



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 05:09 AM UTC

PDB ID : 9EUG / pdb_00009eug
EMDB ID : EMD-19969
Title : Cryo-EM structure of Staphylococcus aureus bacteriophage phi812 baseplate in the pre-contraction state - core, wedge module, and proximal tail proteins
Authors : Binovsky, J.; Siborova, M.; Baska, R.; Pichel-Beleiro, A.; Skubnik, K.; Novacek, J.; van Raaij, M.J.; Plevka, P.
Deposited on : 2024-03-27
Resolution : 4.50 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

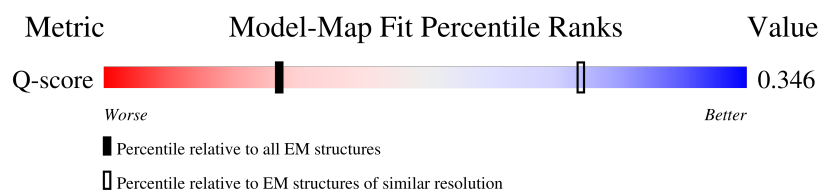
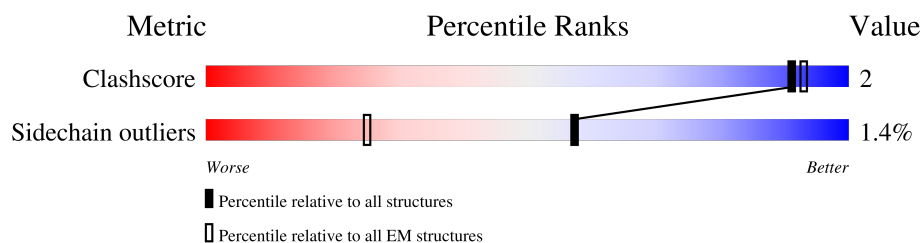
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2937 (4.00 - 5.00)

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	295	5% 49% 48%
2	B	848	33% 63%
3	C	348	13% 95% 5%
3	D	348	14% 94% 6%
3	I	348	14% 88% 11%

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Mol	Chain	Length	Quality of chain
3	K	348	12% 96% .
4	E	808	11% 67% 5% 27%
5	F	174	11% 83% 5% 11%
5	G	174	18% 82% 6% . 12%
6	H	1019	. 10% . 90%
6	J	1019	10% 90%
7	L	234	14% 84% 7% 9%
7	O	234	12% 86% 9%
8	M	263	16% 79% 12% 10%
8	N	263	16% 81% 9% 10%
9	P	587	8% 87% 8%
9	Q	587	9% 89% 8%
9	T	587	20% 89% 9%
9	U	587	17% 88% 9%
9	X	587	55% 86% 10%
9	Y	587	53% 86% 10%
10	R	142	11% 96% ..
10	S	142	12% 96% ..
10	V	142	22% 92% 6% .
10	W	142	23% 87% 11% .
10	Z	142	38% 94% ..
10	a	142	46% 95% ..

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 62523 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 NlpC/P60 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	153	Total	C	N	O	S	0	0
			1267	833	192	237	5		

- Molecule 2 is a protein called GP-PDE domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	310	Total	C	N	O	S	0	0
			2470	1560	401	502	7		

- Molecule 3 is a protein called Baseplate component.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	348	Total	C	N	O	S	0	0
			2760	1734	459	560	7		
3	D	348	Total	C	N	O	S	0	0
			2760	1734	459	560	7		
3	I	347	Total	C	N	O	S	0	0
			2752	1729	458	559	6		
3	K	347	Total	C	N	O	S	0	0
			2752	1729	458	559	6		

- Molecule 4 is a protein called Peptidase C51 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	586	Total	C	N	O	S	0	0
			4764	3042	786	919	17		

- Molecule 5 is a protein called Baseplate component.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	154	Total	C	N	O	S	0	0
			1248	803	200	241	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	153	Total	C	N	O	S	0	0
			1240	799	198	239	4		

- Molecule 6 is a protein called TmpF.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	105	Total	C	N	O	S	0	0
			870	549	153	167	1		
6	J	105	Total	C	N	O	S	0	0
			870	549	153	167	1		

- Molecule 7 is a protein called Baseplate wedge subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	212	Total	C	N	O	S	0	0
			1694	1060	290	339	5		
7	O	212	Total	C	N	O	S	0	0
			1694	1060	290	339	5		

- Molecule 8 is a protein called Putative baseplate component.

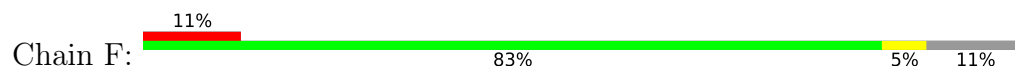
Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	238	Total	C	N	O	S	0	0
			1878	1164	335	375	4		
8	N	238	Total	C	N	O	S	0	0
			1878	1164	335	375	4		

- Molecule 9 is a protein called Major tail sheath protein.

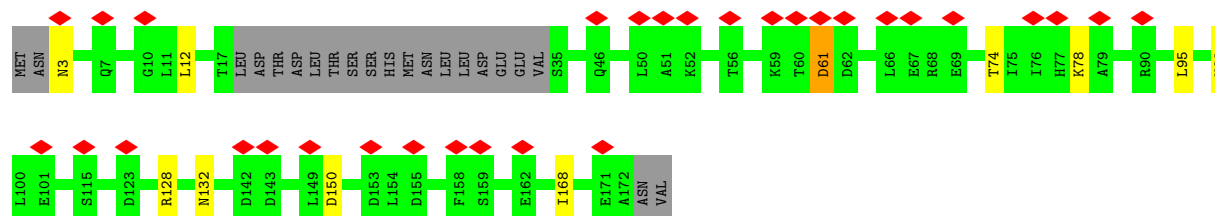
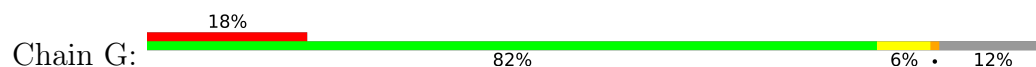
Mol	Chain	Residues	Atoms					AltConf	Trace
9	P	538	Total	C	N	O	S	0	0
			4200	2646	711	836	7		
9	Q	538	Total	C	N	O	S	0	0
			4200	2646	711	836	7		
9	T	536	Total	C	N	O	S	0	0
			4189	2640	711	831	7		
9	U	536	Total	C	N	O	S	0	0
			4189	2640	711	831	7		
9	X	531	Total	C	N	O	S	0	0
			4151	2617	704	823	7		
9	Y	531	Total	C	N	O	S	0	0
			4151	2617	704	823	7		

- Molecule 10 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	R	139	Total	C	N	O	S	0	0
			1091	685	183	219	4		
10	S	139	Total	C	N	O	S	0	0
			1091	685	183	219	4		
10	V	139	Total	C	N	O	S	0	0
			1091	685	183	219	4		
10	W	139	Total	C	N	O	S	0	0
			1091	685	183	219	4		
10	Z	139	Total	C	N	O	S	0	0
			1091	685	183	219	4		
10	a	139	Total	C	N	O	S	0	0
			1091	685	183	219	4		



- Molecule 5: Baseplate component



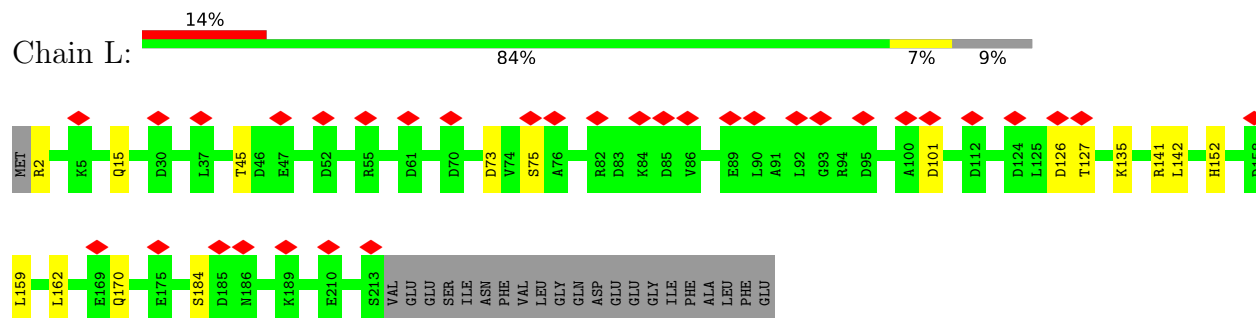
- Molecule 6: TmpF



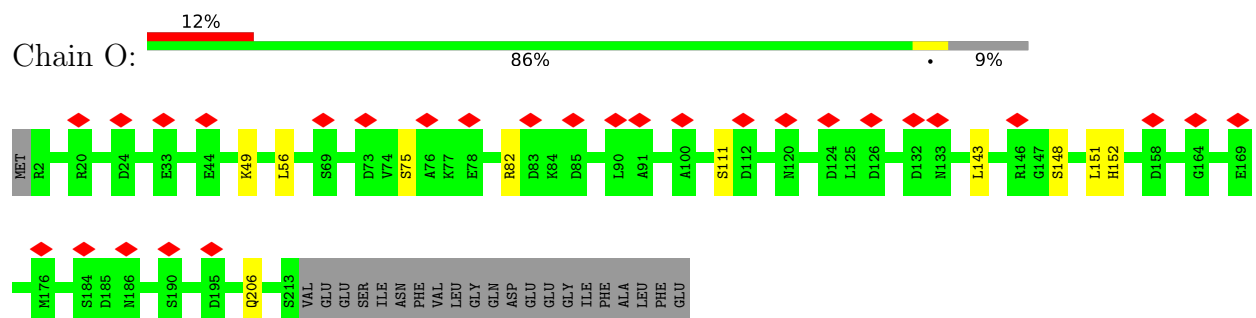


LYS	PRO	ARG	LEU	ASN	THR	ASP	VAL	ARG	VAL	TYR	ILE	ILE	ARG	PRO	TYR	GLY	ASP	SER	PHE	THR	ILE	SER	ASN	LYS	VAL	ASN	ARG	VAL	ARG	ILE	GLU	LEU	VAL	TYR	ASN	ASN	ASN	PRO	ASN	PHE	GLU	ASN	LEU	PRO	THR	THR	ILE	TYR	PRO	SER	LYS	ILE	ASN	VAL	GLY	VAL	ALA	GLU	VAL	LYS	GLY	PHE	SER	ILE	ALA	LYS	LEU	LYS	ASP	TYR	GLY	THR	GLU	LEU	ASP	TYR
GLU	PRO	ILE	ARG	LEU	ASN	GLY	THR	ARG	TYR	LYS	GLU	LEU	ILE	VAL	GLU	GLY	SER	PHE	LYS	ASN	ASN	VAL	ASN	ILE	GLU	ASN	PHE	ARG	ILE	SER	LEU	VAL	GLU	TYR	ASN	ASN	ASN	PRO	ASN	PHE	GLU	ASN	LEU	PRO	THR	THR	ILE	TYR	PRO	SER	LYS	ILE	ASN	VAL	GLY	VAL	ALA	GLU	VAL	LYS	GLY	PHE	SER	ILE	ALA	LYS	LEU	LYS	ASP	TYR	GLY	THR	GLU	LEU	ASP	TYR

