



wwPDB EM Validation Summary Report ⓘ

Apr 7, 2025 – 02:37 PM EDT

PDB ID : 9CUY / pdb_00009cuy
EMDB ID : EMD-45953
Title : Bacteriophage PhiTE extended baseplate
Authors : Hodgkinson-Bean, J.; Ayala, R.
Deposited on : 2024-07-26
Resolution : 3.24 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:

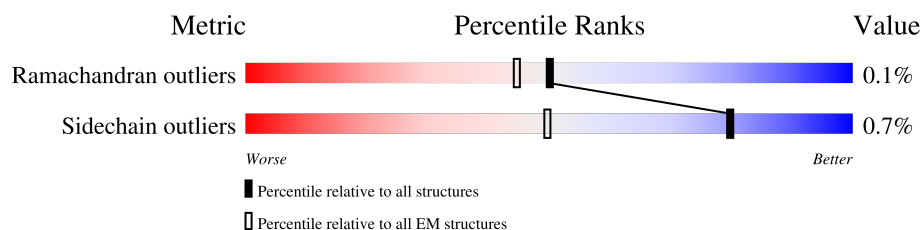
EMDB validation analysis : 0.0.1.dev117
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) :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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY


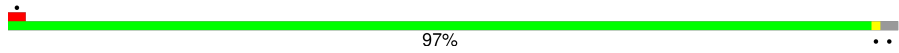
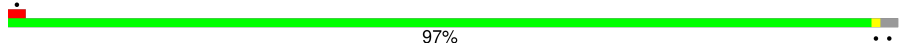
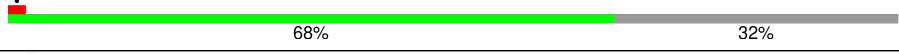
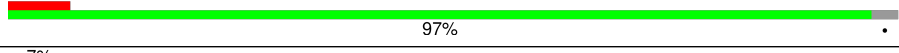
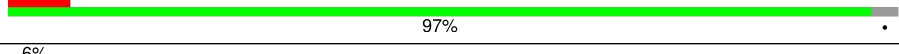
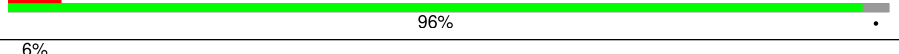
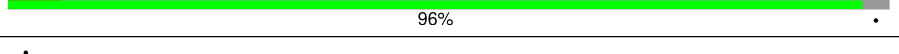
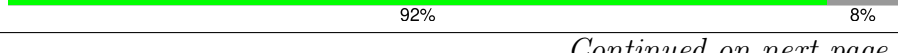
The reported resolution of this entry is 3.24 Å.

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.




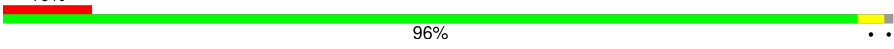
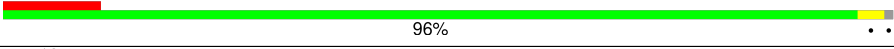
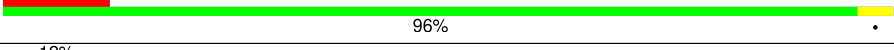
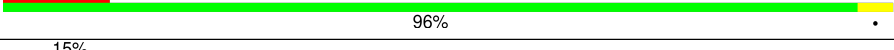

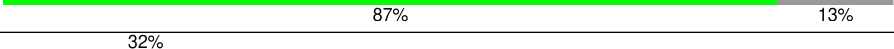
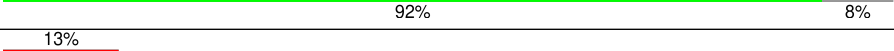
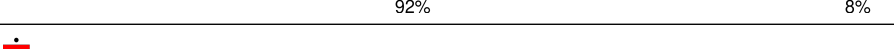
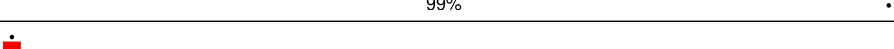
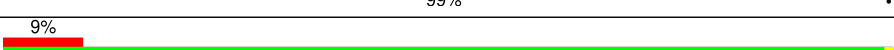
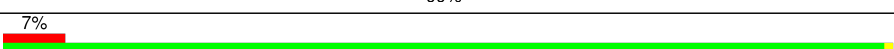
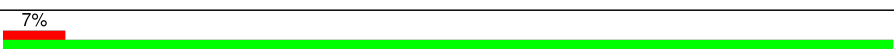
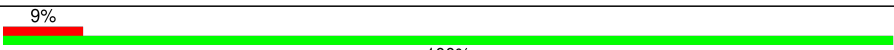











Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$. 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	R	494	
1	S	494	
1	T	494	
1	U	494	
2	A	473	
2	B	473	
2	C	473	
2	D	473	
2	E	473	



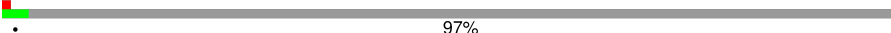
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Mol	Chain	Length	Quality of chain
2	F	473	
3	G	156	
3	H	156	
3	I	156	
3	J	156	
4	K	284	
4	L	284	
5	X	330	
6	Y	247	
7	O	165	
7	P	165	
8	M	112	
8	N	112	
9	m	163	
9	n	163	
10	g	793	
10	h	793	
10	i	793	
10	j	793	
10	k	793	
10	l	793	
11	a	554	
11	b	554	
11	c	554	
11	d	554	

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Mol	Chain	Length	Quality of chain
11	e	554	 16%84%
11	f	554	 16%84%
12	W	811	 97%

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 63911 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 Wedge 2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	T	484	Total	C	N	O	S	0	0
			3703	2322	620	749	12		
1	S	484	Total	C	N	O	S	0	0
			3703	2322	620	749	12		
1	R	336	Total	C	N	O	S	0	0
			2596	1630	442	517	7		
1	U	336	Total	C	N	O	S	0	0
			2596	1630	442	517	7		

- Molecule 2 is a protein called Tail sheath protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	461	Total	C	N	O	S	0	0
			3434	2163	587	670	14		
2	C	457	Total	C	N	O	S	0	0
			3397	2138	582	663	14		
2	E	435	Total	C	N	O	S	0	0
			3254	2056	556	629	13		
2	B	461	Total	C	N	O	S	0	0
			3434	2163	587	670	14		
2	D	457	Total	C	N	O	S	0	0
			3397	2138	582	663	14		
2	F	435	Total	C	N	O	S	0	0
			3254	2056	556	629	13		

- Molecule 3 is a protein called Tail tube protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	156	Total	C	N	O	S	0	0
			1180	744	204	230	2		
3	H	154	Total	C	N	O	S	0	0
			1171	739	202	228	2		
3	I	156	Total	C	N	O	S	0	0
			1180	744	204	230	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	154	Total	C	N	O	S	0	0
			1171	739	202	228	2		

- Molecule 4 is a protein called Tube initiator protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	249	Total	C	N	O	S	0	0
			1959	1197	355	404	3		
4	L	248	Total	C	N	O	S	0	0
			1950	1191	353	403	3		

- Molecule 5 is a protein called Hub protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	X	305	Total	C	N	O	S	0	0
			2376	1497	401	471	7		

- Molecule 6 is a protein called Putative baseplate assembly protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Y	228	Total	C	N	O	S	0	0
			1726	1076	300	343	7		

- Molecule 7 is a protein called Wedge 1 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	165	Total	C	N	O	S	0	0
			1285	817	218	247	3		
7	P	165	Total	C	N	O	S	0	0
			1285	817	218	247	3		

- Molecule 8 is a protein called Spacer protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	112	Total	C	N	O	S	0	0
			920	591	153	172	4		
8	M	112	Total	C	N	O	S	0	0
			920	591	153	172	4		

- Molecule 9 is a protein called Sheath initiator protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	n	163	Total	C	N	O	S	0	0
			1329	860	217	248	4		
9	m	163	Total	C	N	O	S	0	0
			1329	860	217	248	4		

- Molecule 10 is a protein called Putative tail fiber protein.

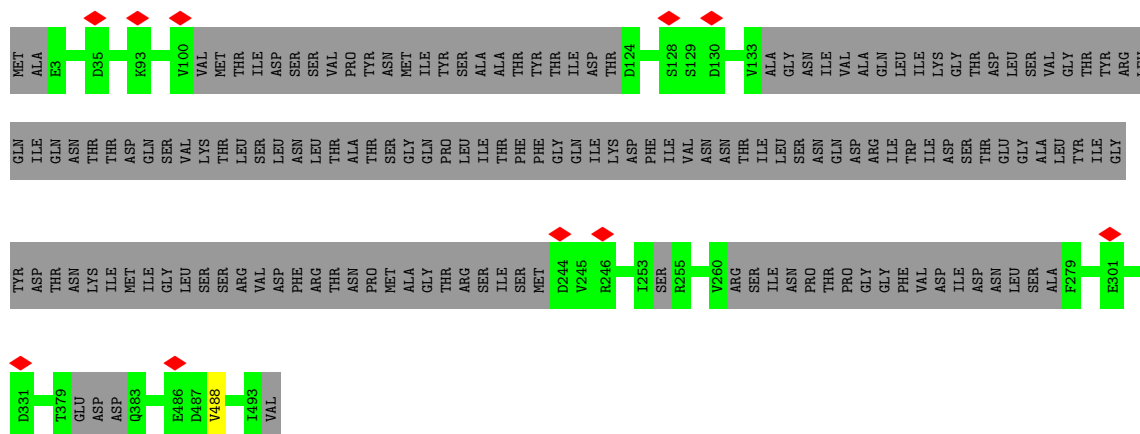
Mol	Chain	Residues	Atoms					AltConf	Trace
10	g	135	Total	C	N	O	S	0	0
			1057	678	174	204	1		
10	i	153	Total	C	N	O	S	0	0
			1184	748	199	235	2		
10	h	153	Total	C	N	O	S	0	0
			1188	751	199	236	2		
10	j	135	Total	C	N	O	S	0	0
			1057	678	174	204	1		
10	k	153	Total	C	N	O	S	0	0
			1184	748	199	235	2		
10	l	153	Total	C	N	O	S	0	0
			1188	751	199	236	2		

- Molecule 11 is a protein called Short tail fiber.

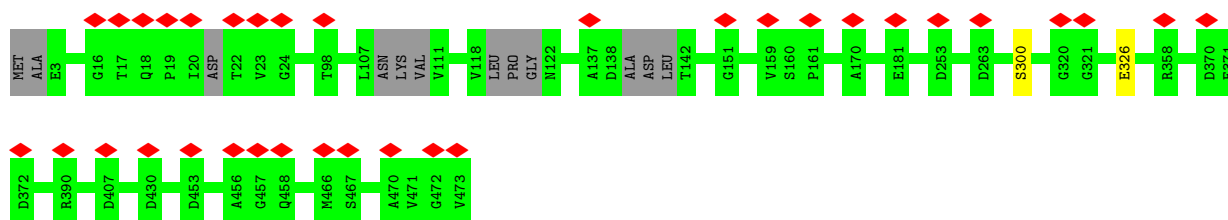
Mol	Chain	Residues	Atoms					AltConf	Trace
11	c	90	Total	C	N	O	S	0	0
			716	460	121	134	1		
11	a	90	Total	C	N	O	S	0	0
			716	460	121	134	1		
11	b	90	Total	C	N	O	S	0	0
			716	460	121	134	1		
11	f	90	Total	C	N	O	S	0	0
			716	460	121	134	1		
11	d	90	Total	C	N	O	S	0	0
			716	460	121	134	1		
11	e	90	Total	C	N	O	S	0	0
			716	460	121	134	1		

- Molecule 12 is a protein called Putative tape measure protein.

