



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 01:03 PM UTC

PDB ID : 8CG4 / pdb_00008cg4
EMDB ID : EMD-16630
Title : The organise full-length structure of the fungal non-reducing polyketide synthase (NR-PKS) PksA
Authors : Munoz-Hernandez, H.; Maier, T.
Deposited on : 2023-02-03
Resolution : 2.60 Å(reported)

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

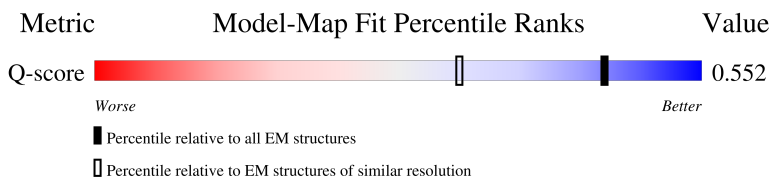
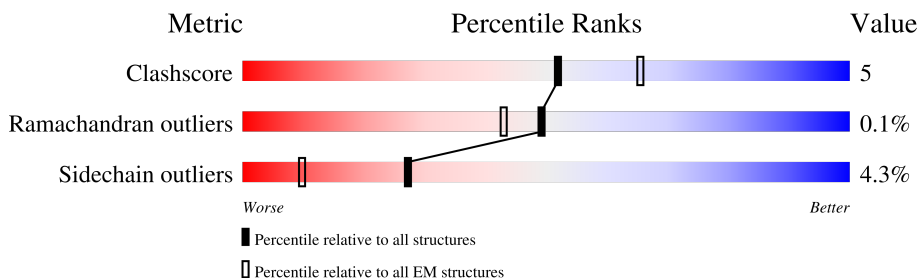
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8728 (2.10 - 3.10)

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	2170	
1	B	2170	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 38440 atoms, of which 19118 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 Norsolorinic acid synthase.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1252	Total	C	H	N	O	S	0	0
			19220	6083	9559	1693	1821	64		
1	B	1252	Total	C	H	N	O	S	0	0
			19220	6083	9559	1693	1821	64		

There are 122 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-60	MET	-	initiating methionine	UNP Q12053
A	-59	ALA	-	expression tag	UNP Q12053
A	-58	HIS	-	expression tag	UNP Q12053
A	-57	HIS	-	expression tag	UNP Q12053
A	-56	HIS	-	expression tag	UNP Q12053
A	-55	HIS	-	expression tag	UNP Q12053
A	-54	HIS	-	expression tag	UNP Q12053
A	-53	HIS	-	expression tag	UNP Q12053
A	-52	HIS	-	expression tag	UNP Q12053
A	-51	HIS	-	expression tag	UNP Q12053
A	-50	HIS	-	expression tag	UNP Q12053
A	-49	HIS	-	expression tag	UNP Q12053
A	-48	GLY	-	expression tag	UNP Q12053
A	-47	SER	-	expression tag	UNP Q12053
A	-46	THR	-	expression tag	UNP Q12053
A	-45	SER	-	expression tag	UNP Q12053
A	-44	GLY	-	expression tag	UNP Q12053
A	-43	SER	-	expression tag	UNP Q12053
A	-42	GLY	-	expression tag	UNP Q12053
A	-41	GLU	-	expression tag	UNP Q12053
A	-40	GLN	-	expression tag	UNP Q12053
A	-39	LYS	-	expression tag	UNP Q12053
A	-38	LEU	-	expression tag	UNP Q12053
A	-37	ILE	-	expression tag	UNP Q12053
A	-36	SER	-	expression tag	UNP Q12053
A	-35	GLU	-	expression tag	UNP Q12053

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-34	GLU	-	expression tag	UNP Q12053
A	-33	ASP	-	expression tag	UNP Q12053
A	-32	LEU	-	expression tag	UNP Q12053
A	-31	GLY	-	expression tag	UNP Q12053
A	-30	SER	-	expression tag	UNP Q12053
A	-29	THR	-	expression tag	UNP Q12053
A	-28	SER	-	expression tag	UNP Q12053
A	-27	GLY	-	expression tag	UNP Q12053
A	-26	SER	-	expression tag	UNP Q12053
A	-25	GLY	-	expression tag	UNP Q12053
A	-24	ASP	-	expression tag	UNP Q12053
A	-23	TYR	-	expression tag	UNP Q12053
A	-22	LYS	-	expression tag	UNP Q12053
A	-21	ASP	-	expression tag	UNP Q12053
A	-20	ASP	-	expression tag	UNP Q12053
A	-19	ASP	-	expression tag	UNP Q12053
A	-18	ASP	-	expression tag	UNP Q12053
A	-17	LYS	-	expression tag	UNP Q12053
A	-16	LEU	-	expression tag	UNP Q12053
A	-15	THR	-	expression tag	UNP Q12053
A	-14	SER	-	expression tag	UNP Q12053
A	-13	LEU	-	expression tag	UNP Q12053
A	-12	TYR	-	expression tag	UNP Q12053
A	-11	LYS	-	expression tag	UNP Q12053
A	-10	LYS	-	expression tag	UNP Q12053
A	-9	ALA	-	expression tag	UNP Q12053
A	-8	GLY	-	expression tag	UNP Q12053
A	-7	LEU	-	expression tag	UNP Q12053
A	-6	GLU	-	expression tag	UNP Q12053
A	-5	ASN	-	expression tag	UNP Q12053
A	-4	LEU	-	expression tag	UNP Q12053
A	-3	TYR	-	expression tag	UNP Q12053
A	-2	PHE	-	expression tag	UNP Q12053
A	-1	GLN	-	expression tag	UNP Q12053
A	0	GLY	-	expression tag	UNP Q12053
B	-60	MET	-	initiating methionine	UNP Q12053
B	-59	ALA	-	expression tag	UNP Q12053
B	-58	HIS	-	expression tag	UNP Q12053
B	-57	HIS	-	expression tag	UNP Q12053
B	-56	HIS	-	expression tag	UNP Q12053
B	-55	HIS	-	expression tag	UNP Q12053
B	-54	HIS	-	expression tag	UNP Q12053

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-53	HIS	-	expression tag	UNP Q12053
B	-52	HIS	-	expression tag	UNP Q12053
B	-51	HIS	-	expression tag	UNP Q12053
B	-50	HIS	-	expression tag	UNP Q12053
B	-49	HIS	-	expression tag	UNP Q12053
B	-48	GLY	-	expression tag	UNP Q12053
B	-47	SER	-	expression tag	UNP Q12053
B	-46	THR	-	expression tag	UNP Q12053
B	-45	SER	-	expression tag	UNP Q12053
B	-44	GLY	-	expression tag	UNP Q12053
B	-43	SER	-	expression tag	UNP Q12053
B	-42	GLY	-	expression tag	UNP Q12053
B	-41	GLU	-	expression tag	UNP Q12053
B	-40	GLN	-	expression tag	UNP Q12053
B	-39	LYS	-	expression tag	UNP Q12053
B	-38	LEU	-	expression tag	UNP Q12053
B	-37	ILE	-	expression tag	UNP Q12053
B	-36	SER	-	expression tag	UNP Q12053
B	-35	GLU	-	expression tag	UNP Q12053
B	-34	GLU	-	expression tag	UNP Q12053
B	-33	ASP	-	expression tag	UNP Q12053
B	-32	LEU	-	expression tag	UNP Q12053
B	-31	GLY	-	expression tag	UNP Q12053
B	-30	SER	-	expression tag	UNP Q12053
B	-29	THR	-	expression tag	UNP Q12053
B	-28	SER	-	expression tag	UNP Q12053
B	-27	GLY	-	expression tag	UNP Q12053
B	-26	SER	-	expression tag	UNP Q12053
B	-25	GLY	-	expression tag	UNP Q12053
B	-24	ASP	-	expression tag	UNP Q12053
B	-23	TYR	-	expression tag	UNP Q12053
B	-22	LYS	-	expression tag	UNP Q12053
B	-21	ASP	-	expression tag	UNP Q12053
B	-20	ASP	-	expression tag	UNP Q12053
B	-19	ASP	-	expression tag	UNP Q12053
B	-18	ASP	-	expression tag	UNP Q12053
B	-17	LYS	-	expression tag	UNP Q12053
B	-16	LEU	-	expression tag	UNP Q12053
B	-15	THR	-	expression tag	UNP Q12053
B	-14	SER	-	expression tag	UNP Q12053
B	-13	LEU	-	expression tag	UNP Q12053
B	-12	TYR	-	expression tag	UNP Q12053

