Full wwPDB EM Validation Report ⓘ

Apr 21, 2025 – 02:36 PM JST

PDB ID	:	8X9X / pdb_00008x9x
EMDB ID	:	EMD-38187
Title	:	C-hexon capsomer of the VZV C-Capsid
Authors	:	Nan, W.; Lei, C.; Xiangxi, W.
Deposited on	:	2023-12-01
Resolution	:	3.10 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:

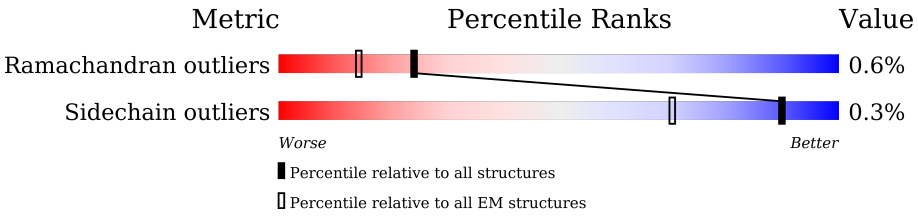
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 3.10 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=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	1369	97%
1	C	1369	97%
1	D	1369	97%
1	E	1369	97%
1	F	1369	97%
1	H	1369	97%
2	B	94	89% 11%
2	G	94	89% 10%
2	L	94	90% 9%

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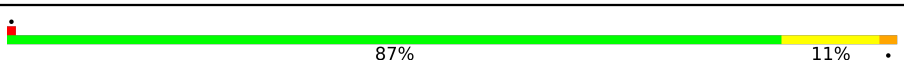
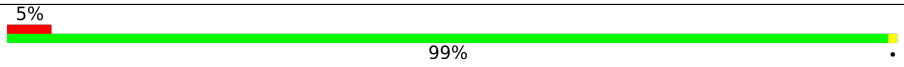
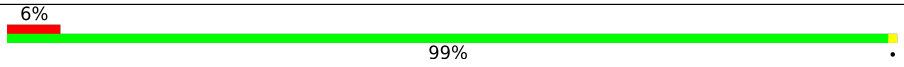
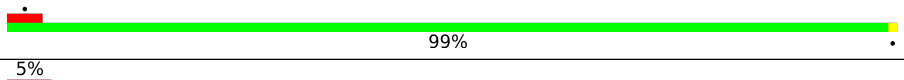
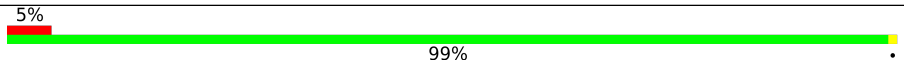
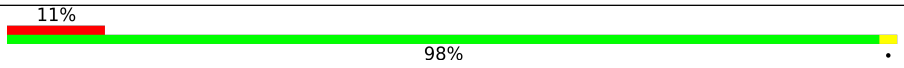
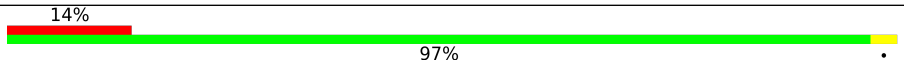
Mol	Chain	Length	Quality of chain
2	Q	94	
2	V	94	
2	g	94	
3	I	256	
3	K	256	
4	N	263	
4	P	263	
5	S	306	
5	U	306	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 78435 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 capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1331	Total	C	N	O	S	0	0
			10325	6541	1808	1910	66		
1	C	1331	Total	C	N	O	S	0	0
			10325	6541	1808	1910	66		
1	D	1331	Total	C	N	O	S	0	0
			10330	6543	1811	1910	66		
1	E	1331	Total	C	N	O	S	0	0
			10325	6541	1808	1910	66		
1	F	1331	Total	C	N	O	S	0	0
			10325	6541	1808	1910	66		
1	H	1331	Total	C	N	O	S	0	0
			10325	6541	1808	1910	66		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	814	ALA	GLY	conflict	UNP Q6QCL5
C	814	ALA	GLY	conflict	UNP Q6QCL5
D	814	ALA	GLY	conflict	UNP Q6QCL5
E	814	ALA	GLY	conflict	UNP Q6QCL5
F	814	ALA	GLY	conflict	UNP Q6QCL5
H	814	ALA	GLY	conflict	UNP Q6QCL5

- Molecule 2 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	94	Total	C	N	O	S	0	0
			699	437	135	125	2		
2	G	94	Total	C	N	O	S	0	0
			699	437	135	125	2		
2	L	94	Total	C	N	O	S	0	0
			699	437	135	125	2		
2	Q	94	Total	C	N	O	S	0	0
			699	437	135	125	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	V	94	Total	C	N	O	S	0	0
			699	437	135	125	2		
2	g	94	Total	C	N	O	S	0	0
			699	437	135	125	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	95	ARG	LYS	conflict	UNP U5NQG6
G	95	ARG	LYS	conflict	UNP U5NQG6
L	95	ARG	LYS	conflict	UNP U5NQG6
Q	95	ARG	LYS	conflict	UNP U5NQG6
V	95	ARG	LYS	conflict	UNP U5NQG6
g	95	ARG	LYS	conflict	UNP U5NQG6

- Molecule 3 is a protein called Tri2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	256	Total	C	N	O	S	0	0
			1847	1191	315	333	8		
3	K	256	Total	C	N	O	S	0	0
			1847	1191	315	333	8		

- Molecule 4 is a protein called Tri2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	263	Total	C	N	O	S	0	0
			1975	1269	339	358	9		
4	P	263	Total	C	N	O	S	0	0
			1975	1269	339	358	9		

- Molecule 5 is a protein called Tri1.

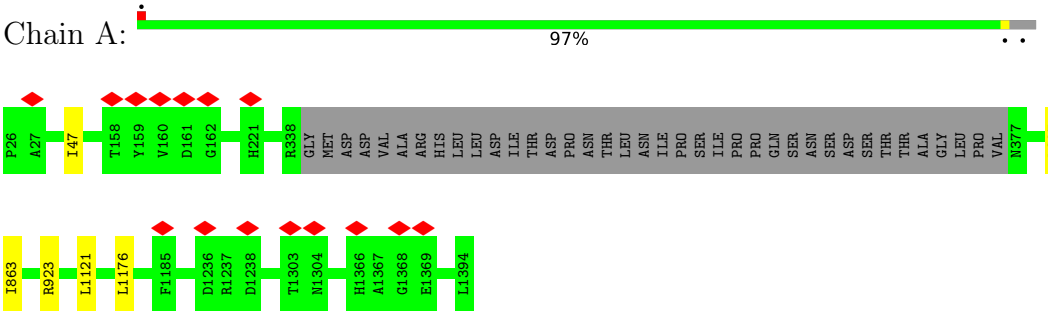
Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	306	Total	C	N	O	S	0	0
			2321	1468	431	409	13		
5	U	306	Total	C	N	O	S	0	0
			2321	1468	431	409	13		

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.

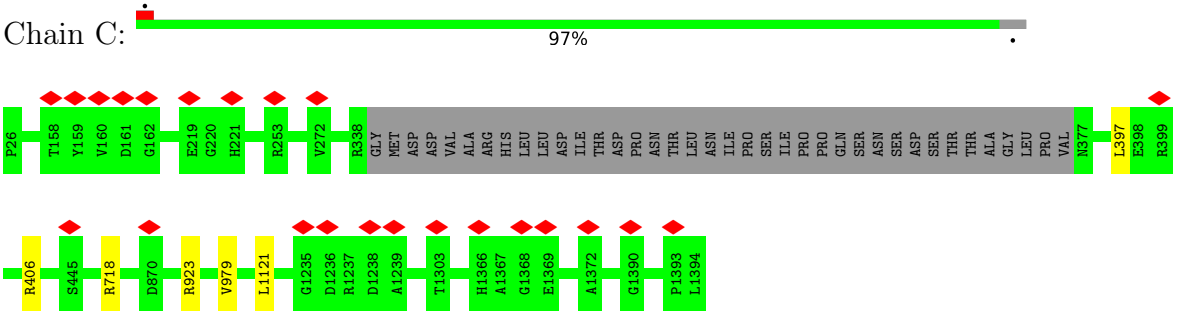
• Molecule 1: Major capsid protein

Chain A:



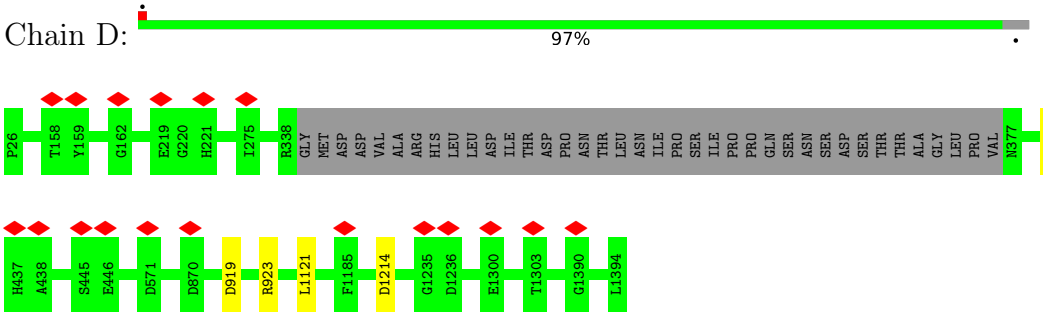
• Molecule 1: Major capsid protein

Chain C:



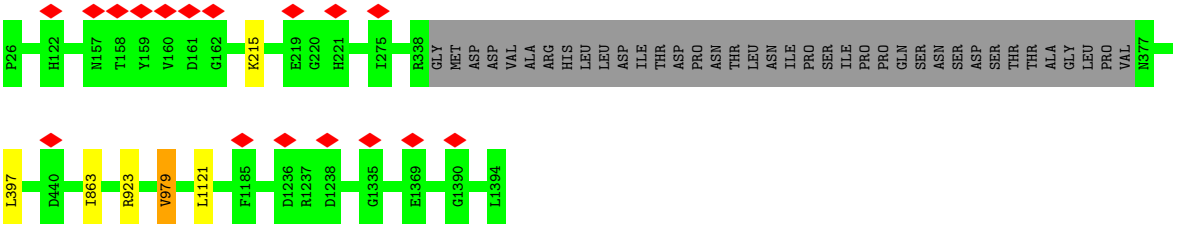
• Molecule 1: Major capsid protein

Chain D:



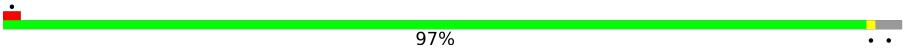
• Molecule 1: Major capsid protein

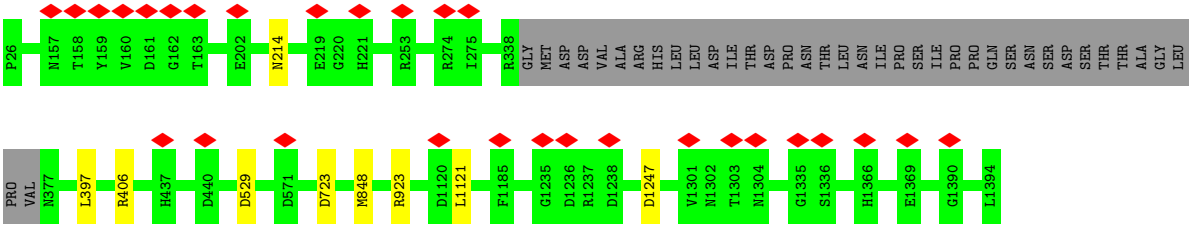
Chain E:



• Molecule 1: Major capsid protein

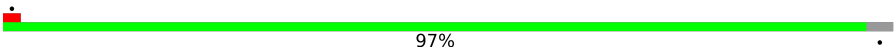
Chain F:

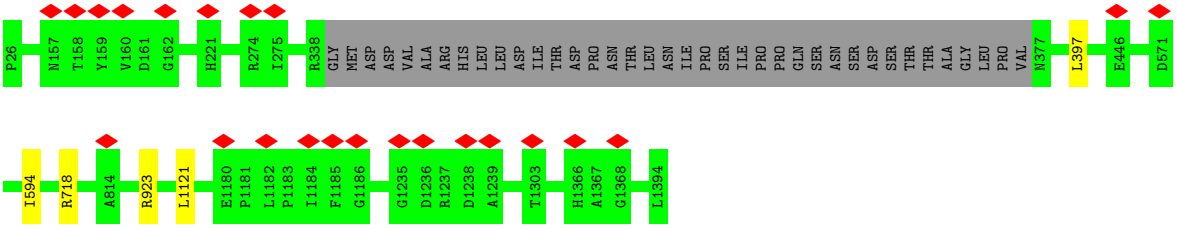




• Molecule 1: Major capsid protein

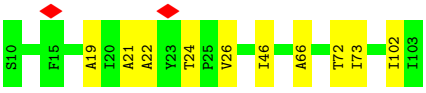
Chain H:





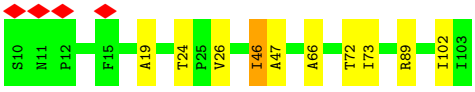
• Molecule 2: Small capsomere-interacting protein

Chain B:



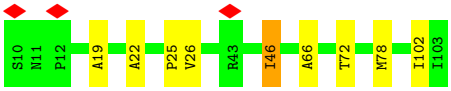
• Molecule 2: Small capsomere-interacting protein

Chain G:



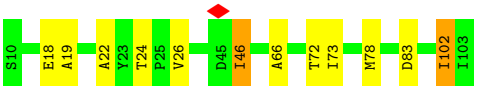
• Molecule 2: Small capsomere-interacting protein

Chain L:



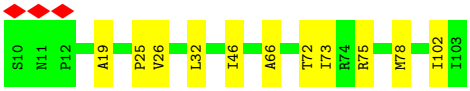
• Molecule 2: Small capsomere-interacting protein

Chain Q:



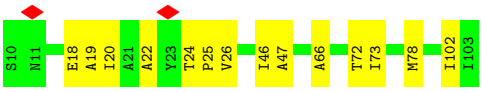
• Molecule 2: Small capsomere-interacting protein

Chain V:



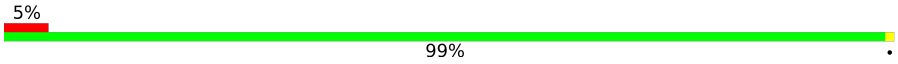
• Molecule 2: Small capsomere-interacting protein

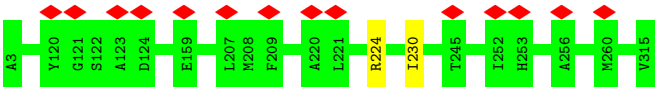
Chain g:



• Molecule 3: Tri2A

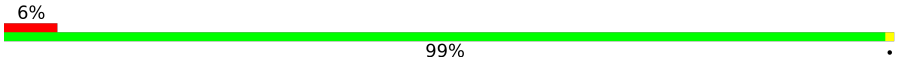
Chain I:

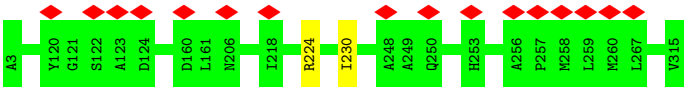




• Molecule 3: Tri2A

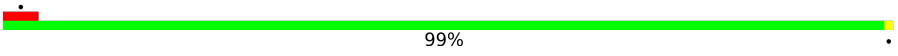
Chain K:

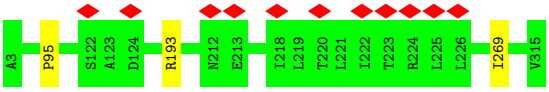




• Molecule 4: Tri2B

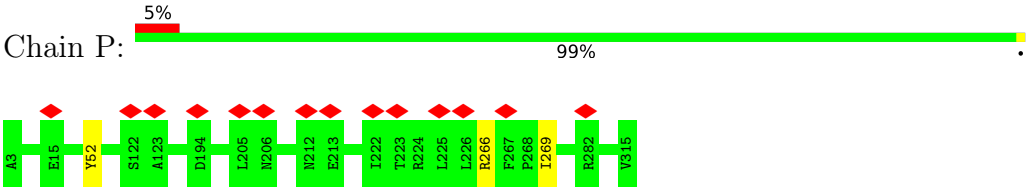
Chain N:





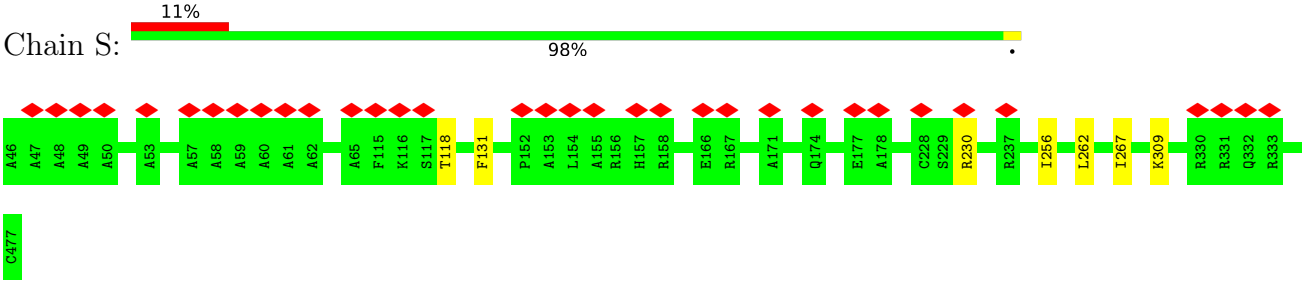
• Molecule 4: Tri2B

Chain P:



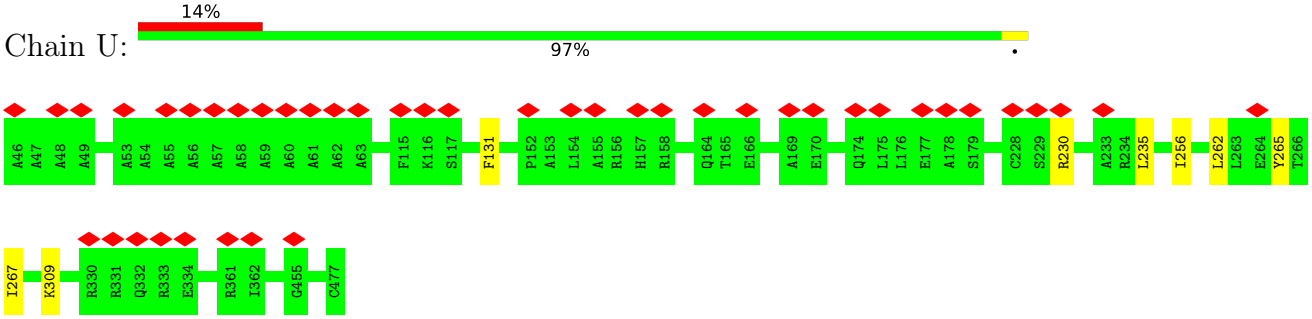
• Molecule 5: Tri1

Chain S:



• Molecule 5: Tri1

Chain U:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1755031	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	0.123	Depositor
Minimum map value	-0.070	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	324.0, 324.0, 324.0	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	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	0.32	0/10575	0.61	6/14415 (0.0%)
1	C	0.32	0/10575	0.62	3/14415 (0.0%)
1	D	0.32	0/10580	0.62	4/14421 (0.0%)
1	E	0.32	0/10575	0.60	4/14415 (0.0%)
1	F	0.32	0/10575	0.62	6/14415 (0.0%)
1	H	0.32	0/10575	0.61	3/14415 (0.0%)
2	B	0.35	0/714	0.94	1/978 (0.1%)
2	G	0.34	0/714	0.94	2/978 (0.2%)
2	L	0.34	0/714	0.93	1/978 (0.1%)
2	Q	0.36	0/714	1.03	3/978 (0.3%)
2	V	0.34	0/714	0.96	2/978 (0.2%)
2	g	0.36	0/714	1.01	2/978 (0.2%)
3	I	0.30	0/1878	0.64	0/2568
3	K	0.29	0/1878	0.62	0/2568
4	N	0.38	1/2010 (0.0%)	0.69	3/2743 (0.1%)
4	P	0.28	0/2010	0.61	0/2743
5	S	0.30	0/2368	0.65	0/3215
5	U	0.30	0/2368	0.66	1/3215 (0.0%)
All	All	0.32	1/80251 (0.0%)	0.64	41/109416 (0.0%)

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	E	0	1
2	B	0	3
2	G	0	1
2	L	0	2
2	Q	0	4
2	g	0	3
4	P	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	15

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	95	PRO	CG-CD	-9.73	1.18	1.50

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	N	95	PRO	N-CD-CG	-10.72	87.11	103.20
4	N	95	PRO	CA-N-CD	-9.47	98.24	111.50
1	F	529	ASP	CB-CG-OD1	7.83	125.35	118.30
1	F	723	ASP	CB-CG-OD1	7.50	125.05	118.30
1	F	1121	LEU	CA-CB-CG	7.25	131.97	115.30
2	g	20	ILE	CG1-CB-CG2	-6.75	96.54	111.40
1	D	1121	LEU	CA-CB-CG	6.71	130.75	115.30
1	D	919	ASP	CB-CG-OD1	6.70	124.33	118.30
1	E	397	LEU	CA-CB-CG	6.70	130.71	115.30
1	E	863	ILE	CG1-CB-CG2	-6.44	97.23	111.40
1	A	863	ILE	CG1-CB-CG2	-6.32	97.49	111.40
1	C	397	LEU	CA-CB-CG	6.31	129.82	115.30
1	F	397	LEU	CA-CB-CG	6.23	129.64	115.30
1	E	1121	LEU	CA-CB-CG	6.19	129.54	115.30
1	A	1121	LEU	CA-CB-CG	6.19	129.53	115.30
2	Q	83	ASP	CB-CG-OD1	6.17	123.85	118.30
1	H	1121	LEU	CA-CB-CG	6.07	129.25	115.30
1	C	1121	LEU	CA-CB-CG	5.95	128.99	115.30
1	F	848	MET	CG-SD-CE	-5.89	90.78	100.20
1	H	397	LEU	CA-CB-CG	5.86	128.78	115.30
1	E	979	VAL	C-N-CA	5.79	136.17	121.70
1	A	1176	LEU	CA-CB-CG	5.78	128.60	115.30
1	C	979	VAL	C-N-CA	5.78	136.14	121.70
4	N	95	PRO	CA-CB-CG	-5.74	93.10	104.00
1	D	397	LEU	CA-CB-CG	5.68	128.37	115.30
1	A	397	LEU	CA-CB-CG	5.67	128.35	115.30
2	g	72	THR	C-N-CA	5.65	135.82	121.70
2	V	32	LEU	CA-CB-CG	5.58	128.14	115.30
1	F	1247	ASP	CB-CG-OD2	5.49	123.24	118.30
2	B	72	THR	C-N-CA	5.45	135.32	121.70
2	G	72	THR	C-N-CA	5.44	135.29	121.70
1	D	1214	ASP	CB-CG-OD1	5.43	123.19	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	102	ILE	CG1-CB-CG2	-5.39	99.54	111.40
2	V	72	THR	C-N-CA	5.38	135.16	121.70
5	U	235	LEU	CA-CB-CG	5.36	127.63	115.30
1	H	594	ILE	CG1-CB-CG2	-5.33	99.67	111.40
2	G	46	ILE	CG1-CB-CG2	-5.29	99.77	111.40
1	A	859	LEU	CA-CB-CG	5.27	127.43	115.30
2	Q	72	THR	C-N-CA	5.16	134.59	121.70
1	A	47	ILE	CG1-CB-CG2	-5.09	100.20	111.40
2	L	72	THR	C-N-CA	5.07	134.37	121.70

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	21	ALA	Peptide
2	B	22	ALA	Peptide
2	B	24	THR	Peptide
1	E	979	VAL	Peptide
2	G	24	THR	Peptide
2	L	22	ALA	Peptide
2	L	46	ILE	Peptide
4	P	52	TYR	Peptide
2	Q	18	GLU	Peptide
2	Q	22	ALA	Peptide
2	Q	24	THR	Peptide
2	Q	46	ILE	Peptide
2	g	18	GLU	Peptide
2	g	22	ALA	Peptide
2	g	24	THR	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	1327/1369 (97%)	1214 (92%)	113 (8%)	0	100 100
1	C	1327/1369 (97%)	1219 (92%)	108 (8%)	0	100 100
1	D	1327/1369 (97%)	1229 (93%)	98 (7%)	0	100 100
1	E	1327/1369 (97%)	1221 (92%)	106 (8%)	0	100 100
1	F	1327/1369 (97%)	1210 (91%)	117 (9%)	0	100 100
1	H	1327/1369 (97%)	1217 (92%)	110 (8%)	0	100 100
2	B	92/94 (98%)	62 (67%)	24 (26%)	6 (6%)	1 6
2	G	92/94 (98%)	59 (64%)	26 (28%)	7 (8%)	1 4
2	L	92/94 (98%)	58 (63%)	27 (29%)	7 (8%)	1 4
2	Q	92/94 (98%)	59 (64%)	26 (28%)	7 (8%)	1 4
2	V	92/94 (98%)	56 (61%)	28 (30%)	8 (9%)	0 4
2	g	92/94 (98%)	63 (68%)	20 (22%)	9 (10%)	0 3
3	I	248/256 (97%)	227 (92%)	20 (8%)	1 (0%)	30 63
3	K	248/256 (97%)	233 (94%)	14 (6%)	1 (0%)	30 63
4	N	257/263 (98%)	240 (93%)	16 (6%)	1 (0%)	30 63
4	P	257/263 (98%)	239 (93%)	17 (7%)	1 (0%)	30 63
5	S	298/306 (97%)	257 (86%)	36 (12%)	5 (2%)	7 30
5	U	298/306 (97%)	261 (88%)	32 (11%)	5 (2%)	7 30
All	All	10120/10428 (97%)	9124 (90%)	938 (9%)	58 (1%)	24 53

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	19	ALA
2	B	66	ALA
2	B	102	ILE
2	G	19	ALA
2	G	66	ALA
2	L	19	ALA
2	L	66	ALA
2	L	102	ILE
2	Q	19	ALA
2	Q	66	ALA
2	Q	102	ILE