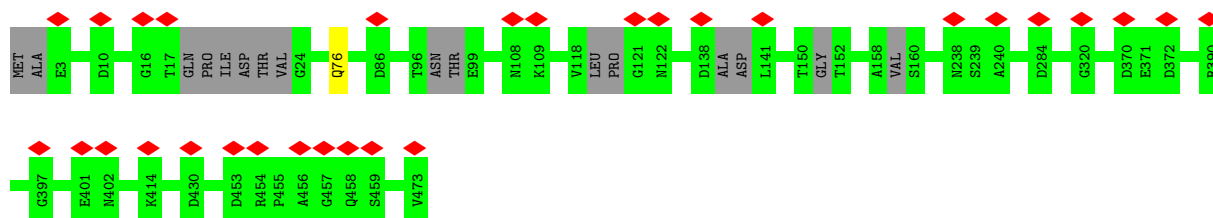
Mol	Chain	Residues	Atoms					AltConf	Trace
12	W	26	Total	C	N	O	S	0	0
			208	128	40	38	2		



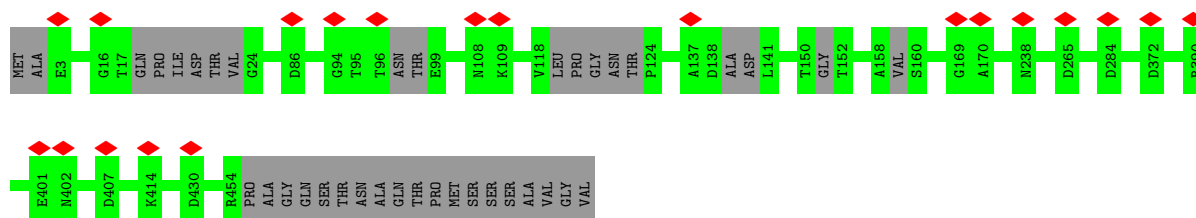
• Molecule 2: Tail sheath protein



• Molecule 2: Tail sheath protein

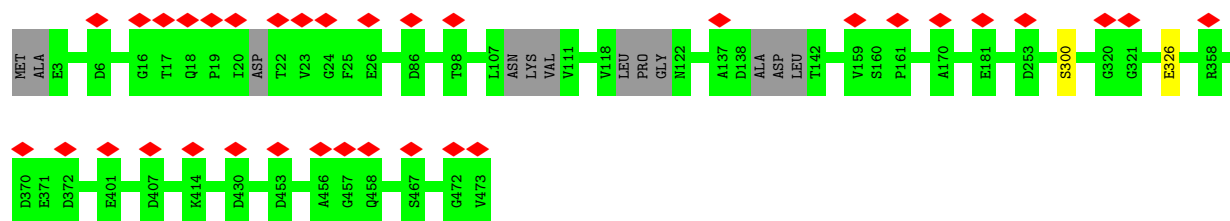


• Molecule 2: Tail sheath protein

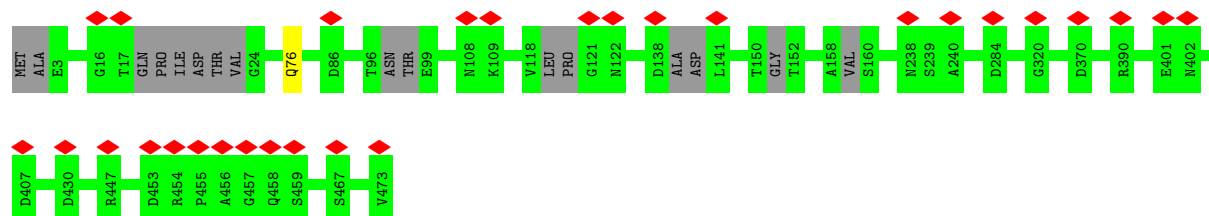


• Molecule 2: Tail sheath protein

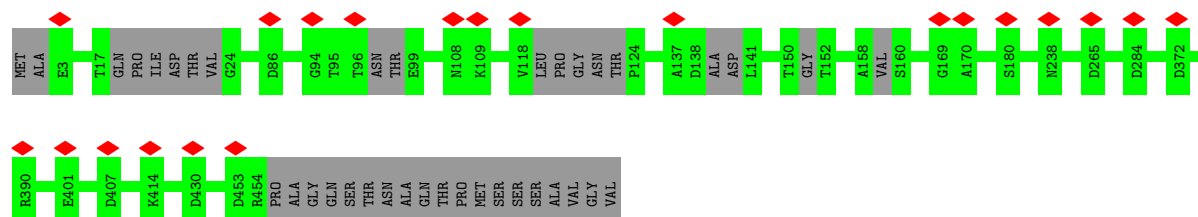
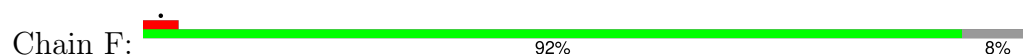




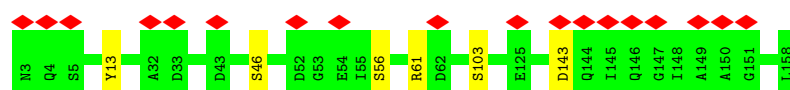
- Molecule 2: Tail sheath protein



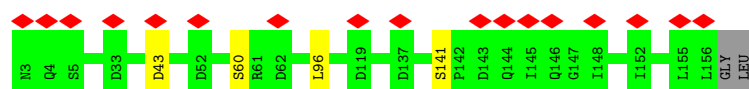
- Molecule 2: Tail sheath protein



- Molecule 3: Tail tube protein

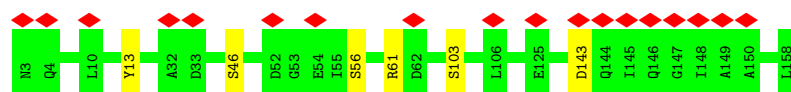


- Molecule 3: Tail tube protein

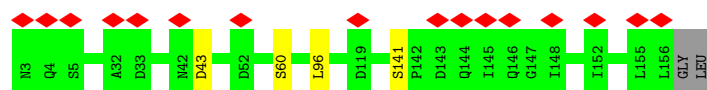


- Molecule 3: Tail tube protein

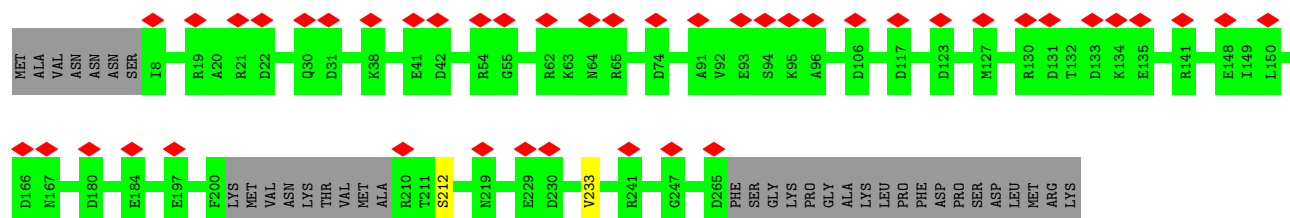
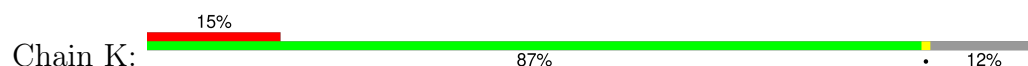




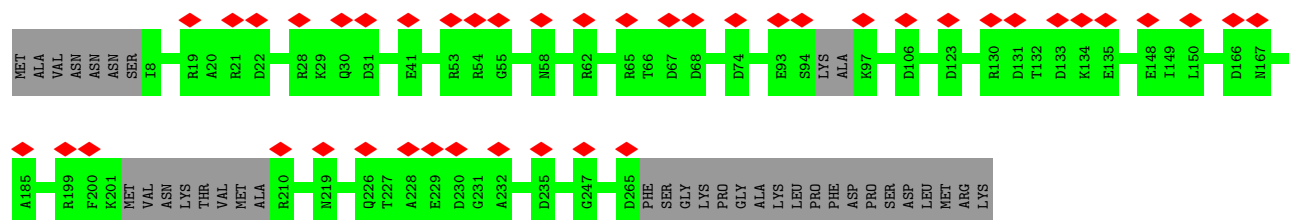
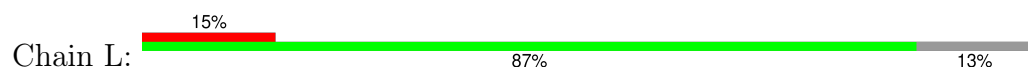
- Molecule 3: Tail tube protein



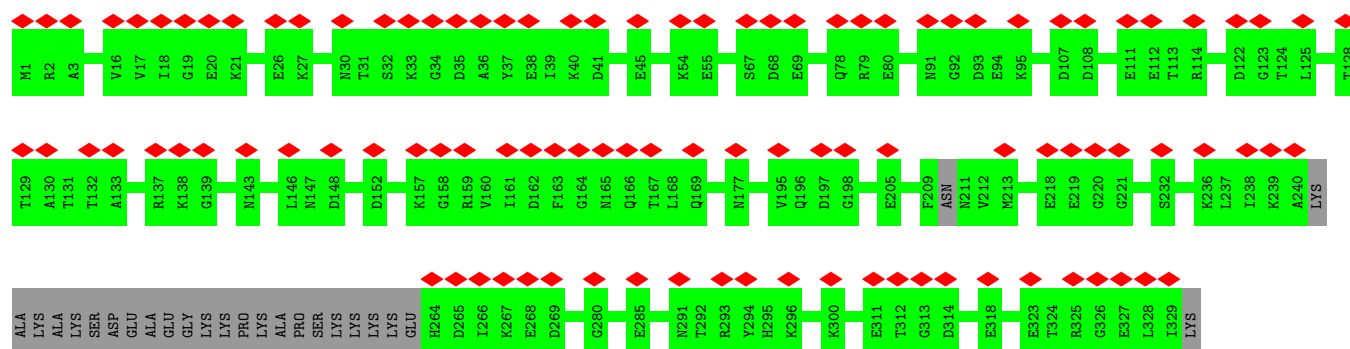
- Molecule 4: Tube initiator protein



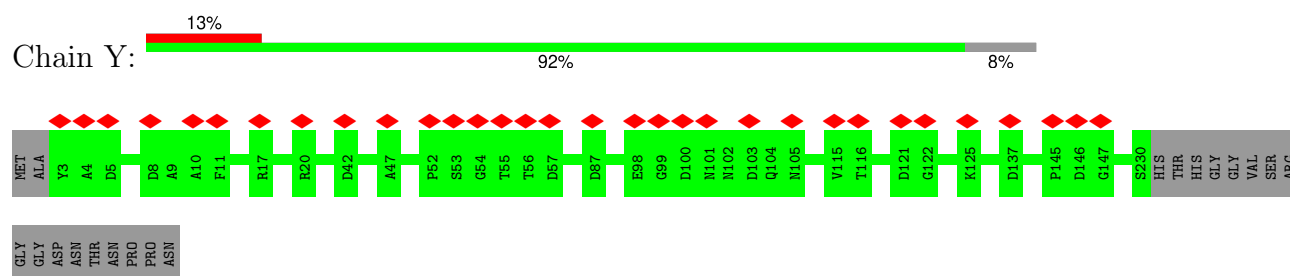
- Molecule 4: Tube initiator protein



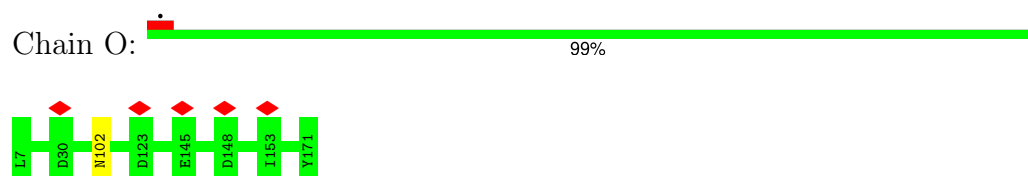
- Molecule 5: Hub protein



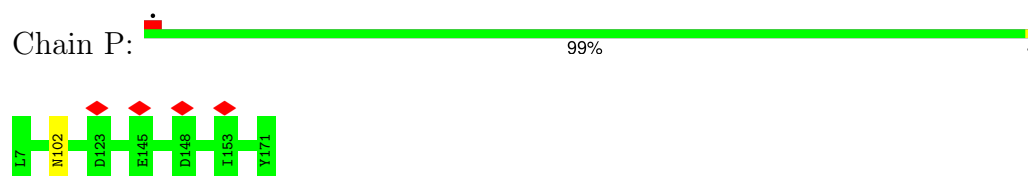
- Molecule 6: Putative baseplate assembly protein



