



wwPDB EM Validation Summary Report ⓘ

Mar 30, 2025 – 04:32 am BST

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 wwPDB EM Validation Summary 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

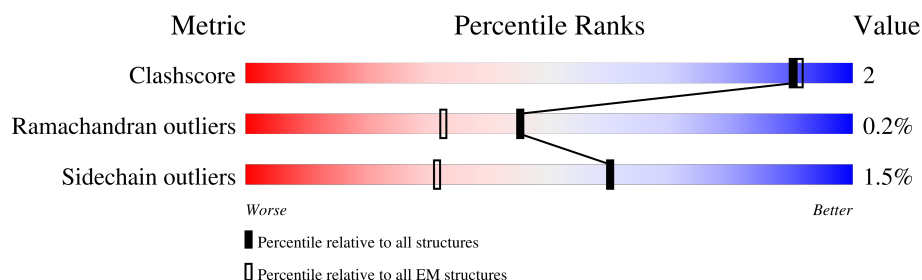
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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)
Clashscore	210492	15764
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 $\leq 5\%$. 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	<div> <div>5%</div> <div>49%</div> <div>48%</div> </div>
2	B	848	<div> <div>32%</div> <div>63%</div> </div>
3	C	348	<div> <div>13%</div> <div>95%</div> </div>
3	D	348	<div> <div>14%</div> <div>94%</div> <div>6%</div> </div>
3	I	348	<div> <div>14%</div> <div>89%</div> <div>11%</div> </div>
3	K	348	<div> <div>12%</div> <div>96%</div> </div>
4	E	808	<div> <div>11%</div> <div>68%</div> <div>5%</div> <div>27%</div> </div>
5	F	174	<div> <div>11%</div> <div>83%</div> <div>6%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
5	G	174	
6	H	1019	
6	J	1019	
7	L	234	
7	O	234	
8	M	263	
8	N	263	
9	P	587	
9	Q	587	
9	T	587	
9	U	587	
9	X	587	
9	Y	587	
10	R	142	
10	S	142	
10	V	142	
10	W	142	
10	Z	142	
10	a	142	

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		

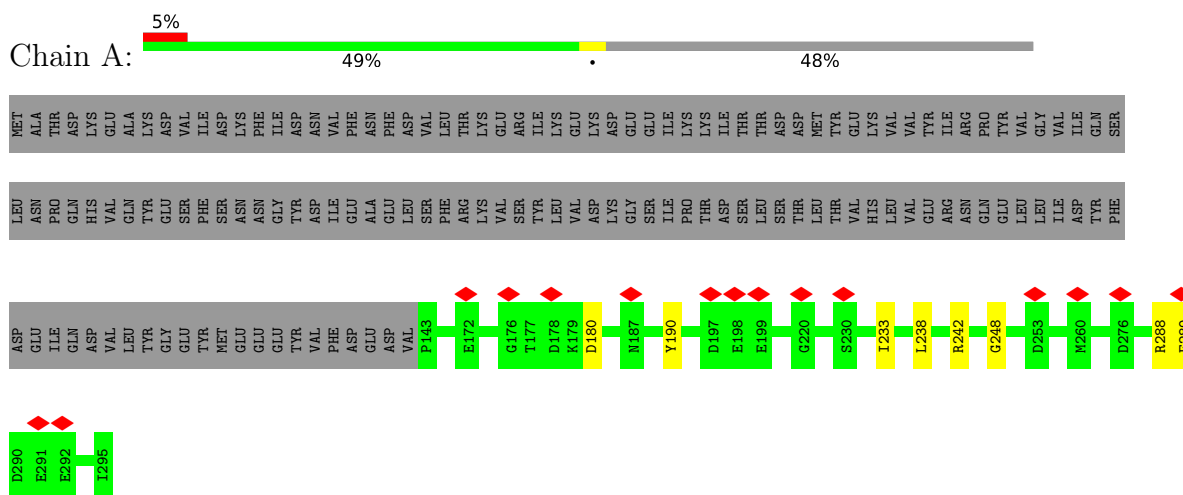
- Molecule 10 is a protein called Capsid protein.

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

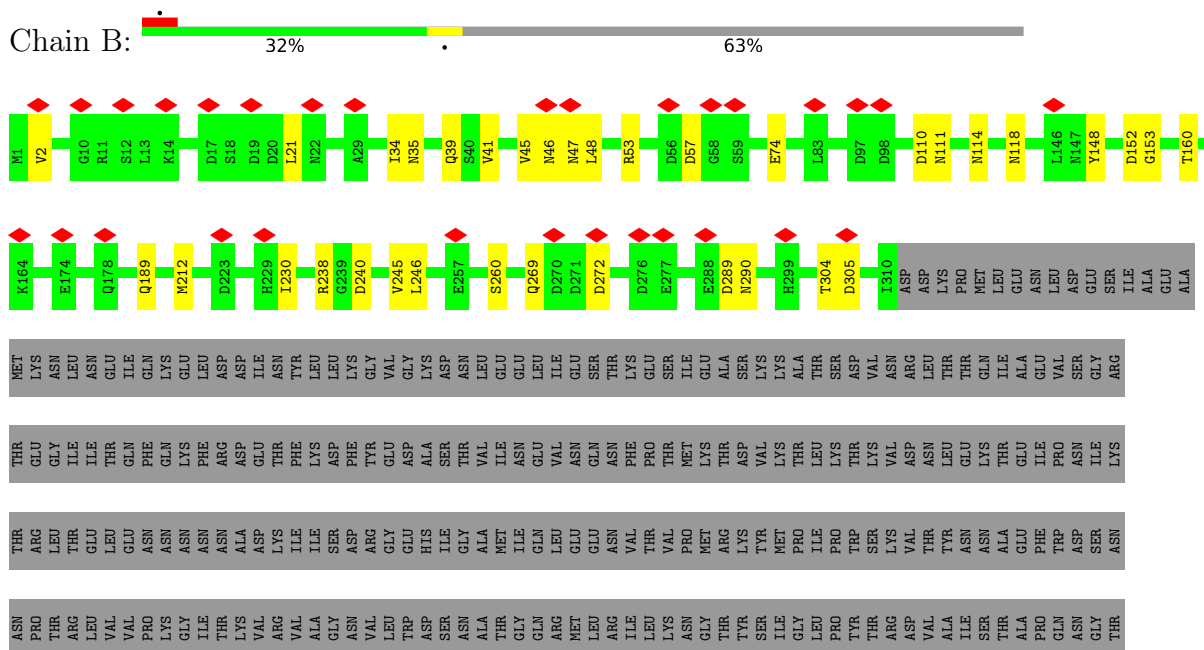
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: NlpC/P60 domain-containing protein

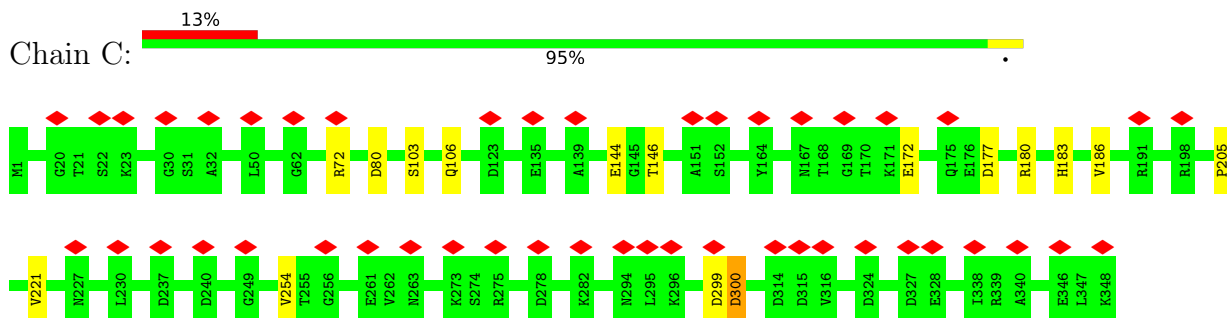


- Molecule 2: GP-PDE domain-containing protein

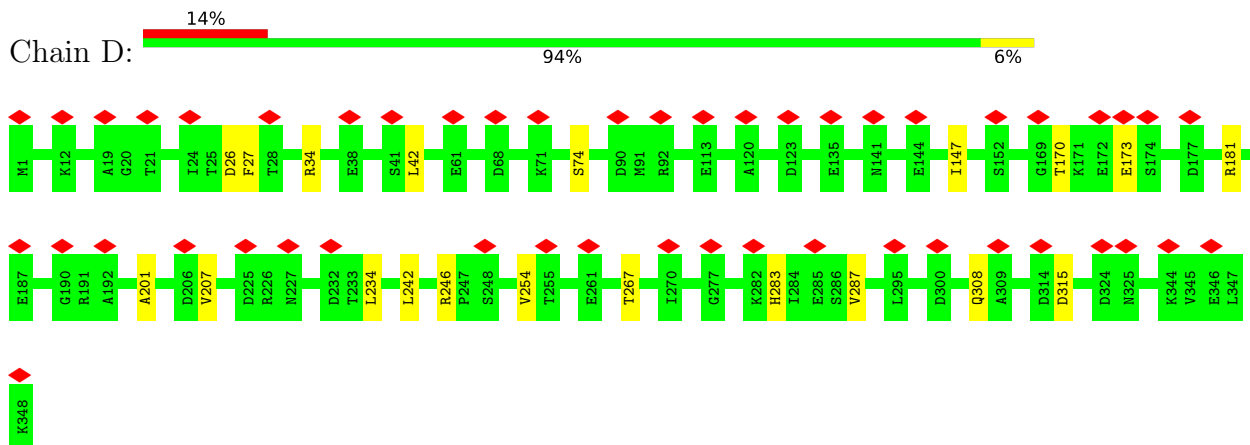


[illegible]

