



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 08:45 AM UTC

PDB ID : 8YVC / pdb_00008yvc
EMDB ID : EMD-39596
Title : Cryo-EM structure of carboxysomal midi-shell:icosahedral assembly from Cso S4A/4B/1A/1B/1C/1D and CsoS2 C-terminal co-expression (T = 19)
Authors : Wang, P.; Li, J.X.; Li, T.P.; Li, K.; Ng, P.C.; Wang, S.M.; Chriscoli, V.; Basle, A.; Marles-Wright, J.; Zhang, Y.Z.; Liu, L.N.
Deposited on : 2024-03-28
Resolution : 3.04 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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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:

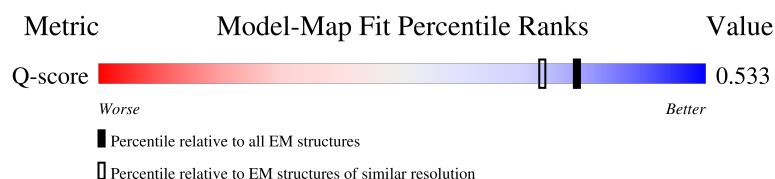
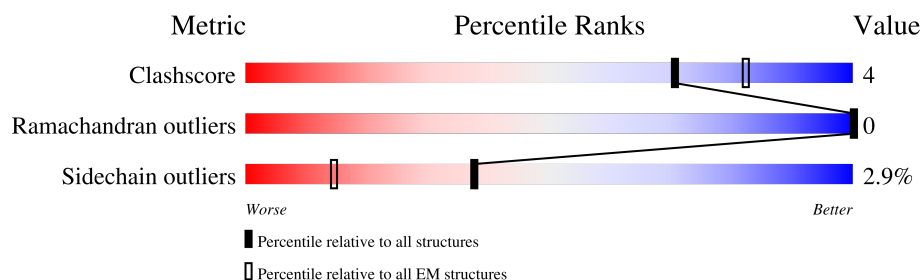
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.04 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.



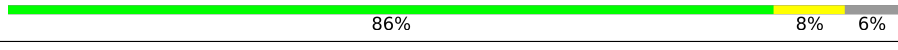
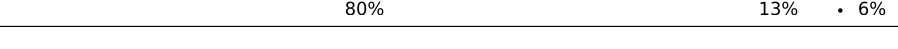
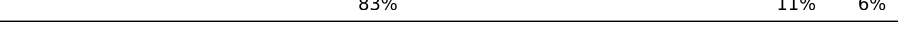
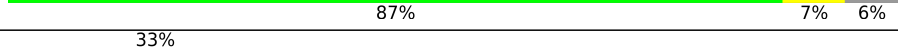
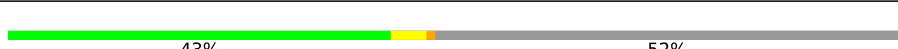
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13952 (2.54 - 3.54)

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	C	98	 76% 18% 6%
1	D	98	 77% 17% 6%
1	E	98	 83% 10% 6%
1	F	98	 73% 20% 6%

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Mol	Chain	Length	Quality of chain
1	G	98	
1	H	98	
1	I	98	
1	J	98	
1	K	98	
1	L	98	
1	M	98	
1	N	98	
1	O	98	
1	P	98	
1	Q	98	
1	R	98	
1	S	98	
1	T	98	
2	U	83	
3	X	279	
3	Y	279	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13952 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 Major carboxysome shell protein CsoS1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	D	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	E	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	F	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	G	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	H	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	I	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	J	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	K	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	L	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	M	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	N	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	O	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	P	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	Q	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	R	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	S	92	Total 656	C 408	N 123	O 122	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	T	92	Total	C	N	O	S	0	0
			656	408	123	122	3		

- Molecule 2 is a protein called Carboxysome shell vertex protein CsoS4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	U	81	Total	C	N	O	S	0	0
			608	386	105	112	5		

- Molecule 3 is a protein called Carboxysome assembly protein CsoS2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	X	77	Total	C	N	O	S	0	0
			556	339	95	119	3		
3	Y	134	Total	C	N	O	S	0	0
			980	591	191	193	5		

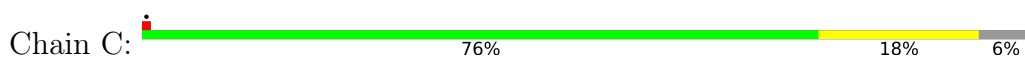
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	591	MET	-	initiating methionine	UNP O85041
Y	591	MET	-	initiating methionine	UNP O85041

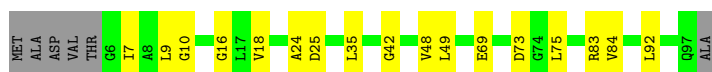
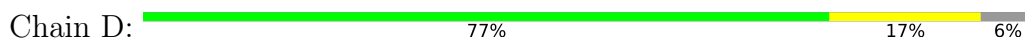
3 Residue-property plots [i](#)

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.

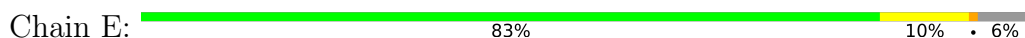
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



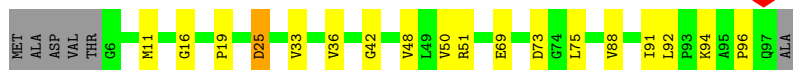
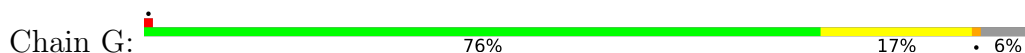
- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



- Molecule 1: Major carboxysome shell protein CsoS1A



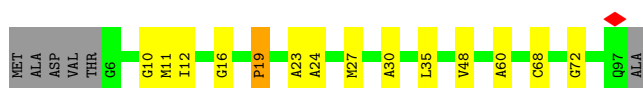
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain H:  86% 8% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain I:  80% 13% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain J:  82% 11% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain K:  82% 12% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain L:  82% 12% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain M:  81% 12% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain N:  77% 15% 6%



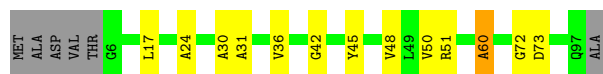
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain O:  83% 11% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain P:  81% 12% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain Q:  85% 9% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain R:  81% 13% 6%



- Molecule 1: Major carboxysome shell protein CsoS1A

Chain S:  82% 12% 6%



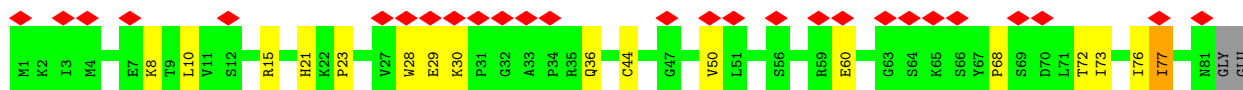
- Molecule 1: Major carboxysome shell protein CsoS1A

Chain T:  87% 7% 6%



- Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain U:  33% 77% 19% 6%



- Molecule 3: Carboxysome assembly protein CsoS2B

ALA	GLY	ASN	THR	MET
GLN	ARG	ASN	ASN	PRO
TRP	ASN	GLN	GLN	THR
ALA	LYS	ALA	GLU	CYS
SER	ALA	ALA	GLN	THR
GLY	GLN	ALA	ASN	SER
ARG	ALA	ALA	PHE	PRO
ASN	PRO	ALA	ALA	GLU
PRO	VAL	VAL	PRO	PRO
SER	VAL	GLY	GLY	GLU
MET	GLN	VAL	GLU	ALA
ARG	PRO	VAL	VAL	GLN
GLY	GLU	M685		SER
ASN	VAL			THR
ALA	VAL	I691		GLU
ARG	ALA			Q607
VAL	THR	P694		S603
VAL	GLN			L609
GLU	GLU	N700		T610
THR	LYS	ARG		Q614
SER	PRO	ILE		
ALA	LEU	THR		V621
PHE	LEU	GLY		
ALA	VAL	ASN		E634
ASN	CYS	ASP		Q636
ARG	ALA	ILE		Q636
ASN	PRO	ALA		L637
VAL	ARG	PRO		I638
PRO	SER	SER		S639
LYS	ASP	GLY		G640
PRO	GLN	R712		
GLU	MET	I713		
LYS	ASP	T714		V644
PRO	ARG			
GLY	VAL	I724		Q647
SER	SER	I725		GLN
LYS	GLY			THR
ILE	GLU	P728		GLY
THR	GLY	E729		CYS
GLY	LYS	F730		LEU
SER	GLU	R731		PRO
SER	ARG	HIS		THR
GLY	CYS	ALA		SER
ASN	ILE	ALA		PRO
THR	THR	GLU		ARG
GLN	GLY	LEU		PHE
GLY	ASP	VAL		ASN
SER	TRP	GLY		GLN
ILE	SER	SER		GLY
THR	VAL	GLN		THR
TYR	ASN	PRO		VAL
SER	LYS	THR		GLN
GLY	HIS	MET		SER
GLY	ILE	MET		MET
ALA	THR	ALA		PHE
ARG	GLY	MET		LYS
THR	THR	ALA		ASN