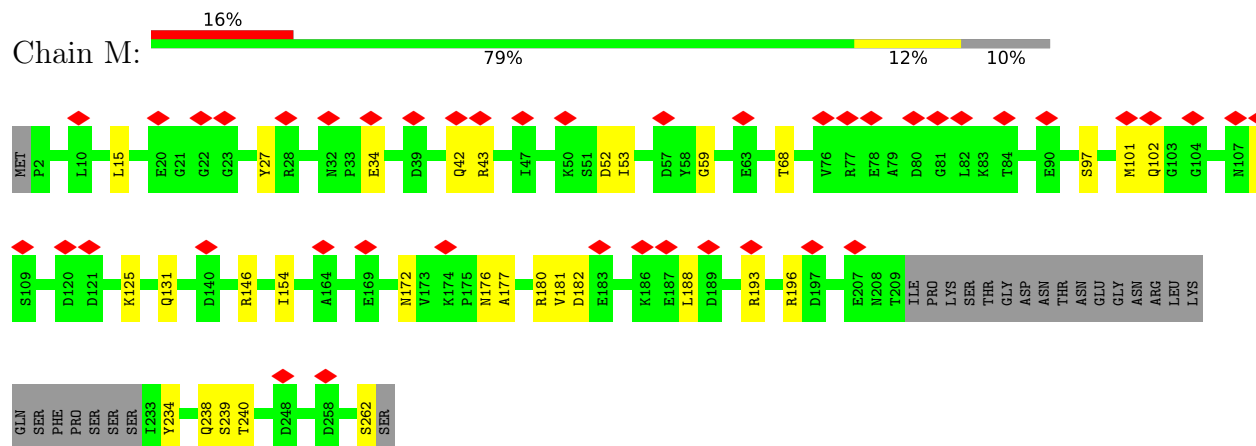
- Molecule 7: Baseplate wedge subunit



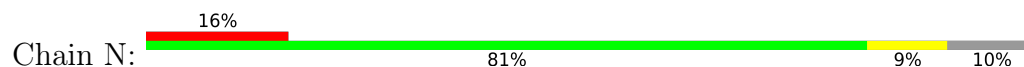
- Molecule 7: Baseplate wedge subunit

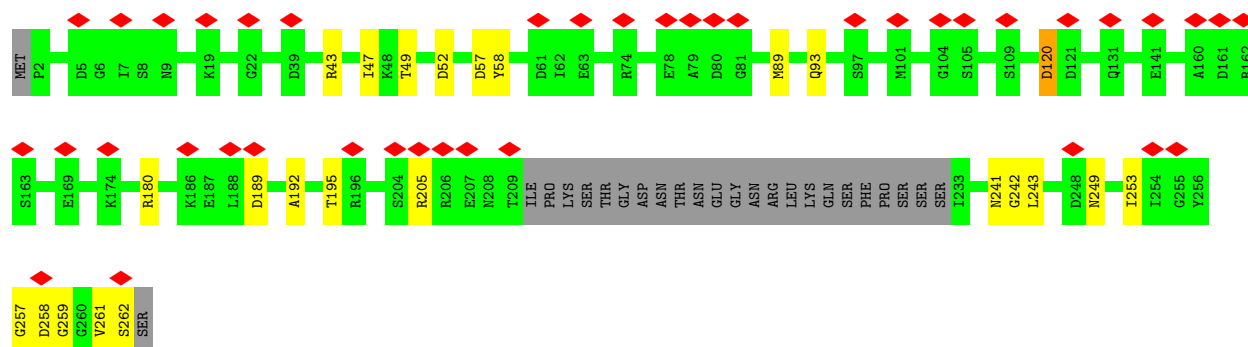


- Molecule 8: Putative baseplate component

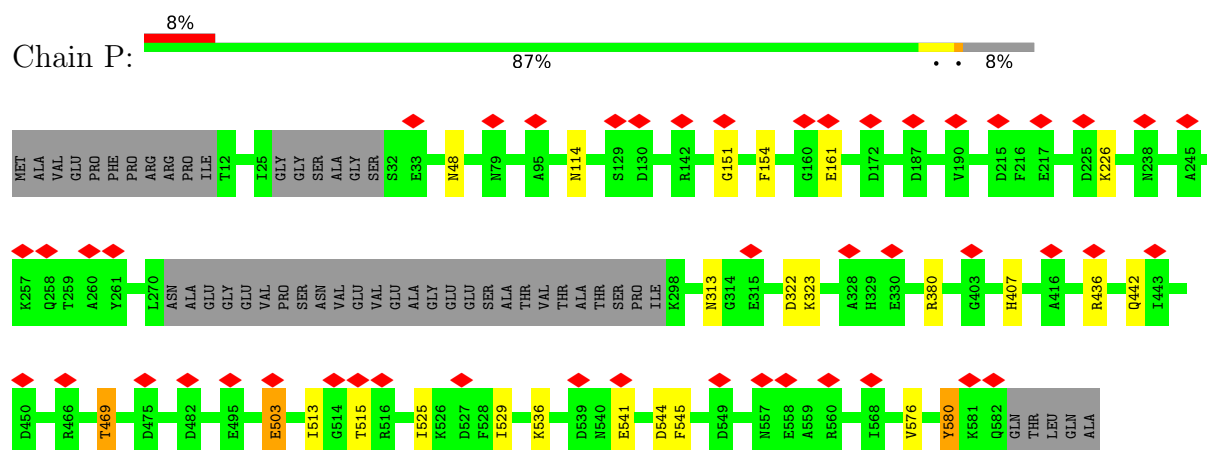


- Molecule 8: Putative baseplate component

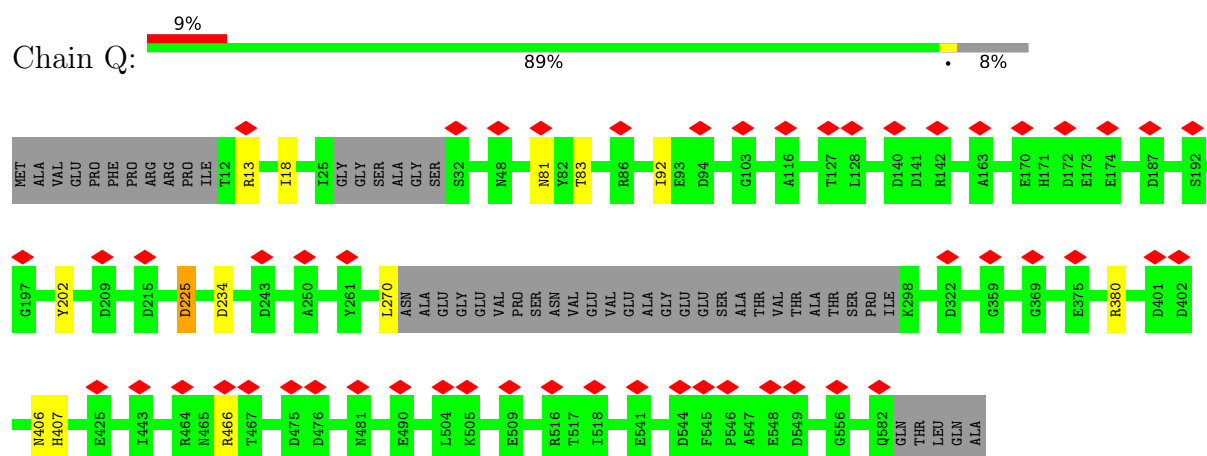




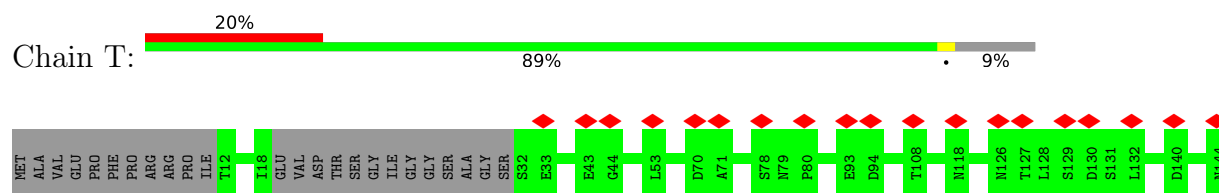
- Molecule 9: Major tail sheath protein

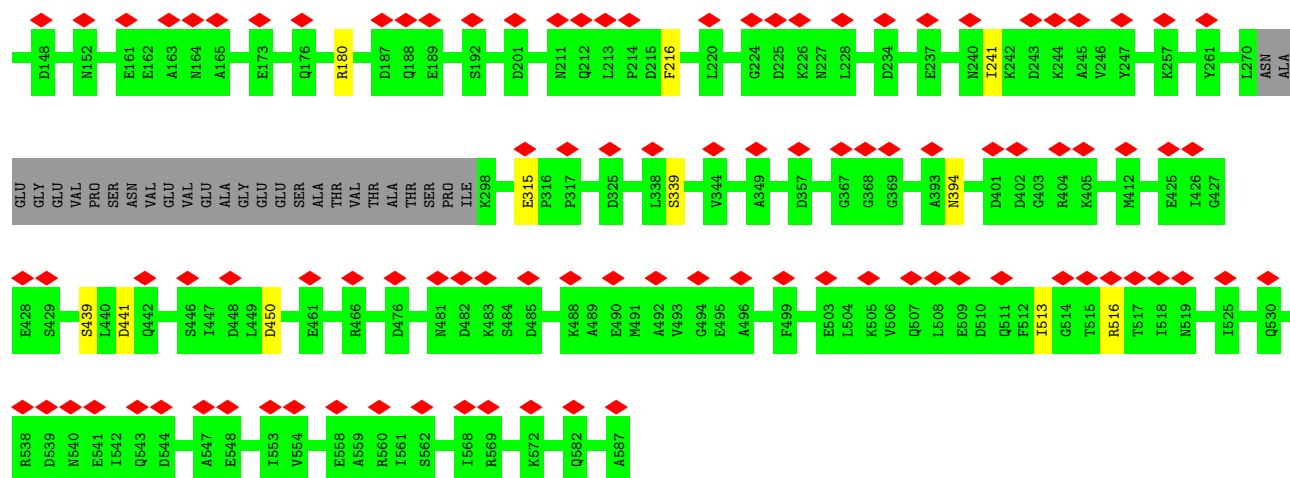


- Molecule 9: Major tail sheath protein

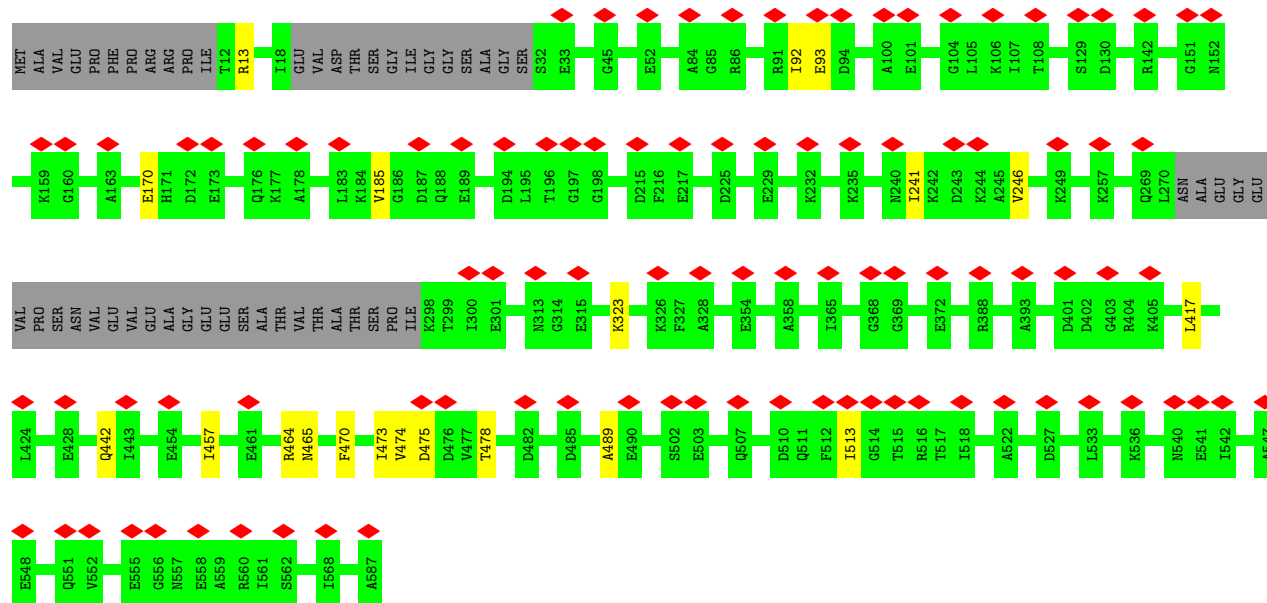
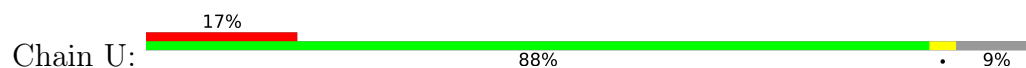


- Molecule 9: Major tail sheath protein

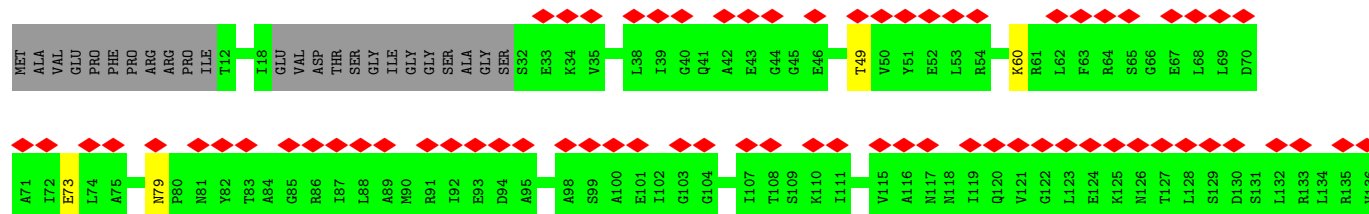
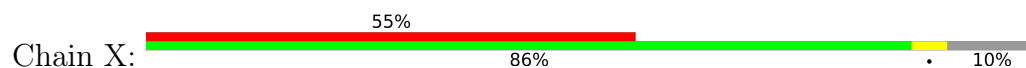