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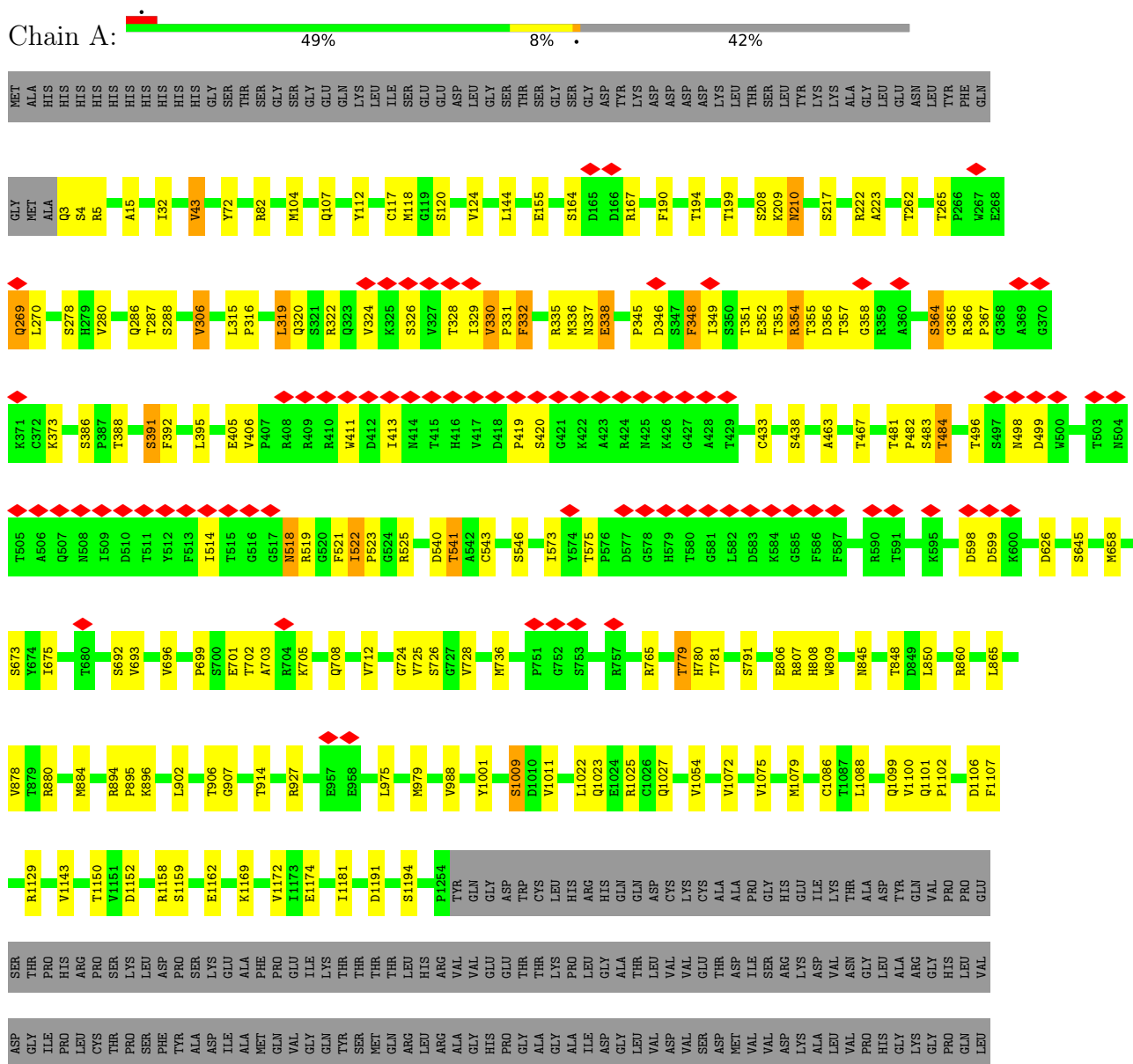
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	LYS	-	expression tag	UNP Q12053
B	-10	LYS	-	expression tag	UNP Q12053
B	-9	ALA	-	expression tag	UNP Q12053
B	-8	GLY	-	expression tag	UNP Q12053
B	-7	LEU	-	expression tag	UNP Q12053
B	-6	GLU	-	expression tag	UNP Q12053
B	-5	ASN	-	expression tag	UNP Q12053
B	-4	LEU	-	expression tag	UNP Q12053
B	-3	TYR	-	expression tag	UNP Q12053
B	-2	PHE	-	expression tag	UNP Q12053
B	-1	GLN	-	expression tag	UNP Q12053
B	0	GLY	-	expression tag	UNP Q12053

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: Norsolorinic acid synthase



[illegible]

- Molecule 1: Norsolorinic acid synthase

[illegible]



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	361377	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.529	Depositor
Minimum map value	-0.251	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.075	Depositor
Map size ($\text{\AA}$)	314.88, 314.88, 314.88	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

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	0.19	0/9884	0.32	0/13444
1	B	0.19	0/9884	0.32	0/13444
All	All	0.19	0/19768	0.32	0/26888

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	338	GLU	Peptide
1	A	541	THR	Peptide
1	B	541	THR	Peptide

5.2 Too-close contacts

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	9661	9559	9569	106	0
1	B	9661	9559	9569	106	0
All	All	19322	19118	19138	208	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.

