580 L581 L582 L583 L584 L585 L586 L587 L588 L589 L590 L591 L592 L593 L594 L595 L596 L597 L598 L599 L600 L601 L602 L603 L604 L605 L606 L607 L608 L609 L610 L611 L612 L613 L614 L615 L616 L617 L618 L619 L620 L621 L622 L623 L624 L625 L626 L627 L628 L629 L630 L631 L632 L633 L634 L635 L63

F640 F647 F653 D654 G665 D668 G670 G674 MET ASP VAL LYS ARG HTS GLY HTS PRO GLN TRP LEU SER ALA GLY GLN THR GLU ALA SER LEU SER SER GLN ARG ALA GLU ASP LYS THR LEU LEU LEU ARG PHE SER LEU ALA HTS PRO LEU TRP

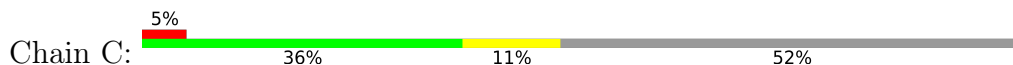
PRO	GLY	HIS	SER	SER	LYS	PHE	LEU	GLY	VAL	GLY	ASP	ALA	ALA	ALA	TRP	GLY	ALA	THR	SER	ALA	ARG	GLY	PRO	SER	THR	PRO	GLY	VAL	LEU	SER	ASN	CYS	THR	SER	PRO	PRO	PRO	GLU	PHE	VAL	HIS	PRO	LEU	LEU	PRO	PRO	PRO
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ASP	LEU	SER	PRO	THR	ALA	PRO	CYS	PRO	ALA	ALA	ALA	THR	ALA	SER	SER	ARG	ILE	ILE	ALA	GLN	ASP	PRO	PRO	SER	SER	VAL	SER	GLY	GLY	THR	GLY	GLY	GLN	LYS	LEU	LEU	ALA	ALA	GLN	LEU	PRO	PRO	GLU	LEU	LEU	SER	SER	ALA	SER	ALA	ALA	GLU	MET	HIS	VAL	ILE	TYR	HIS	LEU	LEU	HIS	FIN
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[illegible]

ASN	LEU	PHE	PRO	GLY	GLY	PHE	GLN	VAL	THR	THR	ASP	THR	GLN	LYS	GLU	PRO	ASP	ARG	ALA	SER	CYS	THR	ASP
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- Molecule 1: Autophagy-related protein 9B



WORLDWIDE
PDB
PROTEIN DATA BANK



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	104050	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	46296	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.950	Depositor
Minimum map value	-2.855	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.076	Depositor
Recommended contour level	0.46	Depositor
Map size (Å)	302.40002, 302.40002, 302.40002	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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	0.13	0/3745	0.34	0/5102
1	B	0.14	0/3745	0.35	0/5102
1	C	0.14	0/3745	0.36	0/5102
All	All	0.14	0/11235	0.35	0/15306

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	3649	0	3736	67	0
1	B	3649	0	3736	80	0
1	C	3649	0	3736	67	0
All	All	10947	0	11208	207	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 9.