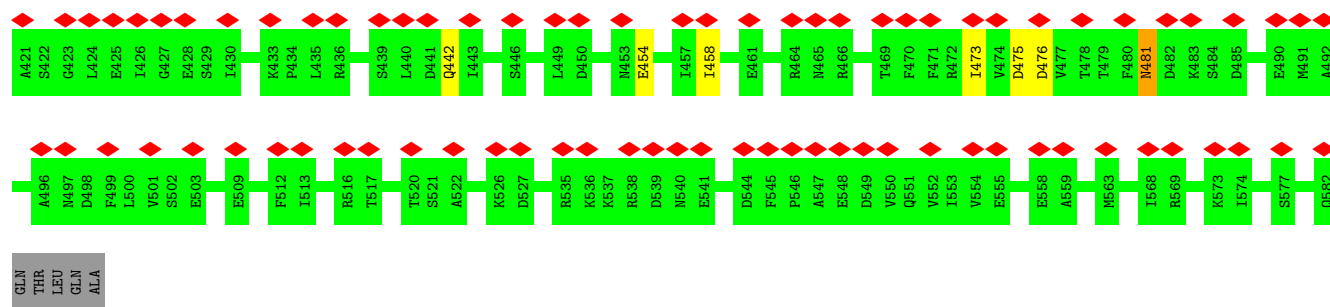
• Molecule 9: Major tail sheath protein



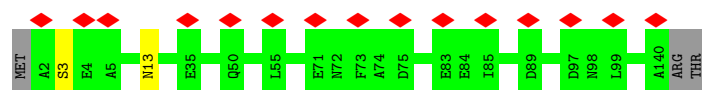
• Molecule 9: Major tail sheath protein



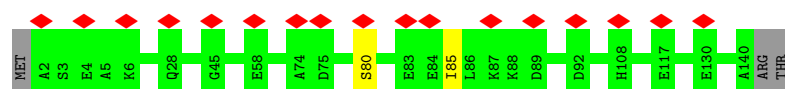




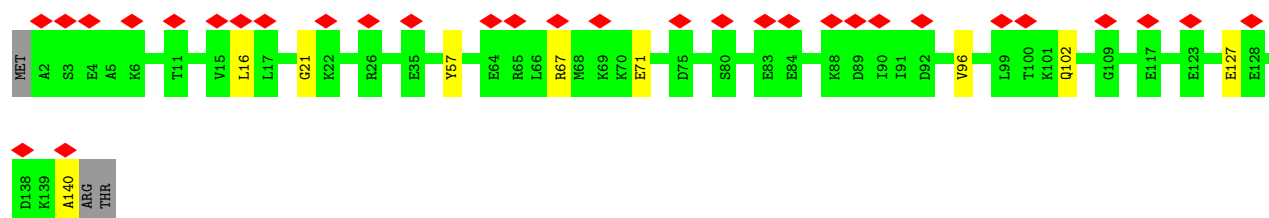
- Molecule 10: Capsid protein



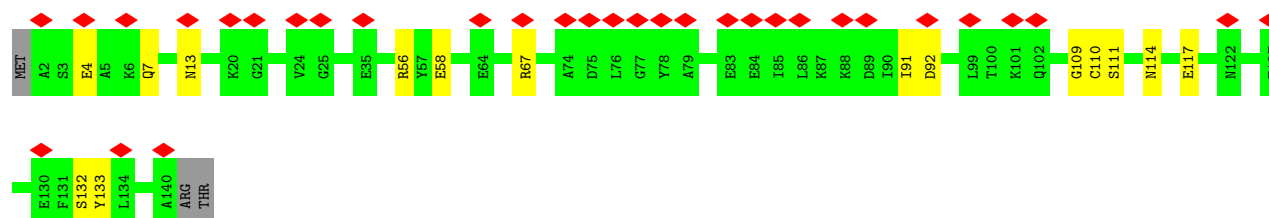
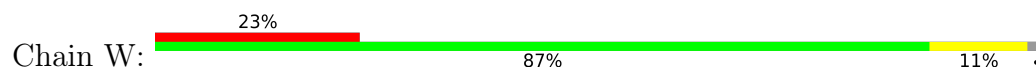
- Molecule 10: Capsid protein



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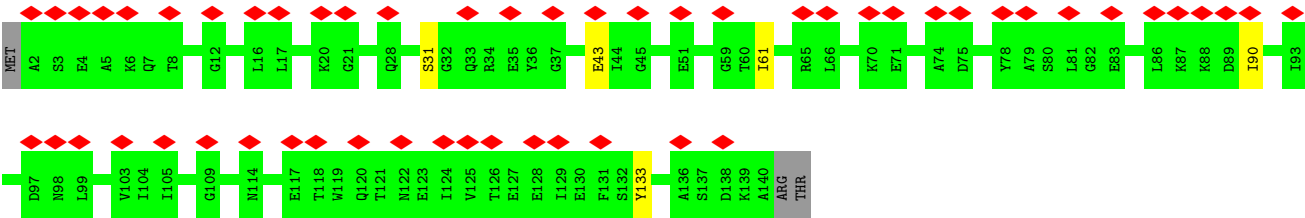


- Molecule 10: Capsid protein

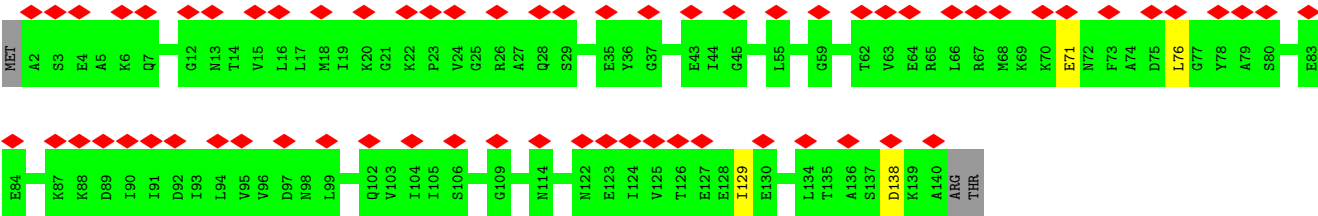


- Molecule 10: Capsid protein





• Molecule 10: Capsid protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	9705	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.110	Depositor
Minimum map value	-0.076	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	903.00006, 903.00006, 903.00006	wwPDB
Map dimensions	840, 840, 840	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.075, 1.075, 1.075	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	0.27	0/1303	0.54	0/1756
2	B	0.27	0/2519	0.54	0/3404
3	C	0.28	0/2803	0.56	0/3794
3	D	0.26	0/2803	0.55	0/3794
3	I	0.28	0/2795	0.57	0/3784
3	K	0.26	0/2795	0.51	0/3784
4	E	0.28	0/4863	0.57	0/6535
5	F	0.29	0/1269	0.57	0/1724
5	G	0.26	0/1261	0.52	0/1713
6	H	0.28	0/883	0.61	0/1186
6	J	0.27	0/883	0.58	0/1186
7	L	0.33	0/1722	0.70	0/2331
7	O	0.38	0/1722	0.69	0/2331
8	M	0.28	0/1907	0.57	0/2565
8	N	0.29	0/1907	0.61	0/2565
9	P	0.30	0/4267	0.60	0/5760
9	Q	0.34	1/4267 (0.0%)	0.63	0/5760
9	T	0.30	0/4256	0.58	0/5745
9	U	0.30	0/4256	0.61	0/5745
9	X	0.27	0/4218	0.56	0/5693
9	Y	0.25	0/4218	0.54	0/5693
10	R	0.40	0/1107	0.72	0/1496
10	S	0.33	0/1107	0.63	0/1496
10	V	0.25	0/1107	0.56	0/1496
10	W	0.25	0/1107	0.56	0/1496
10	Z	0.33	0/1107	0.65	0/1496
10	a	0.27	0/1107	0.59	0/1496
All	All	0.29	1/63559 (0.0%)	0.59	0/85824

