



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:34 AM UTC

PDB ID : 8FW9 / pdb_00008fw9
EMDB ID : EMD-29498
Title : Cryo-EM structure of full-length human NLRC4 inflammasome with C12 symmetry
Authors : Matico, R.E.; Yu, X.; Miller, R.; Somani, S.; Ricketts, M.D.; Kumar, N.; Steele, R.A.; Medley, Q.; Berger, S.; Faustin, B.; Sharma, S.
Deposited on : 2023-01-20
Resolution : 4.46 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:

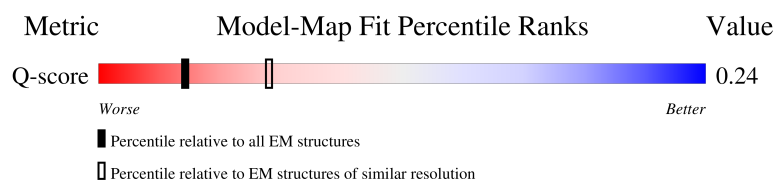
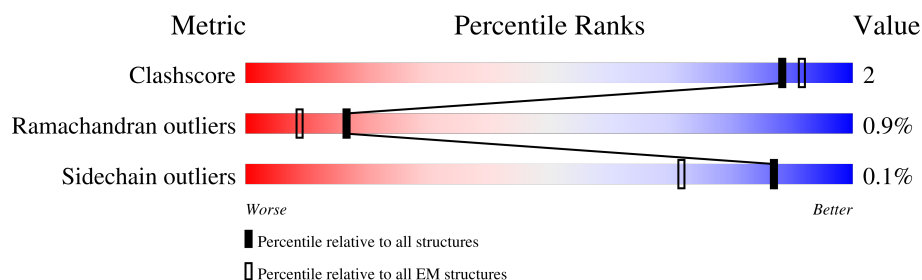
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.46 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	3001 (3.96 - 4.96)

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	1030	
1	B	1030	
1	C	1030	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 21612 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 NLR family CARD domain-containing protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	904	Total	C	N	O	S	0	0
			7204	4608	1220	1339	37		
1	B	904	Total	C	N	O	S	0	0
			7204	4608	1220	1339	37		
1	C	904	Total	C	N	O	S	0	0
			7204	4608	1220	1339	37		

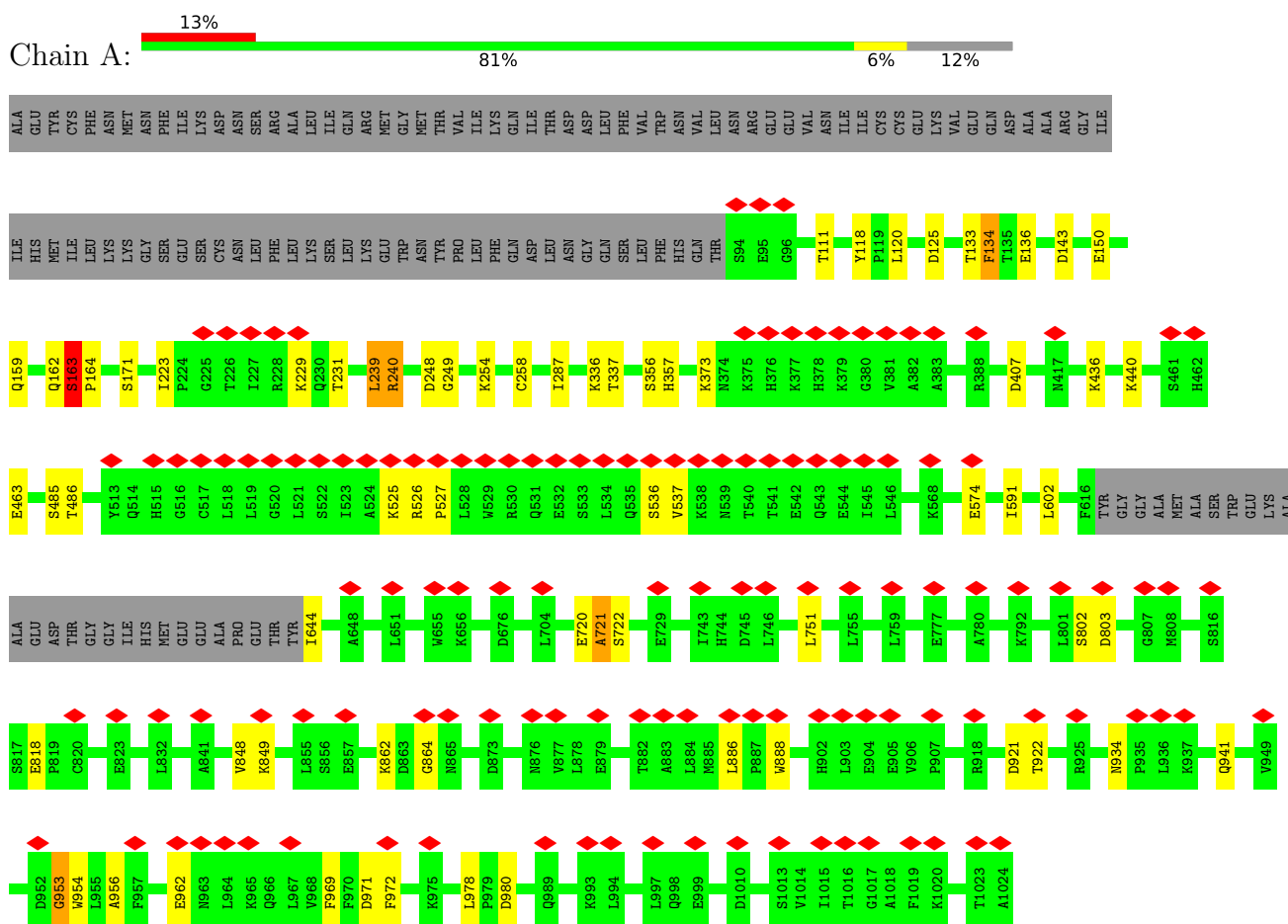
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	ALA	-	expression tag	UNP Q9NPP4
A	-4	GLU	-	expression tag	UNP Q9NPP4
A	-3	TYR	-	expression tag	UNP Q9NPP4
A	-2	CYS	-	expression tag	UNP Q9NPP4
A	-1	PHE	-	expression tag	UNP Q9NPP4
A	0	ASN	-	expression tag	UNP Q9NPP4
B	-5	ALA	-	expression tag	UNP Q9NPP4
B	-4	GLU	-	expression tag	UNP Q9NPP4
B	-3	TYR	-	expression tag	UNP Q9NPP4
B	-2	CYS	-	expression tag	UNP Q9NPP4
B	-1	PHE	-	expression tag	UNP Q9NPP4
B	0	ASN	-	expression tag	UNP Q9NPP4
C	-5	ALA	-	expression tag	UNP Q9NPP4
C	-4	GLU	-	expression tag	UNP Q9NPP4
C	-3	TYR	-	expression tag	UNP Q9NPP4
C	-2	CYS	-	expression tag	UNP Q9NPP4
C	-1	PHE	-	expression tag	UNP Q9NPP4
C	0	ASN	-	expression tag	UNP Q9NPP4

