Full wwPDB EM Validation Report

Oct 7, 2024 – 11:29 AM EDT

PDB ID	:	9B45
EMDB ID	:	EMD-44168
Title	:	Pseudomonas phage Pa193 baseplate complex and tail fiber
Authors	:	Iglesias, S.M.; Cingolani, G.
Deposited on	:	2024-03-20
Resolution	:	3.30 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:

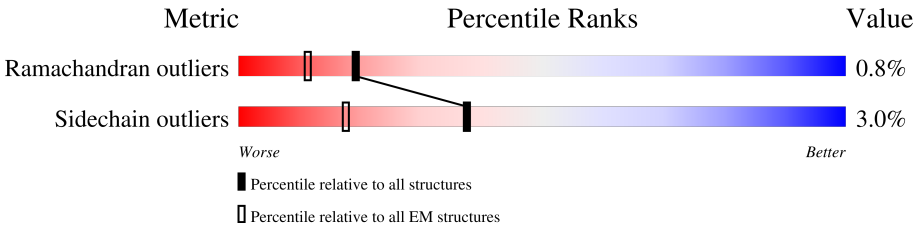
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.30 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	j	417	98%
1	k	417	97%
1	l	417	97%
1	m	417	97%
1	n	417	98%
1	o	417	98%
1	p	417	97%
1	q	417	6% 95% 5%
1	r	417	6% 96%

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Mol	Chain	Length	Quality of chain
1	s	417	96%
1	t	417	5% 96%
1	u	417	5% 96%
2	2	962	5% 34% 65%
2	3	962	6% 35% 65%
2	4	962	6% 33% 65%
3	A	107	94% 5%
3	B	107	94% 5%
3	C	107	95%
3	D	107	94% 5%
3	E	107	96%
3	F	107	94% 5%
4	S	180	93% 6%
4	T	180	93% 6%
4	U	180	91% 6%
5	a	858	98%
5	b	858	98%
5	c	858	98%
6	d	287	96%
6	e	287	97%
6	f	287	97%
7	V	197	94% 5%
7	W	197	94% 5%
7	X	197	94% 5%
8	1	504	96%

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Mol	Chain	Length	Quality of chain
8	v	504	96%
8	w	504	96%
8	x	504	94% 5%
8	y	504	95% 5%
8	z	504	95% 5%
9	M	167	88% 10%
9	N	167	88% 10%
9	O	167	89% 10%
9	P	167	89% 10%
9	Q	167	89% 10%
9	R	167	88% 10%
10	G	116	90% 7%
10	H	116	92% 7%
10	I	116	92% 7%
10	J	116	91% 7%
10	K	116	91% 7%
10	L	116	91% 7%
11	g	221	93%
11	h	221	93%
11	i	221	94%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 104304 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 gp45-a Baseplate wedge 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	j	416	Total	C	N	O	S	0	0
			3028	1897	525	596	10		
1	k	416	Total	C	N	O	S	0	0
			3028	1897	525	596	10		
1	l	416	Total	C	N	O	S	0	0
			3028	1897	525	596	10		
1	m	416	Total	C	N	O	S	0	0
			3028	1897	525	596	10		
1	n	416	Total	C	N	O	S	0	0
			3028	1897	525	596	10		
1	o	416	Total	C	N	O	S	0	0
			3028	1897	525	596	10		
1	q	416	Total	C	N	O	S	0	0
			3027	1897	525	595	10		
1	p	416	Total	C	N	O	S	0	0
			3027	1897	525	595	10		
1	r	416	Total	C	N	O	S	0	0
			3027	1897	525	595	10		
1	s	416	Total	C	N	O	S	0	0
			3027	1897	525	595	10		
1	t	416	Total	C	N	O	S	0	0
			3027	1897	525	595	10		
1	u	416	Total	C	N	O	S	0	0
			3027	1897	525	595	10		

- Molecule 2 is a protein called gp47 Tail fiber.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	340	Total	C	N	O	S	0	0
			2547	1601	450	483	13		
2	3	340	Total	C	N	O	S	0	0
			2547	1601	450	483	13		
2	4	340	Total	C	N	O	S	0	0
			2547	1601	450	483	13		

- Molecule 3 is a protein called gp34 helical bundle.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	106	Total	C	N	O	S	0	0
			854	548	146	154	6		
3	B	106	Total	C	N	O	S	0	0
			854	548	146	154	6		
3	C	106	Total	C	N	O	S	0	0
			854	548	146	154	6		
3	D	106	Total	C	N	O	S	0	0
			854	548	146	154	6		
3	E	106	Total	C	N	O	S	0	0
			854	548	146	154	6		
3	F	106	Total	C	N	O	S	0	0
			854	548	146	154	6		

- Molecule 4 is a protein called gp38 Ripcord-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	170	Total	C	N	O	S	0	0
			1320	823	230	255	12		
4	T	170	Total	C	N	O	S	0	0
			1320	823	230	255	12		
4	U	170	Total	C	N	O	S	0	0
			1320	823	230	255	12		

- Molecule 5 is a protein called gp41 Tape measure protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	a	19	Total	C	N	O	0	0
			146	90	24	32		
5	b	19	Total	C	N	O	0	0
			146	90	24	32		
5	c	19	Total	C	N	O	0	0
			146	90	24	32		

- Molecule 6 is a protein called gp42 Tail hub.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	d	285	Total	C	N	O	S	0	0
			2261	1430	395	423	13		
6	e	285	Total	C	N	O	S	0	0
			2261	1430	395	423	13		
6	f	285	Total	C	N	O	S	0	0
			2261	1430	395	423	13		

- Molecule 7 is a protein called gp39 Ripcord-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	V	188	Total	C	N	O	S	0	0
			1436	906	230	293	7		
7	W	188	Total	C	N	O	S	0	0
			1436	906	230	293	7		
7	X	188	Total	C	N	O	S	0	0
			1436	906	230	293	7		

- Molecule 8 is a protein called gp46 Baseplate wedge 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	v	503	Total	C	N	O	S	0	0
			3844	2448	644	738	14		
8	w	503	Total	C	N	O	S	0	0
			3844	2448	644	738	14		
8	x	503	Total	C	N	O	S	0	0
			3844	2448	644	738	14		
8	y	503	Total	C	N	O	S	0	0
			3844	2448	644	738	14		
8	z	503	Total	C	N	O	S	0	0
			3844	2448	644	738	14		
8	1	503	Total	C	N	O	S	0	0
			3844	2448	644	738	14		

- Molecule 9 is a protein called gp37 Baseplate tube.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	151	Total	C	N	O	S	0	0
			1128	723	181	220	4		
9	N	151	Total	C	N	O	S	0	0
			1128	723	181	220	4		
9	O	151	Total	C	N	O	S	0	0
			1128	723	181	220	4		
9	P	151	Total	C	N	O	S	0	0
			1128	723	181	220	4		
9	Q	151	Total	C	N	O	S	0	0
			1128	723	181	220	4		
9	R	151	Total	C	N	O	S	0	0
			1128	723	181	220	4		

- Molecule 10 is a protein called gp35 Sheath initiator.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	108	Total	C	N	O	S	0	0
			823	510	137	172	4		
10	H	108	Total	C	N	O	S	0	0
			823	510	137	172	4		
10	I	108	Total	C	N	O	S	0	0
			823	510	137	172	4		
10	J	108	Total	C	N	O	S	0	0
			823	510	137	172	4		
10	K	108	Total	C	N	O	S	0	0
			823	510	137	172	4		
10	L	108	Total	C	N	O	S	0	0
			823	510	137	172	4		

- Molecule 11 is a protein called gp44 Tail tip.

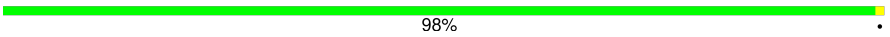
Mol	Chain	Residues	Atoms					AltConf	Trace
11	g	214	Total	C	N	O	S	0	0
			1650	1026	302	317	5		
11	h	214	Total	C	N	O	S	0	0
			1650	1026	302	317	5		
11	i	214	Total	C	N	O	S	0	0
			1650	1026	302	317	5		

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.

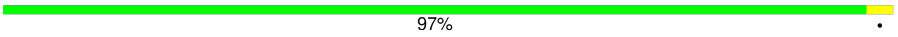
• Molecule 1: gp45-a Baseplate wedge 1

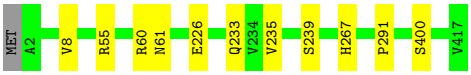
Chain j:



• Molecule 1: gp45-a Baseplate wedge 1

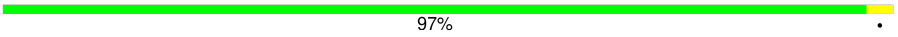
Chain k:





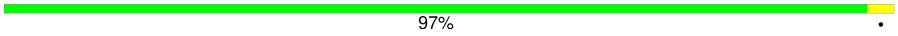
• Molecule 1: gp45-a Baseplate wedge 1

Chain l:



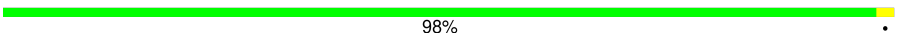
• Molecule 1: gp45-a Baseplate wedge 1

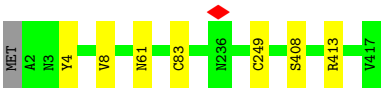
Chain m:



• Molecule 1: gp45-a Baseplate wedge 1

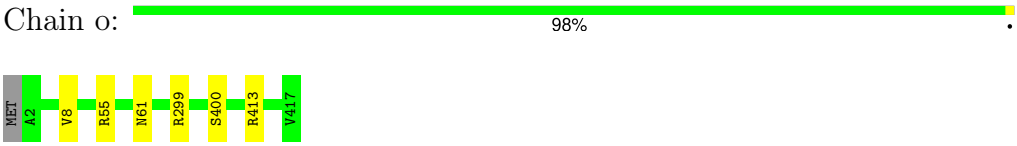
Chain n:





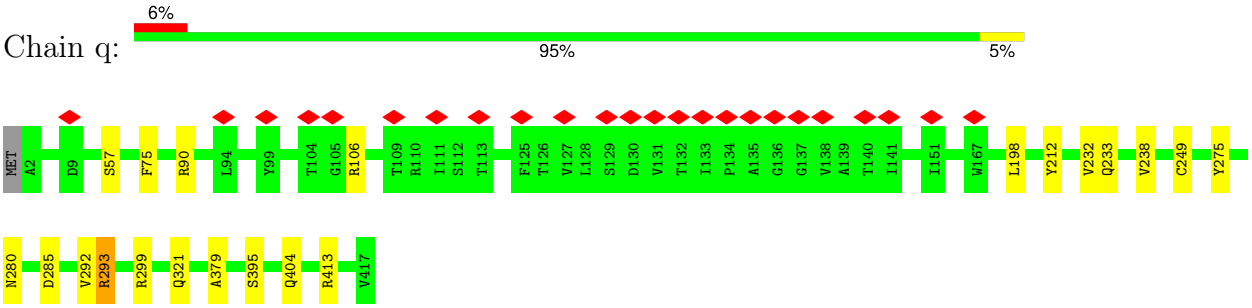
• Molecule 1: gp45-a Baseplate wedge 1

Chain o:



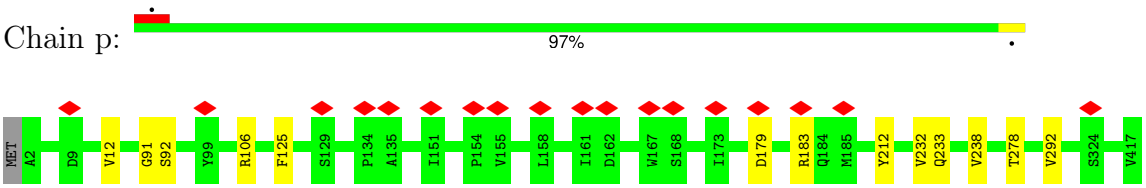
• Molecule 1: gp45-a Baseplate wedge 1

Chain q:



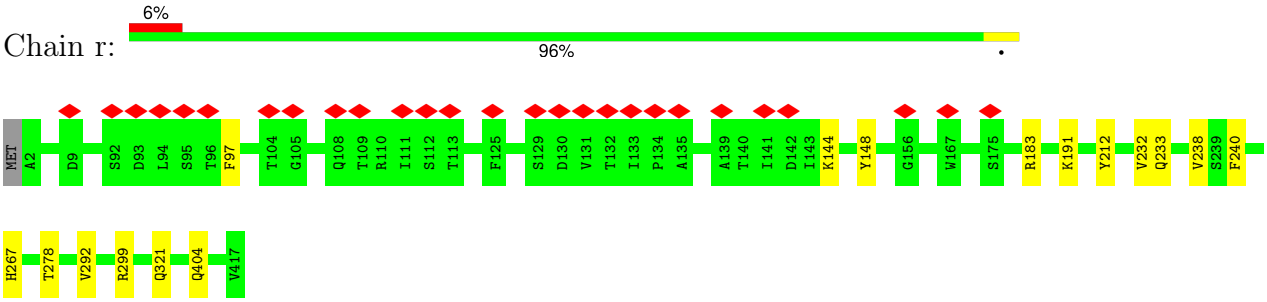
• Molecule 1: gp45-a Baseplate wedge 1

Chain p:



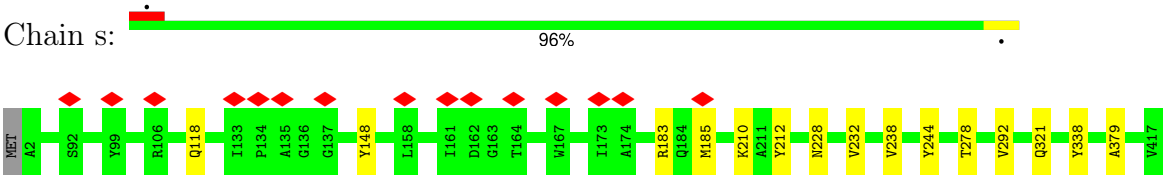
• Molecule 1: gp45-a Baseplate wedge 1

Chain r:



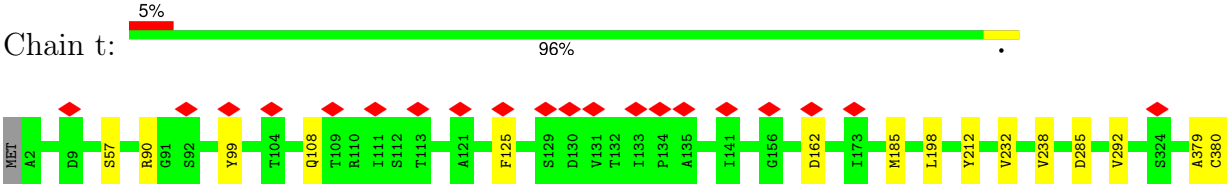
• Molecule 1: gp45-a Baseplate wedge 1

Chain s:

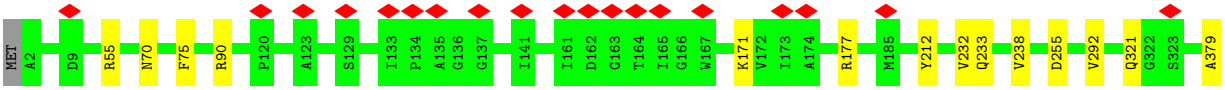


• Molecule 1: gp45-a Baseplate wedge 1

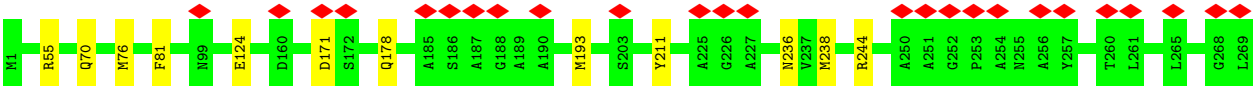
Chain t:

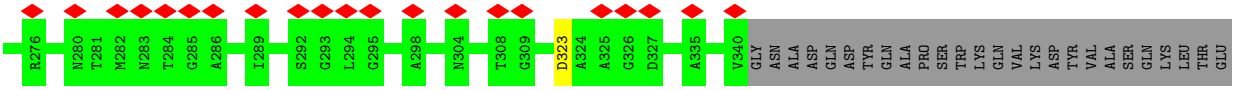


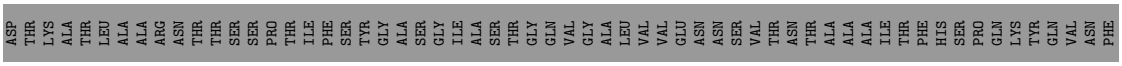
• Molecule 1: gp45-a Baseplate wedge 1



• Molecule 2: gp47 Tail fiber

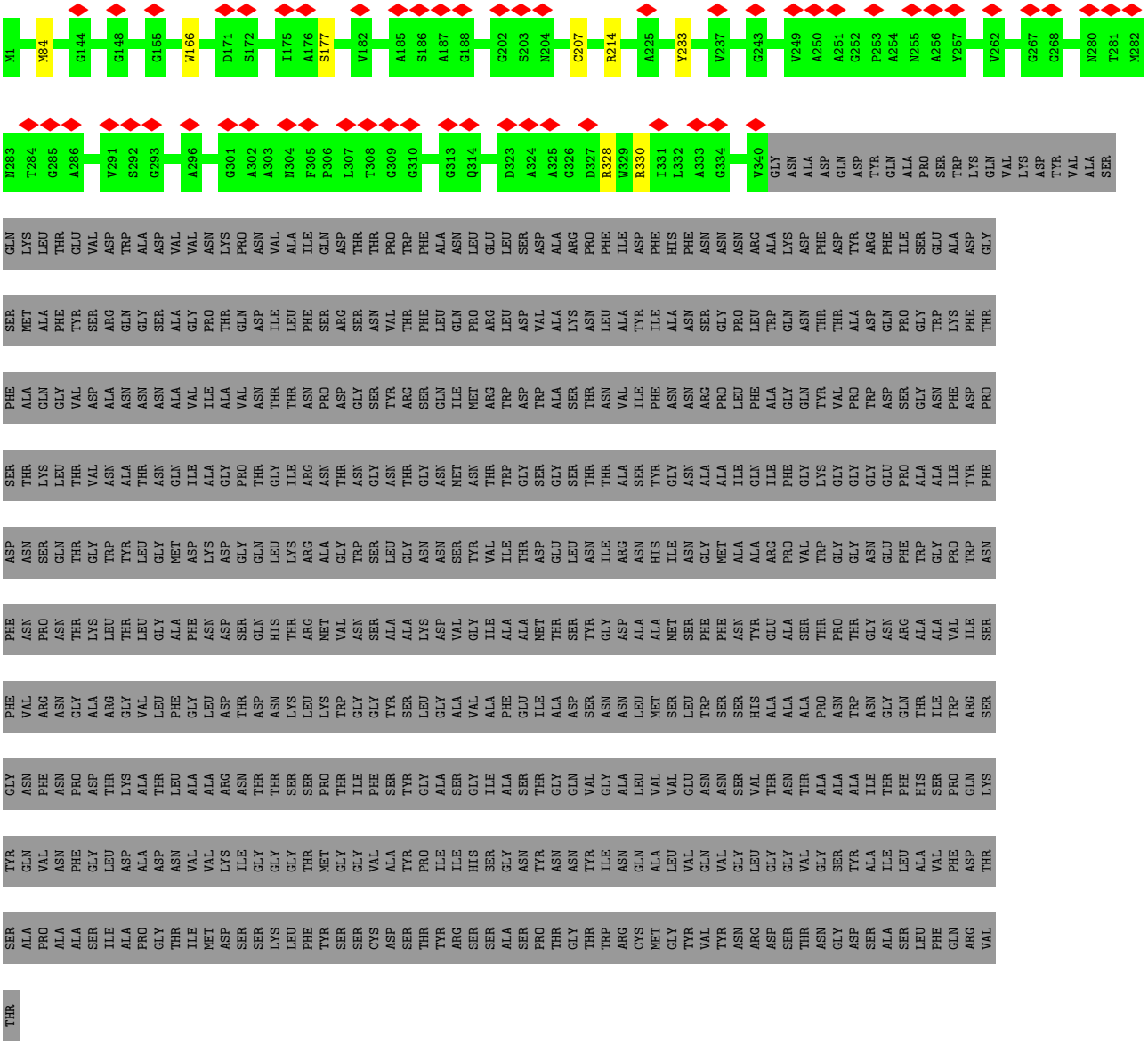






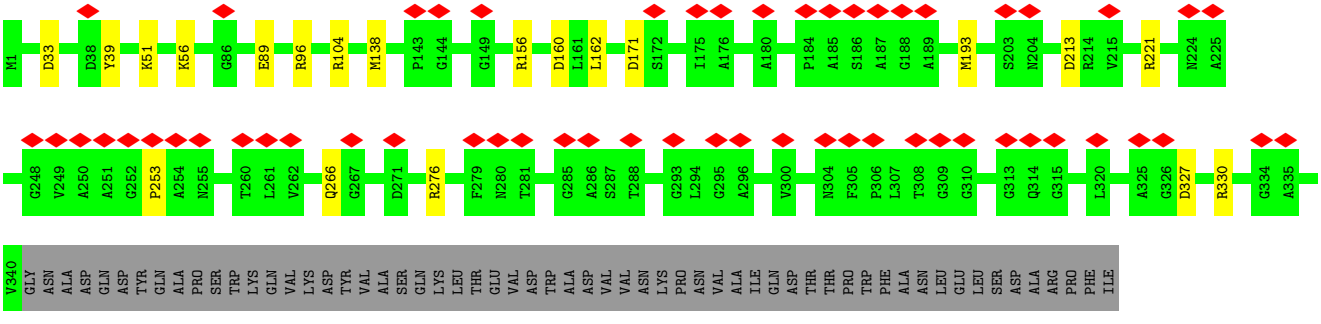
• Molecule 2: gp47 Tail fiber

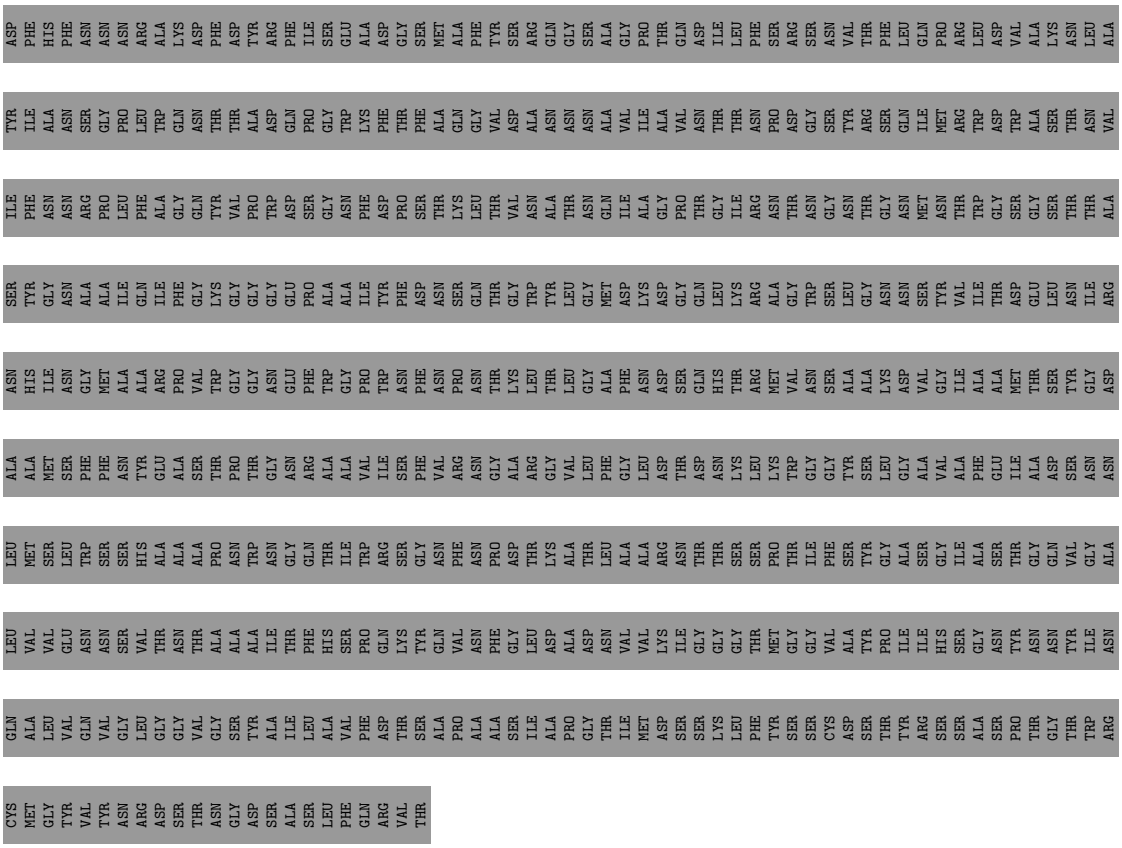
Chain 3:



• Molecule 2: gp47 Tail fiber

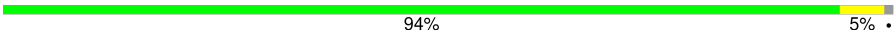
Chain 4:





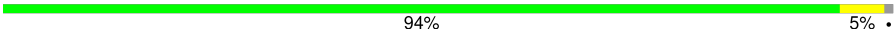
- Molecule 3: gp34 helical bundle

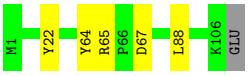
Chain A:



- Molecule 3: gp34 helical bundle

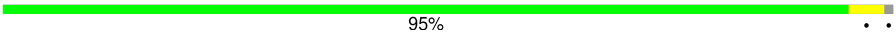
Chain B:

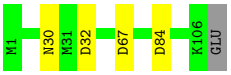




- Molecule 3: gp34 helical bundle

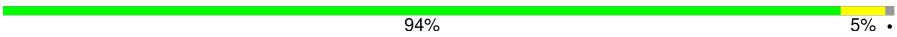
Chain C:

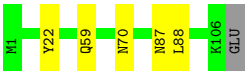




- Molecule 3: gp34 helical bundle

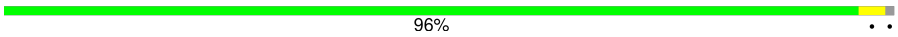
Chain D:





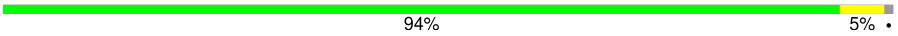
• Molecule 3: gp34 helical bundle

Chain E:



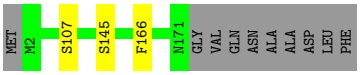
• Molecule 3: gp34 helical bundle

Chain F:



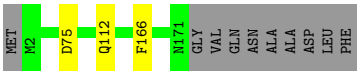
• Molecule 4: gp38 Ripcord-1

Chain S:



• Molecule 4: gp38 Ripcord-1

Chain T:

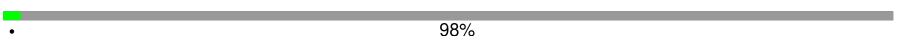


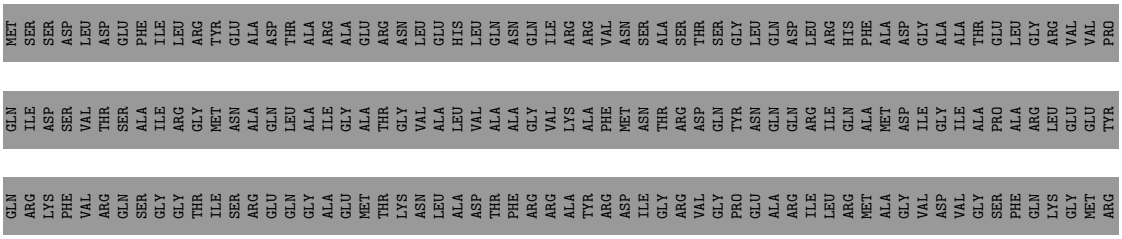
• Molecule 4: gp38 Ripcord-1

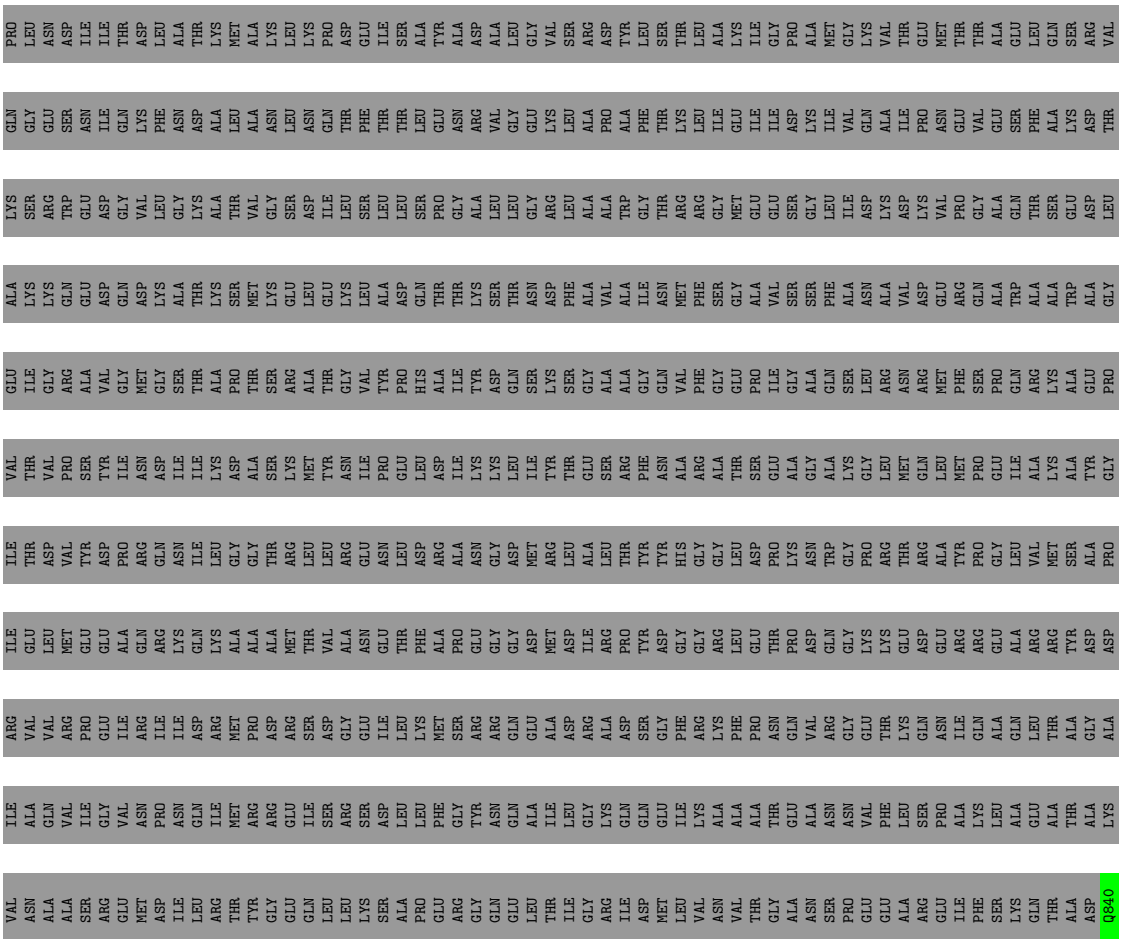
Chain U:

• Molecule 5: gp41 Tape measure protein

Chain a:

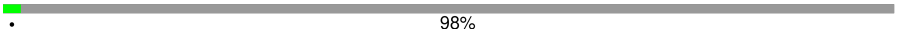


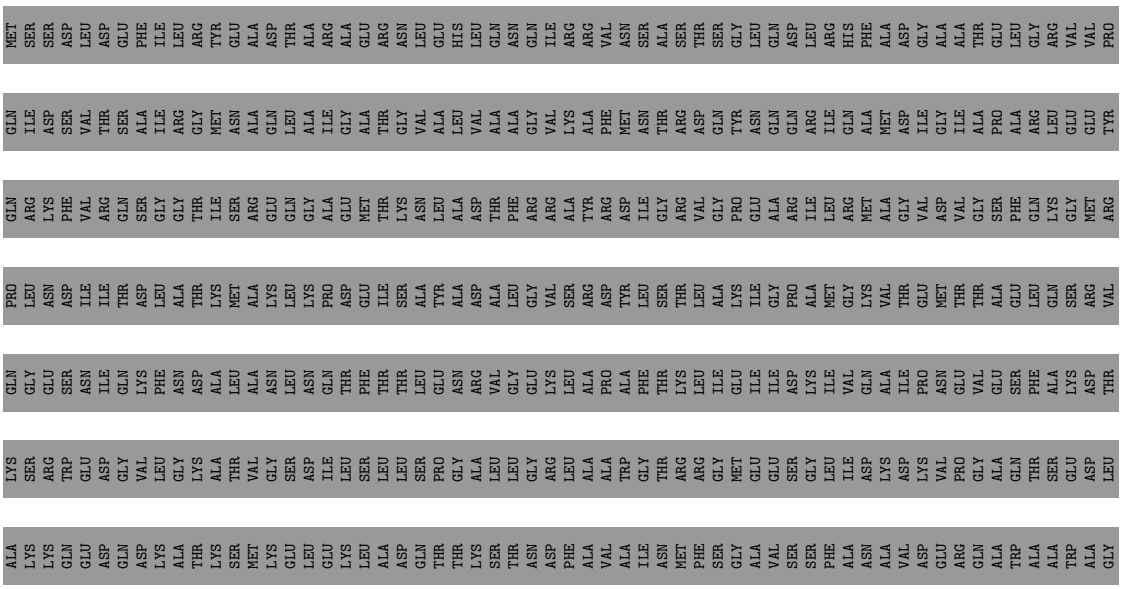




• Molecule 5: gp41 Tape measure protein

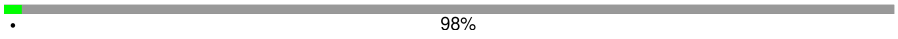
Chain b:

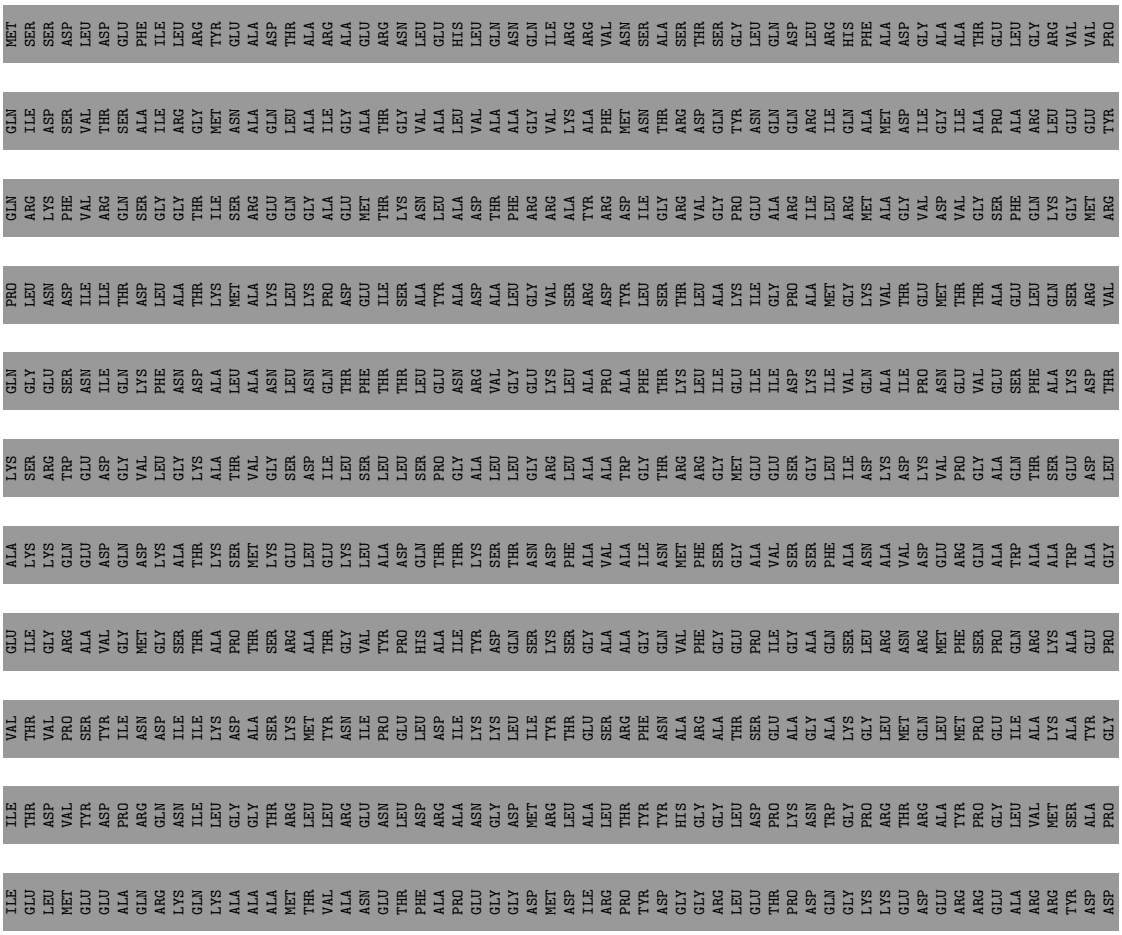


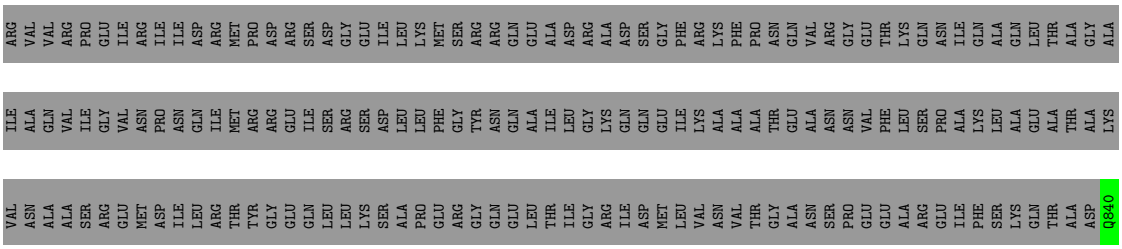


• Molecule 5: gp41 Tape measure protein

Chain c:

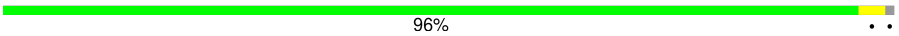


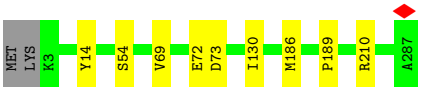




• Molecule 6: gp42 Tail hub

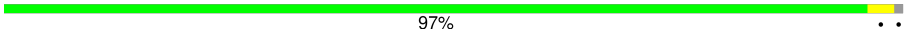
Chain d:





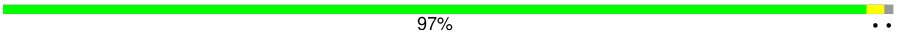
• Molecule 6: gp42 Tail hub

Chain e:



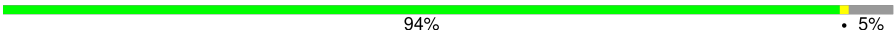
• Molecule 6: gp42 Tail hub

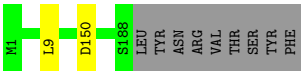
Chain f:



• Molecule 7: gp39 Ripcord-2

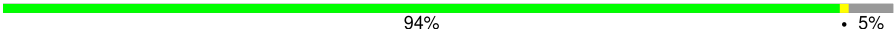
Chain V:

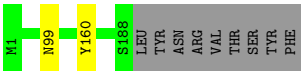




• Molecule 7: gp39 Ripcord-2

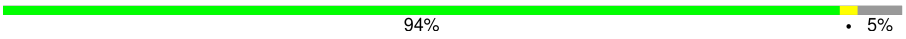
Chain W:

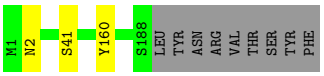




• Molecule 7: gp39 Ripcord-2

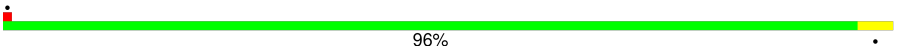
Chain X:

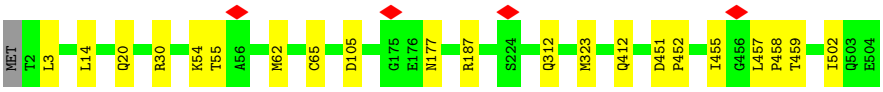




• Molecule 8: gp46 Baseplate wedge 2

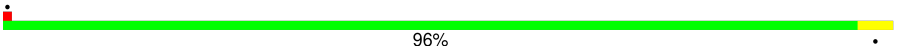
Chain v:

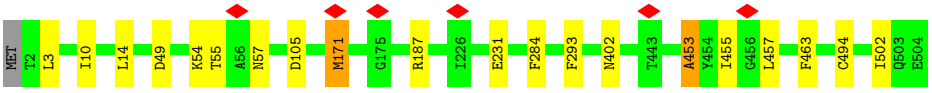




• Molecule 8: gp46 Baseplate wedge 2

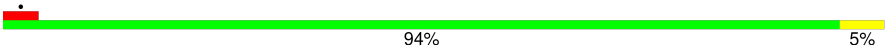
Chain w:

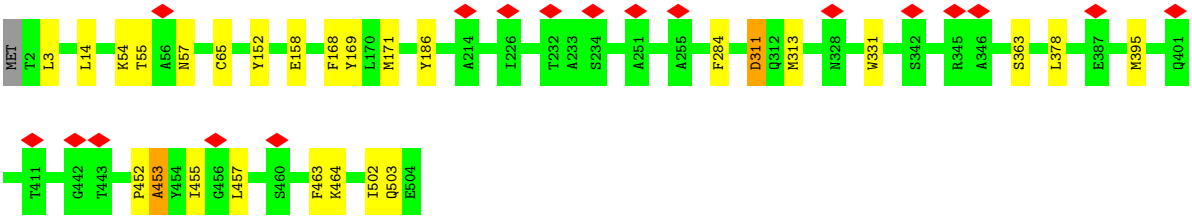




• Molecule 8: gp46 Baseplate wedge 2

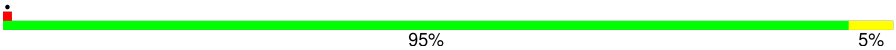
Chain x:

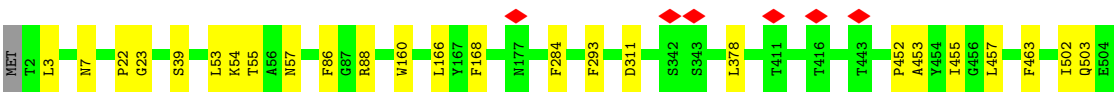




• Molecule 8: gp46 Baseplate wedge 2

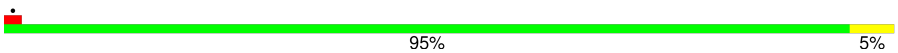
Chain y:

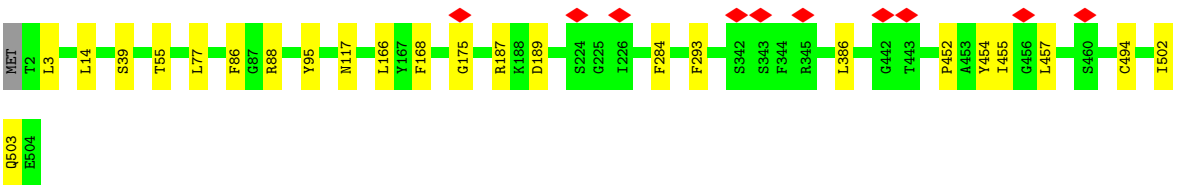




• Molecule 8: gp46 Baseplate wedge 2

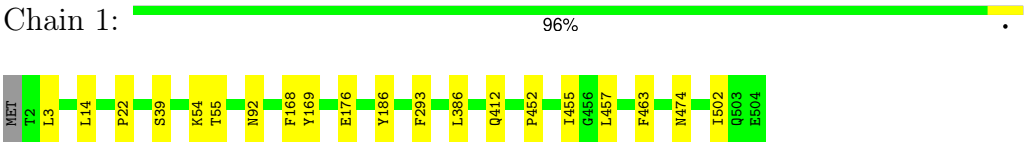
Chain z:





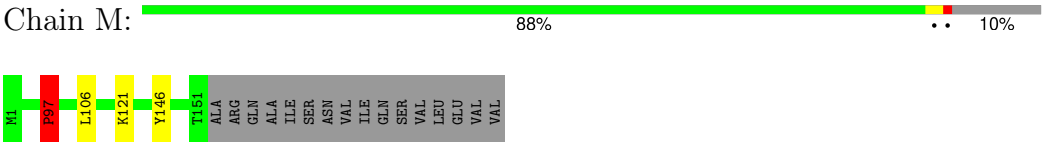
• Molecule 8: gp46 Baseplate wedge 2

Chain 1:



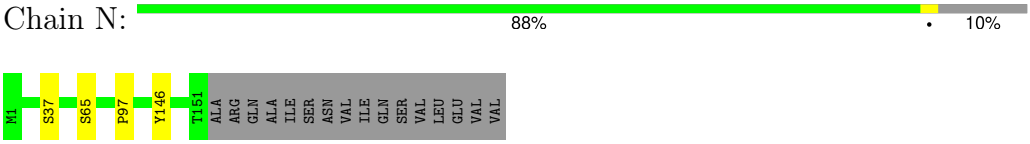
• Molecule 9: gp37 Baseplate tube

Chain M:



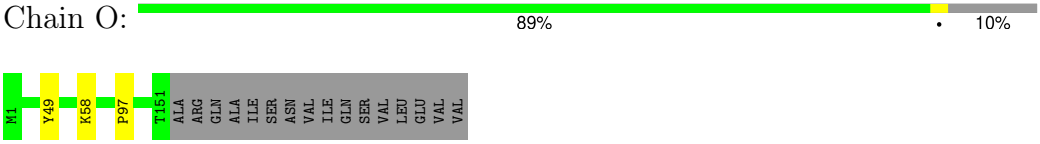
• Molecule 9: gp37 Baseplate tube

Chain N:



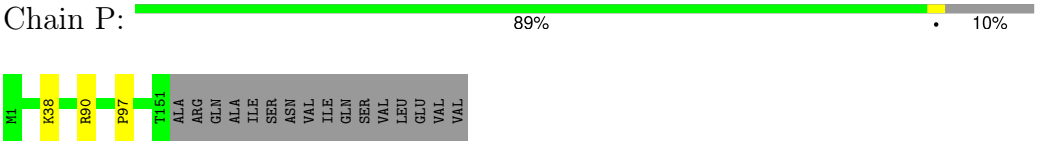
• Molecule 9: gp37 Baseplate tube

Chain O:



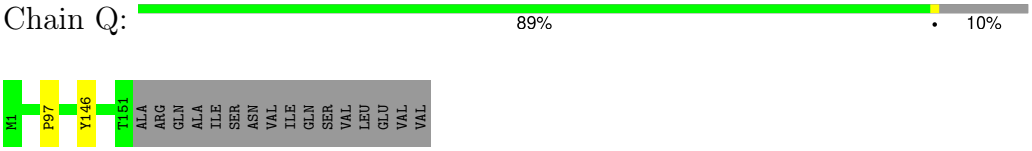
• Molecule 9: gp37 Baseplate tube

Chain P:



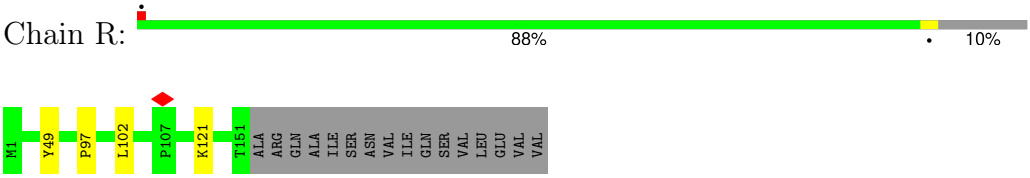
• Molecule 9: gp37 Baseplate tube

Chain Q:



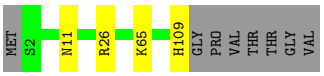
• Molecule 9: gp37 Baseplate tube

Chain R:



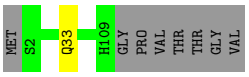
• Molecule 10: gp35 Sheath initiator

Chain G:



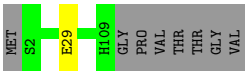
• Molecule 10: gp35 Sheath initiator

Chain H:



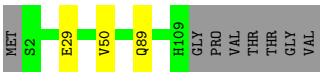
• Molecule 10: gp35 Sheath initiator

Chain I:



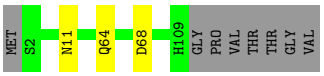
• Molecule 10: gp35 Sheath initiator

Chain J:



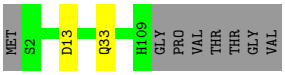
• Molecule 10: gp35 Sheath initiator

Chain K:



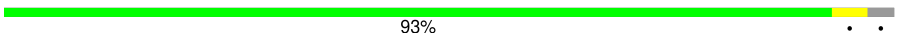
• Molecule 10: gp35 Sheath initiator

Chain L:



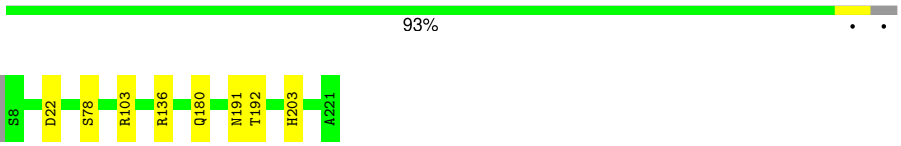
• Molecule 11: gp44 Tail tip

Chain g:



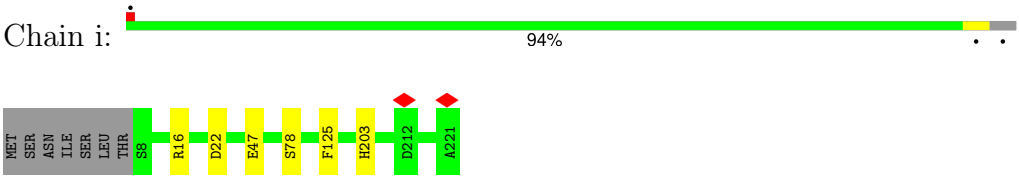
• Molecule 11: gp44 Tail tip

Chain h:



• Molecule 11: gp44 Tail tip

Chain i:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	17175	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	34.4	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	1750	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	34.243	Depositor
Minimum map value	-13.446	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4	Depositor
Map size (Å)	643.2, 643.2, 643.2	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	j	0.28	0/3082	0.51	0/4216
1	k	0.31	0/3082	0.51	0/4216
1	l	0.29	0/3082	0.52	0/4216
1	m	0.29	0/3082	0.51	0/4216
1	n	0.29	0/3082	0.50	0/4216
1	o	0.28	0/3082	0.50	0/4216
1	p	0.30	0/3080	0.58	1/4213 (0.0%)
1	q	0.28	0/3080	0.55	1/4213 (0.0%)
1	r	0.27	0/3080	0.55	0/4213
1	s	0.29	0/3080	0.56	0/4213
1	t	0.28	0/3081	0.56	0/4216
1	u	0.29	0/3080	0.57	0/4213
2	2	0.29	0/2606	0.55	0/3553
2	3	0.27	0/2606	0.54	0/3553
2	4	0.31	0/2606	0.60	2/3553 (0.1%)
3	A	0.29	0/876	0.57	0/1184
3	B	0.31	0/876	0.59	1/1184 (0.1%)
3	C	0.28	0/876	0.56	1/1184 (0.1%)
3	D	0.32	0/876	0.58	0/1184
3	E	0.28	0/876	0.53	0/1184
3	F	0.39	0/876	0.61	0/1184
4	S	0.29	0/1337	0.59	0/1807
4	T	0.31	0/1337	0.60	0/1807
4	U	0.30	0/1337	0.61	1/1807 (0.1%)
5	a	0.29	0/146	0.65	0/198
5	b	0.25	0/146	0.52	0/198
5	c	0.35	0/146	0.71	0/198
6	d	0.29	0/2304	0.57	0/3124
6	e	0.28	0/2304	0.59	0/3124
6	f	0.28	0/2304	0.57	0/3124
7	V	0.31	0/1458	0.60	0/1986
7	W	0.30	0/1458	0.54	0/1986
7	X	0.30	0/1458	0.55	0/1986
8	1	0.33	1/3948 (0.0%)	0.59	1/5398 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
8	v	0.30	0/3948	0.56	0/5398
8	w	0.29	0/3948	0.56	0/5398
8	x	0.31	0/3948	0.57	1/5398 (0.0%)
8	y	0.31	0/3948	0.58	0/5398
8	z	0.31	0/3948	0.57	1/5398 (0.0%)
9	M	0.31	0/1150	0.57	1/1556 (0.1%)
9	N	0.31	0/1150	0.55	0/1556
9	O	0.30	0/1150	0.51	0/1556
9	P	0.30	0/1150	0.54	0/1556
9	Q	0.29	0/1150	0.53	0/1556
9	R	0.31	0/1150	0.53	0/1556
10	G	0.28	0/832	0.56	0/1128
10	H	0.26	0/832	0.49	0/1128
10	I	0.28	0/832	0.53	0/1128
10	J	0.26	0/832	0.51	0/1128
10	K	0.26	0/832	0.51	0/1128
10	L	0.27	0/832	0.53	0/1128
11	g	0.28	0/1682	0.55	0/2288
11	h	0.27	0/1682	0.57	0/2288
11	i	0.30	0/1682	0.58	0/2288
All	All	0.29	1/106408 (0.0%)	0.56	11/145041 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	l	0	1
1	q	0	1
1	t	0	1
2	4	0	1
4	S	0	1
4	U	0	2
5	a	0	1
6	d	0	1
8	w	0	1
8	x	0	1
8	y	0	1
8	z	0	1
11	i	0	1
All	All	0	14

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	1	176	GLU	CB-CG	-5.43	1.41	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	U	48	LEU	CA-CB-CG	5.88	128.83	115.30
1	p	91	GLY	C-N-CA	5.81	136.23	121.70
2	4	253	PRO	N-CD-CG	-5.68	94.67	103.20
9	M	97	PRO	CA-N-CD	-5.64	103.60	111.50
8	1	176	GLU	CA-CB-CG	-5.41	101.49	113.40
1	q	198	LEU	CA-CB-CG	5.38	127.68	115.30
8	z	77	LEU	CA-CB-CG	-5.36	102.96	115.30
3	B	64	TYR	C-N-CA	-5.35	108.32	121.70
2	4	253	PRO	CA-N-CD	-5.34	104.03	111.50
8	x	311	ASP	CB-CA-C	5.20	120.81	110.40
3	C	67	ASP	CB-CG-OD1	5.18	122.96	118.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	4	39	TYR	Peptide
4	S	145	SER	Peptide
4	U	45	ARG	Sidechain
4	U	6	PHE	Peptide
5	a	856	ILE	Peptide
6	d	210	ARG	Sidechain
11	i	16	ARG	Sidechain
1	l	299	ARG	Peptide
1	q	293	ARG	Sidechain
1	t	185	MET	Peptide
8	w	453	ALA	Peptide
8	x	453	ALA	Peptide
8	y	453	ALA	Peptide
8	z	175	GLY	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	j	414/417 (99%)	389 (94%)	24 (6%)	1 (0%)	44	71
1	k	414/417 (99%)	384 (93%)	29 (7%)	1 (0%)	44	71
1	l	414/417 (99%)	386 (93%)	27 (6%)	1 (0%)	44	71
1	m	414/417 (99%)	394 (95%)	19 (5%)	1 (0%)	44	71
1	n	414/417 (99%)	388 (94%)	25 (6%)	1 (0%)	44	71
1	o	414/417 (99%)	390 (94%)	23 (6%)	1 (0%)	44	71
1	p	412/417 (99%)	349 (85%)	55 (13%)	8 (2%)	6	29
1	q	412/417 (99%)	351 (85%)	55 (13%)	6 (2%)	8	33
1	r	412/417 (99%)	356 (86%)	51 (12%)	5 (1%)	11	38
1	s	412/417 (99%)	346 (84%)	60 (15%)	6 (2%)	8	33
1	t	414/417 (99%)	354 (86%)	56 (14%)	4 (1%)	13	42
1	u	412/417 (99%)	348 (84%)	59 (14%)	5 (1%)	11	38
2	2	338/962 (35%)	319 (94%)	18 (5%)	1 (0%)	37	66
2	3	338/962 (35%)	315 (93%)	23 (7%)	0	100	100
2	4	338/962 (35%)	310 (92%)	28 (8%)	0	100	100
3	A	104/107 (97%)	101 (97%)	3 (3%)	0	100	100
3	B	104/107 (97%)	98 (94%)	6 (6%)	0	100	100
3	C	104/107 (97%)	99 (95%)	5 (5%)	0	100	100
3	D	104/107 (97%)	100 (96%)	4 (4%)	0	100	100
3	E	104/107 (97%)	99 (95%)	5 (5%)	0	100	100
3	F	104/107 (97%)	99 (95%)	5 (5%)	0	100	100
4	S	168/180 (93%)	149 (89%)	19 (11%)	0	100	100
4	T	168/180 (93%)	153 (91%)	15 (9%)	0	100	100
4	U	168/180 (93%)	152 (90%)	16 (10%)	0	100	100
5	a	17/858 (2%)	12 (71%)	4 (24%)	1 (6%)	1	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	b	17/858 (2%)	17 (100%)	0	0	100	100
5	c	17/858 (2%)	16 (94%)	1 (6%)	0	100	100
6	d	283/287 (99%)	253 (89%)	27 (10%)	3 (1%)	12	40
6	e	283/287 (99%)	249 (88%)	31 (11%)	3 (1%)	12	40
6	f	283/287 (99%)	249 (88%)	31 (11%)	3 (1%)	12	40
7	V	186/197 (94%)	164 (88%)	22 (12%)	0	100	100
7	W	186/197 (94%)	160 (86%)	26 (14%)	0	100	100
7	X	186/197 (94%)	165 (89%)	21 (11%)	0	100	100
8	1	501/504 (99%)	435 (87%)	58 (12%)	8 (2%)	8	32
8	v	501/504 (99%)	443 (88%)	52 (10%)	6 (1%)	11	38
8	w	501/504 (99%)	448 (89%)	45 (9%)	8 (2%)	8	32
8	x	501/504 (99%)	447 (89%)	46 (9%)	8 (2%)	8	32
8	y	501/504 (99%)	443 (88%)	48 (10%)	10 (2%)	6	28
8	z	501/504 (99%)	441 (88%)	53 (11%)	7 (1%)	9	34
9	M	149/167 (89%)	141 (95%)	6 (4%)	2 (1%)	10	36
9	N	149/167 (89%)	143 (96%)	5 (3%)	1 (1%)	19	50
9	O	149/167 (89%)	146 (98%)	2 (1%)	1 (1%)	19	50
9	P	149/167 (89%)	141 (95%)	7 (5%)	1 (1%)	19	50
9	Q	149/167 (89%)	142 (95%)	6 (4%)	1 (1%)	19	50
9	R	149/167 (89%)	145 (97%)	3 (2%)	1 (1%)	19	50
10	G	106/116 (91%)	96 (91%)	10 (9%)	0	100	100
10	H	106/116 (91%)	95 (90%)	11 (10%)	0	100	100
10	I	106/116 (91%)	94 (89%)	12 (11%)	0	100	100
10	J	106/116 (91%)	93 (88%)	12 (11%)	1 (1%)	14	44
10	K	106/116 (91%)	97 (92%)	9 (8%)	0	100	100
10	L	106/116 (91%)	95 (90%)	11 (10%)	0	100	100
11	g	212/221 (96%)	183 (86%)	29 (14%)	0	100	100
11	h	212/221 (96%)	190 (90%)	22 (10%)	0	100	100
11	i	212/221 (96%)	187 (88%)	25 (12%)	0	100	100
All	All	13730/18483 (74%)	12359 (90%)	1265 (9%)	106 (1%)	19	46