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
2	B	0	1
4	E	0	1
7	O	0	1
8	M	0	1
9	Q	0	2
9	T	0	3
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Q	18	ILE	CG1-CD1	-8.16	1.20	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	53	ARG	Sidechain
4	E	175	ARG	Sidechain
8	M	182	ASP	Sidechain
7	O	82	ARG	Sidechain
9	Q	380	ARG	Sidechain
9	Q	407	HIS	Peptide
9	T	180	ARG	Sidechain
9	T	241	ILE	Peptide
9	T	513	ILE	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	1267	0	1219	3	0
2	B	2470	0	2394	22	0
3	C	2760	0	2729	11	0
3	D	2760	0	2729	10	0
3	I	2752	0	2717	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	2752	0	2717	9	0
4	E	4764	0	4703	26	0
5	F	1248	0	1257	5	0
5	G	1240	0	1251	7	0
6	H	870	0	873	3	0
6	J	870	0	873	1	0
7	L	1694	0	1663	8	0
7	O	1694	0	1663	2	0
8	M	1878	0	1844	18	0
8	N	1878	0	1844	15	0
9	P	4200	0	4156	11	0
9	Q	4200	0	4156	3	0
9	T	4189	0	4150	2	0
9	U	4189	0	4150	7	0
9	X	4151	0	4111	10	0
9	Y	4151	0	4111	14	0
10	R	1091	0	1081	0	0
10	S	1091	0	1081	0	0
10	V	1091	0	1081	3	0
10	W	1091	0	1081	6	0
10	Z	1091	0	1081	0	0
10	a	1091	0	1081	0	0
All	All	62523	0	61796	201	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 (201) 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)
3:C:300:ASP:N	3:C:300:ASP:OD1	2.20	0.74
3:K:191:ARG:NH1	3:K:244:ASP:OD2	2.26	0.69
3:I:335:GLN:N	3:I:335:GLN:OE1	2.27	0.68
3:K:84:GLN:OE1	3:K:158:ARG:NH2	2.28	0.67
3:D:74:SER:OG	3:D:170:THR:O	2.13	0.67
3:C:172:GLU:N	3:C:172:GLU:OE1	2.29	0.66
2:B:46:ASN:O	2:B:47:ASN:ND2	2.29	0.65
2:B:290:ASN:ND2	2:B:305:ASP:OD2	2.29	0.65
3:C:106:GLN:NE2	4:E:206:GLU:O	2.29	0.64
3:K:148:ASN:ND2	3:K:160:VAL:O	2.31	0.64
8:M:97:SER:OG	8:M:101:MET:SD	2.57	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:56:ARG:NH1	10:W:58:GLU:OE1	2.33	0.62
3:I:203:GLN:OE1	3:I:203:GLN:N	2.32	0.62
8:N:180:ARG:NE	8:N:249:ASN:OD1	2.32	0.62
3:I:15:ASP:OD1	8:M:172:ASN:ND2	2.31	0.61
3:D:173:GLU:OE2	3:D:181:ARG:NH1	2.35	0.60
9:T:394:ASN:ND2	9:T:441:ASP:O	2.34	0.59
8:M:172:ASN:O	8:M:234:TYR:N	2.35	0.59
2:B:189:GLN:N	2:B:189:GLN:OE1	2.35	0.59
8:N:89:MET:SD	8:N:93:GLN:NE2	2.75	0.59
10:W:91:ILE:O	10:W:110:CYS:N	2.34	0.59
2:B:45:VAL:N	2:B:48:LEU:O	2.34	0.59
4:E:94:ARG:NE	4:E:244:GLU:OE1	2.34	0.59
8:M:176:ASN:OD1	8:M:180:ARG:NH1	2.36	0.58
8:M:34:GLU:OE1	8:M:146:ARG:NH2	2.37	0.58
3:K:60:GLN:O	3:K:175:GLN:NE2	2.37	0.58
9:Y:304:GLU:N	9:Y:304:GLU:OE1	2.37	0.58
9:P:151:GLY:O	9:P:226:LYS:NZ	2.37	0.57
9:P:544:ASP:OD1	9:P:545:PHE:N	2.37	0.57
7:L:142:LEU:HD21	7:L:159:LEU:HD22	1.86	0.57
8:N:49:THR:OG1	8:N:52:ASP:O	2.15	0.57
2:B:110:ASP:OD1	2:B:111:ASN:N	2.37	0.57
3:C:221:VAL:HB	3:C:254:VAL:HG22	1.85	0.57
3:D:26:ASP:OD1	3:D:27:PHE:N	2.37	0.57
10:W:67:ARG:NH1	10:W:117:GLU:OE2	2.37	0.57
8:N:43:ARG:NH2	8:N:58:TYR:O	2.35	0.56
4:E:174:ARG:NH2	8:N:205:ARG:O	2.39	0.56
1:A:242:ARG:NH2	2:B:152:ASP:OD2	2.40	0.55
9:Y:114:ASN:OD1	9:Y:313:ASN:N	2.38	0.55
1:A:238:LEU:O	1:A:248:GLY:N	2.39	0.55
2:B:240:ASP:OD1	2:B:260:SER:N	2.39	0.55
3:I:76:ARG:NH1	3:I:133:CYS:O	2.40	0.55
2:B:152:ASP:OD1	2:B:153:GLY:N	2.41	0.54
4:E:94:ARG:NH1	4:E:95:LEU:O	2.40	0.54
9:P:114:ASN:OD1	9:P:313:ASN:N	2.39	0.54
4:E:411:THR:OG1	4:E:414:GLU:OE1	2.25	0.54
6:J:80:TYR:CZ	6:J:84:ILE:HD11	2.42	0.54
10:W:92:ASP:OD1	10:W:109:GLY:N	2.39	0.54
2:B:230:ILE:O	2:B:246:LEU:N	2.40	0.54
8:M:238:GLN:O	8:M:239:SER:OG	2.22	0.54
3:C:103:SER:OG	3:C:146:THR:O	2.15	0.53
6:H:96:ASN:OD1	6:H:97:ALA:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:95:LEU:O	5:G:99:VAL:HG23	2.09	0.53
8:M:34:GLU:N	8:M:68:THR:O	2.40	0.53
3:K:302:ILE:HG22	3:K:304:THR:H	1.73	0.53
9:P:513:ILE:O	9:P:515:THR:HG23	2.08	0.53
9:Y:475:ASP:OD1	9:Y:476:ASP:N	2.40	0.53
5:G:128:ARG:O	5:G:132:ASN:ND2	2.41	0.53
3:C:177:ASP:OD1	3:C:180:ARG:NH2	2.42	0.52
3:I:102:THR:O	3:I:149:THR:OG1	2.28	0.52
4:E:228:ASP:O	4:E:231:THR:OG1	2.24	0.52
2:B:114:ASN:O	2:B:118:ASN:ND2	2.42	0.52
3:D:242:LEU:O	3:D:246:ARG:N	2.43	0.52
4:E:74:ILE:HD11	4:E:100:MET:HE3	1.90	0.52
3:I:294:ASN:O	3:I:294:ASN:ND2	2.43	0.52
8:M:42:GLN:NE2	8:M:59:GLY:O	2.43	0.52
3:I:105:ARG:NH2	3:I:145:GLY:O	2.43	0.51
3:I:201:ALA:HB2	3:I:242:LEU:HD21	1.91	0.51
9:Y:193:TYR:OH	9:Y:209:ASP:O	2.06	0.51
5:F:2:ASN:OD1	5:F:3:ASN:N	2.44	0.51
2:B:148:TYR:N	2:B:160:THR:OG1	2.42	0.51
9:X:153:ILE:HD12	9:X:228:LEU:HB2	1.92	0.51
2:B:74:GLU:N	2:B:74:GLU:OE1	2.44	0.51
10:W:4:GLU:OE1	10:W:7:GLN:NE2	2.44	0.51
8:M:102:GLN:O	8:M:108:VAL:HG23	2.11	0.51
7:L:162:LEU:O	7:L:170:GLN:NE2	2.44	0.50
9:Q:225:ASP:N	9:Q:225:ASP:OD1	2.43	0.50
4:E:414:GLU:OE1	4:E:414:GLU:N	2.44	0.50
4:E:540:TYR:O	4:E:543:ASN:ND2	2.45	0.50
7:L:142:LEU:C	7:L:142:LEU:HD23	2.36	0.50
2:B:245:VAL:C	2:B:246:LEU:HD12	2.36	0.50
4:E:227:MET:O	4:E:231:THR:HG23	2.11	0.50
3:I:174:SER:OG	3:I:176:GLU:OE1	2.25	0.50
7:L:73:ASP:OD1	7:L:75:SER:OG	2.26	0.50
8:N:120:ASP:OD1	8:N:120:ASP:N	2.44	0.50
4:E:65:TRP:O	4:E:69:VAL:HG12	2.12	0.49
2:B:289:ASP:OD1	2:B:290:ASN:N	2.45	0.49
4:E:396:GLN:N	4:E:396:GLN:OE1	2.44	0.49
9:Y:204:ASN:HA	9:Y:207:ILE:HD12	1.94	0.49
8:N:189:ASP:O	8:N:192:ALA:N	2.46	0.49
8:N:257:GLY:O	8:N:259:GLY:N	2.46	0.49
5:G:61:ASP:OD1	5:G:61:ASP:N	2.45	0.49
4:E:560:ASP:OD1	4:E:561:LEU:N	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:263:ASN:O	3:I:325:ASN:ND2	2.45	0.48
9:X:458:ILE:HG23	9:X:473:ILE:HD11	1.94	0.48
9:U:474:VAL:HG23	9:U:475:ASP:H	1.78	0.48
9:X:235:LYS:NZ	9:X:237:GLU:OE2	2.42	0.48
8:M:42:GLN:OE1	8:M:43:ARG:N	2.46	0.48
9:P:503:GLU:OE1	9:P:536:LYS:NZ	2.44	0.48
8:M:196:ARG:NH2	8:M:262:SER:O	2.45	0.47
8:M:131:GLN:OE1	8:M:131:GLN:N	2.47	0.47
8:N:261:VAL:O	8:N:262:SER:OG	2.24	0.47
9:Y:172:ASP:O	9:Y:176:GLN:N	2.46	0.47
9:U:93:GLU:O	9:U:323:LYS:NZ	2.46	0.47
3:I:107:GLU:OE1	3:I:107:GLU:N	2.48	0.47
3:K:224:HIS:O	3:K:224:HIS:ND1	2.48	0.47
8:M:177:ALA:O	8:M:181:VAL:HG23	2.15	0.47
10:W:111:SER:N	10:W:132:SER:O	2.44	0.47
7:L:141:ARG:NH2	7:L:184:SER:OG	2.48	0.47
2:B:2:VAL:O	4:E:54:VAL:HG11	2.15	0.47
9:U:464:ARG:NH1	9:U:465:ASN:O	2.43	0.47
5:F:167:LEU:HD23	8:M:240:THR:HG23	1.98	0.46
8:N:241:ASN:OD1	8:N:242:GLY:N	2.48	0.46
2:B:35:ASN:O	2:B:39:GLN:N	2.47	0.46
3:I:221:VAL:O	3:I:254:VAL:HG13	2.15	0.46
8:N:57:ASP:OD1	8:N:58:TYR:N	2.48	0.46
9:P:536:LYS:NZ	9:P:541:GLU:OE1	2.45	0.46
3:I:219:ILE:HG21	3:I:246:ARG:HH22	1.80	0.46
9:Y:458:ILE:CG2	9:Y:473:ILE:HD11	2.46	0.46
3:D:42:LEU:HD23	3:K:16:LYS:HD3	1.97	0.46
10:V:67:ARG:NH1	10:V:127:GLU:OE2	2.46	0.46
9:X:463:VAL:HG21	9:X:472:ARG:HG2	1.97	0.46
3:I:103:SER:OG	3:I:146:THR:HG22	2.16	0.46
8:M:188:LEU:O	8:M:193:ARG:NH1	2.49	0.45
9:U:417:LEU:HD13	9:U:473:ILE:HD13	1.98	0.45
5:G:3:ASN:O	5:G:3:ASN:ND2	2.49	0.45
8:M:52:ASP:OD1	8:M:53:ILE:N	2.49	0.45
9:P:525:ILE:HG22	9:P:529:ILE:HD12	1.98	0.45
9:X:450:ASP:N	9:X:450:ASP:OD1	2.49	0.45
3:C:72:ARG:NH1	3:C:205:PRO:O	2.50	0.45
9:Y:143:PHE:CD2	9:Y:264:ILE:HD12	2.51	0.45
9:Y:454:GLU:O	9:Y:481:ASN:ND2	2.49	0.45
3:K:162:ASN:O	3:K:162:ASN:ND2	2.50	0.45
2:B:269:GLN:NE2	2:B:272:ASP:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:436:THR:HG22	4:E:437:LYS:H	1.80	0.45
3:I:289:ARG:NH1	3:I:341:GLY:O	2.50	0.45
2:B:240:ASP:OD1	2:B:260:SER:OG	2.36	0.44
4:E:264:TRP:O	4:E:564:ARG:NH2	2.51	0.44
10:V:102:GLN:NE2	10:V:140:ALA:O	2.45	0.44
3:K:110:GLN:N	3:K:110:GLN:OE1	2.51	0.44
8:M:125:LYS:O	8:M:154:ILE:N	2.49	0.44
9:X:139:GLN:O	9:X:142:ARG:NH1	2.46	0.44
2:B:57:ASP:OD1	2:B:57:ASP:N	2.50	0.44
4:E:582:SER:O	4:E:598:GLY:N	2.49	0.44
3:I:310:ILE:HD13	3:I:321:VAL:HG21	1.99	0.44
2:B:21:LEU:HD11	4:E:225:GLN:OE1	2.18	0.44
3:D:315:ASP:OD1	3:I:308:GLN:NE2	2.45	0.44
3:C:144:GLU:OE1	3:C:144:GLU:N	2.49	0.44
5:G:78:LYS:NZ	5:G:150:ASP:OD2	2.40	0.44
9:X:226:LYS:O	9:X:257:LYS:NZ	2.50	0.44
3:I:13:LEU:HB3	3:I:37:LEU:HD22	2.00	0.43
7:O:148:SER:O	9:Q:466:ARG:NH1	2.42	0.43
1:A:233:ILE:HD11	1:A:288:ARG:CZ	2.48	0.43
4:E:286:ASP:OD1	4:E:286:ASP:N	2.51	0.43
9:Y:458:ILE:HG23	9:Y:473:ILE:HD11	2.00	0.43
4:E:278:ILE:HD11	8:N:47:ILE:HD12	2.00	0.43
9:X:455:ASN:ND2	9:Y:225:ASP:OD1	2.51	0.43
9:P:322:ASP:OD1	9:P:323:LYS:N	2.51	0.43
3:I:257:VAL:HG22	3:I:337:ILE:HG22	2.00	0.43
5:G:168:ILE:HD11	8:N:243:LEU:HD13	2.00	0.43
3:C:299:ASP:OD1	3:C:300:ASP:N	2.51	0.43
3:D:147:ILE:O	3:D:147:ILE:HG22	2.18	0.43
9:U:241:ILE:HD11	9:U:246:VAL:CG2	2.49	0.43
6:H:76:LYS:HE3	6:H:79:VAL:HG23	2.00	0.43
3:D:320:ASP:OD1	3:I:304:THR:OG1	2.29	0.42
4:E:299:GLY:N	4:E:330:GLU:OE2	2.47	0.42
5:F:16:ASN:O	5:F:17:THR:OG1	2.36	0.42
7:O:49:LYS:HA	7:O:56:LEU:HD23	2.02	0.42
3:D:283:HIS:O	3:D:287:VAL:HG23	2.19	0.42
2:B:212:MET:SD	2:B:212:MET:N	2.93	0.42
5:F:17:THR:HG22	5:F:96:GLN:OE1	2.19	0.42
4:E:47:SER:OG	4:E:50:ASP:OD1	2.32	0.42
9:Q:92:ILE:HG23	9:Q:92:ILE:O	2.19	0.42
7:L:135:LYS:HE3	9:P:580:TYR:CE2	2.55	0.42
9:P:436:ARG:HA	9:P:469:THR:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Y:167:PHE:CD1	9:Y:241:ILE:HD11	2.54	0.42
4:E:191:THR:OG1	4:E:192:ILE:N	2.52	0.42
9:T:516:ARG:NH1	10:V:21:GLY:O	2.53	0.42
9:U:478:THR:N	9:U:489:ALA:O	2.48	0.42
8:M:15:LEU:O	8:M:27:TYR:N	2.51	0.42
2:B:34:ILE:HG13	2:B:41:VAL:HG12	2.02	0.41
9:X:60:LYS:NZ	9:X:73:GLU:OE2	2.51	0.41
3:I:194:ASN:OD1	3:I:194:ASN:N	2.53	0.41
7:L:15:GLN:OE1	7:L:15:GLN:N	2.47	0.41
9:Y:226:LYS:NZ	9:Y:254:ASP:OD2	2.53	0.41
9:U:92:ILE:HG23	9:U:92:ILE:O	2.20	0.41
3:I:94:TYR:OH	9:P:407:HIS:N	2.54	0.41
3:I:182:PHE:O	3:I:186:VAL:HG23	2.21	0.41
3:C:80:ASP:OD1	3:C:80:ASP:N	2.51	0.41
3:C:186:VAL:HG13	6:H:88:LEU:CD1	2.51	0.41
4:E:489:GLU:OE2	4:E:505:LYS:NZ	2.52	0.41
5:F:105:ILE:HG22	5:F:119:LEU:HD22	2.01	0.41
4:E:193:ASP:OD1	4:E:194:ASN:ND2	2.54	0.40
3:I:142:VAL:HG12	3:I:166:PHE:CD2	2.55	0.40
3:D:201:ALA:O	3:D:207:VAL:HG11	2.22	0.40
8:N:195:THR:HG21	8:N:258:ASP:HB3	2.04	0.40
4:E:404:PHE:HD1	4:E:410:VAL:HG23	1.85	0.40
5:G:74:THR:OG1	8:N:253:ILE:O	2.37	0.40
7:L:126:ASP:OD1	7:L:127:THR:N	2.55	0.40
9:X:395:SER:OG	9:X:408:VAL:O	2.40	0.40
9:Y:154:PHE:CD2	9:Y:207:ILE:HG12	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	136/271 (50%)	134 (98%)	2 (2%)	57	70
2	B	279/758 (37%)	278 (100%)	1 (0%)	84	82
3	C	311/311 (100%)	308 (99%)	3 (1%)	68	76
3	D	311/311 (100%)	305 (98%)	6 (2%)	50	66
3	I	310/311 (100%)	308 (99%)	2 (1%)	78	80
3	K	298/311 (96%)	298 (100%)	0	100	100
4	E	523/695 (75%)	521 (100%)	2 (0%)	84	82
5	F	144/164 (88%)	143 (99%)	1 (1%)	76	79
5	G	143/164 (87%)	141 (99%)	2 (1%)	59	71
6	H	95/928 (10%)	93 (98%)	2 (2%)	47	65
6	J	95/928 (10%)	94 (99%)	1 (1%)	65	74
7	L	190/209 (91%)	186 (98%)	4 (2%)	47	65
7	O	190/209 (91%)	184 (97%)	6 (3%)	34	55
8	M	205/228 (90%)	205 (100%)	0	100	100
8	N	205/228 (90%)	204 (100%)	1 (0%)	81	81
9	P	458/495 (92%)	449 (98%)	9 (2%)	48	65
9	Q	458/495 (92%)	450 (98%)	8 (2%)	53	67
9	T	456/495 (92%)	451 (99%)	5 (1%)	65	74
9	U	456/495 (92%)	449 (98%)	7 (2%)	57	70
9	X	452/495 (91%)	443 (98%)	9 (2%)	48	65
9	Y	452/495 (91%)	446 (99%)	6 (1%)	61	72
10	R	119/122 (98%)	117 (98%)	2 (2%)	53	67
10	S	119/122 (98%)	117 (98%)	2 (2%)	53	67
10	V	119/122 (98%)	115 (97%)	4 (3%)	32	54
10	W	119/122 (98%)	116 (98%)	3 (2%)	42	62
10	Z	119/122 (98%)	114 (96%)	5 (4%)	26	48
10	a	119/122 (98%)	115 (97%)	4 (3%)	32	54
All	All	6881/9728 (71%)	6784 (99%)	97 (1%)	57	71