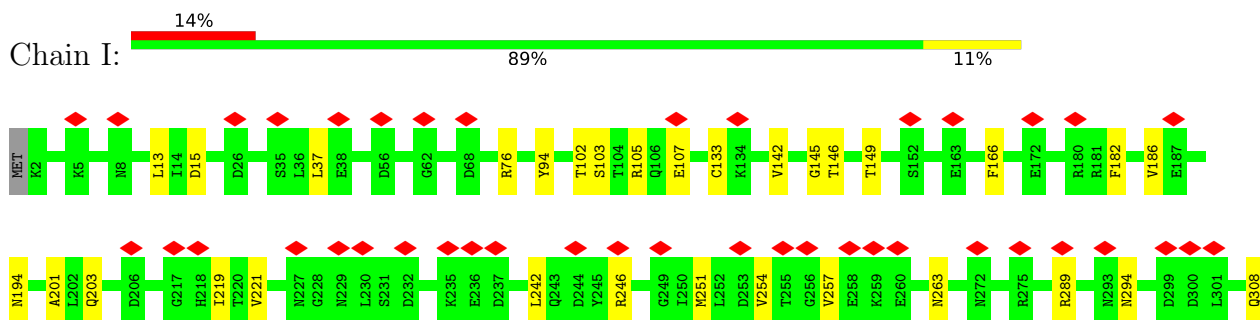
- Molecule 3: Baseplate component

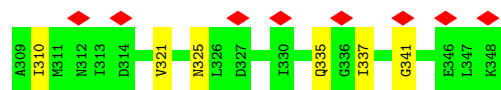


- Molecule 3: Baseplate component

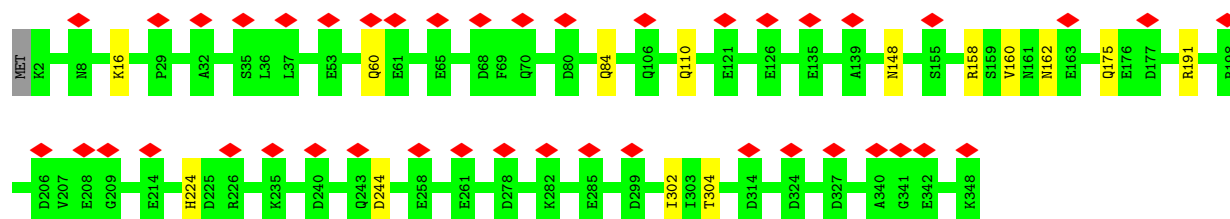


- Molecule 3: Baseplate component

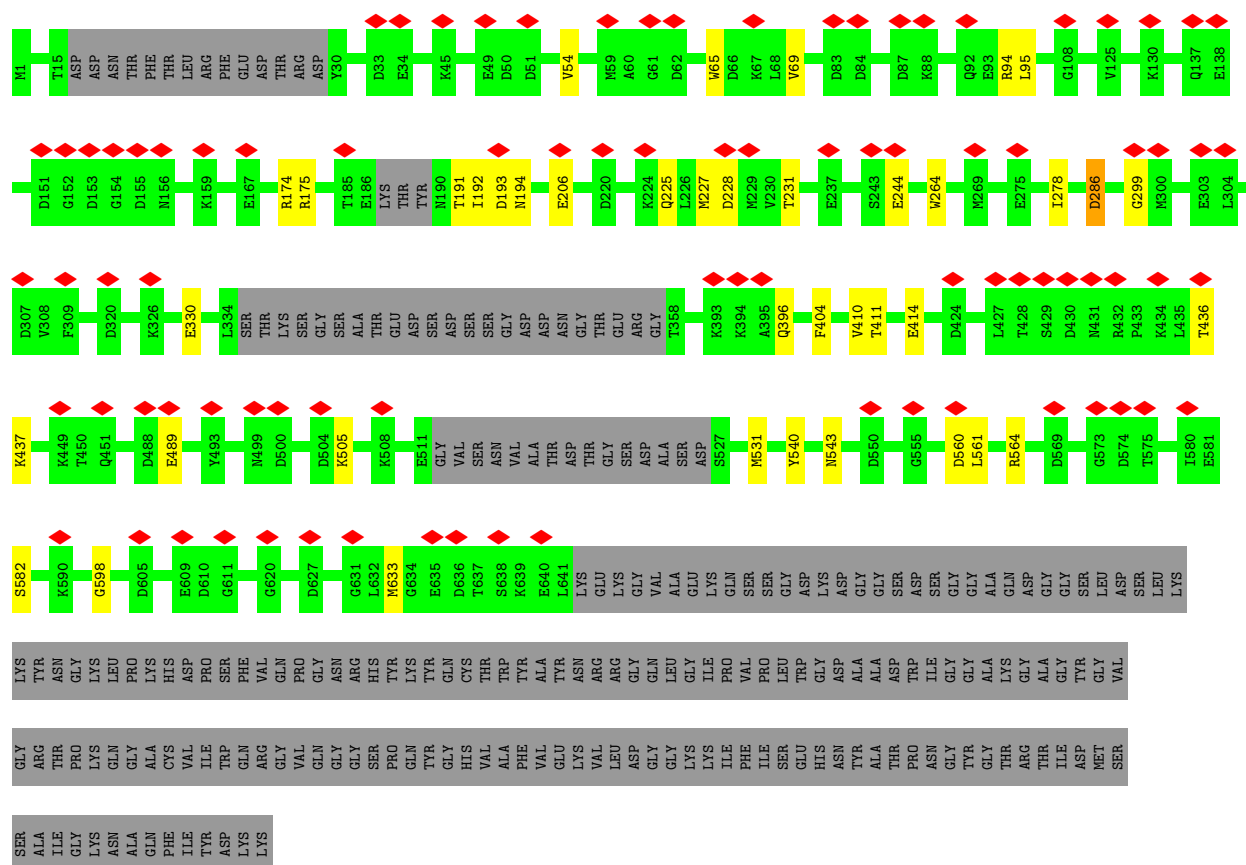




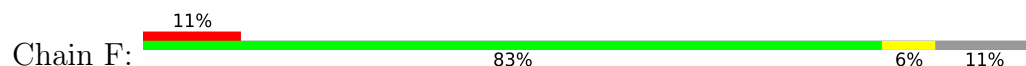
• Molecule 3: Baseplate component

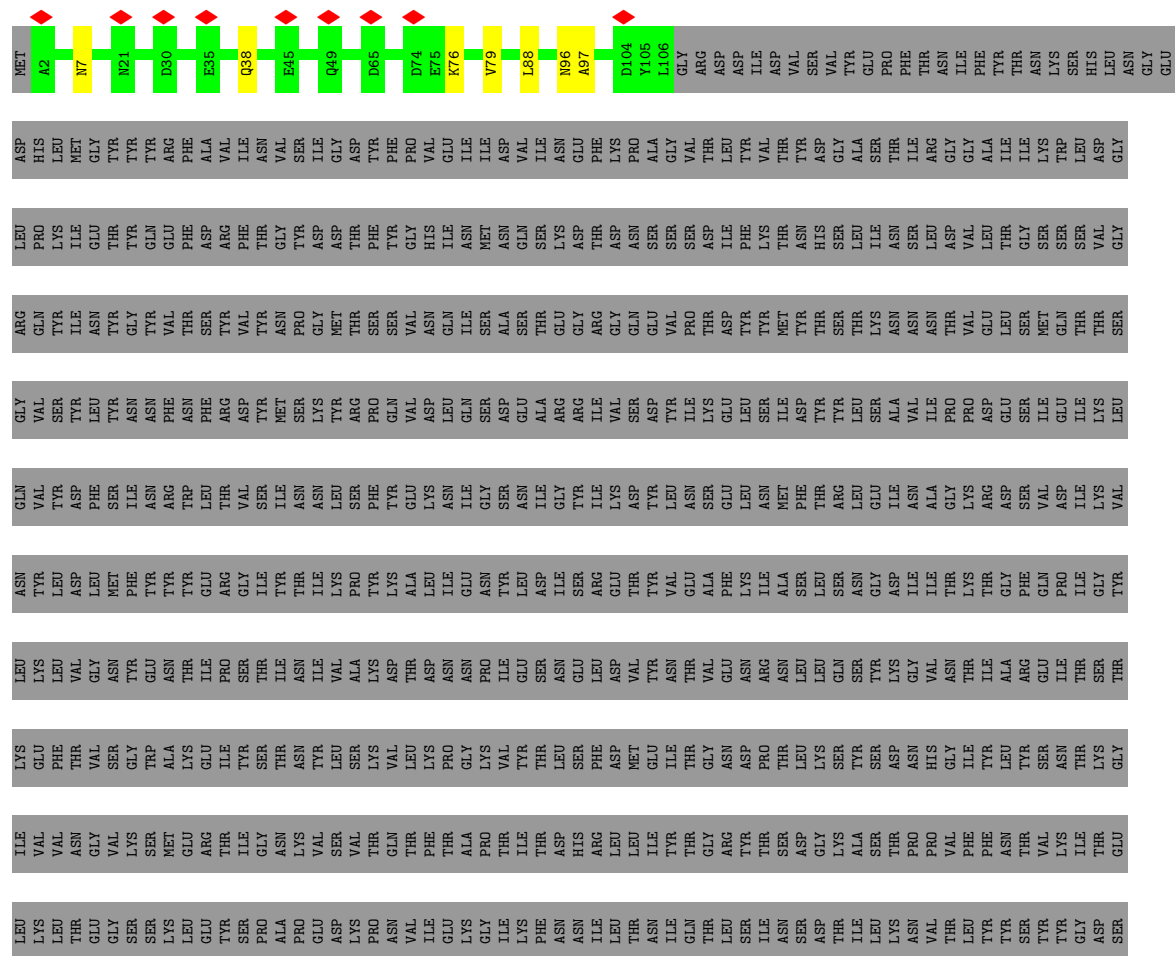


• Molecule 4: Peptidase C51 domain-containing protein




• Molecule 5: Baseplate component

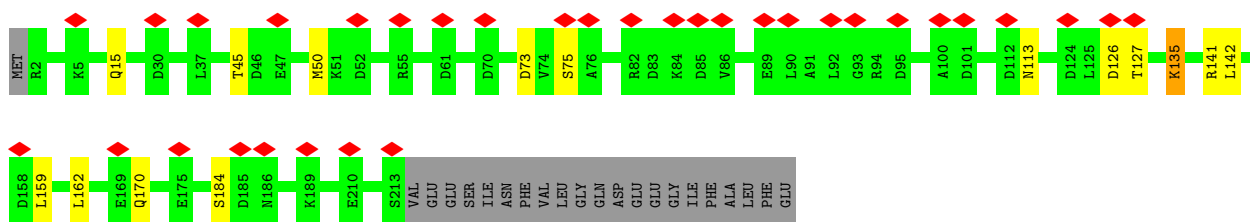




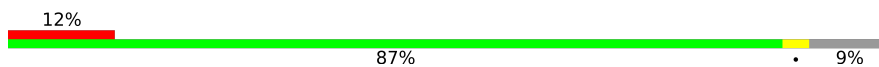
THR	LEU	GLY	ASP	PRO	SER	ARG	LEU	ILE	SER	GLY	THR	ARG	LEU	LYS	GLU	LEU	VAL	GLU	THR	SER	GLY	PHE	SER	ASN	ASN	VAL	ASP	ASN	ARG	ILE	LYS	VAL	ILE	ASP	SER	ILE	PRO	TYR	GLU	PHE	GLU	ASN	ASN	GLU	PRO	THR	PHE	ILE	TYR	ILE	PRO	LYS	ASN	GLY	ILE	PHE	VAL	GLY	ARG	GLU	VAL	GLU	THR	GLY	PHE	ILE	ALA	LYS	PRO	ASP	TYR
GLY	LEU	TYR	GLY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