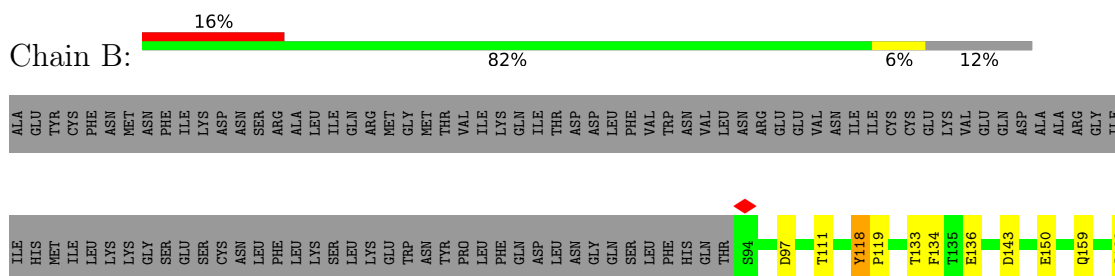
3 Residue-property plots

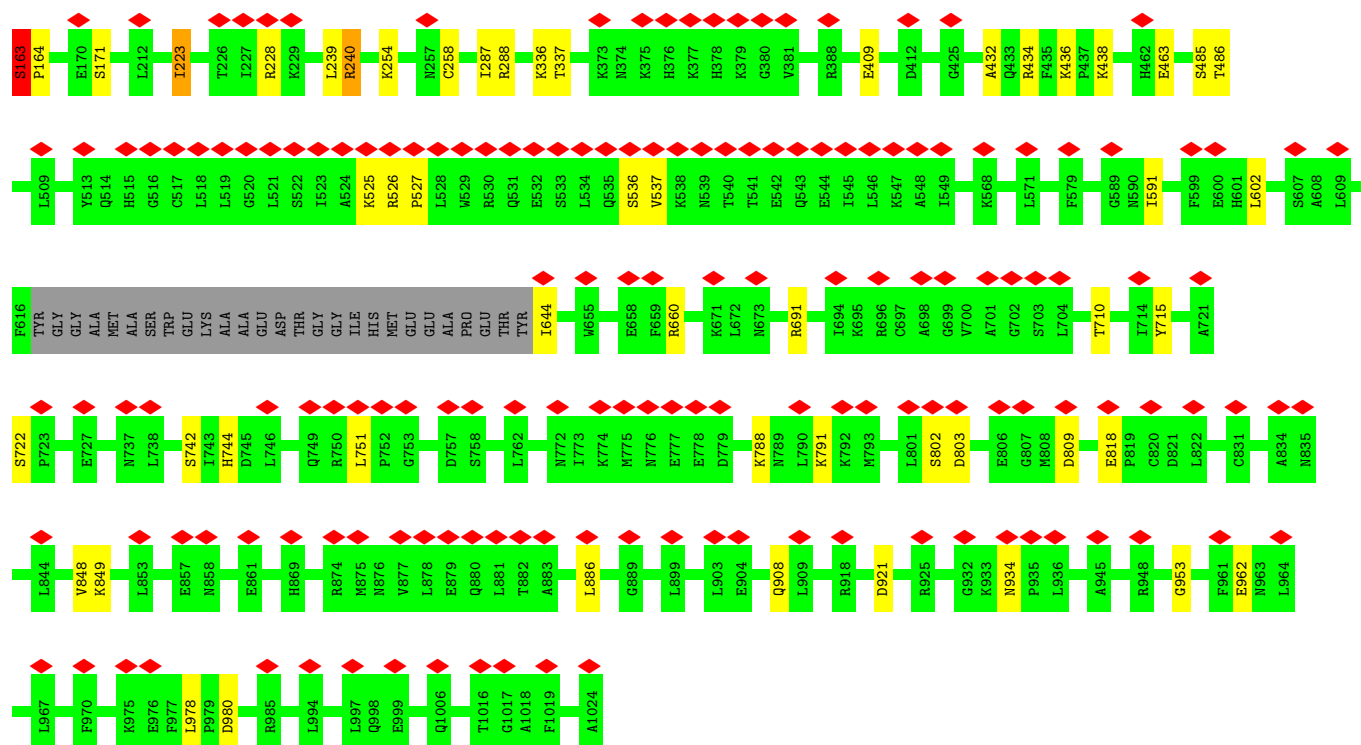
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: NLR family CARD domain-containing protein 4

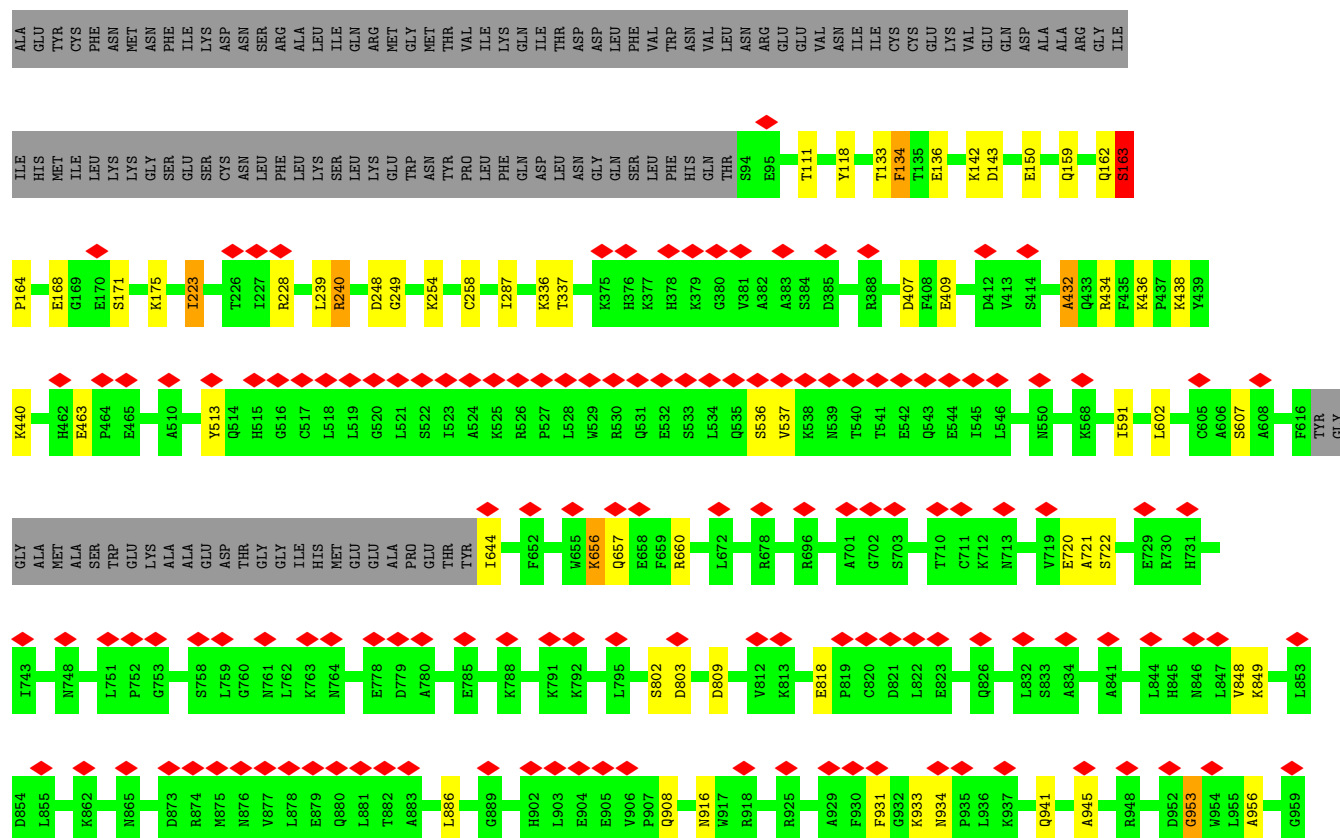
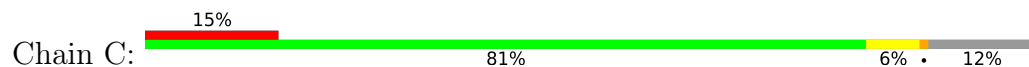


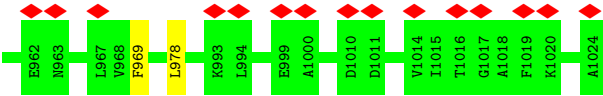
• Molecule 1: NLR family CARD domain-containing protein 4





• Molecule 1: NLR family CARD domain-containing protein 4





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21406	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.408	Depositor
Minimum map value	-0.201	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.084	Depositor
Map size ($\text{\AA}$)	455.04, 455.04, 455.04	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.948, 0.948, 0.948	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	0.66	0/7337	0.88	41/9897 (0.4%)
1	B	0.64	0/7337	0.87	40/9897 (0.4%)
1	C	0.65	0/7337	0.87	38/9897 (0.4%)
All	All	0.65	0/22011	0.87	119/29691 (0.4%)

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	1
1	B	0	1
1	C	0	1
All	All	0	3

There are no bond length outliers.