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Mol	Chain	Res	Type
2	V	19	ALA
2	V	66	ALA
2	V	102	ILE
2	g	19	ALA
2	g	102	ILE
5	S	267	ILE
5	U	267	ILE
2	B	46	ILE
2	G	46	ILE
2	G	47	ALA
2	G	102	ILE
2	L	46	ILE
2	Q	46	ILE
2	V	46	ILE
2	g	46	ILE
2	g	47	ALA
2	g	66	ALA
3	I	230	ILE
5	S	118	THR
2	L	78	MET
2	Q	78	MET
3	K	230	ILE
5	U	131	PHE
2	B	26	VAL
2	g	78	MET
2	G	26	VAL
2	L	26	VAL
2	V	78	MET
5	S	131	PHE
5	S	262	LEU
5	U	265	TYR
2	Q	26	VAL
2	V	26	VAL
5	U	256	ILE
5	U	262	LEU
4	N	269	ILE
2	L	25	PRO
2	B	73	ILE
2	G	73	ILE
2	g	26	VAL
2	g	73	ILE
4	P	269	ILE

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Mol	Chain	Res	Type
2	Q	73	ILE
2	V	25	PRO
2	V	73	ILE
2	g	25	PRO
5	S	256	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1106/1158 (96%)	1105 (100%)	1 (0%)	92 97
1	C	1106/1158 (96%)	1103 (100%)	3 (0%)	91 95
1	D	1107/1158 (96%)	1106 (100%)	1 (0%)	92 97
1	E	1106/1158 (96%)	1104 (100%)	2 (0%)	92 96
1	F	1106/1158 (96%)	1103 (100%)	3 (0%)	91 95
1	H	1106/1158 (96%)	1104 (100%)	2 (0%)	92 96
2	B	69/73 (94%)	69 (100%)	0	100 100
2	G	69/73 (94%)	68 (99%)	1 (1%)	62 81
2	L	69/73 (94%)	69 (100%)	0	100 100
2	Q	69/73 (94%)	69 (100%)	0	100 100
2	V	69/73 (94%)	68 (99%)	1 (1%)	62 81
2	g	69/73 (94%)	69 (100%)	0	100 100
3	I	188/218 (86%)	187 (100%)	1 (0%)	86 92
3	K	188/218 (86%)	187 (100%)	1 (0%)	86 92
4	N	214/224 (96%)	213 (100%)	1 (0%)	86 92
4	P	214/224 (96%)	213 (100%)	1 (0%)	86 92
5	S	225/238 (94%)	223 (99%)	2 (1%)	75 88
5	U	225/238 (94%)	223 (99%)	2 (1%)	75 88
All	All	8305/8746 (95%)	8283 (100%)	22 (0%)	90 95

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	923	ARG
1	C	406	ARG
1	C	718	ARG
1	C	923	ARG
1	D	923	ARG
1	E	215	LYS
1	E	923	ARG
1	F	214	ASN
1	F	406	ARG
1	F	923	ARG
2	G	89	ARG
1	H	718	ARG
1	H	923	ARG
2	V	75	ARG
3	I	224	ARG
3	K	224	ARG
4	N	193	ARG
4	P	266	ARG
5	S	230	ARG
5	S	309	LYS
5	U	230	ARG
5	U	309	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	GLN
2	B	71	ASN
1	C	217	GLN
1	C	653	ASN
1	C	1321	GLN
1	D	175	GLN
1	D	740	ASN
1	D	1058	GLN
1	E	1037	ASN

5.3.3 RNA

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	U	3
5	S	3
3	K	3
3	I	3
4	N	2
4	P	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	U	65:ALA	C	115:PHE	N	36.22
1	S	65:ALA	C	115:PHE	N	35.71
1	N	226:LEU	C	266:ARG	N	28.62
1	P	226:LEU	C	266:ARG	N	28.12
1	K	236:LEU	C	244:VAL	N	20.95
1	I	236:LEU	C	244:VAL	N	20.57
1	K	260:MET	C	267:LEU	N	18.89
1	I	260:MET	C	267:LEU	N	18.54
1	N	163:ALA	C	175:ASP	N	17.38
1	P	163:ALA	C	175:ASP	N	16.78
1	U	179:SER	C	192:ARG	N	13.18

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	U	362:ILE	C	428:CYS	N	13.14
1	S	179:SER	C	192:ARG	N	13.04
1	S	362:ILE	C	428:CYS	N	12.77
1	I	161:LEU	C	206:ASN	N	12.44
1	K	161:LEU	C	206:ASN	N	12.18

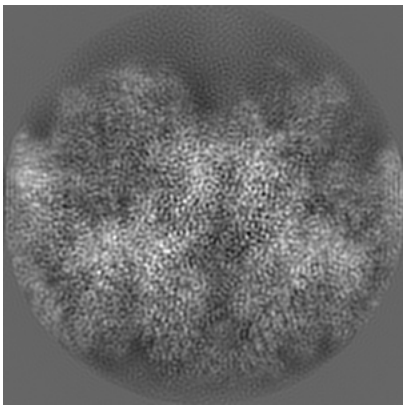
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38187. These allow visual inspection of the internal detail of the map and identification of artifacts.

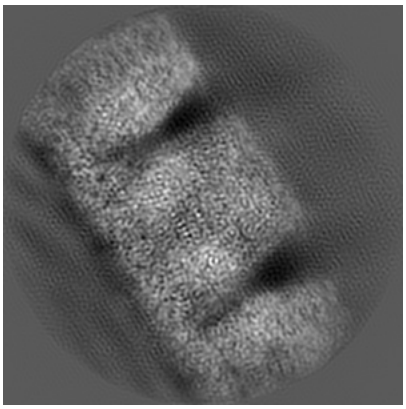
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

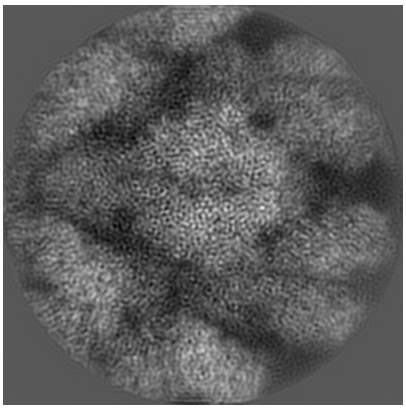
6.1.1 Primary map



X

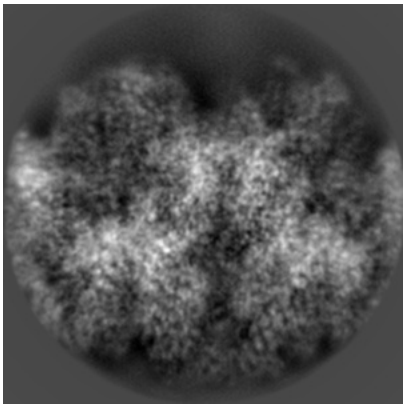


Y

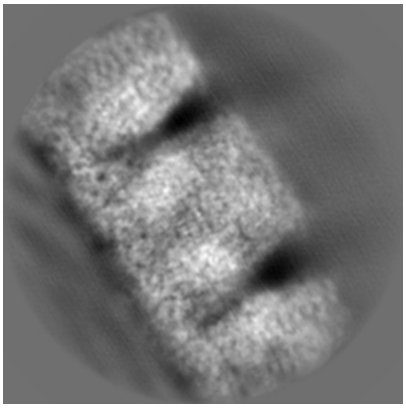


Z

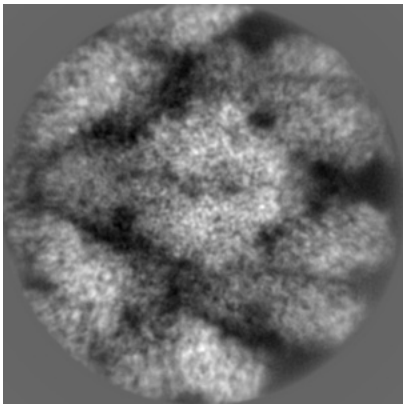
6.1.2 Raw map



X



Y

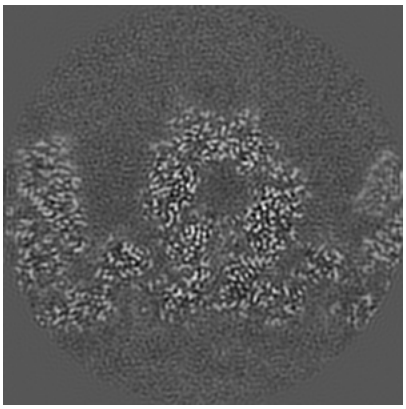


Z

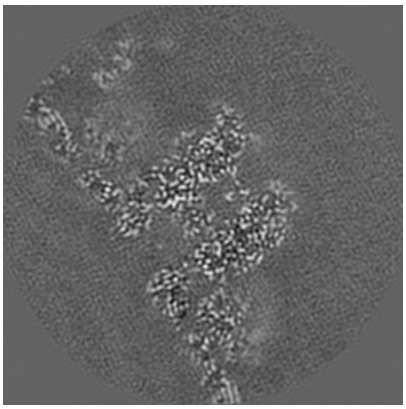
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