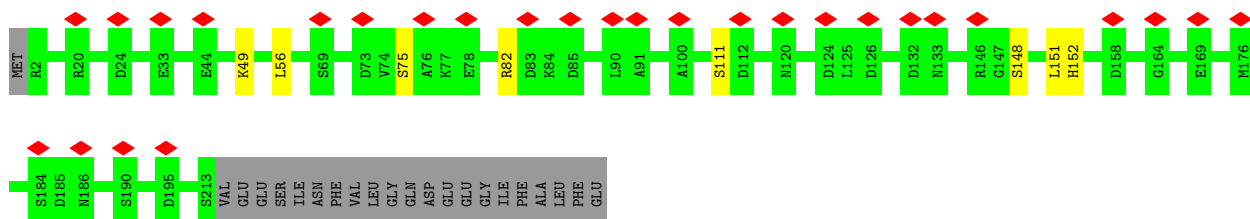
- Molecule 7: Baseplate wedge subunit

Chain L: 




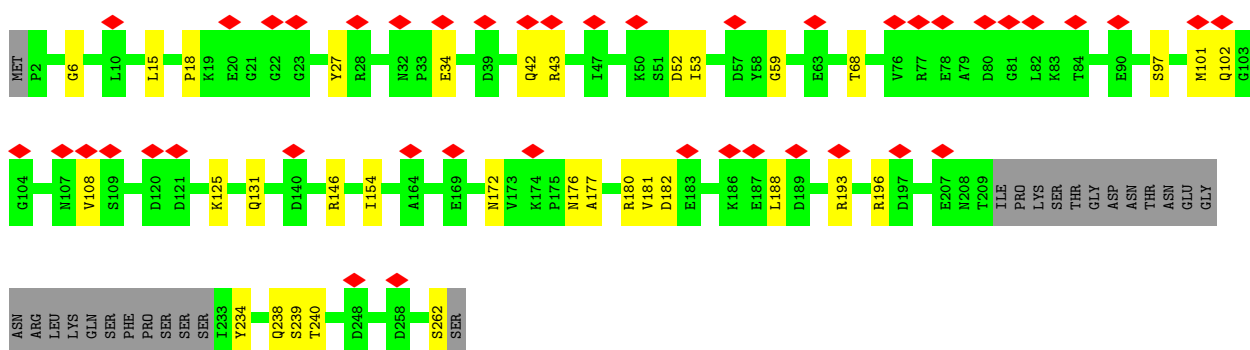
- Molecule 7: Baseplate wedge subunit

Chain O: 




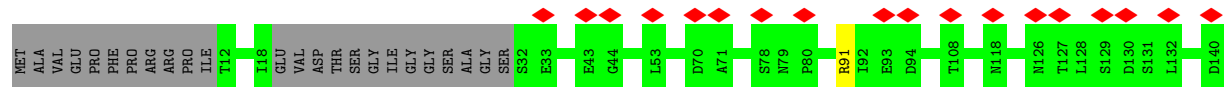
- Molecule 8: Putative baseplate component

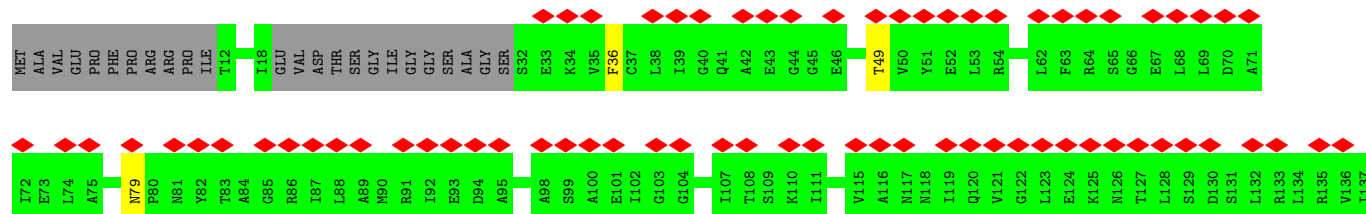
Chain M: 



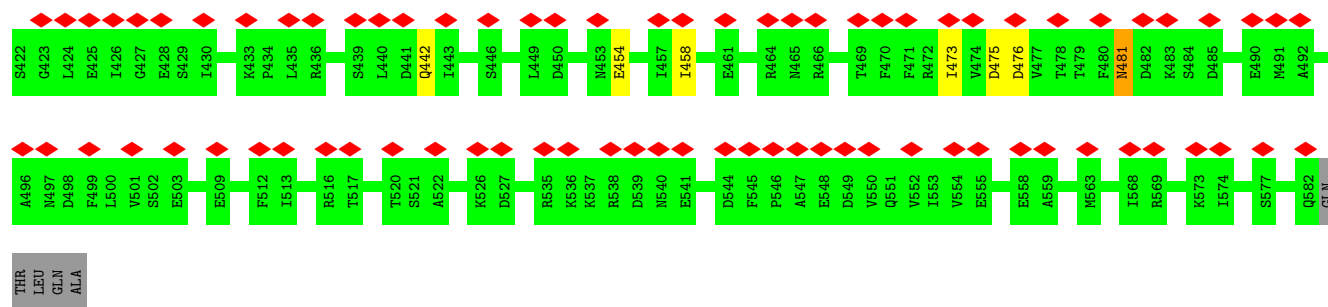
- Molecule 8: Putative baseplate component

Chain N: 

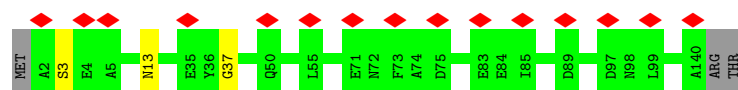




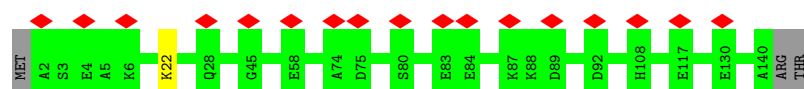




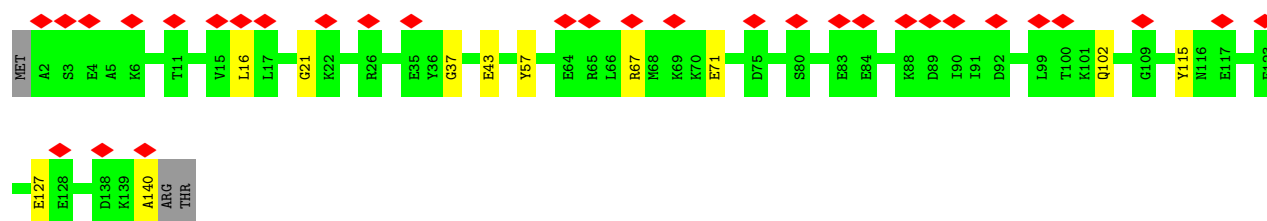
- Molecule 10: Capsid protein



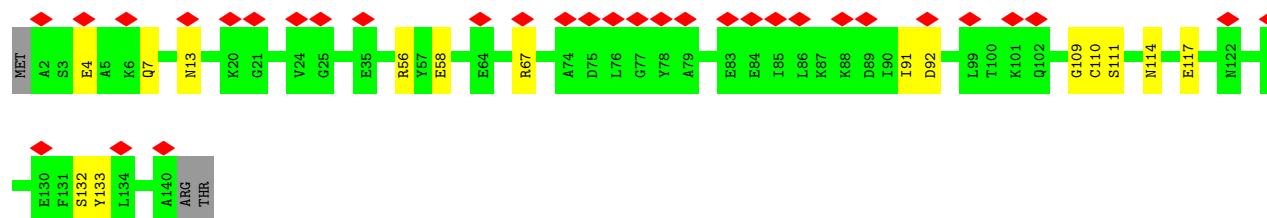
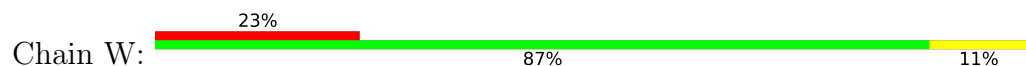
- Molecule 10: Capsid protein