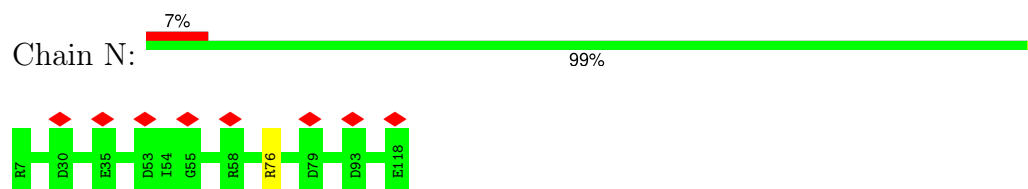
- Molecule 7: Wedge 1 protein



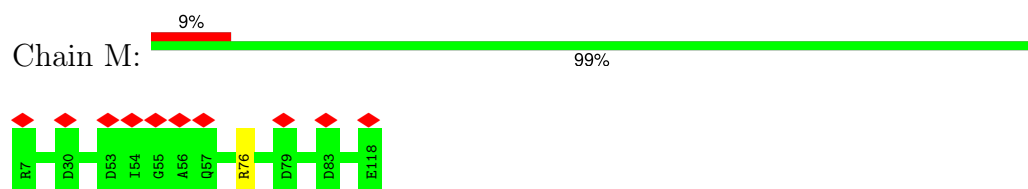
- Molecule 7: Wedge 1 protein



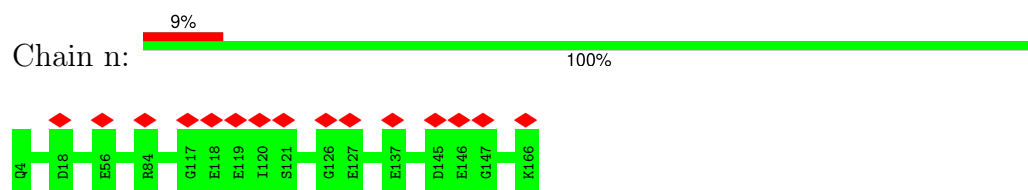
- Molecule 8: Spacer protein



- Molecule 8: Spacer protein

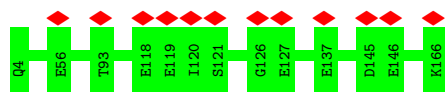


- Molecule 9: Sheath initiator protein



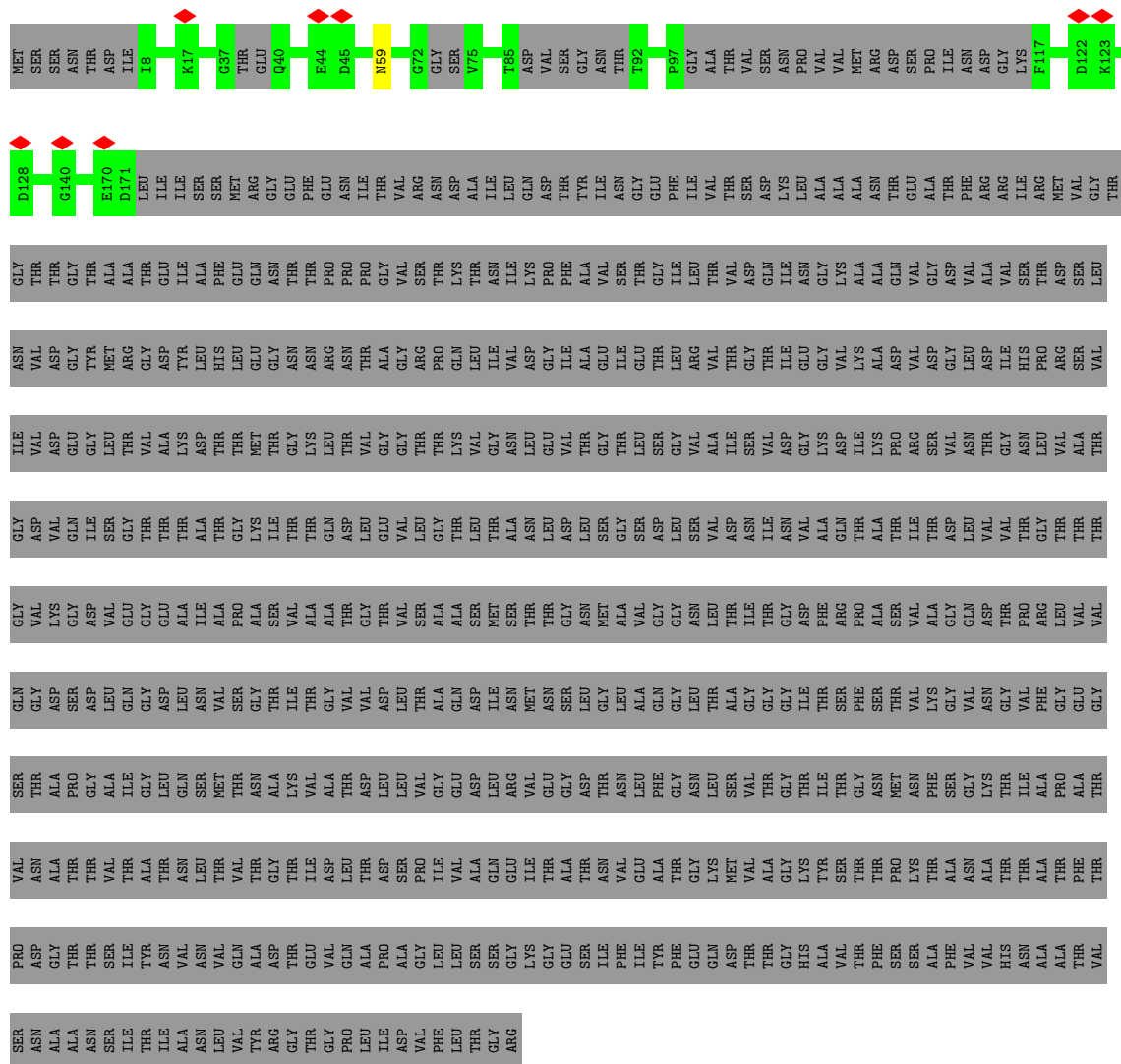
- Molecule 9: Sheath initiator protein





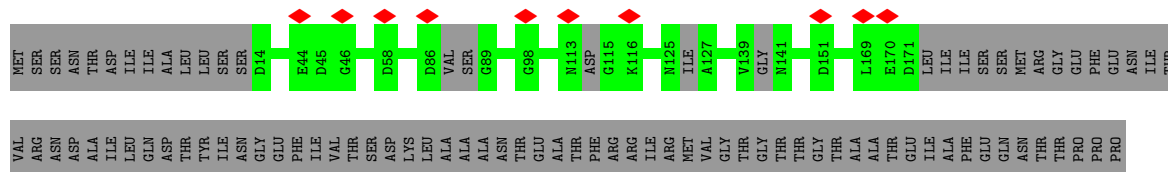
• Molecule 10: Putative tail fiber protein

Chain g: 17% 83%



• Molecule 10: Putative tail fiber protein

Chain i: 19% 81%

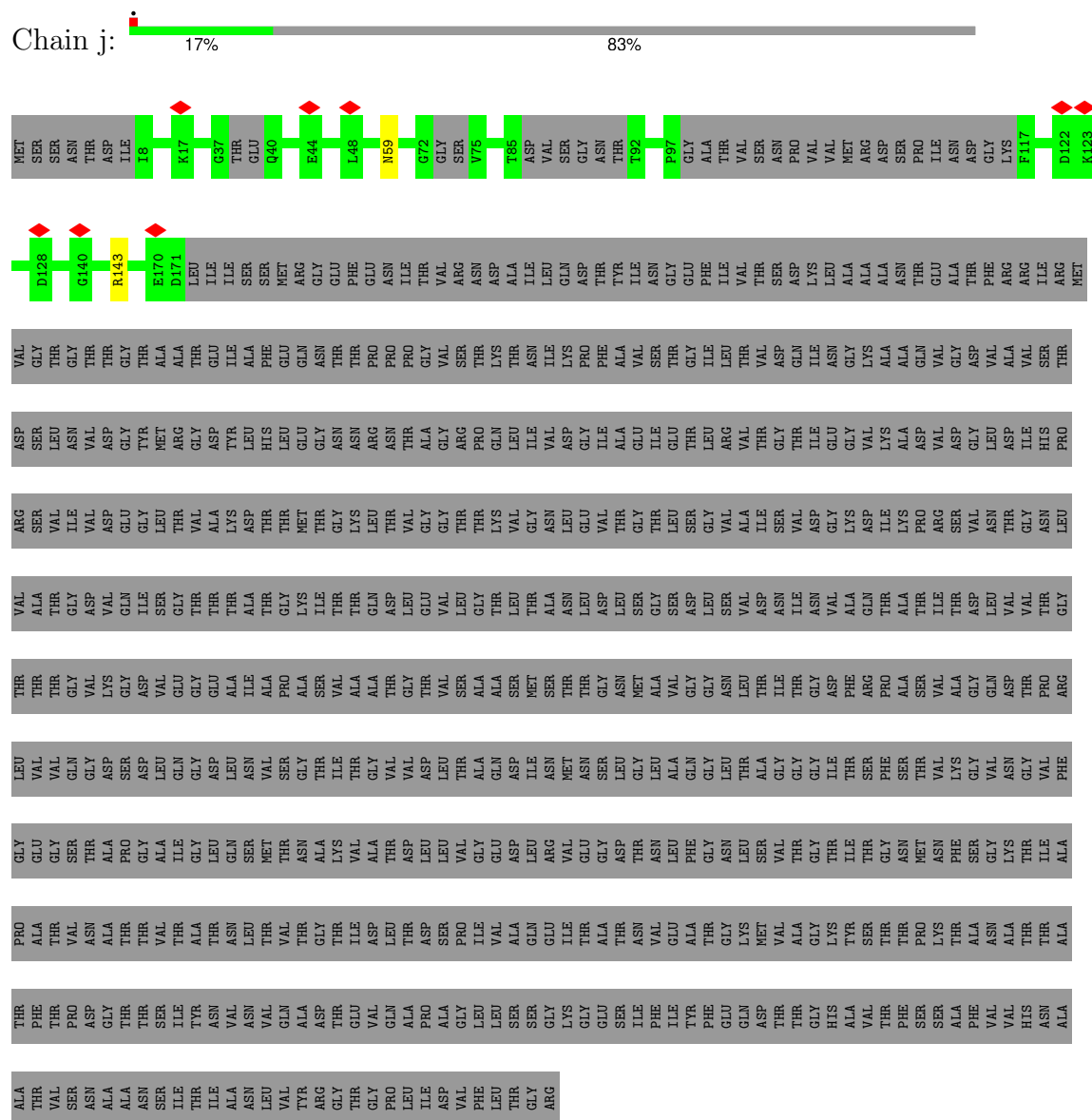


- Molecule 10: Putative tail fiber protein

[illegible]

[illegible]

- Molecule 10: Putative tail fiber protein



- Molecule 10: Putative tail fiber protein







[illegible]

- Molecule 11: Short tail fiber

Chain b: 16% 84%

[illegible]

- Molecule 11: Short tail fiber

Chain f:  16% 84%

[illegible]

[illegible]