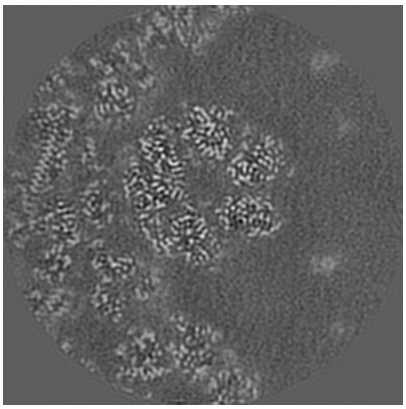
6.2.1 Primary map



X Index: 120

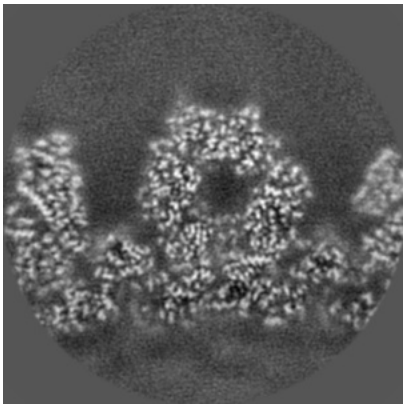


Y Index: 120

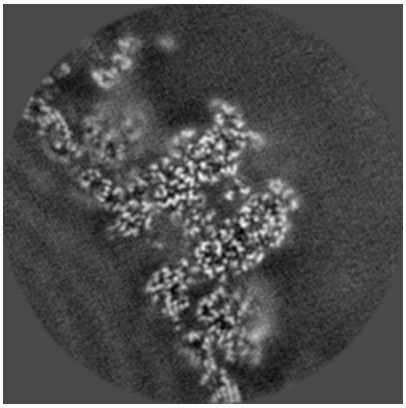


Z Index: 120

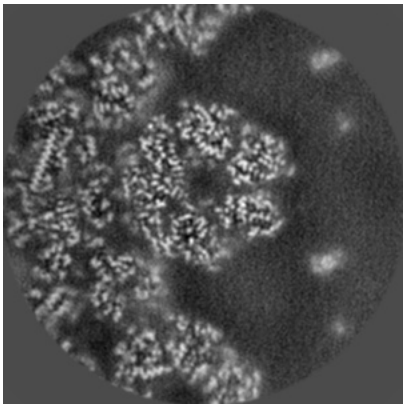
6.2.2 Raw map



X Index: 120



Y Index: 120

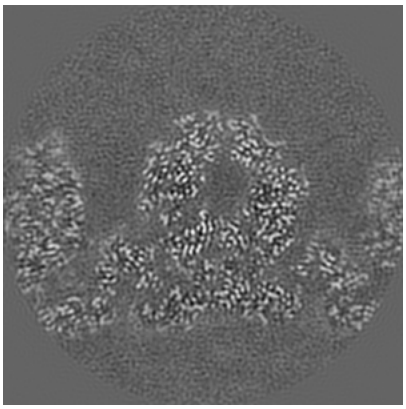


Z Index: 120

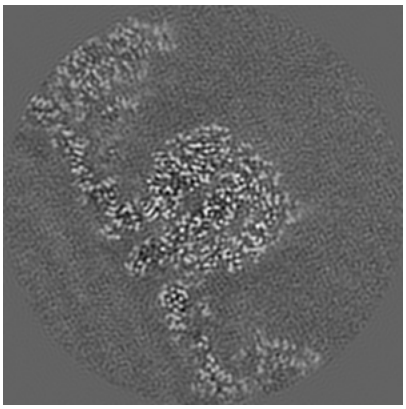
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

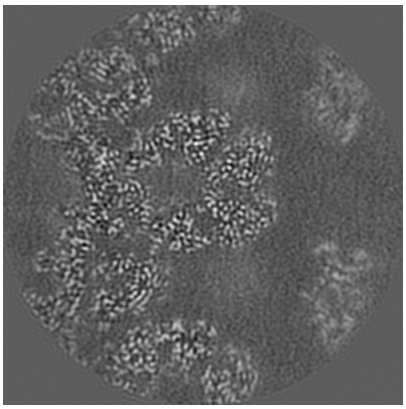
6.3.1 Primary map



X Index: 123

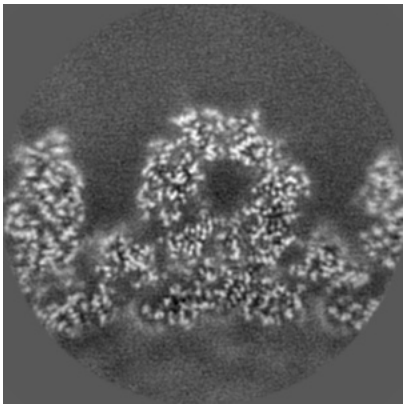


Y Index: 109

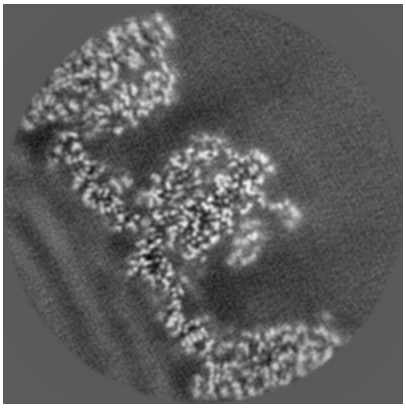


Z Index: 108

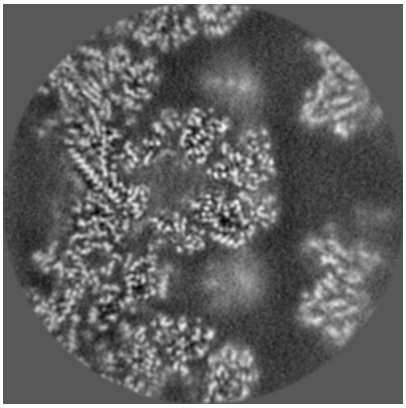
6.3.2 Raw map



X Index: 122



Y Index: 101

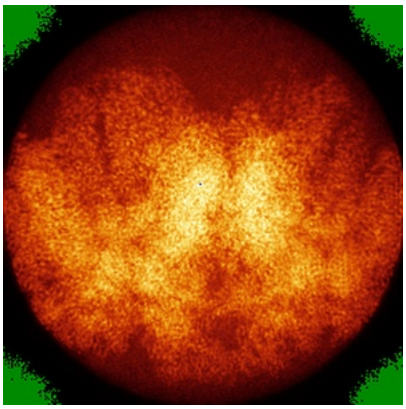


Z Index: 105

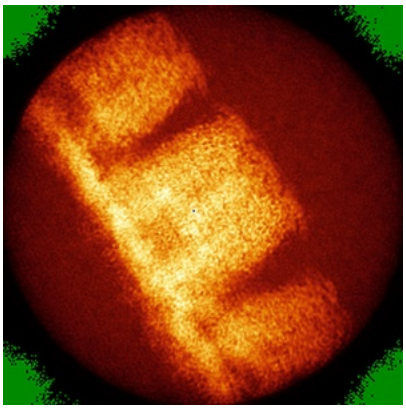
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

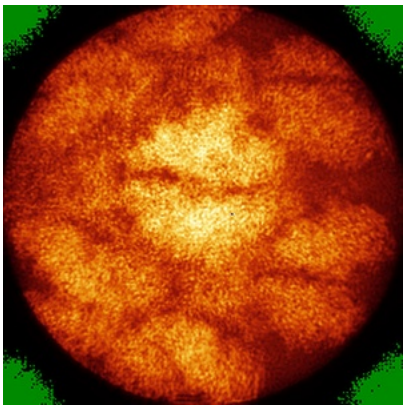
6.4.1 Primary map



X

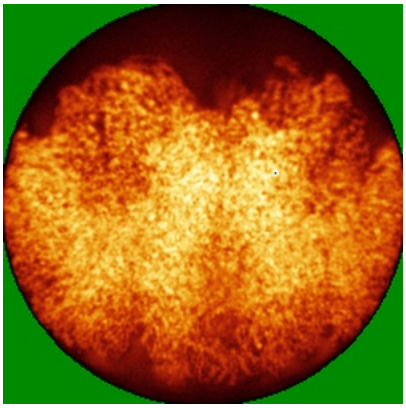


Y

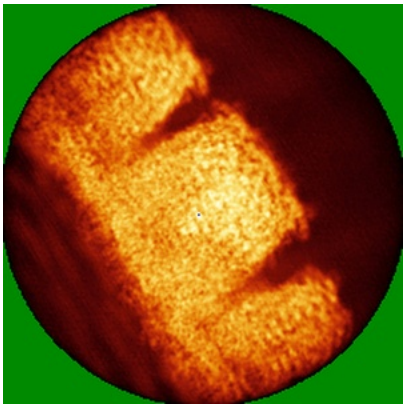


Z

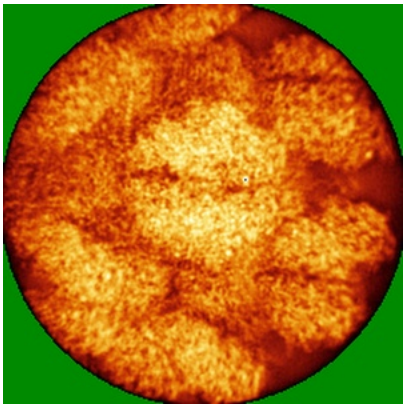
6.4.2 Raw map



X



Y

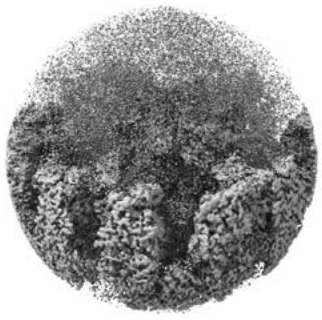


Z

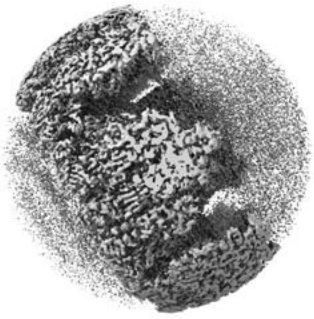
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

