Full wwPDB EM Validation Report

Apr 7, 2025 – 02:38 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 Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

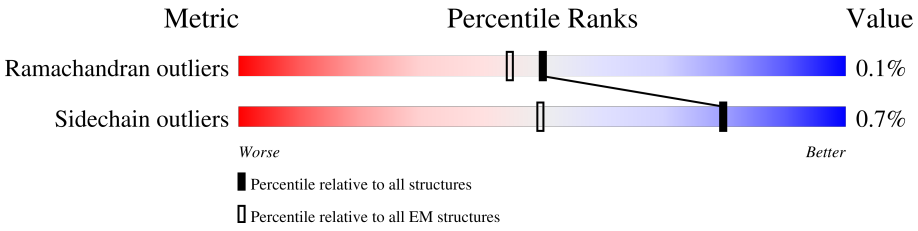
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: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

1 Overall quality at a glance (i)

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 <=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	68% 32%
1	S	494	97%
1	T	494	97%
1	U	494	68% 32%
2	A	473	7% 97%
2	B	473	7% 97%
2	C	473	6% 96%
2	D	473	6% 96%
2	E	473	92% 8%

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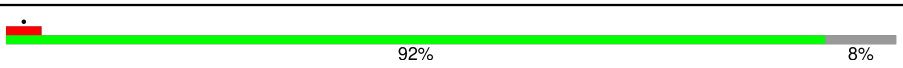
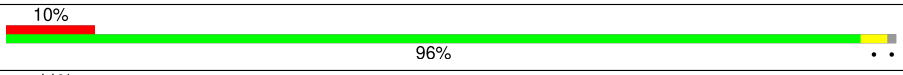
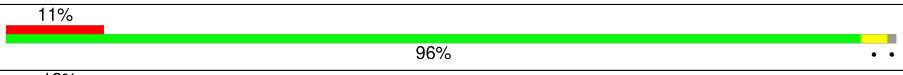
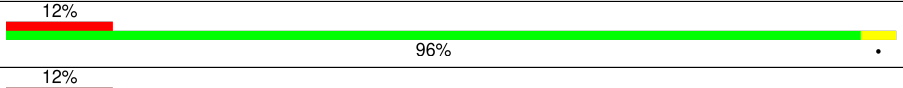
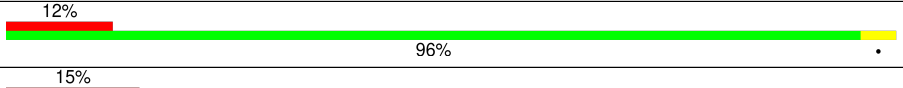
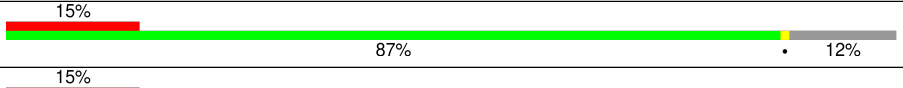
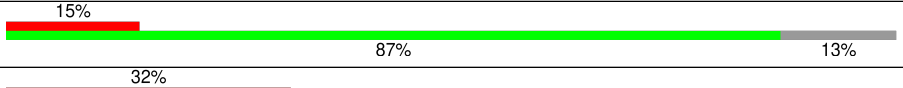
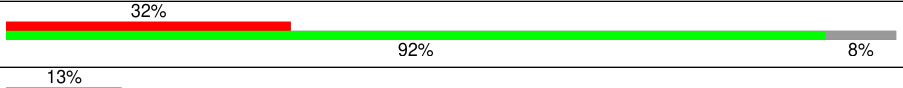
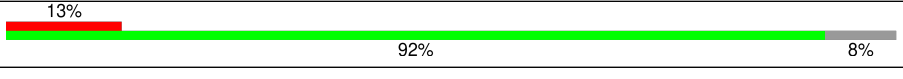
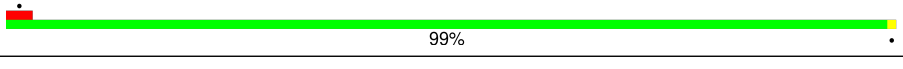
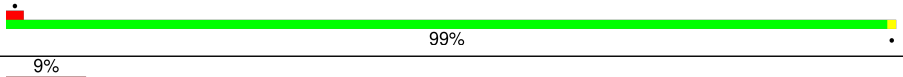
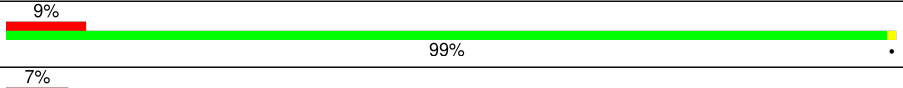
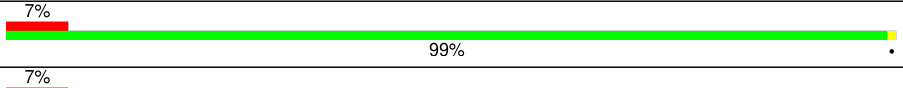
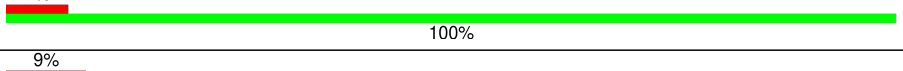
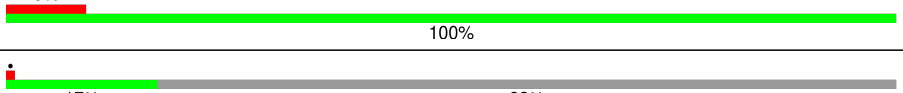
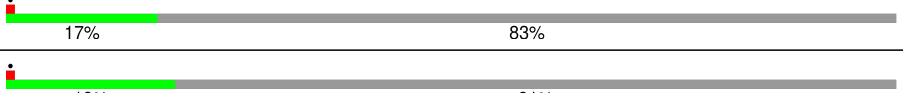
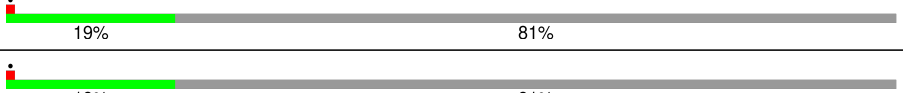
Mol	Chain	Length	Quality of chain
2	F	473	
3	G	156	
3	H	156	
3	I	156	
3	J	156	
4	K	284	
4	L	284	
5	X	330	
6	Y	247	
7	O	165	
7	P	165	
8	M	112	
8	N	112	
9	m	163	
9	n	163	
10	g	793	
10	h	793	
10	i	793	
10	j	793	
10	k	793	
10	l	793	
11	a	554	
11	b	554	
11	c	554	
11	d	554	

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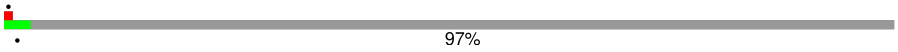
Mol	Chain	Length	Quality of chain
11	e	554	
11	f	554	
12	W	811	

2 Entry composition

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.

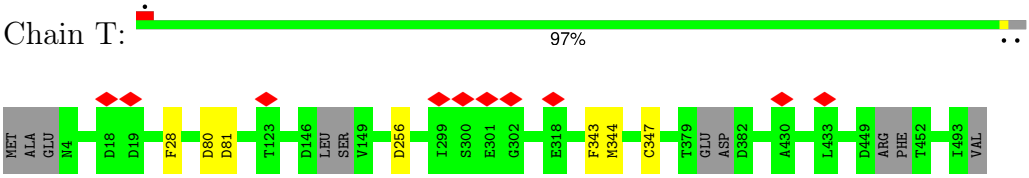
Mol	Chain	Residues	Atoms					AltConf	Trace
12	W	26	Total	C	N	O	S	0	0
			208	128	40	38	2		

3 Residue-property plots (i)

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

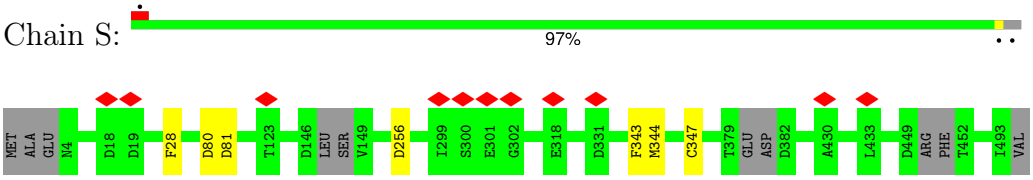
• Molecule 1: Wedge 2 protein

Chain T:



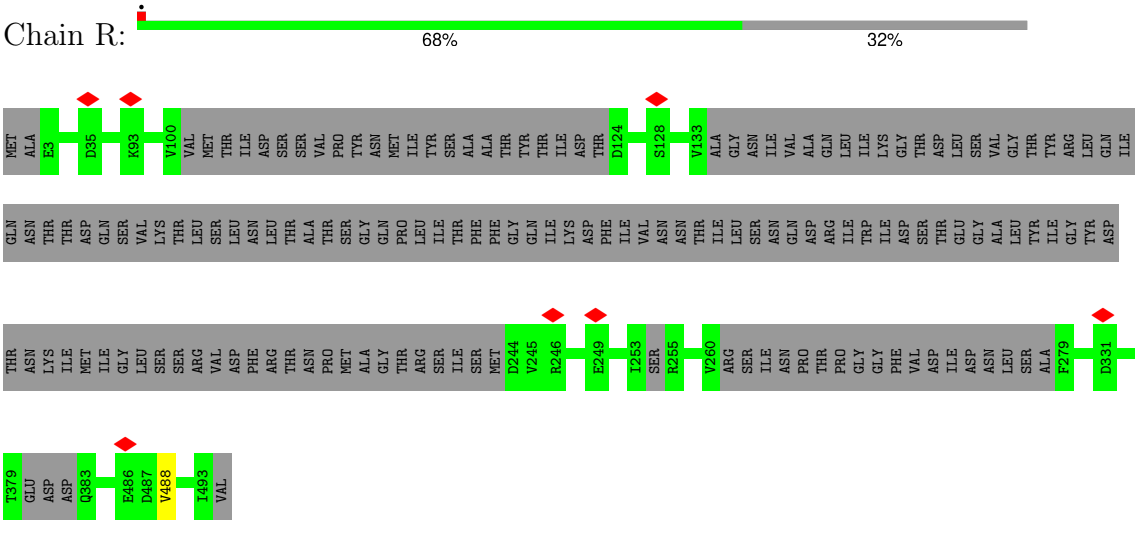
• Molecule 1: Wedge 2 protein

Chain S:



• Molecule 1: Wedge 2 protein

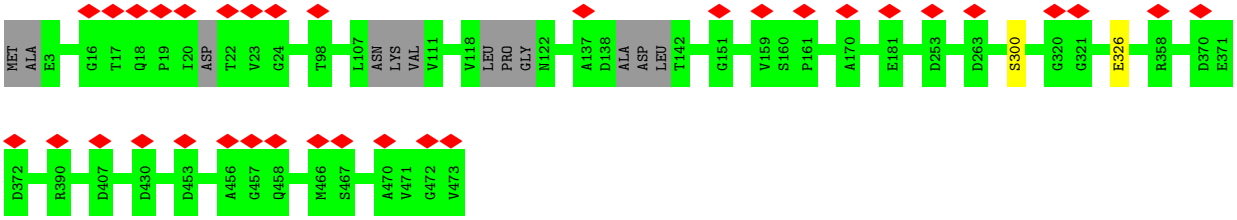
Chain R:



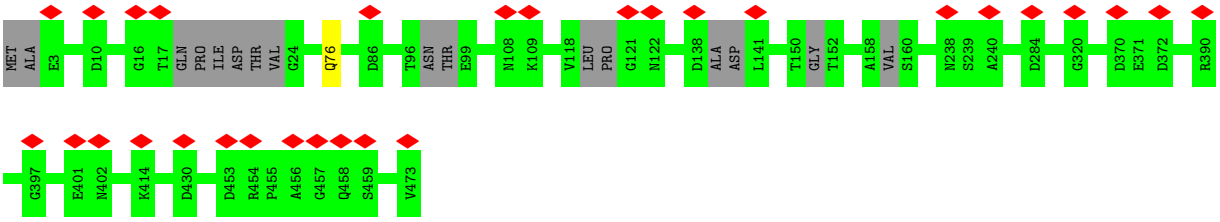
• Molecule 1: Wedge 2 protein

Chain U:

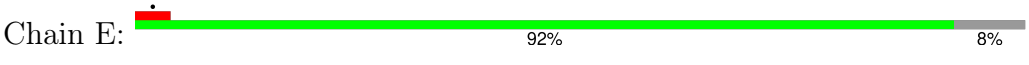
• Molecule 2: Tail sheath protein

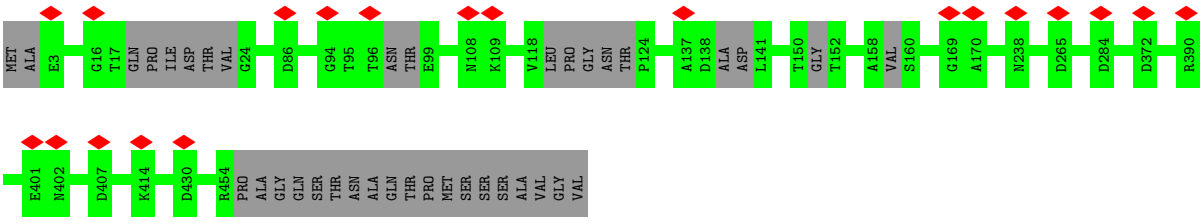


• Molecule 2: Tail sheath protein

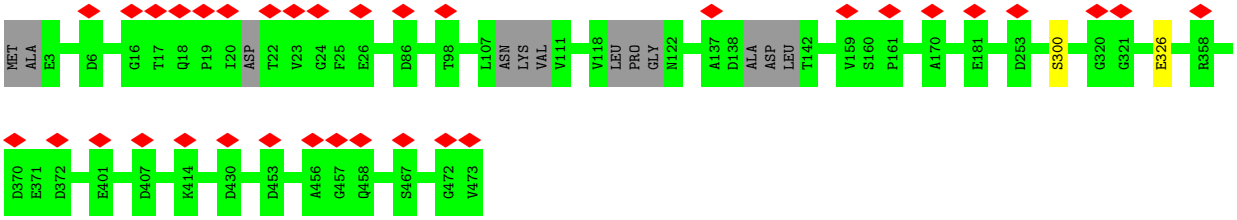


• Molecule 2: Tail sheath protein

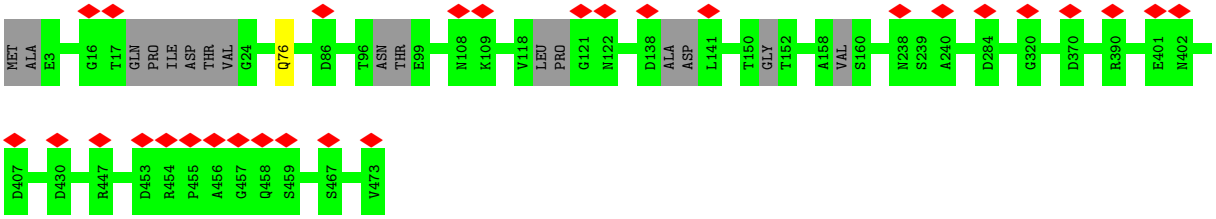




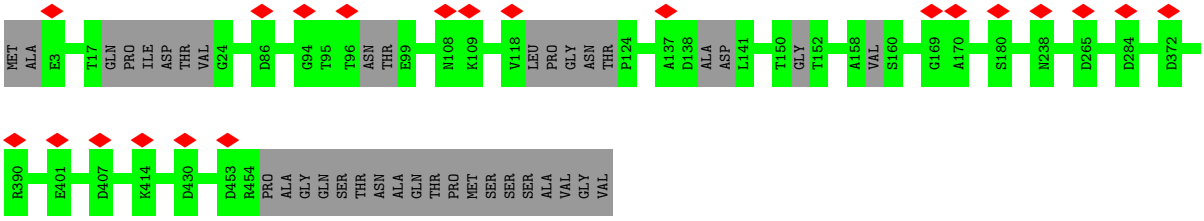
• Molecule 2: Tail sheath protein



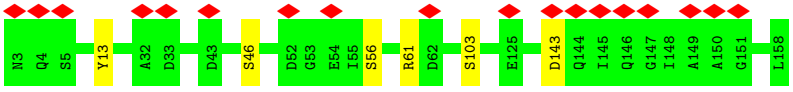
• Molecule 2: Tail sheath protein



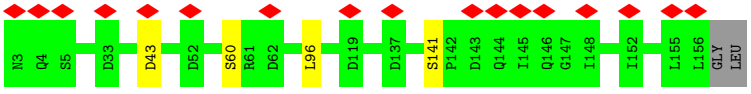
• Molecule 2: Tail sheath protein



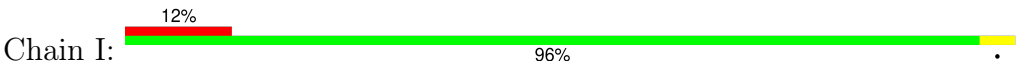
• Molecule 3: Tail tube protein

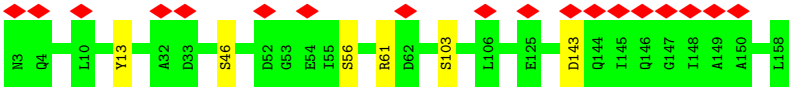


• Molecule 3: Tail tube protein



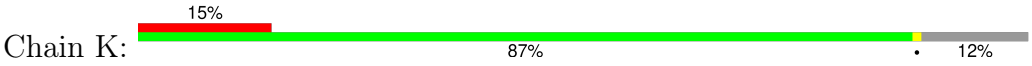
• Molecule 3: Tail tube protein

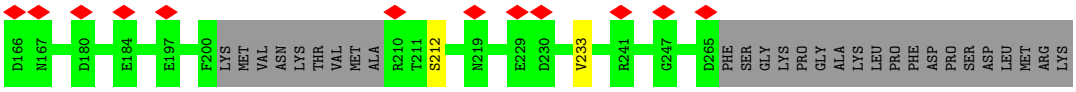




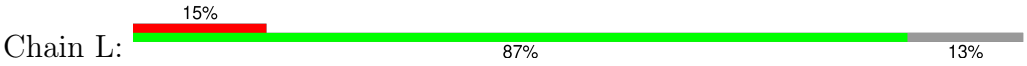
• Molecule 3: Tail tube protein

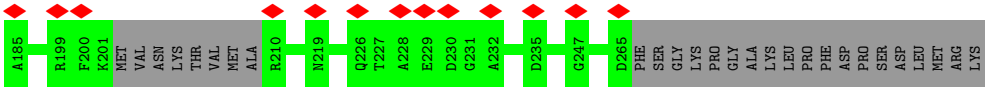
• Molecule 4: Tube initiator protein



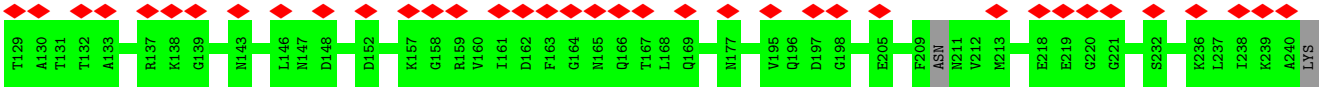


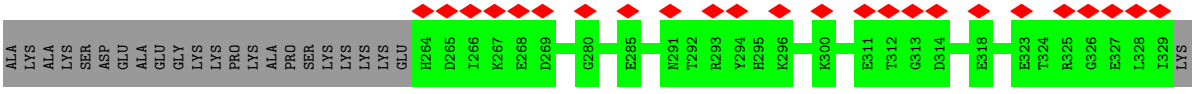
• Molecule 4: Tube initiator protein





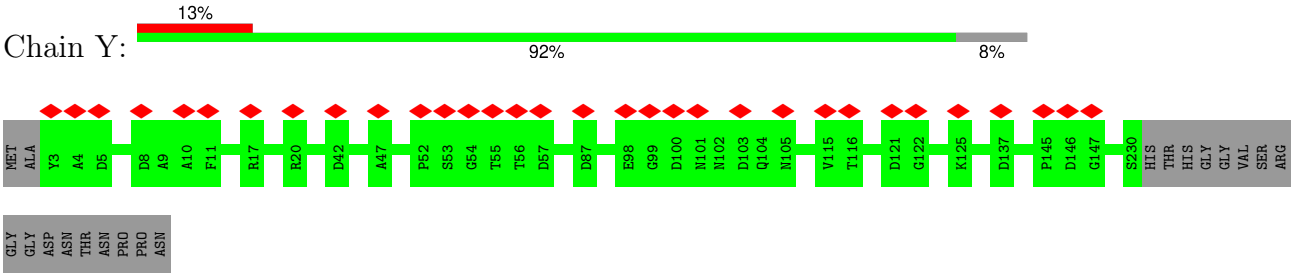
• Molecule 5: Hub protein





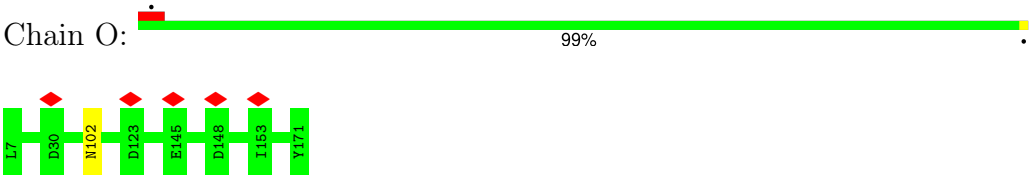
• Molecule 6: Putative baseplate assembly protein

Chain Y:



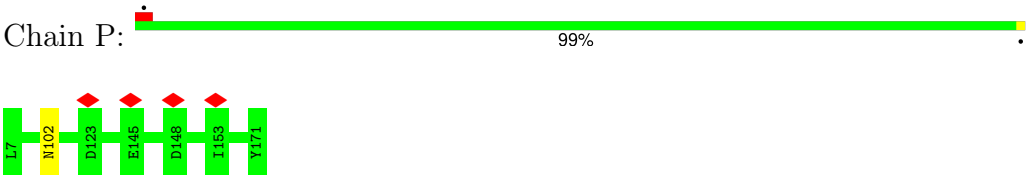
• Molecule 7: Wedge 1 protein

Chain O:



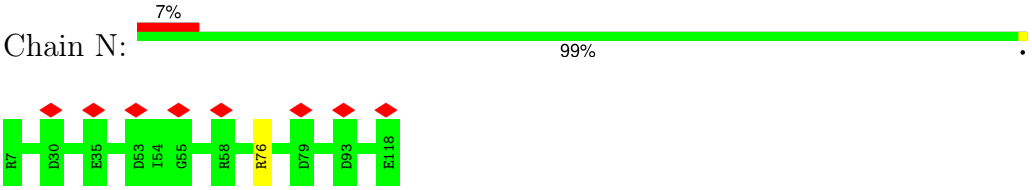
• Molecule 7: Wedge 1 protein

Chain P:



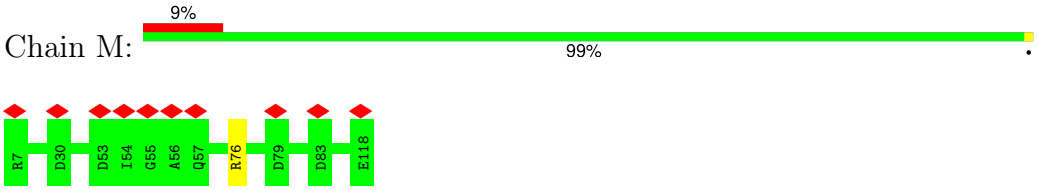
• Molecule 8: Spacer protein

Chain N:



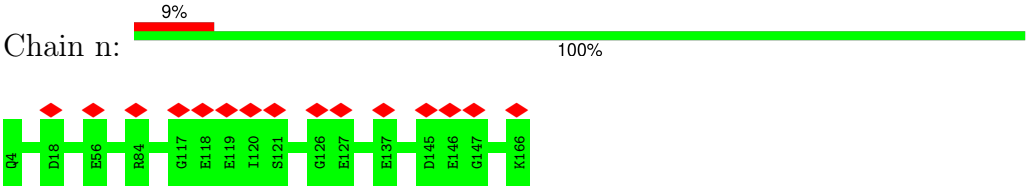
• Molecule 8: Spacer protein

Chain M:



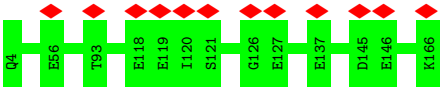
• Molecule 9: Sheath initiator protein

Chain n:



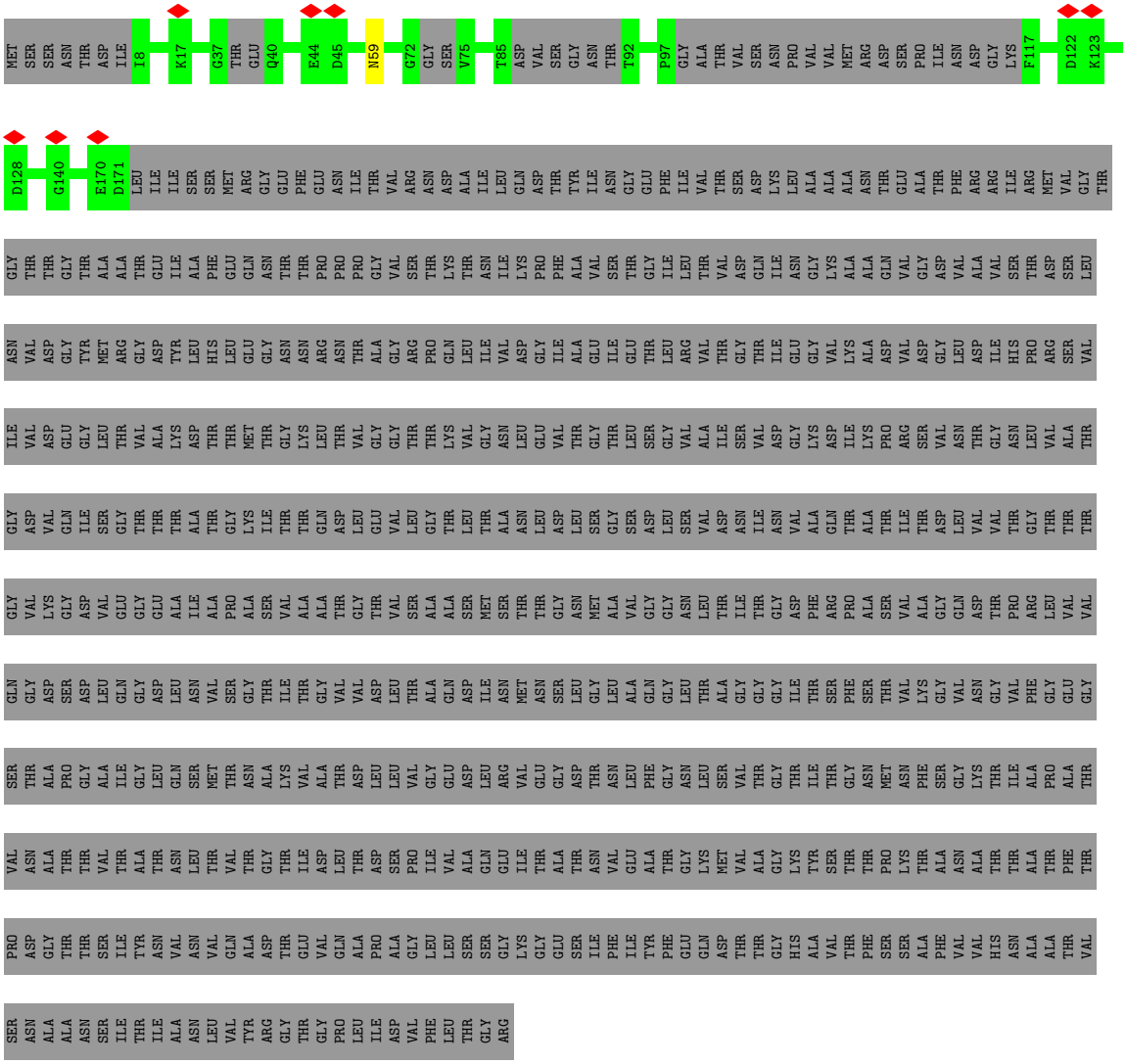
• Molecule 9: Sheath initiator protein

Chain m:



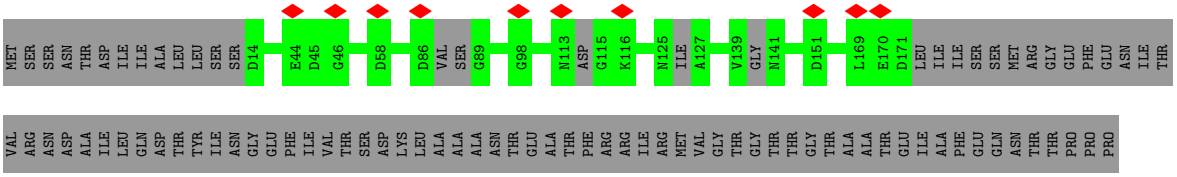
• Molecule 10: Putative tail fiber protein

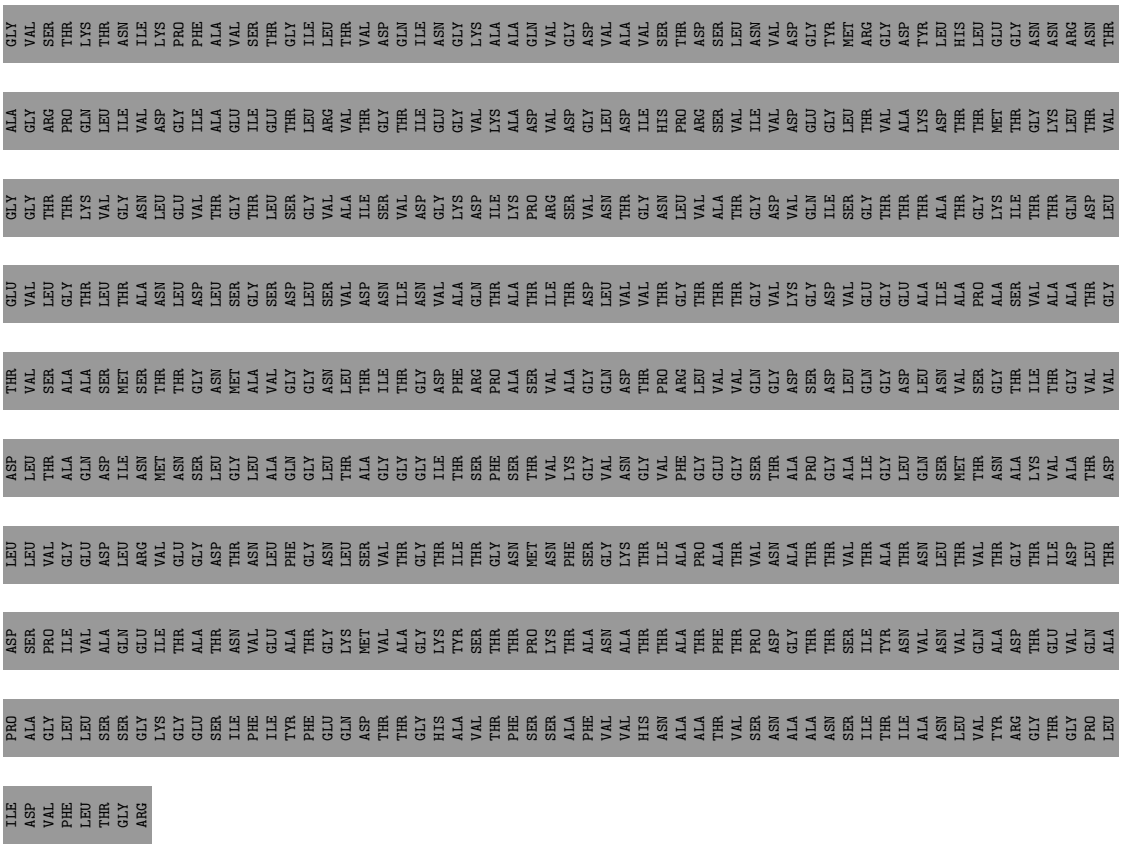
Chain g:



• Molecule 10: Putative tail fiber protein

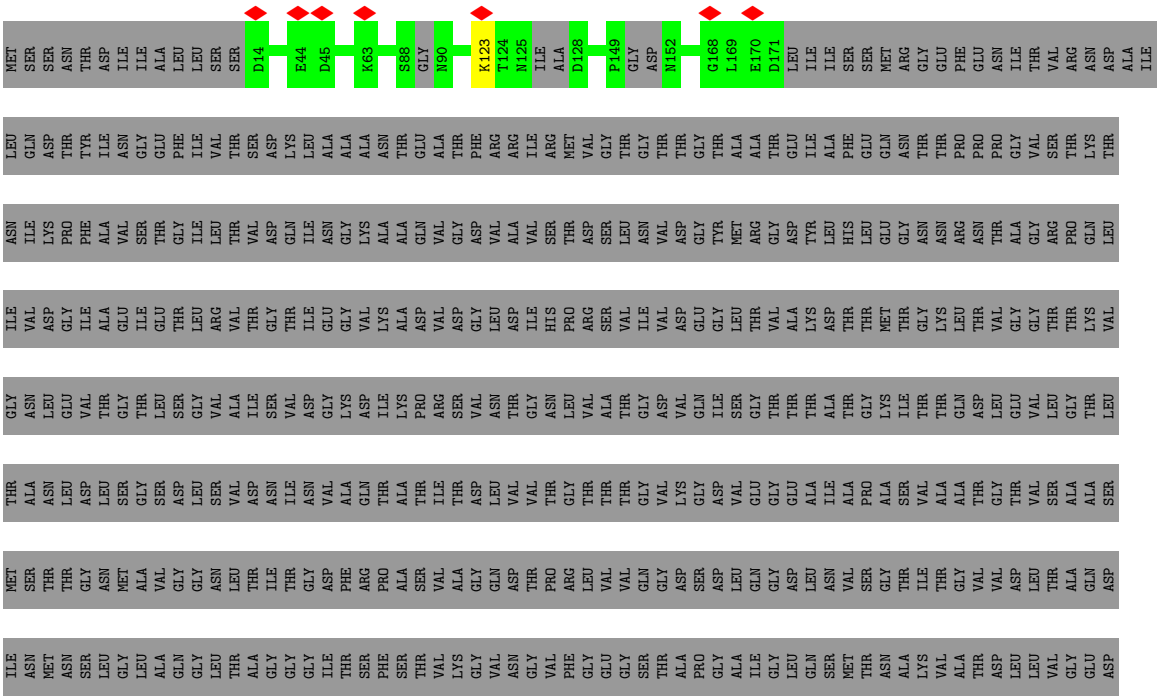
Chain i:

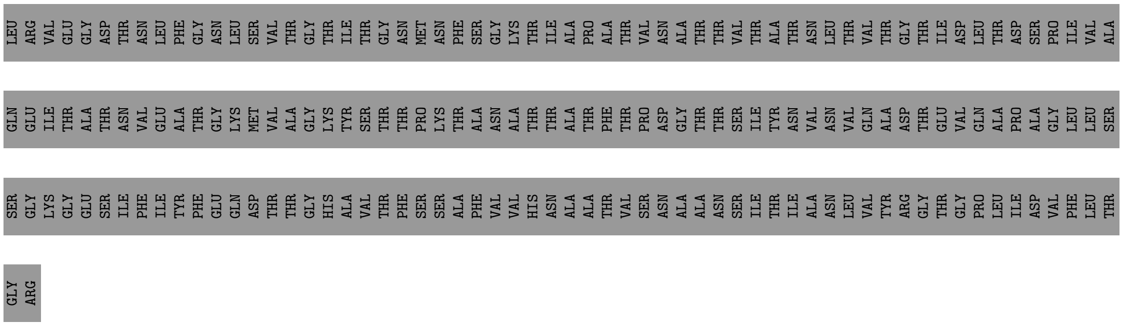




• Molecule 10: Putative tail fiber protein

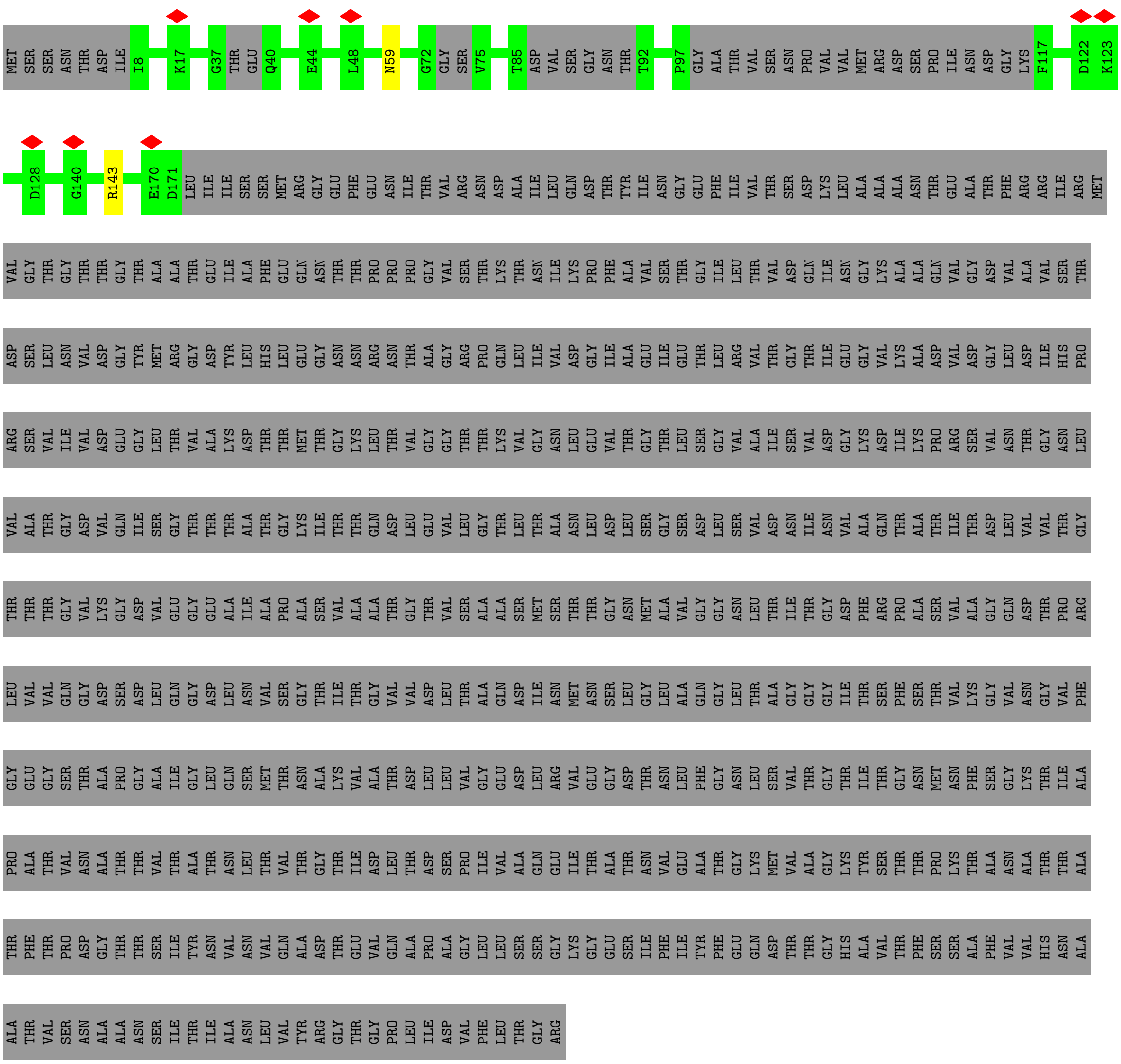
Chain h:





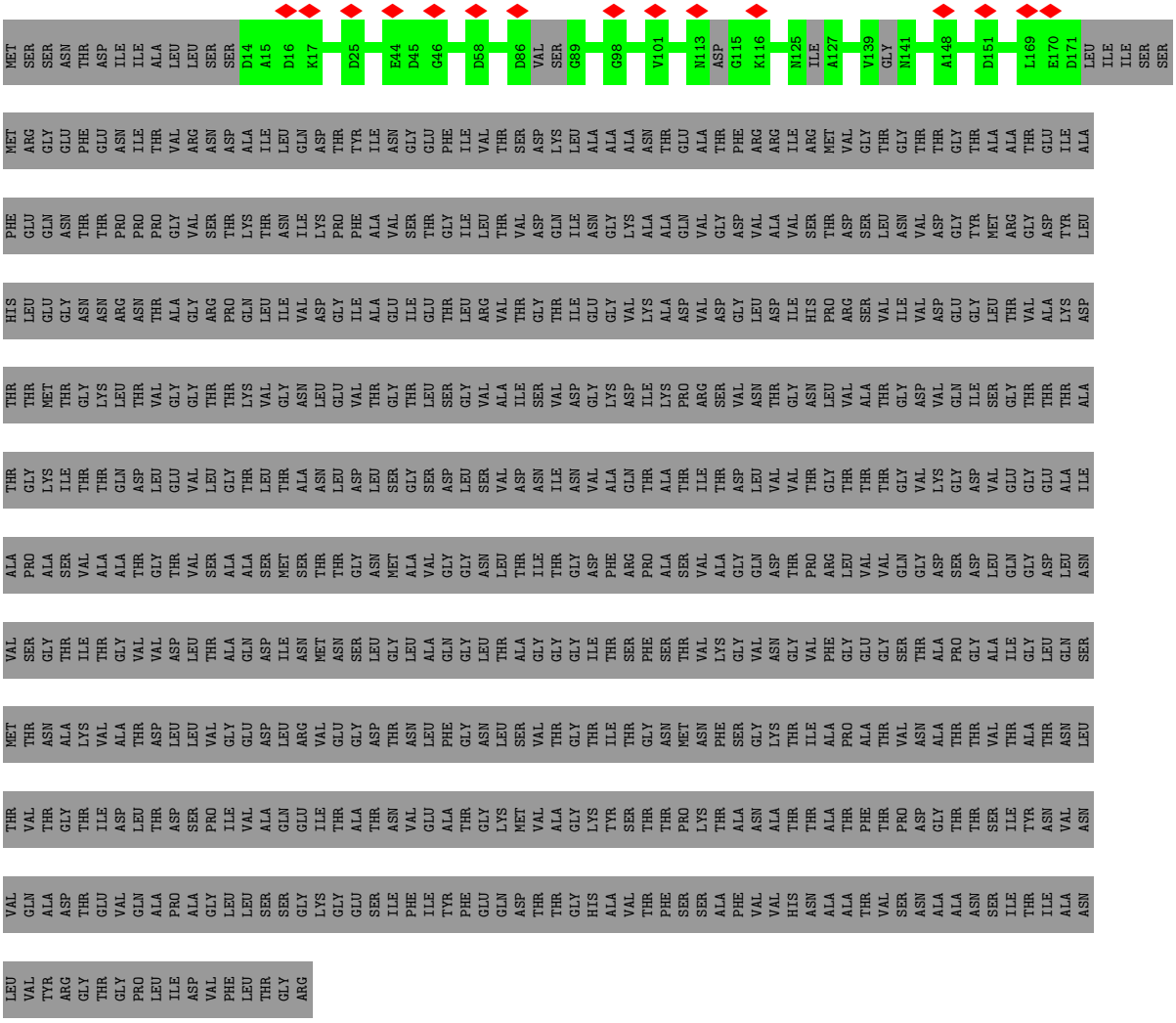
- Molecule 10: Putative tail fiber protein

Chain j:



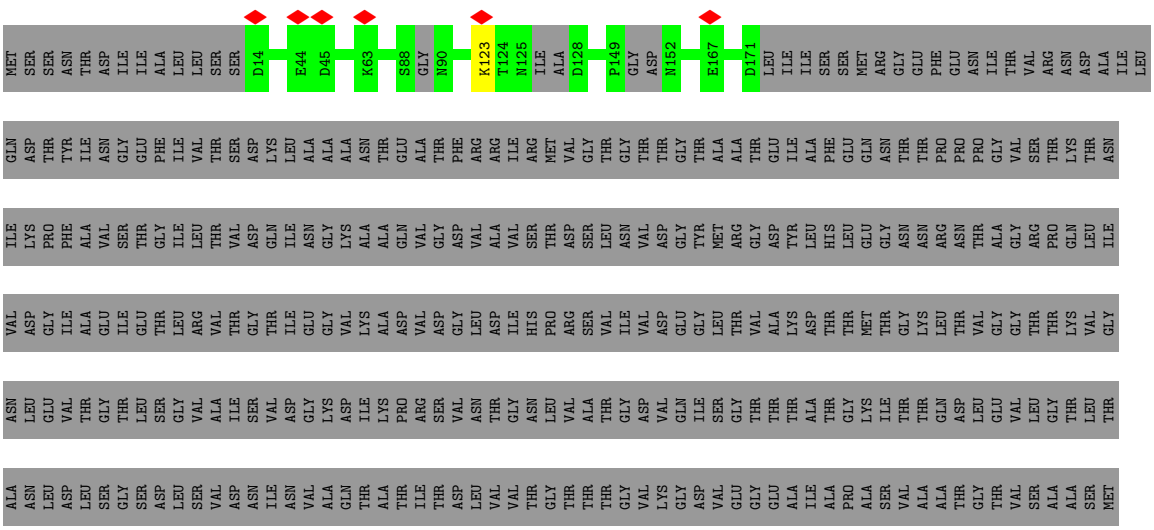
- Molecule 10: Putative tail fiber protein

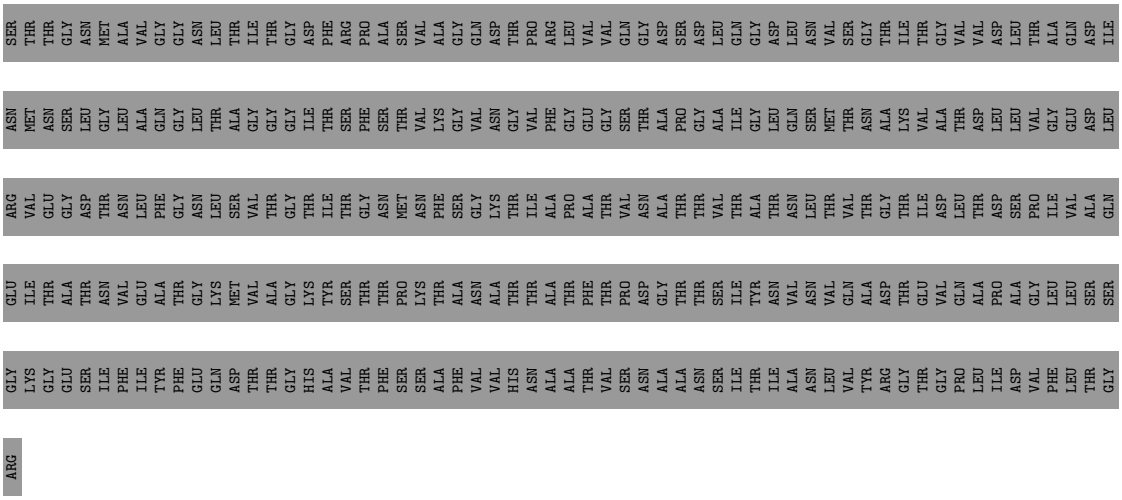
Chain k:



• Molecule 10: Putative tail fiber protein

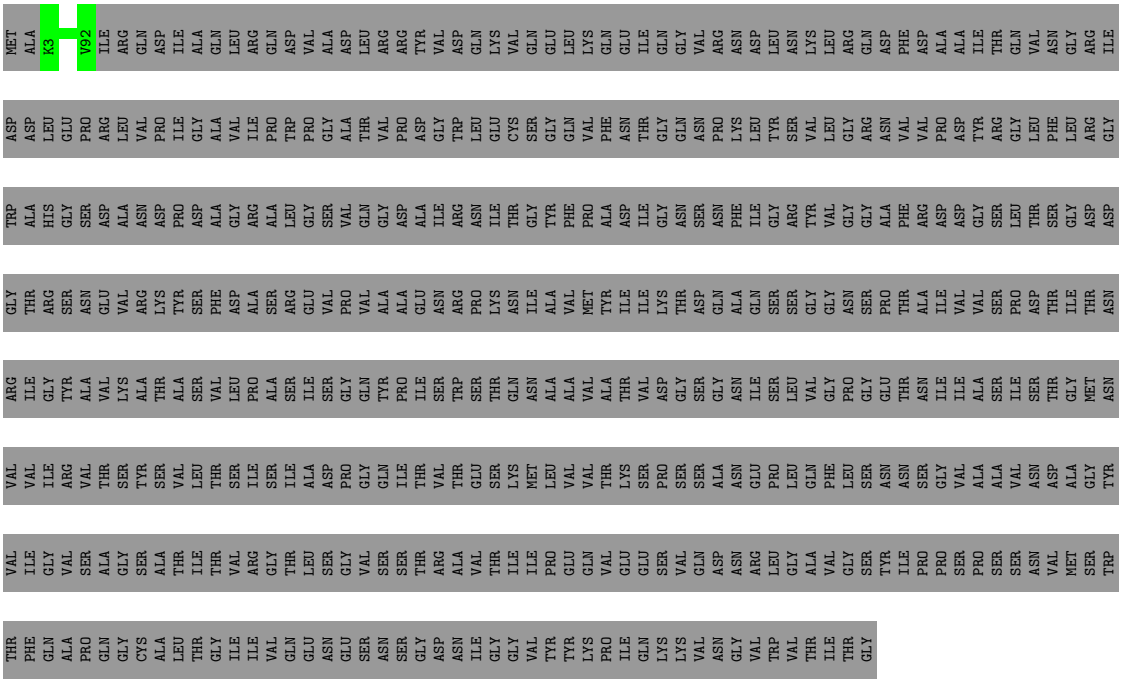
Chain l:





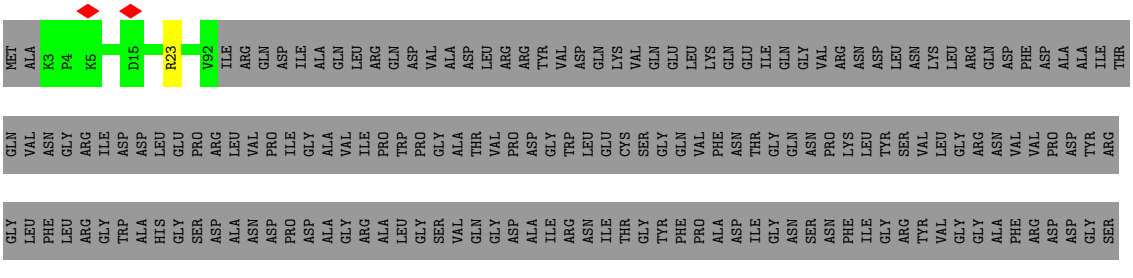
• Molecule 11: Short tail fiber

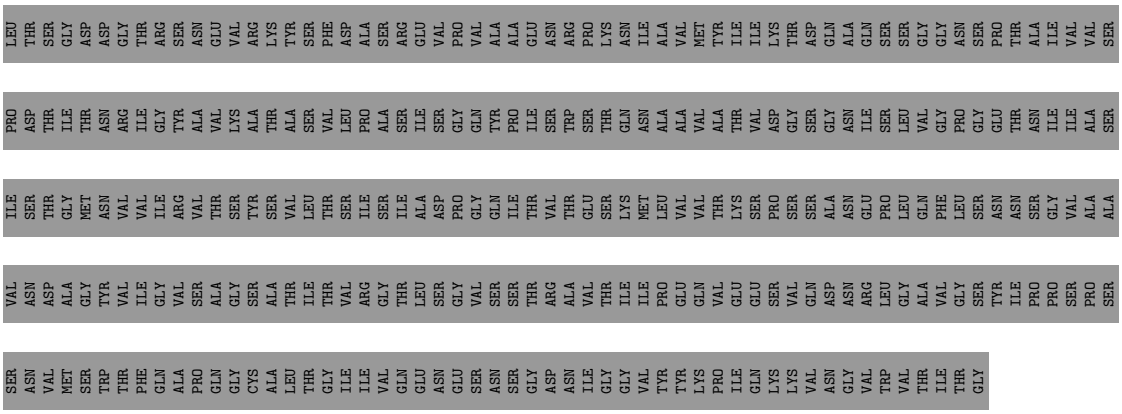
Chain c:



• Molecule 11: Short tail fiber

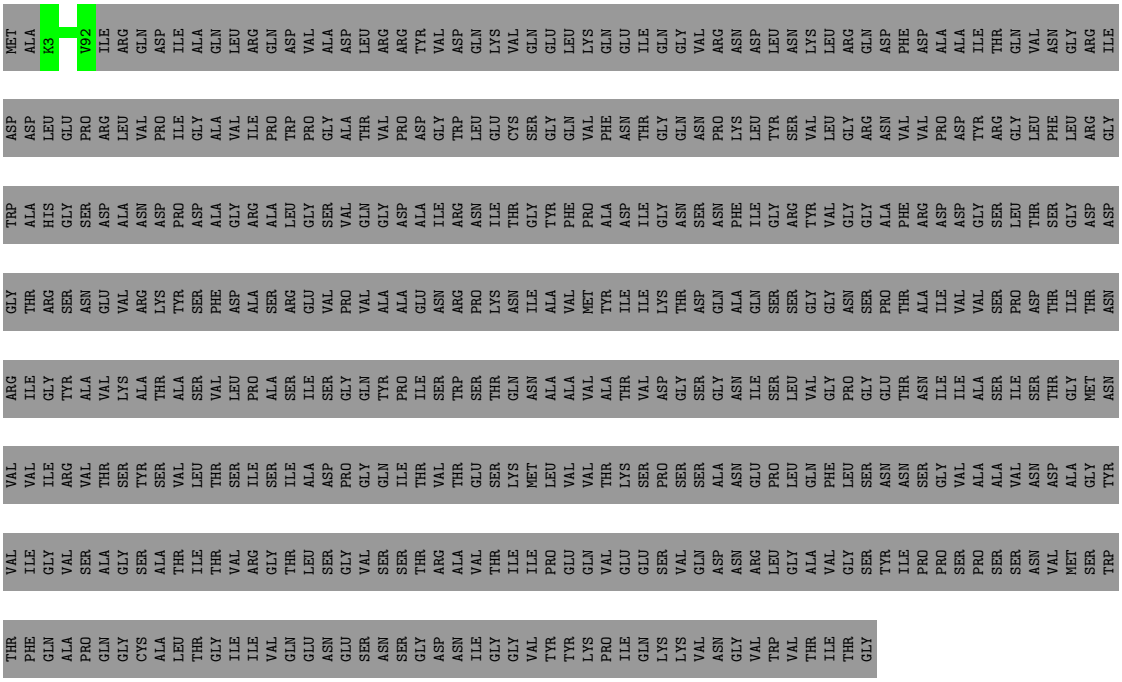
Chain a:





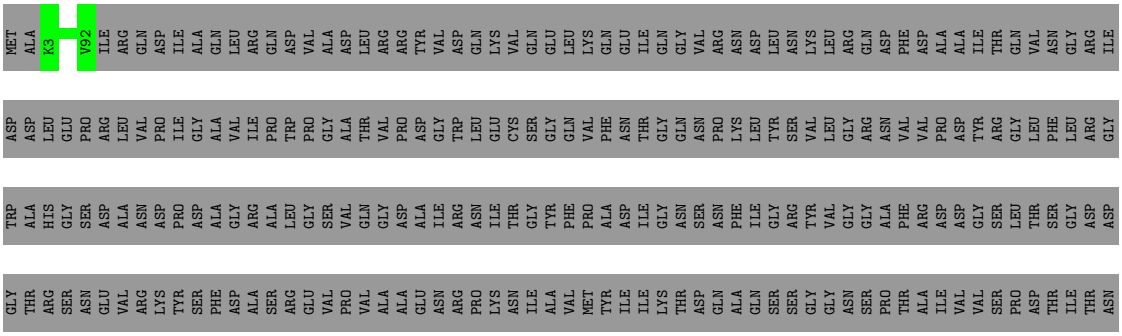
• Molecule 11: Short tail fiber

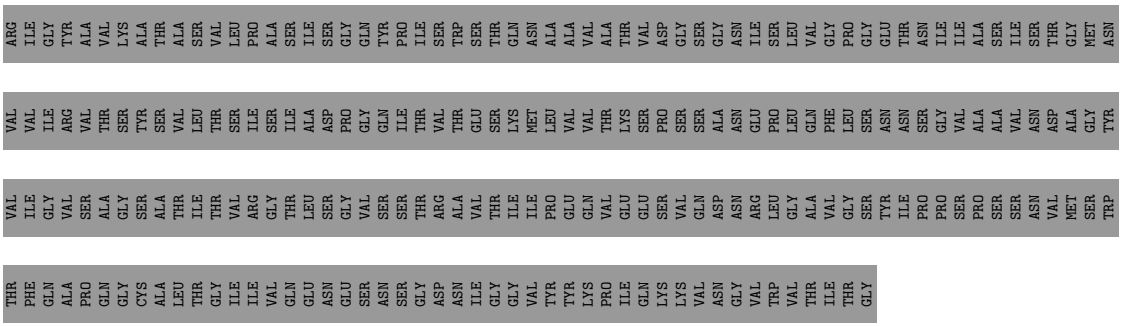
Chain b:



• Molecule 11: Short tail fiber

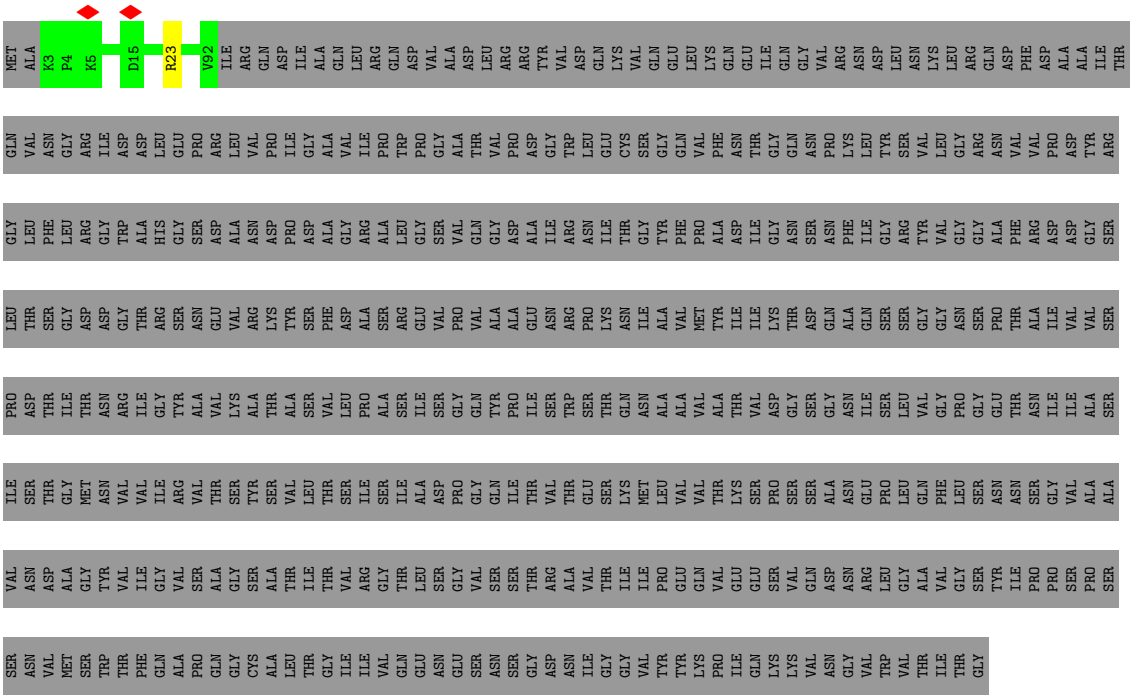
Chain f:





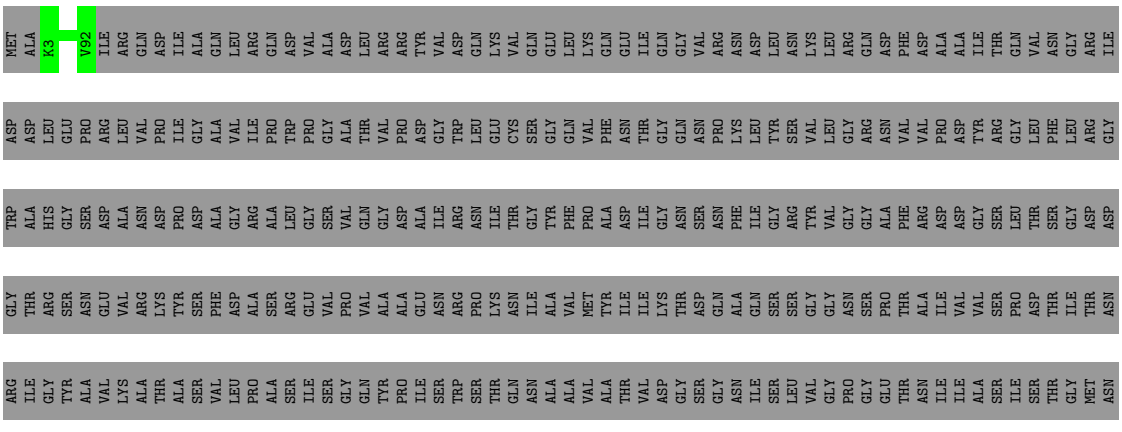
• Molecule 11: Short tail fiber

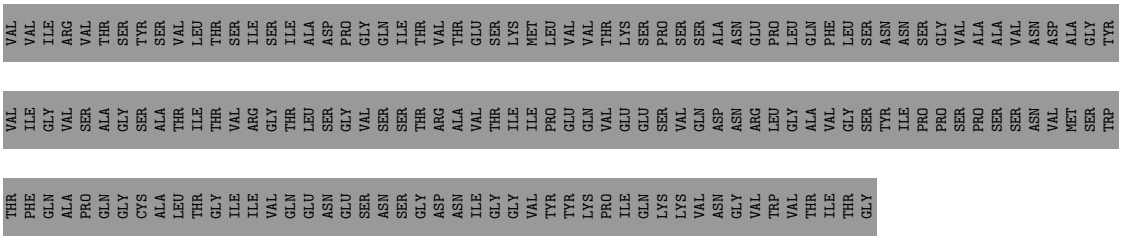
Chain d:



• Molecule 11: Short tail fiber

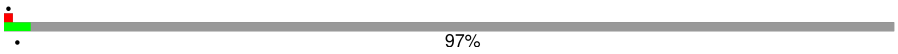
Chain e:

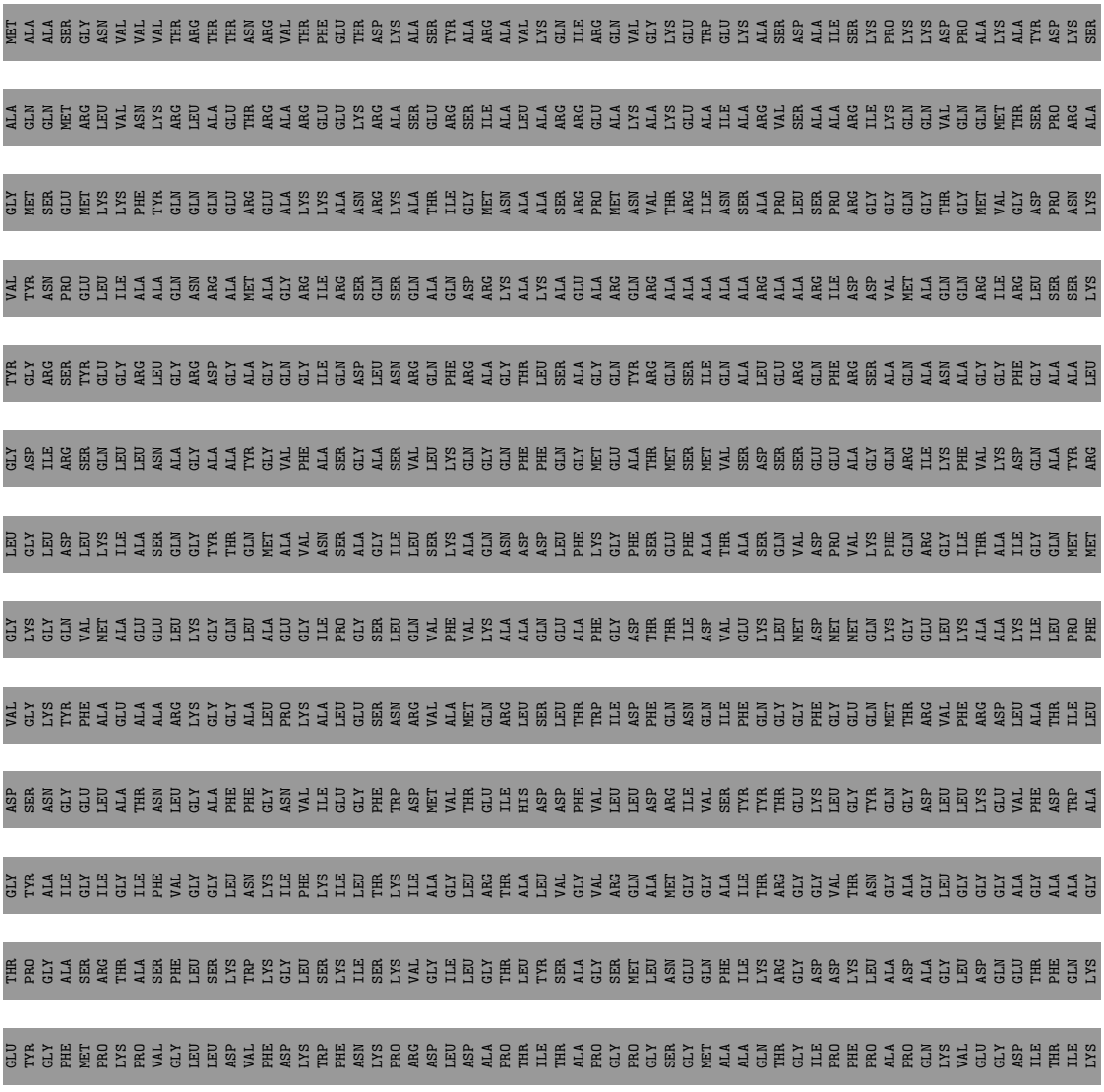




• Molecule 12: Putative tape measure protein

Chain W:





4 Experimental information (i)

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 ($e^-/Å^2$)	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

All (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
3	I	143	ASP
4	K	212	SER
4	K	233	VAL
1	R	488	VAL
1	U	488	VAL

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	T	28	PHE
1	T	80	ASP
1	T	81	ASP
1	T	256	ASP
1	T	343	PHE
1	T	344	MET
1	T	347	CYS
1	S	28	PHE
1	S	80	ASP
1	S	81	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S	256	ASP
1	S	343	PHE
1	S	344	MET
1	S	347	CYS
2	C	76	GLN
3	J	13	TYR
3	J	46	SER
3	J	56	SER
3	J	61	ARG
3	J	103	SER
3	H	43	ASP
3	H	60	SER
3	H	96	LEU
3	H	141	SER
2	D	76	GLN
3	I	13	TYR
3	I	46	SER
3	I	56	SER
3	I	61	ARG
3	I	103	SER
3	G	43	ASP
3	G	60	SER
3	G	96	LEU
3	G	141	SER
7	O	102	ASN
7	P	102	ASN
8	N	76	ARG
8	M	76	ARG
10	g	59	ASN
10	h	123	LYS
11	a	23	ARG
10	j	59	ASN
10	j	143	ARG
10	l	123	LYS
11	d	23	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	T	111	ASN
1	T	329	ASN
1	T	367	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S	111	ASN
1	S	329	ASN
1	S	367	ASN
2	A	278	ASN
2	C	386	ASN
2	E	386	ASN
3	J	99	GLN
3	H	99	GLN
3	H	117	GLN
2	B	439	ASN
2	D	386	ASN
2	D	463	GLN
2	F	386	ASN
3	I	44	ASN
3	I	99	GLN
3	G	99	GLN
4	K	219	ASN
5	X	188	ASN
6	Y	108	GLN
6	Y	195	GLN
6	Y	199	GLN
7	O	162	HIS
1	R	453	GLN
7	P	37	ASN
7	P	162	HIS
1	U	57	GLN
1	U	453	GLN
8	M	57	GLN
9	n	96	GLN
9	n	141	GLN
9	m	85	GLN
9	m	96	GLN
9	m	141	GLN
10	g	59	ASN
12	W	803	ASN
10	j	21	GLN
10	j	59	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

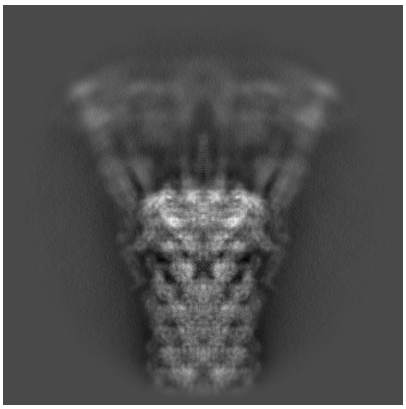
6 Map visualisation

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.