Chain Y: 43% . . 52%

T727	LEU	CYS
R735	PRO	LEU
GLU	THR	THR
LEU	THR	THR
VAL	ARG	THR
GLY	PHE	PRO
SER	ASN	GLU
PRO	GLN	PRO
GLN	THR	GLU
PRO	GLY	ALA
MET	ASN	GLN
ALA	VAL	GLN
ALA	VAL	SER
ALA	GLN	GLU
ALA	SER	GLN
ALA	MET	SER
ALA	GLY	GLN
ARG	PHE	LEU
ARG	LYS	THR
ASN	ASN	CYS
LYS	THR	GLU
ALA	ASN	GLN
ALA	GLN	GLY
ALA	PRO	ILE
ALA	GLU	ILE
PRO	GLN	SER
VAL	ASN	GLY
VAL	PHE	THR
GLN	ALA	SER
PRO	PRO	VAL
GLU	GLY	ASP
VAL	GLU	ALA
VAL	VAL	SER
ALA	VAL	ASP
ALA	MET	LEU
THR	PRO	VAL
GLN	THR	VAL
GLU	THR	THR
GLU	ASP	GLY
K770	PHE	ASN
	ILE	ILE
	GLN	GLY
	THR	GLU
	PRO	GLN
	ALA	GLN
	ARG	LEU
	SER	LEU
	ALA	ILE
	GLN	SER
	ASN	GLY
	ARG	ASP
	ASN	ALA
	I702	ALA
	T703	TYR
		VAL
	I707	GLY
		ALA
	I713	GLN
	T714	GLN
		THR
		CYS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5119	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 ($e^-/\text{\AA}^2$)	50.0	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.485	Depositor
Minimum map value	-0.581	Depositor
Average map value	0.018	Depositor
Map value standard deviation	0.136	Depositor
Recommended contour level	0.2	Depositor
Map size ($\text{\AA}$)	547.9384, 547.9384, 547.9384	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.3046153, 1.3046153, 1.3046153	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	C	0.84	1/662 (0.2%)	1.25	3/897 (0.3%)
1	D	0.91	0/662	1.38	5/897 (0.6%)
1	E	0.94	0/662	1.43	7/897 (0.8%)
1	F	1.02	0/662	1.56	7/897 (0.8%)
1	G	0.83	1/662 (0.2%)	1.26	3/897 (0.3%)
1	H	0.88	0/662	1.33	3/897 (0.3%)
1	I	0.94	2/662 (0.3%)	1.33	4/897 (0.4%)
1	J	0.93	0/662	1.36	4/897 (0.4%)
1	K	0.78	0/662	1.22	5/897 (0.6%)
1	L	0.89	0/662	1.38	1/897 (0.1%)
1	M	0.81	0/662	1.28	2/897 (0.2%)
1	N	0.91	1/662 (0.2%)	1.44	6/897 (0.7%)
1	O	0.96	0/662	1.34	1/897 (0.1%)
1	P	0.87	2/662 (0.3%)	1.30	3/897 (0.3%)
1	Q	0.92	0/662	1.37	5/897 (0.6%)
1	R	0.86	1/662 (0.2%)	1.36	4/897 (0.4%)
1	S	0.84	0/662	1.29	4/897 (0.4%)
1	T	0.80	0/662	1.15	1/897 (0.1%)
2	U	1.02	0/620	1.65	10/843 (1.2%)
3	X	0.96	0/560	1.69	8/757 (1.1%)
3	Y	0.96	1/997 (0.1%)	1.59	8/1345 (0.6%)
All	All	0.90	9/14093 (0.1%)	1.39	94/19091 (0.5%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	50	VAL	C-O	-6.96	1.16	1.24
1	I	60	ALA	C-O	-5.95	1.17	1.24
1	I	19	PRO	C-O	-5.90	1.16	1.24
1	C	60	ALA	C-O	-5.52	1.17	1.24
1	N	19	PRO	C-O	-5.44	1.17	1.24
3	Y	714	THR	C-O	-5.37	1.16	1.23
1	G	19	PRO	C-O	-5.32	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	51	ARG	C-O	-5.18	1.17	1.23
1	P	60	ALA	C-O	-5.16	1.18	1.24

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	29	GLU	N-CA-C	-10.56	99.77	111.28
1	J	42	GLY	CA-C-O	-8.39	116.41	122.45
1	M	42	GLY	CA-C-O	-8.32	116.81	122.22
1	G	16	GLY	CA-C-O	-8.07	116.98	122.22
1	N	16	GLY	CA-C-O	-8.03	116.67	122.45
1	E	16	GLY	CA-C-O	-7.97	116.55	122.37
1	F	42	GLY	CA-C-O	-7.97	117.04	122.22
1	Q	16	GLY	CA-C-O	-7.89	117.09	122.22
1	D	16	GLY	CA-C-O	-7.73	116.88	122.45
1	C	42	GLY	CA-C-O	-7.51	117.05	122.23
1	S	31	ALA	CA-C-O	-7.44	113.49	121.45
3	Y	707	ILE	N-CA-C	-7.41	105.49	112.83
2	U	68	PRO	N-CA-CB	-7.41	97.61	102.65
1	N	42	GLY	CA-C-O	-7.19	117.27	122.45
3	X	728	PRO	CB-CA-C	7.19	120.77	111.21
1	K	16	GLY	CA-C-O	-7.00	116.66	122.33
1	R	73	ASP	N-CA-C	-6.81	100.90	110.50
3	X	621	VAL	N-CA-C	-6.77	106.13	112.83
3	Y	727	THR	CB-CA-C	6.57	118.96	109.11
1	P	73	ASP	CB-CA-C	6.55	122.74	110.63
1	C	60	ALA	CA-C-O	-6.37	113.67	120.42
1	I	60	ALA	CA-C-O	-6.37	113.80	120.55
1	R	42	GLY	CA-C-O	-6.36	116.92	121.88
1	S	96	PRO	N-CA-C	-6.36	104.69	113.53
3	X	728	PRO	N-CA-CB	-6.32	97.46	103.34
2	U	30	LYS	N-CA-C	-6.18	102.57	108.13
2	U	36	GLN	CA-C-O	-6.17	114.90	121.88
1	P	42	GLY	CA-C-O	-6.16	116.47	121.77
1	F	8	ALA	CA-C-O	-6.06	114.95	121.56
1	K	42	GLY	CA-C-O	-6.03	118.07	122.23
3	X	694	PRO	CB-CA-C	-6.01	102.83	112.21
1	O	53	GLU	CA-C-O	-6.00	114.96	121.44
1	R	76	VAL	N-CA-C	-6.00	106.40	111.56
1	T	53	GLU	CA-C-O	-5.94	114.97	121.87
1	J	42	GLY	N-CA-C	-5.94	105.98	112.04
2	U	60	GLU	N-CA-C	-5.93	105.53	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	25	ASP	N-CA-C	-5.89	104.77	111.14
1	L	42	GLY	CA-C-O	-5.88	117.30	121.88
1	R	10	GLY	CA-C-O	-5.85	116.48	121.57
1	S	30	ALA	CA-C-O	-5.81	114.72	120.82
1	E	42	GLY	CA-C-O	-5.80	117.19	122.24
1	I	16	GLY	CA-C-O	-5.80	116.78	121.77
1	K	76	VAL	N-CA-C	-5.76	104.90	110.72
1	E	52	GLY	CA-C-O	-5.75	116.02	121.60
1	E	31	ALA	CA-C-O	-5.74	115.31	121.45
1	M	10	GLY	O-C-N	-5.74	118.52	123.80
2	U	28	TRP	CA-CB-CG	5.74	124.50	113.60
1	D	42	GLY	CA-C-O	-5.71	117.28	122.24
1	P	30	ALA	CA-C-O	-5.70	114.83	120.82
1	D	73	ASP	N-CA-C	-5.68	105.61	112.54
1	H	53	GLU	CA-C-O	-5.65	115.40	121.56
3	Y	713	ILE	CB-CA-C	5.63	120.53	111.29
1	E	76	VAL	N-CA-C	-5.62	105.62	111.58
1	K	73	ASP	CB-CA-C	5.61	119.86	109.54
3	X	725	THR	N-CA-C	-5.58	100.86	109.52
1	N	10	GLY	N-CA-C	-5.58	104.56	112.37
2	U	36	GLN	N-CA-C	-5.56	102.67	110.35
1	Q	73	ASP	CB-CA-C	5.51	119.60	109.46
3	Y	723	LEU	N-CA-C	-5.51	106.24	113.12
1	C	45	TYR	CA-C-O	-5.48	115.02	121.16
1	F	53	GLU	CA-C-O	-5.47	115.64	121.94
1	I	30	ALA	CA-C-O	-5.43	115.11	120.82
1	E	53	GLU	CA-C-O	-5.42	115.91	121.87
1	N	42	GLY	N-CA-C	-5.41	106.53	112.04
3	X	636	GLN	N-CA-C	-5.40	106.53	113.01
1	K	73	ASP	N-CA-C	-5.39	102.89	110.50
3	X	725	THR	CA-C-O	-5.38	115.14	121.44
3	Y	788	GLU	N-CA-C	-5.36	103.06	110.35
1	E	30	ALA	CA-C-O	-5.34	115.21	120.82
1	G	42	GLY	CA-C-O	-5.33	117.72	121.88
1	F	16	GLY	CA-C-O	-5.33	116.72	122.05
1	J	50	VAL	CA-C-O	-5.31	115.49	121.75
1	F	24	ALA	CA-C-O	-5.30	114.93	120.55
1	Q	29	LYS	CA-C-O	-5.29	115.26	120.82
2	U	30	LYS	CA-C-O	-5.28	115.59	120.13
3	Y	703	THR	CA-C-O	-5.23	115.51	121.58
1	H	42	GLY	CA-C-O	-5.19	117.31	121.77
1	D	10	GLY	CA-C-O	-5.17	116.22	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	69	GLU	CA-C-O	-5.13	115.43	120.82
1	F	30	ALA	CA-C-O	-5.12	115.44	120.82
1	F	52	GLY	CA-C-O	-5.12	115.73	121.21
1	Q	73	ASP	N-CA-C	-5.12	102.90	110.48
2	U	23	PRO	N-CA-C	-5.12	103.73	111.41
1	N	52	GLY	CA-C-O	-5.11	116.57	121.38
1	I	10	GLY	CA-C-O	-5.11	116.51	121.11
3	Y	774	VAL	N-CA-C	-5.08	105.44	110.62
3	Y	799	ASP	CA-C-O	-5.07	115.45	121.89
2	U	23	PRO	CA-C-O	-5.06	115.60	122.08
3	X	634	GLU	N-CA-C	-5.06	100.03	110.80
1	H	16	GLY	CA-C-O	-5.04	116.85	122.14
1	J	78	ALA	CA-C-O	-5.04	114.49	120.89
1	N	14	THR	CA-C-O	-5.02	115.88	121.51
1	G	25	ASP	CA-C-O	-5.02	115.55	120.82
1	S	45	TYR	CA-C-O	-5.01	115.68	121.19