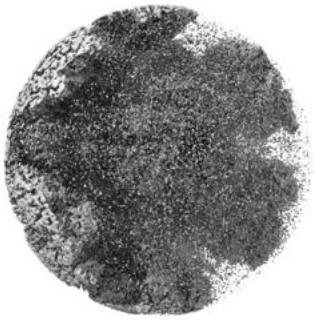
6.5.1 Primary map



X



Y

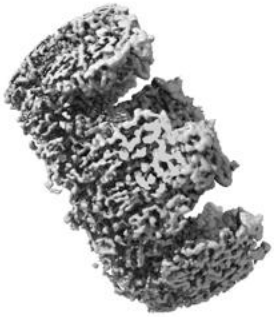


Z

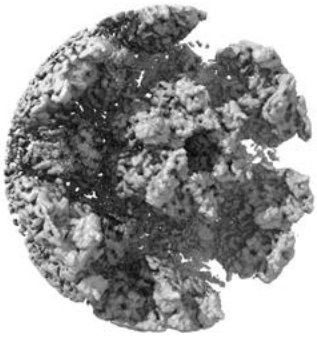
The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

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.

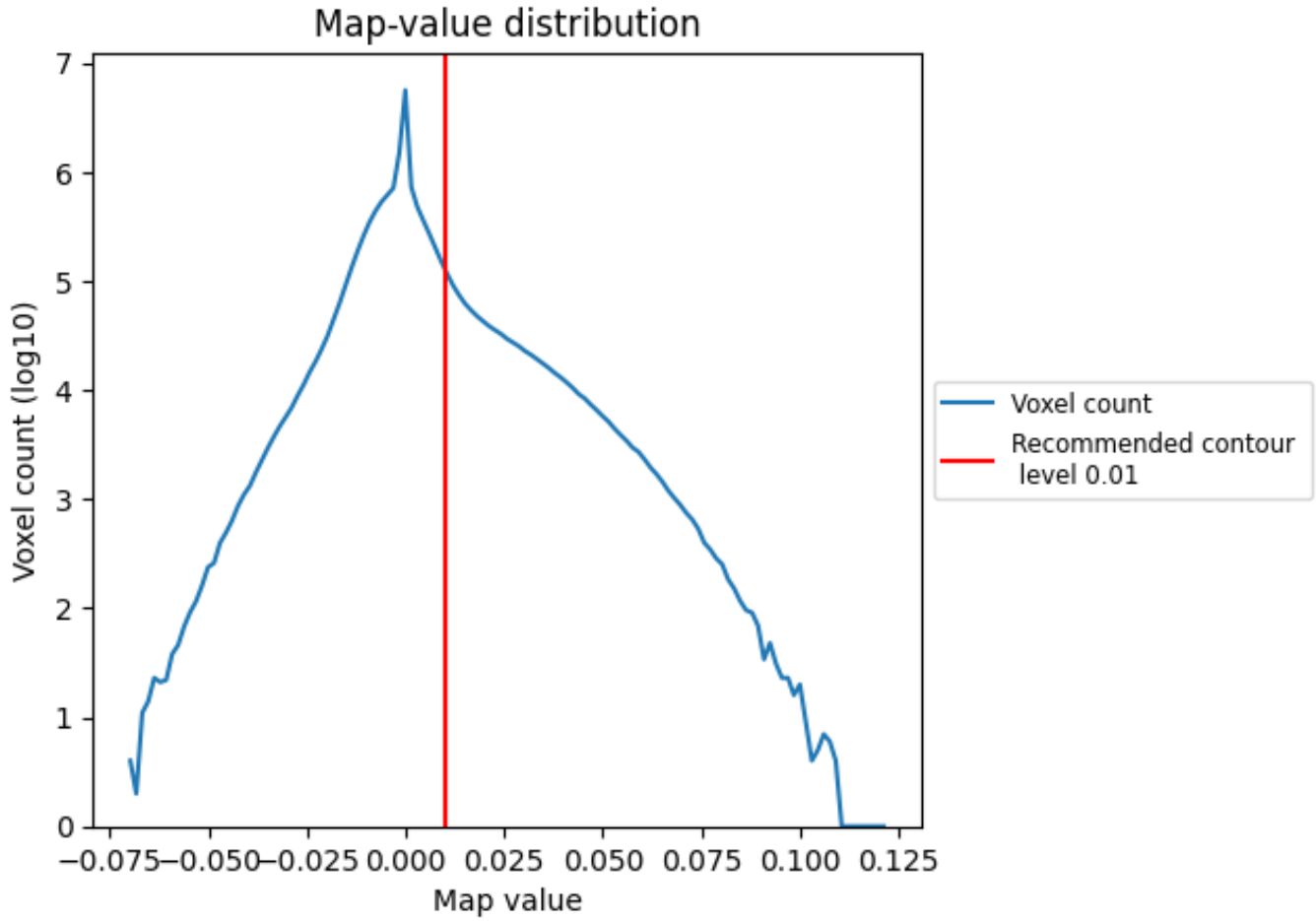
6.6 Mask visualisation (i)

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

7 Map analysis

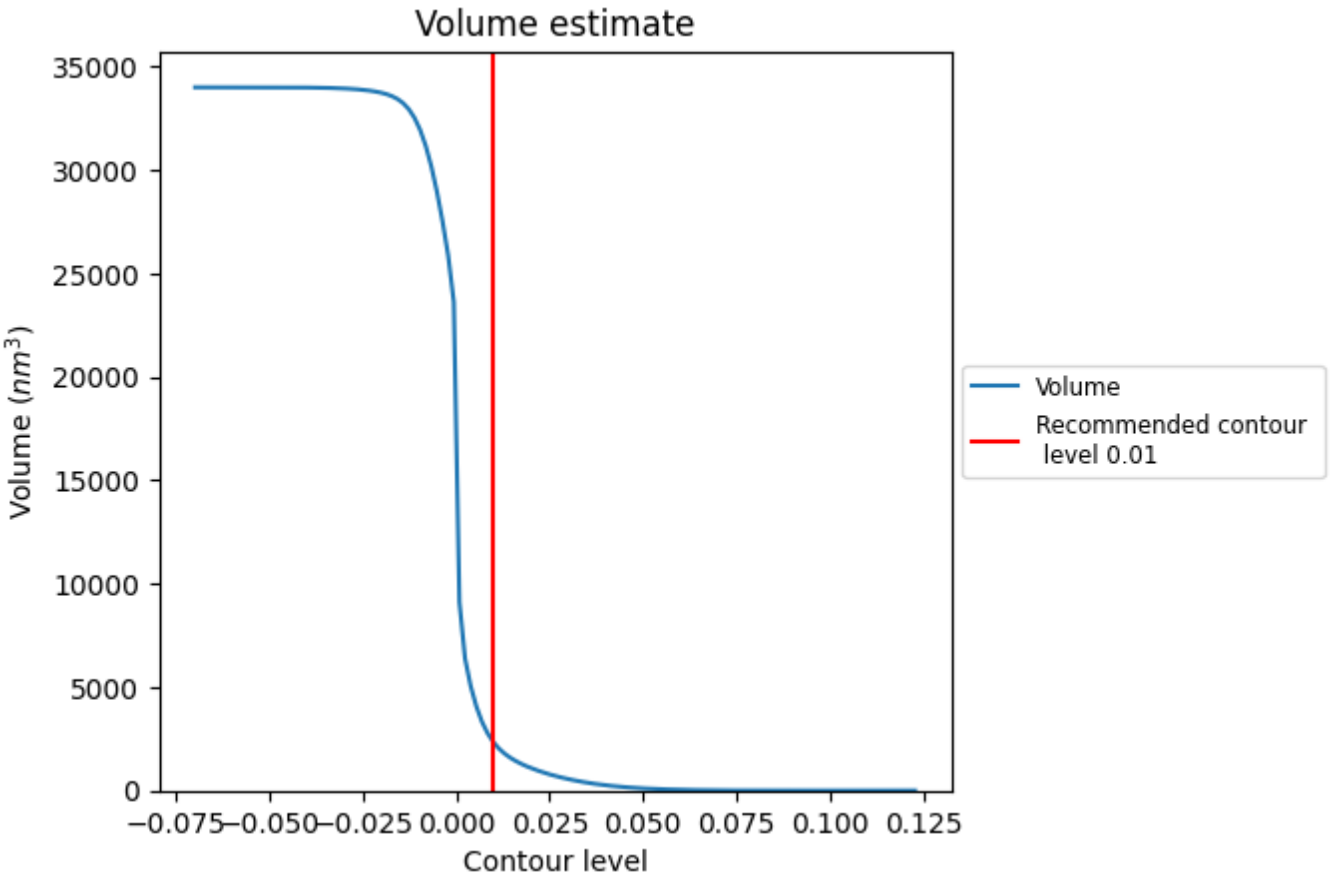
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