All (106) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	k	8	VAL
1	n	8	VAL
1	o	8	VAL
6	d	69	VAL
6	e	69	VAL
6	f	69	VAL
8	v	14	LEU
8	v	452	PRO
8	w	10	ILE
8	w	14	LEU
8	w	453	ALA
8	w	457	LEU
8	x	14	LEU
8	x	452	PRO
8	x	457	LEU
8	y	22	PRO
8	y	457	LEU
8	y	463	PHE
8	z	14	LEU
8	z	457	LEU
8	1	14	LEU
8	1	452	PRO
8	1	457	LEU
1	q	292	VAL
1	q	299	ARG
1	p	92	SER
1	p	183	ARG
1	p	292	VAL
1	r	292	VAL
1	s	292	VAL
1	t	292	VAL
1	u	292	VAL
9	M	97	PRO
9	N	97	PRO
9	O	97	PRO
9	P	97	PRO
9	Q	97	PRO
9	R	97	PRO
1	j	8	VAL
1	l	8	VAL
1	m	8	VAL
8	v	458	PRO
8	w	502	ILE

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Mol	Chain	Res	Type
8	x	455	ILE
8	x	502	ILE
8	y	23	GLY
8	y	452	PRO
8	y	455	ILE
8	y	502	ILE
8	z	452	PRO
8	z	455	ILE
8	z	502	ILE
8	1	502	ILE
1	q	232	VAL
1	q	233	GLN
1	p	232	VAL
1	r	232	VAL
1	s	232	VAL
1	s	379	ALA
8	v	3	LEU
8	v	502	ILE
8	w	3	LEU
8	x	3	LEU
8	y	3	LEU
8	y	503	GLN
8	z	3	LEU
8	z	503	GLN
8	1	3	LEU
8	1	455	ILE
1	r	278	THR
1	t	232	VAL
1	u	232	VAL
8	v	455	ILE
8	w	455	ILE
8	x	503	GLN
1	p	233	GLN
1	s	183	ARG
1	t	379	ALA
1	u	233	GLN
1	u	379	ALA
5	a	857	LEU
6	d	130	ILE
6	e	130	ILE
6	f	130	ILE
8	w	171	MET

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Mol	Chain	Res	Type
8	y	7	ASN
1	q	238	VAL
1	q	379	ALA
1	p	238	VAL
1	r	233	GLN
1	t	238	VAL
1	u	238	VAL
2	2	76	MET
6	d	189	PRO
8	x	453	ALA
8	1	22	PRO
8	1	463	PHE
1	p	278	THR
1	r	238	VAL
1	s	238	VAL
1	s	278	THR
6	e	189	PRO
1	p	12	VAL
6	f	188	MET
10	J	50	VAL
9	M	106	LEU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	j	319/320 (100%)	314 (98%)	5 (2%)	58 76
1	k	319/320 (100%)	309 (97%)	10 (3%)	35 61
1	l	319/320 (100%)	310 (97%)	9 (3%)	38 64
1	m	319/320 (100%)	308 (97%)	11 (3%)	32 59
1	n	319/320 (100%)	313 (98%)	6 (2%)	52 72
1	o	319/320 (100%)	314 (98%)	5 (2%)	58 76
1	p	319/320 (100%)	315 (99%)	4 (1%)	65 79
1	q	319/320 (100%)	305 (96%)	14 (4%)	24 52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	r	319/320 (100%)	308 (97%)	11 (3%)	32	59
1	s	319/320 (100%)	310 (97%)	9 (3%)	38	64
1	t	319/320 (100%)	308 (97%)	11 (3%)	32	59
1	u	319/320 (100%)	309 (97%)	10 (3%)	35	61
2	2	260/753 (34%)	248 (95%)	12 (5%)	23	52
2	3	260/753 (34%)	252 (97%)	8 (3%)	35	61
2	4	260/753 (34%)	242 (93%)	18 (7%)	13	38
3	A	88/89 (99%)	83 (94%)	5 (6%)	17	44
3	B	88/89 (99%)	84 (96%)	4 (4%)	23	52
3	C	88/89 (99%)	85 (97%)	3 (3%)	32	59
3	D	88/89 (99%)	83 (94%)	5 (6%)	17	44
3	E	88/89 (99%)	85 (97%)	3 (3%)	32	59
3	F	88/89 (99%)	83 (94%)	5 (6%)	17	44
4	S	152/159 (96%)	150 (99%)	2 (1%)	65	79
4	T	152/159 (96%)	149 (98%)	3 (2%)	50	71
4	U	152/159 (96%)	148 (97%)	4 (3%)	41	66
5	a	16/688 (2%)	14 (88%)	2 (12%)	3	16
5	b	16/688 (2%)	16 (100%)	0	100	100
5	c	16/688 (2%)	15 (94%)	1 (6%)	15	41
6	d	250/252 (99%)	245 (98%)	5 (2%)	50	71
6	e	250/252 (99%)	245 (98%)	5 (2%)	50	71
6	f	250/252 (99%)	245 (98%)	5 (2%)	50	71
7	V	168/177 (95%)	166 (99%)	2 (1%)	67	80
7	W	168/177 (95%)	166 (99%)	2 (1%)	67	80
7	X	168/177 (95%)	165 (98%)	3 (2%)	54	74
8	1	407/408 (100%)	396 (97%)	11 (3%)	40	65
8	v	407/408 (100%)	392 (96%)	15 (4%)	29	56
8	w	407/408 (100%)	394 (97%)	13 (3%)	34	61
8	x	407/408 (100%)	388 (95%)	19 (5%)	22	51
8	y	407/408 (100%)	393 (97%)	14 (3%)	32	59
8	z	407/408 (100%)	392 (96%)	15 (4%)	29	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	M	124/138 (90%)	121 (98%)	3 (2%)	44	68
9	N	124/138 (90%)	121 (98%)	3 (2%)	44	68
9	O	124/138 (90%)	122 (98%)	2 (2%)	58	76
9	P	124/138 (90%)	122 (98%)	2 (2%)	58	76
9	Q	124/138 (90%)	123 (99%)	1 (1%)	79	87
9	R	124/138 (90%)	121 (98%)	3 (2%)	44	68
10	G	92/98 (94%)	88 (96%)	4 (4%)	25	53
10	H	92/98 (94%)	91 (99%)	1 (1%)	70	82
10	I	92/98 (94%)	91 (99%)	1 (1%)	70	82
10	J	92/98 (94%)	90 (98%)	2 (2%)	47	69
10	K	92/98 (94%)	89 (97%)	3 (3%)	33	60
10	L	92/98 (94%)	90 (98%)	2 (2%)	47	69
11	g	179/186 (96%)	170 (95%)	9 (5%)	20	48
11	h	179/186 (96%)	171 (96%)	8 (4%)	23	52
11	i	179/186 (96%)	174 (97%)	5 (3%)	38	64
All	All	11169/14883 (75%)	10831 (97%)	338 (3%)	37	62

All (338) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	j	55	ARG
1	j	61	ASN
1	j	86	MET
1	j	242	LEU
1	j	380	CYS
1	k	55	ARG
1	k	60	ARG
1	k	61	ASN
1	k	226	GLU
1	k	233	GLN
1	k	235	VAL
1	k	239	SER
1	k	267	HIS
1	k	291	PRO
1	k	400	SER
1	l	4	TYR
1	l	55	ARG

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Mol	Chain	Res	Type
1	l	61	ASN
1	l	86	MET
1	l	97	PHE
1	l	116	ARG
1	l	145	SER
1	l	185	MET
1	l	400	SER
1	m	44	GLN
1	m	55	ARG
1	m	61	ASN
1	m	97	PHE
1	m	145	SER
1	m	180	PRO
1	m	338	TYR
1	m	380	CYS
1	m	400	SER
1	m	408	SER
1	m	413	ARG
1	n	4	TYR
1	n	61	ASN
1	n	83	CYS
1	n	249	CYS
1	n	408	SER
1	n	413	ARG
1	o	55	ARG
1	o	61	ASN
1	o	299	ARG
1	o	400	SER
1	o	413	ARG
2	2	55	ARG
2	2	70	GLN
2	2	81	PHE
2	2	124	GLU
2	2	171	ASP
2	2	178	GLN
2	2	193	MET
2	2	211	TYR
2	2	236	ASN
2	2	238	MET
2	2	244	ARG
2	2	323	ASP
2	3	84	MET

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Mol	Chain	Res	Type
2	3	166	TRP
2	3	177	SER
2	3	207	CYS
2	3	214	ARG
2	3	233	TYR
2	3	328	ARG
2	3	330	ARG
2	4	33	ASP
2	4	51	LYS
2	4	56	LYS
2	4	89	GLU
2	4	96	ARG
2	4	104	ARG
2	4	138	MET
2	4	156	ARG
2	4	160	ASP
2	4	162	LEU
2	4	171	ASP
2	4	193	MET
2	4	213	ASP
2	4	221	ARG
2	4	266	GLN
2	4	276	ARG
2	4	327	ASP
2	4	330	ARG
3	A	46	CYS
3	A	70	ASN
3	A	76	ASP
3	A	102	LEU
3	A	106	LYS
3	B	22	TYR
3	B	65	ARG
3	B	67	ASP
3	B	88	LEU
3	C	30	ASN
3	C	32	ASP
3	C	84	ASP
3	D	22	TYR
3	D	59	GLN
3	D	70	ASN
3	D	87	ASN
3	D	88	LEU

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Mol	Chain	Res	Type
3	E	46	CYS
3	E	70	ASN
3	E	87	ASN
3	F	2	LYS
3	F	17	ASN
3	F	41	ASP
3	F	74	ASP
3	F	87	ASN
4	S	107	SER
4	S	166	PHE
4	T	75	ASP
4	T	112	GLN
4	T	166	PHE
4	U	45	ARG
4	U	49	GLU
4	U	154	LEU
4	U	168	TYR
5	a	850	ASN
5	a	858	TYR
5	c	847	ASP
6	d	14	TYR
6	d	54	SER
6	d	72	GLU
6	d	73	ASP
6	d	186	MET
6	e	12	MET
6	e	14	TYR
6	e	35	ARG
6	e	73	ASP
6	e	186	MET
6	f	14	TYR
6	f	73	ASP
6	f	185	ASP
6	f	186	MET
6	f	188	MET
7	V	9	LEU
7	V	150	ASP
7	W	99	ASN
7	W	160	TYR
7	X	2	ASN
7	X	41	SER
7	X	160	TYR

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Mol	Chain	Res	Type
8	v	20	GLN
8	v	30	ARG
8	v	54	LYS
8	v	55	THR
8	v	62	MET
8	v	65	CYS
8	v	105	ASP
8	v	177	ASN
8	v	187	ARG
8	v	312	GLN
8	v	323	MET
8	v	412	GLN
8	v	451	ASP
8	v	457	LEU
8	v	459	THR
8	w	49	ASP
8	w	54	LYS
8	w	55	THR
8	w	57	ASN
8	w	105	ASP
8	w	171	MET
8	w	187	ARG
8	w	231	GLU
8	w	284	PHE
8	w	293	PHE
8	w	402	ASN
8	w	463	PHE
8	w	494	CYS
8	x	54	LYS
8	x	55	THR
8	x	57	ASN
8	x	65	CYS
8	x	152	TYR
8	x	158	GLU
8	x	168	PHE
8	x	169	TYR
8	x	171	MET
8	x	186	TYR
8	x	284	PHE
8	x	311	ASP
8	x	313	MET
8	x	331	TRP

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Mol	Chain	Res	Type
8	x	363	SER
8	x	378	LEU
8	x	395	MET
8	x	463	PHE
8	x	464	LYS
8	y	39	SER
8	y	53	LEU
8	y	54	LYS
8	y	55	THR
8	y	57	ASN
8	y	86	PHE
8	y	88	ARG
8	y	160	TRP
8	y	166	LEU
8	y	168	PHE
8	y	284	PHE
8	y	293	PHE
8	y	311	ASP
8	y	378	LEU
8	z	39	SER
8	z	55	THR
8	z	86	PHE
8	z	88	ARG
8	z	95	TYR
8	z	117	ASN
8	z	166	LEU
8	z	168	PHE
8	z	187	ARG
8	z	189	ASP
8	z	284	PHE
8	z	293	PHE
8	z	386	LEU
8	z	454	TYR
8	z	494	CYS
8	1	39	SER
8	1	54	LYS
8	1	55	THR
8	1	92	ASN
8	1	168	PHE
8	1	169	TYR
8	1	186	TYR
8	1	293	PHE

Continued on next page...

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Mol	Chain	Res	Type
8	1	386	LEU
8	1	412	GLN
8	1	474	ASN
1	q	57	SER
1	q	75	PHE
1	q	90	ARG
1	q	106	ARG
1	q	212	TYR
1	q	249	CYS
1	q	275	TYR
1	q	280	ASN
1	q	285	ASP
1	q	293	ARG
1	q	321	GLN
1	q	395	SER
1	q	404	GLN
1	q	413	ARG
1	p	106	ARG
1	p	125	PHE
1	p	179	ASP
1	p	212	TYR
1	r	97	PHE
1	r	144	LYS
1	r	148	TYR
1	r	183	ARG
1	r	191	LYS
1	r	212	TYR
1	r	240	PHE
1	r	267	HIS
1	r	299	ARG
1	r	321	GLN
1	r	404	GLN
1	s	118	GLN
1	s	148	TYR
1	s	185	MET
1	s	210	LYS
1	s	212	TYR
1	s	228	ASN
1	s	244	TYR
1	s	321	GLN
1	s	338	TYR
1	t	57	SER

Continued on next page...