All (208) 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:B:546:SER:OG	1:B:724:GLY:O	1.83	0.94
1:A:546:SER:OG	1:A:724:GLY:O	1.90	0.89
1:B:104:MET:SD	1:B:107:GLN:NE2	2.51	0.83
1:A:1129:ARG:NH2	1:A:1152:ASP:OD2	2.11	0.83
1:A:104:MET:SD	1:A:107:GLN:NE2	2.51	0.83
1:A:481:THR:HG1	1:A:484:THR:HG1	1.19	0.80
1:A:335:ARG:NH1	1:A:337:ASN:OD1	2.13	0.80
1:A:3:GLN:N	1:A:326:SER:HG	1.79	0.80
1:B:1129:ARG:NH2	1:B:1152:ASP:OD2	2.16	0.78
1:B:348:PHE:O	1:B:351:THR:N	2.19	0.73
1:A:112:TYR:OH	1:A:322:ARG:NH2	2.23	0.71
1:B:914:THR:HG22	1:B:914:THR:O	1.89	0.71
1:A:914:THR:HG22	1:A:914:THR:O	1.90	0.70
1:B:164:SER:OG	1:B:167:ARG:O	2.08	0.70
1:B:345:PRO:O	1:B:349:ILE:HG23	1.96	0.66
1:B:333:LEU:HD11	1:B:356:ASP:HB2	1.77	0.66
1:B:350:SER:O	1:B:351:THR:HG23	1.96	0.66
1:A:164:SER:OG	1:A:167:ARG:O	2.13	0.65
1:A:496:THR:O	1:A:519:ARG:NH2	2.30	0.65
1:B:336:MET:N	1:B:336:MET:SD	2.71	0.64
1:A:1025:ARG:NH1	1:A:1106:ASP:OD2	2.31	0.64
1:B:541:THR:HG22	1:B:541:THR:O	1.95	0.64
1:A:541:THR:HG22	1:A:541:THR:O	1.98	0.63
1:B:1025:ARG:NH1	1:B:1106:ASP:OD2	2.32	0.63
1:A:336:MET:N	1:A:336:MET:HE3	2.15	0.62
1:B:356:ASP:O	1:B:357:THR:OG1	2.16	0.62
1:B:845:ASN:O	1:B:848:THR:HG23	1.99	0.62
1:B:1023:GLN:O	1:B:1023:GLN:NE2	2.31	0.62
1:B:589:SER:OG	1:B:602:ASP:OD1	2.18	0.62
1:A:518:ASN:OD1	1:A:519:ARG:N	2.32	0.62
1:B:518:ASN:OD1	1:B:519:ARG:N	2.33	0.61
1:A:1023:GLN:O	1:A:1023:GLN:NE2	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:ALA:O	1:A:467:THR:OG1	2.16	0.61
1:A:406:VAL:HG12	1:A:413:ILE:HD11	1.83	0.60
1:B:496:THR:O	1:B:519:ARG:NH2	2.34	0.60
1:B:1027:GLN:O	1:B:1099:GLN:NE2	2.34	0.60
1:B:190:PHE:O	1:B:194:THR:OG1	2.19	0.60
1:A:1027:GLN:O	1:A:1099:GLN:NE2	2.34	0.59
1:B:498:ASN:OD1	1:B:519:ARG:NE	2.35	0.59
1:A:1009:SER:OG	1:B:159:ARG:O	2.21	0.58
1:B:1185:VAL:HG13	1:B:1189:LEU:HD12	1.86	0.58
1:B:43:VAL:HG22	1:B:144:LEU:HD13	1.86	0.58
1:B:463:ALA:O	1:B:467:THR:OG1	2.14	0.57
1:B:598:ASP:OD1	1:B:599:ASP:N	2.38	0.57
1:B:499:ASP:OD2	1:B:575:THR:N	2.36	0.57
1:A:498:ASN:OD1	1:A:519:ARG:NE	2.38	0.56
1:B:626:ASP:O	1:B:807:ARG:NH1	2.33	0.56
1:A:328:THR:HG22	1:A:329:ILE:H	1.71	0.56
1:A:117:CYS:SG	1:A:306:VAL:HG11	2.45	0.56
1:A:352:GLU:OE1	1:A:353:THR:N	2.40	0.55
1:A:356:ASP:O	1:A:357:THR:OG1	2.20	0.55
1:A:598:ASP:OD1	1:A:599:ASP:N	2.39	0.55
1:A:850:LEU:HD11	1:A:878:VAL:HG21	1.89	0.55
1:A:626:ASP:O	1:A:807:ARG:NH1	2.32	0.55
1:B:573:ILE:O	1:B:573:ILE:HG22	2.06	0.55
1:B:351:THR:C	1:B:352:GLU:HG2	2.31	0.54
1:A:120:SER:O	1:A:124:VAL:HG23	2.07	0.54
1:A:352:GLU:OE1	1:A:353:THR:OG1	2.19	0.54
1:A:1001:TYR:HB2	1:A:1011:VAL:HG21	1.88	0.54
1:A:357:THR:HG22	1:A:358:GLY:H	1.71	0.54
1:B:626:ASP:OD1	1:B:860:ARG:NH2	2.41	0.54
1:B:341:SER:O	1:B:345:PRO:HD2	2.08	0.54
1:B:1022:LEU:HD11	1:B:1100:VAL:HG12	1.91	0.53
1:B:117:CYS:SG	1:B:306:VAL:HG11	2.48	0.53
1:A:845:ASN:O	1:A:848:THR:HG23	2.08	0.53
1:A:573:ILE:HG22	1:A:573:ILE:O	2.10	0.52
1:B:701:GLU:O	1:B:702:THR:OG1	2.22	0.52
1:A:72:TYR:OH	1:A:82:ARG:NH2	2.43	0.52
1:A:626:ASP:OD1	1:A:860:ARG:NH2	2.43	0.52
1:B:319:LEU:HD22	1:B:332:PHE:CZ	2.45	0.51
1:B:481:THR:OG1	1:B:484:THR:OG1	2.03	0.51
1:A:914:THR:O	1:A:914:THR:CG2	2.59	0.51
1:B:341:SER:O	1:B:344:LEU:N	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:MET:HG2	1:B:341:SER:HB3	1.93	0.51
1:B:345:PRO:HB3	1:B:353:THR:HG21	1.92	0.51
1:A:1022:LEU:HD11	1:A:1100:VAL:HG12	1.92	0.50
1:B:366:ARG:HG3	1:B:367:PRO:N	2.26	0.50
1:A:366:ARG:HG3	1:A:367:PRO:N	2.26	0.50
1:B:914:THR:O	1:B:914:THR:CG2	2.58	0.50
1:A:692:SER:O	1:A:696:VAL:HG23	2.12	0.50
1:A:499:ASP:OD2	1:A:575:THR:N	2.37	0.49
1:B:692:SER:O	1:B:696:VAL:HG23	2.12	0.49
1:A:701:GLU:O	1:A:702:THR:OG1	2.17	0.49
1:B:575:THR:HG22	1:B:577:ASP:H	1.77	0.49
1:B:699:PRO:O	1:B:765:ARG:NH2	2.44	0.49
1:B:1158:ARG:O	1:B:1162:GLU:HG3	2.12	0.49
1:B:906:THR:OG1	1:B:1174:GLU:OE2	2.29	0.49
1:B:1181:ILE:O	1:B:1185:VAL:HG23	2.12	0.49
1:B:330:VAL:HG12	1:B:331:PRO:HD2	1.93	0.49
1:B:70:GLN:O	1:B:73:VAL:HG22	2.13	0.49
1:B:118:MET:O	1:B:118:MET:HG2	2.12	0.49
1:A:32:ILE:HD11	1:B:32:ILE:HD11	1.95	0.48
1:A:118:MET:O	1:A:118:MET:HG2	2.12	0.48
1:A:330:VAL:HG12	1:A:331:PRO:HD2	1.94	0.48
1:B:806:GLU:N	1:B:806:GLU:OE2	2.47	0.48
1:B:1001:TYR:HB2	1:B:1011:VAL:HG21	1.95	0.48
1:A:117:CYS:O	1:A:118:MET:HB3	2.13	0.47
1:A:4:SER:OG	1:A:5:ARG:N	2.46	0.47
1:A:521:PHE:O	1:A:525:ARG:HB2	2.15	0.47
1:B:117:CYS:O	1:B:118:MET:HB3	2.13	0.47
1:B:335:ARG:NH1	1:B:337:ASN:OD1	2.47	0.47
1:A:1075:VAL:O	1:A:1079:MET:HG3	2.15	0.47
1:A:269:GLN:O	1:A:270:LEU:HD13	2.16	0.46
1:B:519:ARG:NH1	1:B:540:ASP:OD2	2.48	0.46
1:B:392:PHE:CD2	1:B:736:MET:HE1	2.51	0.46
1:A:1088:LEU:C	1:A:1088:LEU:HD13	2.41	0.46
1:B:809:TRP:HA	1:B:809:TRP:CE3	2.50	0.46
1:A:354:ARG:HG3	1:A:355:THR:H	1.80	0.46
1:B:13:GLN:O	1:B:82:ARG:NH1	2.42	0.46
1:B:522:ILE:HB	1:B:523:PRO:CD	2.46	0.46
1:A:315:LEU:O	1:A:319:LEU:HD23	2.16	0.45
1:A:809:TRP:HA	1:A:809:TRP:CE3	2.50	0.45
1:A:330:VAL:HG12	1:A:331:PRO:CD	2.47	0.45
1:A:806:GLU:N	1:A:806:GLU:OE2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1088:LEU:C	1:B:1088:LEU:HD13	2.41	0.45
1:A:209:LYS:O	1:A:210:ASN:CB	2.64	0.45
1:A:514:ILE:HD12	1:B:581:GLY:HA3	1.99	0.45
1:B:259:LEU:O	1:B:291:ARG:NH1	2.50	0.45
1:A:865:LEU:HD21	1:A:894:ARG:NH1	2.31	0.45
1:A:1158:ARG:O	1:A:1162:GLU:HG3	2.16	0.45
1:B:897:SER:O	1:B:898:LYS:C	2.60	0.45
1:A:522:ILE:HB	1:A:523:PRO:CD	2.47	0.45
1:A:1169:LYS:O	1:A:1169:LYS:HG3	2.17	0.44
1:A:15:ALA:HB1	1:A:338:GLU:HG2	2.00	0.44
1:B:319:LEU:HD22	1:B:332:PHE:HZ	1.82	0.44
1:A:906:THR:OG1	1:A:1174:GLU:OE1	2.33	0.44
1:B:543:CYS:HB2	1:B:791:SER:HA	1.99	0.44
1:B:1181:ILE:O	1:B:1181:ILE:HG22	2.18	0.44
1:A:364:SER:OG	1:A:365:GLY:N	2.48	0.44
1:A:392:PHE:CD2	1:A:736:MET:HE1	2.52	0.44
1:B:352:GLU:O	1:B:353:THR:OG1	2.24	0.44
1:B:1106:ASP:OD1	1:B:1106:ASP:N	2.51	0.44
1:A:43:VAL:HG22	1:A:144:LEU:HD13	1.99	0.44
1:A:543:CYS:HB2	1:A:791:SER:HA	1.99	0.44
1:B:174:ILE:HG12	1:B:238:ILE:HD11	1.98	0.44
1:A:357:THR:HG22	1:A:358:GLY:N	2.31	0.44
1:B:343:ILE:HD12	1:B:343:ILE:N	2.33	0.44
1:B:779:THR:OG1	1:B:780:HIS:N	2.51	0.44
1:B:344:LEU:HD22	1:B:348:PHE:HE2	1.83	0.44
1:B:850:LEU:HD11	1:B:878:VAL:HG21	2.00	0.44
1:A:519:ARG:NH1	1:A:540:ASP:OD2	2.49	0.44
1:B:341:SER:O	1:B:345:PRO:CD	2.66	0.44
1:B:522:ILE:HB	1:B:523:PRO:HD3	2.00	0.43
1:A:522:ILE:HB	1:A:523:PRO:HD3	2.01	0.43
1:B:658:MET:HE1	1:B:693:VAL:HG22	2.00	0.43
1:A:1106:ASP:OD1	1:A:1106:ASP:N	2.51	0.43
1:A:1181:ILE:HG22	1:A:1181:ILE:O	2.18	0.43
1:B:1169:LYS:HG3	1:B:1169:LYS:O	2.17	0.43
1:B:269:GLN:O	1:B:270:LEU:HD13	2.19	0.43
1:B:351:THR:O	1:B:352:GLU:HG2	2.18	0.43
1:A:895:PRO:O	1:A:896:LYS:CB	2.67	0.43
1:B:155:GLU:OE2	1:B:155:GLU:HA	2.18	0.43
1:B:319:LEU:HD13	1:B:332:PHE:CE2	2.53	0.43
1:B:1101:GLN:N	1:B:1102:PRO:HD2	2.34	0.43
1:A:320:GLN:O	1:A:324:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:PRO:O	1:A:346:ASP:C	2.61	0.42
1:A:406:VAL:HG12	1:A:413:ILE:CD1	2.48	0.42
1:A:1107:PHE:CE2	1:A:1143:VAL:HG12	2.54	0.42
1:B:521:PHE:O	1:B:525:ARG:HB2	2.18	0.42
1:A:354:ARG:HA	1:A:354:ARG:NE	2.35	0.42
1:A:895:PRO:O	1:A:896:LYS:CG	2.67	0.42
1:B:222:ARG:HG3	1:B:223:ALA:N	2.35	0.42
1:A:975:LEU:O	1:A:979:MET:HG2	2.20	0.42
1:A:1054:VAL:O	1:A:1150:THR:HG22	2.20	0.42
1:A:1169:LYS:HB3	1:A:1169:LYS:NZ	2.35	0.42
1:A:388:THR:OG1	1:A:391:SER:OG	2.33	0.42
1:A:779:THR:OG1	1:A:780:HIS:N	2.52	0.42
1:A:336:MET:HE3	1:A:336:MET:H	1.83	0.41
1:A:345:PRO:O	1:A:349:ILE:HG12	2.20	0.41
1:A:880:ARG:O	1:A:884:MET:HG2	2.20	0.41
1:A:906:THR:HG22	1:A:907:GLY:N	2.35	0.41
1:B:329:ILE:HD12	1:B:351:THR:HG21	2.02	0.41
1:B:1107:PHE:CE2	1:B:1143:VAL:HG12	2.54	0.41
1:A:1101:GLN:N	1:A:1102:PRO:HD2	2.34	0.41
1:B:570:THR:HG22	1:B:610:VAL:HG22	2.02	0.41
1:B:880:ARG:O	1:B:884:MET:HG2	2.20	0.41
1:A:319:LEU:HD23	1:A:319:LEU:H	1.84	0.41
1:B:328:THR:HG22	1:B:329:ILE:N	2.35	0.41
1:B:1191:ASP:OD2	1:B:1191:ASP:N	2.53	0.41
1:B:962:VAL:HG13	1:B:963:VAL:N	2.36	0.41
1:B:997:PHE:HB3	1:B:1011:VAL:HG13	2.03	0.41
1:A:658:MET:HE1	1:A:693:VAL:HG22	2.03	0.41
1:B:414:ASN:HA	1:B:417:VAL:HG23	2.02	0.41
1:A:190:PHE:O	1:A:194:THR:OG1	2.37	0.41
1:A:315:LEU:O	1:A:316:PRO:C	2.63	0.41
1:A:319:LEU:HD13	1:A:332:PHE:CZ	2.56	0.41
1:A:348:PHE:HA	1:A:352:GLU:HB3	2.02	0.41
1:B:353:THR:CG2	1:B:354:ARG:N	2.83	0.41
1:B:419:PRO:O	1:B:420:SER:C	2.63	0.41
1:A:155:GLU:OE2	1:A:155:GLU:HA	2.21	0.41
1:A:482:PRO:HD3	1:B:49:LEU:HD22	2.03	0.41
1:A:1191:ASP:N	1:A:1191:ASP:OD2	2.53	0.41
1:B:596:PRO:O	1:B:597:TYR:C	2.64	0.41
1:B:906:THR:HG22	1:B:907:GLY:N	2.35	0.41
1:B:975:LEU:O	1:B:979:MET:HG2	2.21	0.41
1:A:222:ARG:HG3	1:A:223:ALA:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:699:PRO:O	1:A:765:ARG:NH2	2.45	0.41
1:B:929:ASP:OD2	1:B:977:ASN:ND2	2.51	0.41
1:A:703:ALA:O	1:A:705:LYS:N	2.53	0.40
1:A:902:LEU:HD23	1:A:1172:VAL:HG22	2.04	0.40
1:B:1169:LYS:HB3	1:B:1169:LYS:NZ	2.35	0.40
1:A:366:ARG:HH11	1:A:373:LYS:H	1.69	0.40
1:B:832:LYS:HE2	1:B:886:ILE:HG23	2.03	0.40
1:B:348:PHE:O	1:B:351:THR:O	2.39	0.40
1:A:15:ALA:CB	1:A:338:GLU:HG2	2.52	0.40
1:A:675:ILE:HB	1:A:712:VAL:HG12	2.04	0.40
1:A:419:PRO:O	1:A:420:SER:C	2.64	0.40
1:B:687:ALA:O	1:B:691:GLU:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1250/2170 (58%)	1155 (92%)	94 (8%)	1 (0%)	48	70
1	B	1250/2170 (58%)	1163 (93%)	86 (7%)	1 (0%)	48	70
All	All	2500/4340 (58%)	2318 (93%)	180 (7%)	2 (0%)	49	70