All (207) 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:217:PHE:HB3	1:B:530:GLN:HE21	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:LEU:HD21	1:B:435:TRP:HE1	1.52	0.72
1:C:363:ARG:NH1	1:C:668:ASP:OD1	2.27	0.68
1:B:363:ARG:NH1	1:B:668:ASP:OD1	2.27	0.67
1:C:313:TYR:HE1	1:C:317:LEU:HD22	1.59	0.67
1:C:403:LEU:HD11	1:C:439:VAL:HG12	1.78	0.66
1:A:354:GLU:OE2	1:A:354:GLU:N	2.30	0.65
1:C:399:ASN:OD1	1:C:446:ASN:ND2	2.29	0.65
1:B:221:GLN:O	1:B:225:ILE:HD12	1.96	0.65
1:B:601:PRO:HG2	1:B:619:LEU:HD21	1.78	0.65
1:A:399:ASN:OD1	1:A:446:ASN:ND2	2.30	0.65
1:B:542:LEU:HD11	1:B:558:VAL:HG13	1.79	0.64
1:A:403:LEU:HD21	1:A:435:TRP:HE1	1.63	0.64
1:A:363:ARG:NH1	1:A:668:ASP:OD1	2.31	0.64
1:B:403:LEU:HD11	1:B:439:VAL:HG12	1.80	0.63
1:A:542:LEU:HD11	1:A:558:VAL:HG13	1.80	0.62
1:B:276:ARG:O	1:B:276:ARG:NH1	2.29	0.62
1:C:461:VAL:HG11	1:C:631:LEU:HD13	1.82	0.62
1:B:354:GLU:N	1:B:354:GLU:OE2	2.30	0.61
1:C:221:GLN:O	1:C:225:ILE:HD12	2.01	0.61
1:A:491:HIS:HE1	1:A:502:ARG:CZ	2.14	0.60
1:B:362:LEU:O	1:B:366:ASN:ND2	2.33	0.60
1:A:362:LEU:O	1:A:366:ASN:ND2	2.33	0.60
1:B:234:ARG:HH21	1:B:274:ARG:HE	1.50	0.59
1:A:313:TYR:HE1	1:A:317:LEU:HD12	1.68	0.59
1:B:489:LEU:HD21	1:B:597:MET:HE3	1.84	0.59
1:A:530:GLN:OE1	1:C:217:PHE:HB3	2.03	0.58
1:A:601:PRO:HG2	1:A:619:LEU:HD11	1.84	0.58
1:B:594:LEU:HA	1:B:597:MET:HB3	1.85	0.58
1:A:360:ARG:NH2	1:A:665:GLY:O	2.37	0.58
1:B:234:ARG:HD3	1:B:275:ILE:HA	1.86	0.58
1:A:337:LEU:O	1:A:341:ARG:HG2	2.04	0.57
1:B:360:ARG:NH2	1:B:665:GLY:O	2.38	0.57
1:C:234:ARG:HD3	1:C:275:ILE:HA	1.85	0.56
1:A:327:VAL:HG12	1:A:329:TRP:H	1.70	0.56
1:B:418:LEU:HD12	1:B:419:PRO:HD2	1.88	0.56
1:A:491:HIS:CE1	1:A:502:ARG:CZ	2.89	0.56
1:C:360:ARG:NH2	1:C:665:GLY:O	2.39	0.56
1:B:403:LEU:HD21	1:B:435:TRP:NE1	2.21	0.55
1:A:217:PHE:HB3	1:B:530:GLN:NE2	2.19	0.55
1:A:296:LEU:O	1:A:300:VAL:HG23	2.07	0.55
1:B:337:LEU:O	1:B:341:ARG:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:PRO:O	1:B:477:GLY:N	2.40	0.55
1:C:266:LEU:HD12	1:C:270:GLN:HG2	1.87	0.55
1:C:422:TYR:HE1	1:C:431:LEU:HD22	1.72	0.55
1:C:234:ARG:HE	1:C:274:ARG:HE	1.55	0.55
1:C:213:LEU:O	1:C:217:PHE:HD2	1.89	0.55
1:A:354:GLU:HA	1:A:357:ILE:HD12	1.89	0.55
1:B:327:VAL:HG12	1:B:329:TRP:H	1.72	0.55
1:A:403:LEU:HD11	1:A:439:VAL:HG12	1.89	0.54
1:B:215:ASP:OD2	1:B:299:SER:HB2	2.07	0.54
1:C:479:ARG:HH21	1:C:514:LEU:HD11	1.72	0.54
1:C:594:LEU:HA	1:C:597:MET:HB2	1.89	0.54
1:C:517:ALA:HB2	1:C:586:PRO:HB3	1.91	0.53
1:C:337:LEU:O	1:C:341:ARG:HG2	2.09	0.53
1:B:313:TYR:HE1	1:B:317:LEU:HD12	1.74	0.53
1:C:306:TYR:HA	1:C:309:ILE:HG22	1.91	0.52
1:B:517:ALA:HB2	1:B:586:PRO:HB3	1.91	0.52
1:A:403:LEU:HD21	1:A:435:TRP:NE1	2.24	0.52
1:C:649:ALA:O	1:C:653:ILE:HG12	2.09	0.52
1:C:350:ARG:NH1	1:C:351:PRO:O	2.40	0.51
1:B:314:ARG:HD3	1:B:318:HIS:HA	1.92	0.51
1:C:218:GLN:O	1:C:221:GLN:HB3	2.10	0.51
1:A:479:ARG:HB3	1:A:620:LEU:HD21	1.93	0.51
1:A:461:VAL:HG11	1:A:631:LEU:HD13	1.93	0.50
1:C:260:THR:HG22	1:C:262:SER:H	1.76	0.50
1:A:314:ARG:NH2	1:A:321:PRO:HD3	2.27	0.50
1:A:367:TYR:CE1	1:A:670:CYS:HB3	2.46	0.50
1:B:217:PHE:HD1	1:C:530:GLN:HG3	1.76	0.50
1:A:422:TYR:HE1	1:A:431:LEU:HD22	1.77	0.50
1:A:573:ARG:HD2	1:C:471:ARG:HD3	1.94	0.50
1:B:426:ASP:OD1	1:B:427:GLN:N	2.45	0.50
1:B:426:ASP:OD1	1:B:427:GLN:HG3	2.13	0.49
1:B:511:ALA:O	1:B:515:ARG:HG2	2.12	0.49
1:C:540:ALA:O	1:C:544:VAL:HG12	2.13	0.49
1:B:422:TYR:CE1	1:B:431:LEU:HD22	2.48	0.49
1:B:461:VAL:HG11	1:B:631:LEU:HD13	1.95	0.49
1:B:594:LEU:HD13	1:B:597:MET:HB3	1.95	0.49
1:B:350:ARG:NH1	1:B:356:ASP:OD2	2.46	0.48
1:C:501:ALA:O	1:C:505:ARG:HG3	2.13	0.48
1:B:422:TYR:HE1	1:B:431:LEU:HD22	1.78	0.48
1:A:215:ASP:OD1	1:A:299:SER:HB2	2.14	0.48
1:A:454:LEU:O	1:A:458:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:ARG:HH12	1:B:321:PRO:HD3	1.77	0.48
1:A:362:LEU:HD21	1:A:495:LEU:HD23	1.96	0.48
1:A:517:ALA:HB2	1:A:586:PRO:HB3	1.96	0.48
1:B:260:THR:HG22	1:B:262:SER:H	1.79	0.48
1:B:362:LEU:HD21	1:B:495:LEU:HD23	1.94	0.48
1:C:376:LEU:HD13	1:C:652:ILE:HG12	1.96	0.47
1:A:260:THR:HG22	1:A:262:SER:H	1.80	0.47
1:A:422:TYR:CE1	1:A:431:LEU:HD22	2.50	0.47
1:C:570:THR:HA	1:C:573:ARG:HG2	1.96	0.47
1:A:204:GLN:NE2	1:A:497:HIS:HB3	2.28	0.47
1:C:454:LEU:O	1:C:458:VAL:HG23	2.15	0.47
1:B:570:THR:HA	1:B:573:ARG:HG2	1.97	0.47
1:C:367:TYR:CE1	1:C:670:CYS:HB3	2.50	0.46
1:B:502:ARG:HG2	1:B:505:ARG:NH2	2.31	0.46
1:C:422:TYR:CE1	1:C:431:LEU:HD22	2.49	0.46
1:A:458:VAL:HG22	1:A:631:LEU:HD11	1.98	0.46
1:A:218:GLN:O	1:A:221:GLN:HB3	2.15	0.46
1:C:511:ALA:O	1:C:515:ARG:HG2	2.15	0.46
1:B:223:ILE:HA	1:B:226:VAL:HG12	1.97	0.46
1:B:371:LEU:HD23	1:B:377:LEU:HD21	1.98	0.46
1:C:543:LEU:O	1:C:547:VAL:HG23	2.16	0.46
1:C:205:ARG:HH11	1:C:211:ILE:HG12	1.81	0.46
1:C:213:LEU:O	1:C:217:PHE:CD2	2.68	0.46
1:C:473:PRO:O	1:C:477:GLY:N	2.46	0.46
1:A:196:PHE:HB3	1:A:361:ILE:HD11	1.99	0.45
1:B:196:PHE:HB3	1:B:361:ILE:HD11	1.99	0.45
1:C:215:ASP:OD2	1:C:299:SER:HB2	2.17	0.45
1:C:552:VAL:HG12	1:C:554:ALA:H	1.82	0.45
1:B:367:TYR:CE1	1:B:670:CYS:HB3	2.51	0.45
1:C:481:TRP:CD2	1:C:503:LEU:HD23	2.52	0.45
1:B:483:ARG:NH2	1:B:630:GLU:OE2	2.48	0.45
1:A:471:ARG:HD3	1:B:573:ARG:HD2	1.99	0.44
1:B:365:THR:HB	1:B:490:ARG:HH12	1.82	0.44
1:A:314:ARG:HH22	1:A:321:PRO:HD3	1.81	0.44
1:B:283:LEU:HA	1:B:286:VAL:HG12	1.99	0.44
1:A:200:TYR:CE1	1:A:204:GLN:HG3	2.51	0.44
1:B:221:GLN:HG3	1:B:225:ILE:HD11	1.99	0.44
1:B:428:ARG:NH2	1:B:654:ASP:OD2	2.50	0.44
1:C:296:LEU:O	1:C:300:VAL:HG23	2.18	0.44
1:B:433:ALA:O	1:B:437:ARG:HG2	2.17	0.44
1:C:391:PHE:HZ	1:C:633:SER:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:484:LEU:HG	1:C:488:GLN:OE1	2.17	0.44
1:A:203:HIS:CG	1:A:329:TRP:HD1	2.35	0.44
1:B:196:PHE:CD2	1:B:357:ILE:HG23	2.53	0.44
1:B:411:LEU:HD22	1:B:422:TYR:CE2	2.52	0.44
1:B:485:ALA:O	1:B:489:LEU:HB2	2.18	0.44
1:A:597:MET:O	1:A:599:TYR:N	2.50	0.44
1:C:470:ARG:NH2	1:C:471:ARG:HG2	2.33	0.44
1:C:614:ARG:HA	1:C:614:ARG:HD2	1.77	0.44
1:A:283:LEU:HA	1:A:286:VAL:HG12	2.00	0.43
1:A:552:VAL:HG12	1:A:554:ALA:H	1.83	0.43
1:B:315:GLU:O	1:B:318:HIS:NE2	2.51	0.43
1:A:470:ARG:NH2	1:A:471:ARG:HG2	2.32	0.43
1:A:220:GLY:HA2	1:A:223:ILE:HG22	2.00	0.43
1:A:222:PHE:HA	1:A:225:ILE:HD12	2.00	0.43
1:A:261:LEU:O	1:A:265:ILE:HG12	2.18	0.43
1:A:473:PRO:O	1:A:477:GLY:N	2.44	0.43
1:B:269:ALA:O	1:B:273:GLU:OE1	2.37	0.43
1:B:377:LEU:HB2	1:B:378:PRO:HD3	1.99	0.43
1:C:418:LEU:HD12	1:C:419:PRO:HD2	2.00	0.43
1:A:614:ARG:HA	1:A:614:ARG:HD2	1.73	0.43
1:B:314:ARG:HH22	1:B:321:PRO:HD3	1.84	0.43
1:A:438:THR:O	1:A:441:LEU:HG	2.19	0.43
1:A:649:ALA:O	1:A:653:ILE:HG12	2.19	0.43
1:A:196:PHE:O	1:A:199:ILE:HG22	2.19	0.43
1:A:526:LEU:HD23	1:C:213:LEU:HD11	2.00	0.43
1:A:555:VAL:HG21	1:A:558:VAL:HB	2.01	0.43
1:C:203:HIS:CG	1:C:329:TRP:HD1	2.37	0.43
1:C:438:THR:O	1:C:441:LEU:HG	2.19	0.43
1:B:438:THR:O	1:B:441:LEU:HG	2.18	0.43
1:B:614:ARG:HA	1:B:614:ARG:HD2	1.81	0.43
1:A:371:LEU:HD23	1:A:377:LEU:HD21	2.01	0.42
1:C:315:GLU:O	1:C:318:HIS:NE2	2.52	0.42
1:B:234:ARG:HA	1:B:234:ARG:HE	1.84	0.42
1:C:457:GLN:O	1:C:461:VAL:HG12	2.19	0.42
1:A:196:PHE:CD2	1:A:357:ILE:HG23	2.54	0.42
1:B:526:LEU:O	1:B:530:GLN:HG2	2.19	0.42
1:B:527:LEU:O	1:B:531:LEU:HD23	2.19	0.42
1:C:221:GLN:NE2	1:C:225:ILE:HD11	2.35	0.42
1:C:269:ALA:O	1:C:273:GLU:OE1	2.37	0.42
1:B:379:ALA:HB1	1:B:640:PHE:CE2	2.54	0.42
1:B:205:ARG:HH11	1:B:211:ILE:HG12	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:ARG:HG3	1:B:364:TYR:N	2.34	0.42
1:C:261:LEU:O	1:C:265:ILE:HG12	2.19	0.42
1:C:361:ILE:HG22	1:C:362:LEU:HD22	2.02	0.42
1:C:458:VAL:HG22	1:C:631:LEU:HD11	2.01	0.42
1:A:434:ARG:O	1:A:438:THR:HG23	2.20	0.42
1:C:220:GLY:O	1:C:223:ILE:HG22	2.20	0.42
1:B:552:VAL:HG12	1:B:554:ALA:H	1.85	0.42
1:C:283:LEU:HA	1:C:286:VAL:HG12	2.01	0.42
1:B:543:LEU:O	1:B:547:VAL:HG23	2.20	0.42
1:A:269:ALA:O	1:A:273:GLU:OE1	2.37	0.41
1:A:418:LEU:HD12	1:A:419:PRO:HD2	2.02	0.41
1:C:394:ARG:HG3	1:C:483:ARG:NH2	2.35	0.41
1:A:363:ARG:HG3	1:A:364:TYR:N	2.35	0.41
1:A:457:GLN:O	1:A:461:VAL:HG12	2.20	0.41
1:B:196:PHE:O	1:B:199:ILE:HG22	2.19	0.41
1:B:513:PHE:HB2	1:B:589:LEU:HB3	2.03	0.41
1:C:196:PHE:HB3	1:C:361:ILE:HD11	2.02	0.41
1:B:313:TYR:CE1	1:B:317:LEU:HD12	2.55	0.41
1:A:350:ARG:HD2	1:A:351:PRO:O	2.21	0.41
1:A:372:ALA:HB2	1:A:377:LEU:HD12	2.01	0.41
1:B:213:LEU:HA	1:B:216:VAL:HG12	2.02	0.41
1:C:196:PHE:O	1:C:199:ILE:HG22	2.20	0.41
1:C:529:ARG:HE	1:C:576:ILE:HD11	1.86	0.41
1:A:315:GLU:O	1:A:318:HIS:NE2	2.54	0.41
1:B:435:TRP:CE3	1:B:653:ILE:HD11	2.56	0.41
1:A:204:GLN:HE22	1:A:497:HIS:HB3	1.86	0.41
1:B:354:GLU:HA	1:B:357:ILE:HD12	2.03	0.41
1:B:457:GLN:O	1:B:461:VAL:HG12	2.20	0.41
1:B:566:GLY:O	1:B:570:THR:HG23	2.20	0.41
1:A:306:TYR:HA	1:A:309:ILE:HD12	2.02	0.41
1:B:470:ARG:NH2	1:B:471:ARG:HG2	2.35	0.41
1:A:290:GLY:O	1:A:293:LEU:HG	2.21	0.40
1:B:513:PHE:CE1	1:B:590:LEU:HB2	2.56	0.40
1:C:426:ASP:OD2	1:C:427:GLN:HG3	2.21	0.40
1:B:350:ARG:NH2	1:B:353:THR:OG1	2.49	0.40
1:C:481:TRP:CZ3	1:C:620:LEU:HD12	2.56	0.40
1:C:513:PHE:HB2	1:C:589:LEU:HB3	2.03	0.40
1:C:527:LEU:O	1:C:531:LEU:HD23	2.22	0.40
1:B:422:TYR:CD1	1:B:431:LEU:HD13	2.56	0.40
1:C:234:ARG:HH21	1:C:274:ARG:HE	1.68	0.40
1:B:470:ARG:CZ	1:B:471:ARG:HG2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:LEU:HD22	1:C:422:TYR:OH	2.22	0.40