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	223	ILE	CA-C-N	8.04	128.09	119.89
1	B	223	ILE	C-N-CA	8.04	128.09	119.89
1	B	254	LYS	CA-C-N	7.79	127.51	119.56
1	B	254	LYS	C-N-CA	7.79	127.51	119.56
1	A	818	GLU	CA-C-N	7.60	127.65	119.90
1	A	818	GLU	C-N-CA	7.60	127.65	119.90
1	A	602	LEU	CA-C-N	7.40	127.36	120.03
1	A	602	LEU	C-N-CA	7.40	127.36	120.03
1	A	591	ILE	CA-C-N	7.22	127.22	119.78
1	A	591	ILE	C-N-CA	7.22	127.22	119.78
1	A	254	LYS	CA-C-N	7.15	126.78	119.56
1	A	254	LYS	C-N-CA	7.15	126.78	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	602	LEU	CA-C-N	7.11	127.07	120.03
1	C	602	LEU	C-N-CA	7.11	127.07	120.03
1	B	751	LEU	CA-C-N	7.00	126.25	118.97
1	B	751	LEU	C-N-CA	7.00	126.25	118.97
1	C	818	GLU	CA-C-N	6.97	127.01	119.90
1	C	818	GLU	C-N-CA	6.97	127.01	119.90
1	C	886	LEU	CA-C-N	6.90	126.82	119.85
1	C	886	LEU	C-N-CA	6.90	126.82	119.85
1	C	254	LYS	CA-C-N	6.85	126.48	119.56
1	C	254	LYS	C-N-CA	6.85	126.48	119.56
1	A	436	LYS	CA-C-N	6.80	126.72	119.85
1	A	436	LYS	C-N-CA	6.80	126.72	119.85
1	B	336	LYS	N-CA-C	-6.71	106.05	114.56
1	A	336	LYS	N-CA-C	-6.64	106.12	114.56
1	A	886	LEU	CA-C-N	6.61	126.59	119.78
1	A	886	LEU	C-N-CA	6.61	126.59	119.78
1	A	136	GLU	CA-C-N	6.60	126.56	120.03
1	A	136	GLU	C-N-CA	6.60	126.56	120.03
1	C	336	LYS	N-CA-C	-6.59	106.18	114.56
1	A	722	SER	CA-C-N	6.48	126.40	119.85
1	A	722	SER	C-N-CA	6.48	126.40	119.85
1	C	136	GLU	CA-C-N	6.47	126.43	120.03
1	C	136	GLU	C-N-CA	6.47	126.43	120.03
1	A	934	ASN	CA-C-N	6.40	126.16	119.76
1	A	934	ASN	C-N-CA	6.40	126.16	119.76
1	B	111	THR	CA-C-N	6.39	126.07	119.56
1	B	111	THR	C-N-CA	6.39	126.07	119.56
1	B	886	LEU	CA-C-N	6.36	126.33	120.03
1	B	886	LEU	C-N-CA	6.36	126.33	120.03
1	A	337	THR	CA-C-N	6.36	126.57	119.32
1	A	337	THR	C-N-CA	6.36	126.57	119.32
1	B	136	GLU	CA-C-N	6.35	126.53	120.31
1	B	136	GLU	C-N-CA	6.35	126.53	120.31
1	C	463	GLU	CA-C-N	6.34	126.82	119.47
1	C	463	GLU	C-N-CA	6.34	126.82	119.47
1	B	436	LYS	CA-C-N	6.28	126.19	119.85
1	B	436	LYS	C-N-CA	6.28	126.19	119.85
1	B	591	ILE	CA-C-N	6.28	126.24	119.78
1	B	591	ILE	C-N-CA	6.28	126.24	119.78
1	B	818	GLU	CA-C-N	6.26	126.63	119.93
1	B	818	GLU	C-N-CA	6.26	126.63	119.93
1	B	602	LEU	CA-C-N	6.24	126.21	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	602	LEU	C-N-CA	6.24	126.21	120.03
1	C	436	LYS	CA-C-N	6.22	126.24	119.90
1	C	436	LYS	C-N-CA	6.22	126.24	119.90
1	B	463	GLU	CA-C-N	6.14	126.60	119.47
1	B	463	GLU	C-N-CA	6.14	126.60	119.47
1	C	111	THR	CA-C-N	6.13	125.81	119.56
1	C	111	THR	C-N-CA	6.13	125.81	119.56
1	A	118	TYR	CA-C-N	6.11	125.73	119.56
1	A	118	TYR	C-N-CA	6.11	125.73	119.56
1	A	980	ASP	CA-C-N	6.05	126.22	119.32
1	A	980	ASP	C-N-CA	6.05	126.22	119.32
1	B	258	CYS	CA-C-N	6.04	125.73	119.56
1	B	258	CYS	C-N-CA	6.04	125.73	119.56
1	C	337	THR	CA-C-N	6.03	126.19	119.32
1	C	337	THR	C-N-CA	6.03	126.19	119.32
1	C	722	SER	CA-C-N	6.02	125.94	119.85
1	C	722	SER	C-N-CA	6.02	125.94	119.85
1	A	258	CYS	CA-C-N	5.96	125.64	119.56
1	A	258	CYS	C-N-CA	5.96	125.64	119.56
1	C	258	CYS	CA-C-N	5.96	125.64	119.56
1	C	258	CYS	C-N-CA	5.96	125.64	119.56
1	B	722	SER	CA-C-N	5.93	125.87	119.76
1	B	722	SER	C-N-CA	5.93	125.87	119.76
1	B	978	LEU	CA-C-N	5.88	126.22	119.93
1	B	978	LEU	C-N-CA	5.88	126.22	119.93
1	C	591	ILE	CA-C-N	5.84	125.75	119.85
1	C	591	ILE	C-N-CA	5.84	125.75	119.85
1	A	463	GLU	CA-C-N	5.83	126.23	119.47
1	A	463	GLU	C-N-CA	5.83	126.23	119.47
1	B	337	THR	CA-C-N	5.81	127.11	119.84
1	B	337	THR	C-N-CA	5.81	127.11	119.84
1	A	978	LEU	CA-C-N	5.77	125.53	119.76
1	A	978	LEU	C-N-CA	5.77	125.53	119.76
1	C	934	ASN	CA-C-N	5.75	125.69	119.76
1	C	934	ASN	C-N-CA	5.75	125.69	119.76
1	B	934	ASN	CA-C-N	5.73	125.66	119.76
1	B	934	ASN	C-N-CA	5.73	125.66	119.76
1	C	644	ILE	CA-C-N	5.71	125.47	119.76
1	C	644	ILE	C-N-CA	5.71	125.47	119.76
1	A	111	THR	CA-C-N	5.59	125.43	119.28
1	A	111	THR	C-N-CA	5.59	125.43	119.28
1	A	953	GLY	CA-C-N	5.55	131.68	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	953	GLY	C-N-CA	5.55	131.68	121.70
1	B	644	ILE	CA-C-N	5.34	125.24	119.85
1	B	644	ILE	C-N-CA	5.34	125.24	119.85
1	A	751	LEU	CA-C-N	5.28	125.54	119.83
1	A	751	LEU	C-N-CA	5.28	125.54	119.83
1	C	513	TYR	N-CA-C	-5.25	107.54	114.31
1	B	118	TYR	CA-C-N	5.25	125.05	119.28
1	B	118	TYR	C-N-CA	5.25	125.05	119.28
1	C	978	LEU	CA-C-N	5.22	125.47	119.83
1	C	978	LEU	C-N-CA	5.22	125.47	119.83
1	A	223	ILE	CA-C-N	5.21	125.21	119.90
1	A	223	ILE	C-N-CA	5.21	125.21	119.90
1	C	953	GLY	CA-C-N	5.18	131.02	121.70
1	C	953	GLY	C-N-CA	5.18	131.02	121.70
1	A	644	ILE	CA-C-N	5.15	125.60	120.14
1	A	644	ILE	C-N-CA	5.15	125.60	120.14
1	B	980	ASP	CA-C-N	5.12	126.24	119.84
1	B	980	ASP	C-N-CA	5.12	126.24	119.84
1	B	953	GLY	N-CA-C	-5.09	101.11	113.18
1	C	223	ILE	CA-C-N	5.08	125.02	119.78
1	C	223	ILE	C-N-CA	5.08	125.02	119.78
1	C	118	TYR	CA-C-N	5.01	124.79	119.28
1	C	118	TYR	C-N-CA	5.01	124.79	119.28

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	163	SER	Peptide
1	B	163	SER	Peptide
1	C	163	SER	Peptide

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	7204	0	7307	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	7204	0	7307	27	0
1	C	7204	0	7307	27	0
All	All	21612	0	21921	83	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 2.