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	249	ILE
1	A	289	PHE
2	B	304	THR
3	C	183	HIS
3	C	210	VAL
3	C	337	ILE
3	D	34	ARG
3	D	234	LEU
3	D	254	VAL
3	D	267	THR
3	D	308	GLN
3	D	326	LEU
4	E	531	MET
4	E	633	MET
5	F	90	ARG
5	G	12	LEU
5	G	61	ASP
6	H	7	ASN
6	H	38	GLN
3	I	203	GLN
3	I	331	ILE
6	J	25	ASN
7	L	2	ARG
7	L	45	THR
7	L	101	ASP
7	L	152	HIS
8	N	120	ASP
7	O	75	SER
7	O	111	SER
7	O	143	LEU
7	O	151	LEU
7	O	152	HIS
7	O	206	GLN
9	P	48	ASN
9	P	154	PHE
9	P	161	GLU
9	P	380	ARG
9	P	442	GLN
9	P	469	THR
9	P	503	GLU
9	P	576	VAL
9	P	580	TYR
9	Q	13	ARG

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Mol	Chain	Res	Type
9	Q	81	ASN
9	Q	83	THR
9	Q	202	TYR
9	Q	225	ASP
9	Q	234	ASP
9	Q	270	LEU
9	Q	406	ASN
10	R	3	SER
10	R	13	ASN
10	S	80	SER
10	S	85	ILE
9	T	216	PHE
9	T	315	GLU
9	T	339	SER
9	T	439	SER
9	T	450	ASP
9	U	13	ARG
9	U	170	GLU
9	U	185	VAL
9	U	442	GLN
9	U	457	ILE
9	U	470	PHE
9	U	513	ILE
10	V	16	LEU
10	V	57	TYR
10	V	71	GLU
10	V	96	VAL
10	W	13	ASN
10	W	114	ASN
10	W	133	TYR
9	X	49	THR
9	X	79	ASN
9	X	154	PHE
9	X	201	ASP
9	X	202	TYR
9	X	228	LEU
9	X	231	SER
9	X	234	ASP
9	X	479	THR
9	Y	92	ILE
9	Y	121	VAL
9	Y	154	PHE

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Mol	Chain	Res	Type
9	Y	381	GLN
9	Y	442	GLN
9	Y	481	ASN
10	Z	31	SER
10	Z	43	GLU
10	Z	61	ILE
10	Z	90	ILE
10	Z	133	TYR
10	a	71	GLU
10	a	76	LEU
10	a	129	ILE
10	a	138	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	HIS
2	B	47	ASN
2	B	96	ASN
2	B	118	ASN
2	B	147	ASN
2	B	211	ASN
2	B	217	GLN
2	B	228	ASN
2	B	247	ASN
2	B	290	ASN
3	C	175	GLN
3	C	312	ASN
3	D	148	ASN
3	D	175	GLN
4	E	305	ASN
4	E	431	ASN
5	F	130	ASN
5	G	3	ASN
5	G	164	GLN
6	H	7	ASN
6	H	33	ASN
3	I	263	ASN
3	I	329	ASN
6	J	3	ASN
6	J	17	ASN
6	J	25	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	J	38	GLN
3	K	73	GLN
3	K	141	ASN
8	M	191	ASN
8	N	9	ASN
8	N	93	GLN
8	N	117	ASN
7	O	10	HIS
7	O	106	ASN
7	O	139	GLN
7	O	160	HIS
9	P	188	GLN
9	P	530	GLN
9	P	582	GLN
9	Q	48	ASN
9	Q	497	ASN
10	S	98	ASN
9	T	117	ASN
9	T	149	ASN
9	U	149	ASN
9	U	212	GLN
9	U	269	GLN
9	U	329	HIS
9	U	342	GLN
9	U	376	GLN
9	U	442	GLN
9	U	497	ASN
9	U	557	ASN
10	V	52	HIS
10	V	98	ASN
10	V	108	HIS
10	W	7	GLN
10	W	98	ASN
9	X	164	ASN
9	X	204	ASN
9	X	386	ASN
9	X	442	GLN
9	Y	240	ASN
10	a	108	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.

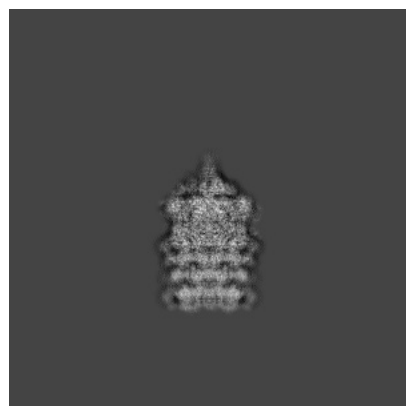
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19969. These allow visual inspection of the internal detail of the map and identification of artifacts.

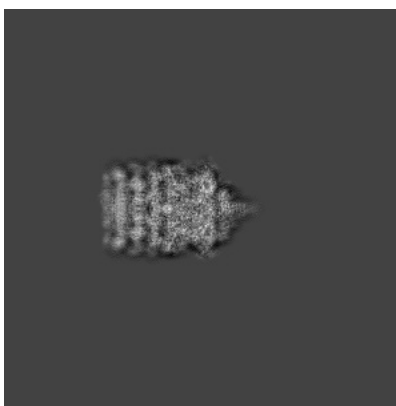
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

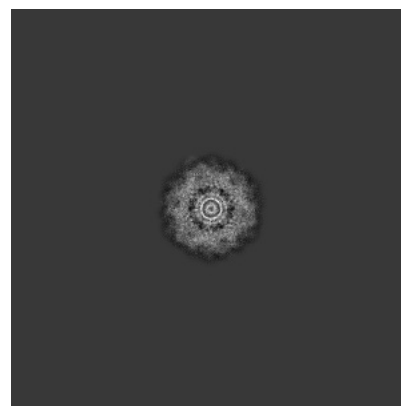
6.1.1 Primary map



X



Y

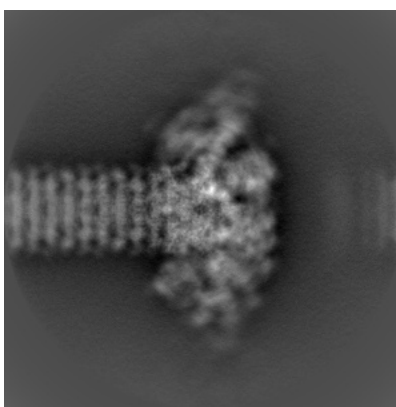


Z

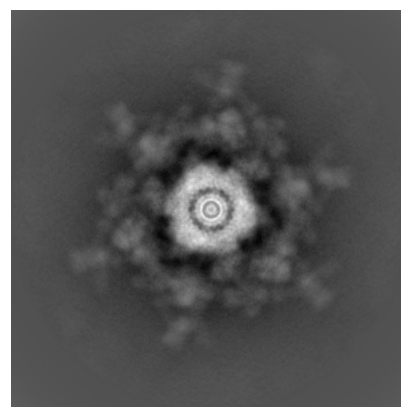
6.1.2 Raw map



X



Y

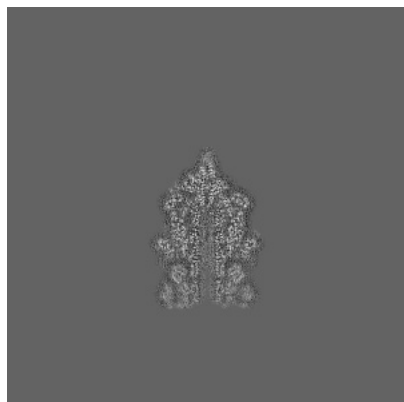


Z

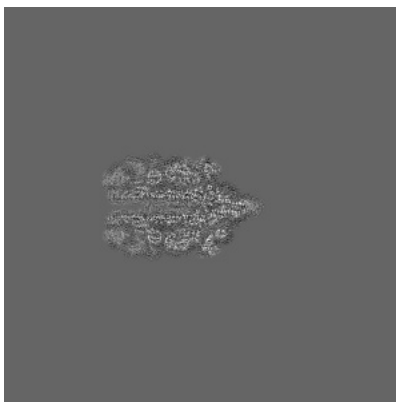
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

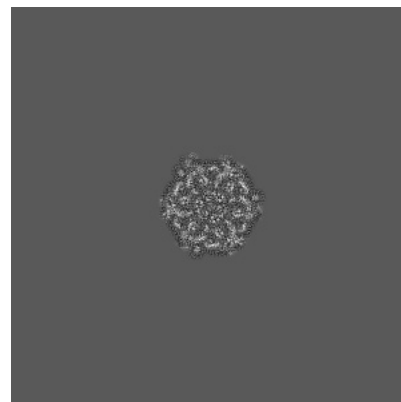
6.2.1 Primary map



X Index: 420

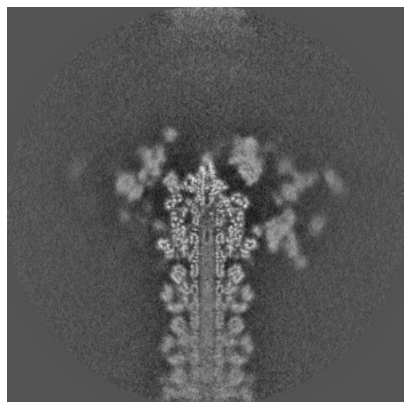


Y Index: 420

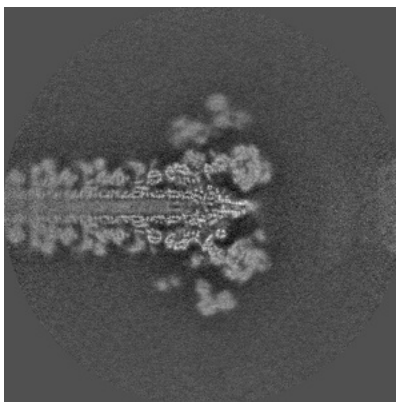


Z Index: 420

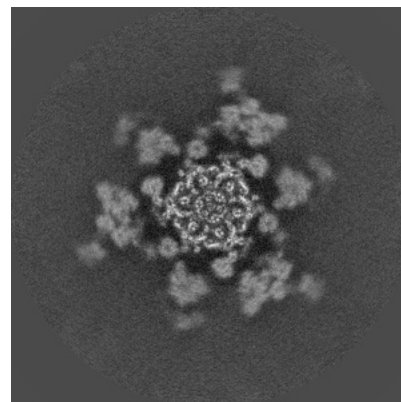
6.2.2 Raw map



X Index: 420



Y Index: 420

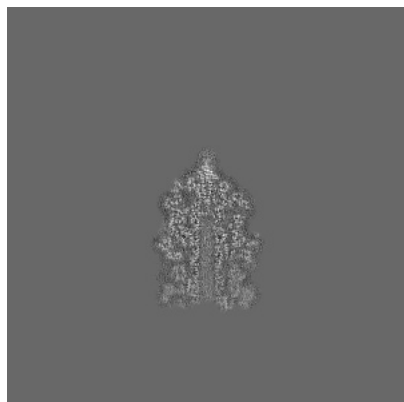


Z Index: 420

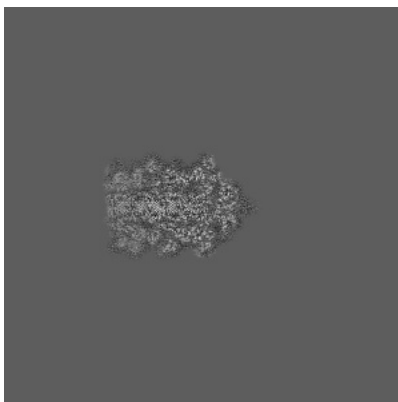
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