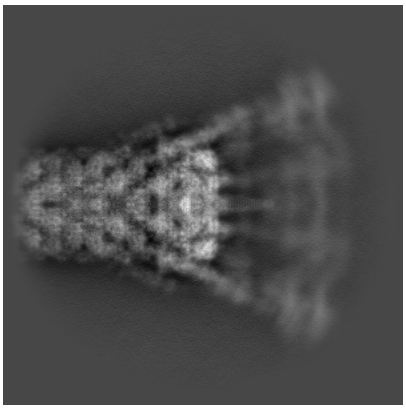
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

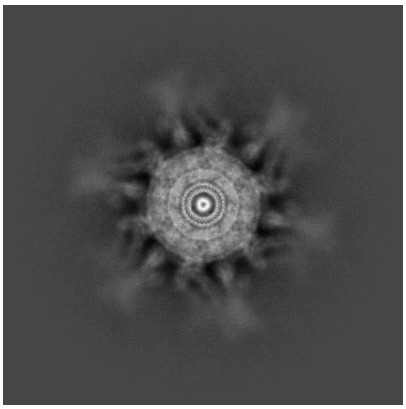
6.1.1 Primary map



X

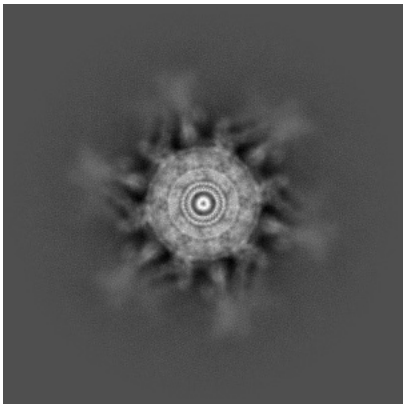


Y

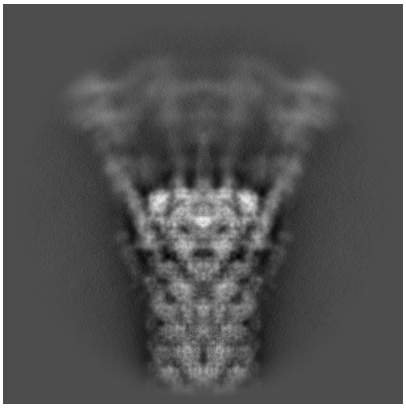


Z

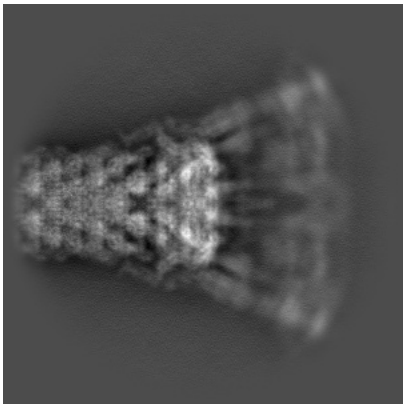
6.1.2 Raw map



X



Y

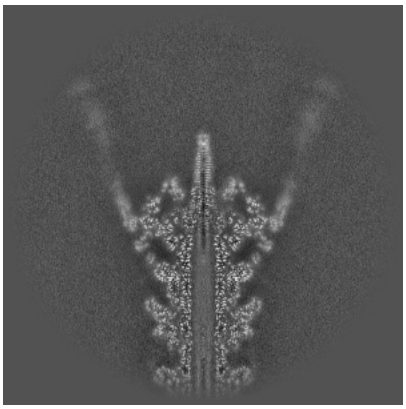


Z

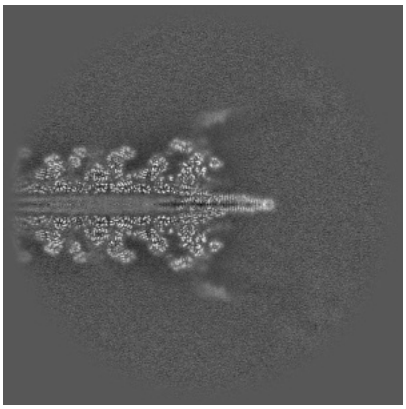
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

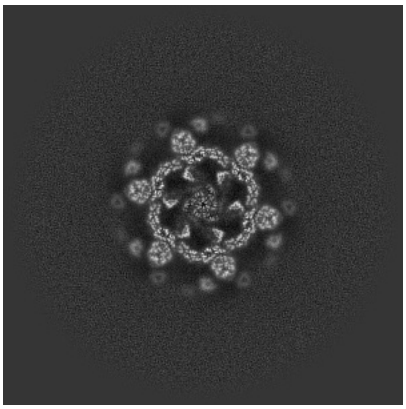
6.2.1 Primary map



X Index: 256

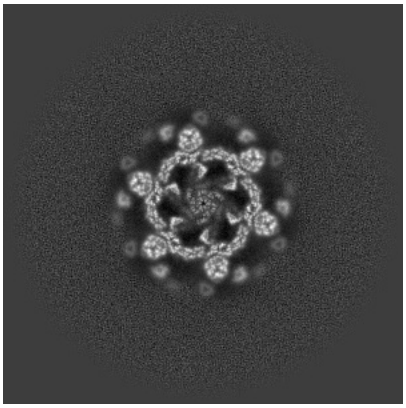


Y Index: 256

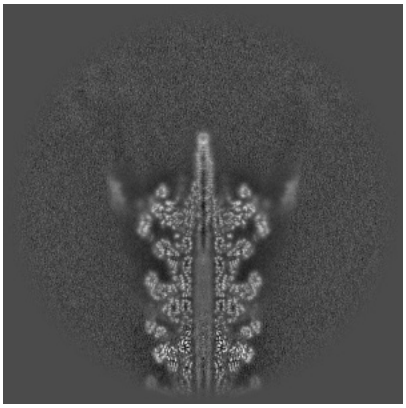


Z Index: 256

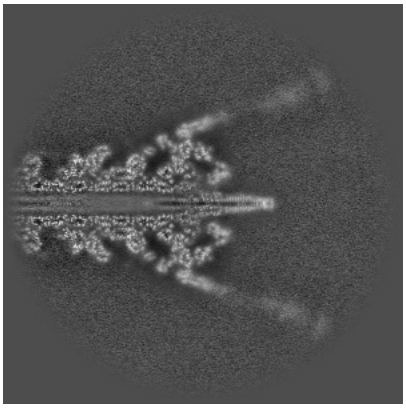
6.2.2 Raw map



X Index: 256



Y Index: 256

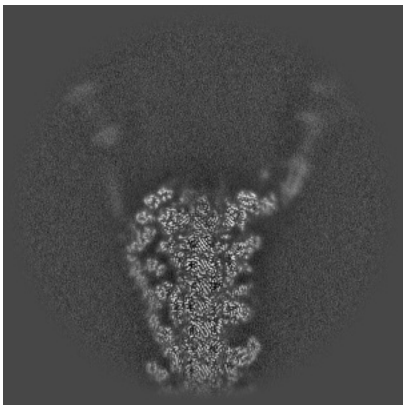


Z Index: 256

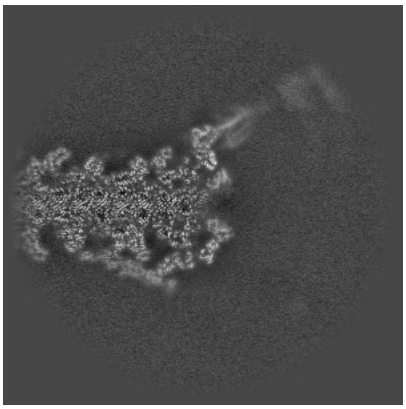
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

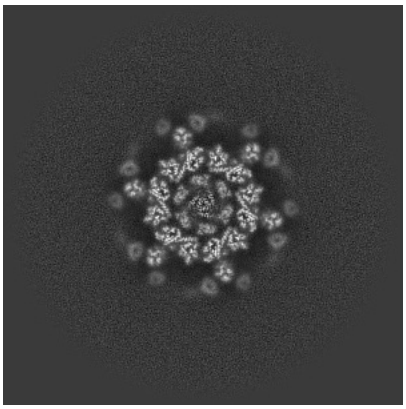
6.3.1 Primary map



X Index: 239

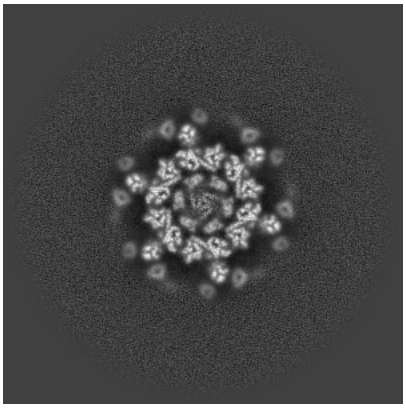


Y Index: 238

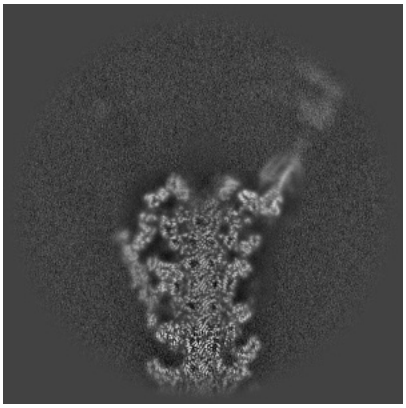


Z Index: 265

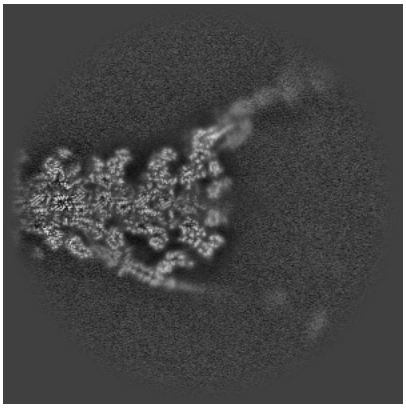
6.3.2 Raw map



X Index: 265



Y Index: 238

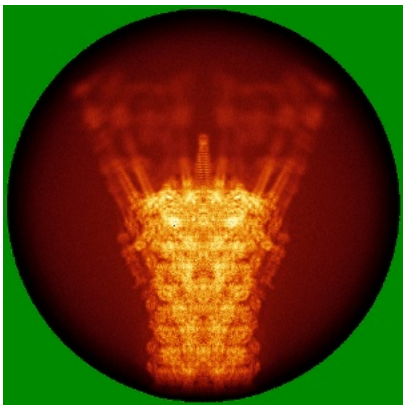


Z Index: 231

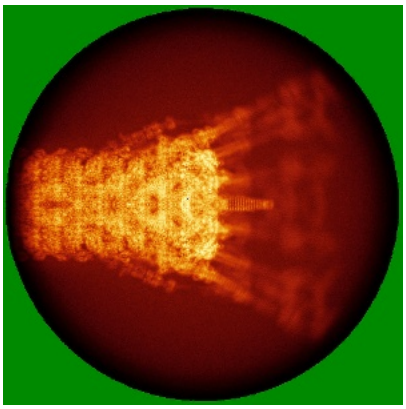
The images above show the largest variance slices of the map in three orthogonal directions.

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

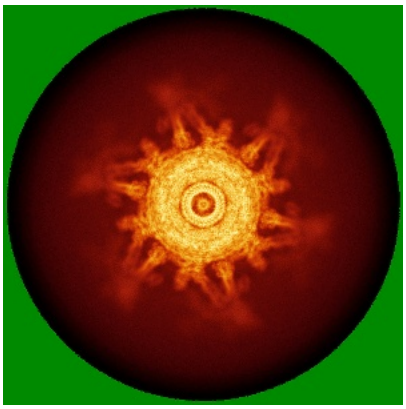
6.4.1 Primary map



X

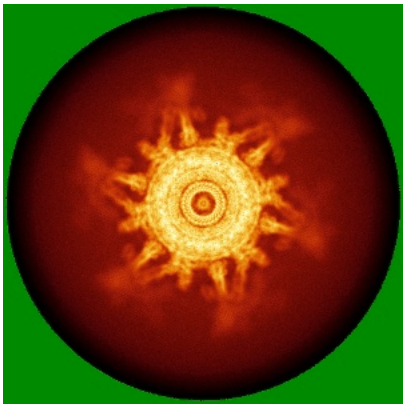


Y

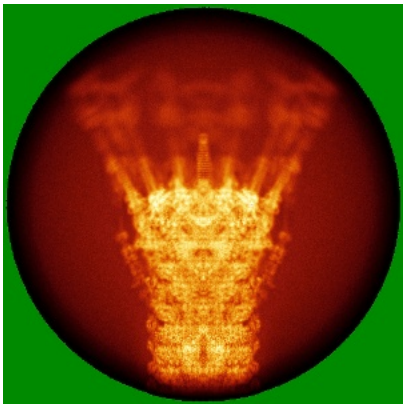


Z

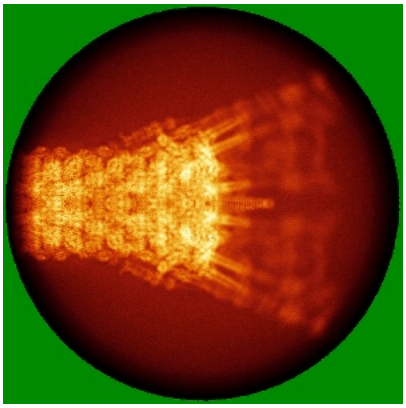
6.4.2 Raw map



X



Y

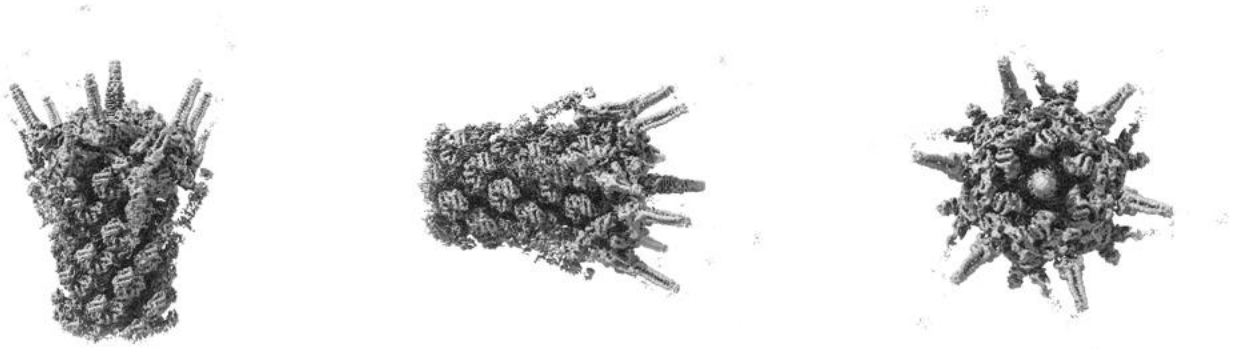


Z

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)