All (83) 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:485:SER:OG	1:B:486:THR:N	2.35	0.59
1:C:407:ASP:OD1	1:C:440:LYS:NZ	2.38	0.56
1:C:656:LYS:HG2	1:C:657:GLN:H	1.72	0.55
1:A:407:ASP:OD1	1:A:440:LYS:NZ	2.40	0.54
1:A:720:GLU:O	1:A:721:ALA:C	2.50	0.54
1:A:485:SER:OG	1:A:486:THR:N	2.33	0.53
1:B:409:GLU:OE2	1:B:438:LYS:NZ	2.41	0.52
1:A:133:THR:O	1:A:134:PHE:C	2.54	0.51
1:B:962:GLU:N	1:B:962:GLU:OE1	2.43	0.50
1:B:239:LEU:O	1:B:240:ARG:HB3	2.11	0.50
1:B:742:SER:OG	1:B:744:HIS:NE2	2.37	0.50
1:B:133:THR:O	1:B:134:PHE:C	2.55	0.50
1:C:175:LYS:NZ	1:C:248:ASP:OD2	2.35	0.50
1:C:848:VAL:O	1:C:849:LYS:HB2	2.12	0.49
1:C:536:SER:OG	1:C:537:VAL:N	2.45	0.49
1:C:239:LEU:O	1:C:240:ARG:HB3	2.12	0.49
1:B:691:ARG:NE	1:B:715:TYR:OH	2.45	0.48
1:C:162:GLN:C	1:C:163:SER:O	2.52	0.48
1:B:848:VAL:O	1:B:849:LYS:HB2	2.13	0.48
1:C:223:ILE:O	1:C:228:ARG:NH1	2.45	0.48
1:C:409:GLU:OE2	1:C:438:LYS:NZ	2.45	0.48
1:C:656:LYS:HG2	1:C:657:GLN:N	2.28	0.48
1:A:962:GLU:N	1:A:962:GLU:OE1	2.46	0.47
1:C:916:ASN:H	1:C:945:ALA:HB3	1.80	0.47
1:B:536:SER:OG	1:B:537:VAL:N	2.47	0.46
1:C:239:LEU:O	1:C:240:ARG:CB	2.63	0.46
1:C:720:GLU:O	1:C:721:ALA:C	2.56	0.46
1:B:239:LEU:O	1:B:240:ARG:CB	2.64	0.45
1:C:953:GLY:N	1:C:956:ALA:H	2.13	0.45
1:B:97:ASP:OD1	1:B:97:ASP:N	2.49	0.45
1:C:931:PHE:C	1:C:933:LYS:HB3	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:848:VAL:O	1:A:849:LYS:HB2	2.16	0.45
1:A:953:GLY:N	1:A:956:ALA:H	2.15	0.45
1:A:536:SER:OG	1:A:537:VAL:N	2.49	0.45
1:B:809:ASP:OD1	1:B:809:ASP:N	2.46	0.45
1:B:223:ILE:O	1:B:228:ARG:NH1	2.50	0.44
1:A:120:LEU:O	1:A:373:LYS:NZ	2.45	0.44
1:A:525:LYS:O	1:A:526:ARG:C	2.59	0.44
1:B:525:LYS:O	1:B:526:ARG:C	2.60	0.44
1:C:809:ASP:OD1	1:C:809:ASP:N	2.49	0.44
1:A:163:SER:HB2	1:A:164:PRO:CD	2.48	0.44
1:A:574:GLU:OE1	1:A:574:GLU:N	2.47	0.44
1:C:248:ASP:OD1	1:C:249:GLY:N	2.50	0.43
1:C:432:ALA:O	1:C:434:ARG:N	2.51	0.43
1:A:802:SER:OG	1:A:803:ASP:N	2.51	0.43
1:A:941:GLN:HG2	1:A:969:PHE:CE2	2.53	0.43
1:A:125:ASP:OD2	1:B:288:ARG:NH2	2.49	0.43
1:B:163:SER:CB	1:B:164:PRO:CD	2.96	0.43
1:A:888:TRP:CD1	1:A:888:TRP:C	2.96	0.43
1:A:921:ASP:OD1	1:A:922:THR:N	2.52	0.43
1:A:162:GLN:C	1:A:163:SER:O	2.62	0.43
1:A:163:SER:CB	1:A:164:PRO:CD	2.97	0.43
1:A:862:LYS:C	1:A:864:GLY:H	2.26	0.43
1:B:162:GLN:C	1:B:163:SER:O	2.60	0.43
1:C:941:GLN:HG2	1:C:969:PHE:CE2	2.54	0.43
1:A:239:LEU:O	1:A:240:ARG:HB3	2.18	0.42
1:A:526:ARG:HB3	1:A:527:PRO:HD3	2.01	0.42
1:A:526:ARG:N	1:A:527:PRO:CD	2.82	0.42
1:B:802:SER:OG	1:B:803:ASP:N	2.51	0.42
1:B:526:ARG:N	1:B:527:PRO:CD	2.82	0.42
1:A:248:ASP:OD1	1:A:249:GLY:N	2.52	0.42
1:B:432:ALA:O	1:B:434:ARG:N	2.52	0.42
1:A:143:ASP:OD1	1:A:143:ASP:C	2.62	0.42
1:C:159:GLN:OE1	1:C:159:GLN:N	2.49	0.42
1:C:143:ASP:OD1	1:C:143:ASP:C	2.62	0.42
1:B:921:ASP:N	1:B:921:ASP:OD1	2.51	0.42
1:B:118:TYR:HA	1:B:119:PRO:HD2	1.92	0.42
1:C:133:THR:O	1:C:134:PHE:C	2.61	0.41
1:C:142:LYS:NZ	1:C:168:GLU:OE1	2.51	0.41
1:C:607:SER:O	1:C:660:ARG:NH1	2.53	0.41
1:C:802:SER:OG	1:C:803:ASP:N	2.52	0.41
1:A:159:GLN:OE1	1:A:159:GLN:N	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ASP:C	1:B:143:ASP:OD1	2.63	0.41
1:A:953:GLY:HA2	1:A:954:TRP:C	2.46	0.41
1:A:971:ASP:O	1:A:972:PHE:C	2.64	0.41
1:B:159:GLN:OE1	1:B:159:GLN:N	2.49	0.41
1:A:229:LYS:C	1:A:231:THR:H	2.29	0.41
1:B:163:SER:HB2	1:B:164:PRO:CD	2.51	0.41
1:C:848:VAL:O	1:C:849:LYS:CB	2.68	0.41
1:B:788:LYS:O	1:B:791:LYS:NZ	2.54	0.40
1:A:356:SER:O	1:A:357:HIS:C	2.64	0.40
1:C:163:SER:CB	1:C:164:PRO:CD	2.99	0.40
1:B:526:ARG:HB3	1:B:527:PRO:HD3	2.02	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	900/1030 (87%)	845 (94%)	47 (5%)	8 (1%)	14	49
1	B	900/1030 (87%)	849 (94%)	44 (5%)	7 (1%)	16	53
1	C	900/1030 (87%)	846 (94%)	46 (5%)	8 (1%)	14	49
All	All	2700/3090 (87%)	2540 (94%)	137 (5%)	23 (1%)	16	49

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	SER
1	A	240	ARG
1	B	240	ARG
1	B	660	ARG
1	C	240	ARG
1	A	239	LEU

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Mol	Chain	Res	Type
1	A	721	ALA
1	B	171	SER
1	B	908	GLN
1	C	134	PHE
1	C	171	SER
1	C	908	GLN
1	B	163	SER
1	C	432	ALA
1	A	150	GLU
1	A	287	ILE
1	C	163	SER
1	A	134	PHE
1	B	150	GLU
1	C	150	GLU
1	B	287	ILE
1	C	287	ILE
1	A	163	SER

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	808/917 (88%)	808 (100%)	0	100	100
1	B	808/917 (88%)	807 (100%)	1 (0%)	88	88
1	C	808/917 (88%)	807 (100%)	1 (0%)	88	88
All	All	2424/2751 (88%)	2422 (100%)	2 (0%)	87	88

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	710	THR
1	C	656	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	HIS
1	A	550	ASN
1	A	693	GLN
1	B	286	HIS
1	B	372	GLN
1	B	693	GLN
1	B	998	GLN
1	C	116	ASN
1	C	145	HIS
1	C	378	HIS
1	C	601	HIS
1	C	693	GLN
1	C	869	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.

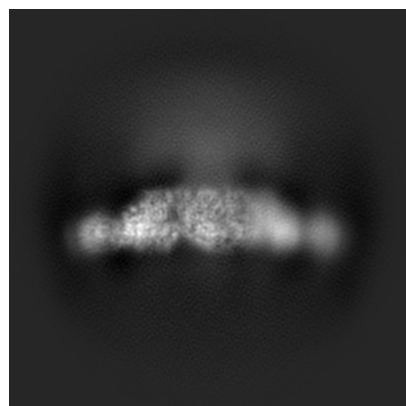
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29498. These allow visual inspection of the internal detail of the map and identification of artifacts.

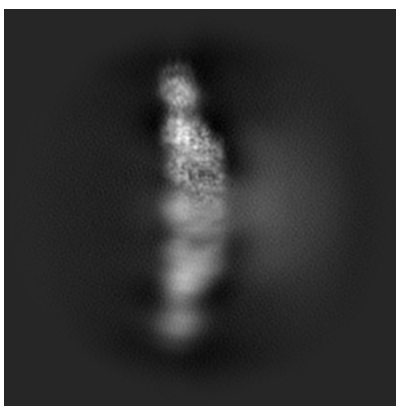
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