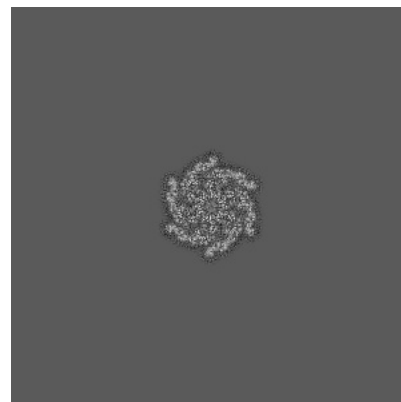
6.3.1 Primary map



X Index: 427



Y Index: 440

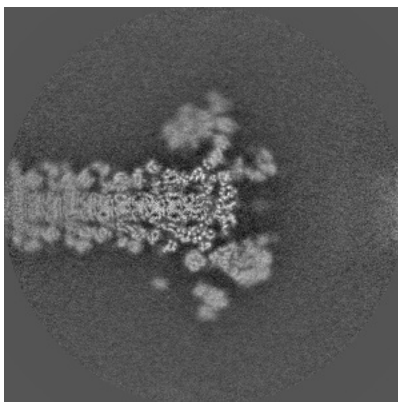


Z Index: 346

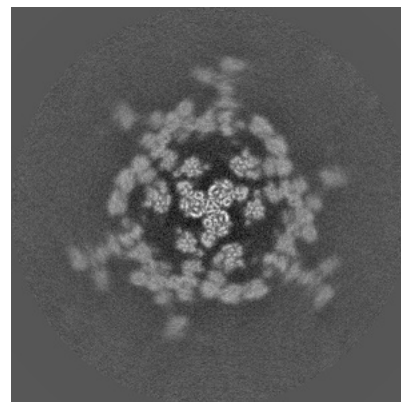
6.3.2 Raw map



X Index: 450



Y Index: 440

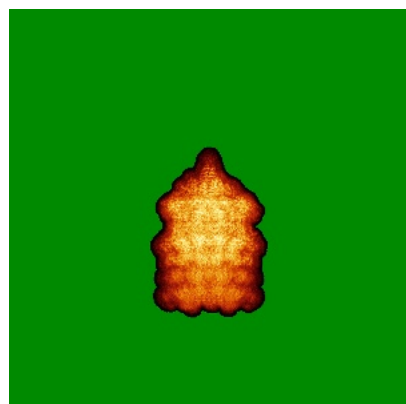


Z Index: 461

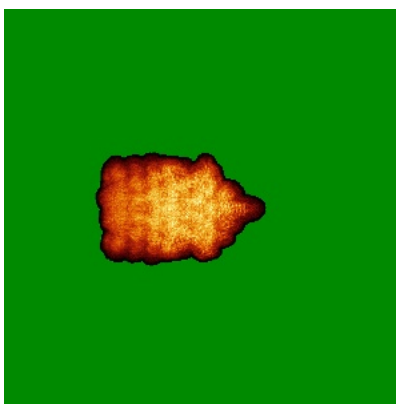
The images above show the largest variance slices of the map in three orthogonal directions.

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

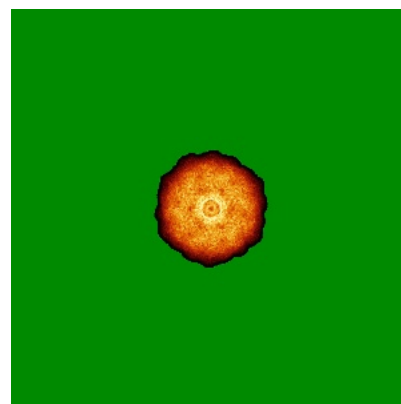
6.4.1 Primary map



X

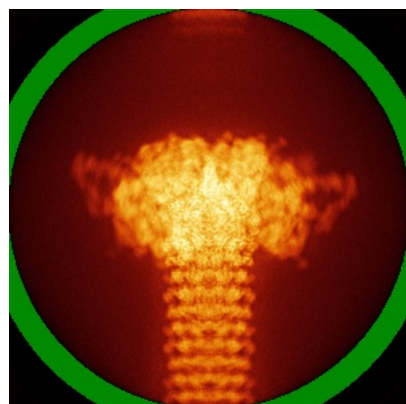


Y

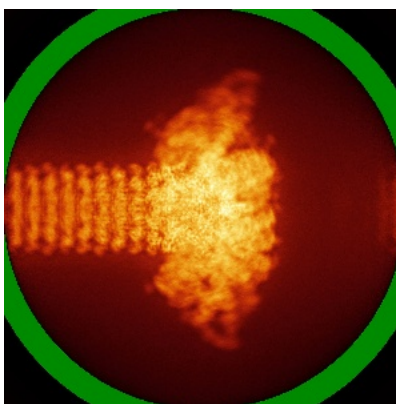


Z

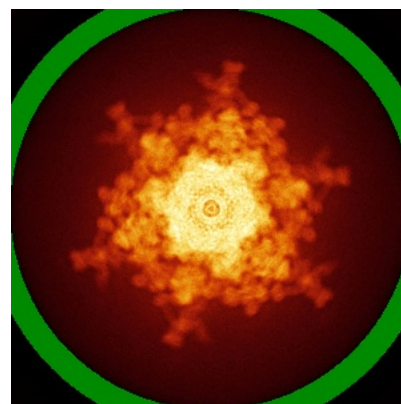
6.4.2 Raw map



X



Y

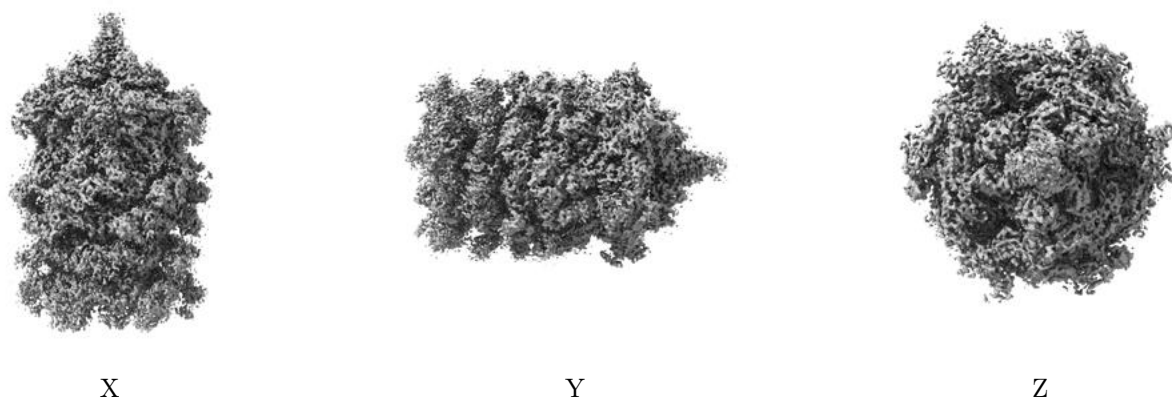


Z

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.

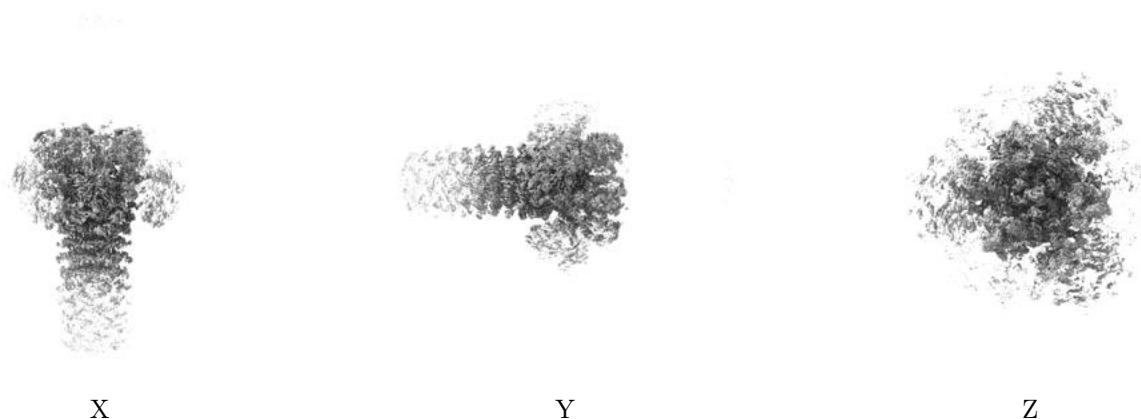
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

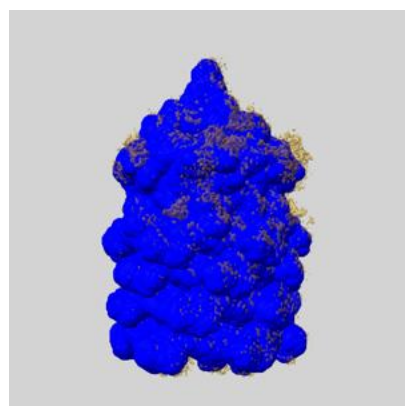
6.6 Mask visualisation [i](#)

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

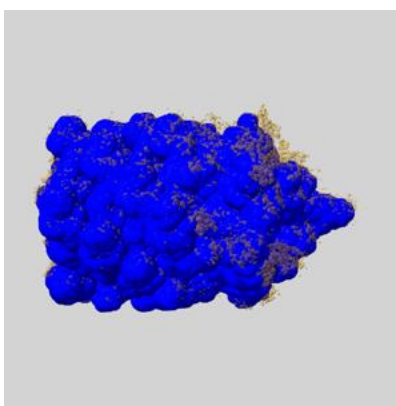
A mask typically either:

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

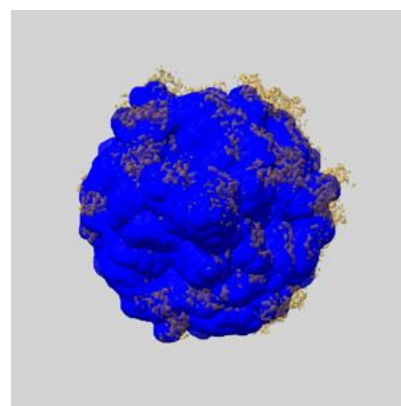
6.6.1 emd_19969_msk_1.map [i](#)