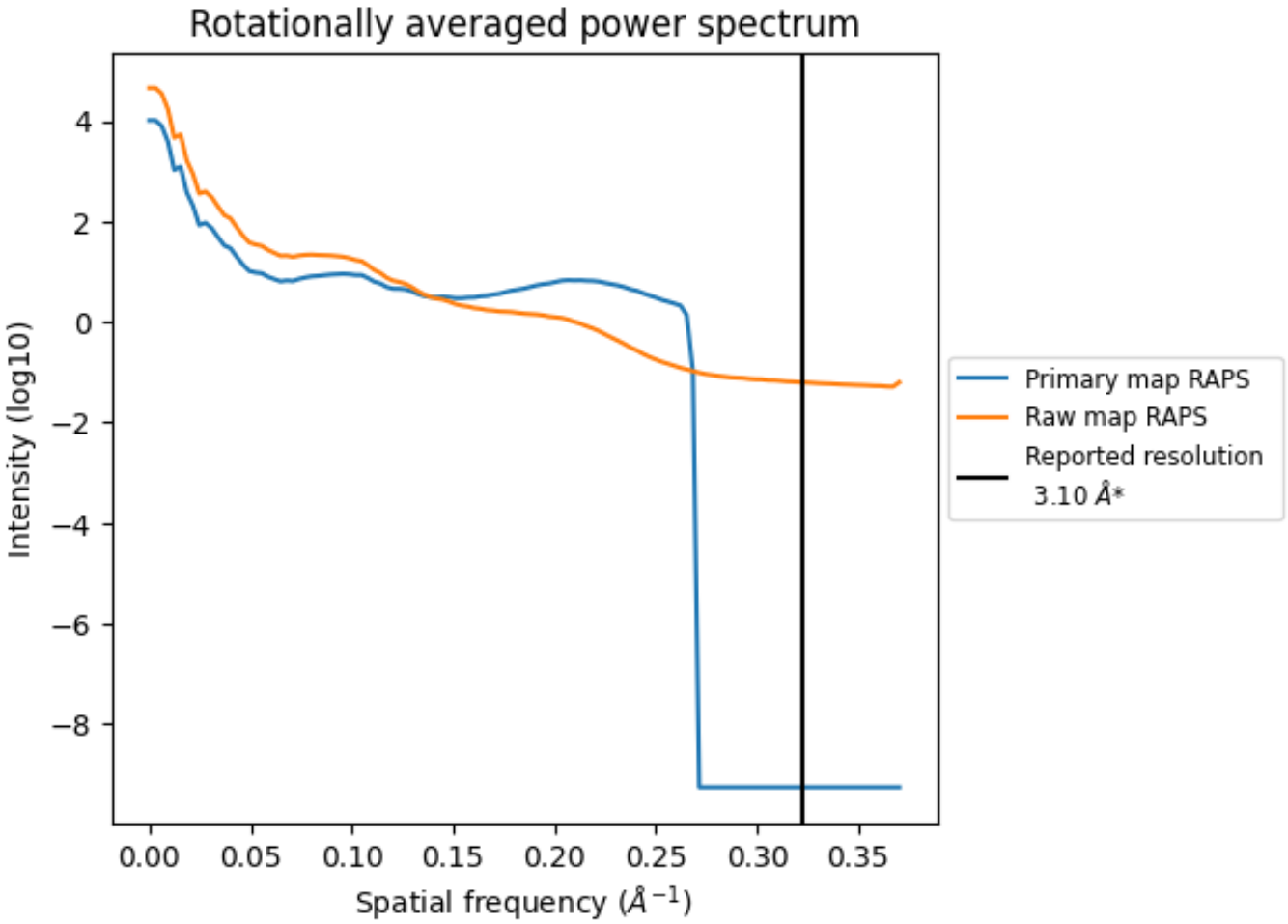
7.2 Volume estimate



The volume at the recommended contour level is 2347 nm^3; this corresponds to an approximate mass of 2120 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 (i)

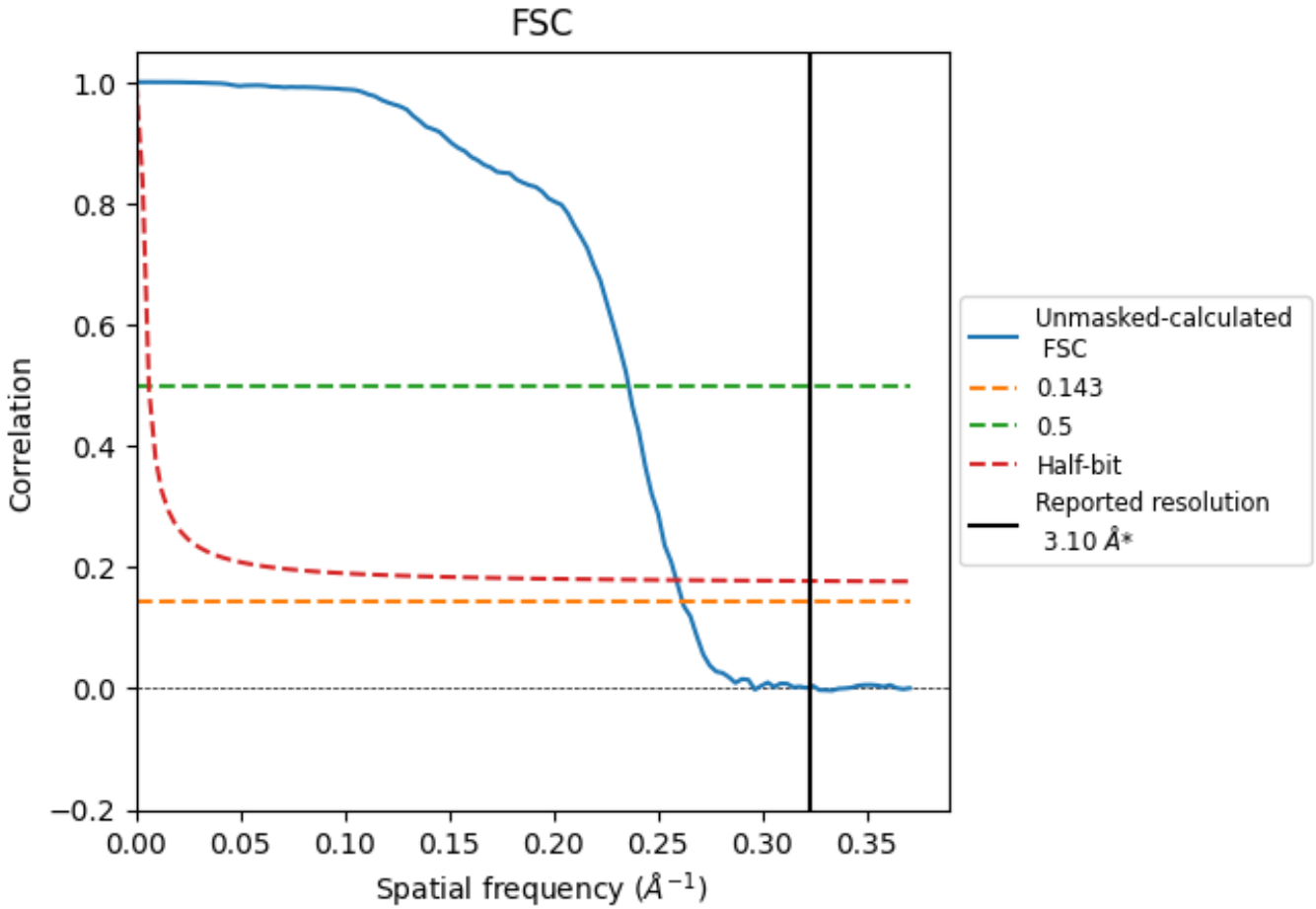


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

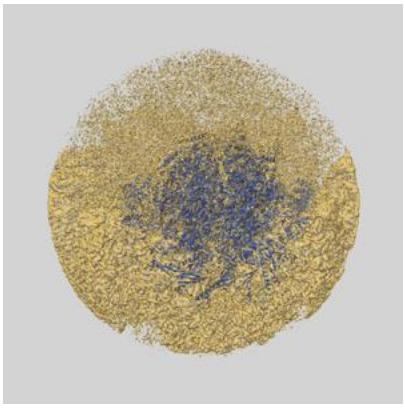
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.82	4.24	3.87

*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 3.82 differs from the reported value 3.1 by more than 10 %

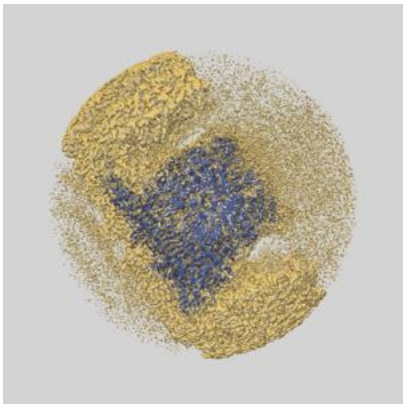
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38187 and PDB model 8X9X. Per-residue inclusion information can be found in section 3 on page 6.