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	447/960 (47%)	433 (97%)	14 (3%)	0	100	100
1	B	447/960 (47%)	435 (97%)	12 (3%)	0	100	100
1	C	447/960 (47%)	435 (97%)	12 (3%)	0	100	100
All	All	1341/2880 (47%)	1303 (97%)	38 (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	379/801 (47%)	379 (100%)	0	100	100
1	B	379/801 (47%)	379 (100%)	0	100	100
1	C	379/801 (47%)	379 (100%)	0	100	100
All	All	1137/2403 (47%)	1137 (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 (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	333	GLN
1	A	366	ASN
1	A	399	ASN
1	A	446	ASN
1	A	557	HIS
1	A	596	HIS
1	A	658	HIS
1	B	366	ASN
1	B	530	GLN
1	B	557	HIS
1	C	221	GLN
1	C	557	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 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.

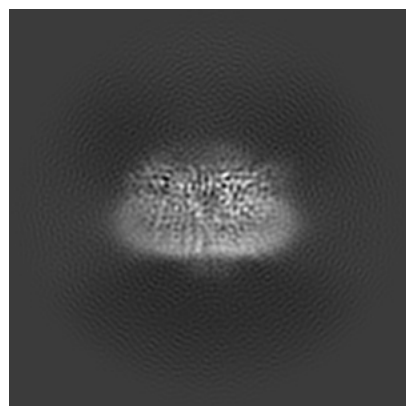
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17789. These allow visual inspection of the internal detail of the map and identification of artifacts.

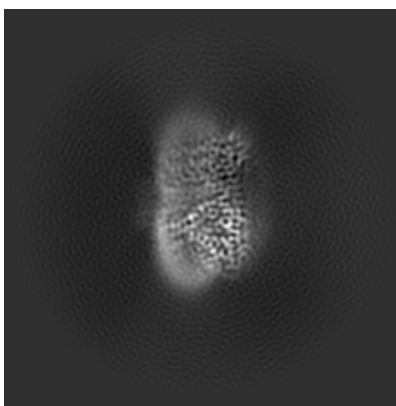
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