- Molecule 10: Capsid protein

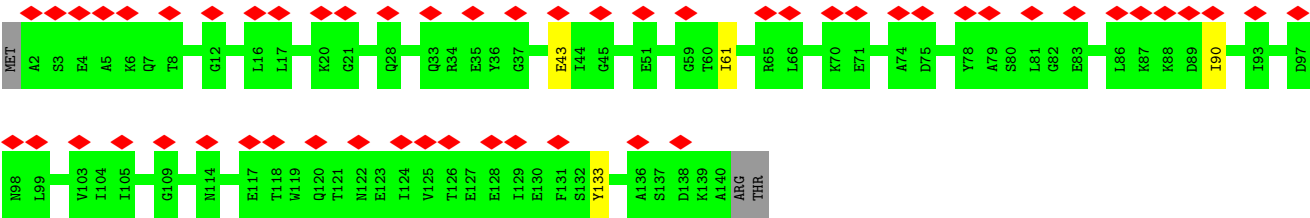


- Molecule 10: Capsid protein

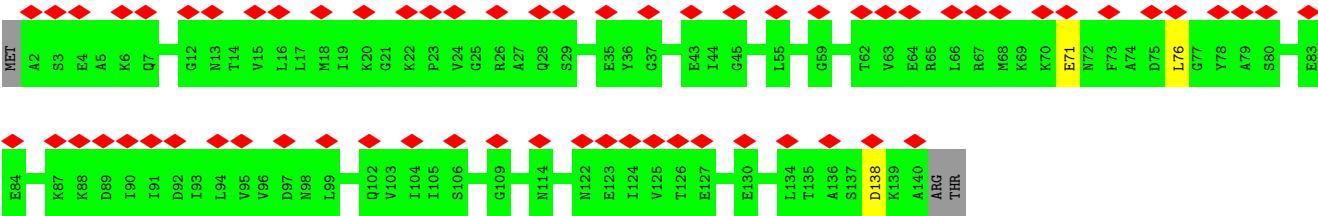


- Molecule 10: Capsid protein





• 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 ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.39	1/1303 (0.1%)	0.64	1/1756 (0.1%)
2	B	0.35	0/2519	0.66	0/3404
3	C	0.34	0/2803	0.66	2/3794 (0.1%)
3	D	0.33	0/2803	0.65	0/3794
3	I	0.34	0/2795	0.66	0/3784
3	K	0.33	0/2795	0.63	0/3784
4	E	0.35	0/4863	0.65	0/6535
5	F	0.33	0/1269	0.65	0/1724
5	G	0.34	0/1261	0.60	0/1713
6	H	0.33	0/883	0.68	0/1186
6	J	0.33	0/883	0.67	0/1186
7	L	0.36	0/1722	0.73	1/2331 (0.0%)
7	O	0.38	0/1722	0.69	0/2331
8	M	0.35	0/1907	0.70	0/2565
8	N	0.34	0/1907	0.72	1/2565 (0.0%)
9	P	0.36	0/4267	0.69	0/5760
9	Q	0.36	0/4267	0.68	0/5760
9	T	0.34	0/4256	0.65	0/5745
9	U	0.35	0/4256	0.68	0/5745
9	X	0.33	0/4218	0.67	0/5693
9	Y	0.32	0/4218	0.65	0/5693
10	R	0.39	0/1107	0.72	0/1496
10	S	0.35	0/1107	0.69	0/1496
10	V	0.33	0/1107	0.70	0/1496
10	W	0.32	0/1107	0.66	0/1496
10	Z	0.36	0/1107	0.69	0/1496
10	a	0.32	0/1107	0.69	0/1496
All	All	0.34	1/63559 (0.0%)	0.67	5/85824 (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
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)
1	A	190	TYR	CE2-CZ	-5.25	1.31	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	300	ASP	CB-CG-OD1	-5.97	112.92	118.30
3	C	300	ASP	CB-CG-OD2	5.73	123.46	118.30
1	A	180	ASP	CB-CG-OD2	5.69	123.42	118.30
7	L	135	LYS	CD-CE-NZ	5.37	124.06	111.70
8	N	50	LYS	CD-CE-NZ	5.01	123.22	111.70

There are no chirality outliers.

5 of 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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2470	0	2394	22	0
3	C	2760	0	2729	11	0
3	D	2760	0	2729	9	0
3	I	2752	0	2717	22	0
3	K	2752	0	2717	9	0
4	E	4764	0	4703	24	0
5	F	1248	0	1257	5	0
5	G	1240	0	1251	6	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	14	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	9	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	195	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.

The worst 5 of 195 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

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	151/295 (51%)	143 (95%)	8 (5%)	0	100	100
2	B	308/848 (36%)	282 (92%)	26 (8%)	0	100	100
3	C	346/348 (99%)	328 (95%)	18 (5%)	0	100	100
3	D	346/348 (99%)	328 (95%)	18 (5%)	0	100	100
3	I	345/348 (99%)	329 (95%)	16 (5%)	0	100	100
3	K	345/348 (99%)	333 (96%)	12 (4%)	0	100	100
4	E	576/808 (71%)	536 (93%)	40 (7%)	0	100	100
5	F	150/174 (86%)	143 (95%)	7 (5%)	0	100	100
5	G	149/174 (86%)	141 (95%)	8 (5%)	0	100	100
6	H	103/1019 (10%)	98 (95%)	5 (5%)	0	100	100
6	J	103/1019 (10%)	99 (96%)	3 (3%)	1 (1%)	13	49
7	L	210/234 (90%)	199 (95%)	11 (5%)	0	100	100
7	O	210/234 (90%)	193 (92%)	17 (8%)	0	100	100
8	M	234/263 (89%)	216 (92%)	16 (7%)	2 (1%)	14	51
8	N	234/263 (89%)	220 (94%)	14 (6%)	0	100	100
9	P	532/587 (91%)	493 (93%)	38 (7%)	1 (0%)	44	78
9	Q	532/587 (91%)	502 (94%)	29 (6%)	1 (0%)	44	78
9	T	530/587 (90%)	502 (95%)	28 (5%)	0	100	100
9	U	530/587 (90%)	499 (94%)	29 (6%)	2 (0%)	30	68
9	X	525/587 (89%)	488 (93%)	34 (6%)	3 (1%)	22	60
9	Y	525/587 (89%)	492 (94%)	33 (6%)	0	100	100
10	R	137/142 (96%)	127 (93%)	9 (7%)	1 (1%)	19	56
10	S	137/142 (96%)	126 (92%)	11 (8%)	0	100	100
10	V	137/142 (96%)	130 (95%)	6 (4%)	1 (1%)	19	56
10	W	137/142 (96%)	132 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	Z	137/142 (96%)	132 (96%)	5 (4%)	0	100	100
10	a	137/142 (96%)	132 (96%)	5 (4%)	0	100	100
All	All	7806/11097 (70%)	7343 (94%)	451 (6%)	12 (0%)	45	78

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	X	260	ALA
8	M	6	GLY
9	U	242	LYS
9	Q	178	ALA
9	X	249	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	136/271 (50%)	135 (99%)	1 (1%)	81	87
2	B	279/758 (37%)	278 (100%)	1 (0%)	89	90
3	C	311/311 (100%)	310 (100%)	1 (0%)	91	91
3	D	311/311 (100%)	306 (98%)	5 (2%)	58	74
3	I	310/311 (100%)	309 (100%)	1 (0%)	91	91
3	K	310/311 (100%)	310 (100%)	0	100	100
4	E	523/695 (75%)	520 (99%)	3 (1%)	84	88
5	F	144/164 (88%)	142 (99%)	2 (1%)	62	75
5	G	143/164 (87%)	141 (99%)	2 (1%)	62	75
6	H	95/928 (10%)	93 (98%)	2 (2%)	48	67
6	J	95/928 (10%)	93 (98%)	2 (2%)	48	67
7	L	190/209 (91%)	187 (98%)	3 (2%)	58	74
7	O	190/209 (91%)	186 (98%)	4 (2%)	48	67
8	M	205/228 (90%)	205 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	N	205/228 (90%)	201 (98%)	4 (2%)	50	68
9	P	458/495 (92%)	447 (98%)	11 (2%)	44	63
9	Q	458/495 (92%)	449 (98%)	9 (2%)	50	68
9	T	456/495 (92%)	450 (99%)	6 (1%)	65	77
9	U	456/495 (92%)	447 (98%)	9 (2%)	50	68
9	X	452/495 (91%)	439 (97%)	13 (3%)	37	58
9	Y	452/495 (91%)	447 (99%)	5 (1%)	70	80
10	R	119/122 (98%)	117 (98%)	2 (2%)	56	72
10	S	119/122 (98%)	118 (99%)	1 (1%)	79	84
10	V	119/122 (98%)	114 (96%)	5 (4%)	25	47
10	W	119/122 (98%)	116 (98%)	3 (2%)	42	62
10	Z	119/122 (98%)	115 (97%)	4 (3%)	32	53
10	a	119/122 (98%)	116 (98%)	3 (2%)	42	62
All	All	6893/9728 (71%)	6791 (98%)	102 (2%)	60	75

5 of 102 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	T	339	SER
10	V	57	TYR
10	a	71	GLU
9	T	450	ASP
9	U	464	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
9	P	118	ASN
10	V	108	HIS
9	U	442	GLN
3	I	263	ASN
8	N	93	GLN

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](#)

There are no chain breaks in this entry.

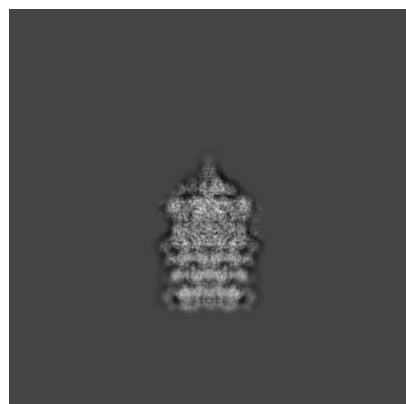
6 Map visualisation [i](#)

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.

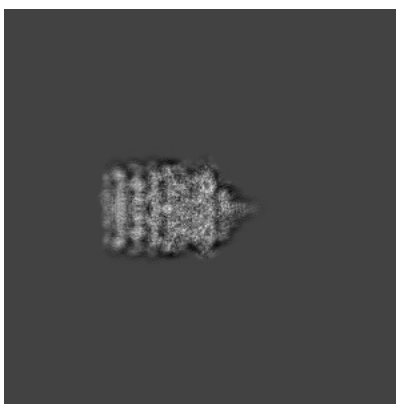
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