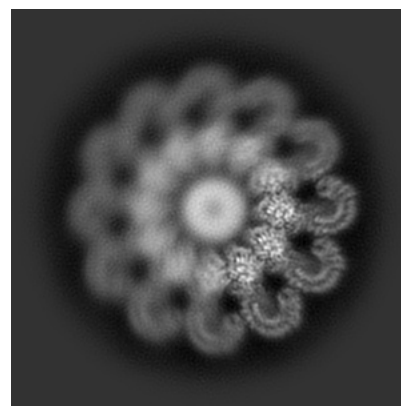
6.1.1 Primary map



X

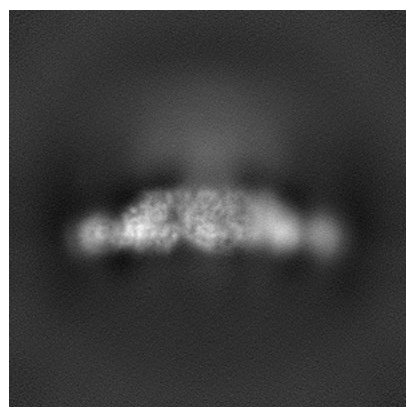


Y

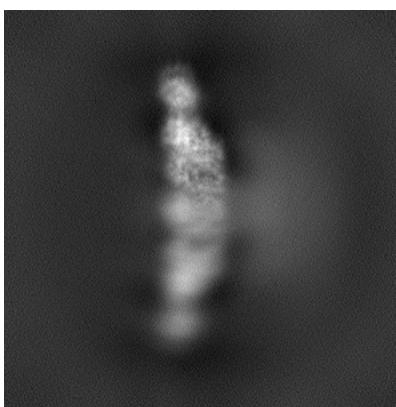


Z

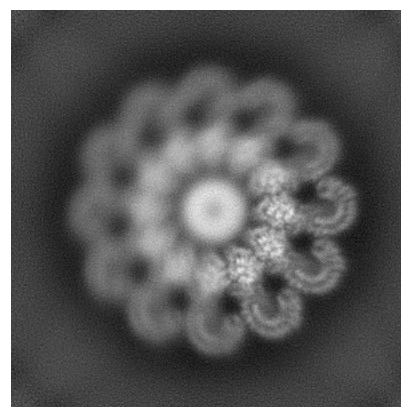
6.1.2 Raw map



X



Y

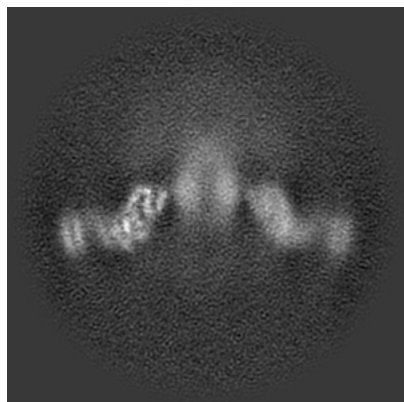


Z

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

6.2 Central slices [i](#)

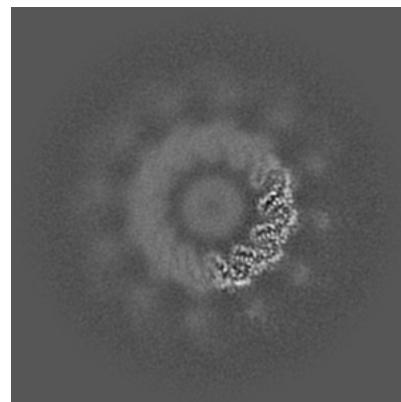
6.2.1 Primary map



X Index: 240

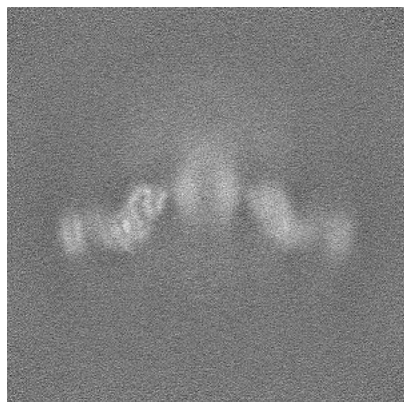


Y Index: 240

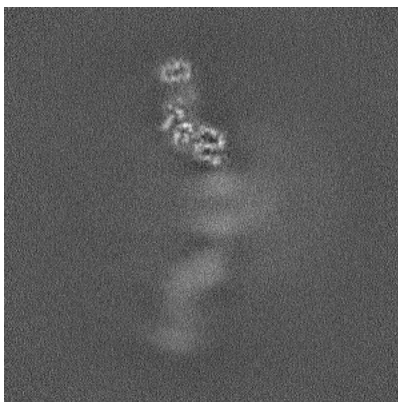


Z Index: 240

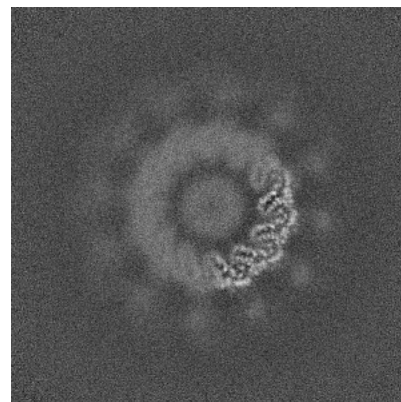
6.2.2 Raw map



X Index: 240



Y Index: 240

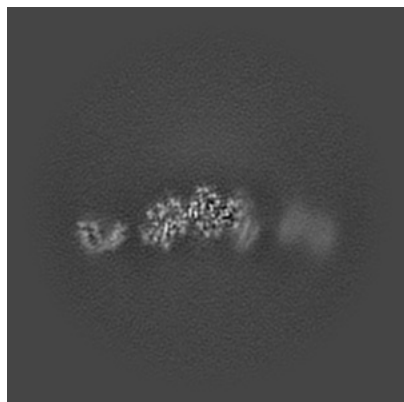


Z Index: 240

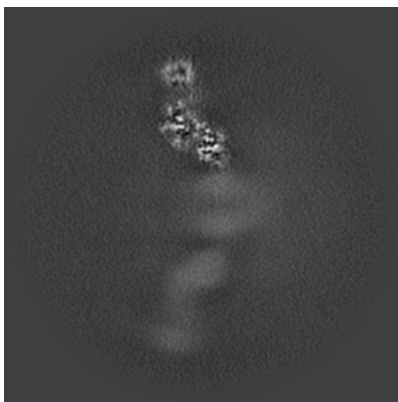
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

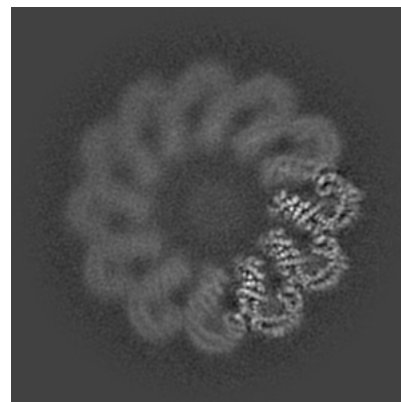
6.3.1 Primary map



X Index: 323

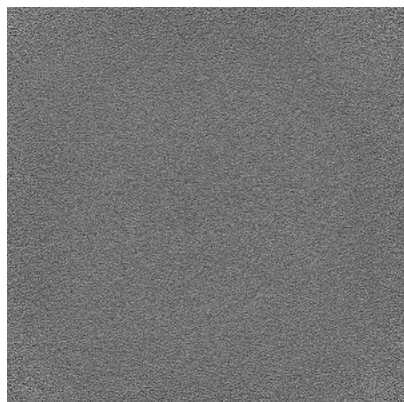


Y Index: 236

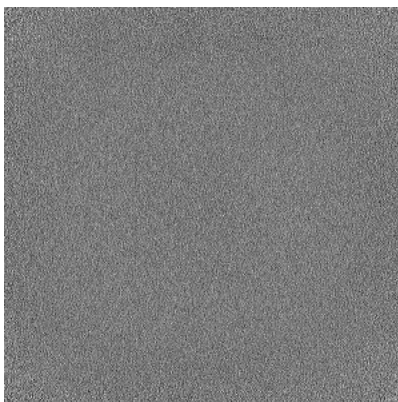


Z Index: 210

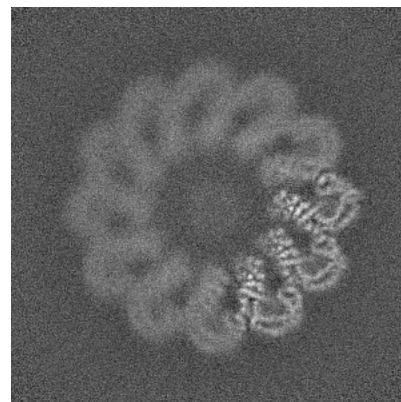
6.3.2 Raw map



X Index: 0



Y Index: 0

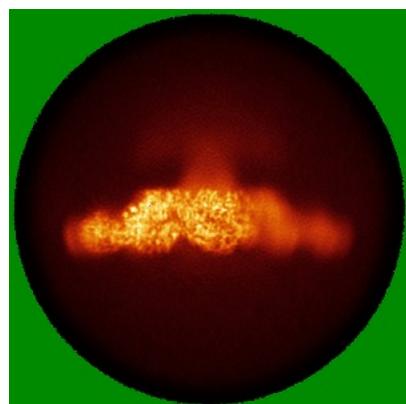


Z Index: 211

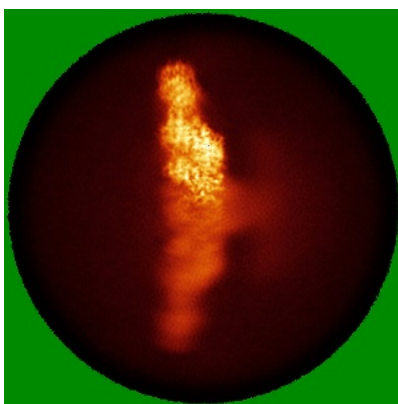
The images above show the largest variance slices of the map in three orthogonal directions.