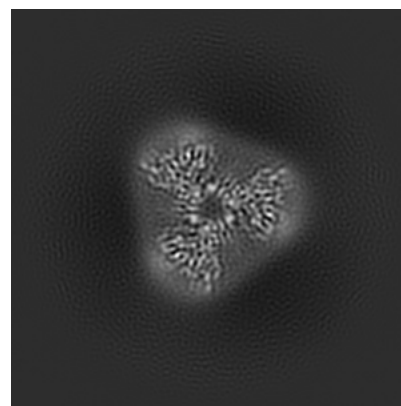
6.1.1 Primary map



X

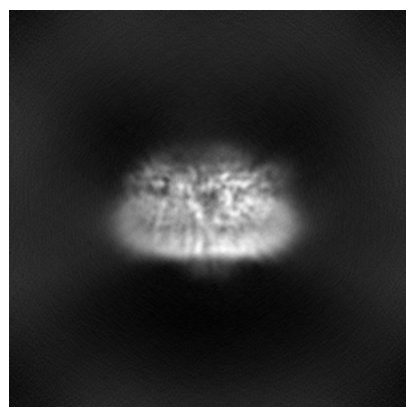


Y

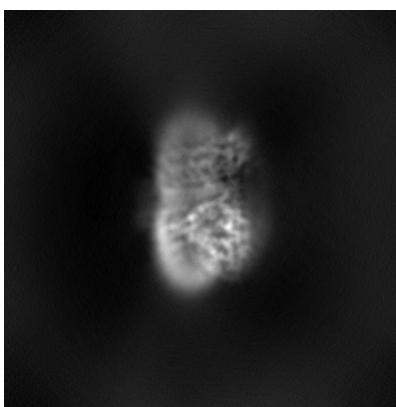


Z

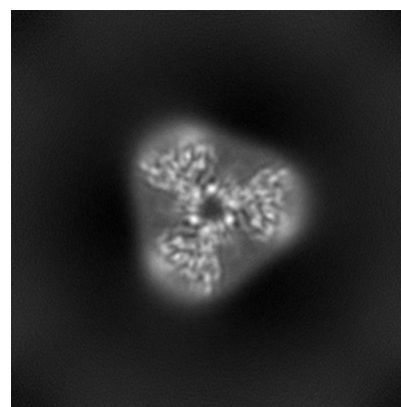
6.1.2 Raw map



X



Y

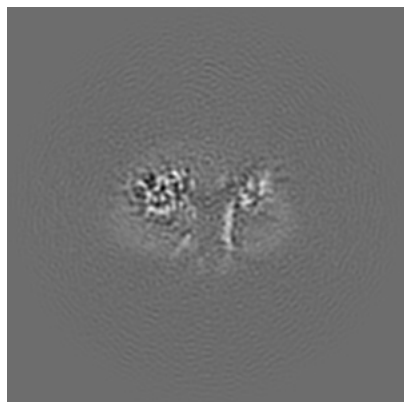


Z

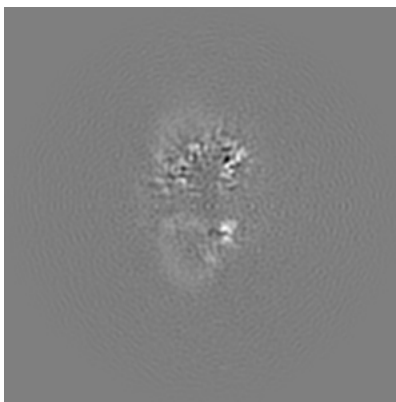
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

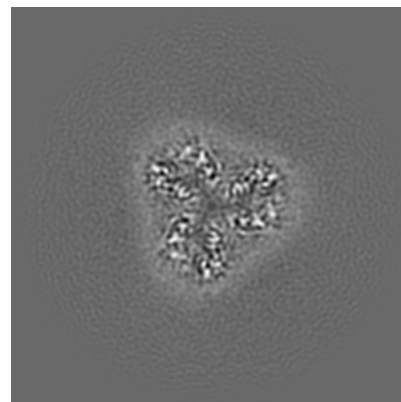
6.2.1 Primary map



X Index: 140

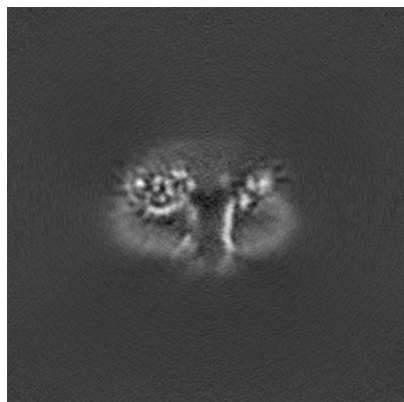


Y Index: 140

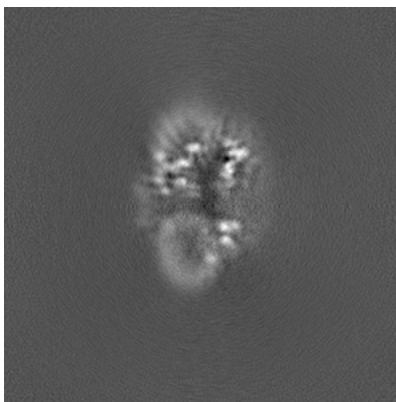


Z Index: 140

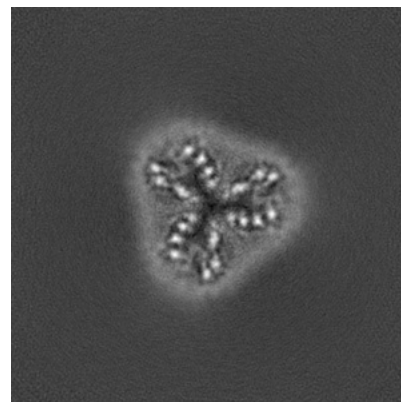
6.2.2 Raw map



X Index: 140



Y Index: 140

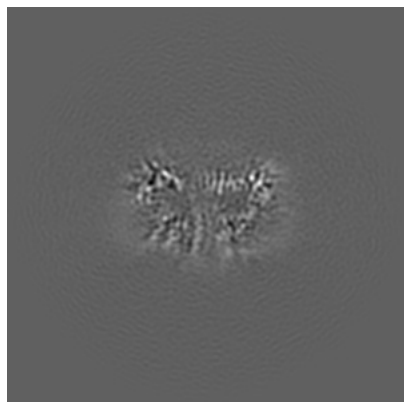


Z Index: 140

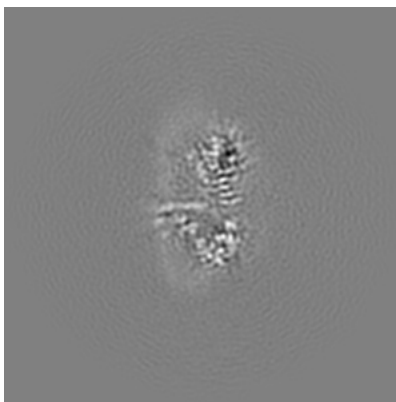
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