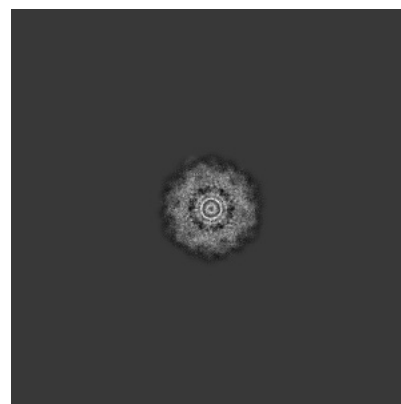
6.1.1 Primary map



X



Y

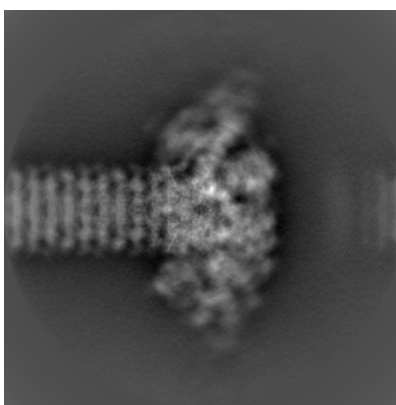


Z

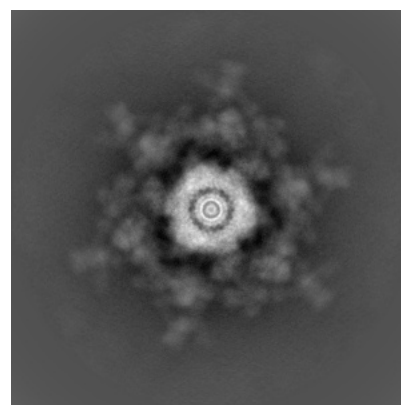
6.1.2 Raw map



X



Y

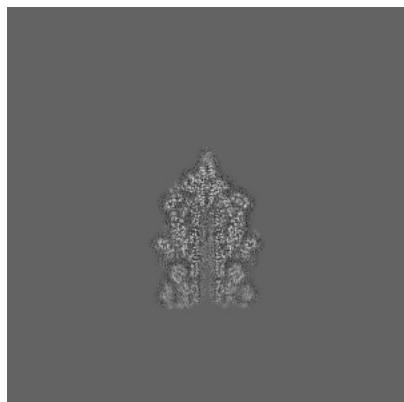


Z

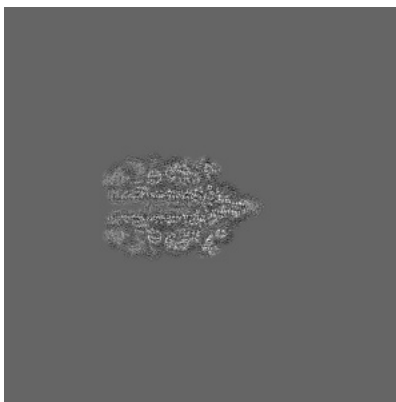
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

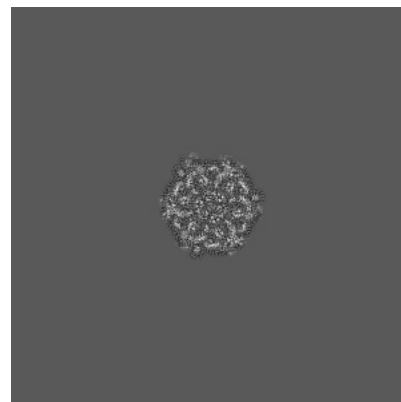
6.2.1 Primary map



X Index: 420

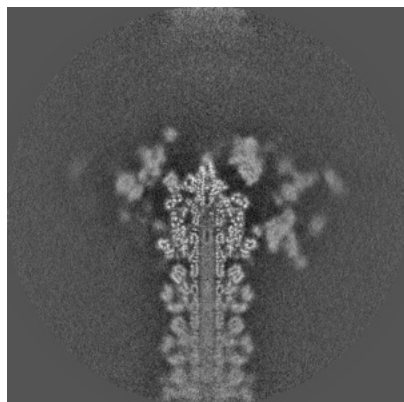


Y Index: 420

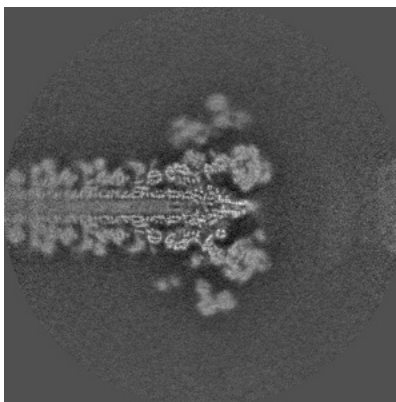


Z Index: 420

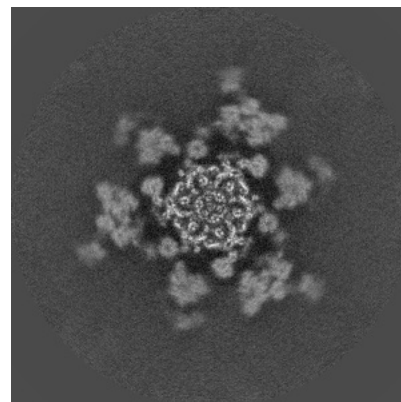
6.2.2 Raw map



X Index: 420



Y Index: 420

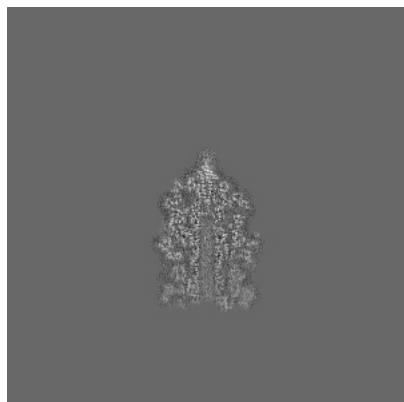


Z Index: 420

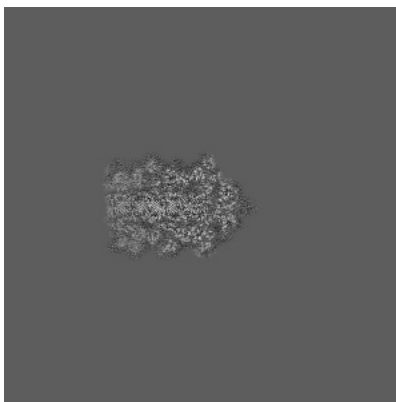
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

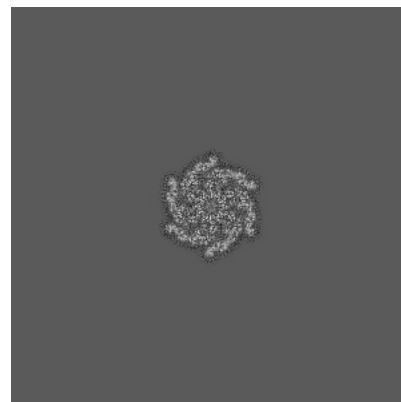
6.3.1 Primary map



X Index: 427



Y Index: 440

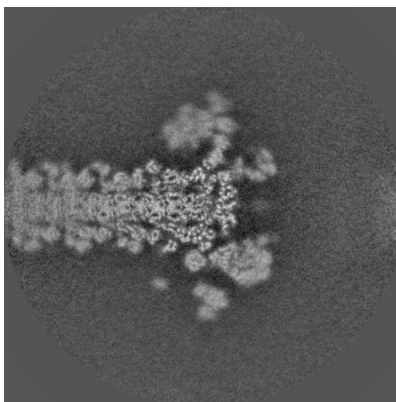


Z Index: 346

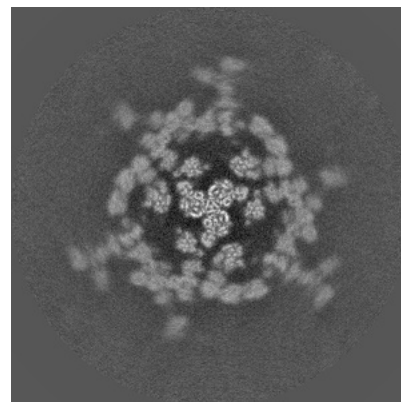
6.3.2 Raw map



X Index: 450



Y Index: 440

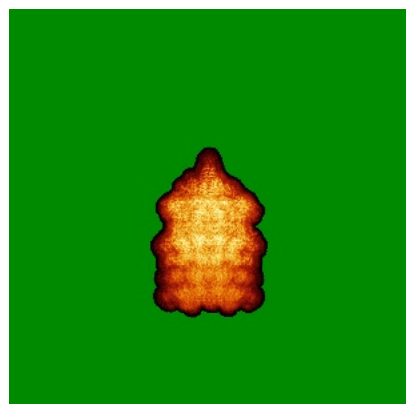


Z Index: 461

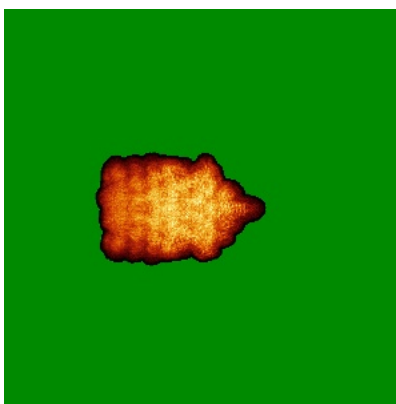
The images above show the largest variance slices of the map in three orthogonal directions.