There are no chirality outliers.

There are no planarity outliers.

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	C	656	0	677	10	0
1	D	656	0	677	6	0
1	E	656	0	677	3	0
1	F	656	0	677	8	0
1	G	656	0	677	9	0
1	H	656	0	677	2	0
1	I	656	0	677	8	0
1	J	656	0	677	8	0
1	K	656	0	677	4	0
1	L	656	0	677	7	0
1	M	656	0	677	9	0
1	N	656	0	677	8	0
1	O	656	0	677	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	656	0	677	7	0
1	Q	656	0	677	3	0
1	R	656	0	677	5	0
1	S	656	0	677	7	0
1	T	656	0	677	3	0
2	U	608	0	625	5	0
3	X	556	0	539	8	0
3	Y	980	0	956	5	0
All	All	13952	0	14306	99	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 4.

All (99) 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:J:88:VAL:HG21	1:N:25:ASP:HA	1.76	0.67
3:X:610:THR:HB	3:X:614:GLN:OE1	1.93	0.67
1:J:72:GLY:HA2	1:M:77:ALA:HB2	1.75	0.67
1:I:23:ALA:HB2	1:I:68:CYS:SG	2.40	0.62
1:P:31:ALA:HB3	1:P:60:ALA:HB2	1.84	0.58
1:M:80:ILE:HG23	3:Y:797:GLY:O	2.04	0.57
1:C:25:ASP:HA	1:H:88:VAL:HG21	1.86	0.57
2:U:44:CYS:SG	2:U:73:ILE:HG21	2.45	0.56
1:S:94:LYS:O	1:S:95:ALA:C	2.48	0.56
1:R:12:ILE:HG23	1:R:75:LEU:HD11	1.88	0.56
1:J:31:ALA:HB3	1:J:60:ALA:HB2	1.89	0.55
1:P:45:TYR:CE1	3:X:694:PRO:CB	2.90	0.54
1:F:12:ILE:HG23	1:F:75:LEU:HD12	1.88	0.53
1:D:24:ALA:HB2	1:D:48:VAL:HG21	1.90	0.52
1:O:23:ALA:HB2	1:O:68:CYS:SG	2.48	0.52
1:S:68:CYS:SG	1:S:75:LEU:CD1	2.98	0.51
1:K:25:ASP:HA	1:L:88:VAL:HG21	1.93	0.51
1:R:68:CYS:SG	1:R:75:LEU:HD13	2.50	0.51
1:G:51:ARG:HG3	1:G:51:ARG:HH11	1.76	0.51
1:O:88:VAL:HG21	1:R:25:ASP:HA	1.92	0.50
2:U:50:VAL:HG12	2:U:76:ILE:HG12	1.92	0.50
1:P:36:VAL:HG11	1:P:51:ARG:HG3	1.93	0.50
1:I:24:ALA:HB2	1:I:48:VAL:HG11	1.92	0.50
1:D:9:LEU:HD11	1:D:49:LEU:HD23	1.94	0.49
1:M:59:ALA:HB1	3:Y:788:GLU:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:7:ILE:HD12	1:N:83:ARG:CG	2.42	0.49
1:D:25:ASP:HA	1:G:88:VAL:HG21	1.93	0.49
1:N:23:ALA:HB2	1:N:68:CYS:SG	2.53	0.49
1:N:62:ARG:NH1	3:X:728:PRO:HB2	2.28	0.49
1:C:11:MET:HE2	1:F:18:VAL:HG13	1.94	0.48
1:I:72:GLY:HA2	1:N:77:ALA:HB2	1.94	0.48
1:M:66:ASP:OD1	3:Y:792:ARG:NH1	2.46	0.48
2:U:77:ILE:HD12	2:U:77:ILE:N	2.29	0.48
1:C:68:CYS:HA	1:C:71:VAL:HG12	1.95	0.48
1:I:12:ILE:HD12	1:I:27:MET:SD	2.53	0.48
1:T:37:GLY:HA2	1:T:96:PRO:HA	1.96	0.48
1:L:83:ARG:HG3	2:U:76:ILE:HD13	1.95	0.48
1:P:24:ALA:HB2	1:P:48:VAL:HG11	1.95	0.48
1:J:24:ALA:HB2	1:J:48:VAL:HG21	1.95	0.48
1:O:62:ARG:CZ	3:X:638:ILE:HG21	2.44	0.47
1:J:35:LEU:CD1	1:J:48:VAL:HG23	2.44	0.47
1:N:8:ALA:HB3	1:N:57:VAL:HG21	1.97	0.47
1:O:44:GLY:HA3	3:X:691:ILE:HD13	1.95	0.47
1:K:69:GLU:OE2	1:K:70:ARG:NH1	2.48	0.47
1:N:62:ARG:HD2	3:X:729:GLU:C	2.40	0.47
1:P:72:GLY:CA	1:S:77:ALA:HB2	2.45	0.47
1:J:72:GLY:CA	1:M:77:ALA:HB2	2.44	0.47
1:Q:45:TYR:CE1	1:Q:76:VAL:HG21	2.49	0.47
1:R:12:ILE:HD12	1:R:75:LEU:HD11	1.97	0.46
1:S:68:CYS:SG	1:S:75:LEU:HD13	2.56	0.46
1:C:36:VAL:C	1:C:96:PRO:HD3	2.40	0.46
1:F:12:ILE:HG21	1:F:23:ALA:HB1	1.98	0.45
1:I:19:PRO:HG3	1:I:72:GLY:HA3	1.99	0.45
1:C:11:MET:HB3	1:F:18:VAL:HG22	1.98	0.45
1:H:22:GLU:HG2	1:H:71:VAL:HG21	1.97	0.45
1:G:51:ARG:HG3	1:G:51:ARG:NH1	2.31	0.45
1:P:72:GLY:HA2	1:S:77:ALA:HB2	1.98	0.45
1:K:94:LYS:HB2	1:K:94:LYS:HE2	1.83	0.45
1:I:24:ALA:HB1	1:I:35:LEU:HD11	1.98	0.44
1:E:88:VAL:HG21	1:G:25:ASP:HA	1.98	0.44
1:C:75:LEU:HD11	1:C:78:ALA:HB2	2.00	0.44
1:F:62:ARG:HA	3:X:724:ILE:HD11	2.00	0.44
1:I:35:LEU:HD21	1:I:48:VAL:HG13	2.00	0.44
1:N:12:ILE:HG23	1:N:75:LEU:HD11	1.99	0.44
1:Q:84:VAL:HG23	1:Q:89:GLU:OE2	2.18	0.44
2:U:77:ILE:HD12	2:U:77:ILE:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:69:GLU:OE1	3:Y:775:CYS:HB2	2.18	0.43
1:D:18:VAL:HG22	1:G:11:MET:HB3	1.99	0.43
1:G:33:VAL:HB	1:G:50:VAL:HB	1.99	0.43
1:E:58:ASN:CB	3:Y:707:ILE:HD12	2.49	0.43
1:G:36:VAL:O	1:G:96:PRO:HA	2.19	0.43
1:G:92:LEU:O	1:G:94:LYS:HG3	2.19	0.43
1:I:11:MET:HB3	1:L:18:VAL:HG22	2.00	0.43
1:P:17:LEU:N	1:S:13:GLU:OE2	2.50	0.43
1:Q:15:ARG:CZ	1:Q:76:VAL:HG22	2.49	0.43
1:D:35:LEU:HD21	1:G:91:ILE:CG2	2.49	0.43
1:K:12:ILE:HD12	1:K:27:MET:SD	2.58	0.43
1:L:9:LEU:HD23	1:L:11:MET:HE2	2.01	0.42
1:O:79:HIS:CE1	3:X:640:GLY:CA	3.01	0.42
1:C:41:VAL:HG13	1:F:46:VAL:CG2	2.49	0.42
1:E:15:ARG:CZ	1:E:76:VAL:HG22	2.50	0.42
1:T:12:ILE:HD12	1:T:27:MET:SD	2.60	0.42
1:C:84:VAL:HG11	1:C:92:LEU:HD11	2.00	0.42
1:L:33:VAL:HB	1:L:50:VAL:HB	2.01	0.42
1:J:35:LEU:HD13	1:J:48:VAL:HG23	2.00	0.42
1:M:36:VAL:C	1:M:96:PRO:HD3	2.43	0.42
1:F:49:LEU:HD12	1:F:93:PRO:HD2	2.00	0.42
1:J:18:VAL:HG22	1:M:11:MET:HB3	2.01	0.42
1:S:81:ILE:HG22	1:S:83:ARG:O	2.20	0.41
1:O:41:VAL:HB	1:O:45:TYR:HB2	2.01	0.41
1:L:37:GLY:HA2	1:L:96:PRO:HA	2.03	0.41
1:T:41:VAL:HB	1:T:45:TYR:HB2	2.03	0.41
1:L:35:LEU:HD12	1:L:49:LEU:O	2.21	0.41
1:M:25:ASP:OD1	1:M:25:ASP:C	2.63	0.41
1:D:7:ILE:HD11	1:D:83:ARG:HG3	2.01	0.40
1:C:57:VAL:HG12	1:C:80:ILE:HG23	2.03	0.40
1:C:88:VAL:HG21	1:F:25:ASP:HA	2.02	0.40
1:O:35:LEU:HD11	1:O:48:VAL:HG13	2.02	0.40
1:R:68:CYS:HA	1:R:71:VAL:HG12	2.03	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	C	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	D	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	E	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	F	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	G	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	H	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	I	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	J	90/98 (92%)	90 (100%)	0	0	100	100
1	K	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	L	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	M	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	N	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	O	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	P	90/98 (92%)	90 (100%)	0	0	100	100
1	Q	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	R	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	S	90/98 (92%)	87 (97%)	3 (3%)	0	100	100
1	T	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
2	U	79/83 (95%)	74 (94%)	5 (6%)	0	100	100
3	X	71/279 (25%)	68 (96%)	3 (4%)	0	100	100
3	Y	130/279 (47%)	128 (98%)	2 (2%)	0	100	100
All	All	1900/2405 (79%)	1858 (98%)	42 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	C	63/67 (94%)	62 (98%)	1 (2%)	55	76
1	D	63/67 (94%)	60 (95%)	3 (5%)	23	54
1	E	63/67 (94%)	62 (98%)	1 (2%)	55	76
1	F	63/67 (94%)	59 (94%)	4 (6%)	16	45
1	G	63/67 (94%)	59 (94%)	4 (6%)	16	45
1	H	63/67 (94%)	61 (97%)	2 (3%)	34	64
1	I	63/67 (94%)	63 (100%)	0	100	100
1	J	63/67 (94%)	61 (97%)	2 (3%)	34	64
1	K	63/67 (94%)	61 (97%)	2 (3%)	34	64
1	L	63/67 (94%)	63 (100%)	0	100	100
1	M	63/67 (94%)	60 (95%)	3 (5%)	23	54
1	N	63/67 (94%)	61 (97%)	2 (3%)	34	64
1	O	63/67 (94%)	63 (100%)	0	100	100
1	P	63/67 (94%)	63 (100%)	0	100	100
1	Q	63/67 (94%)	63 (100%)	0	100	100
1	R	63/67 (94%)	60 (95%)	3 (5%)	23	54
1	S	63/67 (94%)	63 (100%)	0	100	100
1	T	63/67 (94%)	63 (100%)	0	100	100
2	U	66/67 (98%)	60 (91%)	6 (9%)	9	31
3	X	61/223 (27%)	56 (92%)	5 (8%)	10	35
3	Y	103/223 (46%)	101 (98%)	2 (2%)	50	73
All	All	1364/1719 (79%)	1324 (97%)	40 (3%)	38	67