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	ASN
1	B	352	GLU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1060/1823 (58%)	1013 (96%)	47 (4%)	25	50
1	B	1060/1823 (58%)	1015 (96%)	45 (4%)	26	52
All	All	2120/3646 (58%)	2028 (96%)	92 (4%)	27	51

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	VAL
1	A	199	THR
1	A	208	SER
1	A	217	SER
1	A	262	THR
1	A	265	THR
1	A	269	GLN
1	A	278	SER
1	A	280	VAL
1	A	286	GLN
1	A	287	THR
1	A	288	SER
1	A	306	VAL
1	A	319	LEU
1	A	330	VAL
1	A	332	PHE
1	A	348	PHE
1	A	351	THR
1	A	354	ARG
1	A	364	SER
1	A	386	SER
1	A	391	SER
1	A	395	LEU
1	A	405	GLU
1	A	411	TRP
1	A	433	CYS
1	A	438	SER

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Mol	Chain	Res	Type
1	A	483	SER
1	A	484	THR
1	A	518	ASN
1	A	522	ILE
1	A	645	SER
1	A	673	SER
1	A	708	GLN
1	A	725	VAL
1	A	726	SER
1	A	728	VAL
1	A	779	THR
1	A	781	THR
1	A	808	HIS
1	A	927	ARG
1	A	988	VAL
1	A	1009	SER
1	A	1072	VAL
1	A	1086	CYS
1	A	1159	SER
1	A	1194	SER
1	B	199	THR
1	B	208	SER
1	B	217	SER
1	B	262	THR
1	B	265	THR
1	B	269	GLN
1	B	278	SER
1	B	280	VAL
1	B	287	THR
1	B	288	SER
1	B	306	VAL
1	B	330	VAL
1	B	341	SER
1	B	351	THR
1	B	386	SER
1	B	391	SER
1	B	395	LEU
1	B	398	LYS
1	B	411	TRP
1	B	433	CYS
1	B	438	SER
1	B	483	SER

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Mol	Chain	Res	Type
1	B	484	THR
1	B	505	THR
1	B	518	ASN
1	B	522	ILE
1	B	645	SER
1	B	664	THR
1	B	673	SER
1	B	725	VAL
1	B	726	SER
1	B	728	VAL
1	B	779	THR
1	B	781	THR
1	B	808	HIS
1	B	910	SER
1	B	988	VAL
1	B	989	THR
1	B	1009	SER
1	B	1072	VAL
1	B	1106	ASP
1	B	1133	HIS
1	B	1159	SER
1	B	1194	SER
1	B	1241	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	181	GLN
1	A	233	HIS
1	A	796	ASN
1	A	840	GLN
1	A	938	GLN
1	A	940	HIS
1	A	947	HIS
1	B	50	GLN
1	B	181	GLN
1	B	323	GLN
1	B	796	ASN
1	B	840	GLN
1	B	940	HIS
1	B	947	HIS

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Mol	Chain	Res	Type
1	B	1210	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.

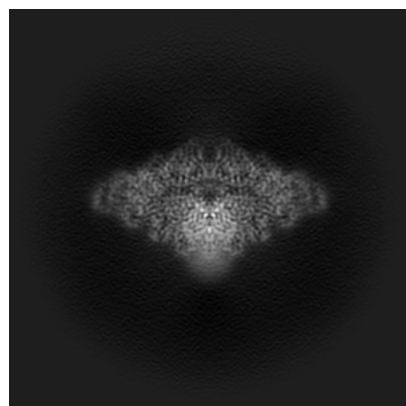
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16630. These allow visual inspection of the internal detail of the map and identification of artifacts.