- Molecule 11: Short tail fiber

Chain d:  16% 84%

VAL	ILE	PRO	LEU	GLY	GLN	
ASN	SER	ASP	THR	LEU	VAL	MET
ASP	THR	THR	SER	PHE	ASN	ALA
ALA	MET	ILE	GLY	LEU	ARG	K3
GLY	MET	THR	ASP	ARG	GLY	K5
TYR	ASN	ASN	ASP	GLY	ILE	
VAL	VAL	ARG	GLY	TRP	ASP	
ILE	VAL	ILE	THR	ALA	ASP	D15
GLY	ILE	GLY	ARG	HIS	LEU	R23
ALA	ARG	TYR	SER	GLY	GLU	
SER	VAL	ALA	ASN	SER	PRO	
ALA	THR	VAL	GLU	ASP	ARG	V92
GLY	SER	LYS	VAL	ALA	LEU	
SER	TYR	ALA	ARG	ASN	VAL	ARG
ALA	SER	THR	LYS	ASP	GLN	ARG
THR	VAL	ALA	TYR	PRO	ILE	ASP
ILE	LEU	SER	SER	ASP	GLY	ILE
THR	THR	VAL	PHE	ALA	ALA	ALA
SER	SER	LEU	ASP	GLY	VAL	GLN
VAL	ILE	PRO	ALA	ARG	ILE	LEU
ARG	ILE	PRO	ALA	ALA	ARG	ARG
THR	THR	ILE	GLU	GLY	TRP	GLN
THR	ILE	SER	ARG	LEU	TRP	GLN
GLY	ASP	ILE	VAL	SER	PRO	ASP
GLY	PRO	GLY	PRO	VAL	GLY	VAL
VAL	GLN	GLN	VAL	GLN	ALA	ALA
SER	GLY	ILE	ALA	GLY	THR	ASP
SER	ILE	PRO	GLU	ASP	VAL	ASP
THR	THR	ILE	ASN	ILE	GLY	ALA
ARG	VAL	SER	ASN	ILE	GLY	ASP
ALA	THR	THR	ARG	ARG	TRP	VAL
VAL	GLU	GLU	VAL	PHE	GLN	GLU
GLN	VAL	VAL	VAL	PRO	VAL	LEU
THR	THR	ALA	TYR	ALA	PHE	LYS
LYS	LYS	THR	ILE	ASP	ASN	GLN
PRO	SER	VAL	ILE	ILE	THR	GLY
SER	PRO	ASP	LYS	GLY	GLY	ILE
SER	SER	GLY	THR	ASN	GLN	GLN
ALA	ALA	GLY	GLN	SER	VAL	GLY
ASN	ASN	ALA	ALA	PHE	LYS	ARG
VAL	GLU	ILE	GLN	ILE	ASN	ASN
LEU	PRO	SER	SER	GLY	TYR	ASP
GLY	LEU	LEU	SER	ARG	SER	LEU
THR	ALA	VAL	GLY	TYR	VAL	ASN
GLY	PHE	GLY	GLY	VAL	LEU	LYS
THR	GLY	PRO	ASN	GLY	GLY	LEU
GLY	SER	GLY	SER	GLY	ARG	ARG
TYR	ASN	GLU	PRO	ALA	ASN	GLN
ILE	ASN	THR	THR	PHE	VAL	ASP
PRO	ASN	ILE	ALA	VAL	VAL	PHE
PRO	GLY	ILE	THR	ASP	ASP	ASP
SER	VAL	VAL	VAL	GLY	PRO	ALA
STR	ALA	SER	STR	STR	ARG	ILE

- Molecule 11: Short tail fiber

Chain e:  16% 84%

ARG	ILE	GLY	THR	GLY	TRP	ASP	MET
ILE	GLY	ARG	THR	ARG	ALA	ASP	ALA
TYR	TYR	ASN	ASN	HIS	GLU	ASP	K3
ALA	ALA	ASN	SER	SER	PRO	ARG	V92
VAL	VAL	GLU	ASP	ASP	ASP	ILE	ILE
LYS	VAL	VAL	ALA	ALA	LEU	ARG	ARG
ALA	ALA	ARG	ASN	ASN	VAL	GLN	GLN
THR	THR	LYS	ASP	ASP	PRO	ASP	ASP
ALA	THR	TYR	PRO	PRO	ILE	ILE	ILE
SER	SER	SER	SER	SER	GLY	GLY	GLN
VAL	VAL	PHE	ALA	ALA	ALA	ALA	GLN
LEU	LEU	ASP	ASP	GLY	VAL	VAL	LEU
PRO	PRO	ALA	ALA	ARG	ILE	ILE	ARG
ALA	SER	ALA	SER	ALA	PRO	GLN	GLN
SER	ARG	ARG	ARG	LEU	TRP	ASP	ASP
ILE	ILE	GLU	GLU	GLY	PRO	VAL	VAL
SER	SER	VAL	VAL	SER	GLY	ALA	ALA
GLY	GLY	PRO	VAL	VAL	ALA	ASP	ASP
GLN	GLN	VAL	GLN	THR	THR	LEU	LEU
TYR	TYR	ALA	GLY	GLY	VAL	ARG	ARG
PRO	PRO	ALA	ALA	ASP	PRO	GLY	GLN
ILE	ILE	GLU	GLU	ALA	ASP	TYR	TYR
SER	SER	ASN	ASN	ILE	ILE	GLY	VAL
TRP	TRP	ARG	ARG	ARG	TRP	ASP	ASP
SER	SER	PRO	PRO	ASN	LEU	GLN	GLN
THR	THR	THR	LYS	ILE	GLY	LYS	LYS
GLN	GLN	ASN	ASN	THR	CYS	VAL	VAL
ASN	ASN	ILE	ILE	GLY	SER	GLN	GLN
ALA	ALA	ALA	ALA	TYR	GLY	GLU	GLU
ALA	VAL	VAL	VAL	PHE	GLN	LEU	LEU
VAL	VAL	MET	PRO	PRO	VAL	LYS	LYS
THR	THR	TYR	ALA	ALA	PHE	ARG	ARG
THR	THR	ILE	ILE	ASP	ASN	GLY	GLY
VAL	VAL	ILE	ILE	ILE	THR	ILE	ILE
ASP	ASP	LYS	LYS	GLY	GLY	GLN	GLN
GLY	GLY	THR	THR	ASN	GLN	GLY	GLY
SER	SER	ASP	ASP	SER	ASN	VAL	VAL
GLY	GLY	GLN	GLN	ASN	PRO	ARG	ARG
ASN	ASN	ALA	ALA	PHE	LYS	ASN	ASN
ILE	ILE	GLN	GLN	ILE	LEU	ASP	ASP
SER	SER	SER	SER	GLY	TYR	LEU	LEU
LEU	LEU	SER	SER	ARG	SER	ASN	ASN
VAL	VAL	GLY	GLY	THR	VAL	LYS	LYS
GLY	GLY	GLY	GLY	VAL	GLY	LEU	LEU
PRO	PRO	ASN	SER	GLY	GLY	ARG	ARG
GLU	GLU	PRO	ALA	ALA	ASN	GLN	GLN
THR	THR	THR	THR	PHE	VAL	PHE	PHE
THR	THR	ILE	ILE	ASP	VAL	ASP	ASP
SER	SER	SER	SER	GLY	TYR	ILE	ILE
ILE	ILE	PRO	PRO	SER	ARG	THR	THR
ILE	ILE	THR	THR	LEU	GLY	GLN	GLN
THR	THR	ASP	ASP	THR	LEU	VAL	VAL
THR	THR	ILE	ILE	SER	PHE	ASN	ASN
GLY	GLY	ILE	ILE	GLY	GLY	GLY	GLY
MET	MET	THR	THR	ASN	ASP	ARG	ARG
ASN	ASN	ASN	ASN	ASP	GLY	GLY	ILE

THR	PHE	GLN	ALA	PRO	GLN	GLY	CYS	ALA	LEU	THR	GLY	ILE	ILE	VAL	GLN	GLU	ASN	ASN	SER	SER	GLY	ASP	ASN	ASN	ILE	GLY	GLY	VAL	VAL	TYR	TYR	LYS	PRO	ILE	GLN	LYS	LYS	VAL	ASN	GLY	VAL	TRP	VAL	THR	THR	ILE	THR	GLY
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- Molecule 12: Putative tape measure protein

Chain W:  97%

GLU	TYR	GLY	PHE	MET	PRO	LYS	PRO	VAL	GLY	LEU	LEU	ASP	VAL	PHE	ASP	LYS	TRP	PHE	ASN	LYS	PRO	ARG	ASP	ASP	ALA	ALA	ALA	PRO	GLY	GLY	PRO	GLY	SER	GLY	MET	ALA	ALA	GLN	THR	GLY	ILE	PRO	PHE	PRO	ALA	GLN	VAL	LYS	GLU	GLY	ASP	ILE	THR	ILE	LYS
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[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16480	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	22.643	Depositor
Minimum map value	-10.403	Depositor
Average map value	0.015	Depositor
Map value standard deviation	1.080	Depositor
Recommended contour level	6.5	Depositor
Map size (Å)	710.144, 710.144, 710.144	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.387, 1.387, 1.387	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	R	0.25	0/2634	0.51	0/3569
1	S	0.25	0/3760	0.51	0/5112
1	T	0.25	0/3760	0.51	0/5112
1	U	0.25	0/2634	0.51	0/3569
2	A	0.26	0/3497	0.46	0/4757
2	B	0.26	0/3497	0.47	0/4757
2	C	0.27	0/3457	0.47	0/4697
2	D	0.27	0/3457	0.48	0/4697
2	E	0.27	0/3312	0.48	0/4498
2	F	0.27	0/3312	0.48	0/4498
3	G	0.26	0/1191	0.50	0/1623
3	H	0.26	0/1191	0.51	0/1623
3	I	0.29	0/1200	0.54	0/1635
3	J	0.29	0/1200	0.53	0/1635
4	K	0.25	0/1984	0.54	0/2676
4	L	0.27	0/1974	0.59	0/2662
5	X	0.26	0/2416	0.52	0/3267
6	Y	0.26	0/1761	0.50	0/2391
7	O	0.27	0/1307	0.54	0/1771
7	P	0.27	0/1307	0.54	0/1771
8	M	0.24	0/944	0.53	0/1283
8	N	0.25	0/944	0.53	0/1283
9	m	0.26	0/1361	0.49	0/1843
9	n	0.26	0/1361	0.49	0/1843
10	g	0.31	0/1083	0.47	0/1478
10	h	0.30	0/1217	0.49	0/1663
10	i	0.29	0/1212	0.47	0/1654
10	j	0.31	0/1083	0.47	0/1478
10	k	0.29	0/1212	0.47	0/1654
10	l	0.30	0/1217	0.49	0/1663
11	a	0.25	0/733	0.41	0/997
11	b	0.26	0/733	0.44	0/997
11	c	0.25	0/733	0.41	0/997
11	d	0.25	0/733	0.41	0/997

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	e	0.26	0/733	0.44	0/997
11	f	0.25	0/733	0.40	0/997
12	W	0.36	0/210	0.54	0/282
All	All	0.26	0/65093	0.49	0/88426

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	R	324/494 (66%)	309 (95%)	14 (4%)	1 (0%)	37	67
1	S	476/494 (96%)	445 (94%)	31 (6%)	0	100	100
1	T	476/494 (96%)	445 (94%)	31 (6%)	0	100	100
1	U	324/494 (66%)	309 (95%)	14 (4%)	1 (0%)	37	67
2	A	451/473 (95%)	435 (96%)	14 (3%)	2 (0%)	30	62
2	B	451/473 (95%)	434 (96%)	15 (3%)	2 (0%)	30	62
2	C	443/473 (94%)	427 (96%)	16 (4%)	0	100	100
2	D	443/473 (94%)	428 (97%)	15 (3%)	0	100	100
2	E	421/473 (89%)	396 (94%)	25 (6%)	0	100	100
2	F	421/473 (89%)	396 (94%)	25 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	152/156 (97%)	149 (98%)	3 (2%)	0	100	100
3	H	152/156 (97%)	148 (97%)	4 (3%)	0	100	100
3	I	154/156 (99%)	145 (94%)	8 (5%)	1 (1%)	22	54
3	J	154/156 (99%)	145 (94%)	8 (5%)	1 (1%)	22	54
4	K	245/284 (86%)	231 (94%)	12 (5%)	2 (1%)	16	48
4	L	242/284 (85%)	232 (96%)	10 (4%)	0	100	100
5	X	299/330 (91%)	287 (96%)	12 (4%)	0	100	100
6	Y	226/247 (92%)	208 (92%)	18 (8%)	0	100	100
7	O	163/165 (99%)	154 (94%)	9 (6%)	0	100	100
7	P	163/165 (99%)	155 (95%)	8 (5%)	0	100	100
8	M	110/112 (98%)	108 (98%)	2 (2%)	0	100	100
8	N	110/112 (98%)	108 (98%)	2 (2%)	0	100	100
9	m	161/163 (99%)	153 (95%)	8 (5%)	0	100	100
9	n	161/163 (99%)	153 (95%)	8 (5%)	0	100	100
10	g	125/793 (16%)	119 (95%)	6 (5%)	0	100	100
10	h	145/793 (18%)	135 (93%)	10 (7%)	0	100	100
10	i	143/793 (18%)	132 (92%)	11 (8%)	0	100	100
10	j	125/793 (16%)	119 (95%)	6 (5%)	0	100	100
10	k	143/793 (18%)	132 (92%)	11 (8%)	0	100	100
10	l	145/793 (18%)	134 (92%)	11 (8%)	0	100	100
11	a	88/554 (16%)	86 (98%)	2 (2%)	0	100	100
11	b	88/554 (16%)	87 (99%)	1 (1%)	0	100	100
11	c	88/554 (16%)	85 (97%)	3 (3%)	0	100	100
11	d	88/554 (16%)	86 (98%)	2 (2%)	0	100	100
11	e	88/554 (16%)	87 (99%)	1 (1%)	0	100	100
11	f	88/554 (16%)	85 (97%)	3 (3%)	0	100	100
12	W	24/811 (3%)	23 (96%)	1 (4%)	0	100	100
All	All	8100/16356 (50%)	7710 (95%)	380 (5%)	10 (0%)	50	78