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	48	VAL

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Mol	Chain	Res	Type
1	D	75	LEU
1	D	84	VAL
1	D	92	LEU
1	E	54	THR
1	F	48	VAL
1	F	50	VAL
1	F	76	VAL
1	F	84	VAL
1	G	48	VAL
1	G	69	GLU
1	G	73	ASP
1	G	75	LEU
1	H	73	ASP
1	H	79	HIS
1	J	14	THR
1	J	48	VAL
1	K	32	GLU
1	K	48	VAL
1	M	34	ARG
1	M	73	ASP
1	M	80	ILE
1	N	7	ILE
1	N	83	ARG
1	R	14	THR
1	R	35	LEU
1	R	50	VAL
2	U	8	LYS
2	U	10	LEU
2	U	15	ARG
2	U	21	HIS
2	U	72	THR
2	U	77	ILE
3	X	608	SER
3	X	614	GLN
3	X	644	VAL
3	X	713	ILE
3	X	714	THR
3	Y	774	VAL
3	Y	796	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	85	HIS
1	I	58	ASN
1	L	58	ASN
1	M	79	HIS
1	N	79	HIS
1	O	85	HIS
1	R	58	ASN
2	U	21	HIS
3	X	692	GLN
3	X	699	GLN
3	Y	805	HIS
3	Y	857	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.

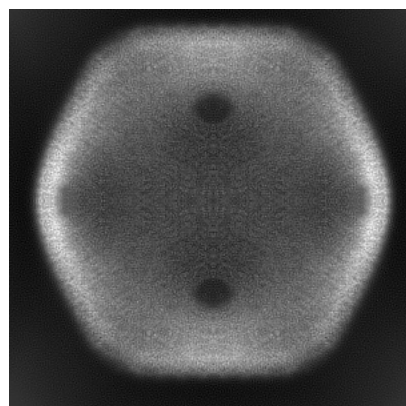
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39596. These allow visual inspection of the internal detail of the map and identification of artifacts.

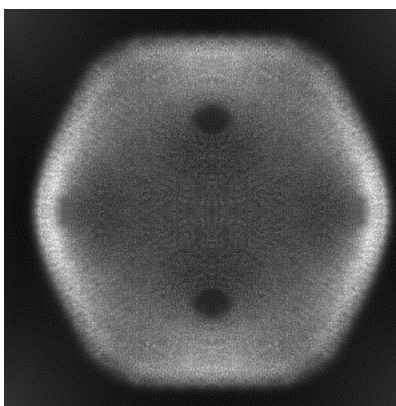
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