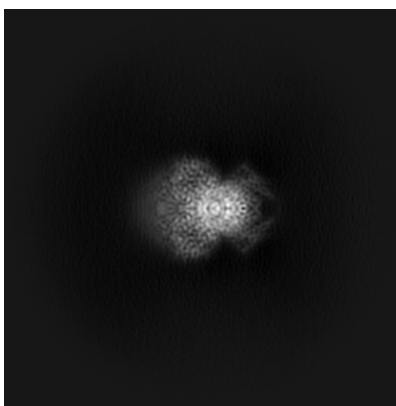
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

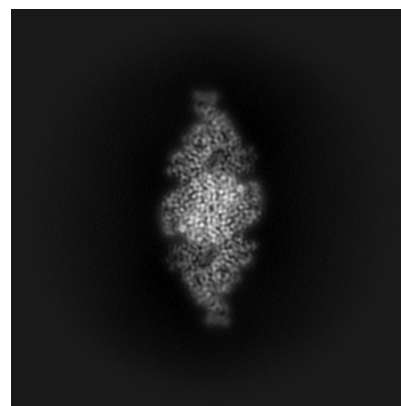
6.1.1 Primary map



X

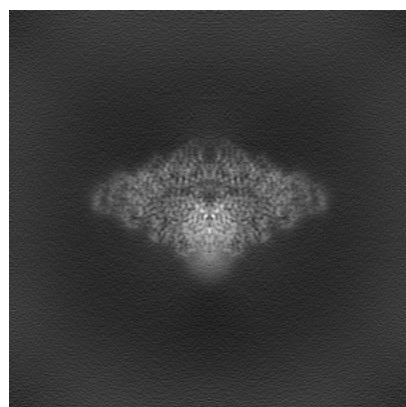


Y

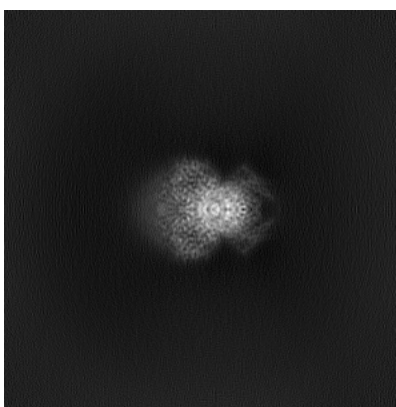


Z

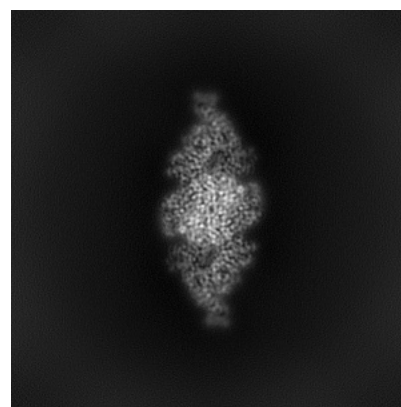
6.1.2 Raw map



X



Y

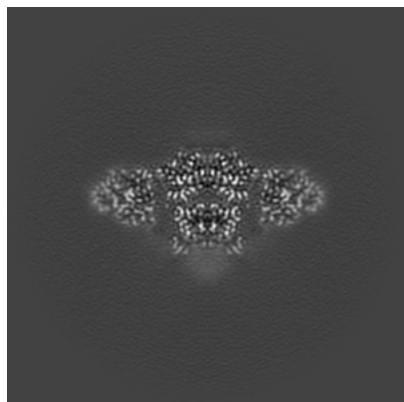


Z

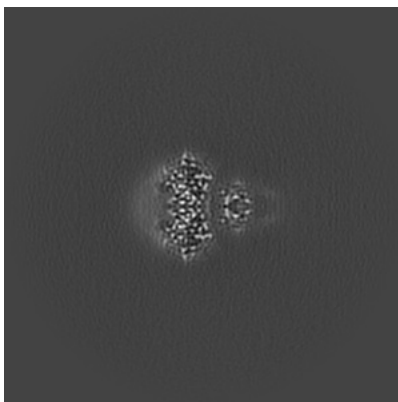
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

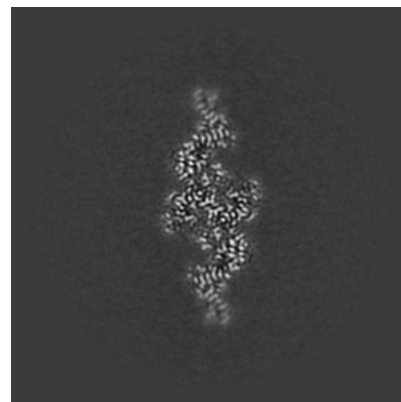
6.2.1 Primary map



X Index: 192

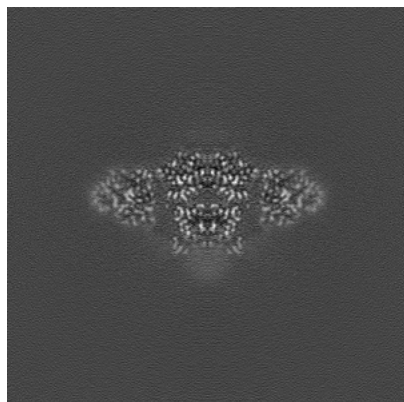


Y Index: 192

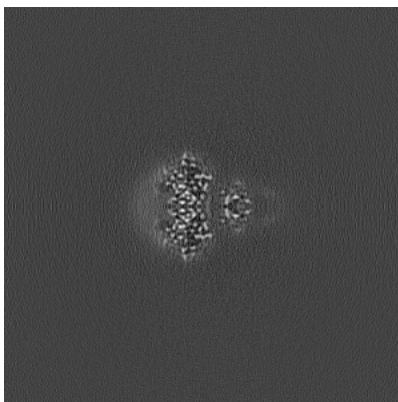


Z Index: 192

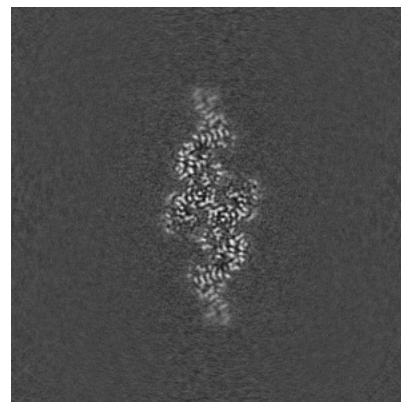
6.2.2 Raw map



X Index: 192



Y Index: 192

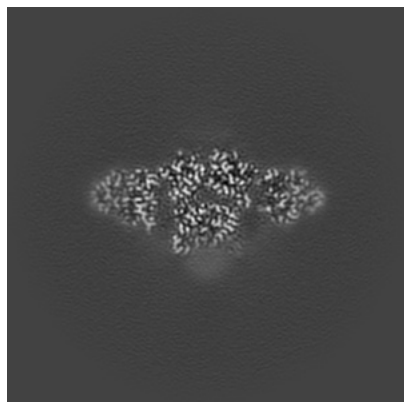


Z Index: 192

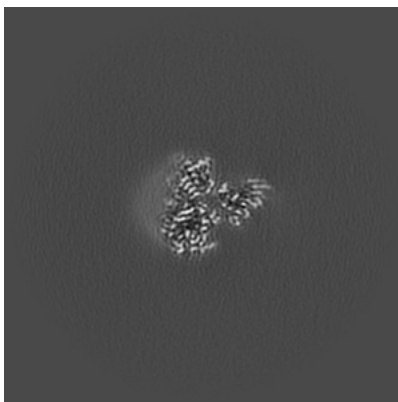
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