X



Y

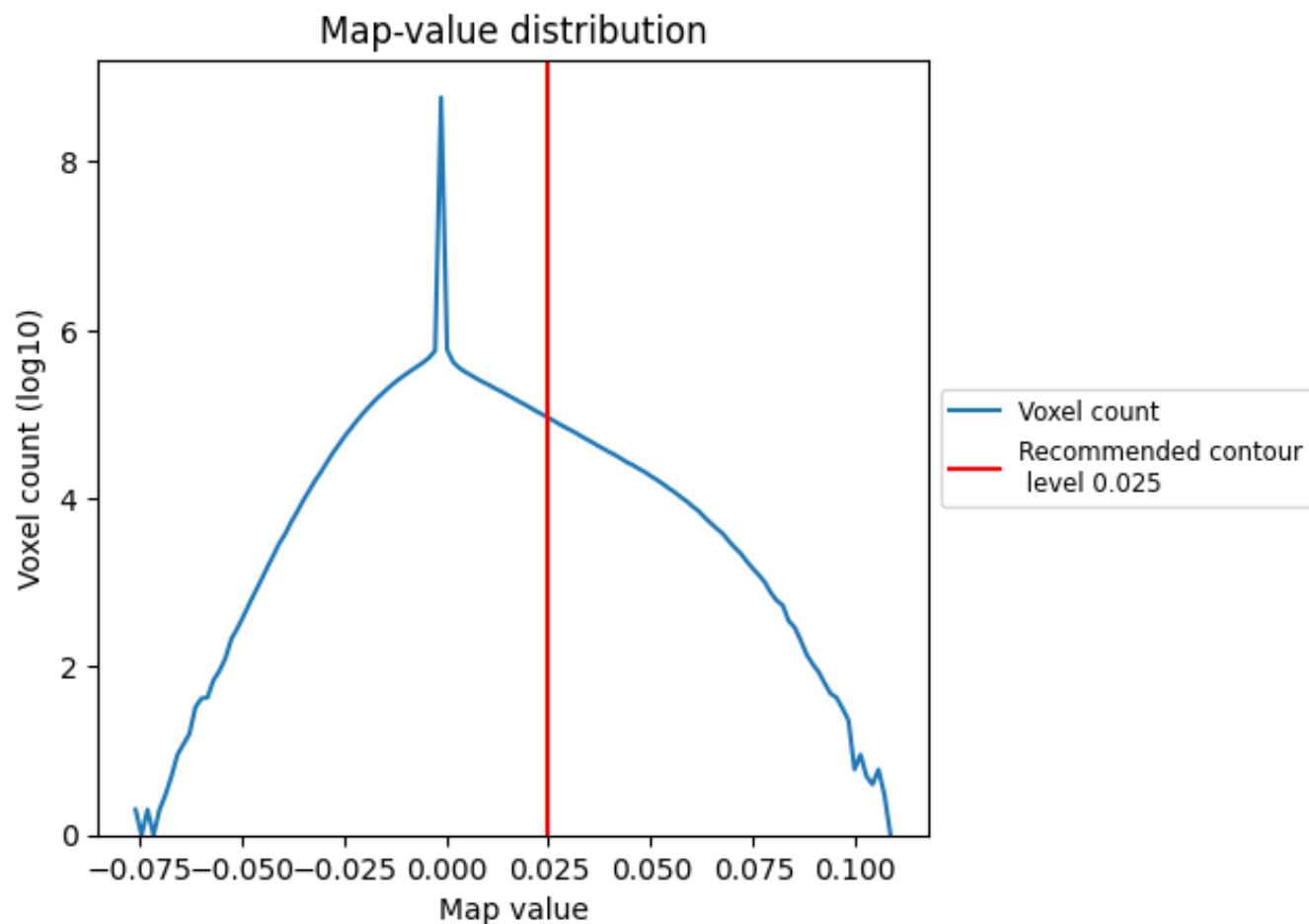


Z

7 Map analysis [i](#)

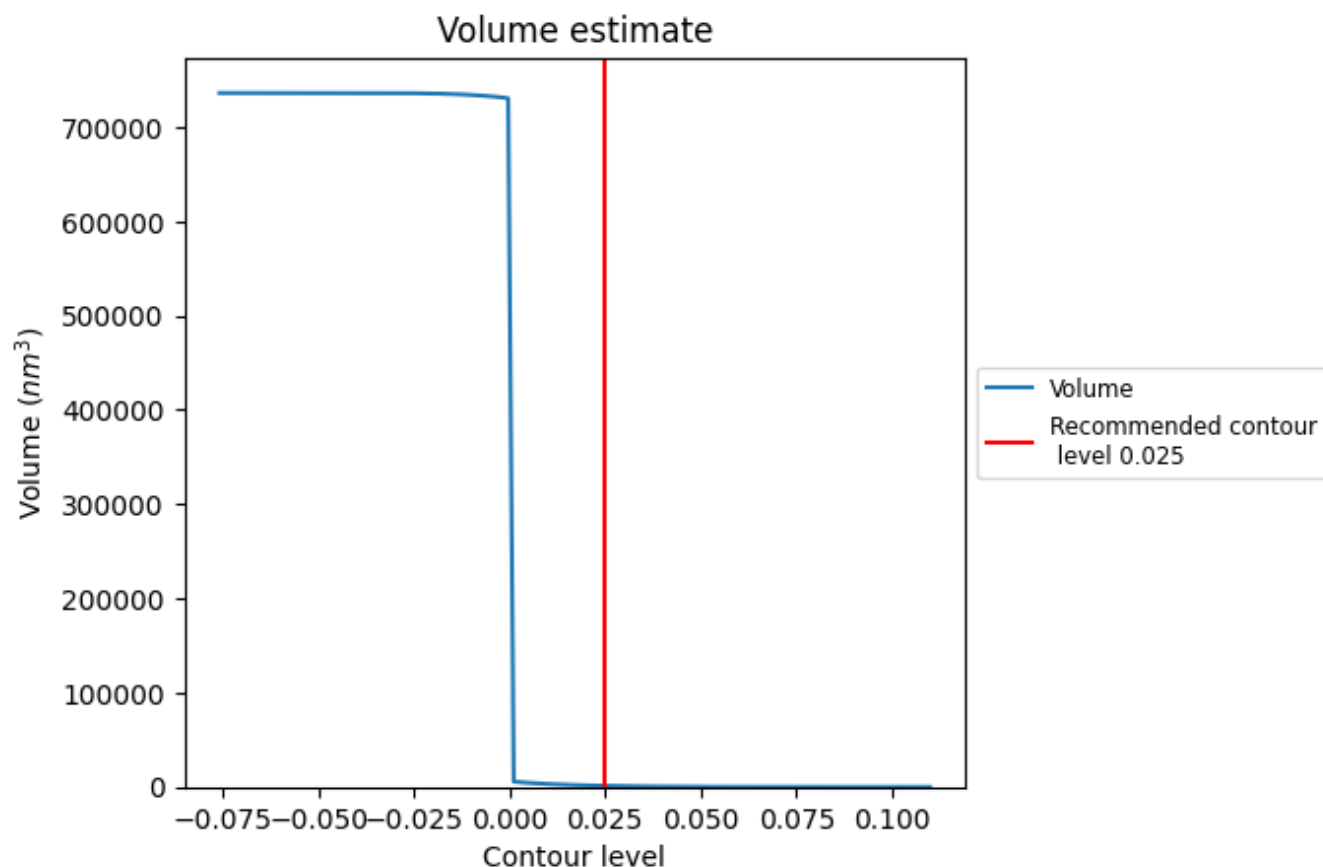
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

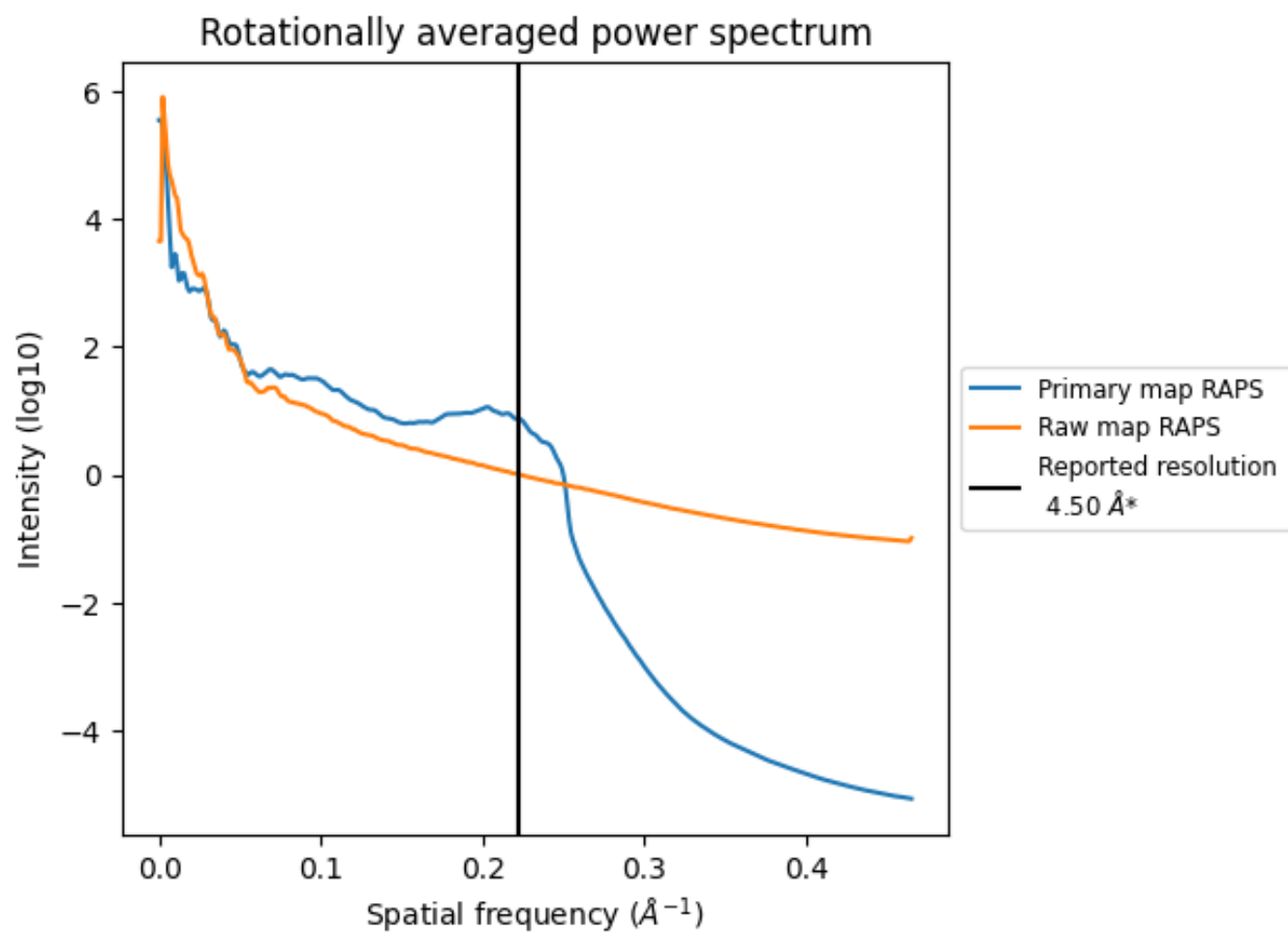
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1199 nm^3 ; this corresponds to an approximate mass of 1083 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 ⓘ

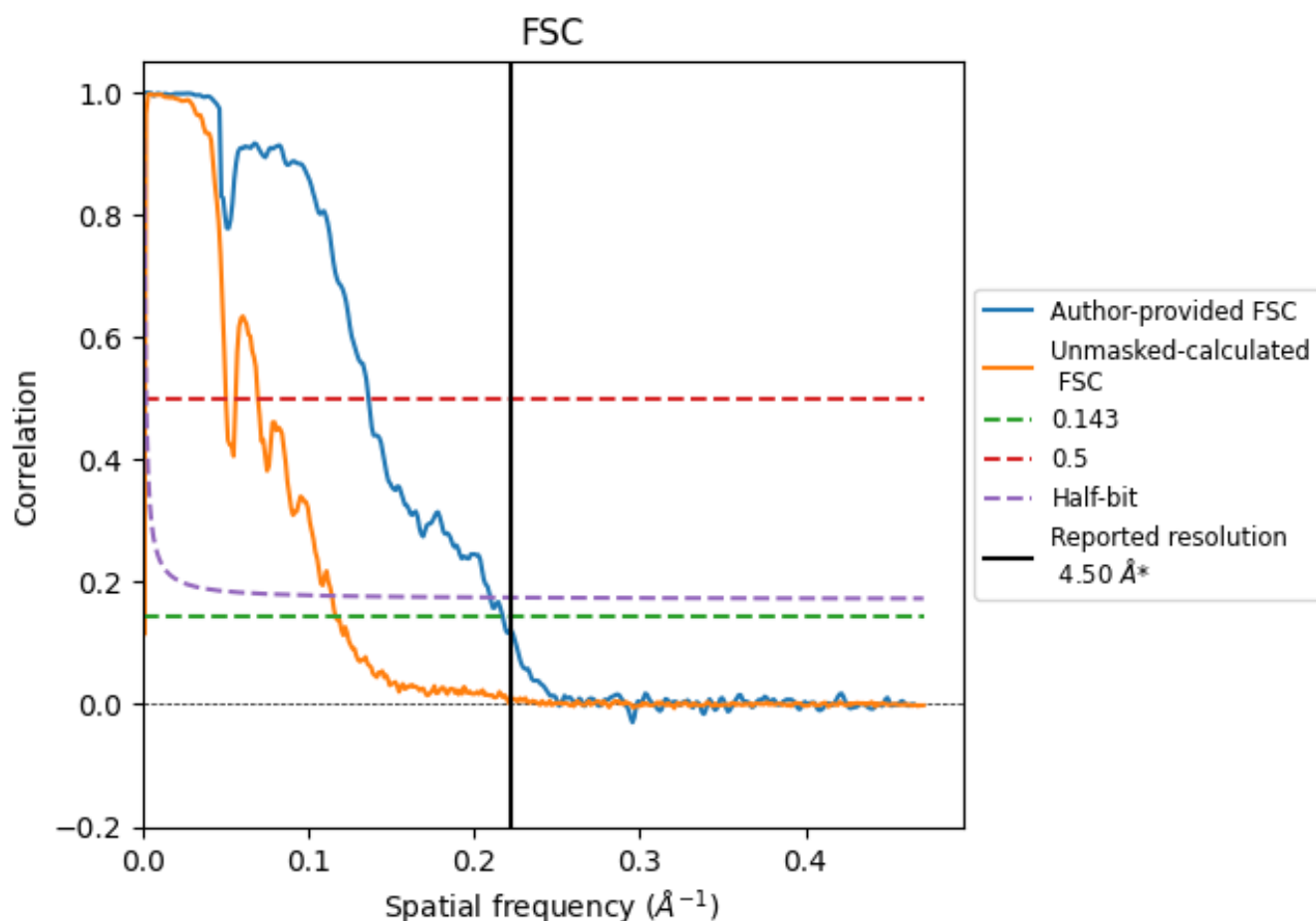


*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

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 0.222 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.60	7.33	4.76
Unmasked-calculated*	833.33	625.00	555.56