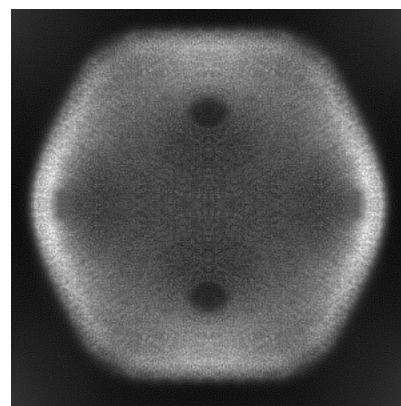
6.1.1 Primary map



X

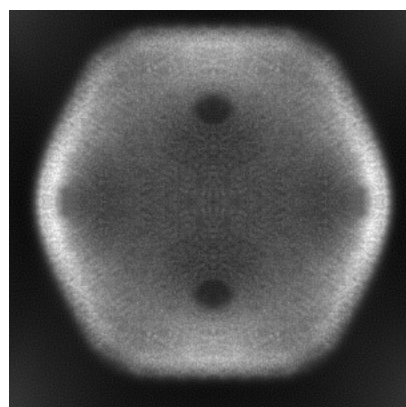


Y

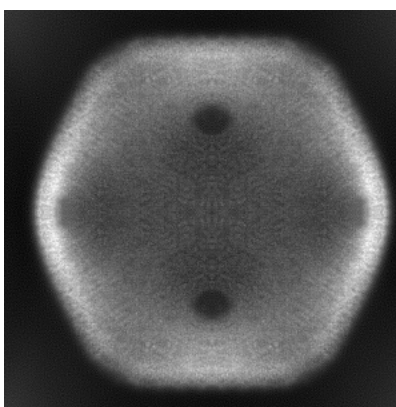


Z

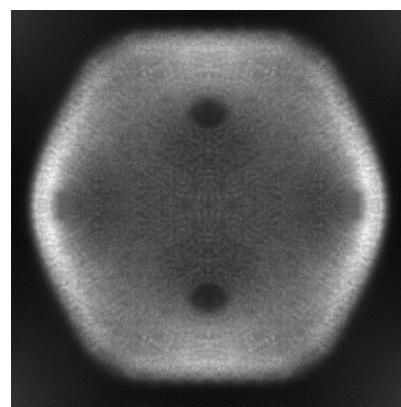
6.1.2 Raw map



X



Y

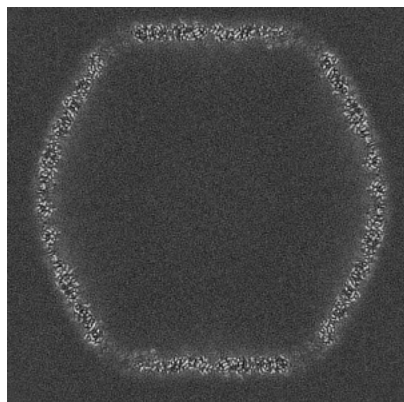


Z

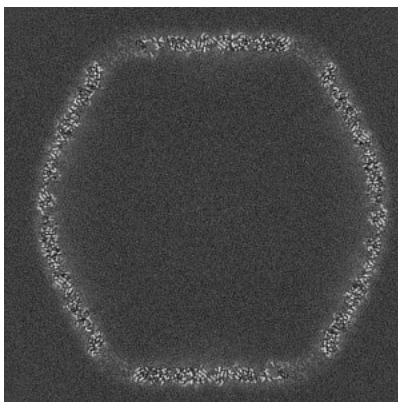
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

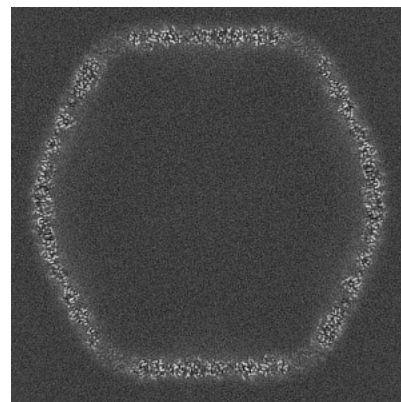
6.2.1 Primary map



X Index: 210

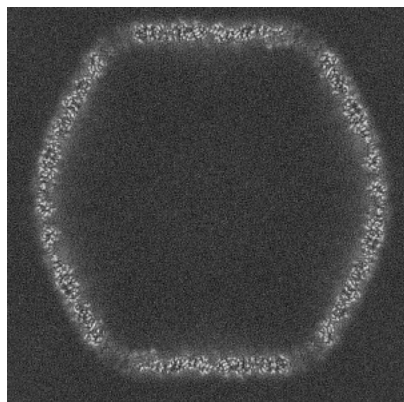


Y Index: 210

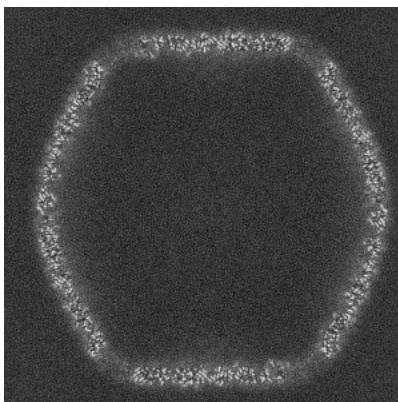


Z Index: 210

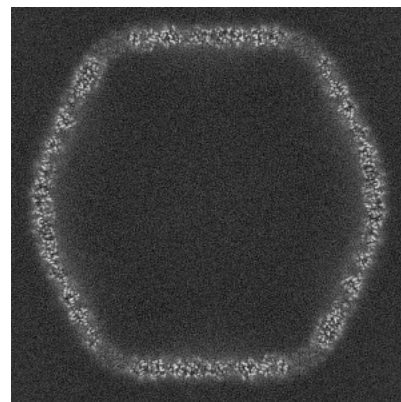
6.2.2 Raw map



X Index: 210



Y Index: 210

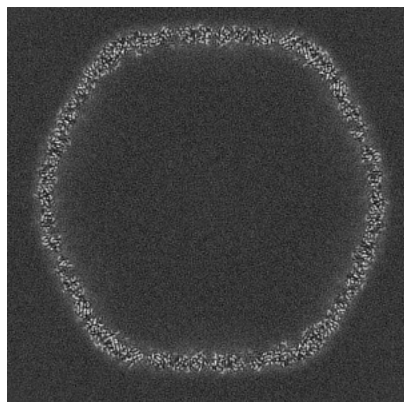


Z Index: 210

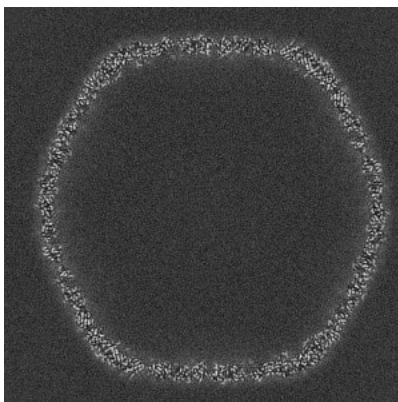
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

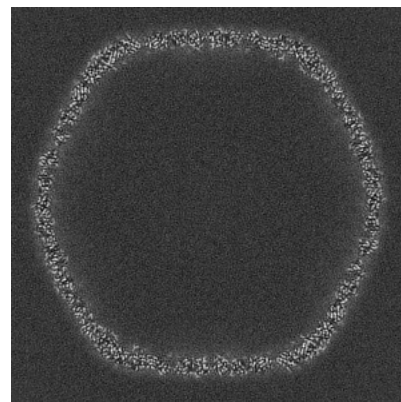
6.3.1 Primary map



X Index: 235

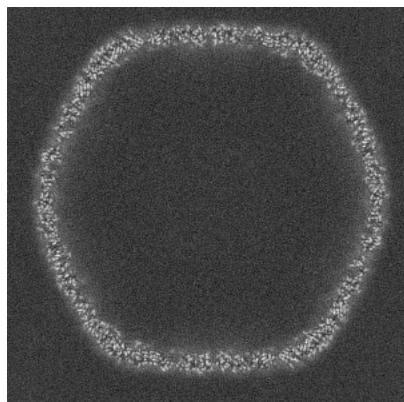


Y Index: 242

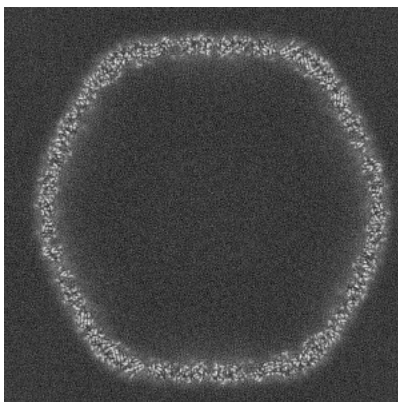


Z Index: 190

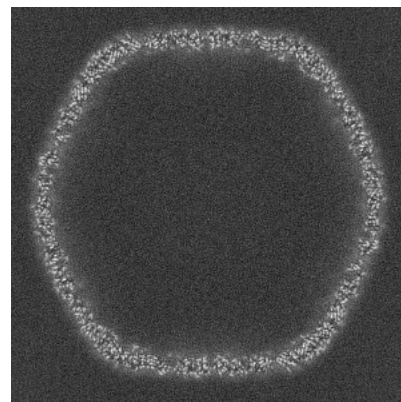
6.3.2 Raw map



X Index: 179



Y Index: 242

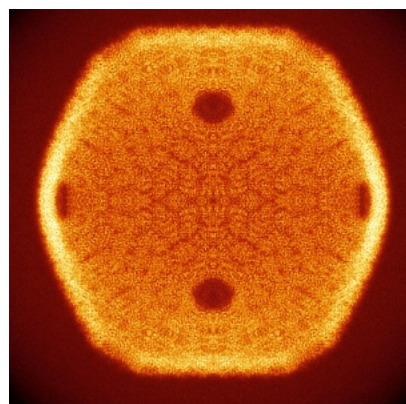


Z Index: 190

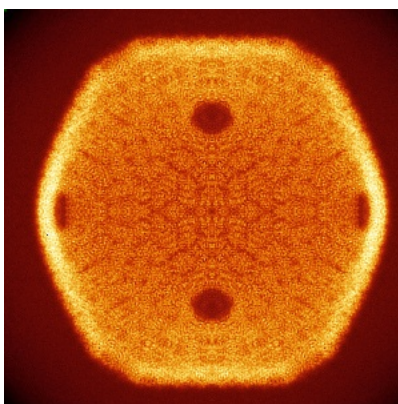
The images above show the largest variance slices of the map in three orthogonal directions.