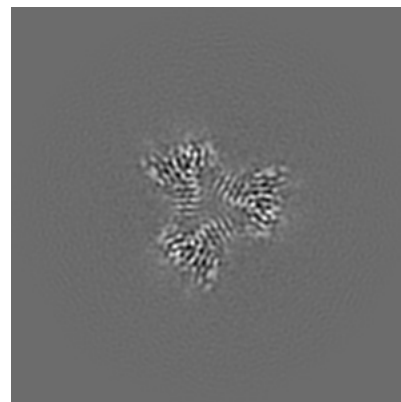
6.3.1 Primary map



X Index: 129

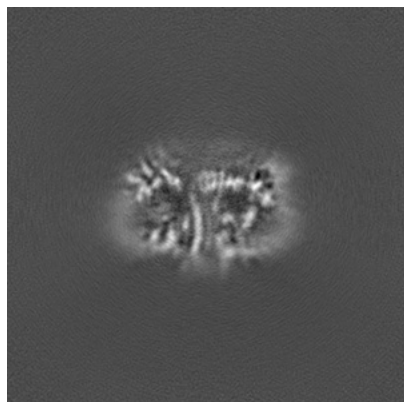


Y Index: 155

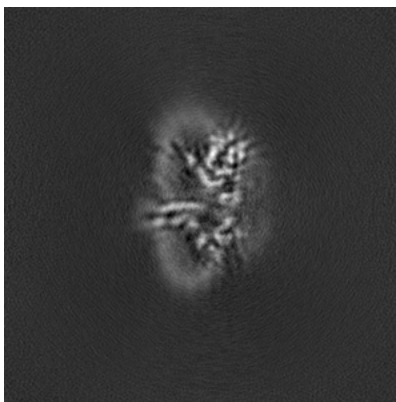


Z Index: 156

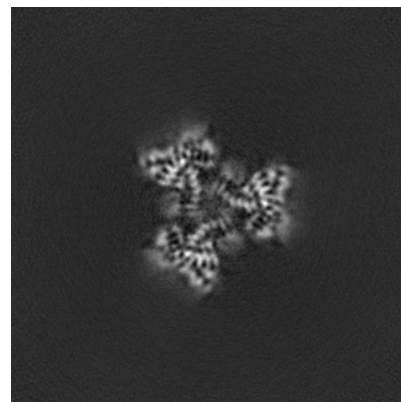
6.3.2 Raw map



X Index: 128



Y Index: 153

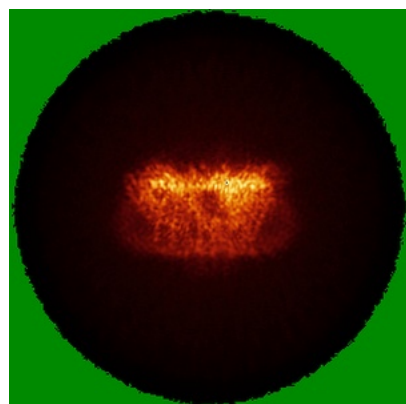


Z Index: 158

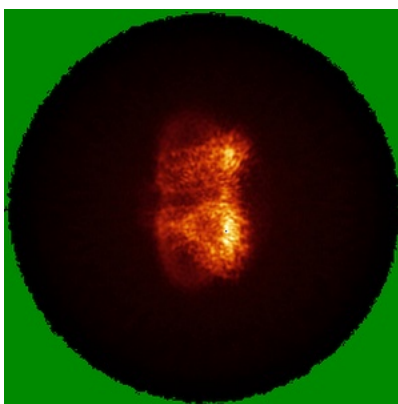
The images above show the largest variance slices of the map in three orthogonal directions.

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

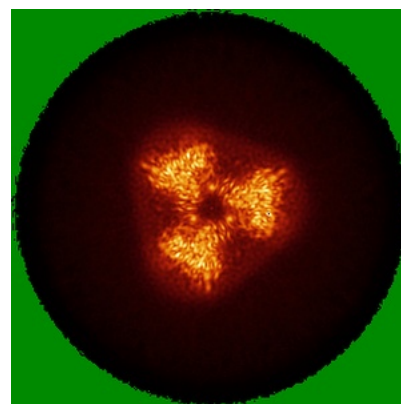
6.4.1 Primary map



X

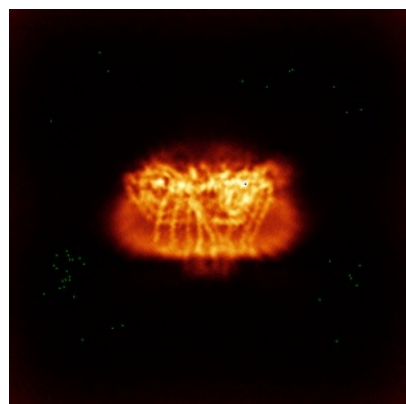


Y

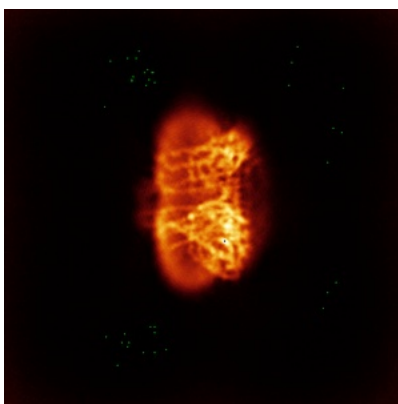


Z

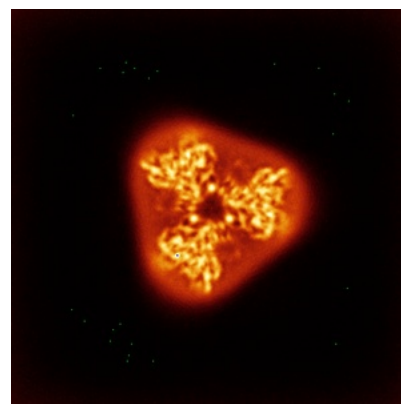
6.4.2 Raw map



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.

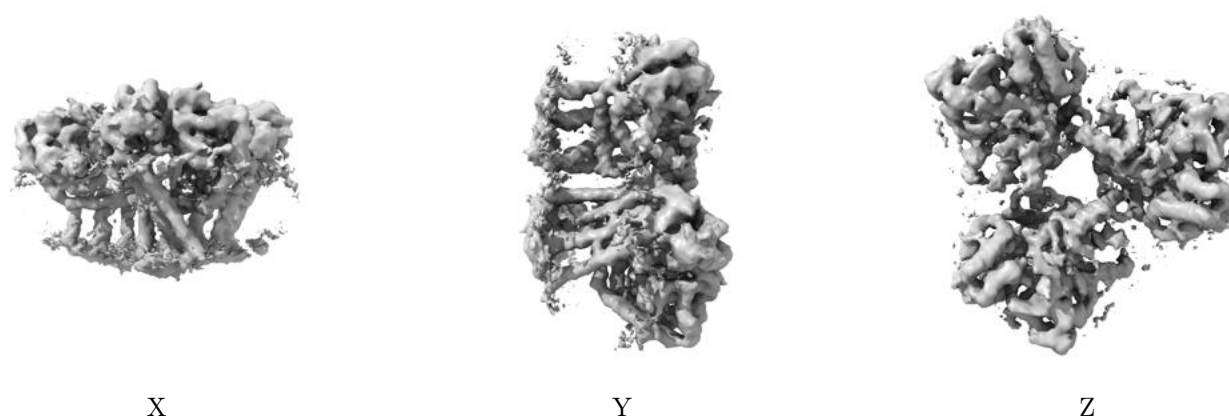
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.46. 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



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.

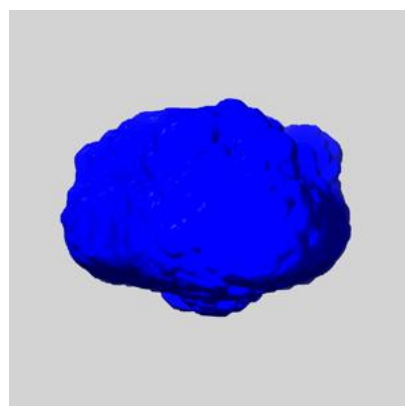
6.6 Mask visualisation [i](#)

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

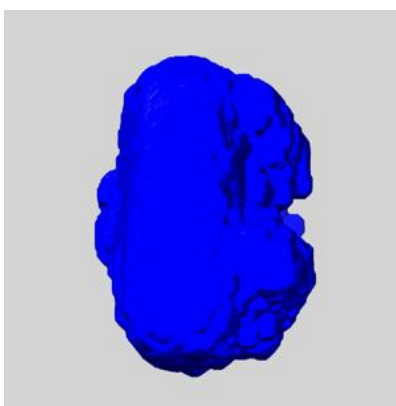
A mask typically either:

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

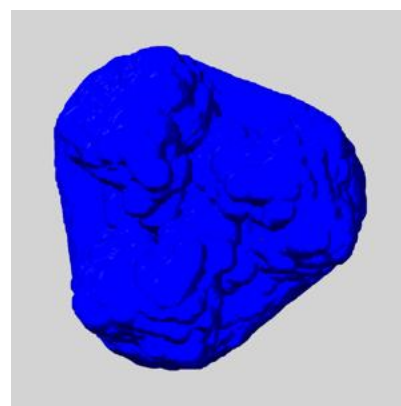
6.6.1 emd_17789_msk_1.map [i](#)