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	300	SER

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Mol	Chain	Res	Type
2	B	300	SER
2	A	326	GLU
3	J	143	ASP
2	B	326	GLU

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	R	278/425 (65%)	278 (100%)	0	100	100
1	S	407/425 (96%)	400 (98%)	7 (2%)	56	76
1	T	407/425 (96%)	400 (98%)	7 (2%)	56	76
1	U	278/425 (65%)	278 (100%)	0	100	100
2	A	363/384 (94%)	363 (100%)	0	100	100
2	B	363/384 (94%)	363 (100%)	0	100	100
2	C	356/384 (93%)	355 (100%)	1 (0%)	91	95
2	D	356/384 (93%)	355 (100%)	1 (0%)	91	95
2	E	340/384 (88%)	340 (100%)	0	100	100
2	F	340/384 (88%)	340 (100%)	0	100	100
3	G	125/126 (99%)	121 (97%)	4 (3%)	34	62
3	H	125/126 (99%)	121 (97%)	4 (3%)	34	62
3	I	125/126 (99%)	120 (96%)	5 (4%)	27	57
3	J	125/126 (99%)	120 (96%)	5 (4%)	27	57
4	K	214/244 (88%)	214 (100%)	0	100	100
4	L	213/244 (87%)	213 (100%)	0	100	100
5	X	262/282 (93%)	262 (100%)	0	100	100
6	Y	188/202 (93%)	188 (100%)	0	100	100
7	O	138/147 (94%)	137 (99%)	1 (1%)	81	90
7	P	138/147 (94%)	137 (99%)	1 (1%)	81	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	M	101/101 (100%)	100 (99%)	1 (1%)	73	85
8	N	101/101 (100%)	100 (99%)	1 (1%)	73	85
9	m	145/145 (100%)	145 (100%)	0	100	100
9	n	145/145 (100%)	145 (100%)	0	100	100
10	g	117/637 (18%)	116 (99%)	1 (1%)	75	87
10	h	134/637 (21%)	133 (99%)	1 (1%)	81	90
10	i	132/637 (21%)	132 (100%)	0	100	100
10	j	117/637 (18%)	115 (98%)	2 (2%)	56	76
10	k	132/637 (21%)	132 (100%)	0	100	100
10	l	134/637 (21%)	133 (99%)	1 (1%)	81	90
11	a	75/453 (17%)	74 (99%)	1 (1%)	65	81
11	b	75/453 (17%)	75 (100%)	0	100	100
11	c	75/453 (17%)	75 (100%)	0	100	100
11	d	75/453 (17%)	74 (99%)	1 (1%)	65	81
11	e	75/453 (17%)	75 (100%)	0	100	100
11	f	75/453 (17%)	75 (100%)	0	100	100
12	W	23/617 (4%)	23 (100%)	0	100	100
All	All	6872/13423 (51%)	6827 (99%)	45 (1%)	80	90

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	I	61	ARG
7	P	102	ASN
3	I	103	SER
3	G	96	LEU
8	M	76	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	U	57	GLN
9	m	141	GLN
1	U	453	GLN
9	n	141	GLN

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Mol	Chain	Res	Type
12	W	803	ASN

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.

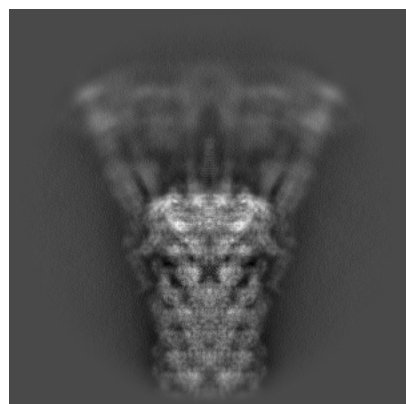
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45953. These allow visual inspection of the internal detail of the map and identification of artifacts.

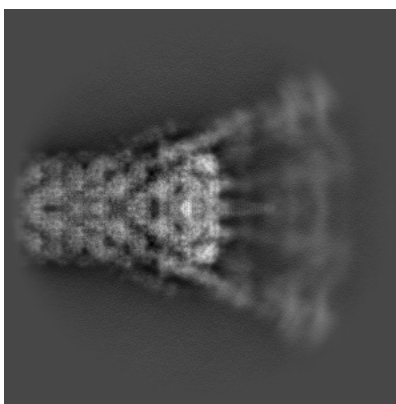
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

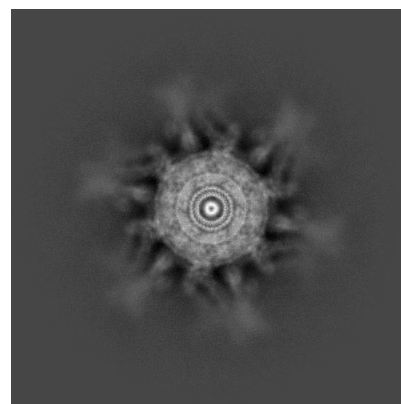
6.1.1 Primary map



X

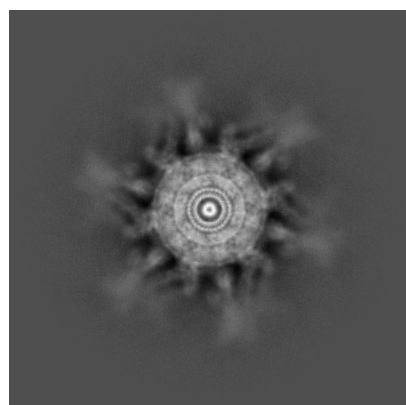


Y

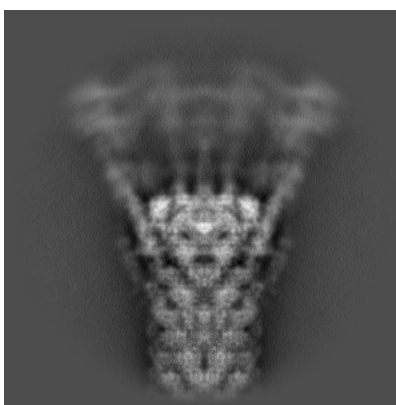


Z

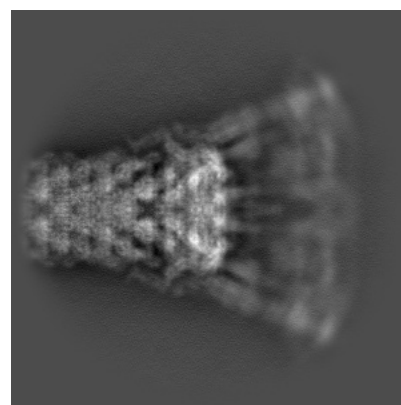
6.1.2 Raw map



X



Y

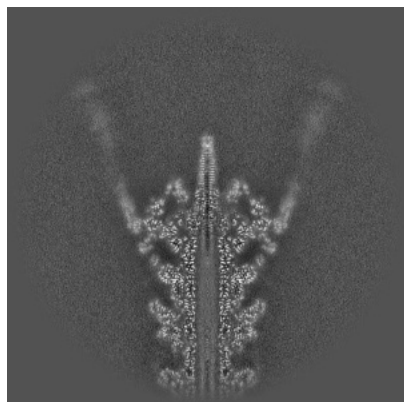


Z

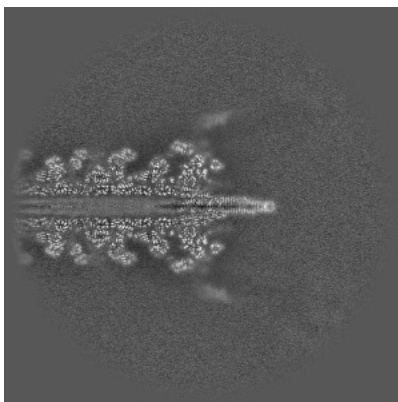
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

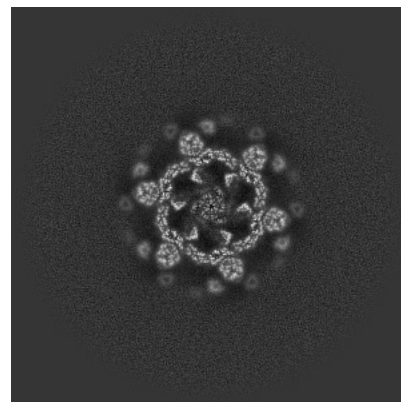
6.2.1 Primary map



X Index: 256

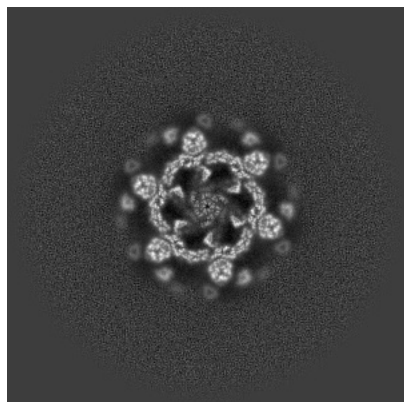


Y Index: 256

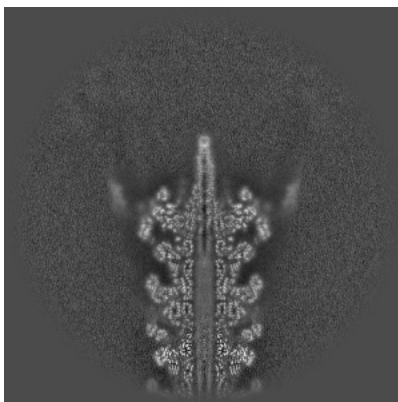


Z Index: 256

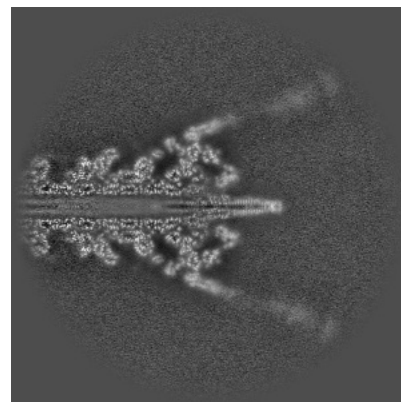
6.2.2 Raw map



X Index: 256



Y Index: 256

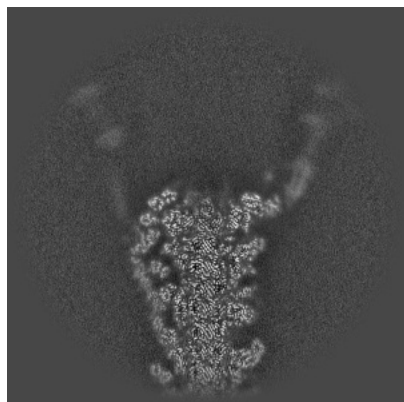


Z Index: 256

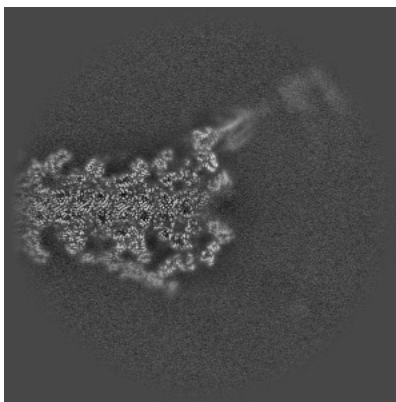
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