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Mol	Chain	Res	Type
1	t	90	ARG
1	t	99	TYR
1	t	108	GLN
1	t	125	PHE
1	t	162	ASP
1	t	198	LEU
1	t	212	TYR
1	t	285	ASP
1	t	380	CYS
1	t	399	MET
1	u	55	ARG
1	u	70	ASN
1	u	75	PHE
1	u	90	ARG
1	u	171	LYS
1	u	177	ARG
1	u	212	TYR
1	u	255	ASP
1	u	321	GLN
1	u	404	GLN
9	M	97	PRO
9	M	121	LYS
9	M	146	TYR
9	N	37	SER
9	N	65	SER
9	N	146	TYR
9	O	49	TYR
9	O	58	LYS
9	P	38	LYS
9	P	90	ARG
9	Q	146	TYR
9	R	49	TYR
9	R	102	LEU
9	R	121	LYS
10	G	11	ASN
10	G	26	ARG
10	G	65	LYS
10	G	109	HIS
10	H	33	GLN
10	I	29	GLU
10	J	29	GLU
10	J	89	GLN

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Mol	Chain	Res	Type
10	K	11	ASN
10	K	64	GLN
10	K	68	ASP
10	L	13	ASP
10	L	33	GLN
11	g	22	ASP
11	g	42	GLN
11	g	47	GLU
11	g	103	ARG
11	g	112	LEU
11	g	136	ARG
11	g	180	GLN
11	g	201	ASN
11	g	203	HIS
11	h	22	ASP
11	h	78	SER
11	h	103	ARG
11	h	136	ARG
11	h	180	GLN
11	h	191	ASN
11	h	192	THR
11	h	203	HIS
11	i	22	ASP
11	i	47	GLU
11	i	78	SER
11	i	125	PHE
11	i	203	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	j	196	ASN
1	j	332	GLN
1	l	118	GLN
1	m	321	GLN
1	o	228	ASN
2	2	70	GLN
2	4	30	ASN
2	4	60	GLN
2	4	67	GLN
2	4	209	GLN
2	4	264	GLN

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Mol	Chain	Res	Type
2	4	280	ASN
3	A	59	GLN
3	B	35	ASN
3	B	59	GLN
4	S	36	ASN
4	S	46	HIS
4	U	46	HIS
4	U	141	ASN
6	d	58	GLN
6	d	184	GLN
6	e	58	GLN
6	e	118	GLN
7	V	68	ASN
7	X	163	GLN
8	v	12	GLN
8	v	99	GLN
8	v	312	GLN
8	w	7	ASN
8	x	401	GLN
8	z	7	ASN
1	q	227	ASN
1	p	321	GLN
1	r	280	ASN
1	s	228	ASN
1	s	267	HIS
1	s	332	GLN
1	t	108	GLN
1	u	268	ASN
10	G	12	ASN
10	H	12	ASN
10	J	46	ASN
10	K	12	ASN
11	g	203	HIS
11	i	107	GLN

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	p	1
1	q	1
1	s	1
1	u	1
1	r	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	p	184:GLN	C	185:MET	N	8.90
1	q	184:GLN	C	185:MET	N	7.08
1	s	184:GLN	C	185:MET	N	5.61
1	u	184:GLN	C	185:MET	N	5.37
1	r	184:GLN	C	185:MET	N	5.33

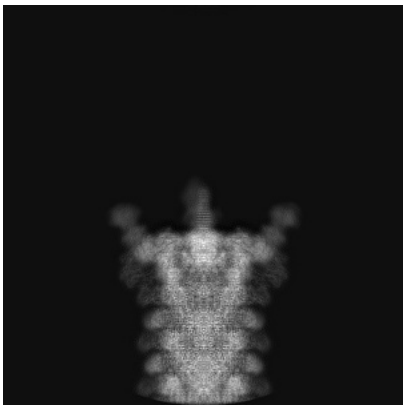
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44168. These allow visual inspection of the internal detail of the map and identification of artifacts.

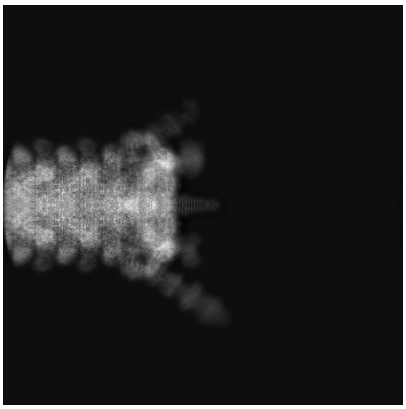
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

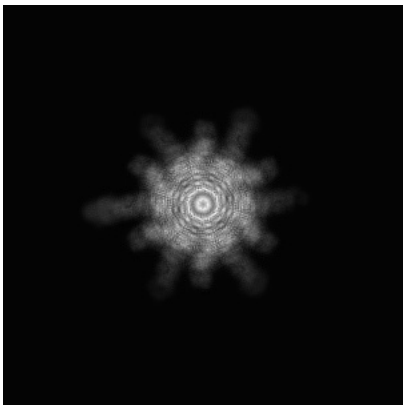
6.1.1 Primary map



X

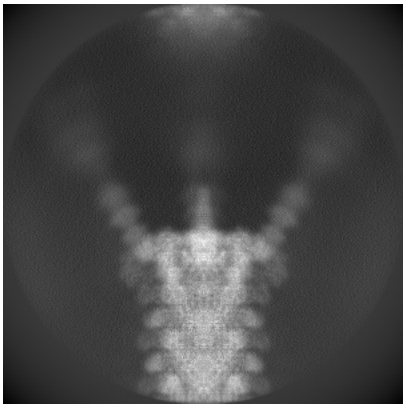


Y

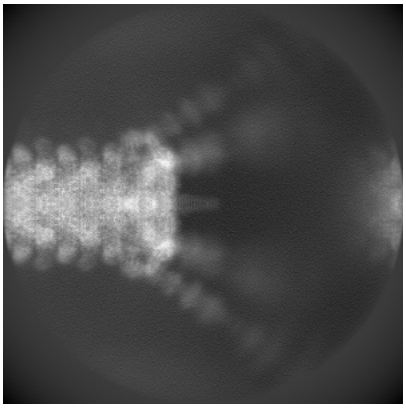


Z

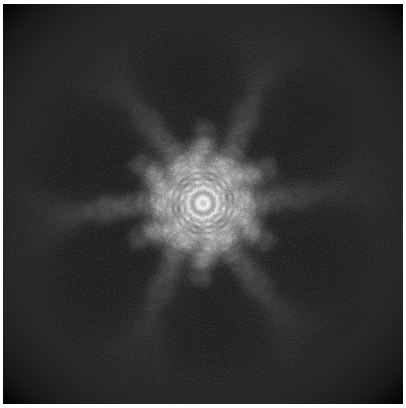
6.1.2 Raw map



X



Y

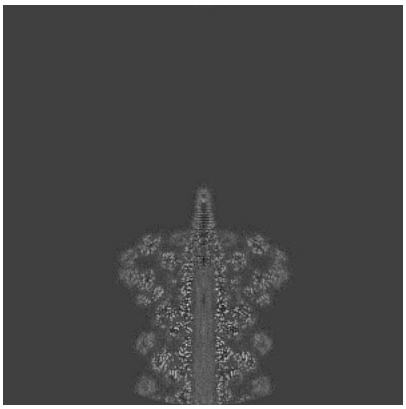


Z

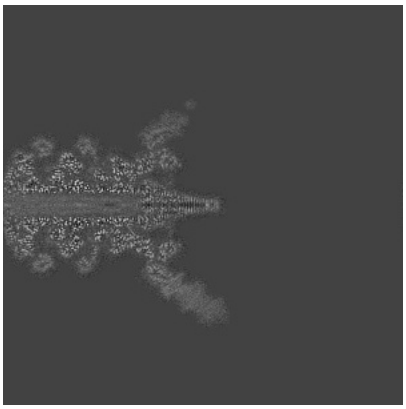
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

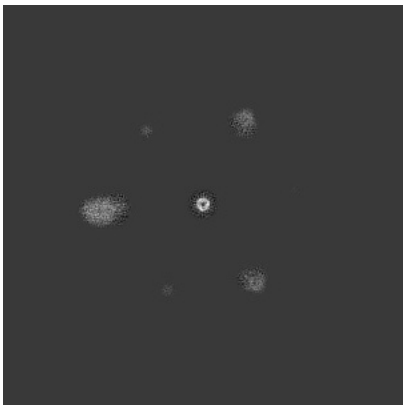
6.2.1 Primary map



X Index: 240

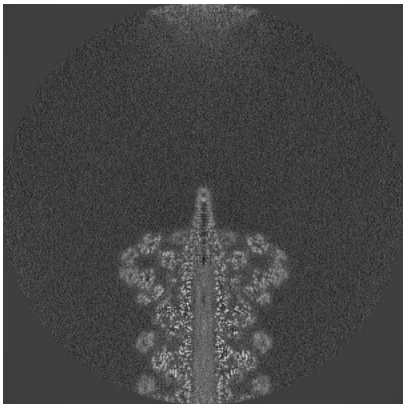


Y Index: 240

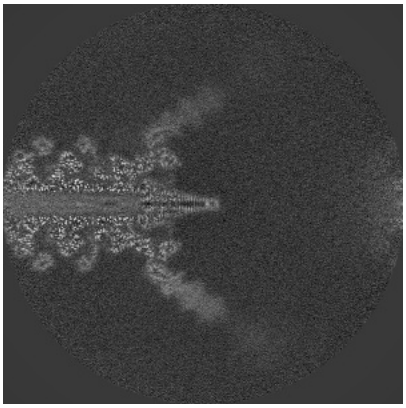


Z Index: 240

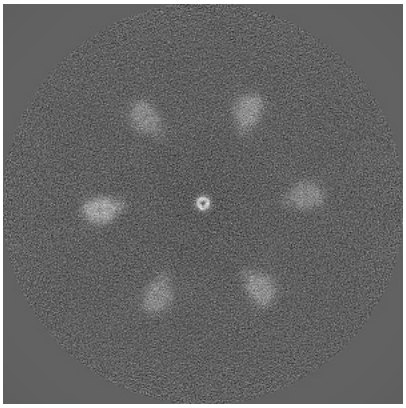
6.2.2 Raw map



X Index: 240



Y Index: 240

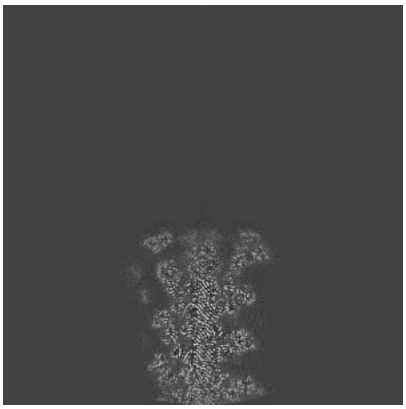


Z Index: 240

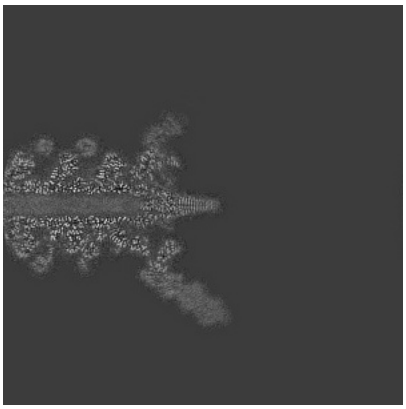
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

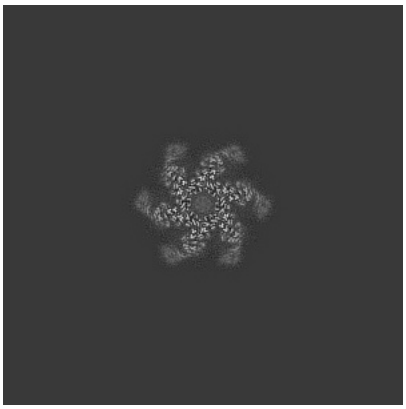
6.3.1 Primary map



X Index: 222

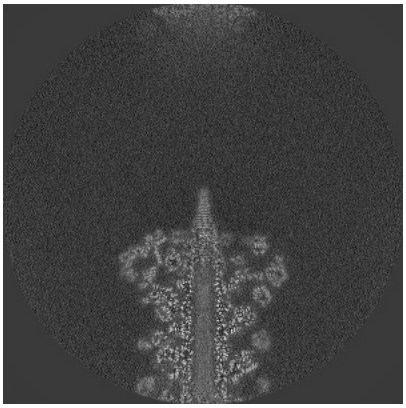


Y Index: 236

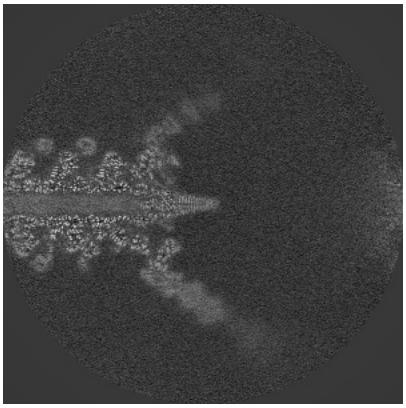


Z Index: 94

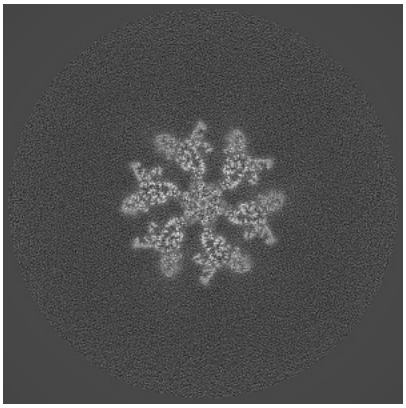
6.3.2 Raw map



X Index: 245



Y Index: 236

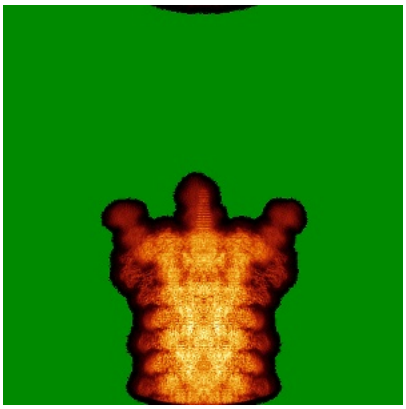


Z Index: 180

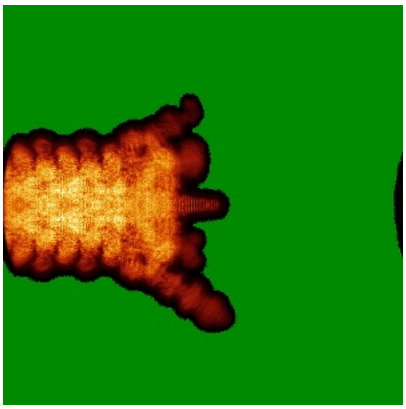
The images above show the largest variance slices of the map in three orthogonal directions.