X



Y

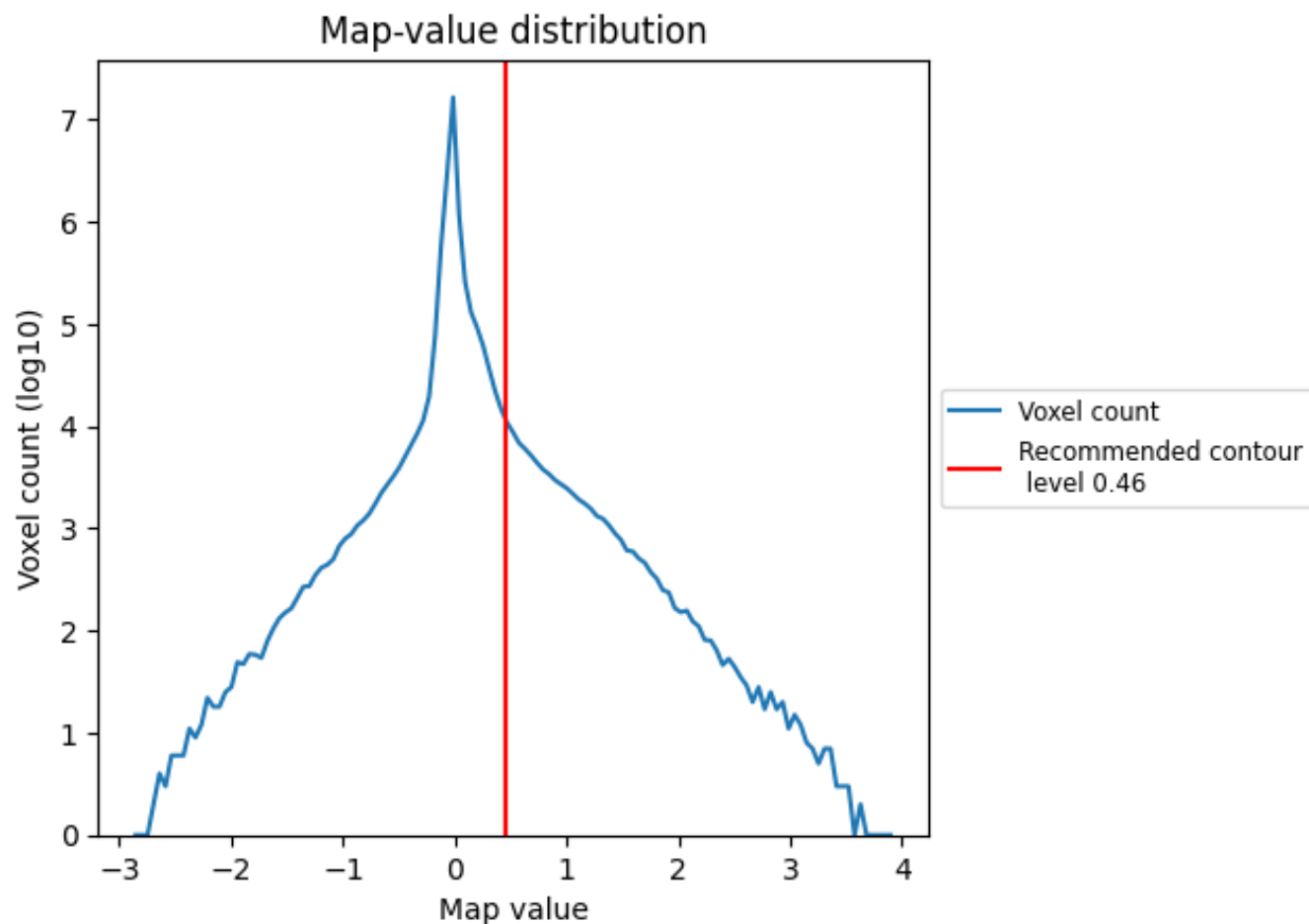


Z

7 Map analysis [i](#)

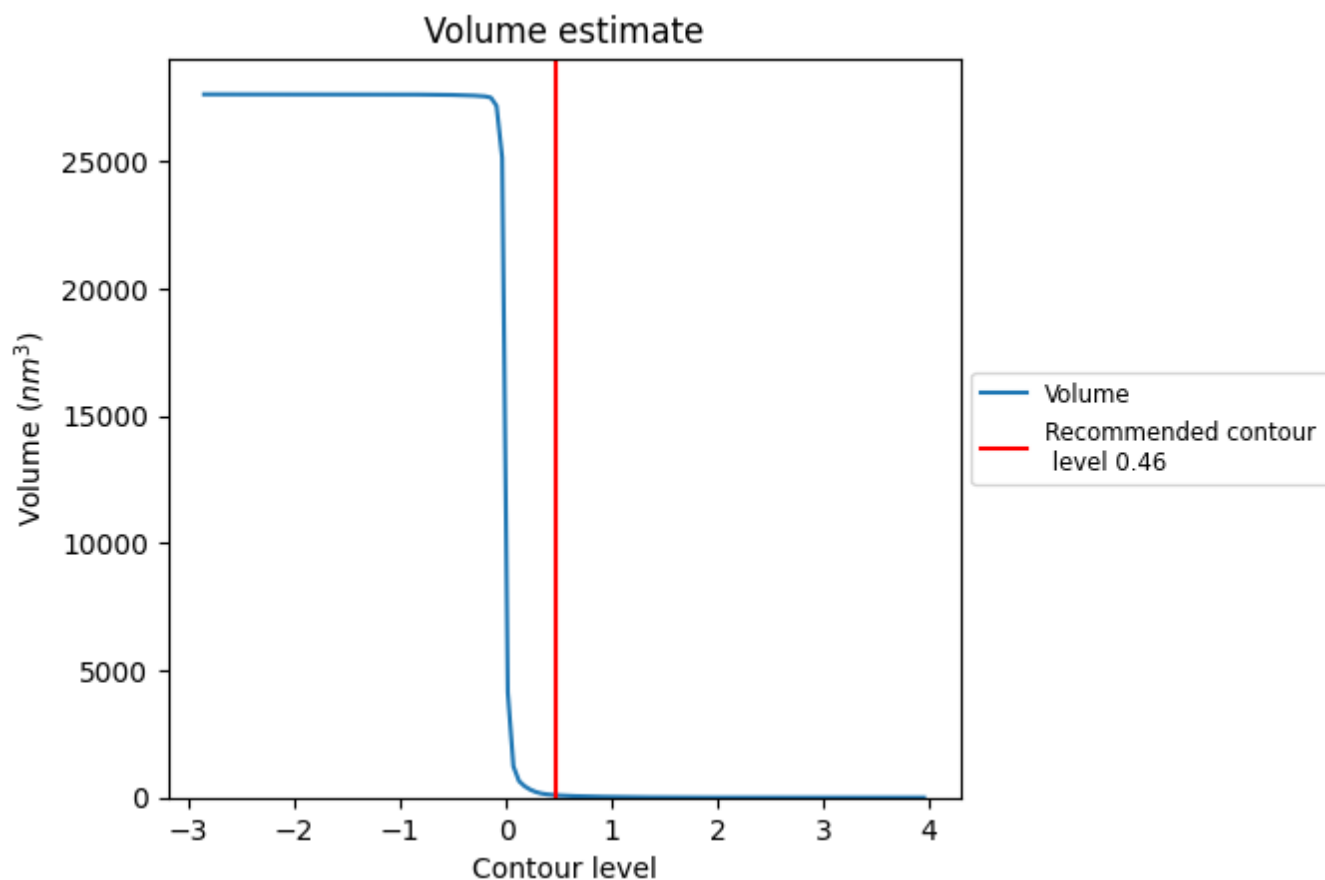
This section contains the results of statistical analysis of the map.

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.