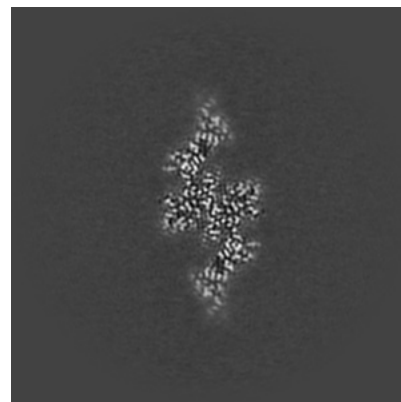
6.3.1 Primary map



X Index: 194

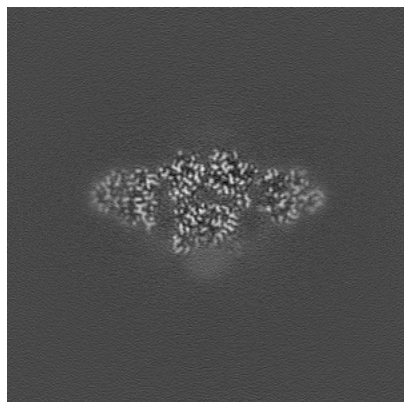


Y Index: 200

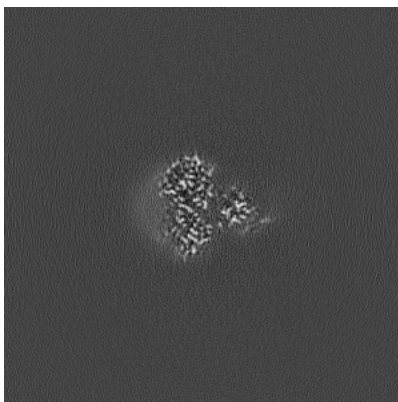


Z Index: 187

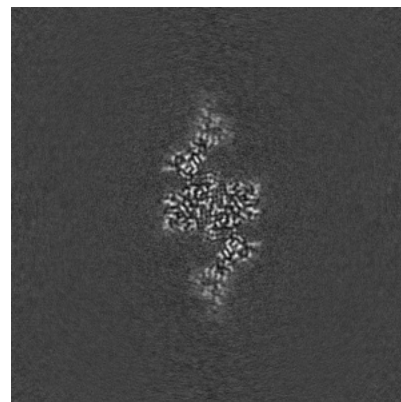
6.3.2 Raw map



X Index: 194



Y Index: 187

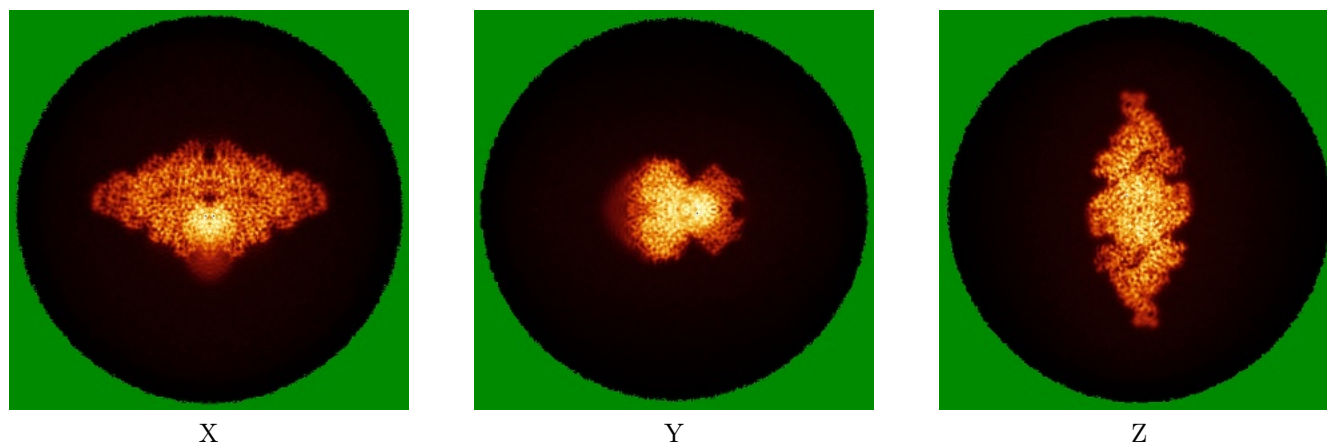


Z Index: 186

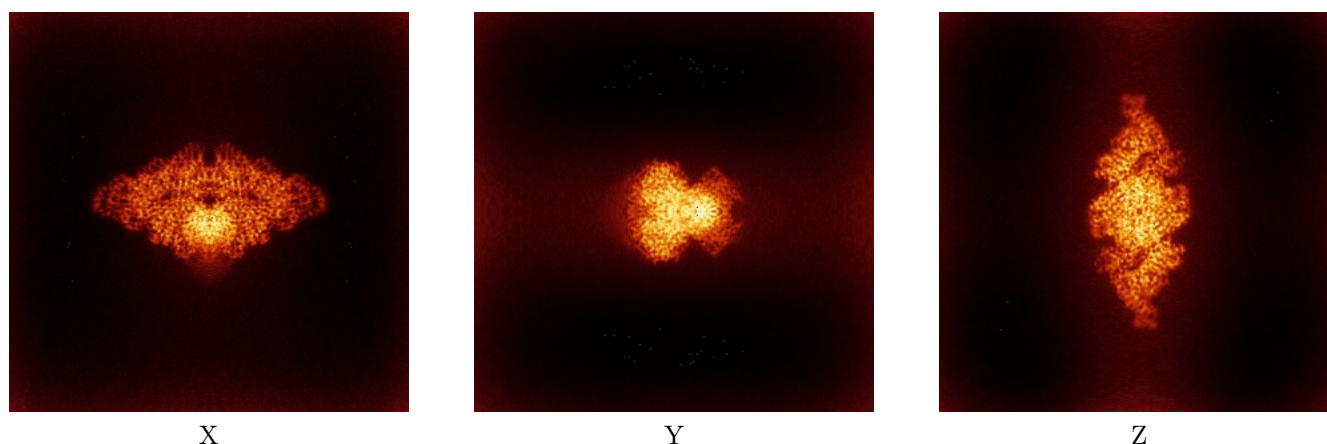
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

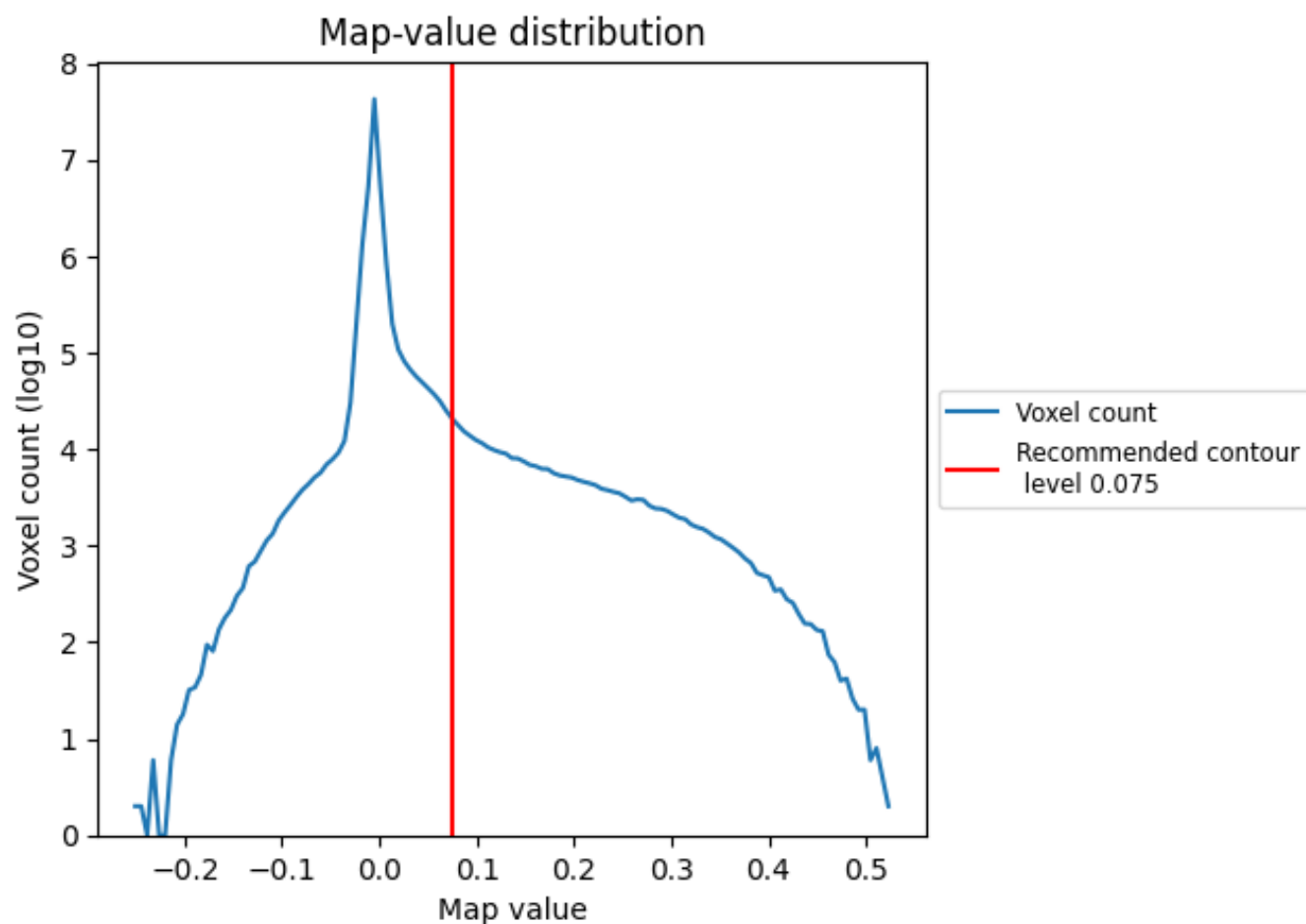
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