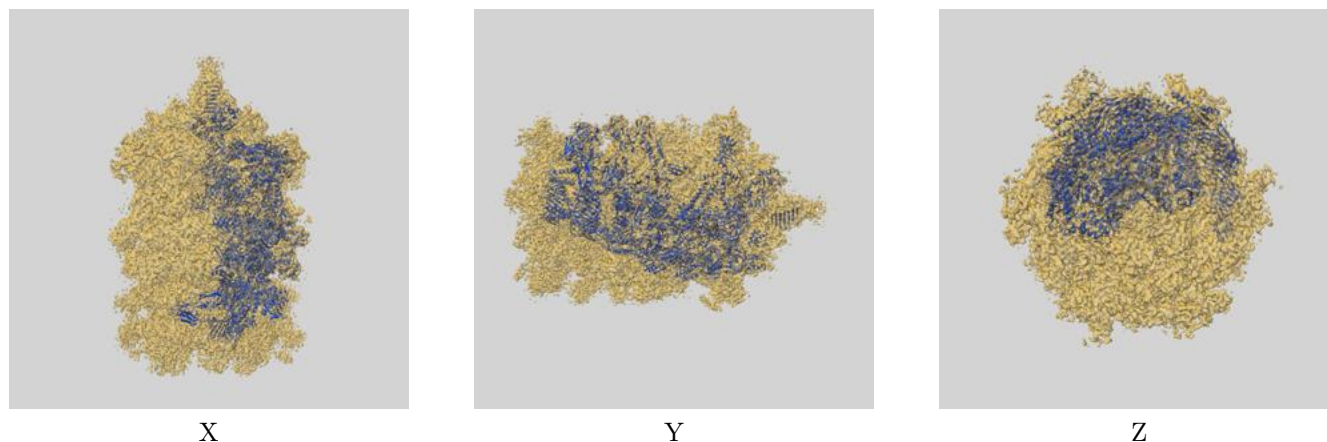
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 833.33 differs from the reported value 4.5 by more than 10 %

9 Map-model fit [i](#)

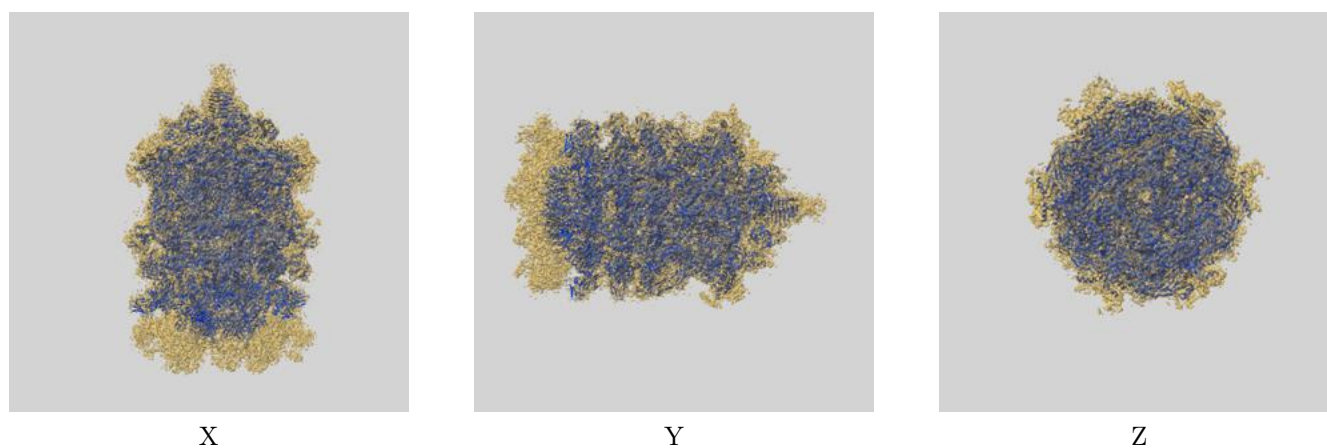
This section contains information regarding the fit between EMDB map EMD-19969 and PDB model 9EUG. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

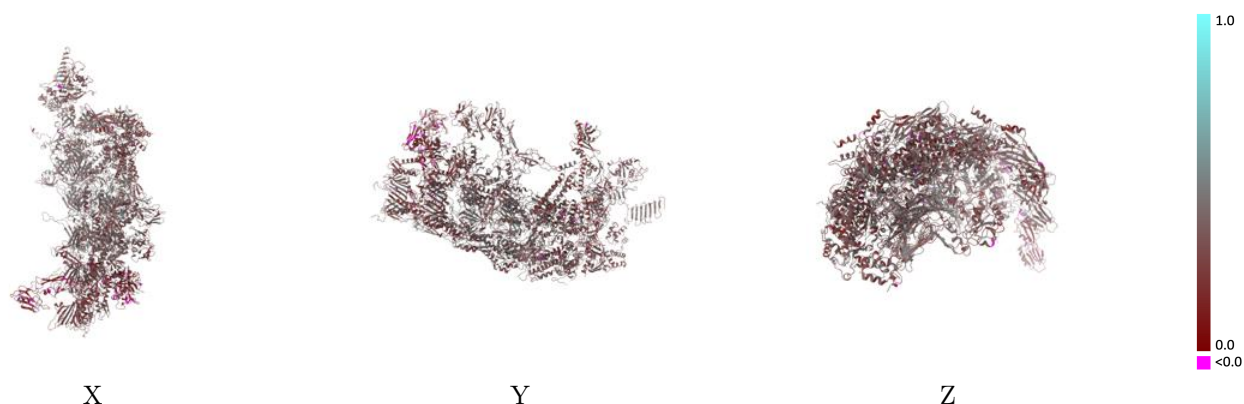


9.1.2 Map-model assembly overlay [i](#)



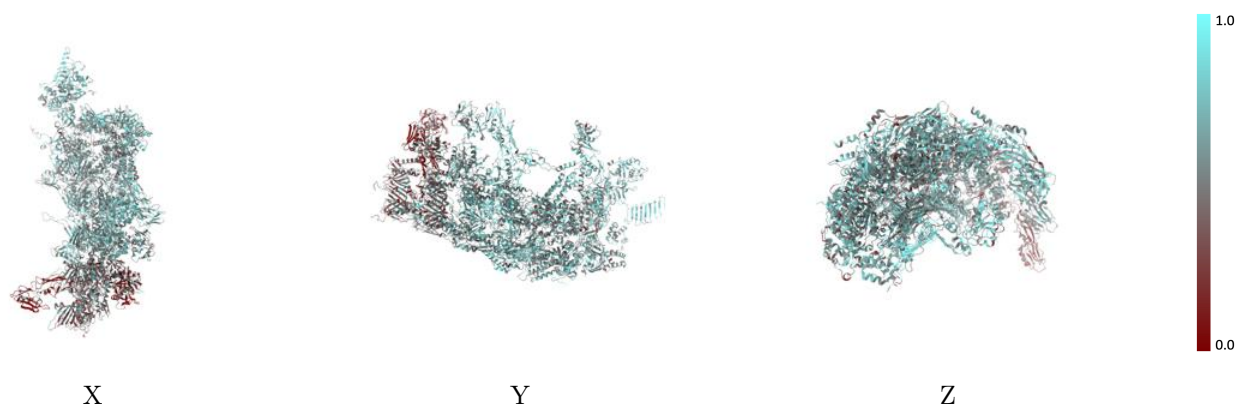
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



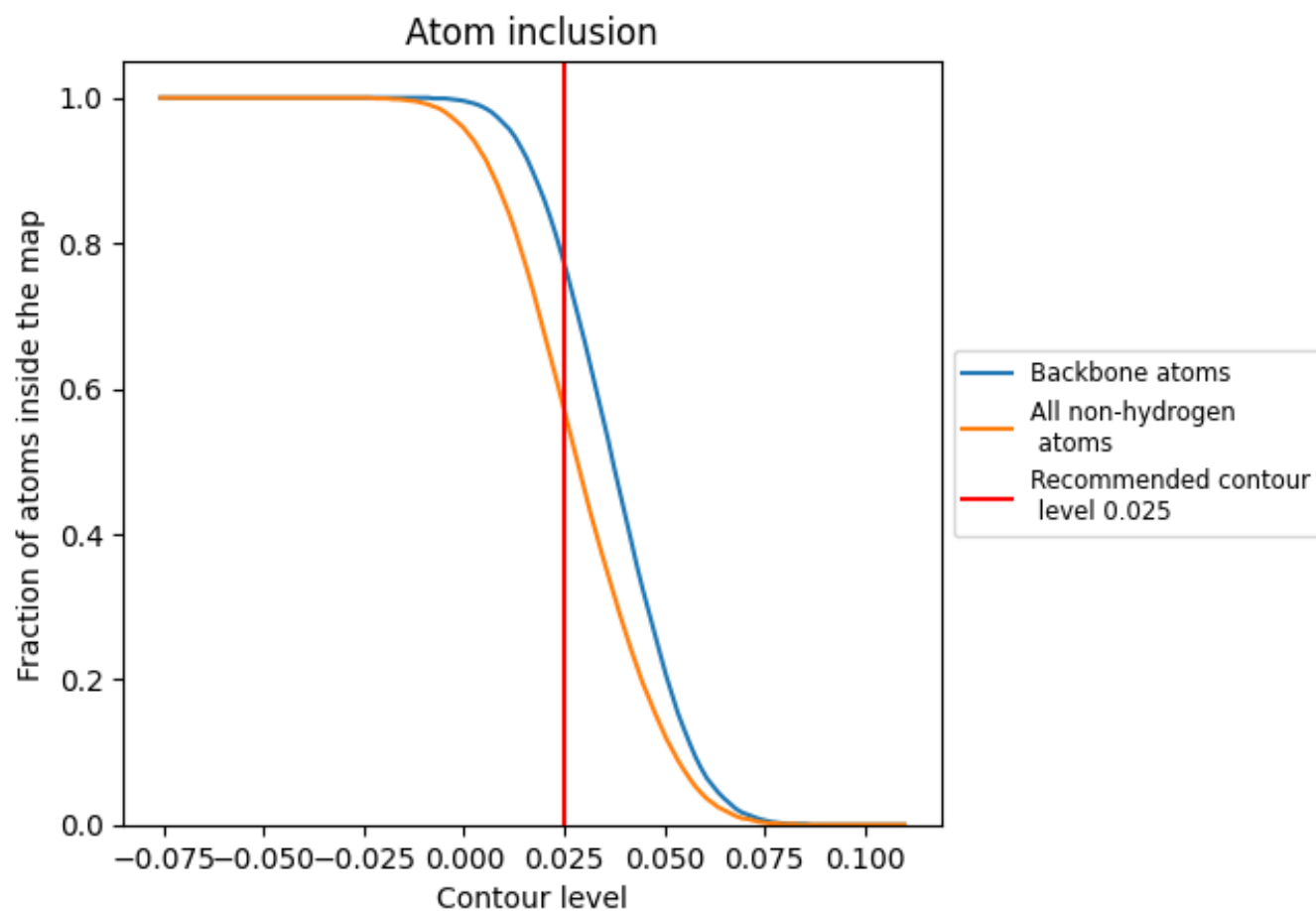
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 57% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5710	 0.3460
A	 0.6380	 0.3250
B	 0.6570	 0.3690
C	 0.6170	 0.3460
D	 0.6280	 0.3460
E	 0.5980	 0.3640
F	 0.6200	 0.3530
G	 0.5760	 0.3070
H	 0.6490	 0.3360
I	 0.6120	 0.3160
J	 0.6470	 0.3460
K	 0.6270	 0.3340
L	 0.6230	 0.3730
M	 0.5830	 0.3600
N	 0.5900	 0.3690
O	 0.6220	 0.3880
P	 0.6590	 0.3850
Q	 0.6530	 0.3760
R	 0.6360	 0.4030
S	 0.6330	 0.4140
T	 0.5630	 0.3550
U	 0.5750	 0.3590
V	 0.5430	 0.3840
W	 0.5440	 0.4000
X	 0.3400	 0.2610
Y	 0.3410	 0.2560
Z	 0.4470	 0.3520
a	 0.4240	 0.3240