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

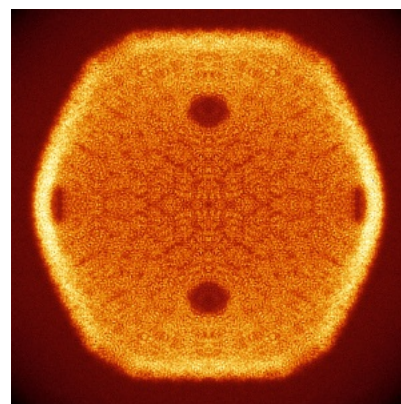
6.4.1 Primary map



X

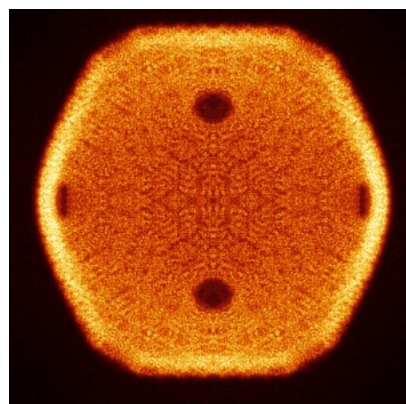


Y

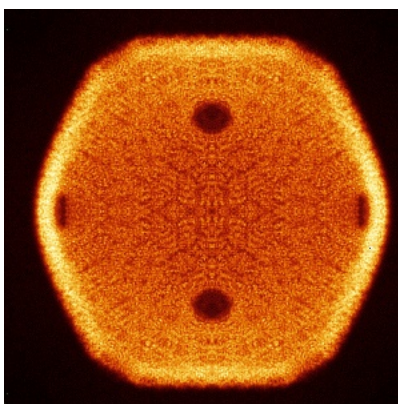


Z

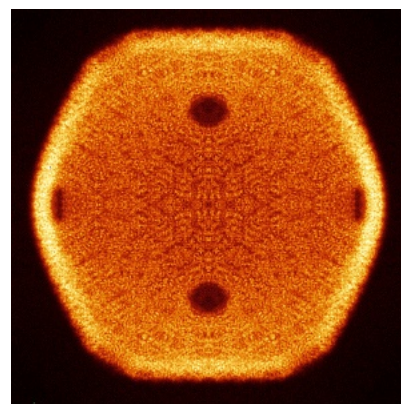
6.4.2 Raw map



X



Y

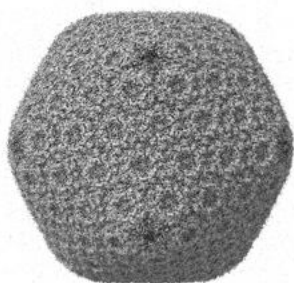


Z

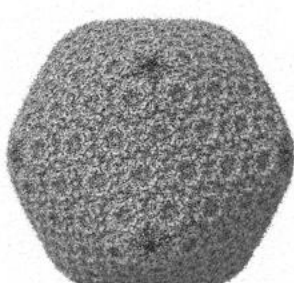
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

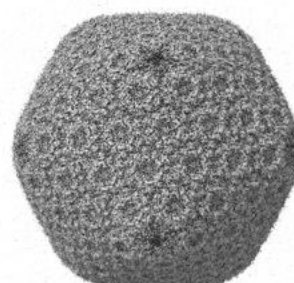
6.5.1 Primary map



X



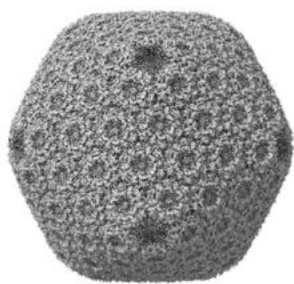
Y



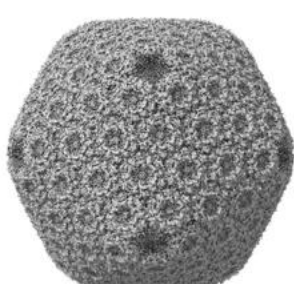
Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

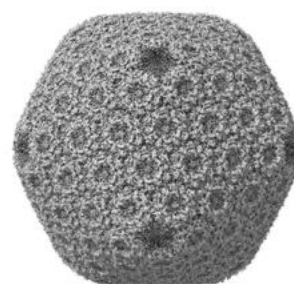
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

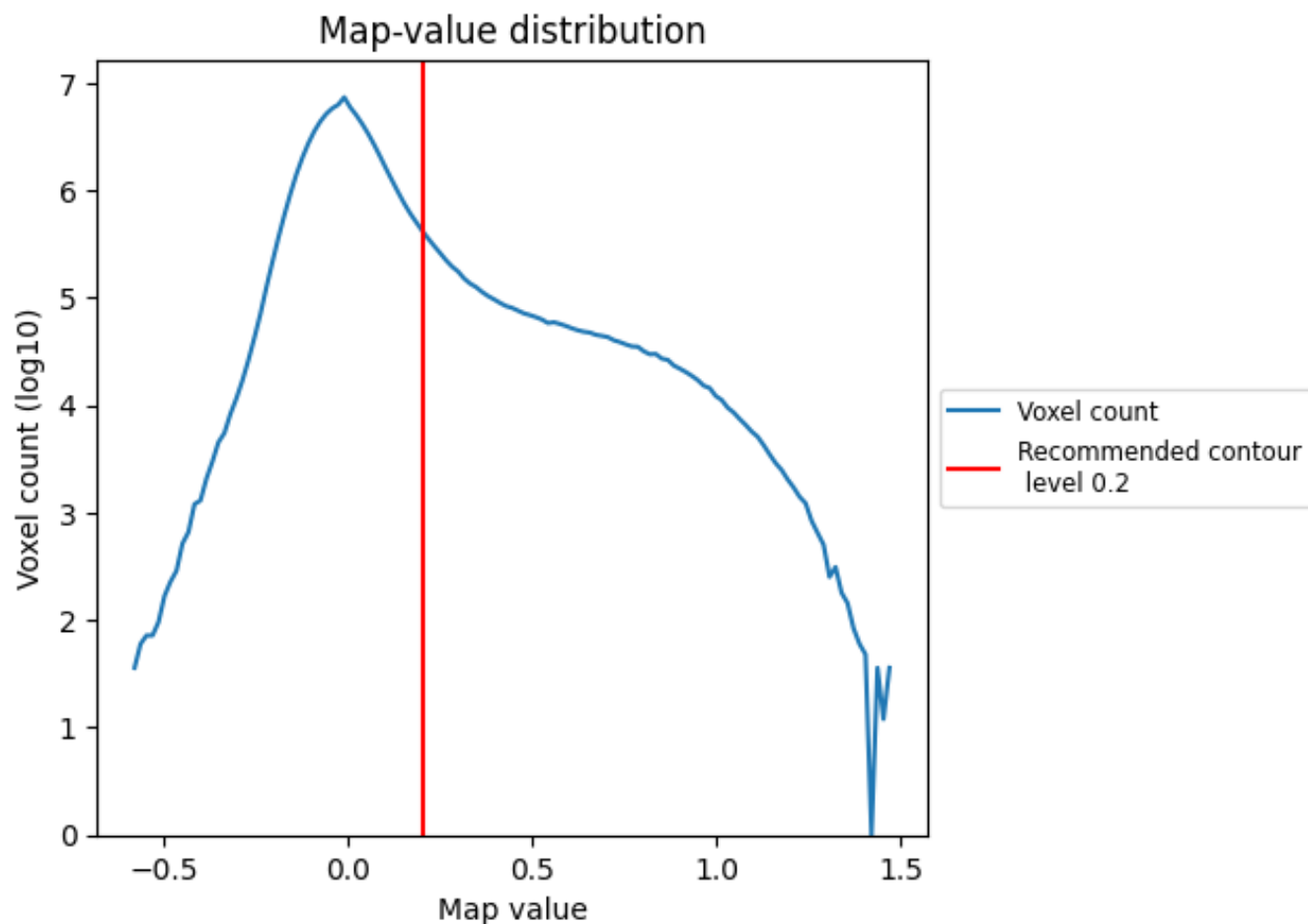
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