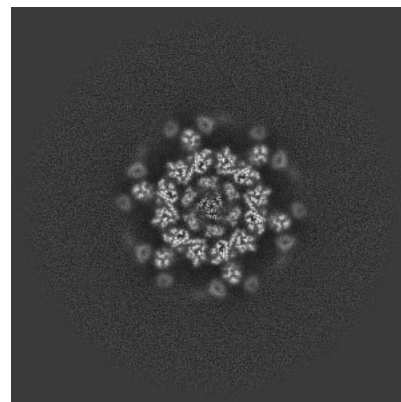
6.3.1 Primary map



X Index: 239

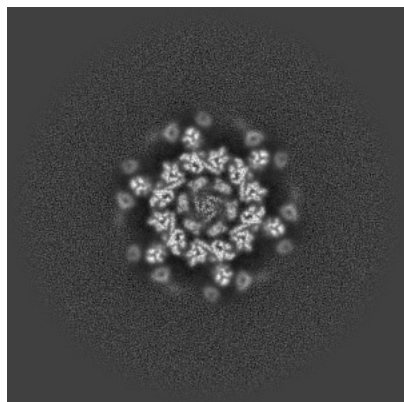


Y Index: 238

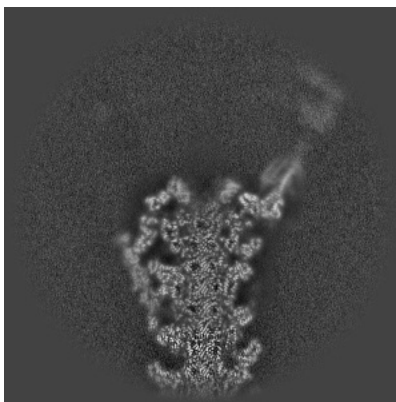


Z Index: 265

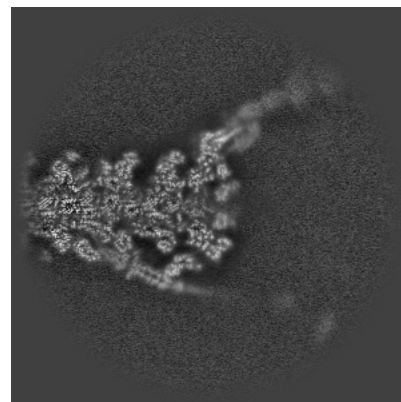
6.3.2 Raw map



X Index: 265



Y Index: 238

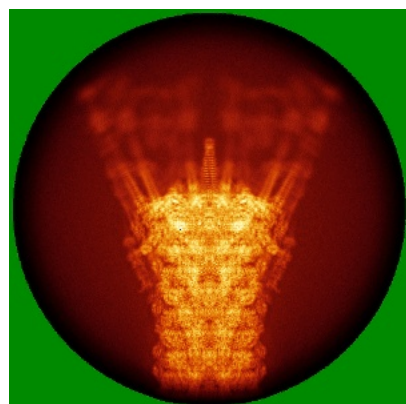


Z Index: 231

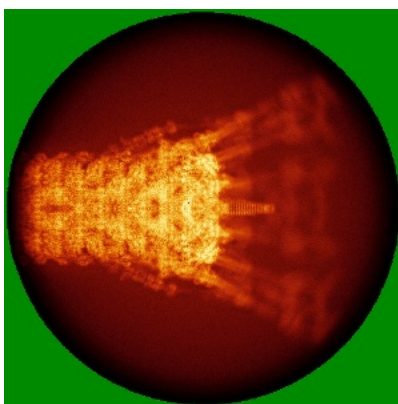
The images above show the largest variance slices of the map in three orthogonal directions.

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

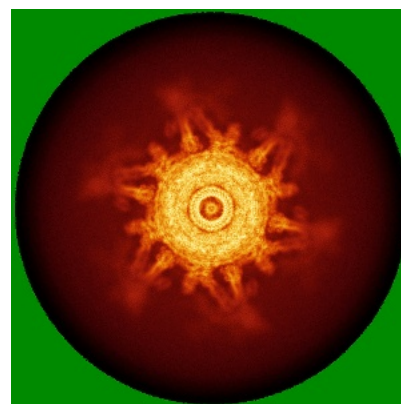
6.4.1 Primary map



X

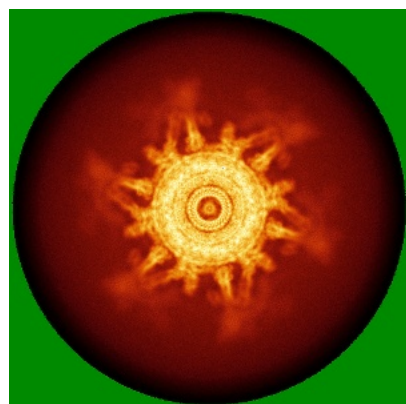


Y

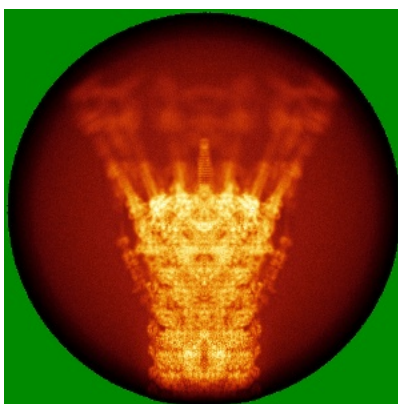


Z

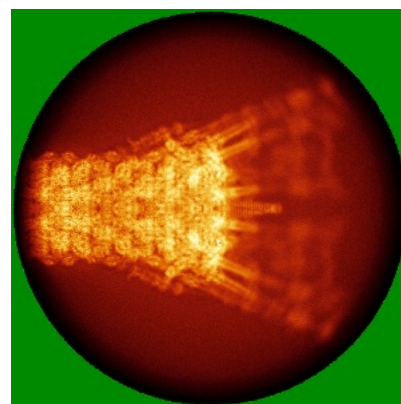
6.4.2 Raw map



X



Y

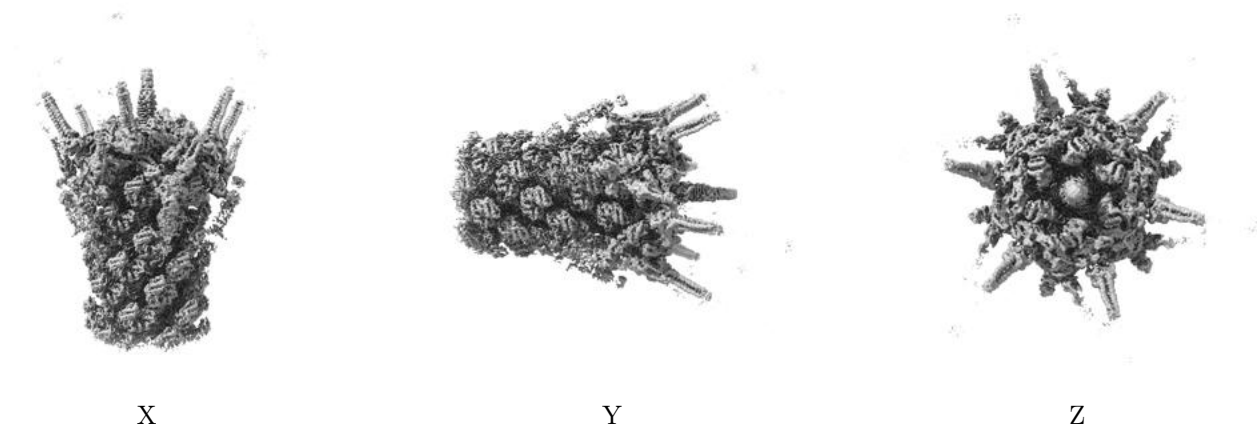


Z

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.

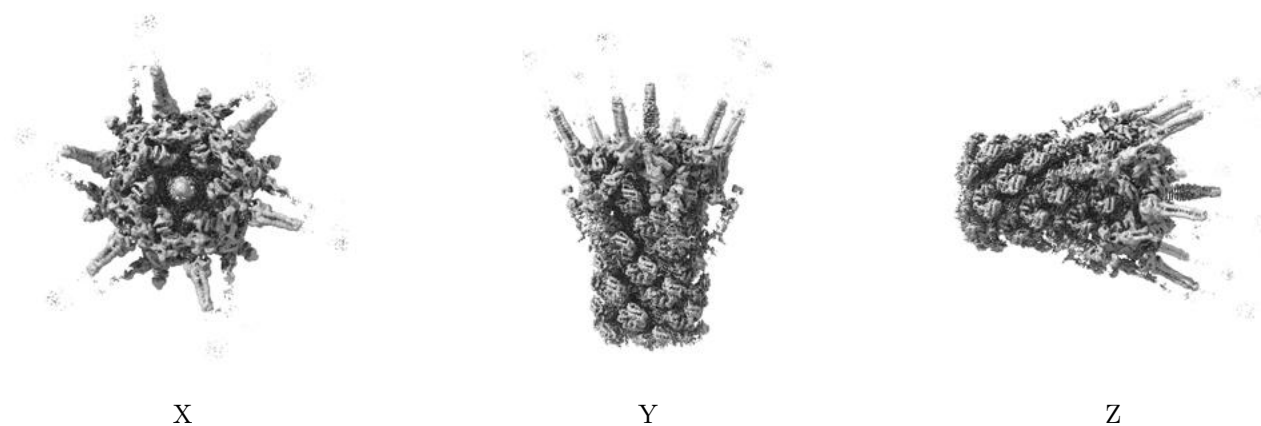
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 6.5. 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.

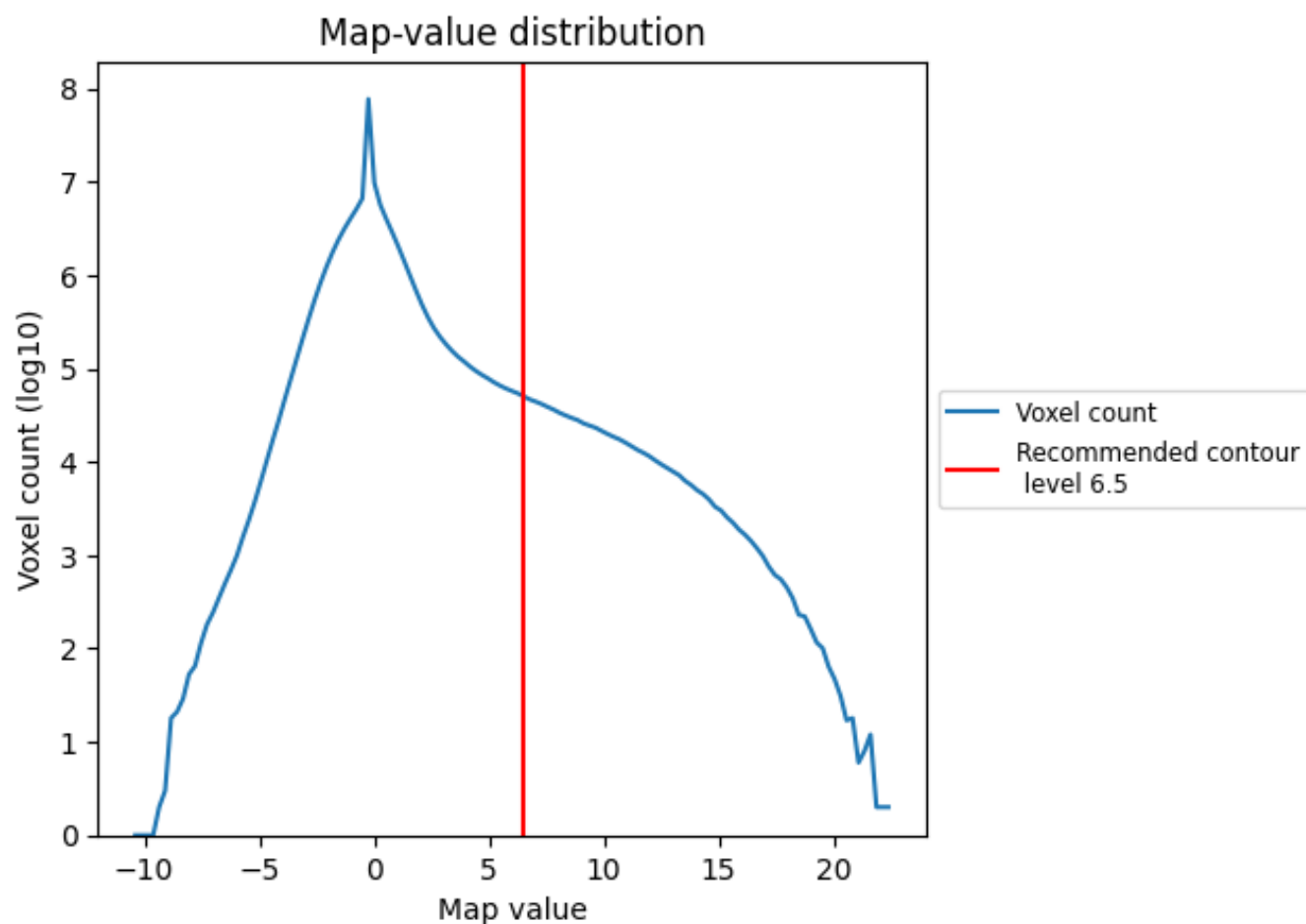
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