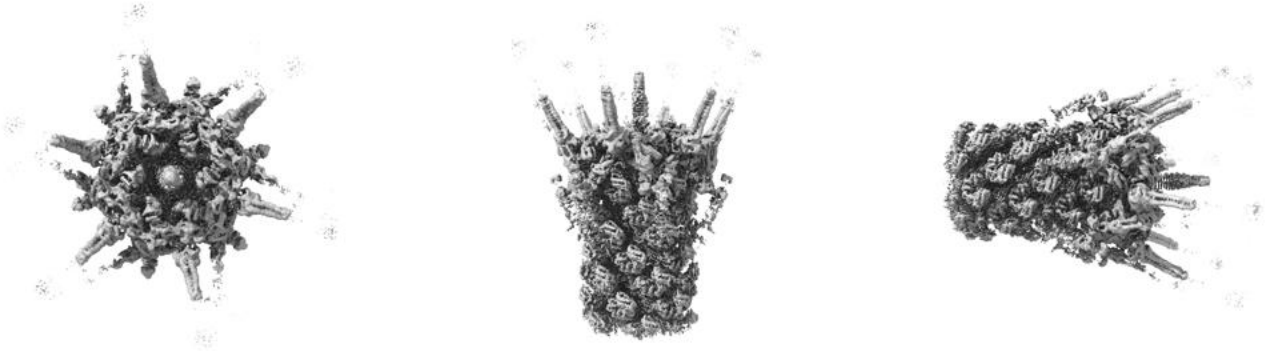
6.5.1 Primary map



X Y Z

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



X Y Z

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

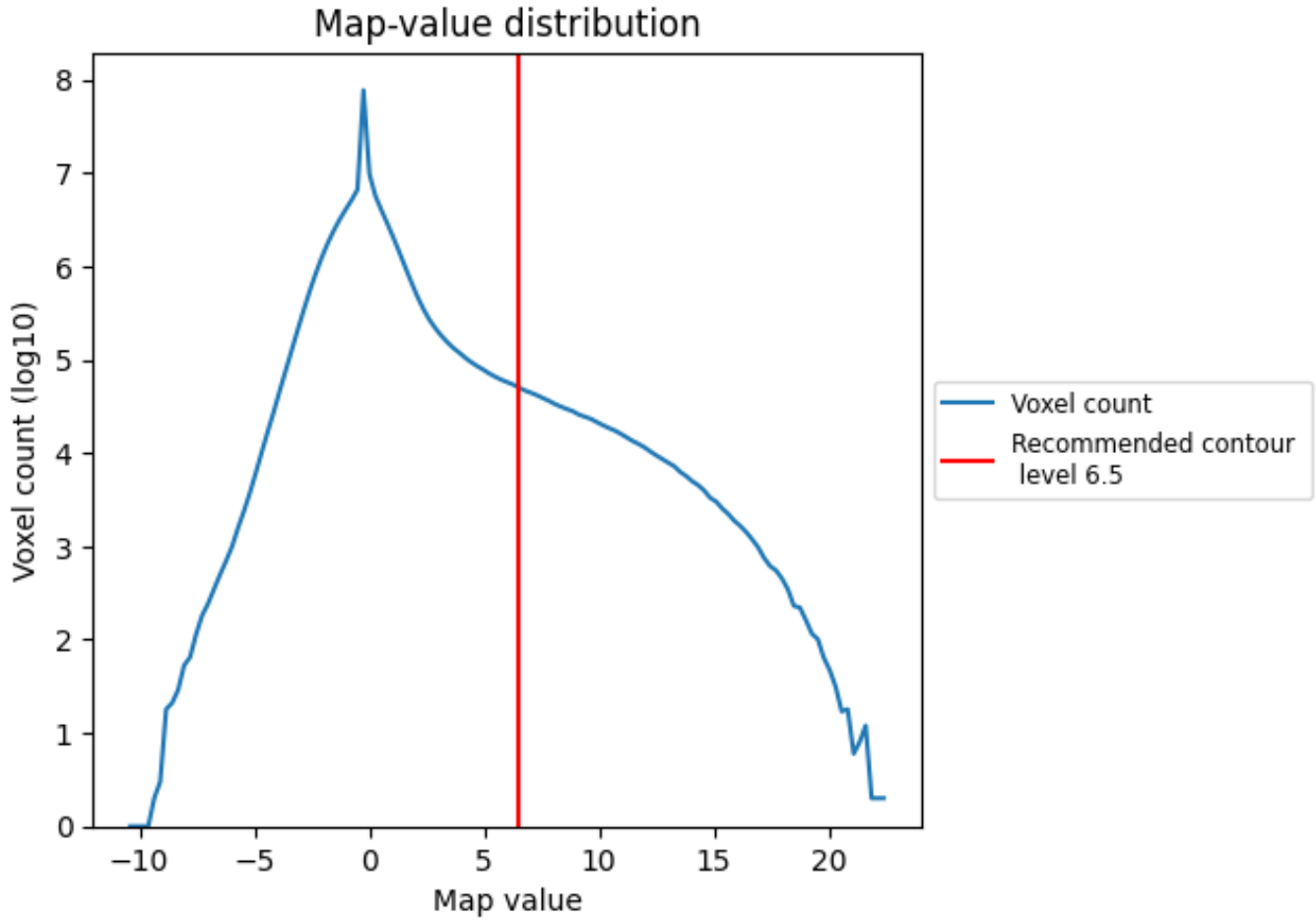
6.6 Mask visualisation (i)

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

7 Map analysis

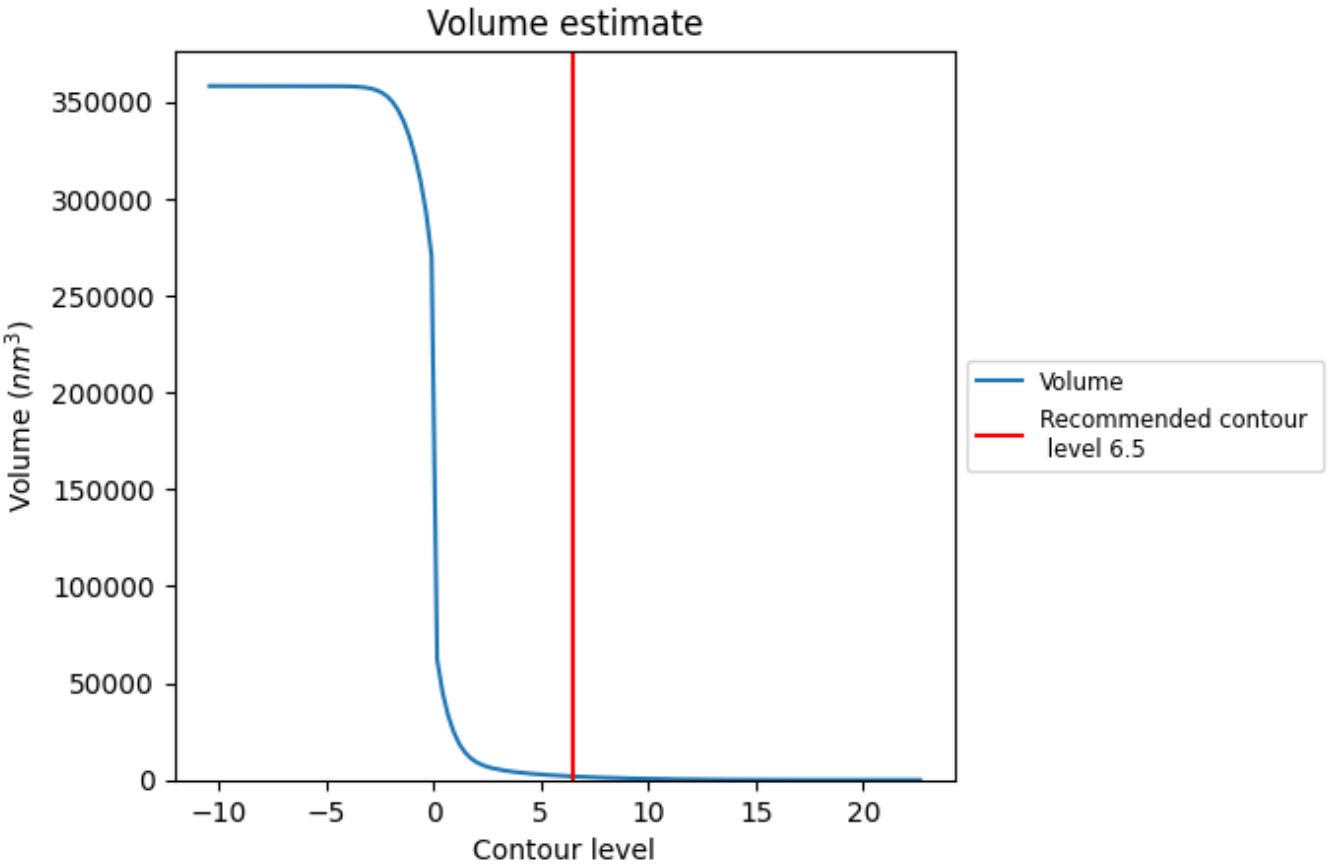
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

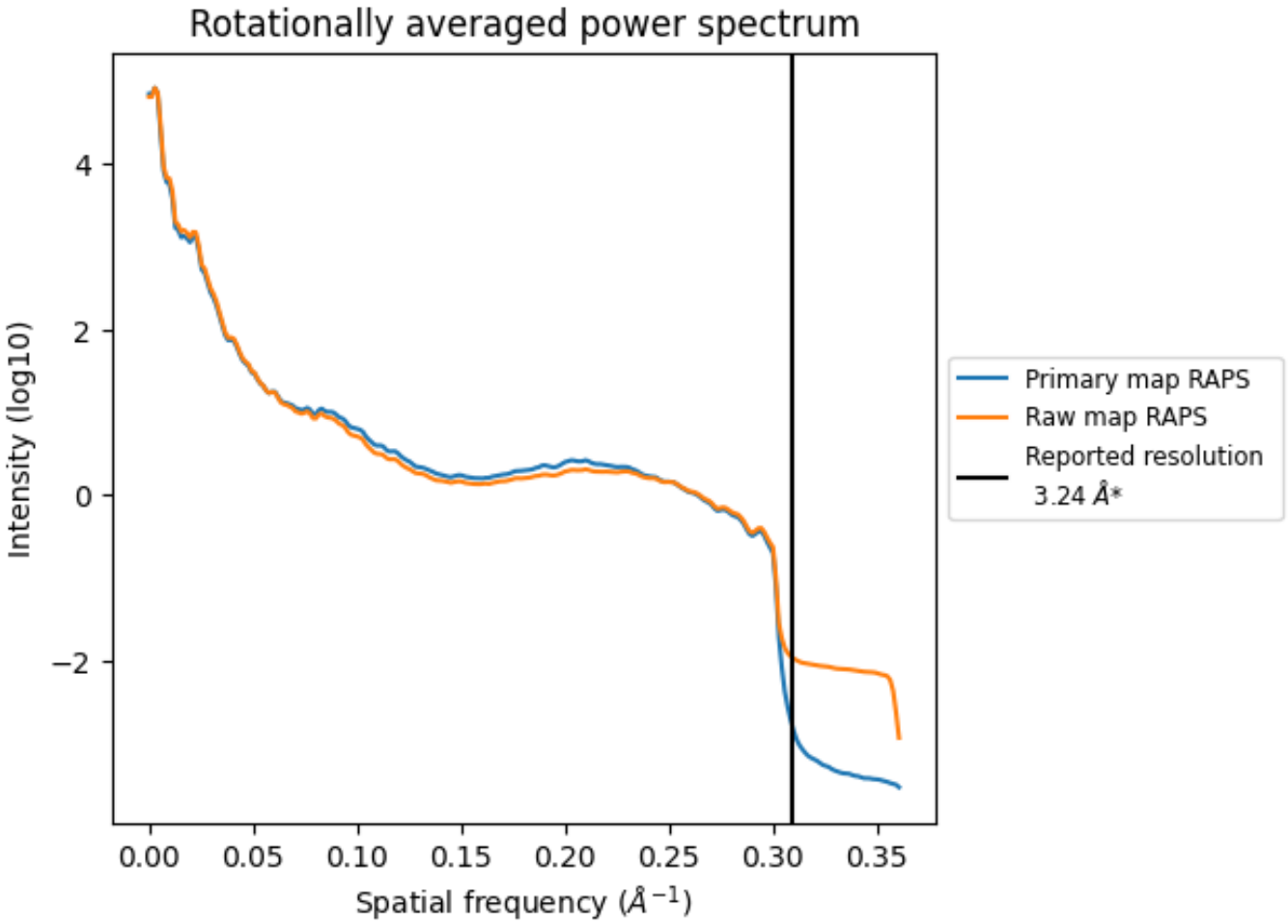
7.2 Volume estimate



The volume at the recommended contour level is 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 (i)