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

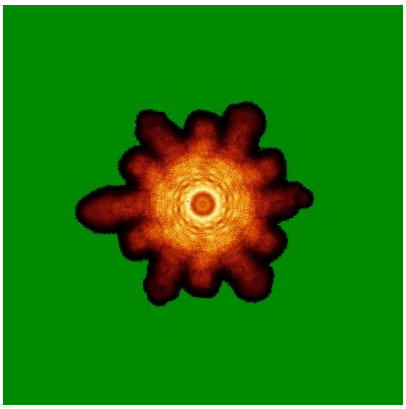
6.4.1 Primary map



X

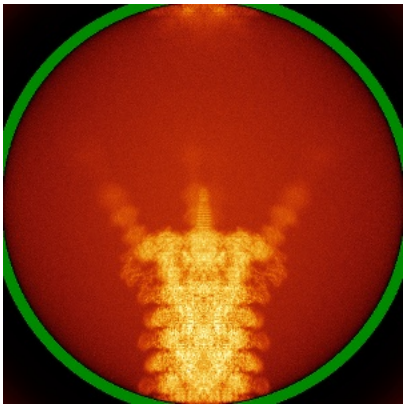


Y

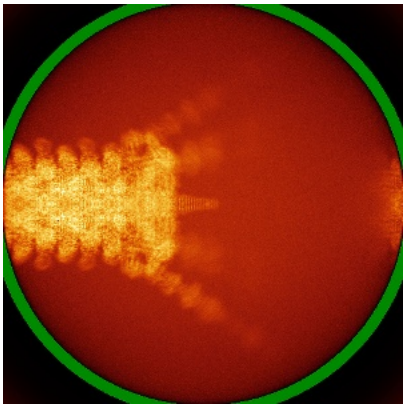


Z

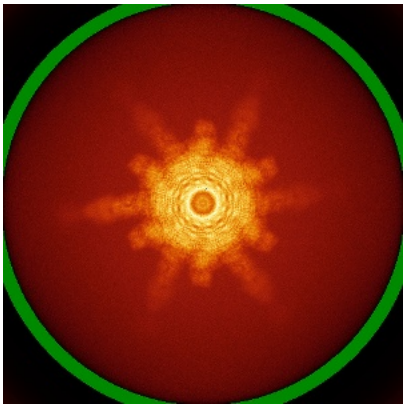
6.4.2 Raw map



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.

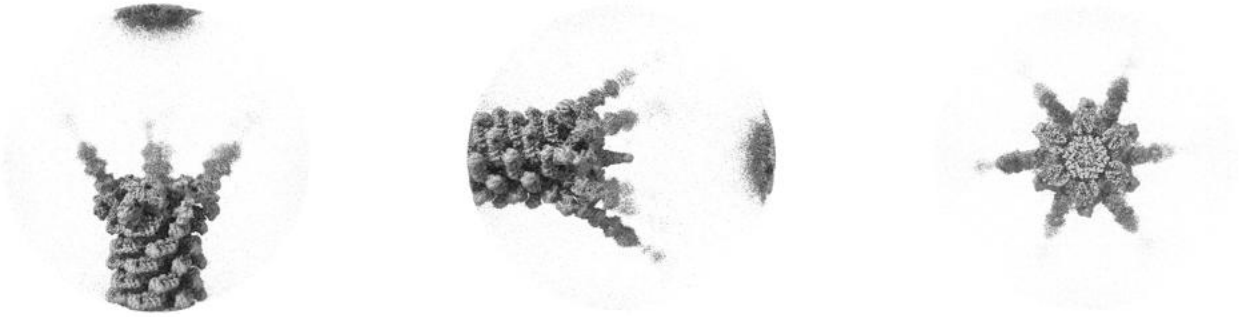
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 4.0. 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.

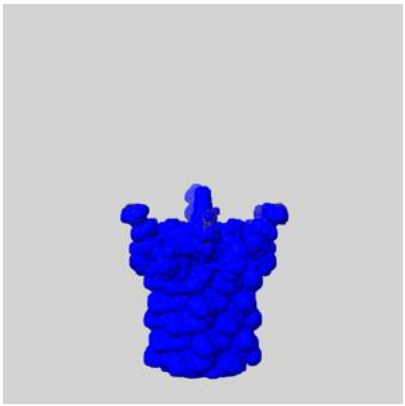
6.6 Mask visualisation (i)

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

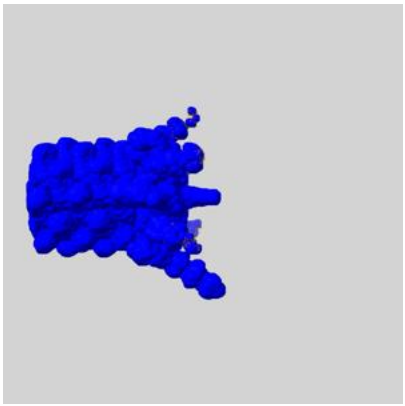
A mask typically either:

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

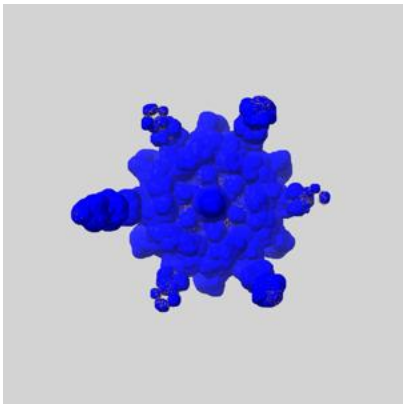
6.6.1 emd_44168_msk_1.map (i)



X



Y

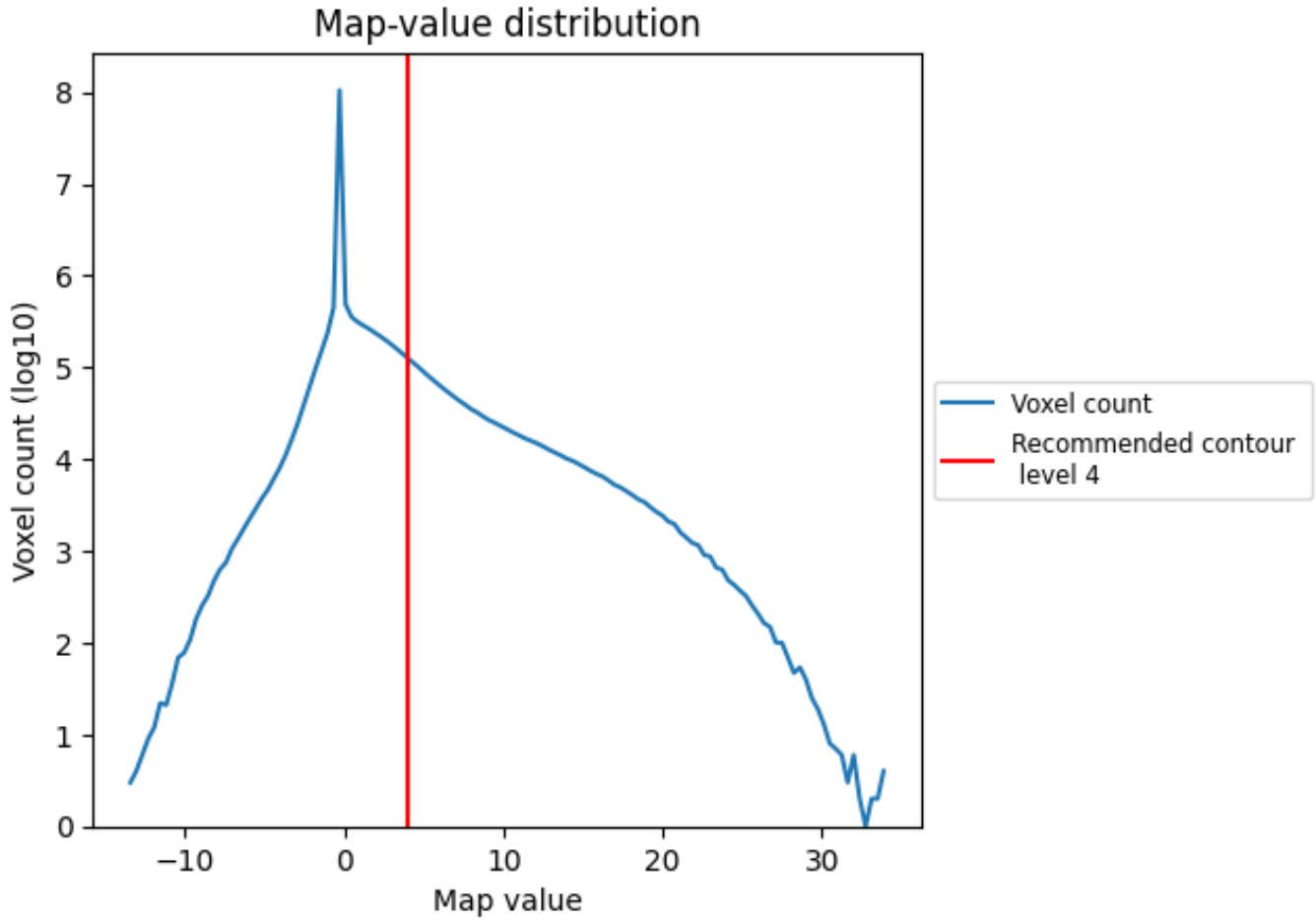


Z

7 Map analysis

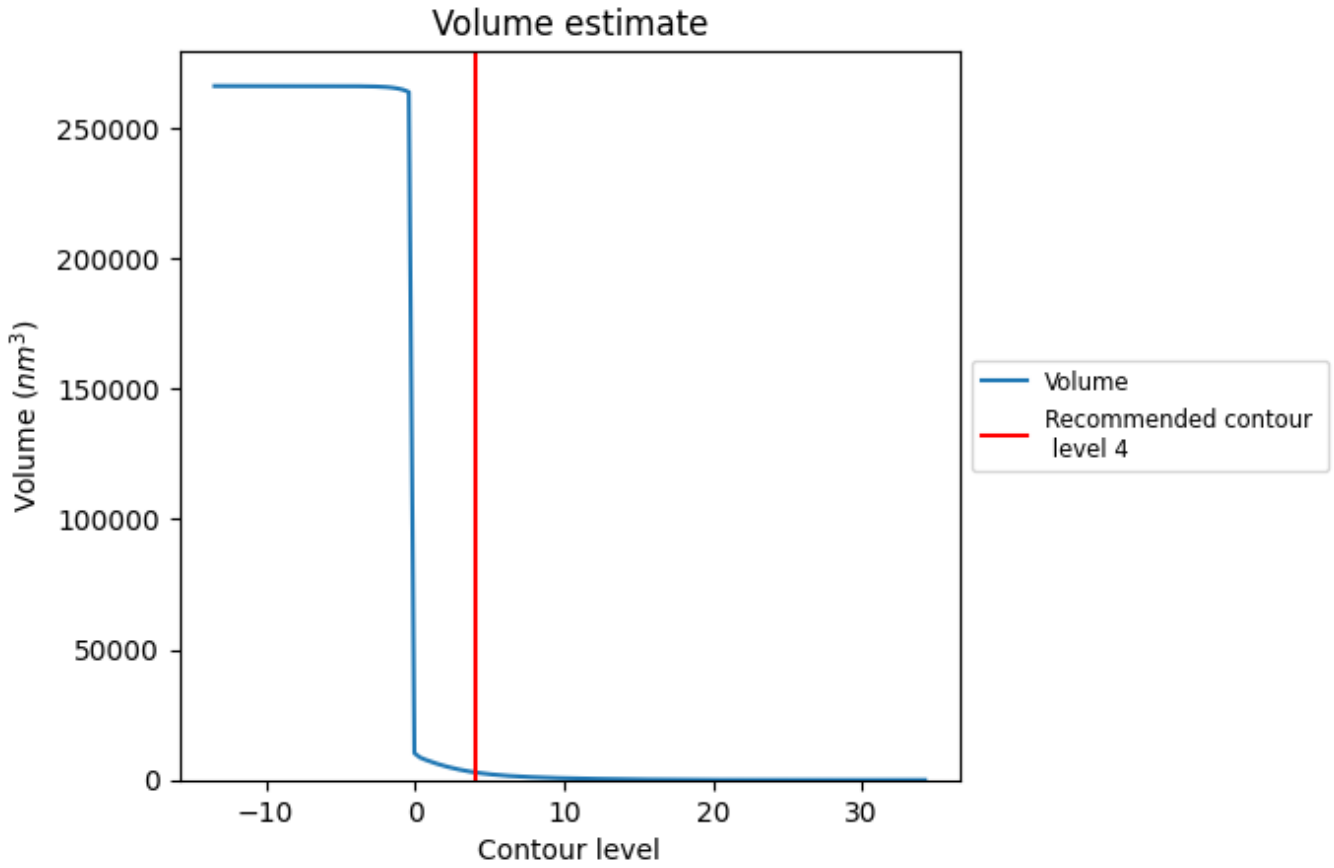
This section contains the results of statistical analysis of the map.

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.

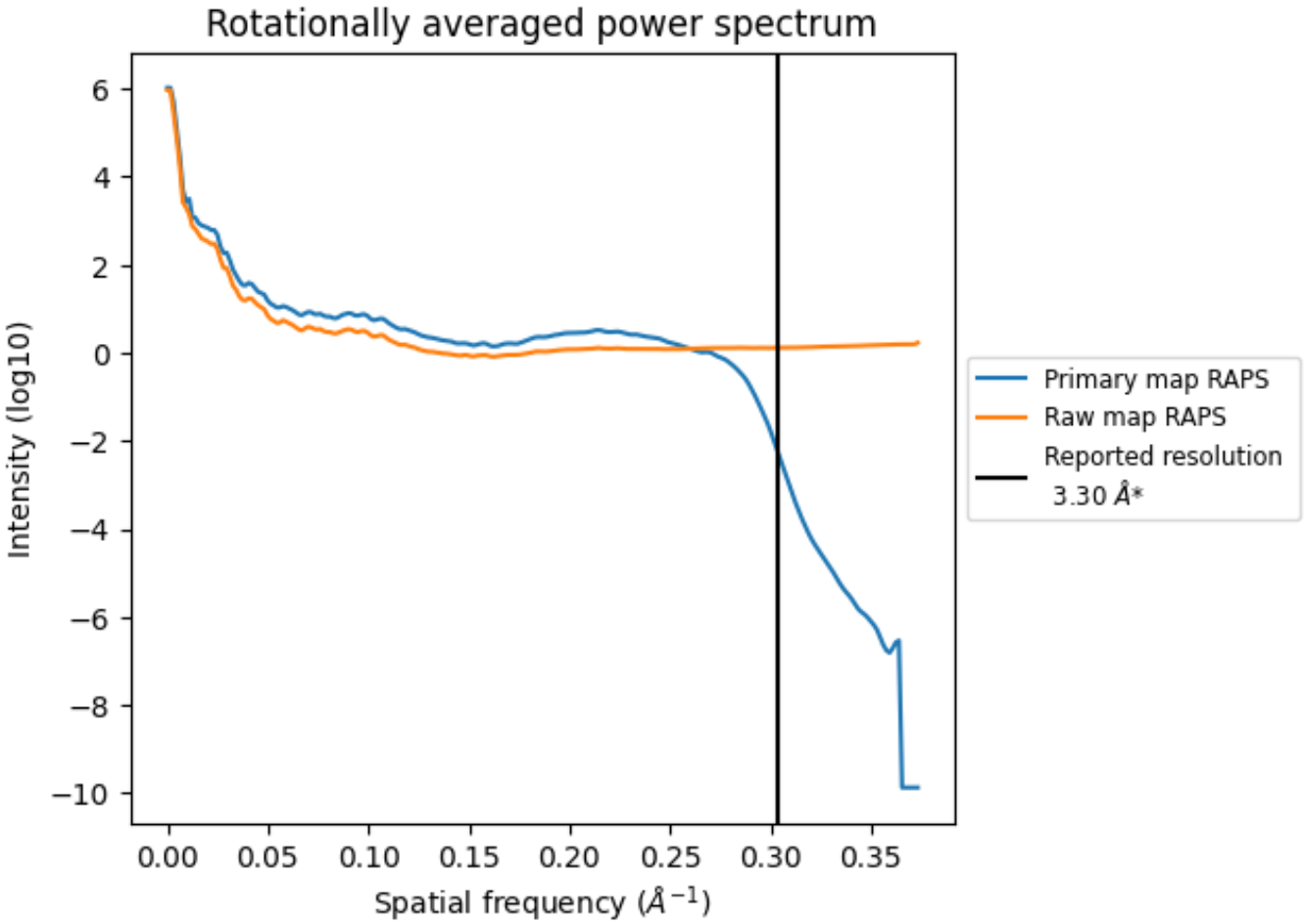
7.2 Volume estimate



The volume at the recommended contour level is 2941 nm^3; this corresponds to an approximate mass of 2657 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)