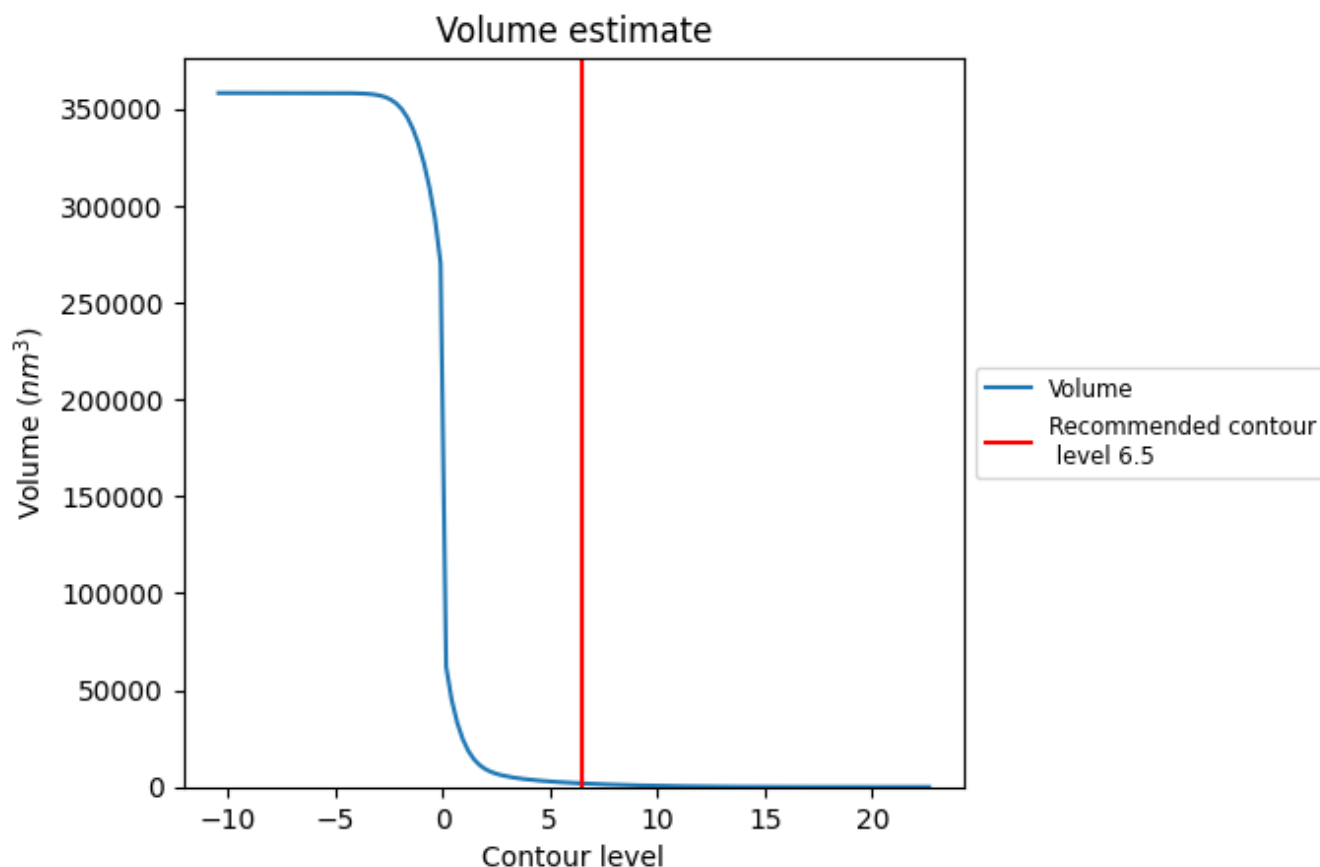
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

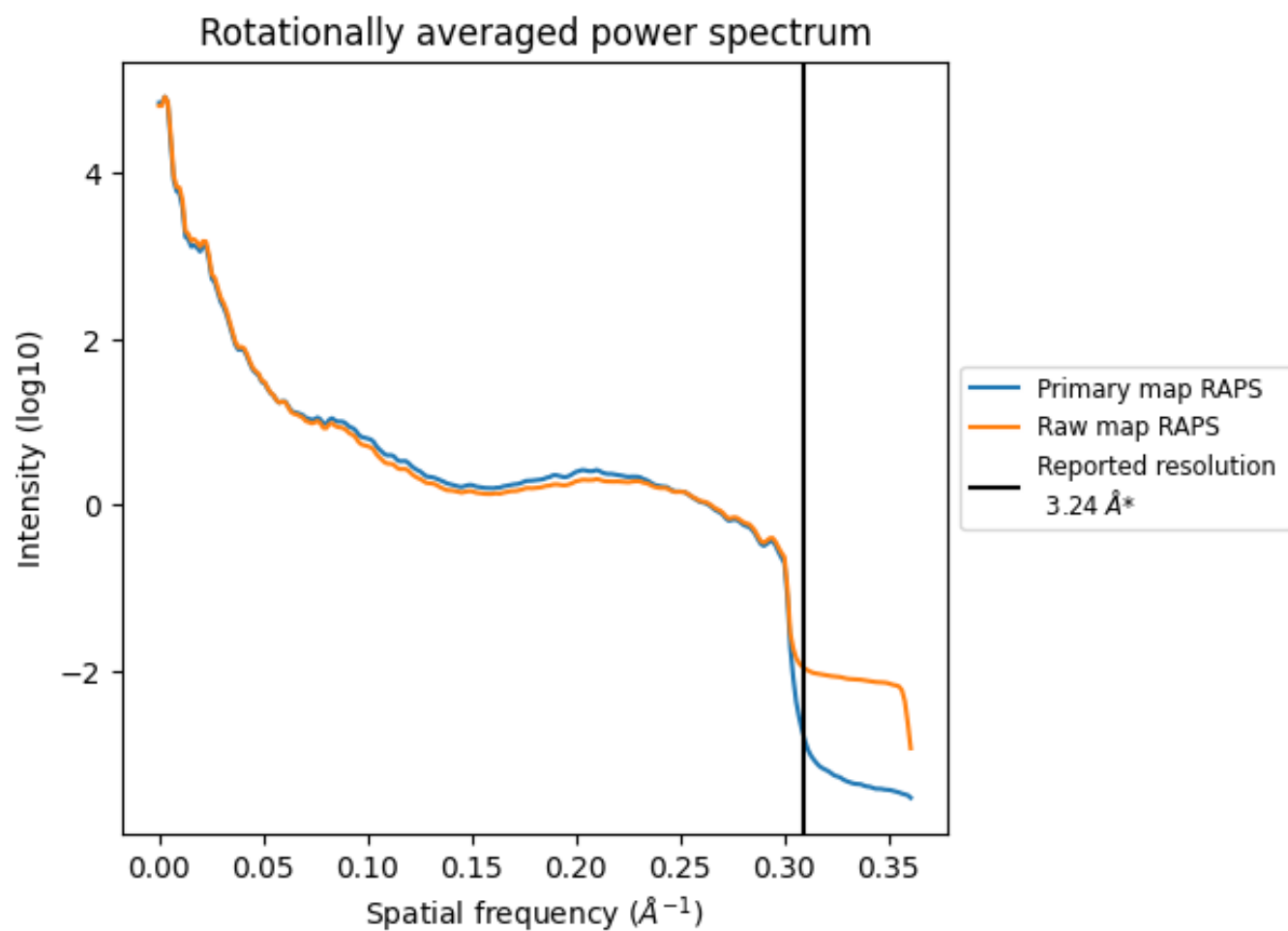
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1848 nm^3 ; this corresponds to an approximate mass of 1670 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 ⓘ

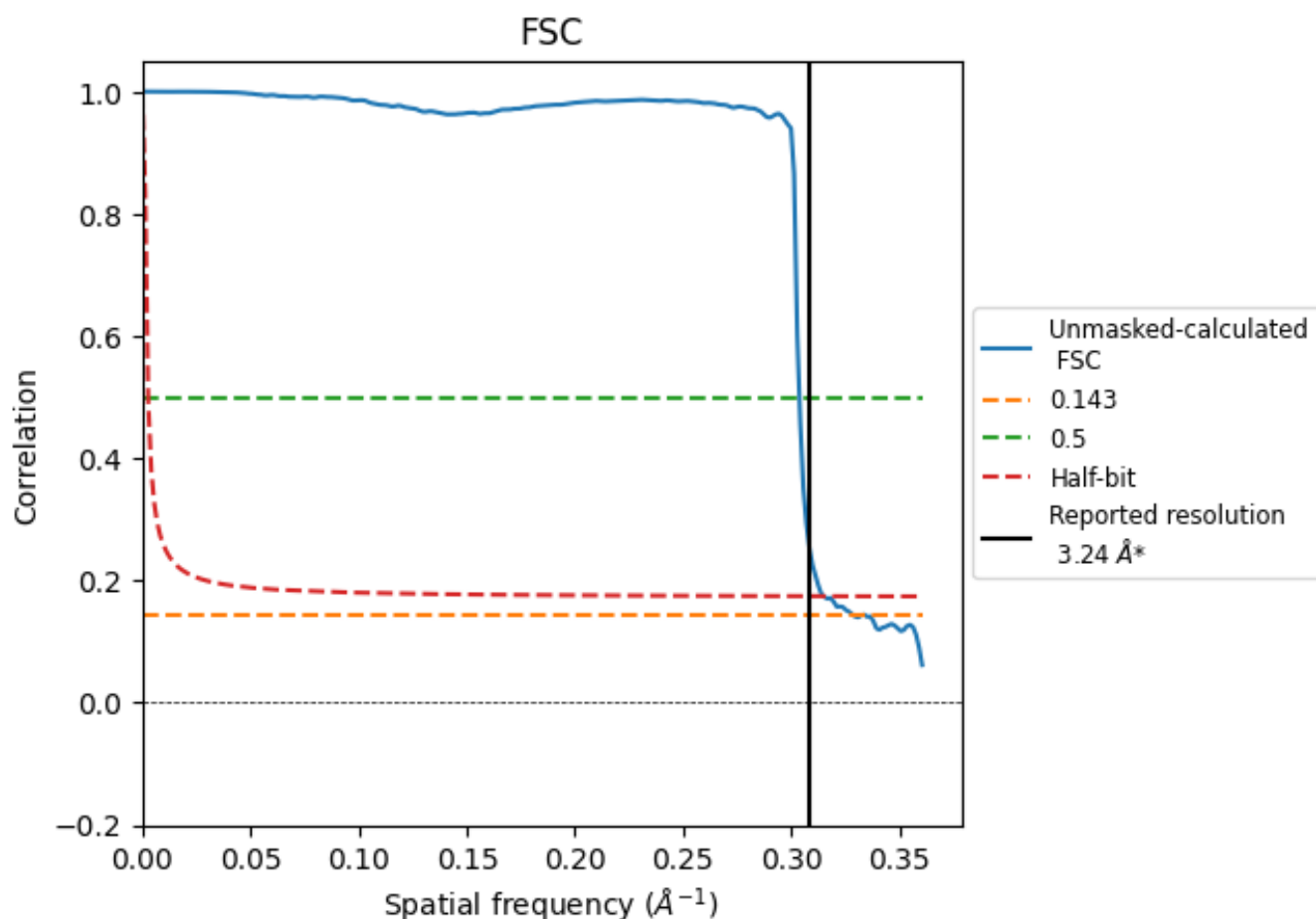


*Reported resolution corresponds to spatial frequency of 0.309 Å⁻¹

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 0.309 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.24	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.04	3.29	3.17