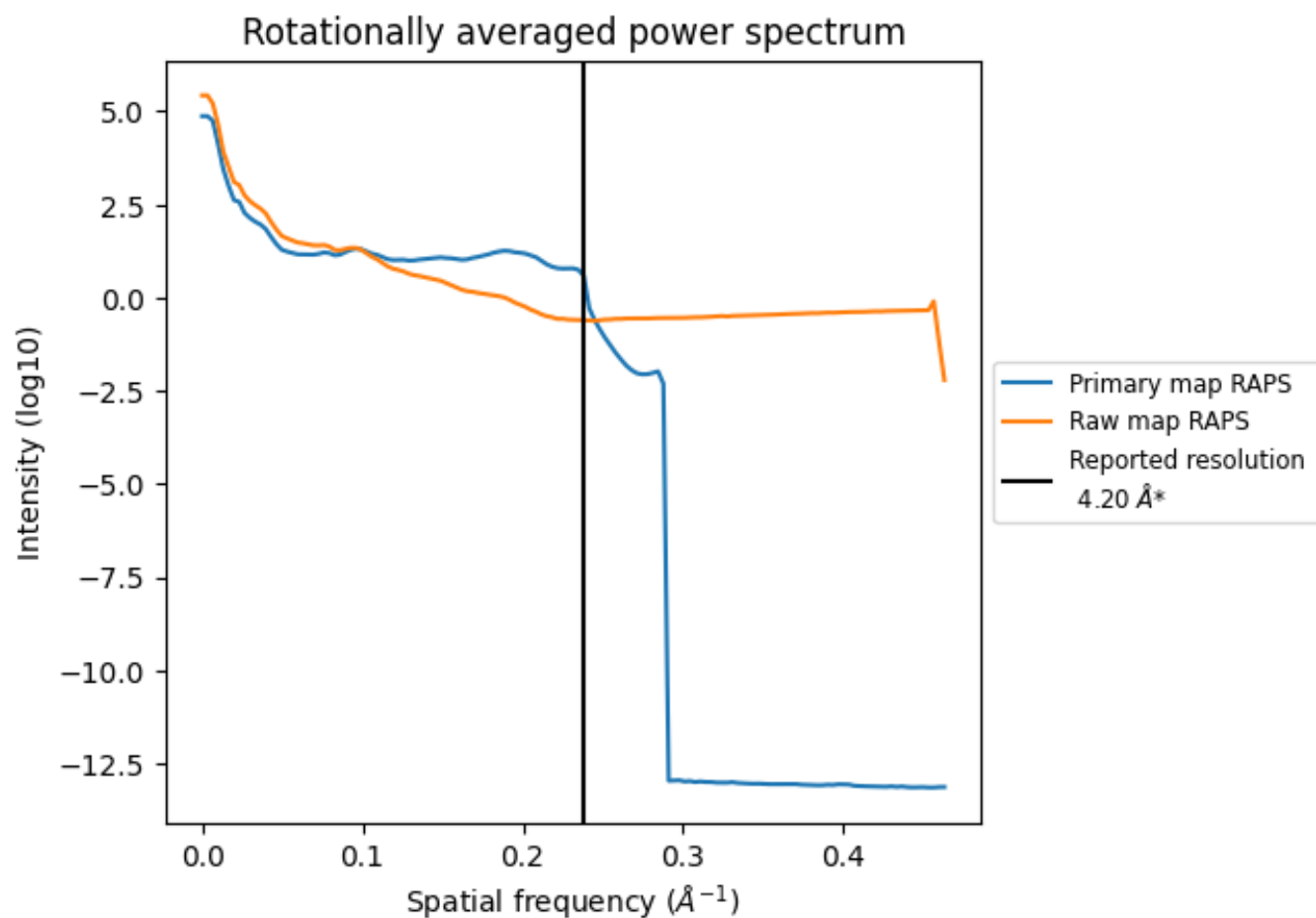
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 97 nm^3 ; this corresponds to an approximate mass of 87 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 ⓘ

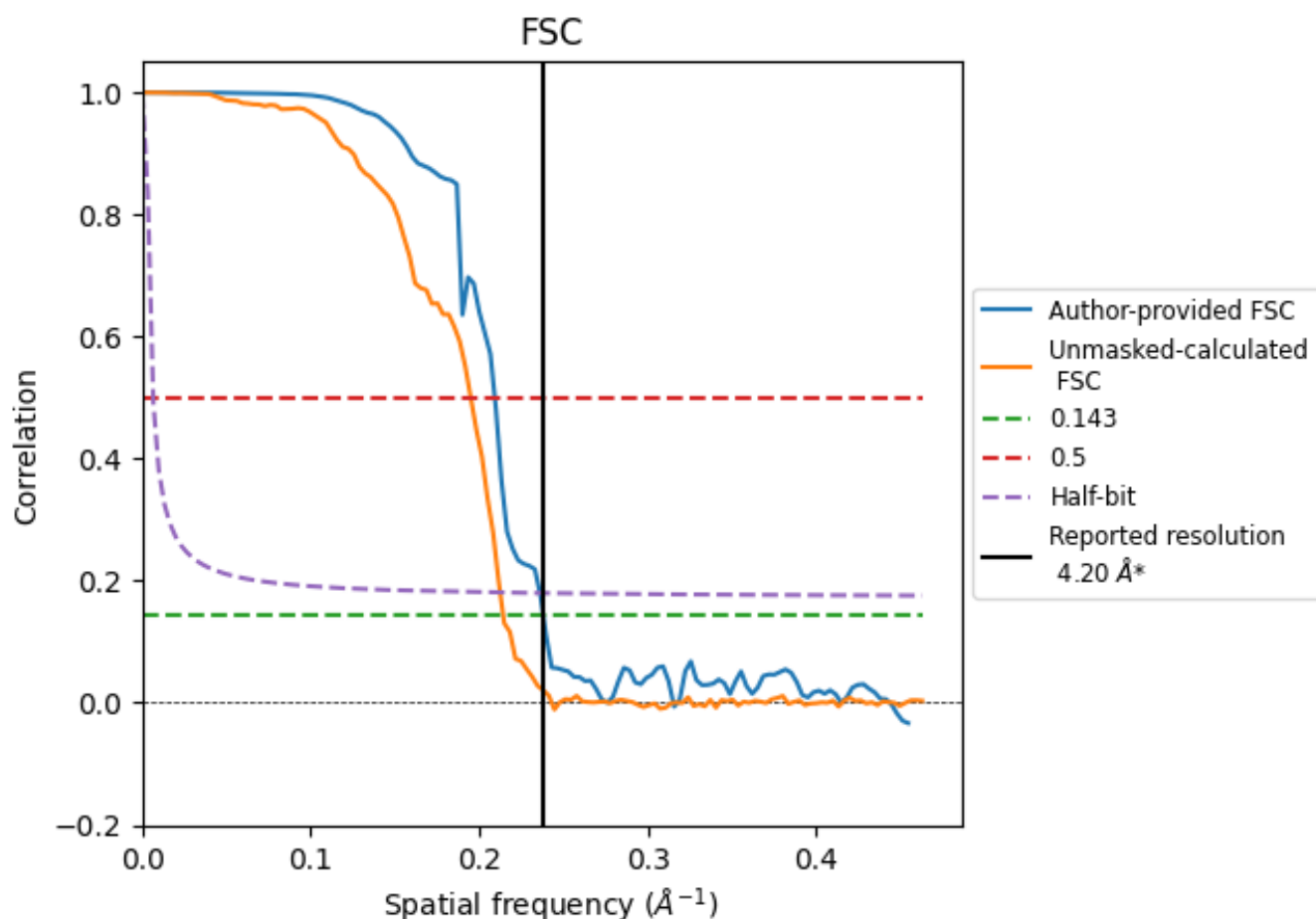


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

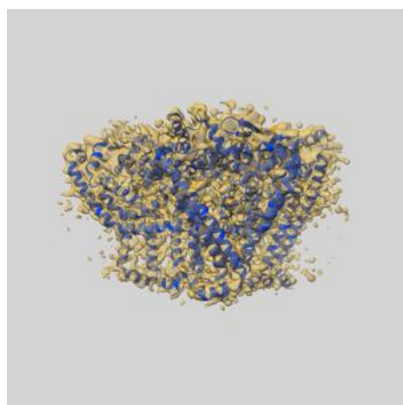
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.20	4.78	4.23
Unmasked-calculated*	4.67	5.13	4.71

*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 4.67 differs from the reported value 4.2 by more than 10 %

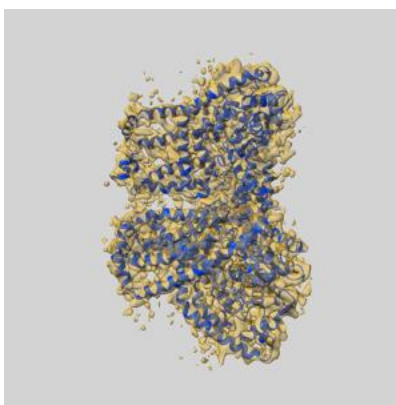
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17789 and PDB model 8POE. Per-residue inclusion information can be found in section 3 on page 7.