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

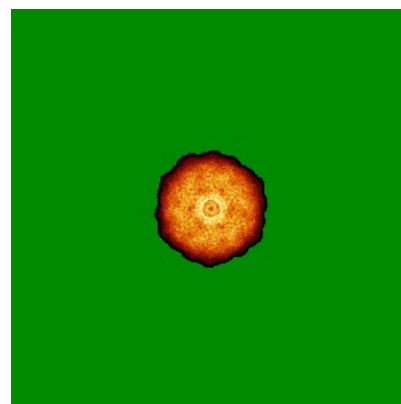
6.4.1 Primary map



X

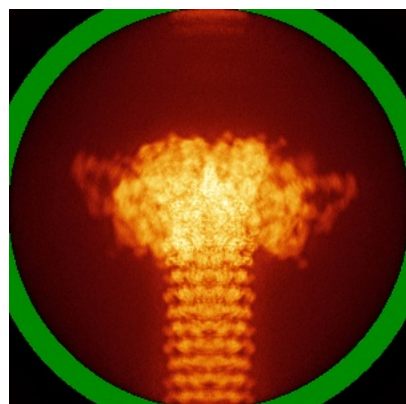


Y

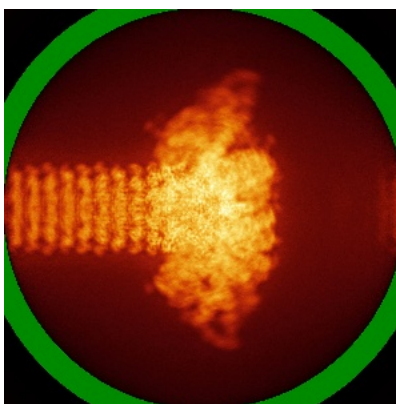


Z

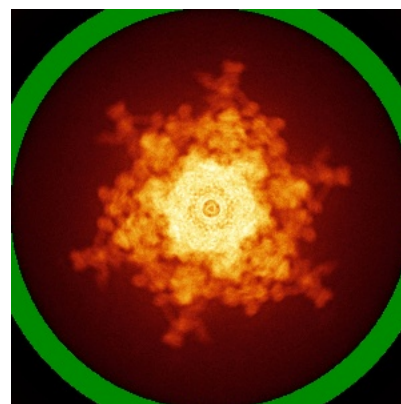
6.4.2 Raw map



X



Y

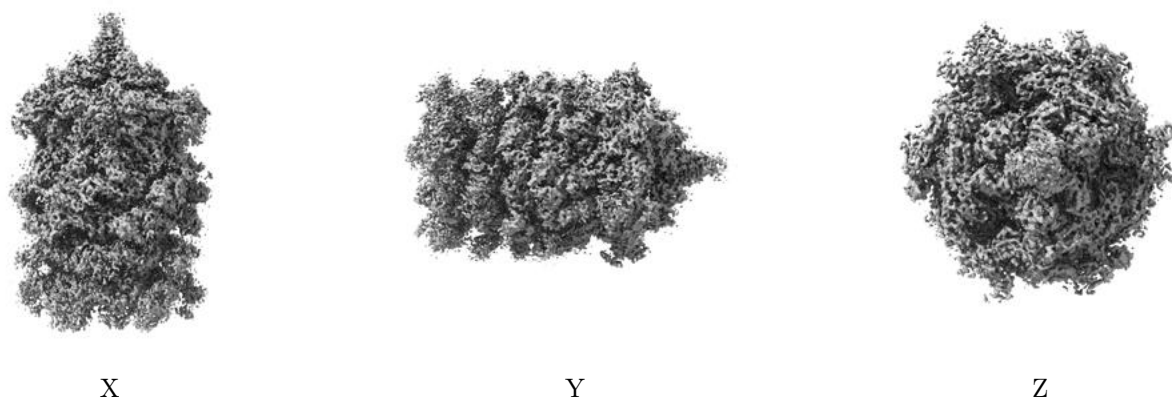


Z

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.

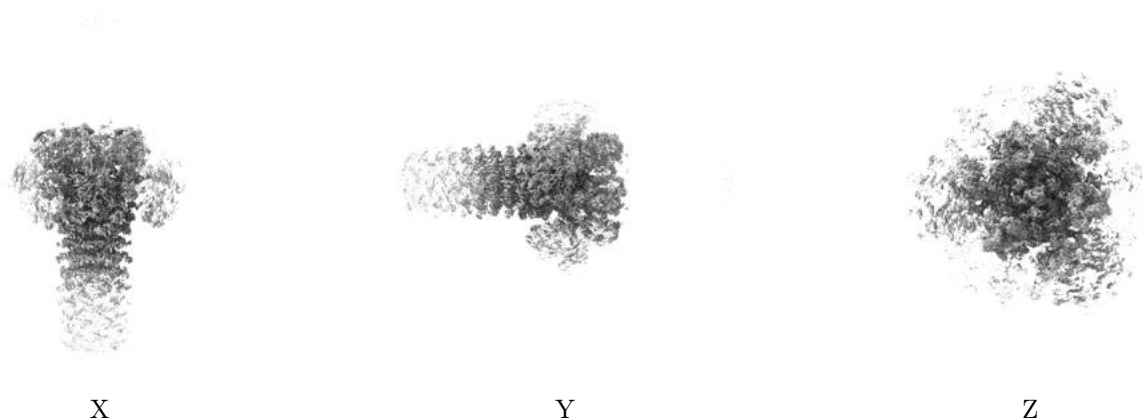
6.5 Orthogonal surface views [i](#)

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.

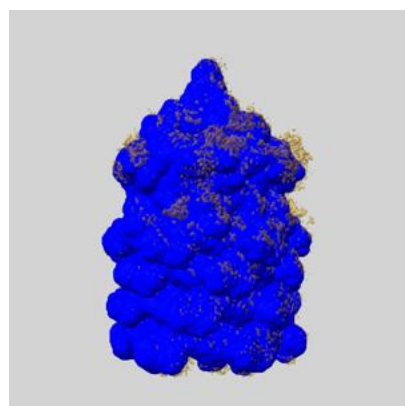
6.6 Mask visualisation [i](#)

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

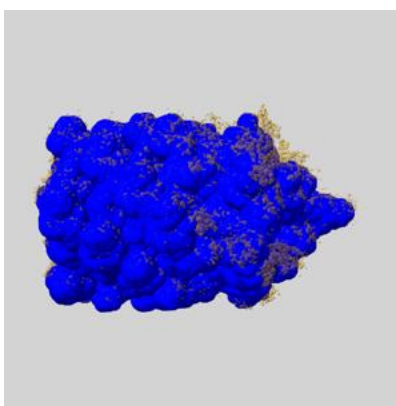
A mask typically either:

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

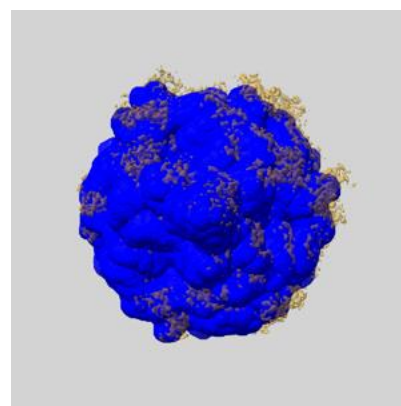
6.6.1 emd_19969_msk_1.map [i](#)