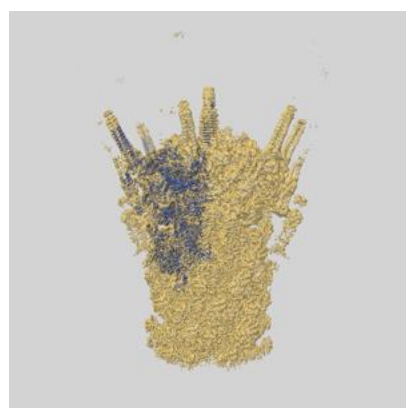
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

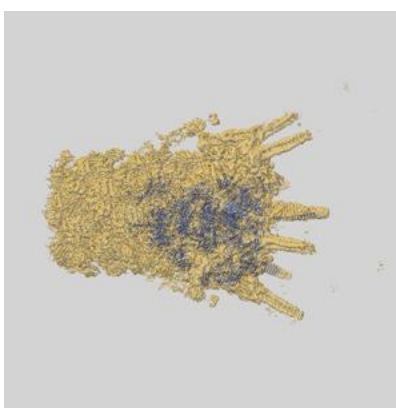
This section contains information regarding the fit between EMDB map EMD-45953 and PDB model 9CUY. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlays

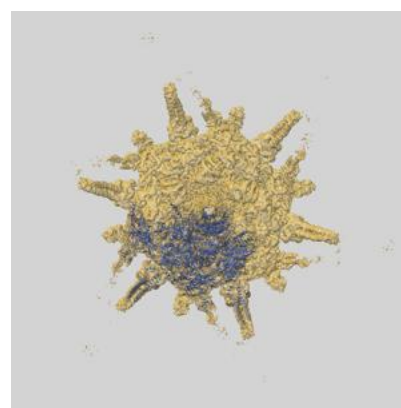
9.1.1 Map-model overlay [i](#)



X

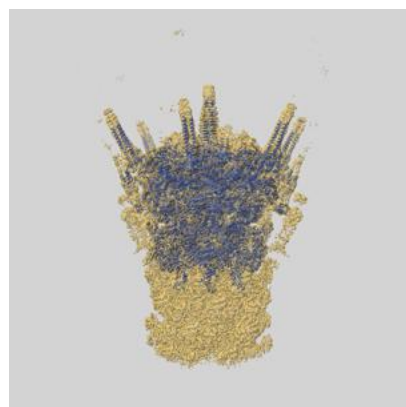


Y

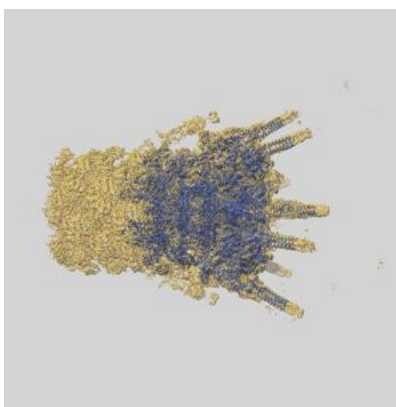


Z

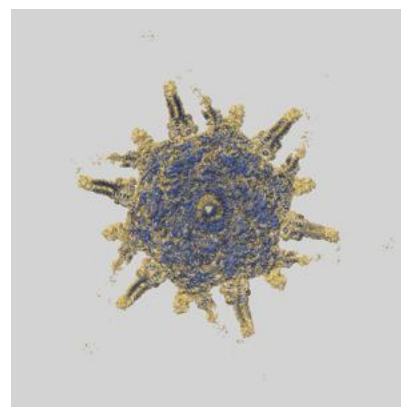
9.1.2 Map-model assembly overlay [i](#)



X



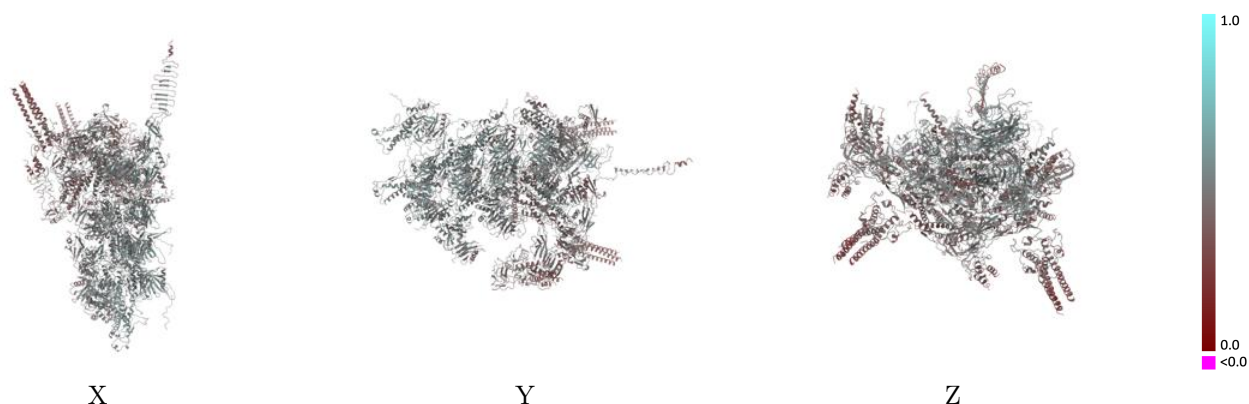
Y



Z

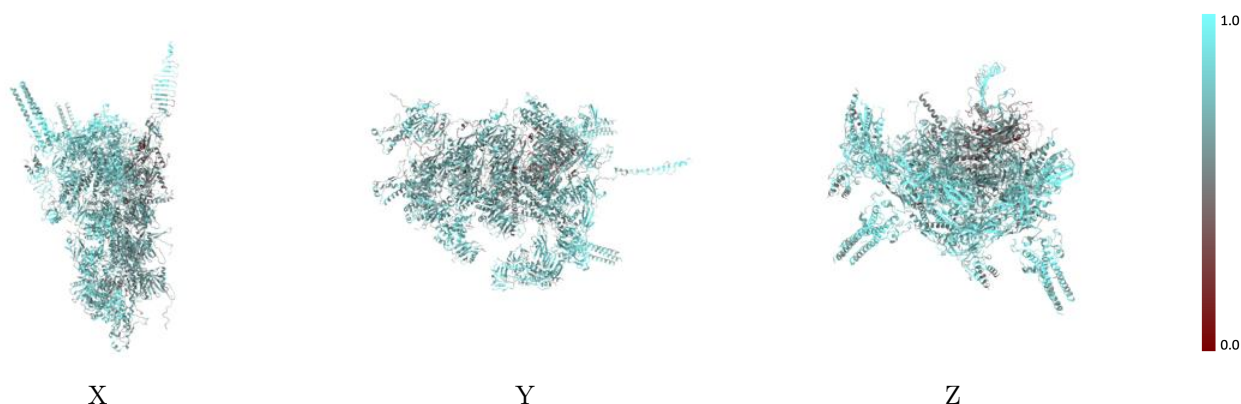
The images above show the 3D surface view of the map at the recommended contour level 6.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



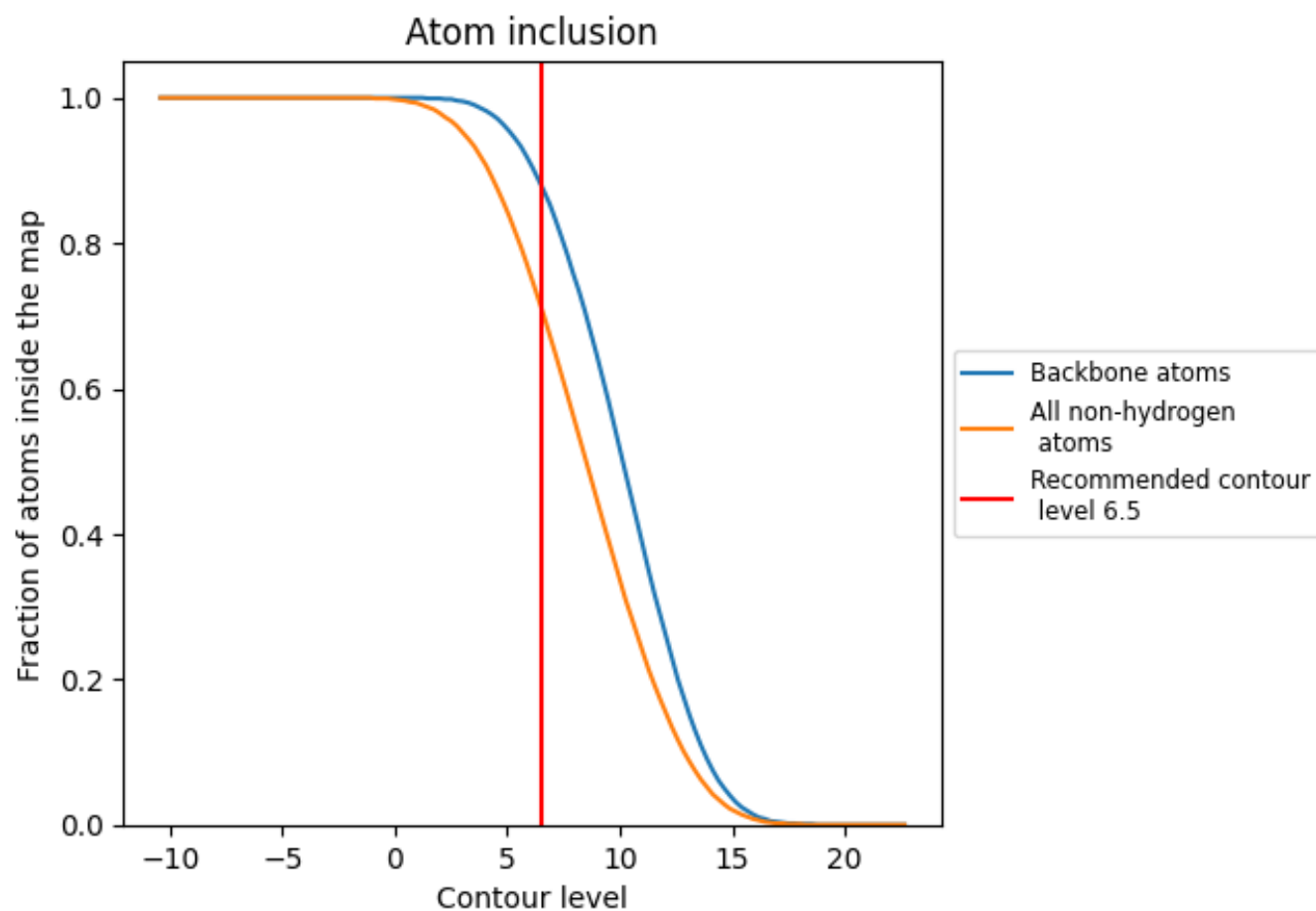
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6.5).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 71% 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 (6.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7120	 0.4590
A	 0.6980	 0.4960
B	 0.6990	 0.4920
C	 0.7280	 0.4920
D	 0.7300	 0.4900
E	 0.7250	 0.4840
F	 0.7280	 0.4830
G	 0.5990	 0.4970
H	 0.5950	 0.4940
I	 0.6150	 0.5110
J	 0.6170	 0.5110
K	 0.5610	 0.4680
L	 0.5690	 0.4730
M	 0.7190	 0.5070
N	 0.7180	 0.5080
O	 0.7480	 0.4550
P	 0.7510	 0.4540
R	 0.8030	 0.4320
S	 0.7900	 0.4430
T	 0.7860	 0.4390
U	 0.8030	 0.4290
W	 0.4310	 0.4880
X	 0.4690	 0.4980
Y	 0.6400	 0.4510
a	 0.8000	 0.3800
b	 0.8110	 0.3730
c	 0.7980	 0.3620
d	 0.8120	 0.3760
e	 0.8080	 0.3630
f	 0.7970	 0.3560
g	 0.7670	 0.4050
h	 0.7790	 0.3880
i	 0.7140	 0.4070
j	 0.7630	 0.3980
k	 0.7030	 0.4010



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Chain	Atom inclusion	Q-score
l	 0.7730	 0.3850
m	 0.6760	 0.4730
n	 0.6740	 0.4730