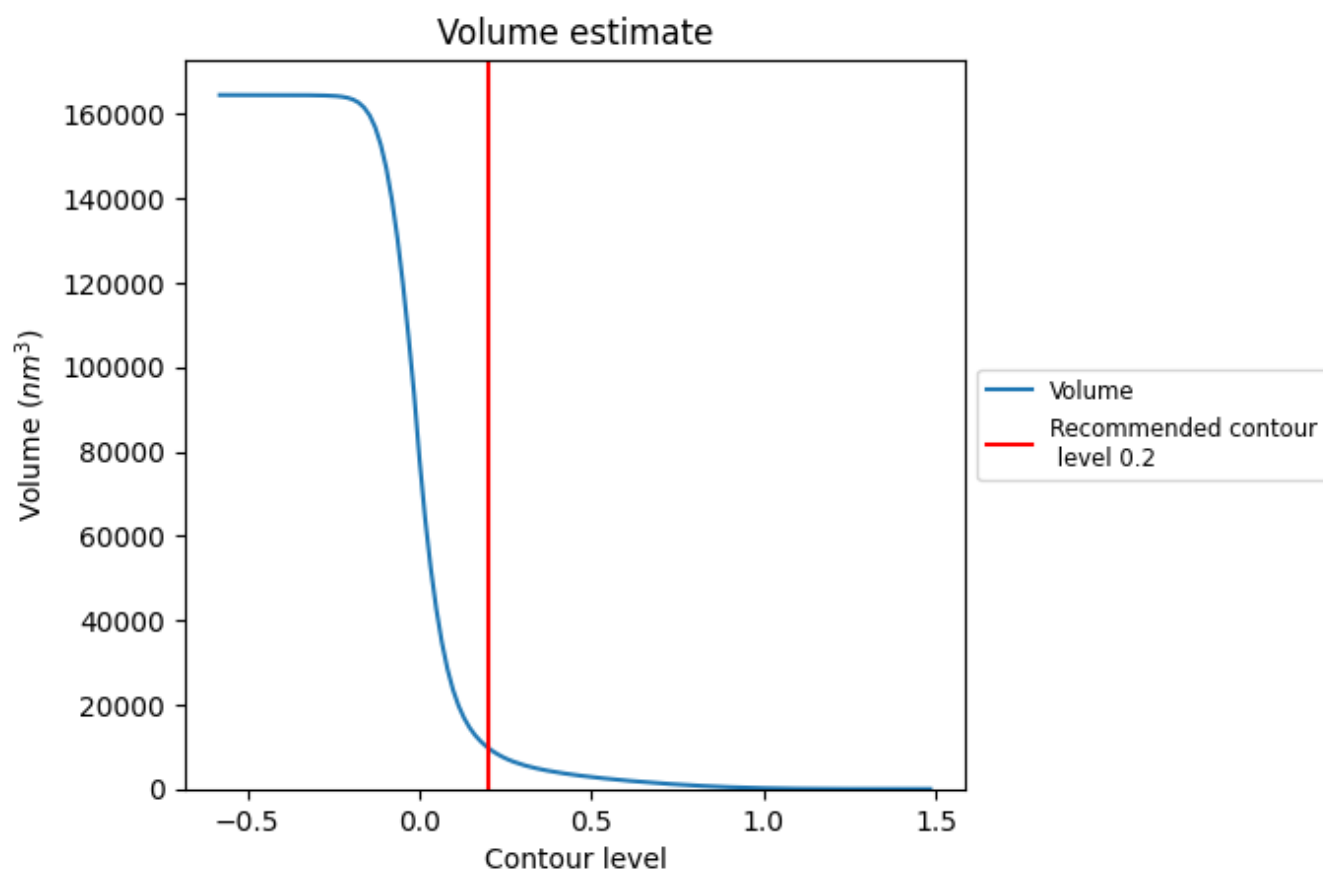
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

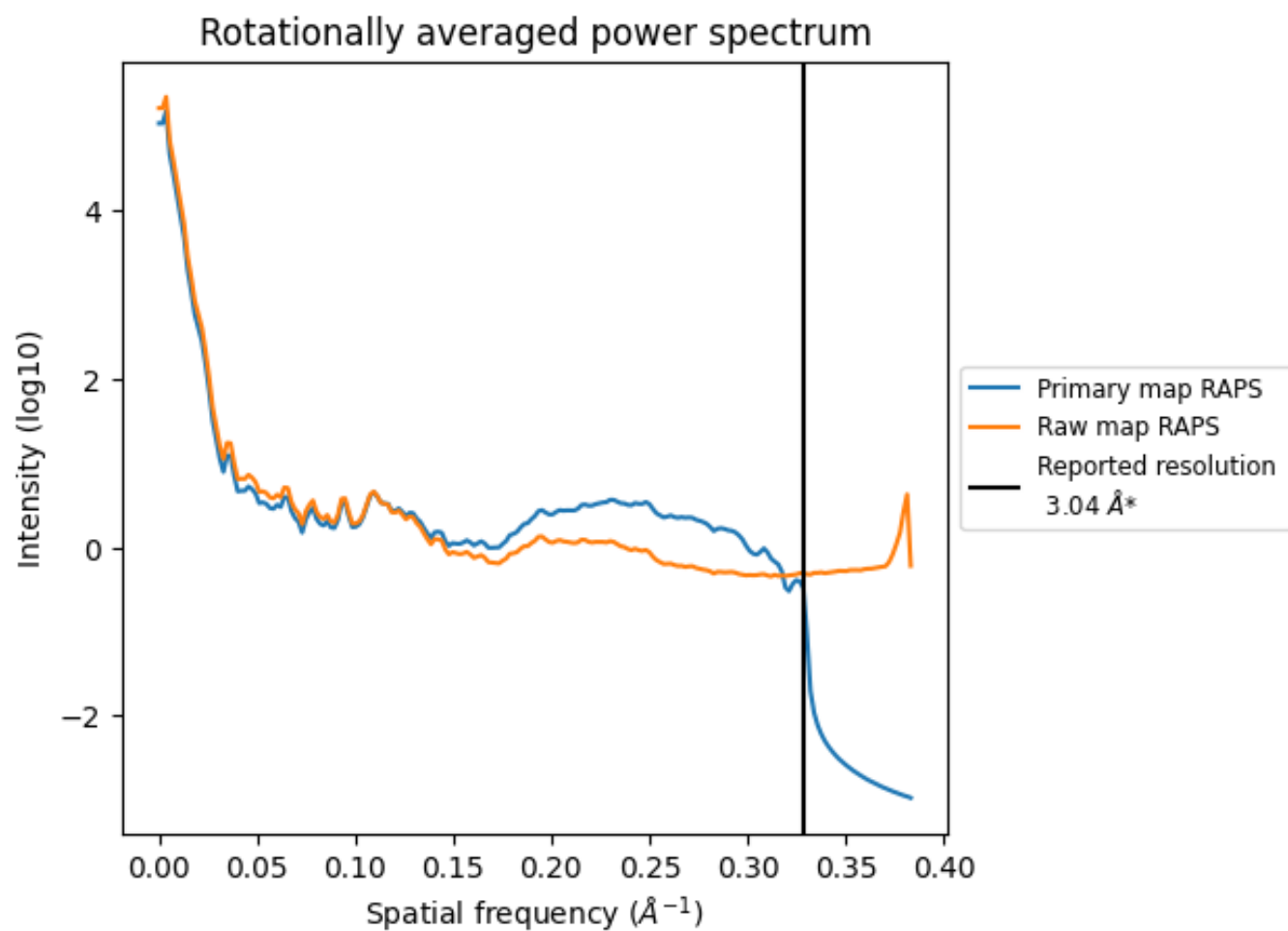
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 9710 nm³; this corresponds to an approximate mass of 8771 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 ⓘ