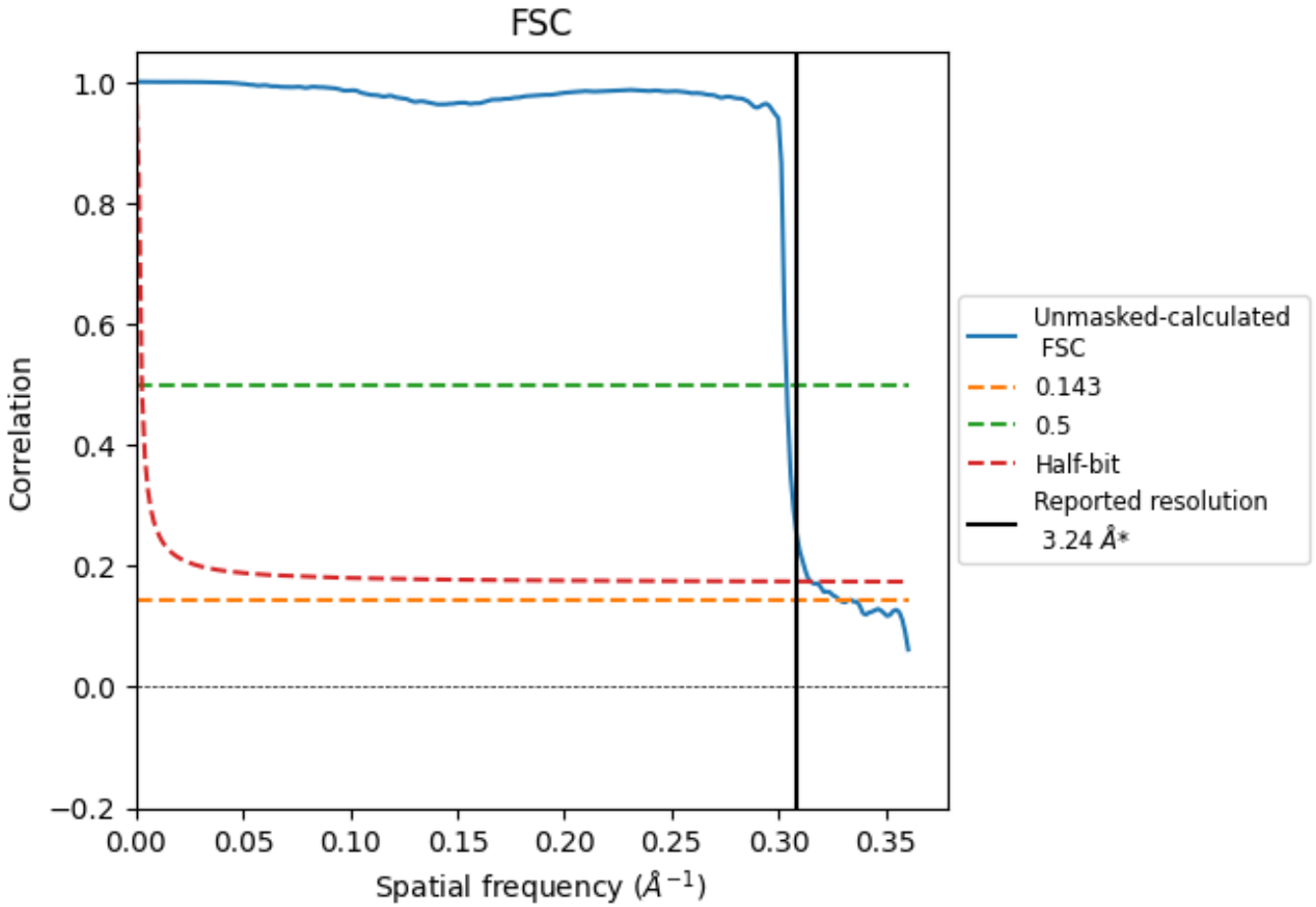


*Reported resolution corresponds to spatial frequency of 0.309 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.309 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

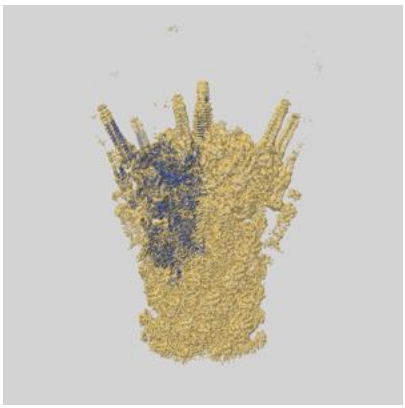
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit

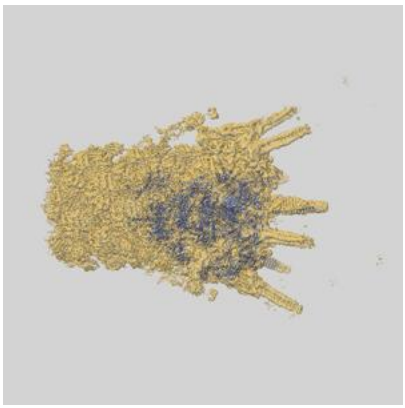
This section contains information regarding the fit between EMDB map EMD-45953 and PDB model 9CUY. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlays

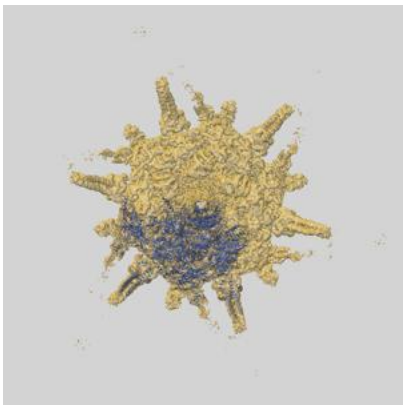
9.1.1 Map-model overlay



X

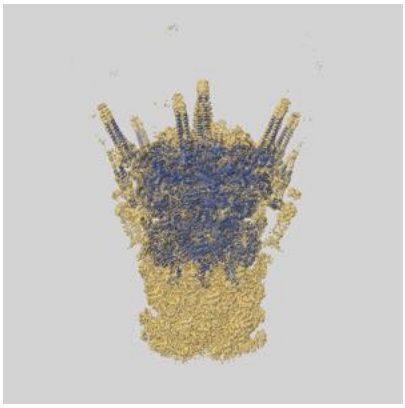


Y

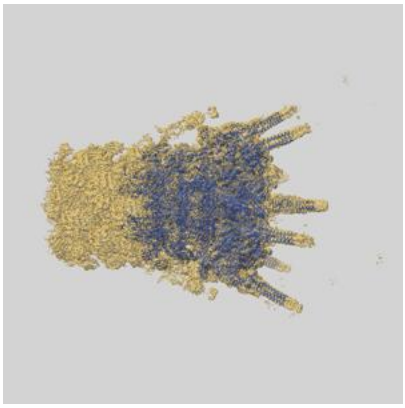


Z

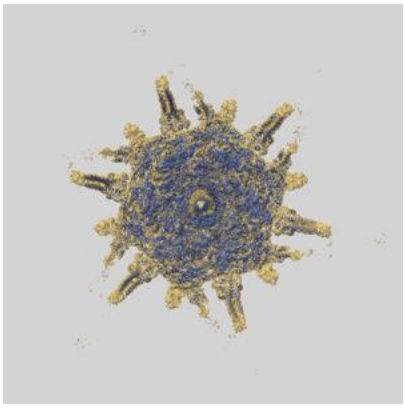
9.1.2 Map-model assembly overlay



X



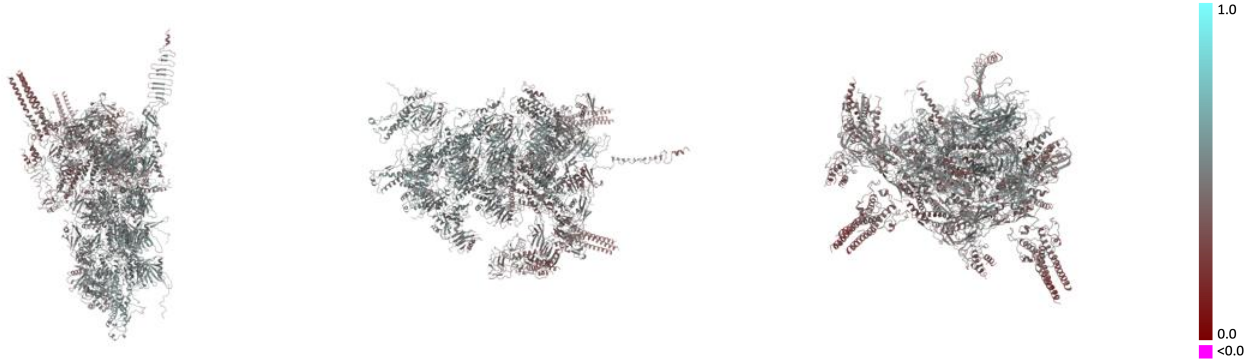
Y



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.

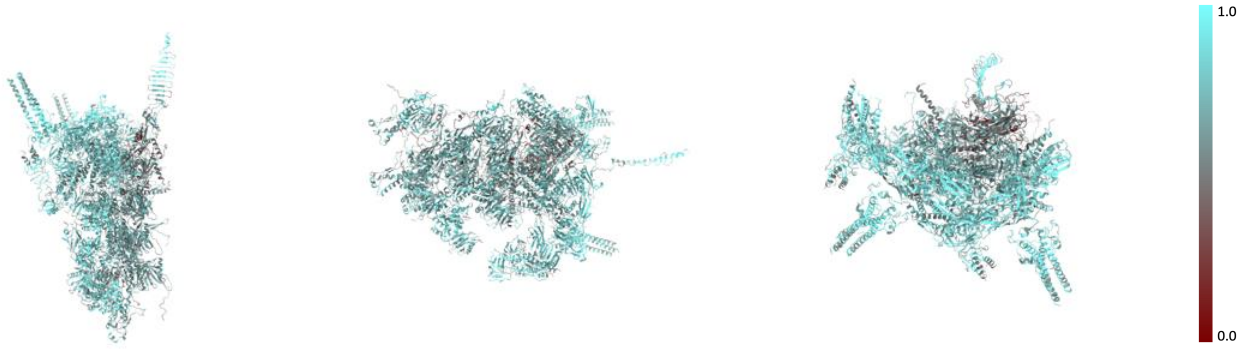
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

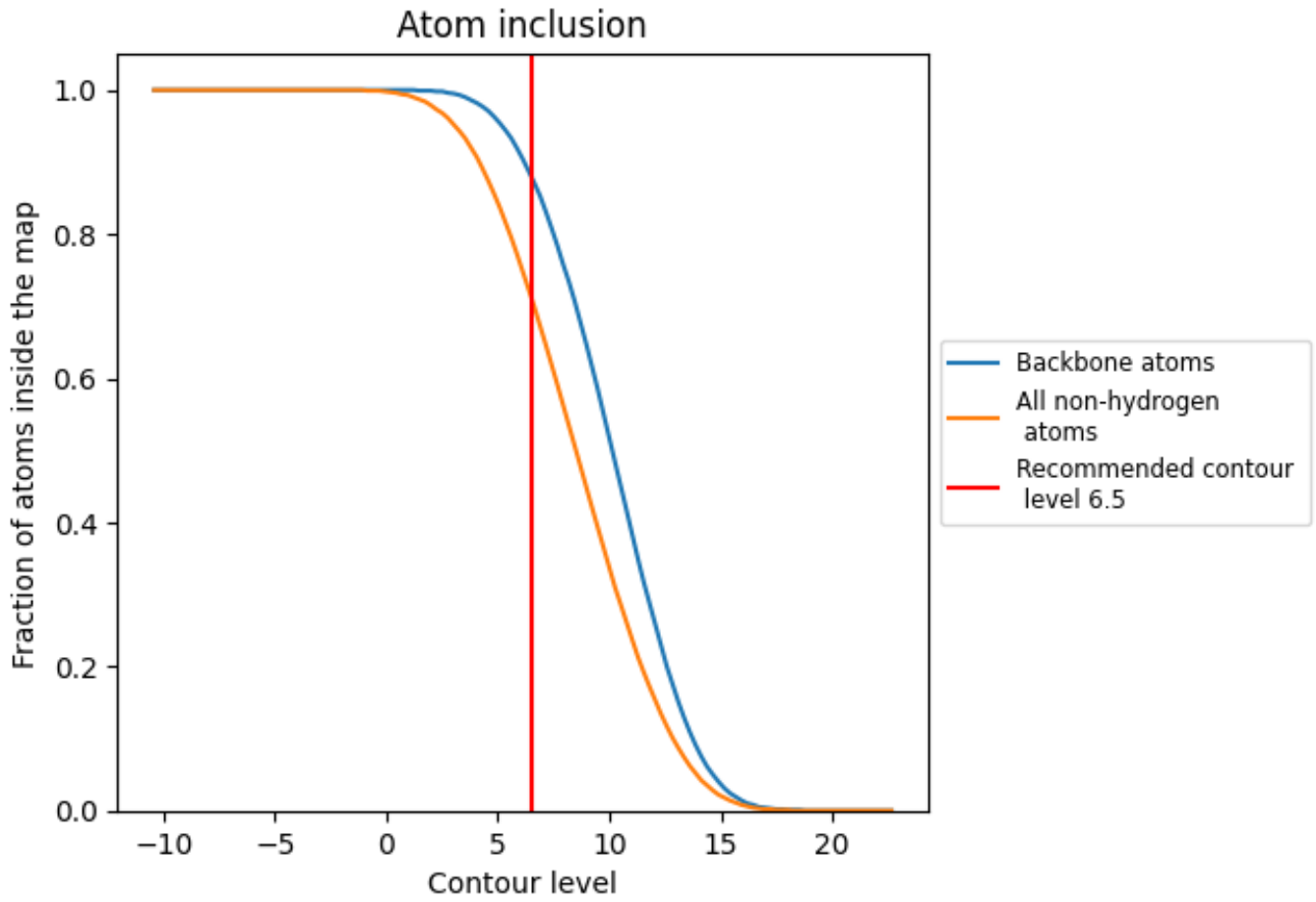
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (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

Continued on next page...

Continued from previous page...

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