X



Y

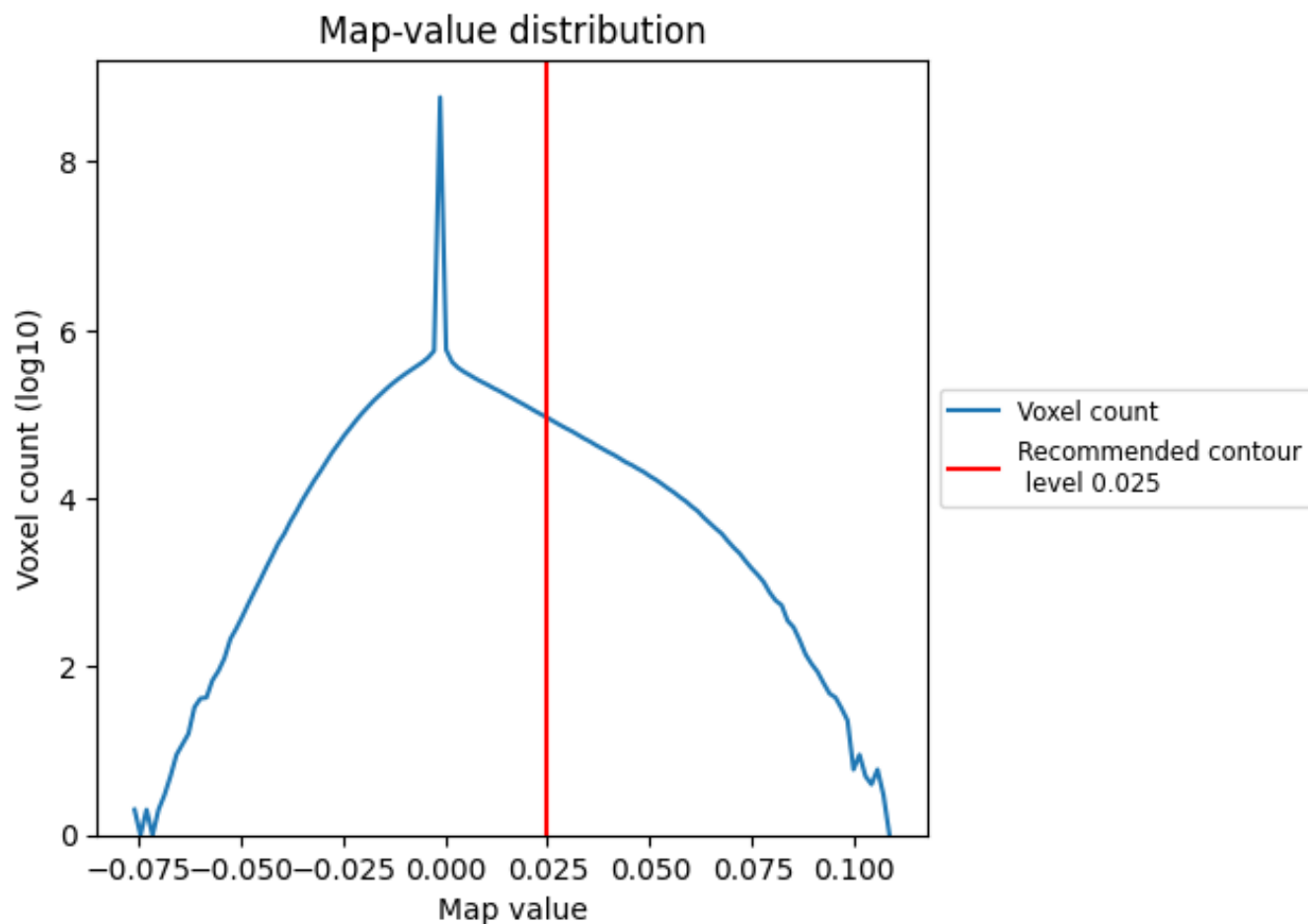


Z

7 Map analysis [i](#)

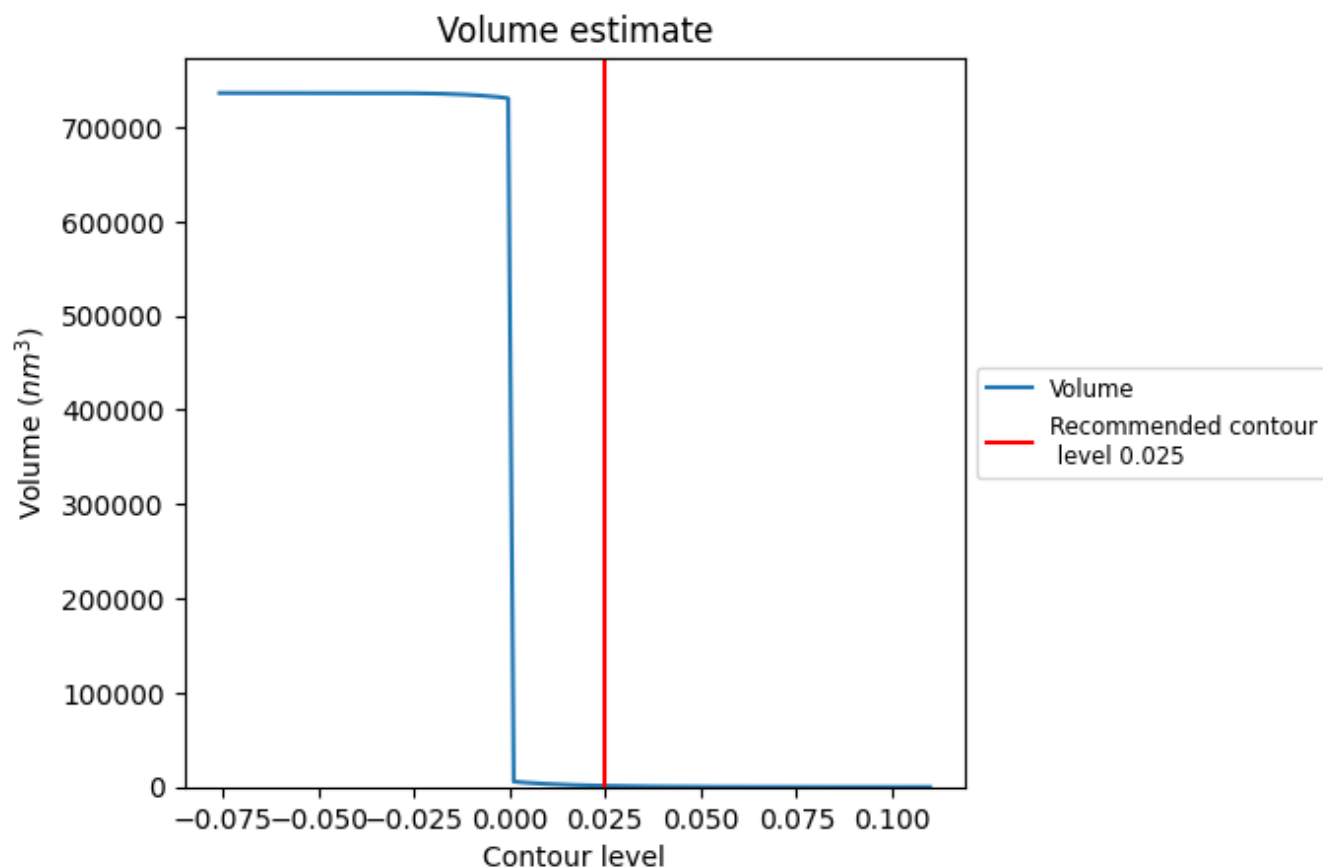
This section contains the results of statistical analysis of the map.

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.

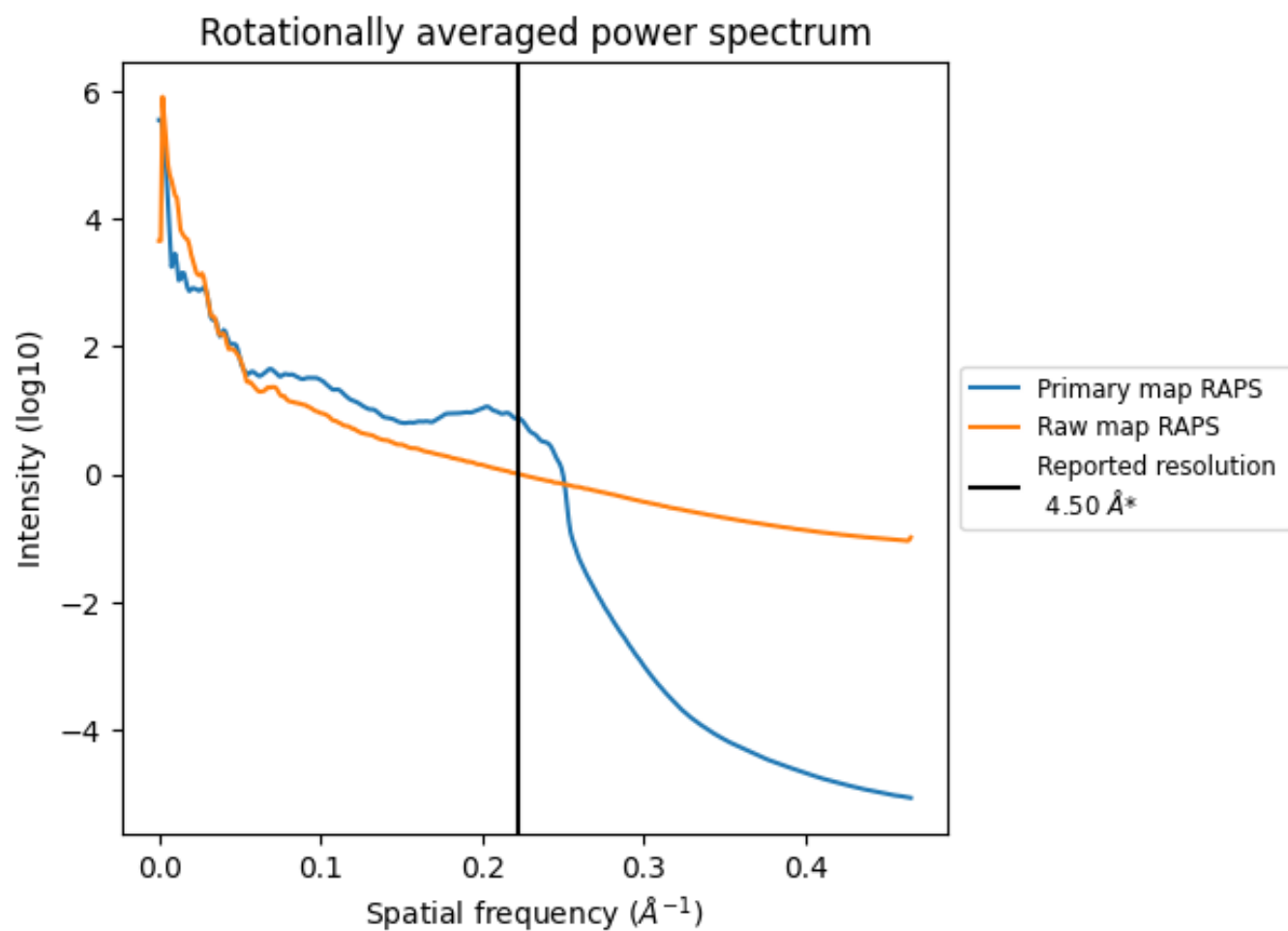
7.2 Volume estimate [i](#)



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 ⓘ

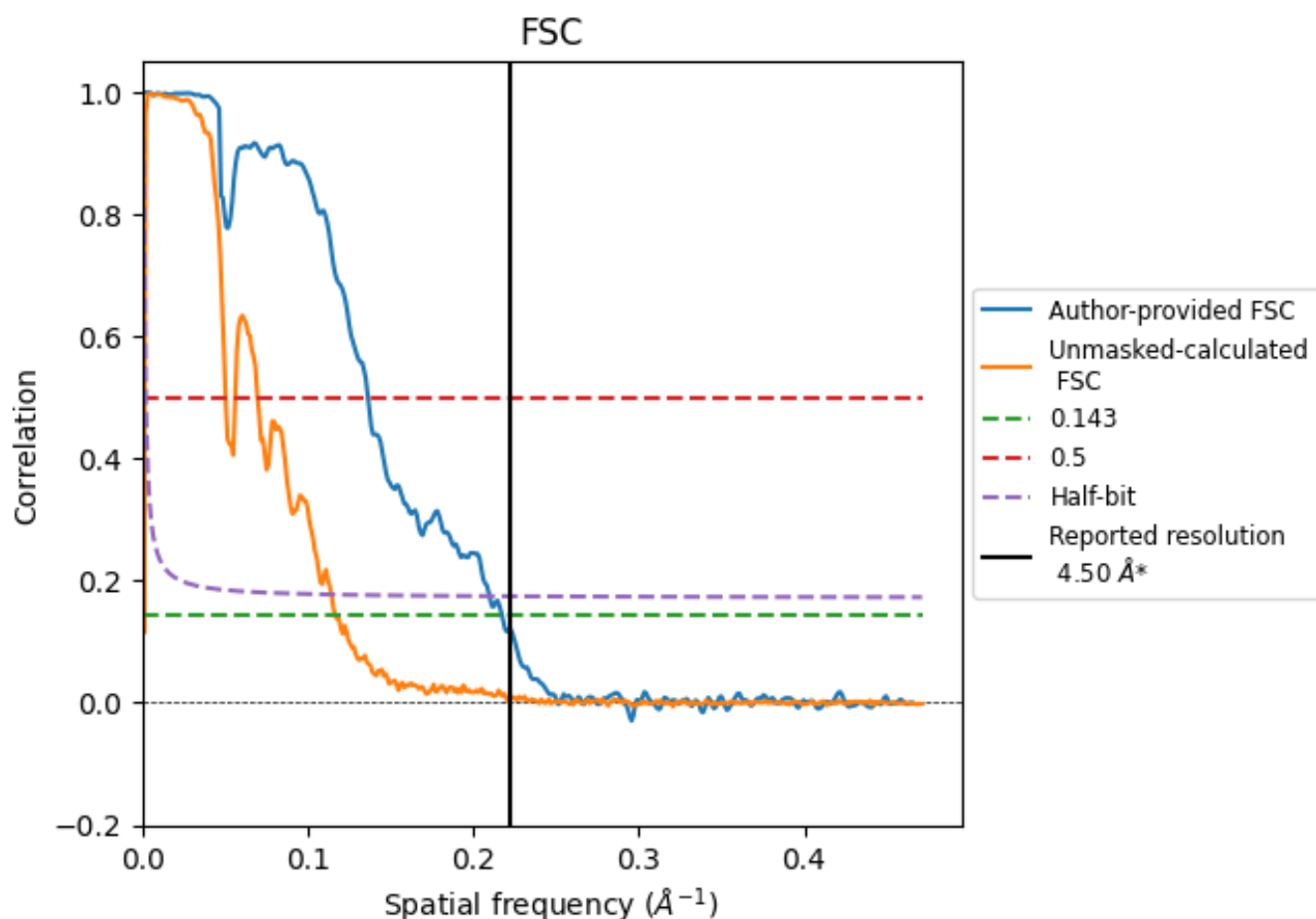


*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

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 Å⁻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

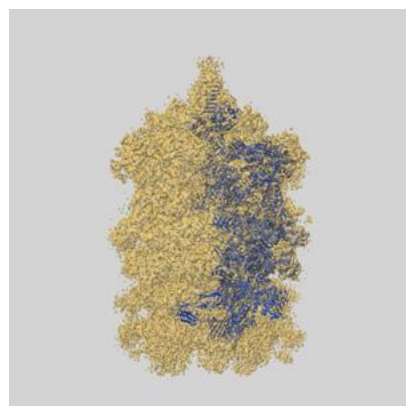
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 833.33 differs from the reported value 4.5 by more than 10 %