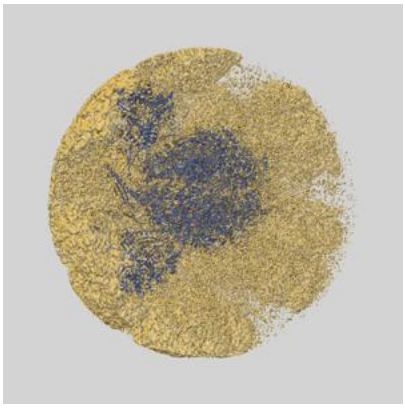
9.1 Map-model overlay



X



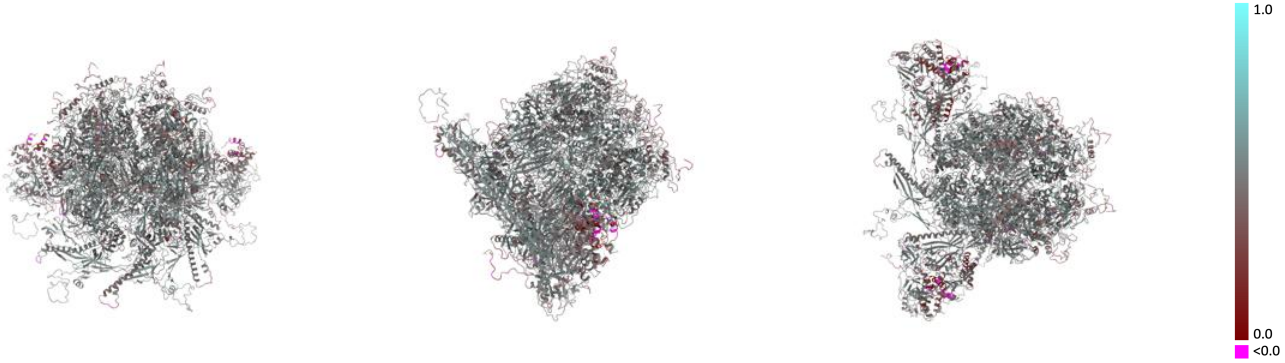
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

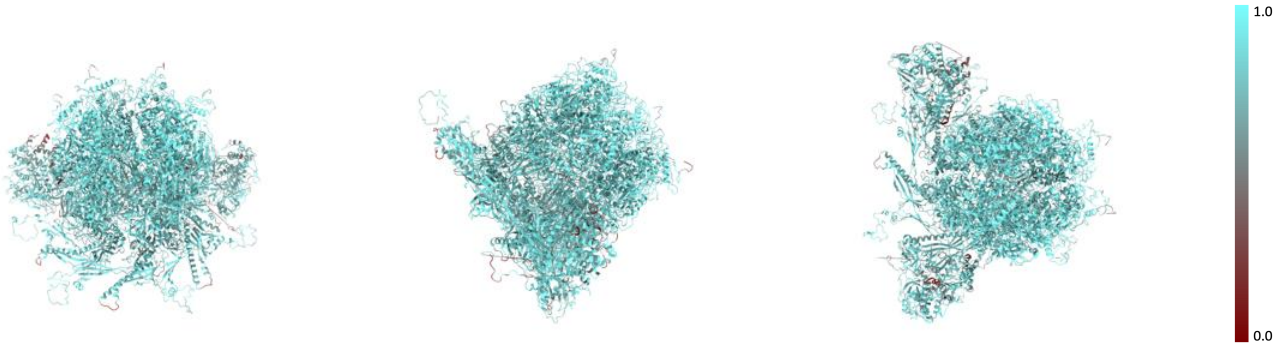
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

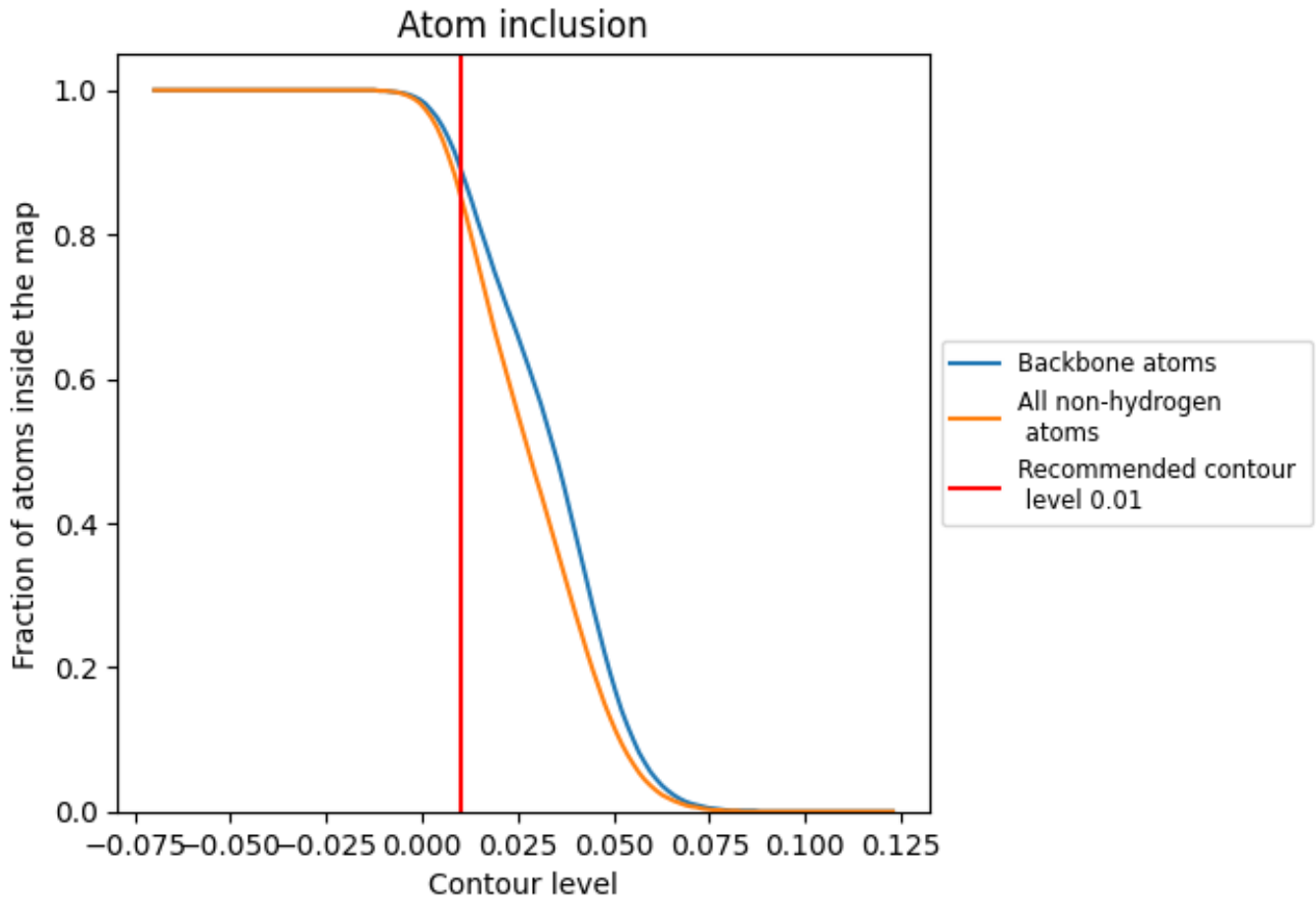
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 86% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8550	0.4720
A	0.8750	0.4890
B	0.8830	0.4030
C	0.8770	0.4870
D	0.8750	0.4910
E	0.8640	0.4850
F	0.8560	0.4820
G	0.8480	0.3840
H	0.8680	0.4860
I	0.7900	0.4430
K	0.7910	0.4280
L	0.8860	0.4040
N	0.7910	0.4410
P	0.7730	0.4190
Q	0.8960	0.3970
S	0.7850	0.4180
U	0.7330	0.3940
V	0.8860	0.3960
g	0.8830	0.3990