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

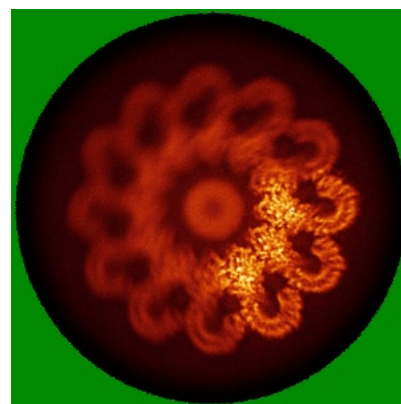
6.4.1 Primary map



X

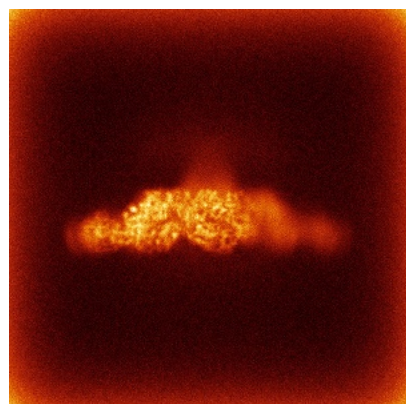


Y

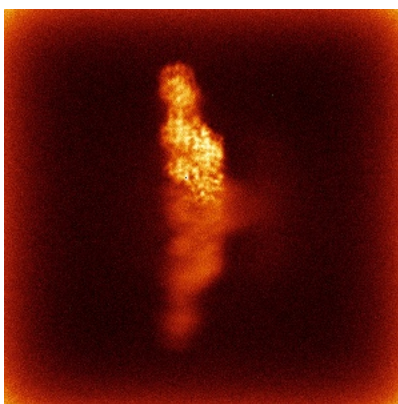


Z

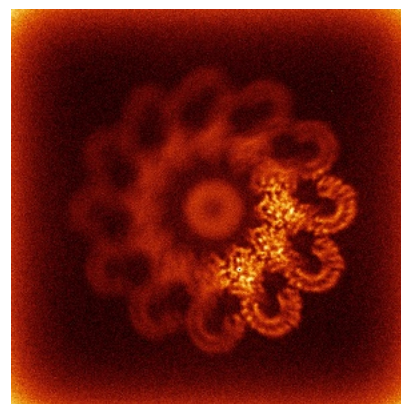
6.4.2 Raw map



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



The images above show the 3D surface view of the map at the recommended contour level 0.084. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

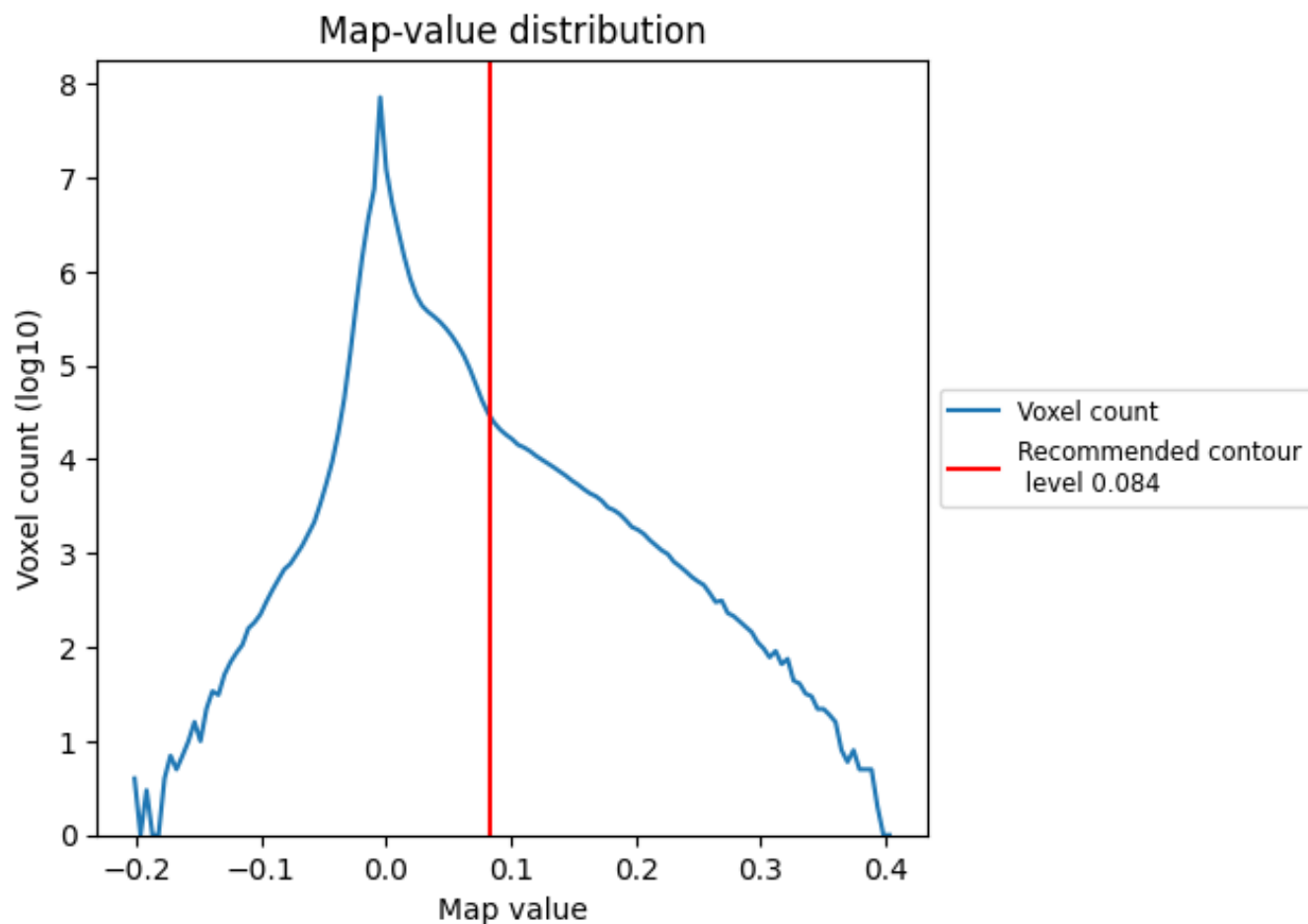
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

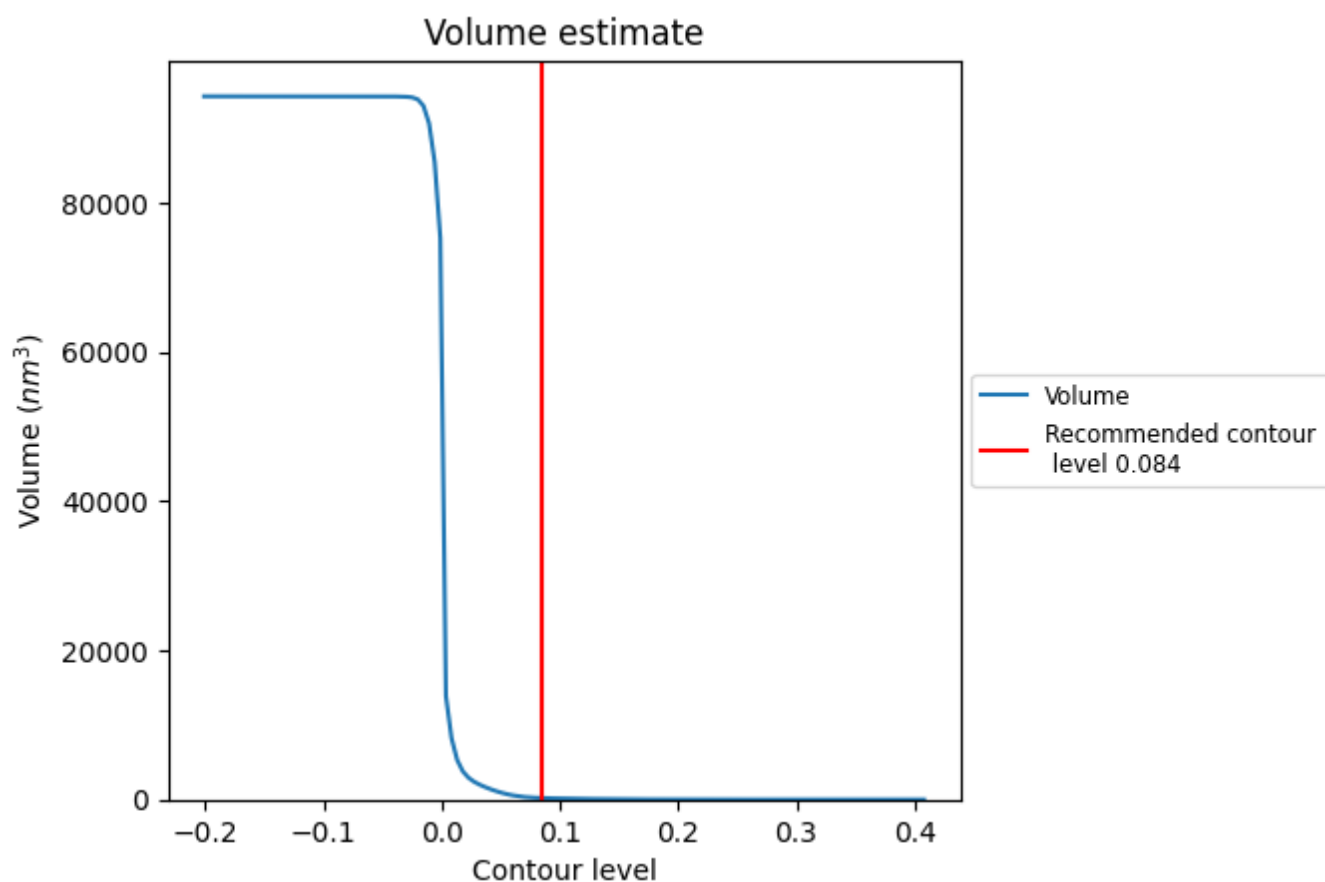
This section contains the results of statistical analysis of the map.