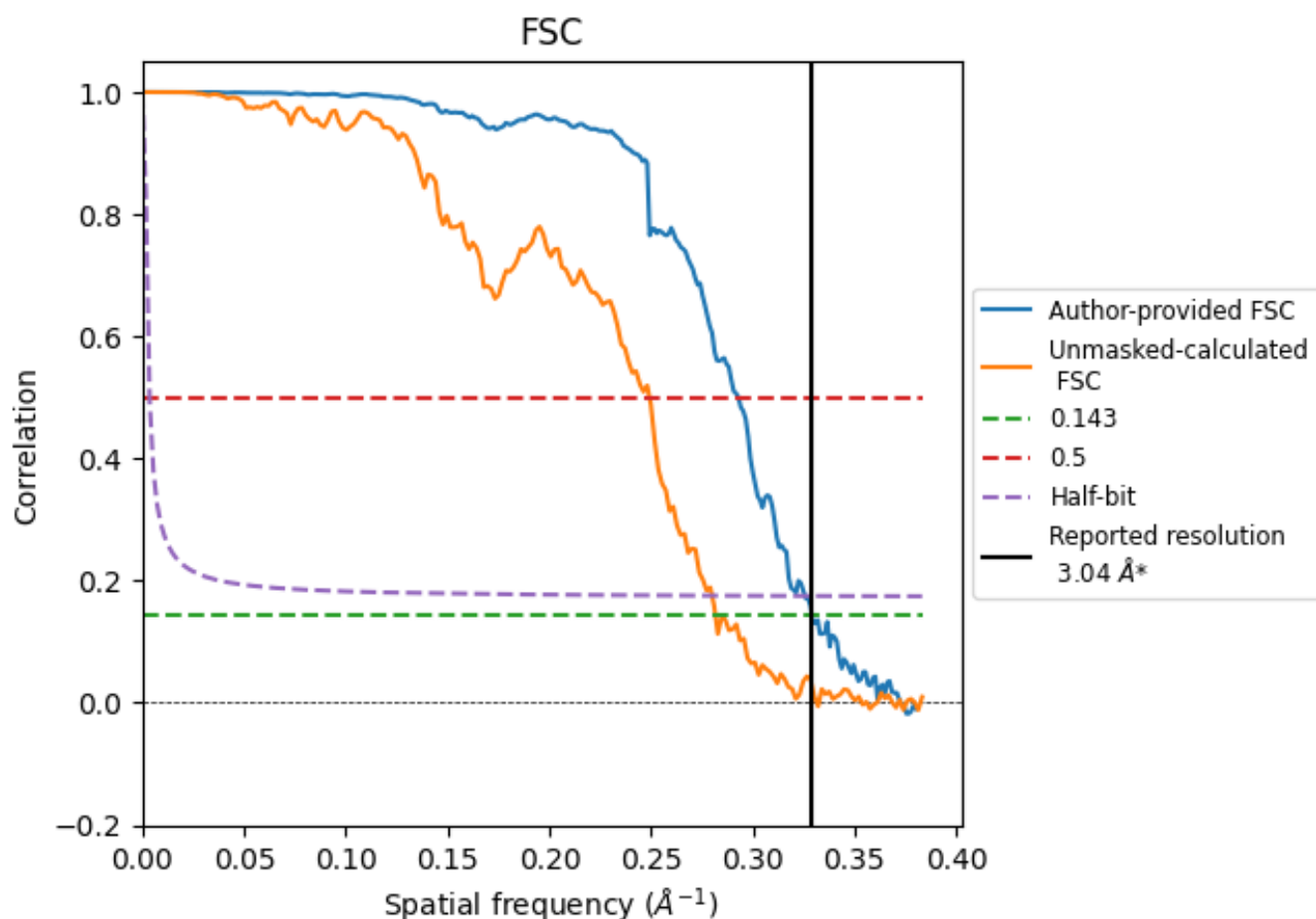


*Reported resolution corresponds to spatial frequency of 0.329 Å⁻¹

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 0.329 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.04	-	-
Author-provided FSC curve	3.04	3.41	3.07
Unmasked-calculated*	3.55	4.01	3.57

*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 3.55 differs from the reported value 3.04 by more than 10 %

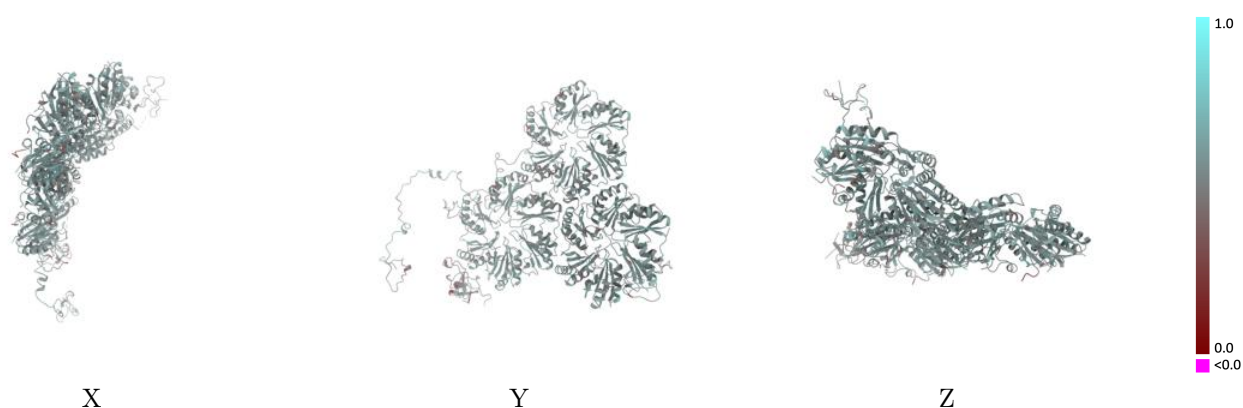
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39596 and PDB model 8YVC. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

This section was not generated.

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



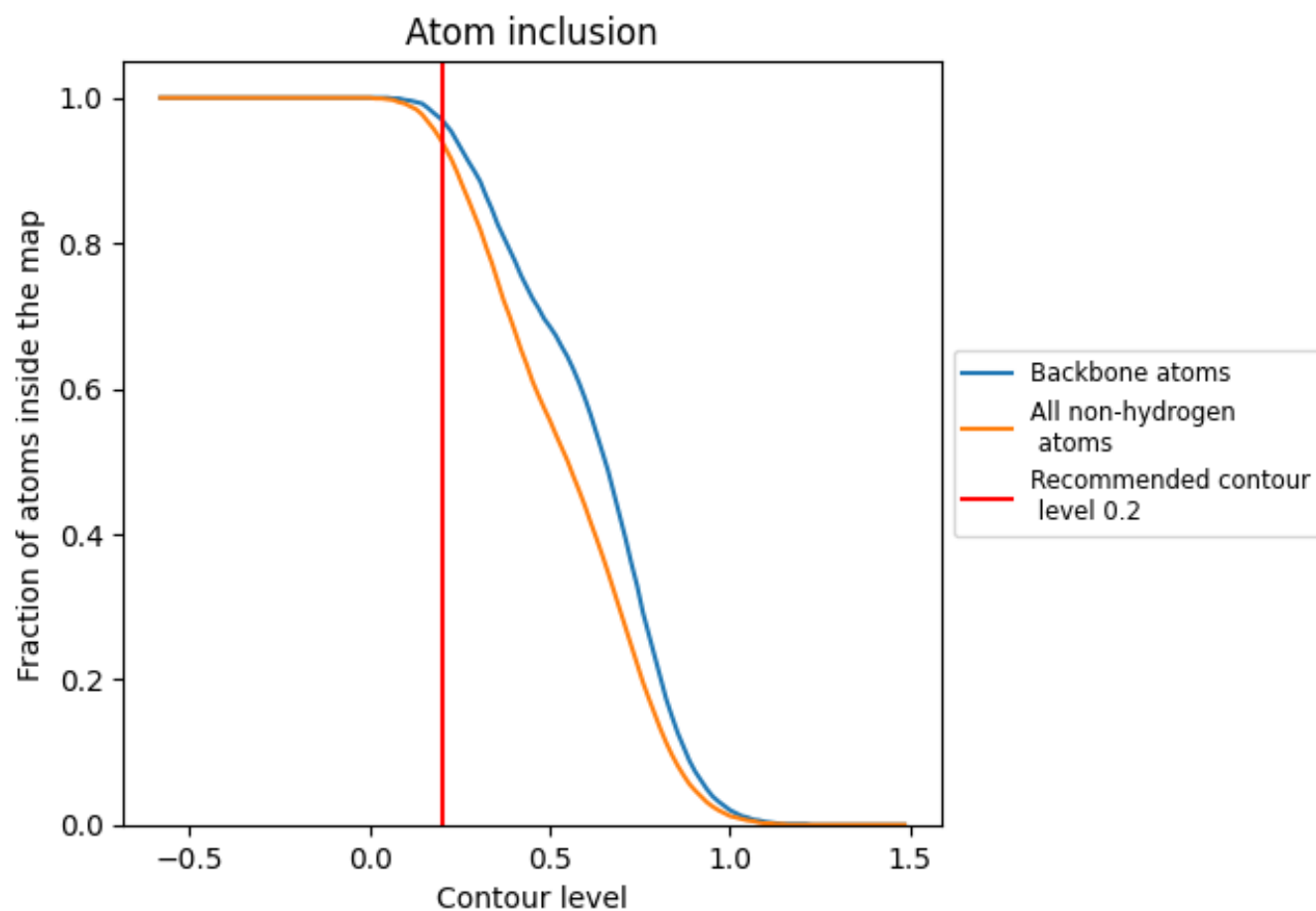
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 94% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9400	 0.5330
C	 0.9530	 0.5430
D	 0.9670	 0.5400
E	 0.9590	 0.5390
F	 0.9780	 0.5590
G	 0.9630	 0.5360
H	 0.9800	 0.5480
I	 0.9660	 0.5500
J	 0.9670	 0.5470
K	 0.9630	 0.5400
L	 0.9750	 0.5350
M	 0.9630	 0.5470
N	 0.9670	 0.5420
O	 0.9630	 0.5410
P	 0.9660	 0.5360
Q	 0.9670	 0.5340
R	 0.9590	 0.5360
S	 0.9610	 0.5410
T	 0.9720	 0.5440
U	 0.5020	 0.4390
X	 0.9070	 0.4900
Y	 0.9120	 0.5030