9 Map-model fit [i](#)

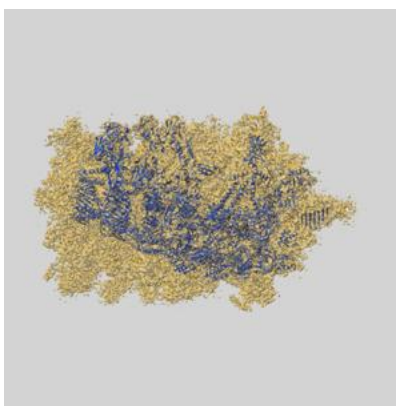
This section contains information regarding the fit between EMDB map EMD-19969 and PDB model 9EUG. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlays

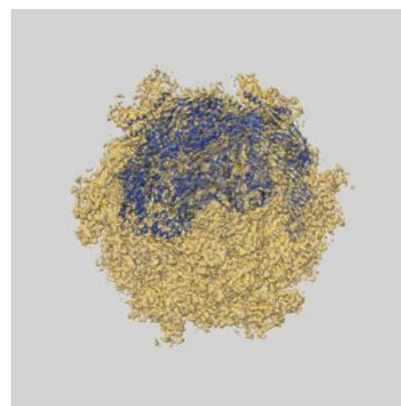
9.1.1 Map-model overlay [i](#)



X

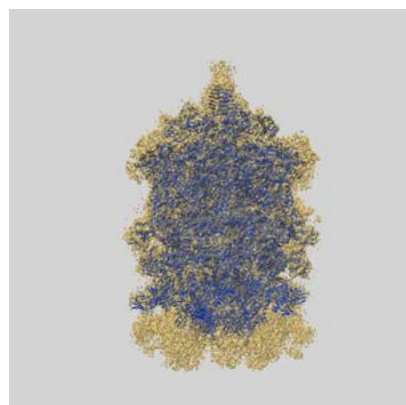


Y

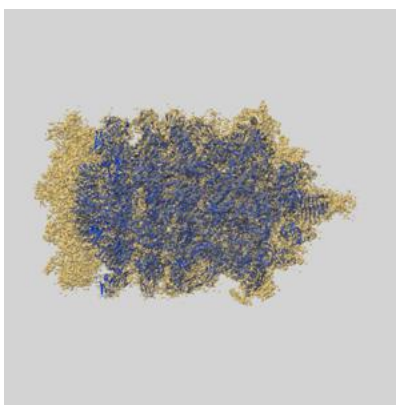


Z

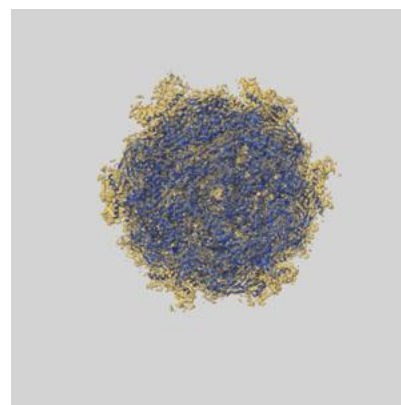
9.1.2 Map-model assembly overlay [i](#)



X



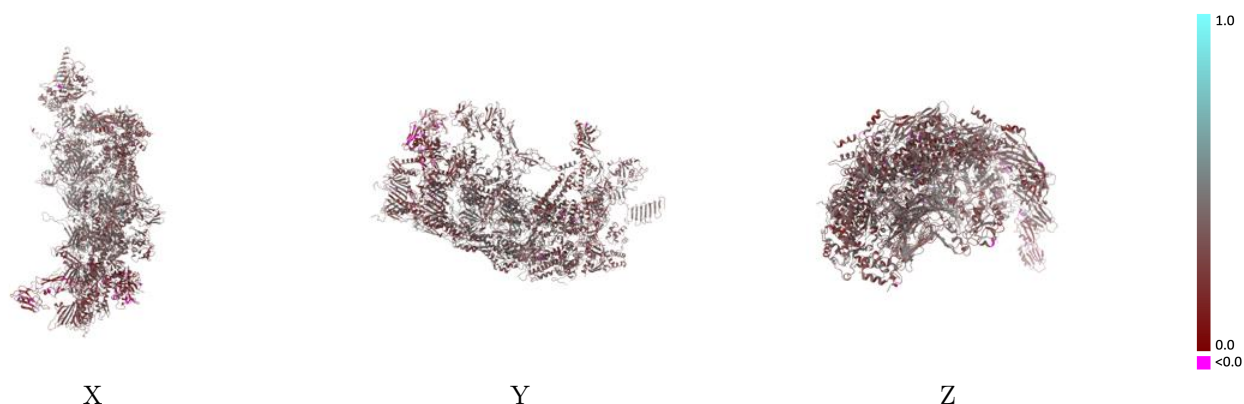
Y



Z

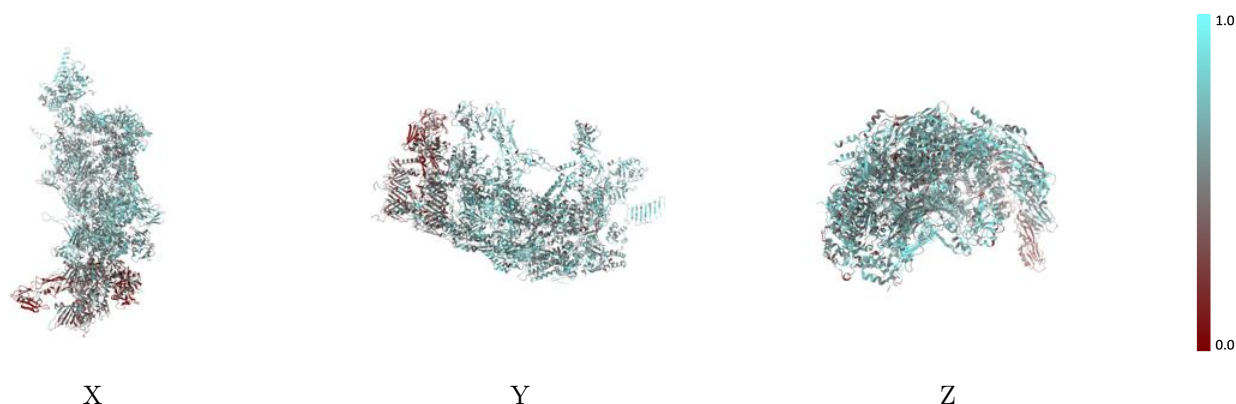
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



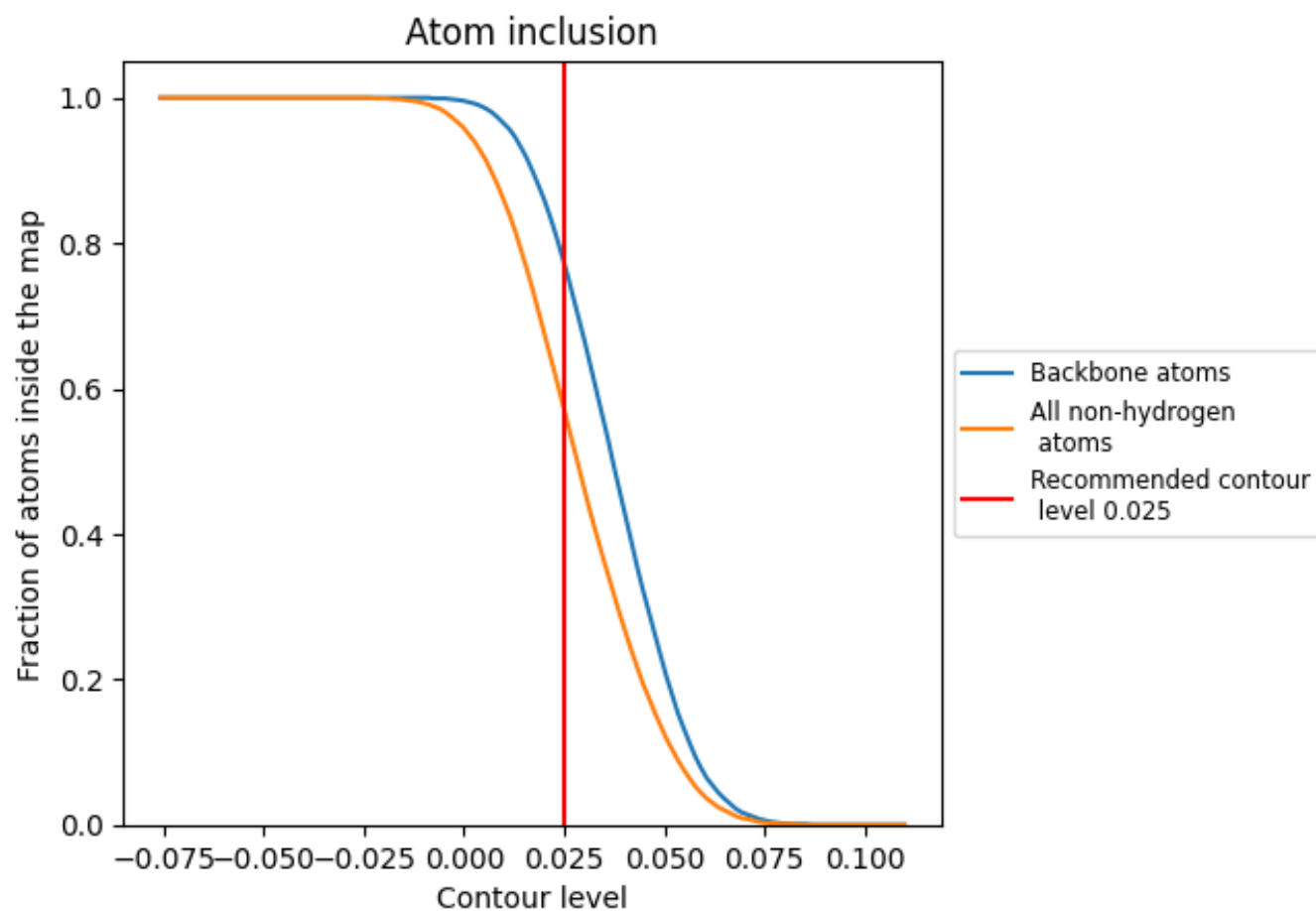
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