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.

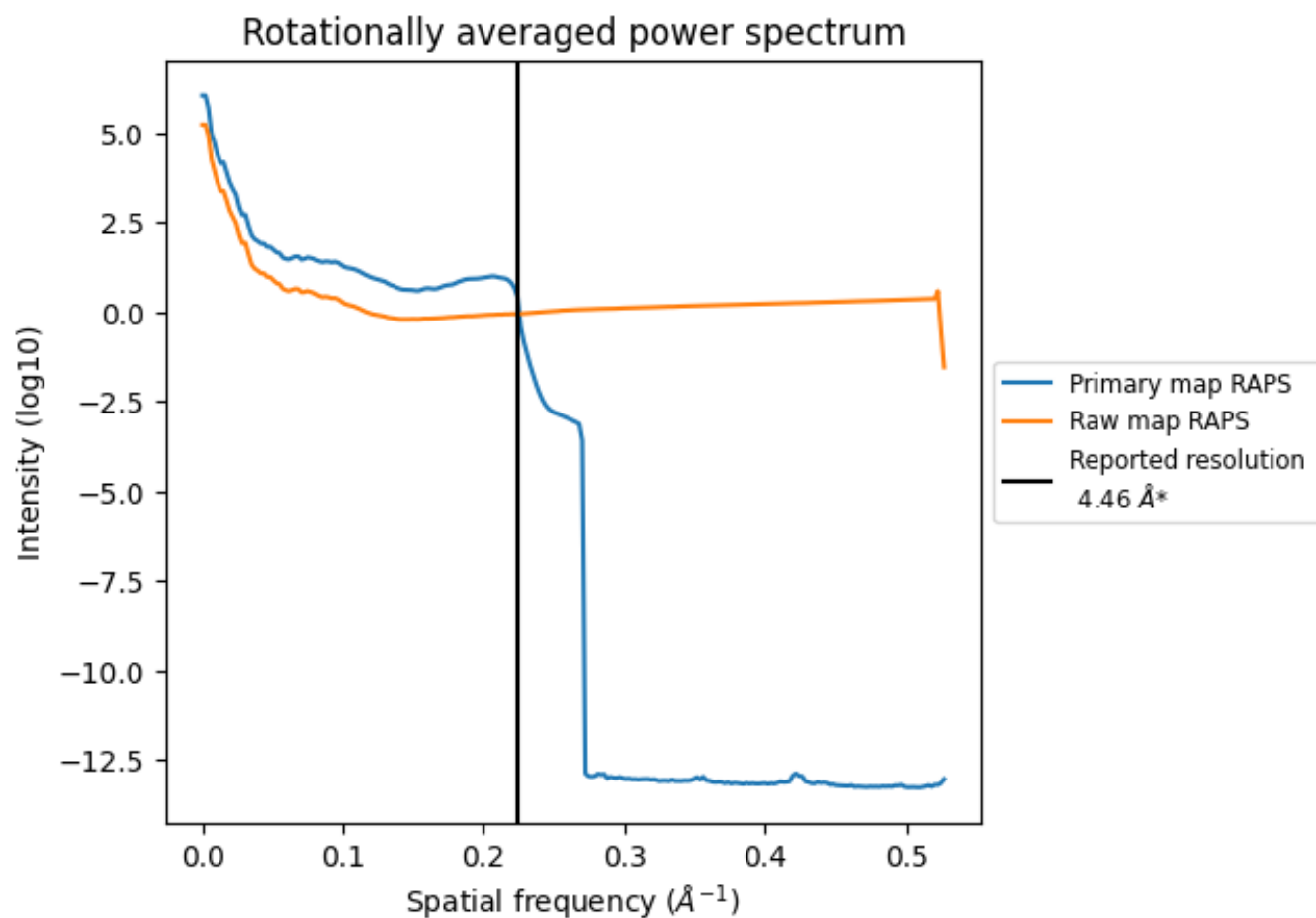
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 208 nm³; this corresponds to an approximate mass of 188 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 ⓘ

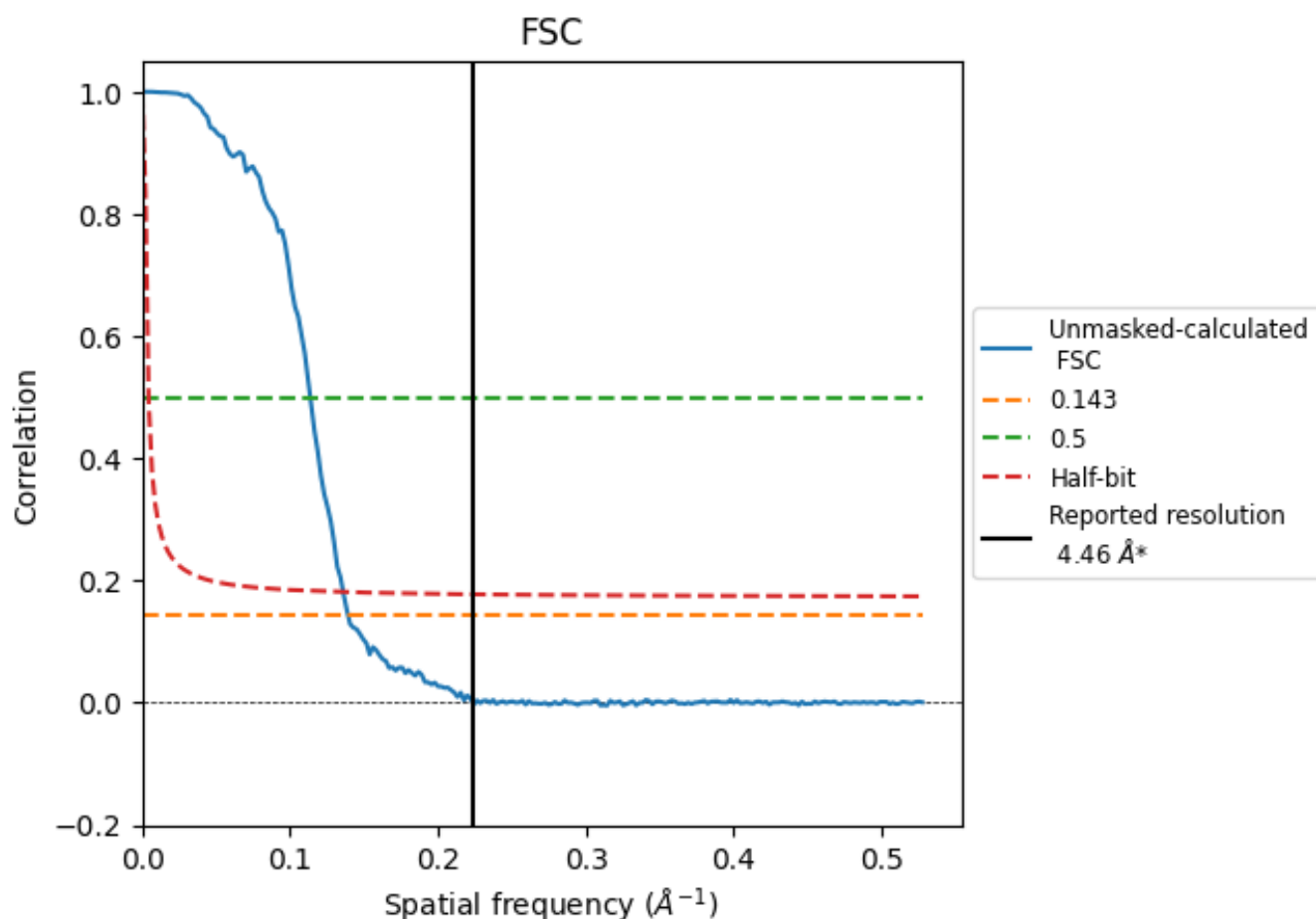


*Reported resolution corresponds to spatial frequency of 0.224 Å⁻¹

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 0.224 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