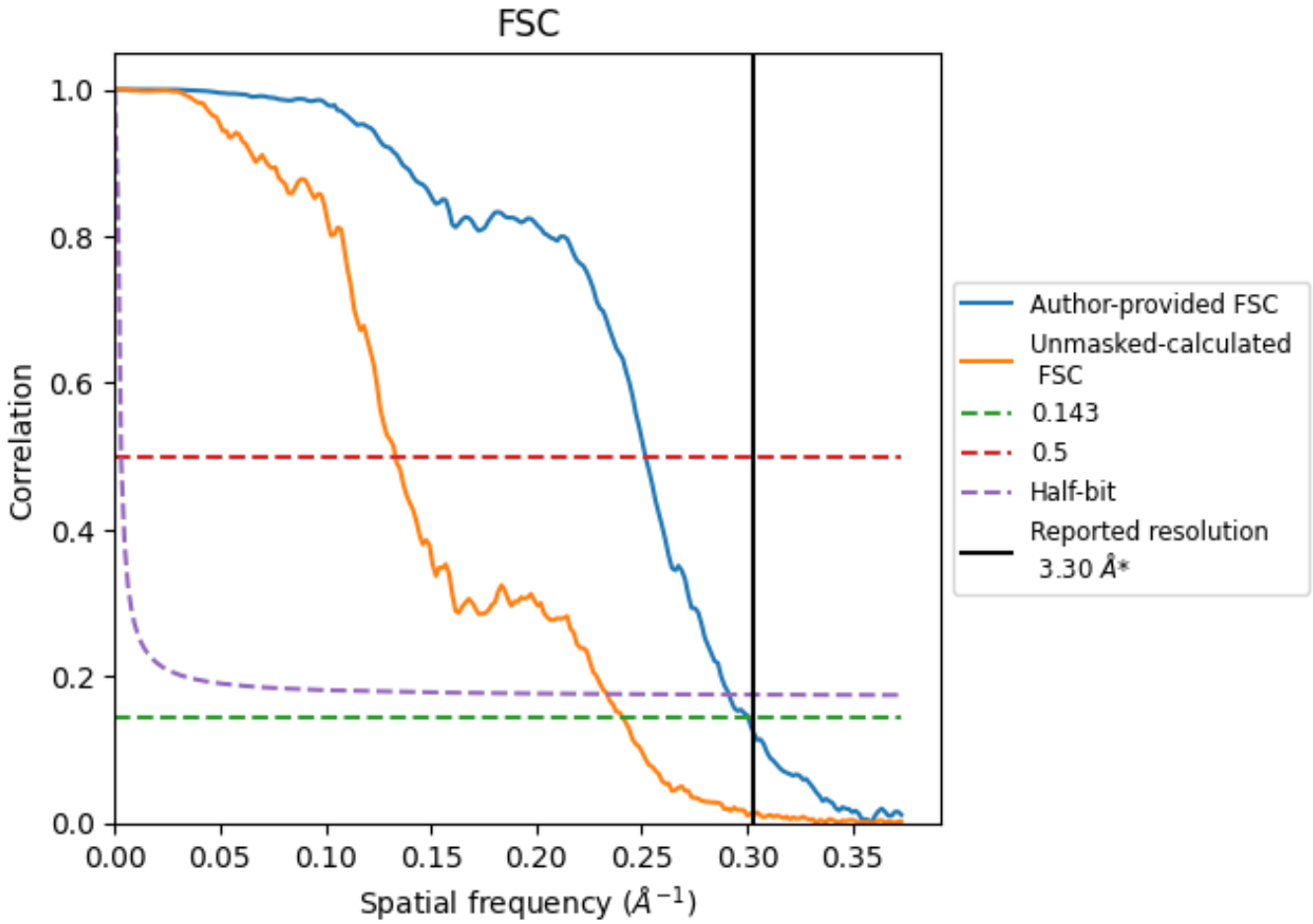


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

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 0.303 Å^{-1}

8.2 Resolution estimates (i)

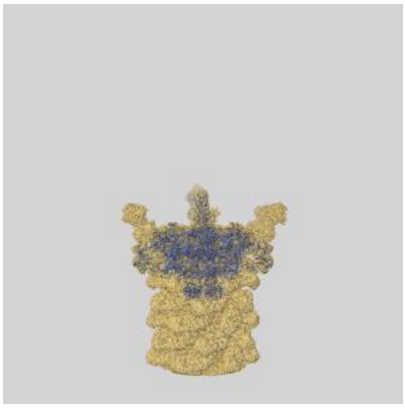
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.33	3.97	3.43
Unmasked-calculated*	4.15	7.51	4.28

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.15 differs from the reported value 3.3 by more than 10 %

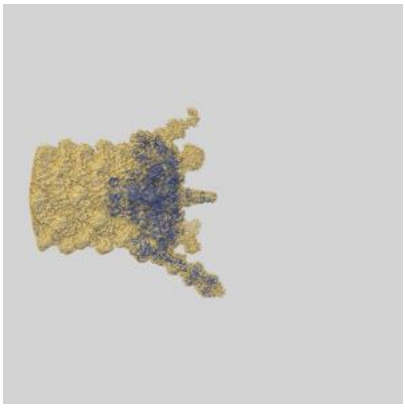
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44168 and PDB model 9B45. Per-residue inclusion information can be found in section 3 on page 9.

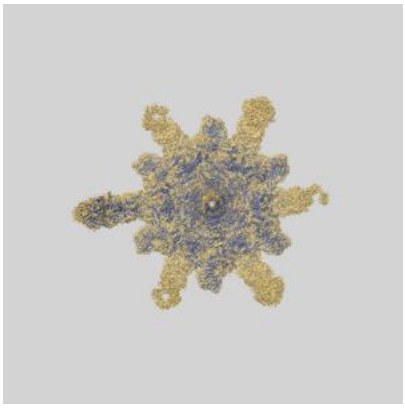
9.1 Map-model overlay



X



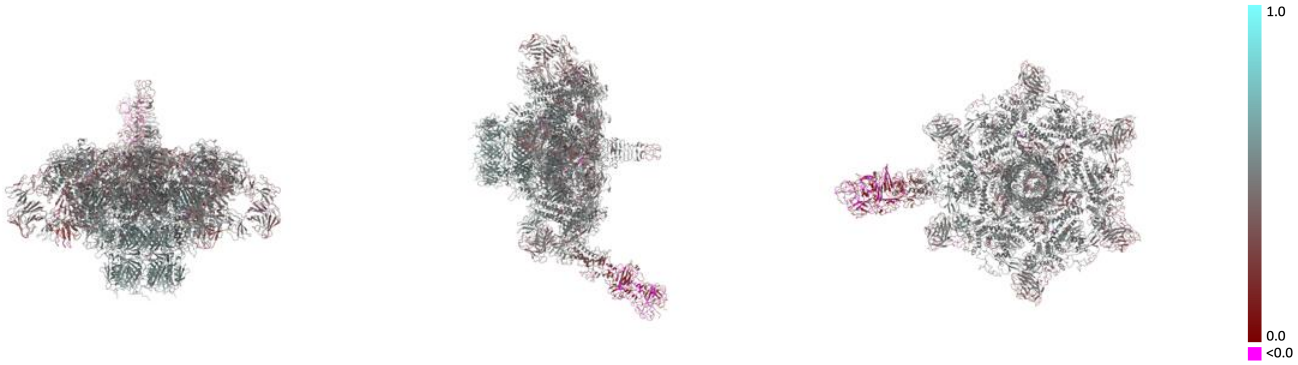
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

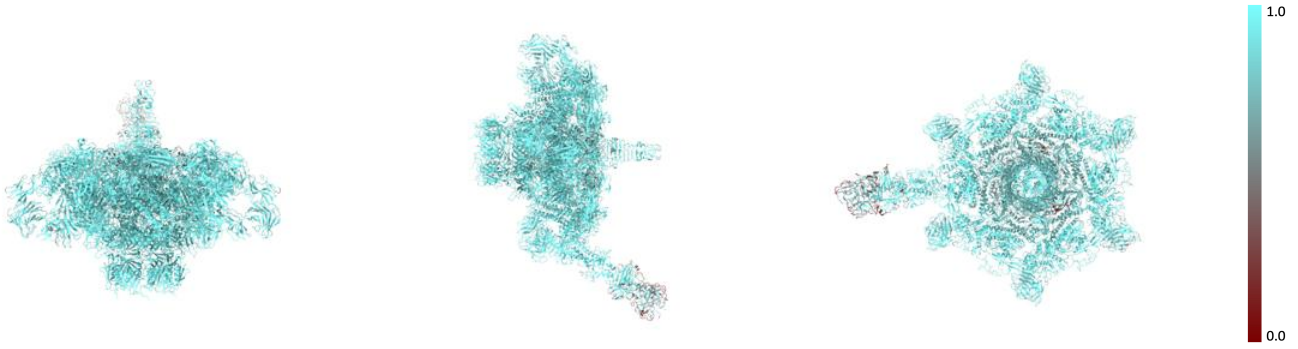
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

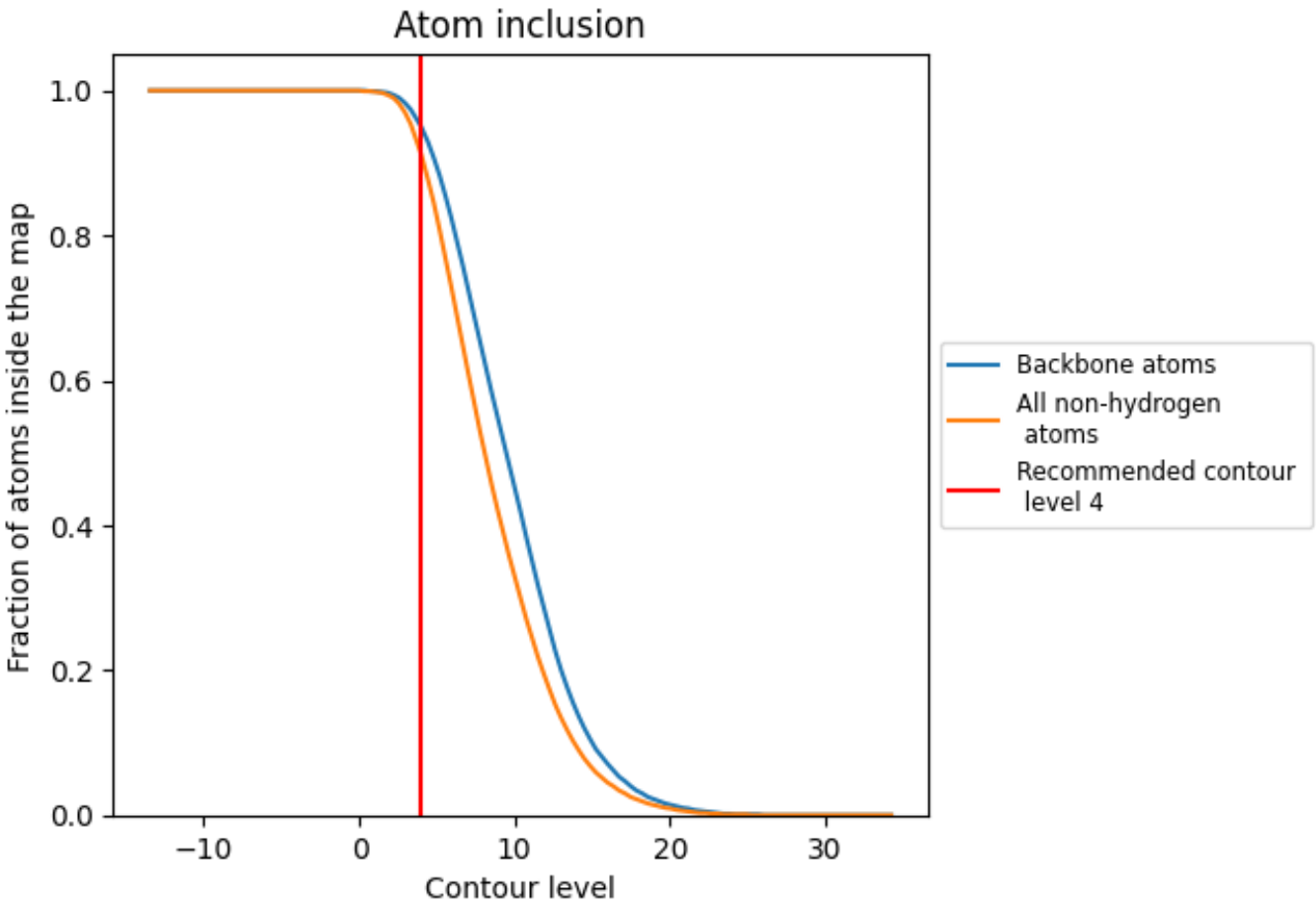
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 91% 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 (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9120	0.4430
1	0.9340	0.4360
2	0.7870	0.2300
3	0.7800	0.2400
4	0.7570	0.2120
A	0.9660	0.5100
B	0.9700	0.5080
C	0.9760	0.5100
D	0.9690	0.5050
E	0.9700	0.5080
F	0.9600	0.5060
G	0.9560	0.5100
H	0.9480	0.5120
I	0.9590	0.5110
J	0.9530	0.5170
K	0.9620	0.5150
L	0.9480	0.5150
M	0.9540	0.5390
N	0.9520	0.5300
O	0.9690	0.5420
P	0.9600	0.5370
Q	0.9570	0.5390
R	0.9570	0.5360
S	0.9580	0.5220
T	0.9550	0.5220
U	0.9490	0.5190
V	0.9290	0.4980
W	0.9250	0.4970
X	0.9310	0.5000
a	0.9240	0.4660
b	0.9240	0.4890
c	0.9380	0.4920
d	0.9350	0.4950
e	0.9310	0.4870
f	0.9340	0.4920

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Chain	Atom inclusion	Q-score
g	0.9310	0.4700
h	0.9290	0.4580
i	0.9230	0.4630
j	0.9530	0.4850
k	0.9450	0.4710
l	0.9340	0.4560
m	0.9420	0.4750
n	0.9540	0.4860
o	0.9640	0.5050
p	0.8740	0.4280
q	0.8650	0.4250
r	0.8570	0.4180
s	0.8850	0.4330
t	0.8630	0.4320
u	0.8900	0.4410
v	0.9270	0.4160
w	0.9080	0.3980
x	0.8650	0.3450
y	0.9000	0.3950
z	0.9020	0.3940