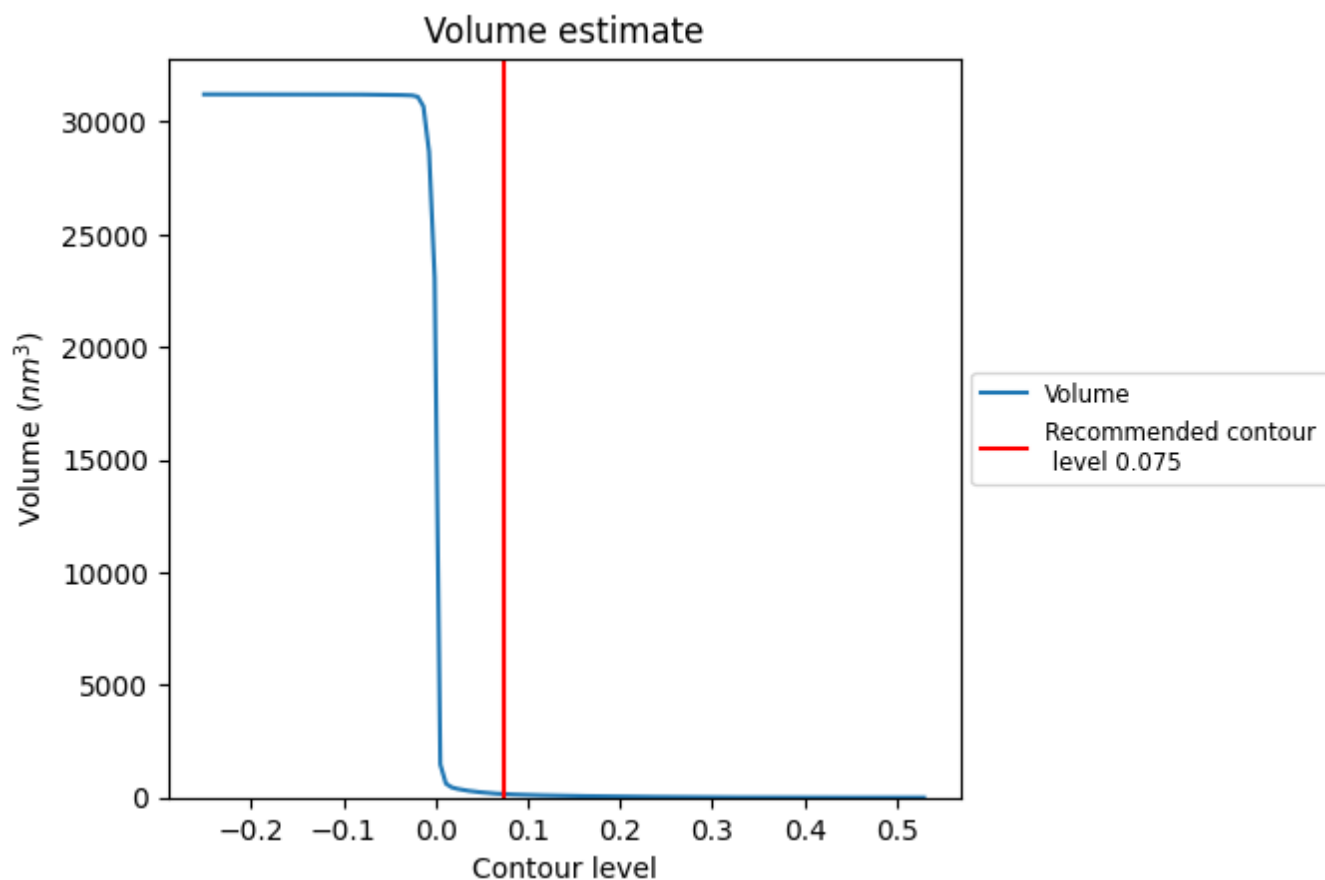
This section contains the results of statistical analysis of the map.

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.

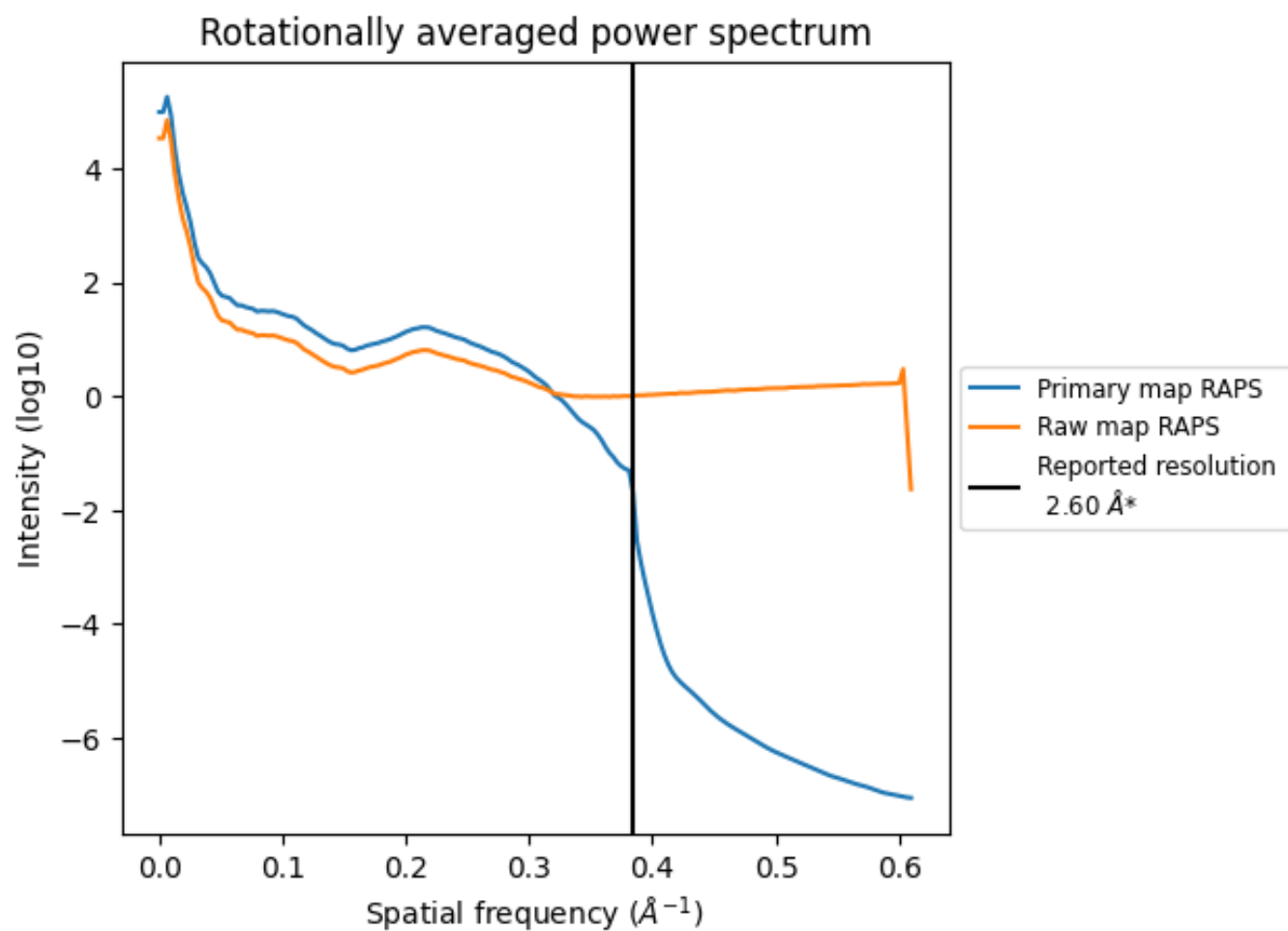
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 153 nm^3 ; this corresponds to an approximate mass of 138 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 ⓘ