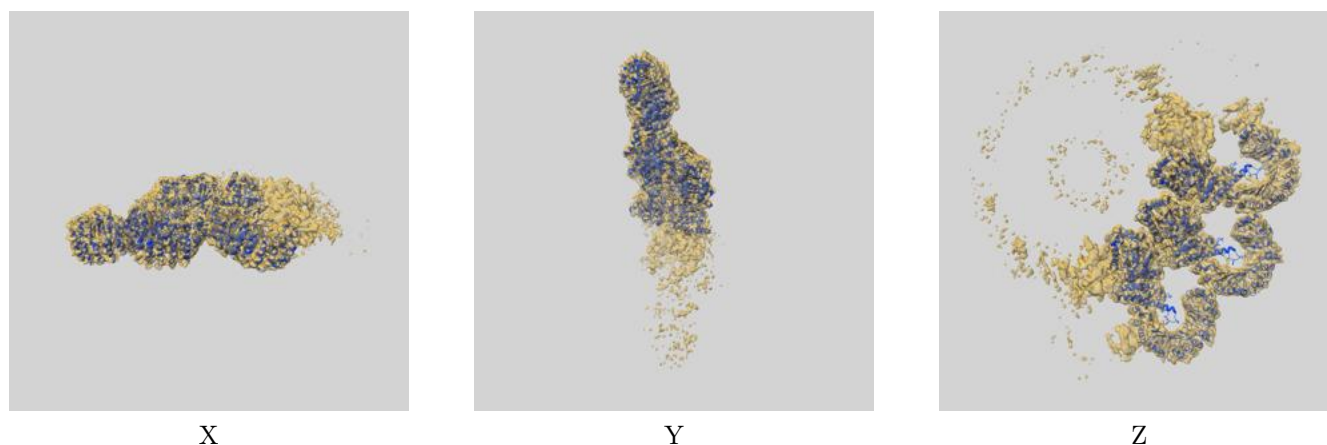
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.46	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.18	8.81	7.36

*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 7.18 differs from the reported value 4.46 by more than 10 %

9 Map-model fit [i](#)

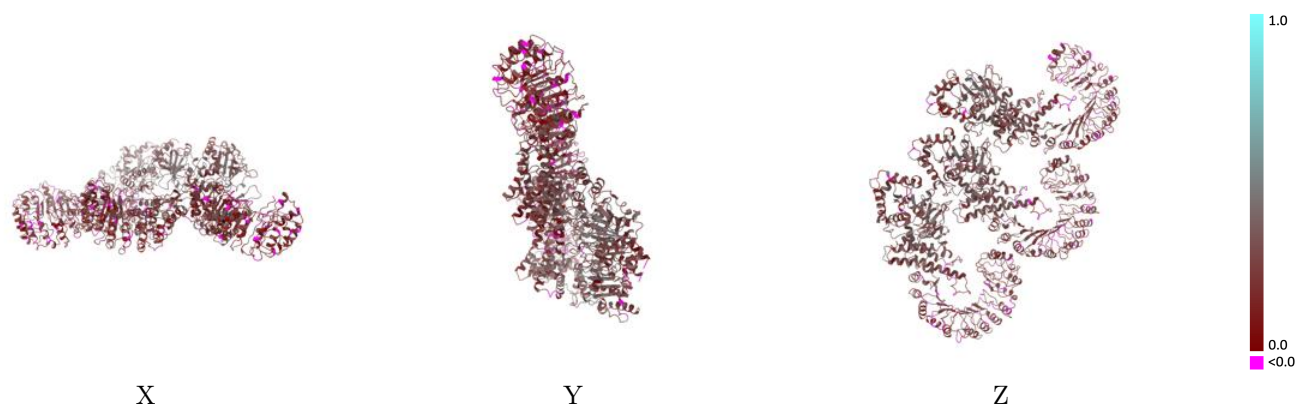
This section contains information regarding the fit between EMDB map EMD-29498 and PDB model 8FW9. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



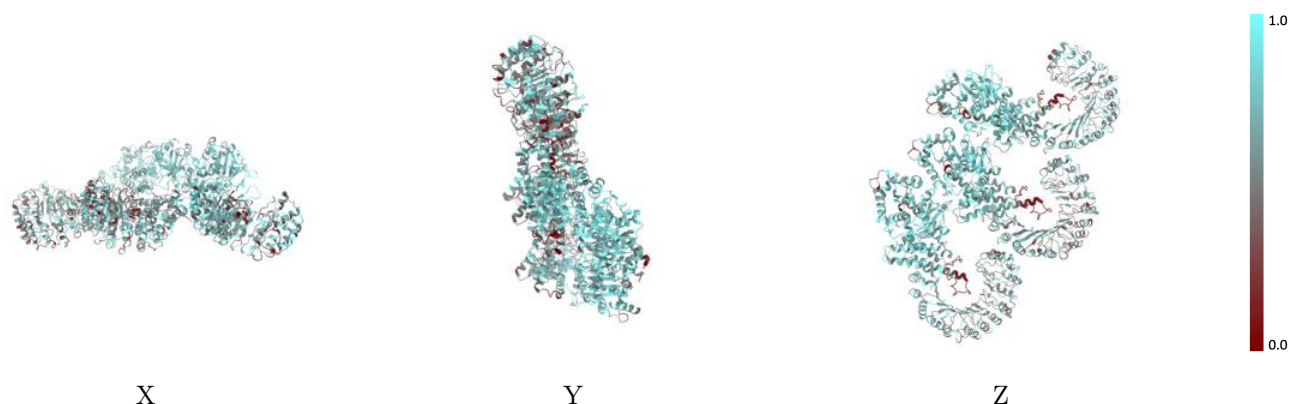
The images above show the 3D surface view of the map at the recommended contour level 0.084 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



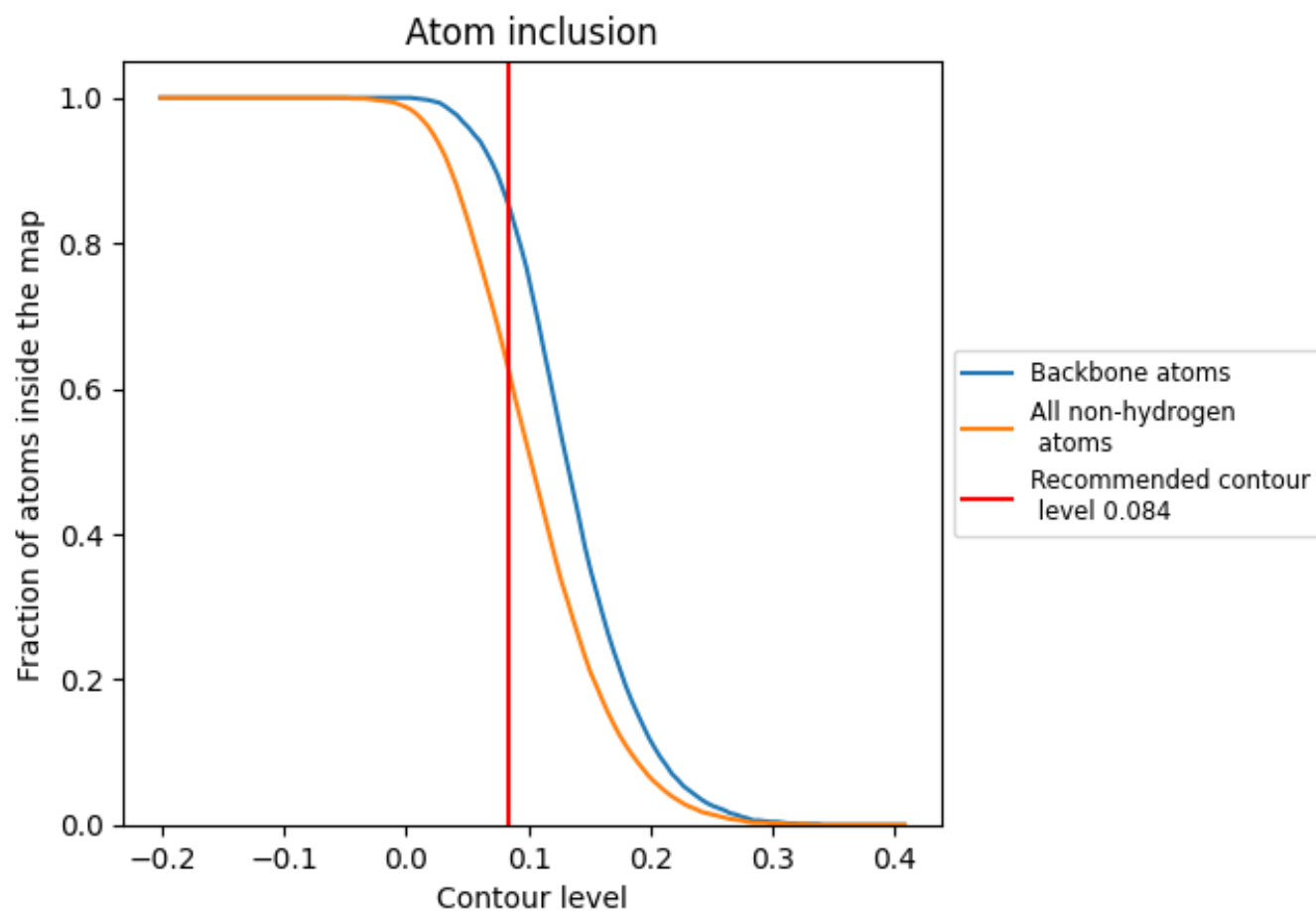
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.084).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 62% 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 (0.084) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6240	0.2400
A	0.6400	0.2410
B	0.6100	0.2450
C	0.6230	0.2330