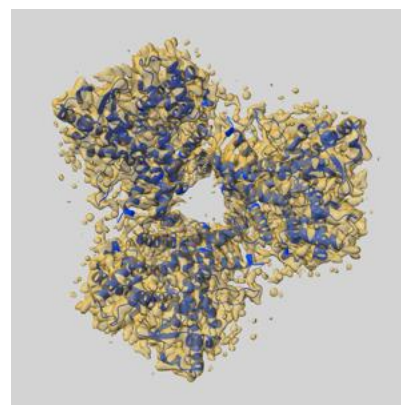
9.1 Map-model overlay [i](#)



X



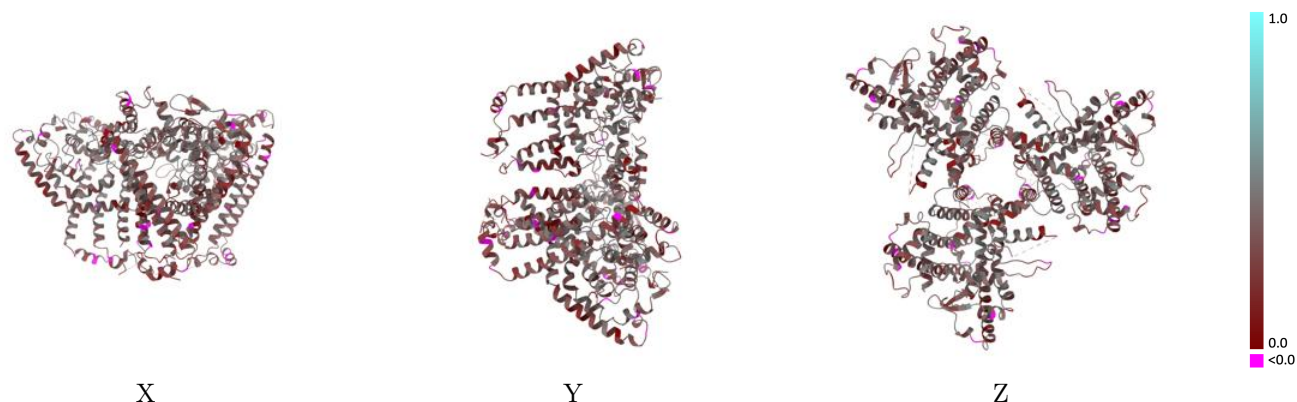
Y



Z

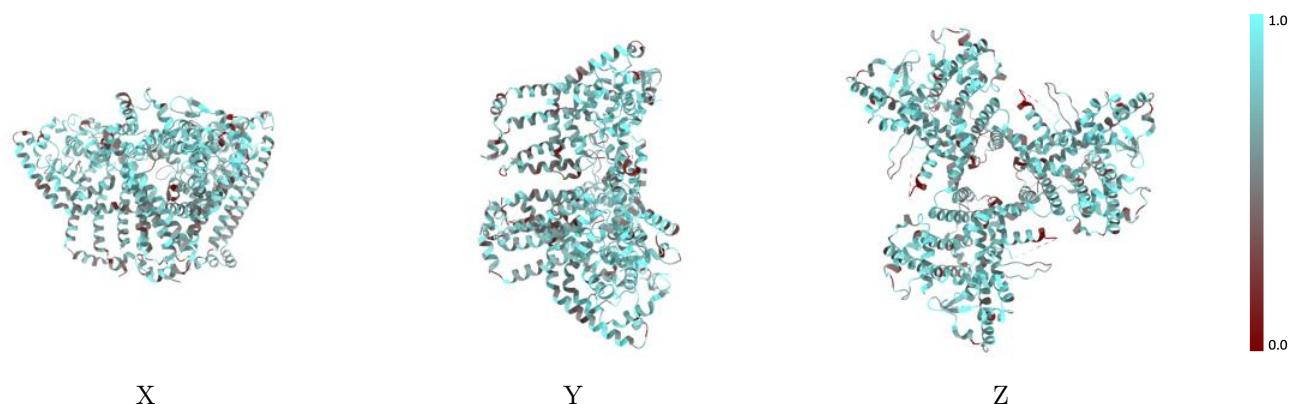
The images above show the 3D surface view of the map at the recommended contour level 0.46 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



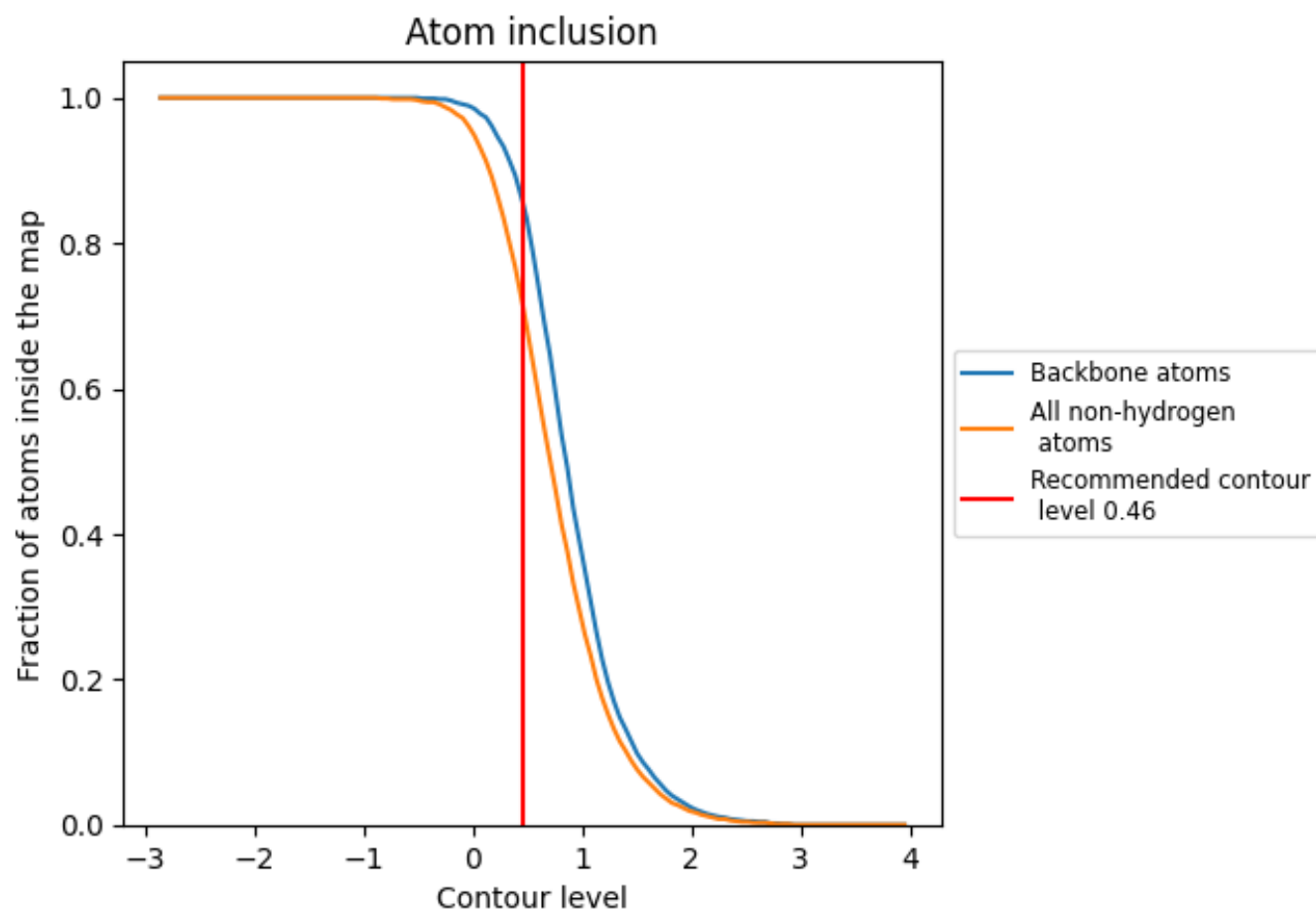
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.46).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 71% 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 (0.46) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7130	0.3330
A	0.7150	0.3330
B	0.7150	0.3330
C	0.7100	0.3330