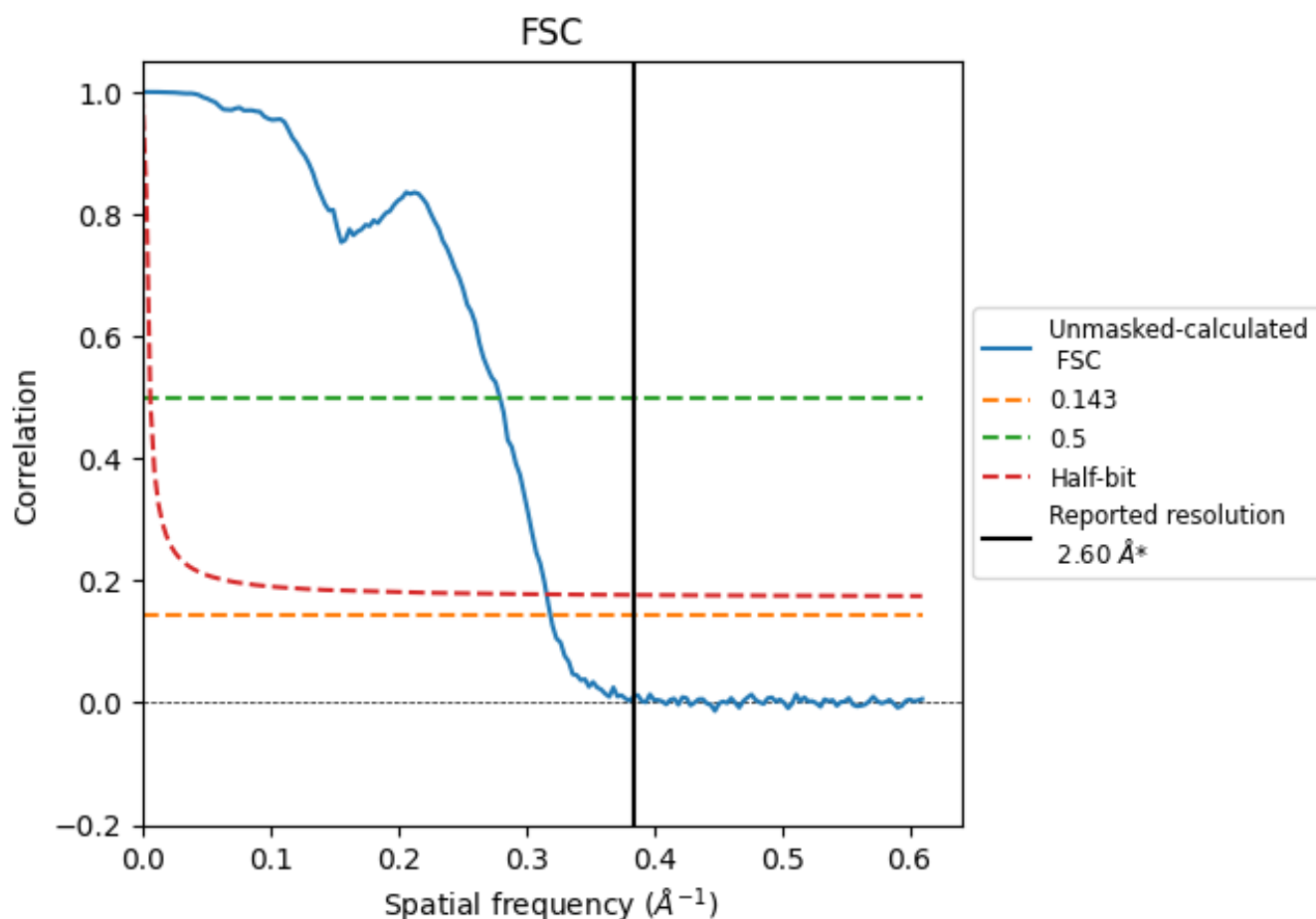


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 $0.385 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

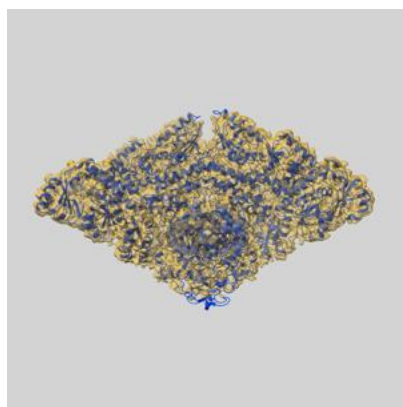
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.13	3.58	3.16

*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 3.13 differs from the reported value 2.6 by more than 10 %

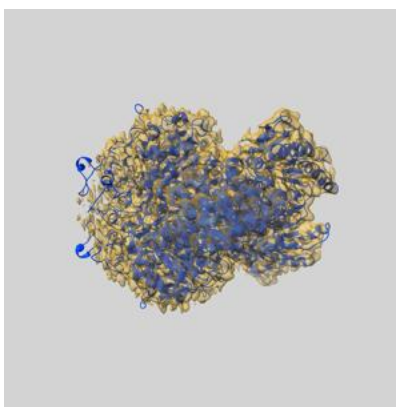
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16630 and PDB model 8CG4. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

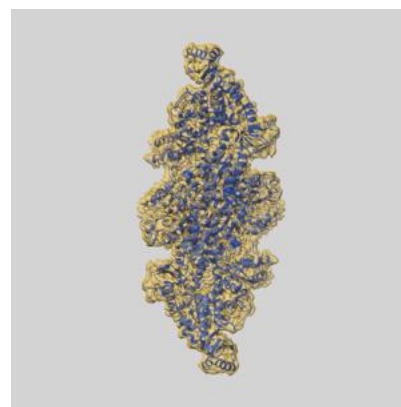
9.1 Map-model overlay [i](#)



X



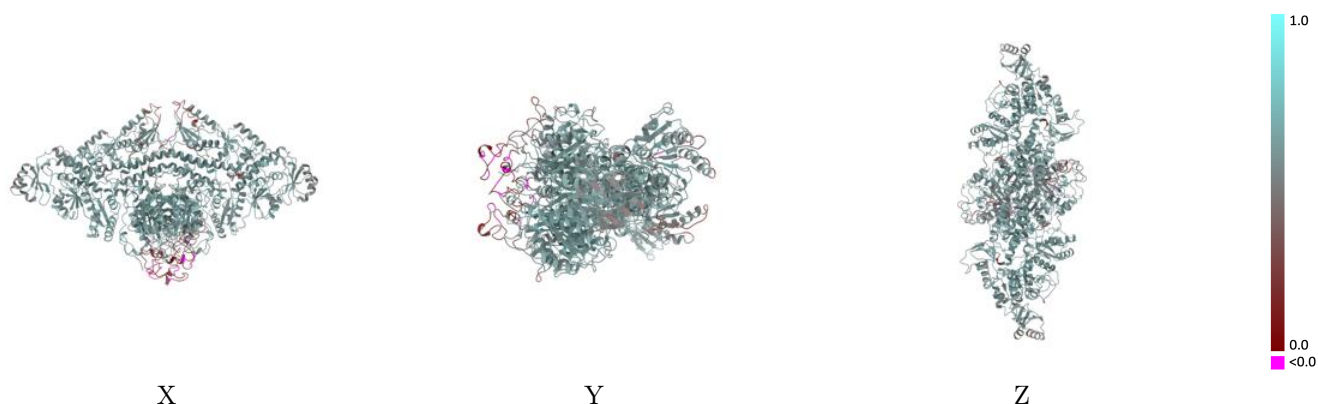
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.075 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](#)

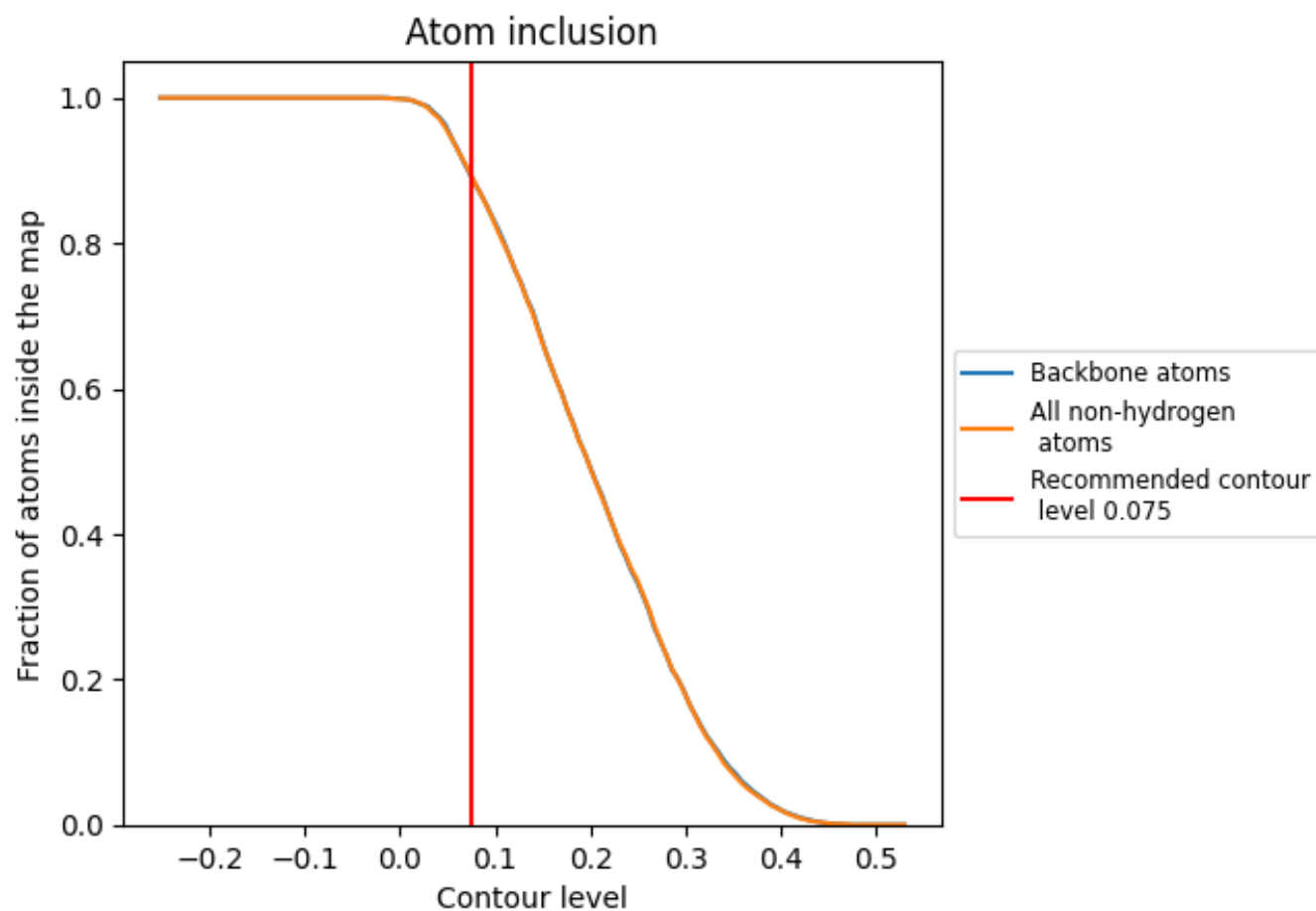


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 89% 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 (0.075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8930	0.5520
A	0.8930	0.5510
B	0.8960	0.5540

